

## NIST-JANAF THERMOCHEMICAL TABLES

**I<sub>1</sub>(g)****A<sub>r</sub> = 126.9045 Iodine (I)****IDEAL GAS**

$$\text{IP}(\text{l}, \text{g}) = 84295.1 \pm 0.2 \text{ cm}^{-1}$$

$$\text{S}^*(298.15 \text{ K}) = 180.786 \pm 0.002 \text{ J K}^{-1} \text{ mol}^{-1}$$

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

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

|                                       |                             | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |           |                                    |                  | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |            |                      |        |
|---------------------------------------|-----------------------------|-----------------------------------------------------------|-----------|------------------------------------|------------------|-------------------------------------------------------|------------|----------------------|--------|
|                                       |                             | $T/K$                                                     |           | $\text{J K}^{-1} \text{ mol}^{-1}$ |                  | $H^\circ - H(T_r)/T$                                  |            | $\text{kJ mol}^{-1}$ |        |
|                                       |                             | $C_p$                                                     | $S^\circ$ | $-[\text{G}^\circ - H(T_r)]T$      | $\Delta H^\circ$ | $\Delta G^\circ$                                      | $\log K_r$ |                      |        |
| Electronic Levels and Quantum Weights |                             | 0                                                         | 0         | 0                                  | -6.197           | 107.164                                               |            |                      |        |
| State                                 | $\epsilon, \text{ cm}^{-1}$ | 100                                                       | 20.786    | 158.979                            | -4.119           | 107.717                                               |            |                      |        |
|                                       | $g_i$                       | 200                                                       | 20.786    | 172.487                            | -2.040           | 107.330                                               | 82.328     |                      |        |
|                                       |                             | 250                                                       | 20.786    | 177.125                            | -1.001           | 107.055                                               | 76.109     | -21.502              |        |
| <sup>2</sup> P <sub>3/2</sub>         | 0.0                         | 298.15                                                    | 20.786    | 180.786                            | 0.               | 106.762                                               | 70.174     | -12.294              |        |
| <sup>2</sup> P <sub>1/2</sub>         | 4                           | 300                                                       | 20.786    | 180.915                            | 0.038            | 106.750                                               | 69.947     | -12.179              |        |
|                                       |                             | 350                                                       | 20.786    | 181.040                            | 1.078            | 106.383                                               | 63.841     | -9.528               |        |
|                                       |                             | 400                                                       | 20.786    | 186.895                            | 2.117            | 98.010                                                | 58.064     | -7.582               |        |
|                                       |                             | 450                                                       | 20.786    | 189.143                            | 3.156            | 97.032                                                | 53.150     | -6.167               |        |
|                                       |                             | 500                                                       | 20.786    | 191.533                            | 4.196            | 75.990                                                | 50.203     | -5.245               |        |
|                                       |                             | 550                                                       | 20.786    | 193.142                            | 5.196            |                                                       |            |                      |        |
|                                       |                             | 600                                                       | 20.786    | 195.323                            | 6.274            | 66.191                                                | 45.027     | -3.920               |        |
|                                       |                             | 700                                                       | 20.786    | 198.577                            | 8.353            | 76.386                                                | 39.818     | -2.971               |        |
|                                       |                             | 800                                                       | 20.786    | 201.502                            | 10.432           | 76.575                                                | 34.880     | -2.238               |        |
|                                       |                             | 900                                                       | 20.789    | 203.751                            | 109.851          | 29.320                                                | -1.702     |                      |        |
|                                       |                             | 1000                                                      | 20.793    | 205.942                            | 191.352          | 24.039                                                | -1.256     |                      |        |
|                                       |                             | 1100                                                      | 20.806    | 207.924                            | 192.770          | 16.669                                                | 18.741     | -0.890               |        |
|                                       |                             | 1200                                                      | 20.824    | 209.735                            | 194.109          | 18.751                                                | 17.275     | -0.584               |        |
|                                       |                             | 1300                                                      | 20.851    | 211.403                            | 20.516           | 8.101                                                 | 8.430      | -0.325               |        |
|                                       |                             | 1400                                                      | 20.889    | 212.949                            | 196.577          | 22.921                                                | 77.574     | 2.762                | -0.103 |
|                                       |                             | 1500                                                      | 20.936    | 214.392                            | 197.717          | 25.013                                                | 77.701     | -2.586               | 0.090  |
|                                       |                             | 1600                                                      | 20.984    | 215.745                            | 198.802          | 27.109                                                | 77.899     | -7.942               | 0.259  |
|                                       |                             | 1700                                                      | 21.062    | 217.020                            | 199.836          | 29.212                                                | 77.894     | -13.304              | 0.409  |
|                                       |                             | 1800                                                      | 21.137    | 218.226                            | 200.825          | 31.322                                                | 77.954     | -18.671              | 0.542  |
|                                       |                             | 1900                                                      | 21.220    | 219.371                            | 201.771          | 33.440                                                | 77.986     | -24.040              | 0.661  |
|                                       |                             | 2000                                                      | 21.308    | 220.461                            | 202.679          | 35.566                                                | 77.992     | -29.410              | 0.768  |
|                                       |                             | 2100                                                      | 21.399    | 221.503                            | 203.550          | 37.701                                                | 77.974     | -34.780              | 0.865  |
|                                       |                             | 2200                                                      | 21.493    | 222.501                            | 204.389          | 39.846                                                | 77.933     | -40.148              | 0.953  |
|                                       |                             | 2300                                                      | 21.588    | 223.458                            | 205.198          | 42.000                                                | 77.875     | -45.514              | 1.034  |
|                                       |                             | 2400                                                      | 21.682    | 224.379                            | 205.977          | 44.163                                                | 77.803     | -50.877              | 1.107  |
|                                       |                             | 2500                                                      | 21.775    | 225.266                            | 206.732          | 46.336                                                | 77.724     | -56.237              | 1.175  |
|                                       |                             | 2600                                                      | 21.865    | 226.142                            | 207.461          | 48.518                                                | 77.643     | -61.594              | 1.237  |
|                                       |                             | 2700                                                      | 21.953    | 226.949                            | 208.168          | 50.709                                                | 77.565     | -66.948              | 1.295  |
|                                       |                             | 2800                                                      | 22.036    | 227.749                            | 208.353          | 52.909                                                | 77.497     | -72.299              | 1.349  |
|                                       |                             | 2900                                                      | 22.116    | 228.523                            | 209.518          | 55.116                                                | 77.447     | -77.648              | 1.389  |
|                                       |                             | 3000                                                      | 22.191    | 229.277                            | 210.164          | 57.132                                                | 77.406     | -82.993              | 1.445  |
|                                       |                             | 3100                                                      | 22.261    | 230.003                            | 210.792          | 59.554                                                | 77.392     | -88.342              | 1.489  |
|                                       |                             | 3200                                                      | 22.327    | 230.711                            | 211.404          | 61.784                                                | 77.403     | -93.688              | 1.529  |
|                                       |                             | 3300                                                      | 22.443    | 232.068                            | 212.580          | 66.261                                                | 77.511     | -99.035              | 1.568  |
|                                       |                             | 3400                                                      | 22.582    | 233.354                            | 213.399          | 68.558                                                | 77.612     | -107.733             | 1.638  |
|                                       |                             | 3500                                                      | 22.494    | 232.720                            | 213.146          |                                                       |            |                      |        |

**Heat Capacity and Entropy**

The adopted value for the enthalpy of formation of I<sub>1</sub>(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  $D_0^\circ(I_1, g) = 12440.06 \pm 0.03 \text{ cm}^{-1}$  ( $148.816 \pm 0.001 \text{ kJ mol}^{-1}$ ). The convergence limit in the absorption spectrum of the  $^3\text{I}_{0+} - ^3\text{I}_{2+}$  system corresponds to dissociation to a ground state iodine atom ( $^3\text{P}_{1/2}$ ) and an excited state iodine atom ( $^3\text{P}_{3/2}$ ).

Using earlier data, the CODATA recommended value<sup>5</sup> was  $12440.9 \pm 1.1 \text{ cm}^{-1}$  from LeRoy,<sup>6</sup> Brown,<sup>7</sup> and LeRoy and Bernstein,<sup>8</sup> and Sitterly,<sup>9</sup> LeRoy,<sup>10</sup> and Bernstein,<sup>11</sup> and a recent study by LeRoy and Bernstein<sup>12</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>

The thermodynamic functions at 298.15 K are in agreement with recent CODATA recommendations<sup>13</sup> except for two minor differences.

First, the entropy differs by  $0.1094 \text{ J K}^{-1} \text{ mol}^{-1}$  because this table uses a standard-state pressure of 1 bar, whereas CODATA recommendations are based on 1 atm. Second, entropy differences of the order of  $0.001 - 0.004 \text{ J K}^{-1} \text{ mol}^{-1}$  for the monatomic halogens arise due to the use of slightly different values for the relative atomic mass and for R; this table uses  $R = 8.31441 \text{ J K}^{-1} \text{ mol}^{-1}$ . Considering these minor changes, this table agrees within the estimated uncertainty with those by Hullgren *et al.*<sup>16</sup> Gurvich *et al.*<sup>17</sup> and Wagner *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>19</sup> and the 1973 values,<sup>19</sup> respectively.

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PREVIOUS: June 1974 (1 atm)

CURRENT: June 1982 (1 bar)

**Iodine (I)****I<sub>1</sub>(g)**

Iodine, Ion ( $I^+$ )

## IDEAL GAS

 $I^+(g)$ 

$$\Delta H^\circ(0\text{ K}) = 1115.557 \pm 0.05 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = 182.642 \pm 0.005 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

| Electronic Levels and Quantum States | $\epsilon, \text{cm}^{-1}$ | Quantum Weights $g$ |
|--------------------------------------|----------------------------|---------------------|
| $3_p$                                | 0.0                        | 5                   |
| $1P_1$                               | 7087.0                     | 3                   |
| $1P_0$                               | 6447.9                     | 1                   |
| $1D_2$                               | 13731                      | 5                   |
| $1S_0$                               | 32629                      | 1                   |

**Enthalpy of Formation**  
 $\Delta H^\circ(I^+, g, 0\text{ K})$  is calculated from  $\Delta H^\circ(I, g, 0\text{ K})^1$  using the spectroscopic value of IP(I) = 84295.1  $\pm 0.2 \text{ cm}^{-1}(1008.39 \pm 0.01 \text{ kJ}\cdot\text{mol}^{-1})$  from Moore.<sup>2</sup> The ionization limit is converted from  $\text{cm}^{-1}$  to  $\text{kJ}\cdot\text{mol}^{-1}$  using the factor,  $1 \text{ cm}^{-1} = 0.01196766 \text{ kJ}\cdot\text{mol}^{-1}$ , which is derived from the 1973 CODATA fundamental constants.<sup>3</sup> Rosenstein *et al.*<sup>4</sup> and Levin and Lias<sup>5</sup> have summarized additional ionization potential and appearance potential data.

$\Delta H^\circ(I^+, g, 298.15\text{ K})$  is calculated from  $\Delta H^\circ(I, g, 0\text{ K})$  by using IP(I) with JANAF<sup>6</sup> enthalpies,  $H^\circ(0\text{ K})\text{-}H^\circ(298.15\text{ K})$ , for  $I(g), I^+(g)$ , and  $e^-$ (ref.).  $\Delta H^\circ(I \rightarrow I^+ + e^-; 298.15\text{ K})$  differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstein *et al.*<sup>4</sup>  $\Delta H^\circ(298.15\text{ K})$  should be changed by  $-6.197 \text{ kJ}\cdot\text{mol}^{-1}$  if it is to be used in the ion convention that excludes the enthalpy of the electron.

## Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,<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  $81040 \text{ cm}^{-1}$  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 study by Moore.<sup>2,6</sup> The reported uncertainty in  $S^\circ$ (298.15 K) is due to uncertainties in the relative ion 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:  $I(g), 3-31-82; e^-$  (ref.), 3-31-82.
- <sup>2</sup>C. E. Moore, U. S. Natl. Bur. Stand., NBS-NBS-34, 8 pp. (1970).
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- <sup>4</sup>H. M. Rosenstein, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Suppl. 1, 783 pp. (1977).
- <sup>5</sup>R. D. Levin and S. G. Lias, U. S. Natl. Bur. Stand., NBS-NBS-71, 634 pp. (1982).
- <sup>6</sup>C. E. Moore, U. S. Natl. Bur. Stand., NBS-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-78-9960, Contract No. F44690-75-1-0048, (1978).

| $T/K$  | $C_v^*$ | $S^\circ - [G^\circ - H^\circ(T)]/T$ | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                  |            |
|--------|---------|--------------------------------------|-------------------------------------------------------|------------------|------------|
|        |         |                                      | $H^\circ - H^\circ(T)$                                | $\Delta H^\circ$ | $\log K_r$ |
| 100    | 0       | 0                                    | -6.197                                                | 1115.557         |            |
| 200    | 20.786  | 159.934                              | -4.119                                                |                  |            |
| 250    | 20.786  | 184.543                              | -2.040                                                |                  |            |
| 298.15 | 20.786  | 182.984                              | -1.001                                                |                  |            |
| 300    | 20.786  | 182.642                              | 0.                                                    | 1121.353         |            |
| 350    | 20.786  | 185.974                              | 0.038                                                 | 1121.379         |            |
| 400    | 20.786  | 183.457                              | 2.117                                                 | 1147.718         |            |
| 450    | 20.786  | 184.184                              | 3.156                                                 | 1147.780         |            |
| 500    | 20.786  | 193.388                              | 4.196                                                 | 1094.777         |            |
| 600    | 20.786  | 197.178                              | 6.274                                                 | 1097.057         |            |
| 700    | 20.787  | 200.382                              | 8.355                                                 | 1099.330         |            |
| 800    | 20.790  | 203.158                              | 10.432                                                | 1011.598         |            |
| 900    | 20.800  | 205.607                              | 19.176                                                | 1031.861         |            |
| 1000   | 20.819  | 207.800                              | 19.208                                                | 14.592           | 1061.119   |
|        |         |                                      |                                                       |                  | 1005.231   |
|        |         |                                      |                                                       |                  | -52.508    |
|        |         |                                      |                                                       |                  |            |
| 1100   | 20.852  | 209.785                              | 194.626                                               | 16.675           | 995.032    |
| 1200   | 21.602  | 195.966                              | 187.634                                               | -39.624          | -42.860    |
| 1300   | 20.974  | 213.777                              | 197.234                                               | 20.857           | -39.137    |
| 1400   | 21.065  | 198.435                              | 22.959                                                | 1115.105         | -33.940    |
| 1500   | 21.176  | 216.292                              | 197.578                                               | 25.070           | 952.353    |
| 1600   | 21.305  | 217.663                              | 200.666                                               | 27.194           | 1119.546   |
| 1700   | 21.450  | 218.939                              | 201.705                                               | 29.332           | 1211.744   |
| 1800   | 21.608  | 220.189                              | 202.658                                               | 31.485           | 123.925    |
| 1900   | 21.776  | 221.362                              | 203.649                                               | 33.654           | 912.088    |
| 2000   | 21.932  | 222.483                              | 204.563                                               | 35.840           | 1128.233   |
| 2100   | 22.134  | 223.559                              | 205.442                                               | 38.045           | 1130.361   |
| 2200   | 22.320  | 224.593                              | 206.289                                               | 40.267           | 1134.477   |
| 2300   | 22.506  | 225.589                              | 207.107                                               | 42.509           | 860.370    |
| 2400   | 22.693  | 226.551                              | 207.897                                               | 44.769           | -19.540    |
| 2500   | 22.879  | 227.481                              | 208.662                                               | 47.047           | 848.403    |
| 2600   | 23.062  | 228.382                              | 209.403                                               | 49.344           | 836.348    |
| 2700   | 23.241  | 229.256                              | 210.122                                               | 51.659           | 824.208    |
| 2800   | 23.416  | 230.104                              | 210.821                                               | 53.992           | 1143.031   |
| 2900   | 23.587  | 230.929                              | 211.500                                               | 56.343           | 1145.175   |
| 3000   | 23.751  | 231.731                              | 212.161                                               | 58.710           | 1147.341   |
| 3100   | 23.910  | 232.513                              | 212.805                                               | 61.093           | 1151.760   |
| 3200   | 24.062  | 233.274                              | 213.433                                               | 63.491           | 1154.019   |
| 3300   | 24.208  | 234.017                              | 214.046                                               | 65.905           | 1156.315   |
| 3400   | 24.346  | 234.741                              | 214.644                                               | 68.333           | 1158.649   |
| 3500   | 24.478  | 235.449                              | 215.228                                               | 70.774           | 1161.022   |
| 3600   | 24.603  | 236.140                              | 215.799                                               | 73.228           | 1163.436   |
| 3700   | 24.720  | 236.816                              | 216.338                                               | 75.694           | 1168.891   |
| 3800   | 24.830  | 237.477                              | 216.905                                               | 78.172           | 1172.683   |
| 3900   | 24.933  | 238.123                              | 217.441                                               | 79.774           | 1170.922   |
| 4000   | 25.049  | 238.736                              | 217.966                                               | 83.050           | 1183.158   |
| 4100   | 25.118  | 239.375                              | 218.481                                               | 83.666           | 1176.112   |
| 4200   | 25.200  | 239.981                              | 218.986                                               | 88.182           | 1178.764   |
| 4300   | 25.276  | 240.575                              | 219.481                                               | 90.705           | 1181.452   |
| 4400   | 25.345  | 241.157                              | 219.967                                               | 93.236           | 1184.176   |
| 4500   | 25.407  | 241.727                              | 220.444                                               | 95.774           | 1185.934   |
| 4600   | 25.464  | 242.296                              | 220.913                                               | 98.318           | 1189.725   |
| 4700   | 25.514  | 242.834                              | 221.373                                               | 100.867          | 1192.546   |
| 4800   | 25.559  | 243.372                              | 221.826                                               | 103.420          | 1195.398   |
| 4900   | 25.598  | 243.872                              | 222.271                                               | 105.978          | 1198.277   |
| 5000   | 25.632  | 244.417                              | 222.709                                               | 108.540          | 1201.184   |
| 5100   | 25.661  | 244.925                              | 223.140                                               | 111.104          | 1204.116   |
| 5200   | 25.685  | 245.423                              | 223.563                                               | 113.672          | 1207.072   |
| 5300   | 25.705  | 245.913                              | 223.980                                               | 116.241          | 1210.052   |
| 5400   | 25.720  | 246.393                              | 224.391                                               | 118.813          | 1213.052   |
| 5500   | 25.732  | 246.863                              | 224.795                                               | 121.385          | 1216.074   |
| 5600   | 25.739  | 247.329                              | 225.194                                               | 123.959          | 1219.115   |
| 5700   | 25.743  | 247.785                              | 225.585                                               | 126.533          | 1222.174   |
| 5800   | 25.747  | 248.233                              | 226.354                                               | 129.249          | 1225.628   |
| 5900   | 25.740  | 248.673                              | 121.107                                               | 131.682          | 1228.342   |
| 6000   | 25.734  | 249.105                              | 226.729                                               | 134.255          | 1231.449   |

CURRENT: June 1982 (1 bar)

PREVIOUS

## NIST-JANAF THERMOCHEMICAL TABLES

 $I_1^-$ (g) $M_r = 126.90505$  Iodine, Ion ( $I^-$ )

## IDEAL GAS

$$EA(I, g) = 3.0591 \pm 0.0004 \text{ eV}$$

$$S^*(298.15 \text{ K}) = 169.260 \pm 0.005 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta H^\circ(0 \text{ K}) = -187.992 \pm 0.4 \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = [-194.59] \text{ kJ} \cdot \text{mol}^{-1}$$

| Electronic State | $\epsilon, \text{cm}^{-1}$ | Quantum Weight $g_e$ |
|------------------|----------------------------|----------------------|
| $I_S^*$          | 0.0                        | 1                    |

## Enthalpy of Formation

$\Delta_f H^\circ(I^-, g, 0 \text{ K})$  is calculated from  $\Delta_f H^\circ(\text{I}, g, 0 \text{ K})^1$  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 Hopf and Lineberger,<sup>2</sup> is based on laser optogalvanic spectroscopy.<sup>5</sup> Additional information on I<sup>-</sup>(g) may be obtained in the critical discussions of Hopf and Lineberger,<sup>2</sup> Rosenstein,<sup>6</sup> and Massey.<sup>7</sup>

$\Delta_f H^\circ(I^-, g, 298.15 \text{ K})$  is obtained from  $\Delta_f H^\circ(\text{I}, g, 0 \text{ K}) - H^\circ(298.15 \text{ K})$ , for I<sup>-</sup>(g). If  $\Delta_f H^\circ(\text{I})$  with JANAF<sup>8</sup> enthalpies,  $H^\circ(0 \text{ K}) - H^\circ(T)$  by using EA(I) with threshold effects discussed by Rosenstein et al.<sup>3</sup>  $\Delta_f H^\circ(298.15 \text{ K})$  differs from a room-temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstein et al.<sup>3</sup>  $\Delta_f H^\circ(298.15 \text{ K})$  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 Hopf and Lineberger,<sup>2,6</sup> Rosenstein 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>7</sup> respectively.

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|  |  | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                                                      | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                                   |
|--|--|-----------------------------------------------------------|------------------------------------------------------|-------------------------------------------------------|-----------------------------------|
|  |  | $T/K$                                                     | $C_p^\circ$                                          | $S^\circ$                                             | $[G^\circ - H^\circ(T)]/T$        |
|  |  |                                                           | $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ | $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  | $\text{kJ} \cdot \text{mol}^{-1}$ |
|  |  | 0                                                         | 0                                                    | 0                                                     | -187.992                          |
|  |  | 100                                                       | 0.786                                                | 146.553                                               | -6.197                            |
|  |  | 200                                                       | 20.786                                               | 160.961                                               | -4.119                            |
|  |  | 250                                                       | 20.786                                               | 165.599                                               | -2.040                            |
|  |  | 298.15                                                    | 20.786                                               | 169.260                                               | -1.001                            |
|  |  | 350                                                       | 20.786                                               | 172.593                                               | 0                                 |
|  |  | 400                                                       | 20.786                                               | 175.348                                               | -194.591                          |
|  |  | 450                                                       | 20.786                                               | 177.817                                               | -221.488                          |
|  |  | 500                                                       | 20.786                                               | 180.007                                               | 38.804                            |
|  |  | 600                                                       | 20.786                                               | 183.796                                               | 38.593                            |
|  |  | 700                                                       | 20.786                                               | 187.001                                               | 33.736                            |
|  |  | 800                                                       | 20.786                                               | 189.776                                               | 32.057                            |
|  |  | 900                                                       | 20.786                                               | 192.224                                               | 30.961                            |
|  |  | 1000                                                      | 20.786                                               | 194.414                                               | 29.902                            |
|  |  | 1100                                                      | 20.786                                               | 196.306                                               | 27.035                            |
|  |  | 1200                                                      | 20.786                                               | 198.204                                               | 24.417                            |
|  |  | 1300                                                      | 20.786                                               | 199.849                                               | 23.720                            |
|  |  | 1400                                                      | 20.786                                               | 201.408                                               | 20.904                            |
|  |  | 1500                                                      | 20.786                                               | 202.842                                               | 20.376                            |
|  |  | 1600                                                      | 20.786                                               | 204.184                                               | 19.715                            |
|  |  | 1700                                                      | 20.786                                               | 205.444                                               | 19.157                            |
|  |  | 1800                                                      | 20.786                                               | 206.632                                               | 18.618                            |
|  |  | 1900                                                      | 20.786                                               | 207.756                                               | 18.002                            |
|  |  | 2000                                                      | 20.786                                               | 208.822                                               | 17.397                            |
|  |  | 2100                                                      | 20.786                                               | 209.836                                               | 16.786                            |
|  |  | 2200                                                      | 20.786                                               | 210.765                                               | 16.177                            |
|  |  | 2300                                                      | 20.786                                               | 211.707                                               | 15.568                            |
|  |  | 2400                                                      | 20.786                                               | 212.612                                               | 15.000                            |
|  |  | 2500                                                      | 20.786                                               | 213.461                                               | 14.455                            |
|  |  | 2600                                                      | 20.786                                               | 214.276                                               | 13.909                            |
|  |  | 2700                                                      | 20.786                                               | 215.050                                               | 13.397                            |
|  |  | 2800                                                      | 20.786                                               | 215.816                                               | 12.807                            |
|  |  | 2900                                                      | 20.786                                               | 216.546                                               | 12.268                            |
|  |  | 3000                                                      | 20.786                                               | 217.250                                               | 11.660                            |
|  |  | 3100                                                      | 20.786                                               | 217.932                                               | 11.060                            |
|  |  | 3200                                                      | 20.786                                               | 218.592                                               | 10.450                            |
|  |  | 3300                                                      | 20.786                                               | 219.231                                               | 9.840                             |
|  |  | 3400                                                      | 20.786                                               | 219.852                                               | 9.230                             |
|  |  | 3500                                                      | 20.786                                               | 220.454                                               | 8.620                             |
|  |  | 3600                                                      | 20.786                                               | 221.040                                               | 8.010                             |
|  |  | 3700                                                      | 20.786                                               | 221.610                                               | 7.399                             |
|  |  | 3800                                                      | 20.786                                               | 222.164                                               | 6.789                             |
|  |  | 3900                                                      | 20.786                                               | 222.704                                               | 6.179                             |
|  |  | 4000                                                      | 20.786                                               | 223.230                                               | 5.569                             |
|  |  | 4100                                                      | 20.786                                               | 223.743                                               | 5.059                             |
|  |  | 4200                                                      | 20.786                                               | 224.244                                               | 4.549                             |
|  |  | 4300                                                      | 20.786                                               | 224.733                                               | 4.039                             |
|  |  | 5000                                                      | 20.786                                               | 227.658                                               | 2.510                             |
|  |  | 5100                                                      | 20.786                                               | 228.280                                               | 2.141                             |
|  |  | 5200                                                      | 20.786                                               | 228.884                                               | 1.831                             |
|  |  | 5300                                                      | 20.786                                               | 229.079                                               | 1.521                             |
|  |  | 5400                                                      | 20.786                                               | 229.468                                               | 1.211                             |
|  |  | 5500                                                      | 20.786                                               | 229.849                                               | 0.901                             |
|  |  | 5600                                                      | 20.786                                               | 230.224                                               | 0.591                             |
|  |  | 5700                                                      | 20.786                                               | 230.592                                               | 0.281                             |
|  |  | 5800                                                      | 20.786                                               | 230.953                                               | -0.091                            |
|  |  | 5900                                                      | 20.786                                               | 231.309                                               | -0.401                            |
|  |  | 6000                                                      | 20.786                                               | 231.658                                               | -0.711                            |

CURRENT: June 1992 (1 bar)

Iodine, Ion ( $I^-$ )

PREVIOUS:

## Potassium Iodide (KI)

M<sub>r</sub> = 166.0028 Potassium Iodide (KI)

## CRYSTAL

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= 106.387 \text{ J K}^{-1} \text{ mol}^{-1} \\ T_{\text{m}} &= 954 \text{ K} \\ \Delta_H^\circ(0 \text{ K}) &= -326.93 \pm 0.4 \text{ kJ mol}^{-1} \\ \Delta_H^\circ(298.15 \text{ K}) &= -327.90 \pm 0.4 \text{ kJ mol}^{-1} \\ \Delta_{\text{sub}}H^\circ &= 24.016 \text{ kJ mol}^{-1} \end{aligned}$$

## 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,  $\Delta_H^\circ(298.15 \text{ K}) = 4.86 \pm 0.03 \text{ kcal mol}^{-1}$ , reported by Parker, and  $\Delta_H^\circ(298.15 \text{ K}) = -60.32$  and  $-13.19 \text{ kcal mol}^{-1}$  for K<sup>+</sup>(aq,  $\infty$ ) and I<sup>-(aq,  $\infty$ )</sup>, respectively, obtained from,<sup>2</sup> we obtain  $\Delta_H^\circ(\text{KI, cr, } 298.15 \text{ K}) = -78.37 \pm 0.1 \text{ kcal mol}^{-1}$ , which is adopted.

| $\Delta_H^\circ, \text{ kcal mol}^{-1}$ (a) | T/°C | n(b)  | Source                               |
|---------------------------------------------|------|-------|--------------------------------------|
| 4.820 ± 0.05                                | 19   | 200   | Thomsen <sup>3</sup>                 |
| 4.897 ± 0.04                                | 25   | 18    | Wust and Lange <sup>4</sup>          |
| 4.873                                       | 25   | 500   | Lange and Martin <sup>5</sup>        |
| 4.790 ± 0.10                                | 20.5 | 600   | Popov et al. <sup>6</sup>            |
| 4.790 ± 0.10                                | 24.5 | 18.5  | Bobylev and Lairsch <sup>7</sup>     |
| 5.020                                       | 25   | 75000 | Kapustinskii and Drakin <sup>8</sup> |
| 4.830 ± 0.07                                |      |       |                                      |

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  $C_p^\circ$  values reported by Scales,<sup>10</sup> 2–7 K. The data of Clusius 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 Koref.<sup>12</sup> The value of  $S^\circ(298.15 \text{ K})$  is derived based on the adopted low temperature heat capacities, using  $S^\circ(2.86 \text{ K}) = 0.033 \text{ cal K}^{-1} \text{ mol}^{-1}$ .

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  $C_p^\circ$ . Enthalpy values used in the curve fit include smooth values calculated from the equation of Skuratov and the value  $H^\circ(954)-H^\circ(298.15) = 9.2 \text{ kcal mol}^{-1}$  from Dworkin. Deviations 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.  $C_p^\circ$  above the melting point is obtained by graphical extrapolation.

## Fusion Data

$T_{\text{m}}$  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  $\Delta_H^\circ(298.15 \text{ K})$  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) is calculated as the enthalpy change for the following reaction: 2KI(cr) = K<sub>2</sub>I(g).

## References

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PREVIOUS December 1961

CURRENT June 1967

## Potassium Iodide (KI)

## Potassium Iodide (KI)

## LIQUID

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

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

$T_{\text{fus}} = 954\text{ K}$

$\Delta_fH^\circ(298.15\text{ K}) = [-312.846] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{fus}}H^\circ = 24.016 \text{ kJ}\cdot\text{mol}^{-1}$

## Enthalpy of Formation

$\Delta_fH^\circ(\text{KI}, 298.15\text{ K})$ , is calculated from  $\Delta_fH^\circ(\text{KI, cr}, 298.15\text{ K})$  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 cal K<sup>-1</sup>·mol<sup>-1</sup> from the enthalpy measurements, 954–1014K, by Dworkin,<sup>1</sup> This C<sub>p</sub><sup>o</sup> value is adopted in the temperature range 298.15 K S<sup>o</sup>(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

The boiling point, T<sub>vap</sub> = 1618 K (1 atm), is calculated as the temperature at which the sum of the partial pressure of KI(g) and K<sub>2</sub>I<sub>2</sub>(g) over KI(l) equals one atmosphere. The value of Δ<sub>vap</sub>H<sup>o</sup> is calculated as the heat required to produce one mole of vapor mixture, which contains 78 percent monomer (KI) and 22 percent dimer (K<sub>2</sub>I<sub>2</sub>) at T<sub>vap</sub>.<sup>2</sup> T<sub>vap</sub> was reported as 1603 and 1590 K by Wartenberg and Albrecht,<sup>2</sup> and Ruff and Mugdan,<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. Mugdan, Z. Anorg. Chem. 117, 147 (1921).

| 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 |                               |                               |
|---------|-----------------------------|------------------------------------------------------------|----------------------------------------------------|-------------------------------|-------------------------------|
|         |                             |                                                            | H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )  | Δ <sub>f</sub> H <sup>o</sup> | Δ <sub>f</sub> G <sup>o</sup> |
| 0       |                             |                                                            |                                                    |                               |                               |
| 298.15  | 72.383                      | 114.098                                                    | 114.098                                            | 0.                            | -312.846                      |
| 200     | 72.383                      | 114.546                                                    | 114.100                                            | 0.134                         | -310.253                      |
| 300     | 72.383                      | 115.369                                                    | 116.359                                            | 0.372                         | -308.881                      |
| 400     | 72.383                      | 151.521                                                    | 122.300                                            | 14.611                        | -303.743                      |
| 500     | 72.383                      | 164.718                                                    | 128.303                                            | 21.849                        | -295.340                      |
| 600     | 72.383                      | 175.876                                                    | 134.223                                            | 29.087                        | -289.329                      |
| 700     | 72.383                      | 185.541                                                    | 140.135                                            | 36.326                        | -282.657                      |
| 800     | 72.383                      | 194.067                                                    | 145.663                                            | 43.564                        | -274.799                      |
| 900     | 72.383                      | 198.285                                                    | 148.523                                            | 47.473                        | -276.282                      |
| 954,000 | 72.383                      | 150.891                                                    | 150.891                                            | —                             | — CRYSTAL <--> LIQUID         |
| 1000    | 72.383                      | 201.693                                                    | 50.802                                             | -330.106                      | -270.169                      |
| 1100    | 72.383                      | 208.592                                                    | 155.928                                            | 58.040                        | -406.794                      |
| 1200    | 72.383                      | 214.890                                                    | 160.491                                            | 65.279                        | -403.551                      |
| 1300    | 72.383                      | 220.684                                                    | 164.902                                            | 72.517                        | -400.320                      |
| 1400    | 72.383                      | 226.048                                                    | 169.080                                            | 79.755                        | -397.104                      |
| 1500    | 72.383                      | 231.042                                                    | 173.046                                            | 86.994                        | -393.909                      |
| 1600    | 72.383                      | 235.714                                                    | 176.819                                            | 94.232                        | -390.740                      |
| 1700    | 72.383                      | 240.102                                                    | 180.413                                            | 101.470                       | -387.602                      |
| 1800    | 72.383                      | 244.239                                                    | 183.845                                            | 108.709                       | -384.499                      |
| 1900    | 72.383                      | 248.153                                                    | 187.128                                            | 115.947                       | -381.435                      |
| 2000    | 72.383                      | 251.866                                                    | 190.273                                            | 123.185                       | -378.411                      |
| 2100    | 72.383                      | 255.397                                                    | 193.291                                            | 130.424                       | -375.428                      |
| 2200    | 72.383                      | 258.764                                                    | 196.191                                            | 137.662                       | -372.485                      |
| 2300    | 72.383                      | 261.982                                                    | 198.982                                            | 144.900                       | -369.581                      |
| 2400    | 72.383                      | 265.063                                                    | 201.671                                            | 152.139                       | -365.713                      |
| 2500    | 72.383                      | 268.017                                                    | 204.267                                            | 159.377                       | -363.879                      |

## Potassium Iodide (KI)

 $M_r = 166.0028$  Potassium Iodide (KI)

## CRYSTAL-LIQUID

0 to 954 K crystal  
above 954 K liquid

Refer to the individual tables for details.

| T/K     | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |         | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |                |                |
|---------|----------------------------------------------------------|---------|---------------------------------------------------|----------------|----------------|
|         | $C_p^*$                                                  | $S^*$   | $-G^*-H^*(T_r)/T_r$                               | $H^*-H^*(T_r)$ | $\Delta_f G^*$ |
| 0       | 0                                                        | 0       | INFINITE                                          | -12.711        | -326.930       |
| 100     | 45.003                                                   | 52.413  | 151.516                                           | -9.920         | -326.028       |
| 200     | 50.518                                                   | 85.772  | 111.148                                           | -5.075         | -324.572       |
| 298.15  | 52.777                                                   | 106.387 | 106.387                                           | 0              | 84.770         |
| 300     | 52.806                                                   | 106.713 | 106.388                                           | -327.900       | 56.592         |
| 400     | 53.932                                                   | 122.054 | 108.472                                           | 5.433          | -322.994       |
| 500     | 53.363                                                   | 134.235 | 112.446                                           | 10.894         | 56.238         |
| 600     | 57.300                                                   | 144.990 | 116.953                                           | 16.522         | 41.859         |
| 700     | 59.777                                                   | 153.503 | 121.543                                           | 22.372         | -304.584       |
| 800     | 62.639                                                   | 161.668 | 126.055                                           | 28.490         | -295.437       |
| 900     | 63.793                                                   | 169.225 | 130.437                                           | 34.909         | -286.448       |
| 954.000 | 67.594                                                   | 173.111 | 132.743                                           | 38.510         | 18.703         |
| 954.000 | 72.383                                                   | 198.285 | 132.43                                            | 62.527         | 16.113         |
| 1000    | 72.383                                                   | 201.693 | 135.837                                           | 65.856         | -313.870       |
| 1100    | 72.383                                                   | 208.592 | 142.143                                           | 73.095         | 32.790         |
| 1200    | 72.383                                                   | 214.890 | 147.946                                           | 80.333         | -270.169       |
| 1300    | 72.383                                                   | 220.684 | 153.322                                           | 87.571         | 14.112         |
| 1400    | 72.383                                                   | 226.048 | 158.327                                           | 94.810         | -12.331        |
| 1500    | 72.383                                                   | 231.042 | 163.010                                           | 102.048        | -246.444       |
| 1600    | 72.383                                                   | 235.714 | 167.410                                           | 109.286        | -233.483       |
| 1700    | 72.383                                                   | 240.102 | 171.558                                           | 116.524        | -220.770       |
| 1800    | 72.383                                                   | 244.239 | 175.482                                           | 123.763        | 9.381          |
| 1900    | 72.383                                                   | 248.153 | 179.205                                           | 131.001        | -160.332       |
| 2000    | 72.383                                                   | 251.866 | 182.746                                           | 138.239        | -148.773       |
| 2100    | 72.383                                                   | 255.397 | 186.122                                           | 145.478        | -137.365       |
| 2200    | 72.383                                                   | 258.764 | 189.348                                           | 152.716        | 3.417          |
| 2300    | 72.383                                                   | 261.982 | 192.437                                           | 159.954        | -126.098       |
| 2400    | 72.383                                                   | 265.063 | 195.399                                           | 167.193        | 2.994          |
| 2500    | 72.383                                                   | 268.017 | 198.245                                           | 174.431        | -114.963       |

Potassium Iodide (KI)

PREVIOUS: CURRENT: June 1967

## Potassium Iodide (KI)

## IDEAL GAS

## $I_1K_1(g)$

$$S^*(298.15 \text{ K}) = 258.283 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^{\circ}(0 \text{ K}) = -122.08 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^{\circ}(298.15 \text{ K}) = -123.52 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$$

| Electronic Level and Quantum Weight |                            | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                            | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |              |
|-------------------------------------|----------------------------|-----------------------------------------------------------|----------------------------|---------------------------------------------------|--------------|
| State                               | $\epsilon, \text{cm}^{-1}$ | $C_p^*$                                                   | $S^* - [G^* - H^*(T_r)]/T$ | $H^* - H^*(T_r)$                                  | $\Delta H^*$ |
| ${}^1\Sigma^+$                      | 0                          | 0                                                         | 0                          | -10.242                                           | -122.081     |
|                                     | 1                          | 1                                                         | 0.000267 $\text{cm}^{-1}$  | -7.165                                            | -137.559     |
|                                     |                            |                                                           |                            | -3.615                                            | -152.295     |
|                                     |                            |                                                           |                            | -1.782                                            | -124.627     |
|                                     |                            |                                                           |                            | 0                                                 | -125.520     |
|                                     |                            |                                                           |                            | -165.932                                          | 29.071       |
|                                     |                            |                                                           |                            | -125.556                                          | -166.182     |
|                                     |                            |                                                           |                            | -128.992                                          | -28.935      |
|                                     |                            |                                                           |                            | -172.775                                          | -25.785      |
|                                     |                            |                                                           |                            | -178.644                                          | -183.644     |
|                                     |                            |                                                           |                            | -139.830                                          | -21.317      |
|                                     |                            |                                                           |                            | -161.576                                          | -186.523     |
|                                     |                            |                                                           |                            | -162.722                                          | -19.486      |
|                                     |                            |                                                           |                            | -163.818                                          | 16.663       |
|                                     |                            |                                                           |                            | -164.891                                          | -14.633      |
|                                     |                            |                                                           |                            | -200.634                                          | -13.100      |
|                                     |                            |                                                           |                            | -205.038                                          | -11.900      |
|                                     |                            |                                                           |                            | -209.321                                          | 10.934       |
|                                     |                            |                                                           |                            | -209.564                                          | -208.881     |
|                                     |                            |                                                           |                            | -247.167                                          | 9.919        |
|                                     |                            |                                                           |                            | -247.330                                          | -205.394     |
|                                     |                            |                                                           |                            | -247.496                                          | -20.892      |
|                                     |                            |                                                           |                            | -247.669                                          | -198.378     |
|                                     |                            |                                                           |                            | -247.834                                          | -194.851     |
|                                     |                            |                                                           |                            | -248.000                                          | -6.785       |
|                                     |                            |                                                           |                            | -248.167                                          | -191.311     |
|                                     |                            |                                                           |                            | -248.282                                          | 6.246        |
|                                     |                            |                                                           |                            | -248.348                                          | -5.769       |
|                                     |                            |                                                           |                            | -248.410                                          | -5.345       |
|                                     |                            |                                                           |                            | -248.476                                          | -184.190     |
|                                     |                            |                                                           |                            | -248.540                                          | -4.965       |
|                                     |                            |                                                           |                            | -248.608                                          | -80.608      |
|                                     |                            |                                                           |                            | -248.676                                          | -177.010     |
|                                     |                            |                                                           |                            | -248.744                                          | -173.396     |
|                                     |                            |                                                           |                            | -248.812                                          | -4.313       |
|                                     |                            |                                                           |                            | -248.879                                          | -169.764     |
|                                     |                            |                                                           |                            | -248.946                                          | -162.114     |
|                                     |                            |                                                           |                            | -248.981                                          | -162.446     |
|                                     |                            |                                                           |                            | -249.049                                          | -158.760     |
|                                     |                            |                                                           |                            | -249.116                                          | 3.317        |
|                                     |                            |                                                           |                            | -249.183                                          | -155.054     |
|                                     |                            |                                                           |                            | -249.250                                          | -151.329     |
|                                     |                            |                                                           |                            | -249.317                                          | -29.928      |
|                                     |                            |                                                           |                            | -249.384                                          | -192.688     |
|                                     |                            |                                                           |                            | -249.451                                          | -2.753       |
|                                     |                            |                                                           |                            | -249.518                                          | -2.591       |
|                                     |                            |                                                           |                            | -249.585                                          | -140.043     |
|                                     |                            |                                                           |                            | -249.652                                          | -140.438     |
|                                     |                            |                                                           |                            | -249.719                                          | -136.543     |
|                                     |                            |                                                           |                            | -249.786                                          | -132.226     |
|                                     |                            |                                                           |                            | -249.853                                          | -128.591     |
|                                     |                            |                                                           |                            | -249.920                                          | -124.378     |
|                                     |                            |                                                           |                            | -249.987                                          | -1.916       |
|                                     |                            |                                                           |                            | -250.053                                          | -120.688     |
|                                     |                            |                                                           |                            | -250.120                                          | -1.804       |
|                                     |                            |                                                           |                            | -250.187                                          | -1.697       |
|                                     |                            |                                                           |                            | -250.254                                          | -1.377       |
|                                     |                            |                                                           |                            | -250.321                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.388                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.455                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.522                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.589                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.656                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.723                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.790                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.857                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.924                                          | -1.345       |
|                                     |                            |                                                           |                            | -250.991                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.058                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.125                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.192                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.259                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.326                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.393                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.460                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.527                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.594                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.661                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.728                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.795                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.862                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.929                                          | -1.345       |
|                                     |                            |                                                           |                            | -251.996                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.063                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.130                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.197                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.264                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.331                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.398                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.465                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.733                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.933                                          | -1.345       |
|                                     |                            |                                                           |                            | -252.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.133                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.333                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -253.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -254.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -255.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -256.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -257.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -258.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -259.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -260.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.932                                          | -1.345       |
|                                     |                            |                                                           |                            | -261.999                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.066                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.132                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.199                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.266                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.332                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.399                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.466                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.532                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.599                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.666                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.732                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.799                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.866                                          | -1.345       |
|                                     |                            |                                                           |                            | -262.932                                          | -1.345       |

## Lithium Iodide (LiI)

## CRYSTAL

 $\text{Li}_1\text{Li}_1(\text{cr})$  $M_r = 133.8455$  Lithium Iodide (LiI)

$$\text{S}^\circ(298.15 \text{ K}) = [85.772] \text{ J K}^{-1}\text{mol}^{-1}$$

$$T_{\text{trs}} = 742 \text{ K}$$

## Enthalpy of Formation

The enthalpy of formation,  $\Delta_f H^\circ(\text{LiI, cr, 298.15 K}) = -64.55 \text{ kcal mol}^{-1}$ , 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,  $\Delta_{\text{sol}} H^\circ(\text{eq, liq}) = -15.130 \pm 75 \text{ cal K}^{-1}\text{mol}^{-1}$  for  $\text{LiI(cr)} \rightarrow \text{LiI(aq,liq)}$  at 298.15 K. The ionic heat of formation,  $\Delta_f H^\circ(\text{Li}^+, \text{aq, } \infty, 298.15 \text{ K}) = -66.49 \text{ kcal mol}^{-1}$  was calculated from  $\Delta H^\circ(\text{LiOH}_4, \infty, 298.15 \text{ K}) = -121.46 \text{ kcal mol}^{-1}$  (see JANAF LiOH(cr) table, Mar 31, 1966) with  $\Delta_f H^\circ(\text{OH}^- \text{aq, } \infty, 298.15 \text{ K}) = -54.97 \text{ kcal mol}^{-1}$  from<sup>2</sup>. The value  $\Delta_f H^\circ(\text{Li}^+, \text{aq, } \infty, 298.15 \text{ K}) = 13.19 \text{ kcal mol}^{-1}$  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  $\text{LiI}(\text{aq, } \infty)$ ,  $\Delta_f H^\circ(\text{298.15 K}) = -79.68 \text{ kcal mol}^{-1}$ .

## Heat Capacity and Entropy

Dworkin<sup>3</sup> has measured the enthalpy changes by the drop method (642–802 K), yielding  $H^\circ(742 \text{ K}) - H^\circ(298.15 \text{ K}) = 6.0 \text{ kcal mol}^{-1}$  for the crystal at the melting point. Heat capacities derived from his data were  $C_p^\circ(692 \text{ K}) = 14.8$  and  $C_p^\circ(772 \text{ K}) = 15.1 \text{ cal K}^{-1}\text{mol}^{-1}$  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,  $S^\circ(298.15 \text{ K}) = 20.5 \text{ cal K}^{-1}\text{mol}^{-1}$ , 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  $\pm 0.5 \text{ cal K}^{-1}\text{mol}^{-1}$  of this value.

Kelley<sup>4</sup> has estimated the heat capacities ( $C_p^\circ = 12.30 + 2.44 \times 10^{-3} \text{ cal K}^{-1}\text{mol}^{-1}$ ) and the entropy,  $S^\circ(298.15 \text{ K}) = 17.50 \text{ cal K}^{-1}\text{mol}^{-1}$ .

## Fusion Data

The selected enthalpy of fusion,  $\Delta H^\circ(823 \text{ K}) = 350 \text{ kcal mol}^{-1}$  was obtained from enthalpy measurements in a drop calorimeter by Dworkin and Bredig.<sup>5</sup>

## References

- <sup>1</sup>V. B. Parker, NSRDS NBS 2, 66 pp. (1965).
- <sup>2</sup>U. S. Natl. 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).

$$\Delta_f H^\circ(298.15 \text{ K}) = -270.08 \pm 0.4 \text{ kJ mol}^{-1}$$

$$\Delta_{\text{sol}} H^\circ = 14.64 \text{ kJ mol}^{-1}$$

|        | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |             |                                        |                                              | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                    |                    |            |
|--------|-----------------------------------------------------------|-------------|----------------------------------------|----------------------------------------------|-------------------------------------------------------|--------------------|--------------------|------------|
|        | $T/\text{K}$                                              | $C_p^\circ$ | $J \cdot \text{K}^{-1}\text{mol}^{-1}$ | $S^\circ - (C^\circ - H^\circ(T)/T)\text{J}$ | $H^\circ - H^\circ(T_r)/T$                            | $\Delta_f H^\circ$ | $\Delta_f G^\circ$ | $\log K_r$ |
| 0      |                                                           |             |                                        |                                              |                                                       |                    |                    |            |
| 100    |                                                           |             |                                        |                                              |                                                       |                    |                    |            |
| 200    | 50.082                                                    | 85.772      | 85.772                                 | 0.                                           | -270.077                                              | -269.665           | 47.244             |            |
| 298.15 | 50.082                                                    | 85.772      | 85.772                                 | 0.093                                        | -270.080                                              | -269.662           | 46.932             |            |
| 300    | 50.187                                                    | 86.082      | 85.773                                 | 0.093                                        | -278.350                                              | -269.208           | 35.155             |            |
| 400    | 53.430                                                    | 100.875     | 87.767                                 | 5.243                                        | -302.910                                              | -264.545           | 27.637             |            |
| 500    | 55.948                                                    | 113.073     | 91.645                                 | 10.714                                       | -302.047                                              | -256.948           | 22.369             |            |
| 600    | 58.560                                                    | 123.499     | 96.104                                 | 16.437                                       | -300.480                                              | -249.523           | 18.620             |            |
| 700    | 62.258                                                    | 132.807     | 100.693                                | 22.480                                       | -299.188                                              | -242.302           | 15.821             |            |
| 800    | 66.107                                                    | 141.363     | 105.248                                | 28.891                                       | -297.185                                              | -235.308           | 13.657             |            |
| 900    | 69.517                                                    | 149.355     | 109.710                                | 35.680                                       | -294.889                                              | -228.553           | 11.938             |            |
| 1000   | 71.965                                                    | 156.815     | 114.052                                | 42.763                                       | -292.399                                              | -222.039           | 10.544             |            |
| 1100   | 73.534                                                    | 163.751     | 118.259                                | 50.042                                       | -289.785                                              | -215.757           | 9.392              |            |
| 1200   | 74.359                                                    | 170.195     | 122.321                                | 57.448                                       | -284.337                                              | -209.697           | 8.426              |            |
| 1300   | 75.375                                                    | 176.196     | 126.237                                | 64.946                                       | -284.337                                              | -203.847           | 7.606              |            |
| 1400   | 75.877                                                    | 181.801     | 130.008                                | 72.510                                       | -281.548                                              | -198.195           | 6.902              |            |
| 1500   | 76.191                                                    | 187.049     | 133.638                                | 80.116                                       | -278.767                                              | -192.729           | 6.292              |            |
| 1600   | 76.191                                                    | 191.966     | 137.132                                | 87.735                                       | -278.767                                              | -182.261           | 5.539              |            |
| 1700   | 76.191                                                    | 196.585     | 140.594                                | 95.354                                       | -42.143                                               | -166.186           | 4.823              |            |
| 1800   | 76.191                                                    | 200.940     | 143.733                                | 102.974                                      | -417.755                                              | -152.304           | 4.187              |            |
| 1900   | 76.191                                                    | 205.060     | 146.553                                | 110.593                                      | -414.303                                              | -138.603           | 3.630              |            |
| 2000   | 76.191                                                    | 208.968     | 149.862                                | 118.212                                      | -410.888                                              | -125.072           | 3.111              |            |
| 2100   | 76.191                                                    | 212.683     | 152.766                                | 125.831                                      | -407.509                                              | -111.702           | 2.652              |            |
| 2200   | 76.191                                                    | 216.229     | 155.570                                | 133.570                                      | -404.165                                              | -400.854           | 2.237              |            |
| 2300   | 76.191                                                    | 219.616     | 158.282                                | 141.059                                      | -397.571                                              | -85.406            | 1.859              |            |
| 2400   | 76.191                                                    | 222.859     | 160.906                                | 148.688                                      | -394.313                                              | -72.466            | 1.514              |            |
| 2500   | 76.191                                                    | 225.969     | 163.446                                |                                              |                                                       |                    |                    |            |

|        | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |             |                                        |                                              | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                    |                    |            |
|--------|-----------------------------------------------------------|-------------|----------------------------------------|----------------------------------------------|-------------------------------------------------------|--------------------|--------------------|------------|
|        | $T/\text{K}$                                              | $C_p^\circ$ | $J \cdot \text{K}^{-1}\text{mol}^{-1}$ | $S^\circ - (C^\circ - H^\circ(T)/T)\text{J}$ | $H^\circ - H^\circ(T_r)/T$                            | $\Delta_f H^\circ$ | $\Delta_f G^\circ$ | $\log K_r$ |
| 0      |                                                           |             |                                        |                                              |                                                       |                    |                    |            |
| 100    |                                                           |             |                                        |                                              |                                                       |                    |                    |            |
| 200    | 50.082                                                    | 85.772      | 85.772                                 | 0.                                           | -270.077                                              | -269.665           | 47.244             |            |
| 298.15 | 50.082                                                    | 85.772      | 85.772                                 | 0.093                                        | -270.080                                              | -269.662           | 46.932             |            |
| 300    | 50.187                                                    | 86.082      | 85.773                                 | 0.093                                        | -278.350                                              | -269.208           | 35.155             |            |
| 400    | 53.430                                                    | 100.875     | 87.767                                 | 5.243                                        | -302.910                                              | -264.545           | 27.637             |            |
| 500    | 55.948                                                    | 113.073     | 91.645                                 | 10.714                                       | -302.047                                              | -256.948           | 22.369             |            |
| 600    | 58.560                                                    | 123.499     | 96.104                                 | 16.437                                       | -300.480                                              | -249.523           | 18.620             |            |
| 700    | 62.258                                                    | 132.807     | 100.693                                | 22.480                                       | -300.814                                              | -249.523           | 18.620             |            |
| 800    | 66.107                                                    | 141.363     | 105.248                                | 28.891                                       | -299.188                                              | -242.302           | 15.821             |            |
| 900    | 69.517                                                    | 149.355     | 109.710                                | 35.680                                       | -297.185                                              | -235.308           | 13.657             |            |
| 1000   | 71.965                                                    | 156.815     | 114.052                                | 42.763                                       | -294.889                                              | -228.553           | 11.938             |            |
| 1100   | 73.534                                                    | 163.751     | 118.259                                | 50.042                                       | -292.399                                              | -222.039           | 10.544             |            |
| 1200   | 74.359                                                    | 170.195     | 122.321                                | 57.448                                       | -289.785                                              | -215.757           | 9.392              |            |
| 1300   | 75.375                                                    | 176.196     | 126.237                                | 64.946                                       | -287.087                                              | -209.697           | 8.426              |            |
| 1400   | 75.877                                                    | 181.801     | 130.008                                | 72.510                                       | -284.337                                              | -203.847           | 7.606              |            |
| 1500   | 76.191                                                    | 187.049     | 133.638                                | 80.116                                       | -281.548                                              | -198.195           | 6.902              |            |
| 1600   | 76.191                                                    | 191.966     | 137.132                                | 87.735                                       | -278.767                                              | -192.729           | 6.292              |            |
| 1700   | 76.191                                                    | 196.585     | 140.594                                | 95.354                                       | -42.143                                               | -180.261           | 5.539              |            |
| 1800   | 76.191                                                    | 200.940     | 143.733                                | 102.974                                      | -417.755                                              | -166.186           | 4.823              |            |
| 1900   | 76.191                                                    | 205.060     | 146.553                                | 110.593                                      | -414.303                                              | -152.304           | 4.187              |            |
| 2000   | 76.191                                                    | 208.968     | 149.862                                | 118.212                                      | -410.888                                              | -138.603           | 3.630              |            |
| 2100   | 76.191                                                    | 212.683     | 152.766                                | 125.831                                      | -407.509                                              | -125.072           | 3.111              |            |
| 2200   | 76.191                                                    | 216.229     | 155.570                                | 133.570                                      | -404.165                                              | -111.702           | 2.652              |            |
| 2300   | 76.191                                                    | 219.616     | 158.282                                | 141.059                                      | -400.854                                              | -98.482            | 2.237              |            |
| 2400   | 76.191                                                    | 222.859     | 160.906                                | 148.688                                      | -397.571                                              | -85.406            | 1.859              |            |
| 2500   | 76.191                                                    | 225.969     | 163.446                                |                                              | -394.313                                              | -72.466            | 1.514              |            |

CURRENT: June 1961

PREVIOUS: September 1961

## Lithium Iodide (LiI)

## Lithium Iodide (LiI)

## LIQUID

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

$$S^\circ(298.15\text{ K}) = [98.6(11) \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}]$$

 $T_{\text{fus}} = 742\text{ K}$ 

$$\Delta_H^\circ(298.15\text{ K}) = [-258.349 \text{ kJ}\cdot\text{mol}^{-1}]$$

$$\Delta_{\text{sub}}H^\circ = 14.644 \text{ kJ}\cdot\text{mol}^{-1}$$

## Enthalpy of Formation

$\Delta_H^\circ(\text{LiI}, 1, 298.15\text{ K})$  is calculated from  $\Delta_H^\circ(\text{Li}, \sigma, 298.15\text{ K})$  by adding the enthalpy of fusion,  $\Delta_{\text{fus}}H^\circ$ , and the difference in enthalpy,  $H^\circ(742\text{ K}) - H^\circ(298.15\text{ K})$ , between the crystal and liquid.

## Heat Capacity and Entropy

Dworkin<sup>1</sup> has derived the heat capacity ( $C_p^\circ = 15.1 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ) 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

$T_{\text{vap}}^{\text{(to monomer only)}} = 1497\text{ K}$  is determined as the temperature at which the fugacity is 1 atm for the reaction  $\text{Li}(g) = \text{LiI}(l)$ . The corresponding enthalpy change ( $\Delta_H^\circ$ ) at boiling point is the enthalpy of vaporization  $\Delta_{\text{vap}}H^\circ$  (to monomer only).  $T_{\text{vap}}^{\text{(to equilibrium mixture)}} = 1447\text{ K}$  is the temperature at which the sum of the calculated partial vapor pressures of  $\text{Li}(g)$  and  $\text{Li}_2\text{I}_2(g)$  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 Mugdan.<sup>2</sup>  $\Delta_{\text{vap}}H^\circ$  (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  $\text{LiI}(g)$  and  $\text{Li}_2\text{I}_2(g)$  tables.

## References

<sup>1</sup>A. S. Dworkin, Oak Ridge National Laboratory, personal communication, (December 1964).

<sup>2</sup>O. Ruff and S. Mugdan, Z. Anorg. Chem. 117, 147 (1921).

 $M_r = 133.8455$  Lithium Iodide (LiI)

|         | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |           |                                        | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                                             |                                             |
|---------|----------------------------------------------------------|-----------|----------------------------------------|-------------------------------------------------------|---------------------------------------------|---------------------------------------------|
|         | $T/K$                                                    | $C^\circ$ | $S^\circ - [G^\circ - H^\circ(T_r)]/T$ | $H^\circ - H^\circ(T_r)$                              | $\Delta_H^\circ$                            | $\Delta_G^\circ$                            |
| 0       |                                                          |           |                                        |                                                       |                                             |                                             |
| 100     |                                                          |           |                                        |                                                       |                                             |                                             |
| 200     | 298.15                                                   | 63.178    | 98.611                                 | 98.611                                                | 0                                           | -258.349                                    |
| 300     | 63.178                                                   | 99.002    | 98.612                                 | 0.117                                                 | -258.328                                    | -261.785                                    |
| 400     | 63.178                                                   | 117.177   | 101.090                                | 6.435                                                 | -265.430                                    | -262.809                                    |
| 500     | 63.178                                                   | 131.273   | 105.770                                | 12.753                                                | -289.143                                    | -259.879                                    |
| 600     | 63.178                                                   | 142.794   | 111.010                                | 19.070                                                | -287.685                                    | -254.163                                    |
| 700     | 63.178                                                   | 152.533   | 116.264                                | 25.388                                                | -286.177                                    | -248.694                                    |
| 742.000 | 63.178                                                   | 156.214   | 118.422                                | 28.042                                                | — CRYSTAL $\leftarrow \rightarrow$ LIQUID — | — CRYSTAL $\leftarrow \rightarrow$ LIQUID — |
| 800     | 63.178                                                   | 160.969   | 121.336                                | 31.705                                                | -284.644                                    | -243.444                                    |
| 900     | 63.178                                                   | 168.410   | 126.162                                | 38.024                                                | -283.113                                    | -238.386                                    |
| 1000    | 63.178                                                   | 175.057   | 130.725                                | 44.342                                                | -283.498                                    | -233.498                                    |
| 1100    | 63.178                                                   | 181.088   | 135.034                                | 50.660                                                | -280.053                                    | -228.764                                    |
| 1200    | 63.178                                                   | 186.586   | 139.104                                | 56.977                                                | -278.527                                    | -224.169                                    |
| 1300    | 63.178                                                   | 191.543   | 142.934                                | 63.295                                                | -277.010                                    | 8.828                                       |
| 1400    | 63.178                                                   | 196.225   | 146.601                                | 69.613                                                | -275.502                                    | -215.348                                    |
| 1500    | 63.178                                                   | 200.683   | 150.063                                | 75.931                                                | -274.005                                    | -211.104                                    |
| 1600    | 63.178                                                   | 204.761   | 153.355                                | 82.249                                                | -272.525                                    | -206.959                                    |
| 1700    | 63.178                                                   | 208.591   | 156.493                                | 88.567                                                | -270.302                                    | -195.730                                    |
| 1800    | 63.178                                                   | 212.02    | 159.489                                | 94.884                                                | -268.116                                    | -182.818                                    |
| 1900    | 63.178                                                   | 215.618   | 162.334                                | 101.202                                               | -261.965                                    | -170.027                                    |
| 2000    | 63.178                                                   | 218.839   | 165.099                                | 107.520                                               | -269.851                                    | -157.349                                    |
| 2100    | 63.178                                                   | 221.941   | 167.733                                | 113.338                                               | -267.773                                    | -144.775                                    |
| 2200    | 63.178                                                   | 224.860   | 170.264                                | 120.156                                               | -265.731                                    | -132.299                                    |
| 2300    | 63.178                                                   | 227.689   | 172.700                                | 126.474                                               | -263.721                                    | -121.141                                    |
| 2400    | 63.178                                                   | 230.378   | 175.048                                | 132.792                                               | -261.739                                    | -119.916                                    |
| 2500    | 63.178                                                   | 232.957   | 177.313                                | 139.109                                               | -259.782                                    | -107.616                                    |

CURRENT June 1966

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## Lithium Iodide (LiI)

## CRYSTAL-LIQUID

 $M_r = 133.8455$  Lithium Iodide (LiI)

0 to 742 K crystal  
above 742 K liquid

Refer to the individual tables for details.

| $T/K$   | $C_v^*$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                          | Standard State Pressure = $P = 0.1\text{ MPa}$ |                                         |
|---------|---------|----------------------------------------------------------|--------------------------|------------------------------------------------|-----------------------------------------|
|         |         | $\text{J K}^{-1}\text{mol}^{-1}$                         | $S^* - [G^* - H^*(T)]/T$ | $H^* - H^*(T_r)$<br>$\text{kJ mol}^{-1}$       | $\Delta H^*$<br>$\text{kJ mol}^{-1}$    |
| 0       |         |                                                          |                          |                                                |                                         |
| 100     |         |                                                          |                          |                                                |                                         |
| 200     | 50.082  | 85.772                                                   | 85.772                   | 0.                                             | -270.077                                |
| 298.15  |         |                                                          |                          |                                                |                                         |
| 300     | 50.187  | 86.082                                                   | 85.773                   | 0.093                                          | -270.080                                |
| 400     | 53.430  | 100.875                                                  | 87.767                   | 5.243                                          | -278.350                                |
| 500     | 55.948  | 113.073                                                  | 91.645                   | 10.714                                         | -302.910                                |
| 600     | 58.660  | 123.499                                                  | 96.104                   | 16.437                                         | -302.047                                |
| 700     | 62.258  | 132.807                                                  | 100.593                  | 22.480                                         | -300.814                                |
| 742.000 | 63.764  | 136.478                                                  | 102.615                  | 25.126                                         | CRYSTAL $\leftarrow \rightarrow$ LIQUID |
| 742.000 | 63.178  | 156.214                                                  | 102.615                  | 39.770                                         | TRANSITION                              |
| 800     | 63.178  | 160.969                                                  | 106.676                  | 43.435                                         | -284.644                                |
| 900     | 63.178  | 168.410                                                  | 113.130                  | 49.732                                         | -243.444                                |
| 1000    | 63.178  | 175.410                                                  | 118.597                  | 56.070                                         | -283.113                                |
| 1100    | 63.178  | 181.088                                                  | 124.372                  | 62.388                                         | -281.582                                |
| 1200    | 63.178  | 186.586                                                  | 129.331                  | 68.706                                         | -280.053                                |
| 1300    | 63.178  | 191.643                                                  | 133.932                  | 75.024                                         | -278.527                                |
| 1400    | 63.178  | 196.325                                                  | 138.224                  | 81.342                                         | -277.010                                |
| 1500    | 63.178  | 200.684                                                  | 142.244                  | 87.659                                         | -275.502                                |
| 1600    | 63.178  | 204.761                                                  | 146.025                  | 93.977                                         | -274.005                                |
| 1700    | 63.178  | 208.591                                                  | 149.594                  | 100.295                                        | -272.525                                |
| 1800    | 63.178  | 212.202                                                  | 152.973                  | 106.613                                        | -271.302                                |
| 1900    | 63.178  | 215.618                                                  | 156.181                  | 112.931                                        | -270.027                                |
| 2000    | 63.178  | 218.859                                                  | 159.234                  | 119.249                                        | -409.851                                |
| 2100    | 63.178  | 221.941                                                  | 162.148                  | 125.566                                        | -407.773                                |
| 2200    | 63.178  | 224.880                                                  | 164.913                  | 131.884                                        | -405.731                                |
| 2300    | 63.178  | 227.689                                                  | 167.601                  | 138.202                                        | -403.721                                |
| 2400    | 63.178  | 230.378                                                  | 170.161                  | 144.520                                        | -401.739                                |
| 2500    | 63.178  | 232.957                                                  | 172.622                  | 150.838                                        | -399.782                                |

PREVIOUS: CURRENT: June 1966

## Lithium Iodide (LiI)

 ${}^1\text{Li}(\text{cr},\text{l})$

## Lithium Iodide (LiI)

## IDEAL GAS

## $\text{LiI(g)}$

$$S^*(298.15 \text{ K}) = 232.262 \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta H^\circ(0 \text{ K}) = -89.09 \pm 8.4 \text{ kJ mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = -91.00 \pm 8.4 \text{ kJ mol}^{-1}$$

| Electronic Level and Quantum State | Weight ε, cm⁻¹ | ω₀ε = 3.39 cm⁻¹ | ω₀ε = 0.00416 cm⁻¹ |
|------------------------------------|----------------|-----------------|--------------------|
| 2*                                 | 0              |                 |                    |
| 1                                  |                |                 |                    |

$$\omega_0 \epsilon = 498.16 \text{ cm}^{-1}$$

$$B_\epsilon = 0.44837 \text{ cm}^{-1}$$

### Enthalpy of Formation

The enthalpy of formation,  $\Delta_f H^\circ(\text{LiI, g}, 298.15 \text{ K}) = -21.75 \pm 2 \text{ kcal mol}^{-1}$ , 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  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{monomer, 298.15 K}) = 43.2 \pm 0.4 \text{ kcal mol}^{-1}$  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 ( $\Omega_{\text{dimer}}/P_{\text{monomer}} = 6$ ) which have been used for 3rd law calculation. Using the same technique, Friedman reported the heats of sublimation as  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{monomer, 722 K}) = 41.9 \pm 0.5 \text{ kcal mol}^{-1}$  and  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{dimer, 722 K}) = 40.8 \pm 0.5 \text{ kcal mol}^{-1}$  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⁻¹ 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>5</sup> In order to have good agreement between the calculated vapor pressure and the observed total vapor pressure, the heats of sublimation have been so chosen as  $\Delta_{\text{sub}} H^\circ(\text{298.15 K}) = 42.8 \text{ kcal mol}^{-1}$  and  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{dimer, 298.15 K}) = 42.6 \text{ kcal mol}^{-1}$  and the heat of dissociation of dimer,  $\Delta H^\circ(\text{cr} \rightarrow \text{monomer, 298.15 K}) = 43.0 \text{ kcal mol}^{-1}$ . 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                                                                                                         | $\Delta_f H^\circ(298.15 \text{ K}), \text{ kcal mol}^{-1}$ |
|----------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------|
| $\text{LiI(cr)} \rightarrow \text{LiI(g)}$                     | Gorokhov<br>Friedman<br>Gorokhov<br>Friedman<br>$\text{Li}_2\text{I}_x(\text{g}) \rightarrow 2 \text{ LiI(g)}$ | 44.7<br>43.9<br>41.3<br>44.1<br>38.8<br>43.7<br>43.2        |
| $\text{2 LiI(cr)} \rightarrow \text{Li}_2\text{I}_x(\text{g})$ | —                                                                                                              | 42.2                                                        |
| $\text{Li}_2\text{I}_x(\text{g}) \rightarrow 2 \text{ LiI(g)}$ | Berkowitz <i>et al.</i>                                                                                        | —                                                           |
| $\text{LiI(g)}$                                                | Friedman<br>Gorokhov                                                                                           | 43.1<br>43.2                                                |

### Heat Capacity and Entropy

The bond distance and the rotational constants ( $B_e$  and  $\nu_e$ ), corrected to the isotopic abundance of 7.4%  $\text{Li}^6$  and 92.6%  $\text{Li}^7$ , were obtained from the microwave studies by Honig *et al.*<sup>6</sup> The vibrational constants ( $\omega_e$  and  $\omega_{e\perp}$ ) were determined from the infrared spectrum by Klempner *et al.*<sup>7</sup> The tabulated thermodynamic functions are in reasonable agreement with those calculated by Wilkins who used slightly different molecular constants.

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## $\text{LiI(g)}$

|        |  | Enthalpy Reference Temperature = T = 298.15 K  |         |                                              |                    | Standard State Pressure = p° = 0.1 MPa |          |                        |                    |
|--------|--|------------------------------------------------|---------|----------------------------------------------|--------------------|----------------------------------------|----------|------------------------|--------------------|
|        |  | $C_p^\circ, \text{ J K}^{-1} \text{ mol}^{-1}$ |         | $S^\circ, \text{ J K}^{-1} \text{ mol}^{-1}$ |                    | $H^\circ - H^\circ(T_1)/T$             |          | $k \text{ J mol}^{-1}$ | $\Delta_f G^\circ$ |
| T/K    |  | 0                                              | 0       | 0                                            | -[G° - H°(T, 1)]/T | 0                                      | -ΔH°     | 0                      | log K <sub>f</sub> |
| 0      |  | 0                                              | 0       | 0                                            | INFINITE           | -9.297                                 | -89.078  | -104.161               | INFINITE           |
| 100    |  | 29.475                                         | 197.607 | 261.437                                      | -6.383             | -88.184                                | -119.720 | -126.588               | 54.408             |
| 200    |  | 32.394                                         | 218.879 | 235.163                                      | -3.297             | -89.405                                | -127.209 | -134.077               | 31.678             |
| 250    |  | 33.663                                         | 226.251 | 232.826                                      | -1.644             | -90.194                                | -127.979 | -134.830               | 21.683             |
| 298.15 |  | 34.572                                         | 231.262 | 232.262                                      | 0.                 | -91.002                                | -134.265 | -135.523               | 23.523             |
| 300    |  | 34.602                                         | 232.476 | 232.262                                      | 0.064              | -91.034                                | -134.534 | -135.824               | 23.424             |
| 350    |  | 33.289                                         | 231.864 | 232.086                                      | 1.812              | -91.935                                | -141.713 | -142.450               | 19.390             |
| 400    |  | 33.798                                         | 242.611 | 233.636                                      | 3.590              | -100.928                               | -148.450 | -149.300               | 17.914             |
| 450    |  | 36.185                                         | 246.851 | 234.873                                      | 5.390              | -102.568                               | -154.327 | -155.327               | 16.483             |
| 500    |  | 36.485                                         | 250.679 | 236.265                                      | 7.207              | -127.342                               | -157.780 | -158.780               | 14.256             |
| 600    |  | 36.521                                         | 257.372 | 239.241                                      | 10.879             | -128.530                               | -163.755 | -164.537               | 12.651             |
| 700    |  | 37.223                                         | 263.088 | 242.250                                      | 14.587             | -129.631                               | -169.537 | -170.166               | 11.437             |
| 800    |  | 37.448                                         | 268.074 | 245.173                                      | 18.321             | -130.683                               | -175.166 | -176.654               | 10.485             |
| 900    |  | 37.627                                         | 272.495 | 247.967                                      | 22.075             | -131.715                               | -180.664 | -181.048               | 9.718              |
| 1000   |  | 37.777                                         | 276.467 | 250.622                                      | 25.845             | -132.732                               | -186.048 | -186.432               | 9.086              |
| 1100   |  | 37.906                                         | 280.074 | 253.138                                      | 29.629             | -133.736                               | -191.131 | -191.523               | 8.554              |
| 1200   |  | 38.022                                         | 283.377 | 253.522                                      | 33.426             | -134.732                               | -196.523 | -197.112               | 8.012              |
| 1300   |  | 38.128                                         | 286.425 | 257.784                                      | 37.234             | -135.725                               | -201.632 | -202.580               | 5.658              |
| 1400   |  | 38.227                                         | 289.254 | 259.932                                      | 41.051             | -136.717                               | -206.665 | -207.587               | 2.164              |
| 1500   |  | 38.321                                         | 291.895 | 261.976                                      | 44.870             | -137.710                               | -211.627 | -212.569               | 7.711              |
| 1600   |  | 38.410                                         | 294.371 | 263.924                                      | 48.715             | -138.712                               | -216.522 | -217.464               | 7.069              |
| 1700   |  | 38.596                                         | 296.702 | 265.784                                      | 52.561             | -284.962                               | -214.178 | -215.126               | 6.584              |
| 1800   |  | 38.580                                         | 298.905 | 267.563                                      | 56.415             | -285.239                               | -210.006 | -210.966               | 6.094              |
| 1900   |  | 38.662                                         | 300.993 | 269.268                                      | 60.277             | -285.543                               | -205.819 | -206.780               | 5.658              |
| 2000   |  | 38.742                                         | 302.978 | 270.903                                      | 64.147             | -285.847                               | -201.614 | -202.576               | 2.163              |
| 2100   |  | 38.821                                         | 304.870 | 272.477                                      | 68.025             | -286.239                               | -197.392 | -198.337               | 4.910              |
| 2200   |  | 38.899                                         | 306.678 | 273.450                                      | 71.911             | -286.629                               | -193.152 | -194.194               | 4.586              |
| 2300   |  | 38.976                                         | 308.469 | 275.450                                      | 75.805             | -287.043                               | -188.874 | -189.820               | 4.290              |
| 2400   |  | 39.052                                         | 310.069 | 276.858                                      | 79.706             | -287.478                               | -184.617 | -185.562               | 4.018              |
| 2500   |  | 39.128                                         | 311.165 | 278.219                                      | 83.615             | -287.930                               | -180.322 | -181.307               | 3.768              |
| 2600   |  | 39.203                                         | 313.201 | 279.535                                      | 87.532             | -288.394                               | -176.009 | -177.009               | 3.536              |
| 2700   |  | 39.277                                         | 314.682 | 280.810                                      | 91.456             | -288.867                               | -171.677 | -172.677               | 3.321              |
| 2800   |  | 39.352                                         | 316.112 | 282.045                                      | 95.387             | -289.324                               | -167.528 | -168.528               | 2.935              |
| 2900   |  | 39.426                                         | 317.494 | 283.244                                      | 99.326             | -289.802                               | -162.962 | -163.962               | 2.761              |
| 3000   |  | 39.499                                         | 318.832 | 284.408                                      | 103.272            | -290.300                               | -158.580 | -159.580               | 2.598              |
| 3100   |  | 39.572                                         | 320.128 | 285.539                                      | 107.226            | -290.771                               | -154.181 | -155.181               | 2.445              |
| 3200   |  | 39.645                                         | 321.386 | 286.640                                      | 111.187            | -291.236                               | -149.768 | -150.768               | 2.102              |
| 3300   |  | 39.718                                         | 322.607 | 287.756                                      | 115.155            | -291.693                               | -145.340 | -146.340               | 2.014              |
| 3400   |  | 39.791                                         | 323.794 | 288.755                                      | 119.131            | -292.140                               | -140.898 | -141.898               | 1.816              |
| 3500   |  | 39.863                                         | 324.948 | 289.773                                      | 123.113            | -292.578                               | -136.443 | -137.443               | 2.036              |
| 3600   |  | 39.936                                         | 326.099 | 290.766                                      | 127.103            | -293.007                               | -131.976 | -132.976               | 1.915              |
| 3700   |  | 40.008                                         | 327.167 | 291.735                                      | 131.100            | -293.426                               | -127.497 | -128.497               | 1.800              |
| 3800   |  | 40.080                                         | 328.225 | 292.681                                      | 135.105            | -293.838                               | -123.007 | -124.007               | 1.691              |
| 3900   |  | 40.152                                         | 329.277 | 293.606                                      | 139.116            | -294.242                               | -118.506 | -119.506               | 1.587              |
| 4000   |  | 40.224                                         | 330.329 | 294.511                                      | 143.135            | -294.641                               | -113.995 | -114.995               | 1.489              |
| 4100   |  | 40.296                                         | 331.289 | 295.396                                      | 147.161            | -295.035                               | -110.474 | -111.474               | 1.395              |
| 4200   |  | 40.368                                         | 332.261 | 296.261                                      | 151.194            | -295.426                               | -109.404 | -110.404               | 1.305              |
| 4300   |  | 40.439                                         | 334.121 | 297.110                                      | 155.235            | -295.821                               | -100.404 | -101.404               | 1.220              |
| 4400   |  | 40.511                                         | 334.142 | 297.941                                      | 159.282            | -296.194                               | -95.836  | -96.836                | 1.138              |
| 4500   |  | 40.583                                         | 335.053 | 298.756                                      | 163.337            | -296.583                               | -91.299  | -92.299                | 1.060              |
| 4600   |  | 40.654                                         | 335.946 | 299.555                                      | 167.399            | -296.980                               | -86.732  | -87.732                | 0.985              |
| 4700   |  | 40.726                                         | 336.821 | 300.338                                      | 171.468            | -297.383                               | -82.158  | -83.158                | 0.913              |
| 4800   |  | 40.797                                         | 337.679 | 301.107                                      | 175.544            | -297.796                               | -77.574  | -78.574                | 0.844              |
| 4900   |  | 40.869                                         | 338.521 | 301.862                                      | 180.627            | -298.222                               | -72.981  | -73.981                | 0.778              |
| 5000   |  | 40.940                                         | 339.347 | 302.604                                      | 183.718            | -298.561                               | -68.380  | -69.380                | 0.714              |
| 5100   |  | 41.011                                         | 340.159 | 303.332                                      | 187.815            | -298.811                               | -63.771  | -64.771                | 0.653              |
| 5200   |  | 41.083                                         | 340.595 | 304.048                                      | 191.920            | -299.111                               | -59.152  | -60.152                | 0.594              |
| 5300   |  | 41.154                                         | 341.739 | 304.752                                      | 196.032            | -299.424                               | -54.523  | -55.523                | 0.537              |
| 5400   |  | 41.225                                         | 342.509 | 305.444                                      | 200.151            | -299.726                               | -50.500  | -51.500                | 0.483              |
| 5500   |  | 41.296                                         | 343.266 | 306.125                                      | 204.277            | -301.145                               | -45.238  | -46.238                | 0.430              |
| 5600   |  | 41.368                                         | 344.011 | 307.795                                      | 208.410            | -302.422                               | -40.579  | -41.579                | 0.379              |
| 5700   |  | 41.439                                         | 344.744 | 307.454                                      | 212.550            | -302.324                               | -35.911  | -36.911                | 0.329              |
| 5800   |  | 41.510                                         | 345.465 | 308.103                                      | 216.698            | -302.962                               | -31.231  | -32.231                | 0.281              |
| 5900   |  | 41.581                                         | 346.275 | 308.743                                      | 220.852            | -303.536                               | -36.541  | -37.541                | 0.235              |
| 6000   |  | 41.652                                         | 346.973 | 309.347                                      | 225.014            | -304.347                               | -21.838  | -22.838                | 0.190              |

CURRENT June 1966 (1 bar)

PREVIOUS June 1966 (1 atm)

## Lithium Iodide (LiI)





## Nitrosyl Iodide (NOI)

## IDEAL GAS

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

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

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

Vibrational Frequencies and Degeneracies

$$v, \text{ cm}^{-1}$$

$$[1780](1)$$

$$[440](1)$$

$$[200](1)$$

Ground State Quantum Weight: 1

$$\alpha = 1$$

Point Group:  $C_s$ 

Bond Distances: O-N = [1.15] Å

N-I = [2.3] Å

Bond Angle: O-N-I = [120]°

Product of the Moments of Inertia:  $I_{\text{A}}I_{\text{B}}I_{\text{C}} = [7.908120 \times 10^{15}] \text{ g}^2 \cdot \text{cm}^6$ 

## Enthalpy of Formation

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

## Heat Capacity and Entropy

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

| T/K    | $J \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ |           | $H^\circ - H^\circ(T_J)/T$    |                  | Standard State Pressure = $P = 0.1 \text{ MPa}$ |                  |
|--------|-----------------------------------------------|-----------|-------------------------------|------------------|-------------------------------------------------|------------------|
|        | $C_p$                                         | $S^\circ$ | $-[C^\circ - H^\circ(T_J)]/T$ | $\Delta H^\circ$ | $k \cdot \text{mol}^{-1}$                       | $\Delta G^\circ$ |
| 0      | 0                                             | 0         | 0                             | -12.107          | 115.300                                         | INFINITE         |
| 100    | 38.203                                        | 236.047   | 322.541                       | -8.629           | 114.349                                         | 110.430          |
| 200    | 44.111                                        | 264.773   | 287.171                       | -4.480           | 113.122                                         | -27.948          |
| 250    | 45.744                                        | 274.803   | 283.726                       | -2.231           | 112.600                                         | -22.032          |
| 298.15 | 46.856                                        | 282.960   | 282.961                       | 0                | 112.131                                         | 104.227          |
| 300    | 46.893                                        | 283.250   | 283.250                       | 0.087            | 112.113                                         | 104.178          |
| 350    | 47.790                                        | 290.548   | 284.822                       | 4.864            | 103.127                                         | 102.894          |
| 400    | 48.566                                        | 296.281   | 284.822                       | 4.864            | 101.875                                         | -13.314          |
| 450    | 49.279                                        | 302.743   | 286.998                       | 7.310            | 102.065                                         | -11.825          |
| 500    | 49.950                                        | 307.930   | 288.388                       | 9.791            | 101.937                                         | -10.845          |
| 600    | 51.181                                        | 317.188   | 292.440                       | 14.849           | 81.066                                          | -9.435           |
| 800    | 52.248                                        | 325.160   | 296.588                       | 20.027           | 81.207                                          | -8.425           |
| 900    | 53.146                                        | 332.197   | 300.311                       | 25.293           | 81.345                                          | -7.667           |
| 1000   | 53.890                                        | 338.301   | 304.451                       | 30.646           | 81.532                                          | -7.076           |
| 1000   | 54.503                                        | 344.212   | 308.146                       | 36.066           | 81.701                                          | -6.603           |
| 1100   | 55.006                                        | 349.431   | 311.665                       | 41.543           | 81.866                                          | -6.214           |
| 1200   | 55.422                                        | 354.236   | 315.015                       | 47.085           | 82.023                                          | -5.890           |
| 1300   | 55.767                                        | 358.686   | 318.205                       | 52.625           | 82.166                                          | -5.615           |
| 1400   | 56.055                                        | 362.829   | 321.246                       | 58.216           | 82.291                                          | 144.177          |
| 1500   | 56.297                                        | 366.705   | 324.149                       | 63.834           | 148.594                                         | 5.174            |
| 1600   | 56.302                                        | 370.345   | 326.924                       | 69.474           | 82.459                                          | -4.995           |
| 1700   | 56.677                                        | 373.776   | 329.580                       | 75.133           | 82.492                                          | 157.413          |
| 1800   | 56.827                                        | 377.020   | 332.126                       | 80.809           | 82.484                                          | 161.820          |
| 1900   | 56.955                                        | 380.996   | 334.571                       | 86.498           | 82.434                                          | 166.229          |
| 2000   | 57.069                                        | 383.020   | 339.592                       | 92.199           | 82.339                                          | 167.641          |
| 2100   | 57.167                                        | 385.807   | 339.183                       | 97.911           | 82.207                                          | 175.059          |
| 2200   | 57.253                                        | 388.469   | 341.163                       | 103.632          | 82.024                                          | 179.486          |
| 2300   | 57.229                                        | 391.015   | 342.467                       | 109.362          | 81.824                                          | 182.920          |
| 2400   | 57.197                                        | 393.457   | 345.899                       | 115.098          | 81.561                                          | 188.365          |
| 2500   | 57.457                                        | 395.801   | 347.463                       | 120.841          | 81.286                                          | 192.820          |
| 2600   | 57.511                                        | 398.056   | 349.367                       | 126.589          | 80.990                                          | 197.288          |
| 2700   | 57.559                                        | 400.227   | 351.211                       | 132.343          | 80.578                                          | 201.767          |
| 2800   | 57.602                                        | 352.999   | 352.999                       | 138.101          | 80.137                                          | 206.258          |
| 2900   | 57.641                                        | 404.343   | 354.343                       | 143.863          | 80.032                                          | 210.759          |
| 3000   | 57.677                                        | 406.298   | 356.422                       | 149.629          | 80.798                                          | -3.796           |
| 3100   | 57.709                                        | 408.190   | 358.061                       | 155.398          | 79.390                                          | 219.797          |
| 3200   | 57.738                                        | 410.022   | 359.556                       | 161.171          | 79.861                                          | 224.331          |
| 3300   | 57.765                                        | 411.799   | 361.210                       | 166.946          | 78.785                                          | 232.962          |
| 3400   | 57.790                                        | 413.524   | 362.723                       | 172.724          | 78.504                                          | 233.427          |
| 3500   | 57.812                                        | 415.200   | 364.199                       | 178.504          | 78.241                                          | 237.988          |
| 3600   | 57.833                                        | 416.829   | 365.638                       | 184.286          | 77.997                                          | 242.555          |
| 3700   | 57.852                                        | 418.414   | 367.043                       | 190.070          | 77.715                                          | 247.129          |
| 3800   | 57.870                                        | 419.957   | 368.415                       | 195.836          | 77.574                                          | 251.710          |
| 3900   | 57.886                                        | 421.450   | 369.756                       | 201.644          | 77.395                                          | 256.295          |
| 4000   | 57.902                                        | 422.926   | 371.067                       | 217.434          | 77.229                                          | 260.884          |
| 4100   | 57.916                                        | 424.356   | 372.250                       | 213.225          | 77.105                                          | 265.476          |
| 4200   | 57.929                                        | 425.751   | 373.605                       | 219.017          | 76.994                                          | 270.477          |
| 4300   | 57.941                                        | 427.115   | 374.333                       | 224.810          | 76.904                                          | -3.519           |
| 4400   | 57.953                                        | 428.447   | 376.037                       | 230.605          | 76.836                                          | -3.337           |
| 4500   | 57.964                                        | 429.749   | 377.216                       | 236.401          | 76.788                                          | -3.315           |
| 4600   | 57.974                                        | 431.023   | 378.372                       | 242.198          | 76.760                                          | -3.460           |
| 4700   | 57.983                                        | 432.270   | 379.505                       | 247.996          | 76.732                                          | -3.433           |
| 4800   | 57.992                                        | 433.491   | 380.617                       | 253.794          | 76.702                                          | -3.276           |
| 4900   | 58.000                                        | 434.687   | 381.709                       | 259.594          | 76.761                                          | -3.222           |
| 5000   | 58.008                                        | 435.859   | 382.780                       | 265.394          | 76.828                                          | -3.222           |
| 5100   | 58.015                                        | 437.008   | 383.832                       | 271.195          | 76.884                                          | -3.190           |
| 5200   | 58.022                                        | 438.134   | 384.866                       | 276.997          | 76.954                                          | -3.175           |
| 5300   | 58.029                                        | 439.240   | 385.881                       | 282.809          | 77.037                                          | -3.160           |
| 5400   | 58.035                                        | 440.324   | 386.879                       | 288.603          | 77.130                                          | 325.277          |
| 5500   | 58.041                                        | 441.389   | 387.861                       | 294.407          | 77.234                                          | -3.133           |
| 5600   | 58.047                                        | 442.435   | 388.826                       | 300.211          | 77.346                                          | 334.464          |
| 5700   | 58.052                                        | 443.463   | 389.775                       | 306.016          | 77.466                                          | 339.054          |
| 5800   | 58.057                                        | 444.472   | 390.710                       | 311.822          | 77.592                                          | 343.642          |
| 5900   | 58.062                                        | 445.465   | 391.659                       | 317.628          | 77.723                                          | 348.228          |
| 6000   | 58.066                                        | 446.441   | 392.434                       | 323.434          | 77.838                                          | 352.812          |

PREVIOUS: December 1966 (1 atm)

CURRENT: December 1966 (1 bar)

## Nitrosyl Iodide (ONI)

## NIST-JANAF THERMOCHEMICAL TABLES

## Sodium Iodide (NaI)

## CRYSTAL

 $M_r = 149.89427$  Sodium Iodide (NaI)

$$\Delta H^\circ(298.15\text{ K}) = 98.500 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

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

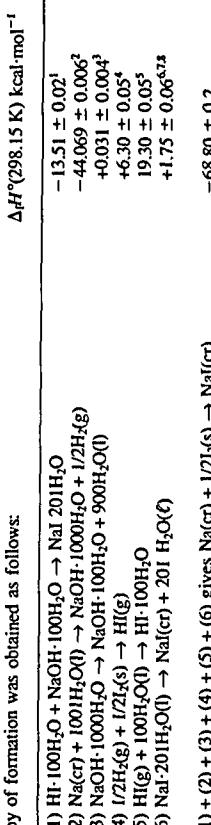
$$\Delta H^\circ(298.15\text{ K}) = -287.34 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = -287.86 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{fus}} H^\circ = 23.598 \text{ kJ}\cdot\text{mol}^{-1}$$

## Enthalpy of Formation

The enthalpy of formation was obtained as follows:



## Heat Capacity and Entropy

Smoothed heat capacities between 3 and 270 K have been presented by Berg and Morrison.<sup>6</sup> Above 270 K the heat capacity was obtained by comparing with  $K(\text{cr})$  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  $T_{\text{fus}}$  and  $\Delta_{\text{fus}} H^\circ$ .

## 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. Wiss and E. Lange, Z. Physik. Chem., **116**, 161 (1925).
- <sup>7</sup>E. Lange and A. I. Robinson, Chem. Revs., **9**, 89 (1931).
- <sup>8</sup>W. T. Berg and J. A. Morrison, Proc. Roy. Soc. (London) **242A**, 467 (1957).
- <sup>9</sup>A. Dworkin and M. Bredig, J. Phys. Chem., **64**, 259 (1960).

 $\text{I}_1\text{Na}_1(\text{cr})$ 

| $T/K$   | $C_p^\circ$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                          |                     | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                      |          |
|---------|-------------|----------------------------------------------------------|--------------------------|---------------------|-------------------------------------------------------|----------------------|----------|
|         |             | $S^\circ - [G^\circ - H^\circ(T_r)]/T$                   | $H^\circ - H^\circ(T_r)$ | $k\text{-mol}^{-1}$ | $\Delta G^\circ$                                      | $\text{kg K,}$       |          |
| 0       | 0           | 0                                                        | -12,523                  | -287,336            | -287,477                                              | -286,336             | INFINITE |
| 100     | 43,032      | 45,601                                                   | -9,749                   | -287,621            | -283,566                                              | -283,593             | 149,581  |
| 200     | 49,852      | 78,103                                                   | 103,207                  | -5,021              | -287,621                                              | -283,566             |          |
| 298.15  | 52,225      | 98,500                                                   | 98,500                   | 0                   | -287,839                                              | -284,572             | 49,856   |
| 300     | 52,258      | 98,823                                                   | 98,501                   | 0.097               | -287,865                                              | -284,551             | 49,545   |
| 400     | 53,806      | 114,077                                                  | 100,570                  | 5,403               | -299,000                                              | -282,898             | 36,943   |
| 500     | 55,020      | 126,213                                                  | 104,526                  | 10,844              | -320,758                                              | -276,772             | 28,914   |
| 600     | 56,233      | 136,353                                                  | 109,008                  | 16,407              | -320,088                                              | -268,035             | 23,315   |
| 700     | 57,363      | 145,106                                                  | 113,554                  | 22,087              | -319,244                                              | -259,424             | 19,258   |
| 800     | 58,492      | 152,840                                                  | 117,950                  | 27,880              | -318,230                                              | -250,945             | 16,385   |
| 900     | 59,580      | 159,573                                                  | 122,255                  | 33,784              | -317,128                                              | -242,598             | 14,080   |
| 933.000 | 59,939      | 161,945                                                  | 123,621                  | 35,756              | ---                                                   | CRYSTAL. <--> LIQUID | ---      |
| 1000    | 60,675      | 166,127                                                  | 126,530                  | 39,796              | -315,904                                              | -24,381              | 12,243   |
| 1100    | 61,764      | 171,961                                                  | 130,217                  | 45,918              | -314,598                                              | -276,297             | 10,746   |
| 1200    | 62,844      | 177,381                                                  | 133,924                  | 52,149              | -315,994                                              | -215,884             | 9,397    |
| 1300    | 63,914      | 182,454                                                  | 137,454                  | 58,487              | -407,663                                              | -8,028               |          |
| 1400    | 64,974      | 187,229                                                  | 140,850                  | 64,931              | -405,241                                              | -183,903             | 6,861    |
| 1500    | 66,024      | 191,748                                                  | 144,093                  | 71,481              | -402,733                                              | -168,180             | 5,357    |
| 1600    | 67,064      | 196,942                                                  | 147,207                  | 78,136              | -400,146                                              | -152,677             | 4,983    |
| 1700    | 68,095      | 200,139                                                  | 150,201                  | 84,894              | -397,484                                              | -157,238             | 4,217    |
| 1800    | 69,116      | 204,960                                                  | 153,985                  | 91,734              | -394,753                                              | -122,008             | 3,541    |
| 1900    | 70,127      | 207,924                                                  | 155,868                  | 98,717              | -391,956                                              | -106,931             | 2,940    |
| 2000    | 71,128      | 211,446                                                  | 158,357                  | 105,779             | -389,093                                              | -92,004              | 2,403    |

PREVIOUS CURRENT: September 1963

## Sodium Iodide (NaI)

**Sodium Iodide (NaI)**

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

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

**Enthalpy of Formation**

$\Delta H^\circ(\text{NaI}, 1, 298.15\text{ K})$  is calculated from that of the crystal by adding  $\Delta_{\text{fus}}H^\circ$  and the difference in enthalpy,  $H^\circ(933\text{ K}) - H^\circ(298.15\text{ K})$ .

**Heat Capacity and Entropy**

$C_p^\circ$  is assumed assuming each atom contributed 7.75 cal·K<sup>-1</sup>·mol<sup>-1</sup>.  $S^\circ(\text{NaI}, 1, 298.15\text{ K})$  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,  $T_{\text{bp}} = 1577\text{ K}$  ( $1 \rightarrow$  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).

**Liquid****I<sub>1</sub>Na(I)**

$$M_r = 149.89427$$

**I<sub>1</sub>Na(I)**

| $\Delta H^\circ(298.15\text{ K}) = [-266.508] \text{ kJ}\cdot\text{mol}^{-1}$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |             |           |                             | Standard State Pressure = $p = 0.1 \text{ MPa}$ |                  |                     |            |
|-------------------------------------------------------------------------------|----------------------------------------------------------|-------------|-----------|-----------------------------|-------------------------------------------------|------------------|---------------------|------------|
|                                                                               | $T/K$                                                    | $C_p^\circ$ | $S^\circ$ | $-[G^\circ - H^\circ(T)]/T$ | $H^\circ - H^\circ(T)$                          | $\Delta H^\circ$ | $\Delta G^\circ$    | $\log K_r$ |
| 0                                                                             |                                                          |             |           |                             | 0.                                              | -266.508         | -269.856            | 47.278     |
| 100                                                                           | 298.15                                                   | 52.225      | 120.754   | 120.754                     | 0.097                                           | -266.514         | -269.876            | 46.990     |
| 200                                                                           | 300                                                      | 52.258      | 121.077   | 120.755                     | 5.403                                           | -277.649         | -270.448            | 35.317     |
| 300                                                                           | 400                                                      | 53.806      | 136.331   | 122.824                     | 10.844                                          | -289.407         | -265.548            | 27.846     |
| 400                                                                           | 500                                                      | 55.020      | 148.468   | 126.780                     | 16.407                                          | -298.737         | -260.036            | 22.638     |
| 500                                                                           | 600                                                      | 56.233      | 158.606   | 131.262                     | 16.407                                          | —                | GLASS <--> LIQUID   | —          |
| 600                                                                           | 600,000                                                  | 56.233      | 158.606   | 131.262                     | 16.407                                          | —                | TRANSITION          | —          |
| 600,000                                                                       | 600,000                                                  | 158.606     | 131.262   | 16.407                      | —                                               | —                | —                   | —          |
| 700                                                                           | 600                                                      | 64.852      | 177.603   | 135.901                     | 22.892                                          | -297.088         | 18.933              | 18.933     |
| 800                                                                           | 600                                                      | 64.852      | 177.653   | 140.542                     | 29.377                                          | -295.401         | -247.635            | 16.469     |
| 900                                                                           | 600                                                      | 64.852      | 184.902   | 145.955                     | 35.862                                          | -293.659         | -241.766            | 14.032     |
| 933,000                                                                       | 933,000                                                  | 191.734     | 146.506   | 146.506                     | 38.002                                          | —                | CRYSTAL <--> LIQUID | —          |
| 1000                                                                          | 64.852                                                   | 191.734     | 149.387   | 149.387                     | 42.347                                          | -292.002         | -236.087            | 12.332     |
| 1200                                                                          | 64.852                                                   | 203.558     | 153.522   | 153.522                     | 48.833                                          | -290.333         | -230.576            | 10.949     |
| 1300                                                                          | 64.852                                                   | 208.749     | 161.208   | 157.460                     | 55.318                                          | -385.474         | -222.776            | 9.697      |
| 1400                                                                          | 64.852                                                   | 213.555     | 164.778   | 164.778                     | 61.803                                          | -382.995         | -209.318            | 8.411      |
| 1500                                                                          | 64.852                                                   | 218.030     | 168.181   | 174.773                     | 74.773                                          | -380.532         | -196.031            | 7.315      |
| 1600                                                                          | 64.852                                                   | 222.215     | 171.428   | 181.259                     | 81.259                                          | -378.089         | -182.959            | 6.371      |
| 1700                                                                          | 64.852                                                   | 226.147     | 174.533   | 187.744                     | 87.744                                          | -375.672         | -170.030            | 5.551      |
| 1800                                                                          | 64.852                                                   | 229.854     | 177.504   | 194.229                     | 94.229                                          | -370.927         | -144.611            | 4.832      |
| 1900                                                                          | 64.852                                                   | 233.360     | 180.352   | 100.714                     | 100.714                                         | -368.607         | -132.101            | 3.632      |
| 2000                                                                          | 64.852                                                   | 236.686     | 183.087   | 107.199                     | 107.199                                         | -366.322         | -119.713            | 3.127      |
| 2100                                                                          | 64.852                                                   | 239.851     | 185.715   | 113.685                     | 113.685                                         | -364.071         | -107.438            | 2.672      |
| 2200                                                                          | 64.852                                                   | 242.867     | 188.245   | 120.170                     | 120.170                                         | -361.854         | -95.269             | 2.262      |
| 2300                                                                          | 64.852                                                   | 245.750     | 190.683   | 126.655                     | 126.655                                         | -359.666         | -83.201             | 1.890      |
| 2400                                                                          | 64.852                                                   | 248.510     | 193.035   | 133.140                     | 133.140                                         | -357.503         | -71.227             | 1.550      |
| 2500                                                                          | 64.852                                                   | 251.158     | 195.308   | 139.625                     | 139.625                                         | -355.360         | -59.343             | 1.240      |
| 2600                                                                          | 64.852                                                   | 253.701     | 197.505   | 146.111                     | 146.111                                         | -353.233         | -47.544             | 0.955      |
| 2700                                                                          | 64.852                                                   | 256.149     | 199.632   | 152.596                     | 152.596                                         | -351.116         | -35.827             | 0.693      |
| 2800                                                                          | 64.852                                                   | 258.507     | 201.693   | 159.081                     | 159.081                                         | -349.005         | -24.188             | 0.451      |
| 2900                                                                          | 64.852                                                   | 260.783     | 203.691   | 163.566                     | 163.566                                         | -346.897         | -12.625             | 0.227      |
| 3000                                                                          | 64.852                                                   | 262.982     | 205.631   | 172.051                     | 172.051                                         | -344.787         | -1.134              | 0.020      |

CURRENT: September 1963

PREVIOUS:

**Sodium Iodide (NaI)****I<sub>1</sub>Na(I)**

## Sodium Iodide (NaI)

**M<sub>r</sub> = 149.89427 Sodium Iodide (NaI)****CRYSTAL-LIQUID**

0 to 933 K crystal  
above 933 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 <sup>*</sup> = 0.1 MPa     |                                                   |                                      |
|---------|------------------------------------------------------------|--------------------------------------------------------|--------------------------------------------------------|---------------------------------------------------|--------------------------------------|
|         | C <sub>p</sub><br>J·K <sup>-1</sup> ·mol <sup>-1</sup>     | S <sup>*</sup><br>J·K <sup>-1</sup> ·mol <sup>-1</sup> | -[G <sup>*</sup> - H <sup>r</sup> (T <sub>r</sub> )]/T | H <sup>r</sup> - H <sup>r</sup> (T <sub>r</sub> ) | kJ·mol <sup>-1</sup>                 |
| 0       | 0                                                          | 0                                                      | INFINITE                                               | -12.523                                           | -287.336                             |
| 100     | 43.032                                                     | 45.001                                                 | 143.089                                                | -9.749                                            | -286.536                             |
| 200     | 49.852                                                     | 78.103                                                 | 103.207                                                | -5.021                                            | -285.621                             |
| 298.15  | 52.225                                                     | 98.500                                                 | 98.500                                                 | 0                                                 | -287.859                             |
| 300     | 52.258                                                     | 98.823                                                 | 98.501                                                 | 0.097                                             | -287.865                             |
| 400     | 53.806                                                     | 114.077                                                | 100.570                                                | 5.403                                             | -299.000                             |
| 500     | 55.020                                                     | 126.213                                                | 104.526                                                | 10.844                                            | -276.772                             |
| 600     | 56.233                                                     | 136.353                                                | 109.008                                                | 16.407                                            | -268.035                             |
| 700     | 57.363                                                     | 145.106                                                | 113.554                                                | 22.087                                            | -259.424                             |
| 800     | 58.492                                                     | 152.840                                                | 117.990                                                | 27.880                                            | -250.945                             |
| 900     | 59.580                                                     | 159.793                                                | 122.255                                                | 33.784                                            | -242.598                             |
| 933.000 | 59.939                                                     | 161.945                                                | 123.621                                                | 35.756                                            | — CRYSTAL <--> LIQUID — TRANSITION — |
| 933.000 | 64.852                                                     | 187.237                                                | 123.621                                                | 59.354                                            |                                      |
| 1000    | 64.852                                                     | 191.734                                                | 128.036                                                | 63.659                                            | -292.002                             |
| 1100    | 64.852                                                     | 197.915                                                | 134.112                                                | 70.184                                            | -290.333                             |
| 1200    | 64.852                                                     | 203.558                                                | 139.667                                                | 76.669                                            | -290.576                             |
| 1300    | 64.852                                                     | 208.749                                                | 144.784                                                | 83.154                                            | -222.776                             |
| 1400    | 64.852                                                     | 213.555                                                | 149.527                                                | 89.639                                            | -382.995                             |
| 1500    | 64.852                                                     | 218.030                                                | 153.946                                                | 96.125                                            | -380.532                             |
| 1600    | 64.852                                                     | 222.215                                                | 158.084                                                | 102.610                                           | -378.089                             |
| 1700    | 64.852                                                     | 226.147                                                | 161.973                                                | 109.095                                           | -373.672                             |
| 1800    | 64.852                                                     | 229.854                                                | 165.642                                                | 115.580                                           | -157.250                             |
| 1900    | 64.852                                                     | 233.356                                                | 169.115                                                | 122.065                                           | -144.611                             |
| 2000    | 64.852                                                     | 236.686                                                | 172.411                                                | 128.551                                           | -132.101                             |
| 2100    | 64.852                                                     | 239.850                                                | 175.548                                                | 135.036                                           | -364.071                             |
| 2200    | 64.852                                                     | 242.867                                                | 178.540                                                | 141.521                                           | -107.438                             |
| 2300    | 64.852                                                     | 245.750                                                | 181.400                                                | 148.006                                           | -95.269                              |
| 2400    | 64.852                                                     | 248.510                                                | 184.139                                                | 154.491                                           | -83.201                              |
| 2500    | 64.852                                                     | 251.158                                                | 186.167                                                | 160.977                                           | -71.227                              |
| 2600    | 64.852                                                     | 253.701                                                | 189.293                                                | 167.462                                           | -35.360                              |
| 2700    | 64.852                                                     | 256.149                                                | 191.724                                                | 173.947                                           | -353.233                             |
| 2800    | 64.852                                                     | 258.507                                                | 194.067                                                | 180.432                                           | -47.544                              |
| 2900    | 64.852                                                     | 260.783                                                | 196.529                                                | 186.917                                           | -351.116                             |
| 3000    | 64.852                                                     | 262.982                                                | 198.514                                                | 193.403                                           | -346.897                             |

LiNa<sub>1</sub>(cr,l)

## Iodine Oxide (IO)

## IDEAL GAS

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

$$D_0^e = 18892 \pm 1500 \text{ cm}^{-1}$$

$$S^*(298.15 \text{ K}) = 239.6 \pm 1 \text{ J K}^{-1} \cdot \text{mol}^{-1}$$

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

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

| State                           | $T_e$    | Electronic Levels and Molecular Constants ( <sup>17</sup> I <sup>16</sup> O), cm <sup>-1</sup> |            |        |            | $\sigma=1$ |        |
|---------------------------------|----------|------------------------------------------------------------------------------------------------|------------|--------|------------|------------|--------|
|                                 |          | $\epsilon_e$                                                                                   | $\omega_e$ | $B_e$  | $\alpha_e$ |            |        |
| X <sup>2</sup> Π <sub>3/2</sub> | 0        | 2                                                                                              | 681.6004   | 4.3699 | 0.340206   | 0.0026296  | 3.6    |
| X <sup>2</sup> Π <sub>1/2</sub> | 2091     | 2                                                                                              | 681.6004   | 4.3699 | 0.340206   | 0.0026296  | 3.6    |
| A <sup>2</sup> Π <sub>3/2</sub> | 21557.81 | 2                                                                                              | 514.507    | 5.52   | 0.27635    | [3.2]      | 2.0723 |
| A <sup>2</sup> Π <sub>1/2</sub> | [24698]  | 2                                                                                              | 514.57     | 5.52   | 0.27635    | [3.2]      | 2.0723 |

Point Group: C<sub>∞v</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 (P<sub>1/2</sub>) + O(D<sub>1</sub>). Coleman *et al.*<sup>1</sup> from their study of the IO spectrum in flames, used a graphical Birge-Sponer 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> (21.72 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-Sponer extrapolation of the first four vibrational levels in the upper state leading to  $D_0^e = 10200 \text{ cm}^{-1}$  for the estimated 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  $D_0^e = 238.5 \pm 25 \text{ kJ} \cdot \text{mol}^{-1}$ . This value was calculated from the assumed equilibrium constant for formation value (relative to the monatomic 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  $D_0^e = 256 \text{ kJ} \cdot \text{mol}^{-1}$  or 21400 cm<sup>-1</sup>.

Herron and Huie<sup>4</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>5</sup>,  $D_0^e = 222 \pm 13 \text{ kJ} \cdot \text{mol}^{-1}$ , and Buss *et al.*<sup>6</sup>,  $D_0^e = 230 \pm 8 \text{ kJ} \cdot \text{mol}^{-1}$ . Ruscic and Berkowitz<sup>7</sup> in determining experimentally the enthalpy of formation and ionization potential of HOBr, inferred a new value for the enthalpy of formation of IO,  $\Delta H^\circ(0, 0 \text{ K}) = 145 \text{ kJ} \cdot \text{mol}^{-1}$ . This value was a mean of the Radlein *et al.*<sup>5</sup> and the spectroscopic results.<sup>1,2</sup> In concurrence with the arguments of Huie, Herron and Laszlo we adopt  $D_0^e = 226 \text{ kJ} \cdot \text{mol}^{-1}$  which leads to  $\Delta H^\circ(0 \text{ K}) = 128 \pm 18 \text{ kJ} \cdot \text{mol}^{-1}$ . Additional data needed for the calculations presented here, e.g., thermal functions for I(g), and I<sub>2</sub>(ref), O(g), and O<sub>2</sub>(ref), are taken from JANAF Thermochemical Tables. A recent photoionization study,<sup>10</sup> confirms our adopted value.

## Heat Capacity and Entropy

The spectroscopic results tabulated above are for the <sup>17</sup>I<sup>16</sup>O isotopomer. 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  $\omega_e$  and  $\omega_a$  are from Bekooy *et al.*<sup>12</sup> and Gillies *et al.*<sup>13</sup> but the value of  $D_e$  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>16</sup> The recent measured value of Gillies *et al.*<sup>11</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.<sup>7</sup> 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>2</sup>Π<sub>3/2</sub>, was provided by Bekooy *et al.*<sup>12</sup> Vaidya<sup>18</sup> and Durie *et al.*<sup>20</sup> We adopt the 21557.81 cm<sup>-1</sup> value of Durie *et al.*<sup>21</sup> Additional excited states have been mentioned by Callear and Metcalf<sup>22</sup> and Saito.<sup>5</sup> The higher states were not included in the thermal function calculations.

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| State  | $T/K$  | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                             |                          |                    | $\sigma=1$ | Standard State Pressure = $p = 0.1 \text{ MPa}$ |            |         |         |
|--------|--------|-----------------------------------------------------------|-----------------------------|--------------------------|--------------------|------------|-------------------------------------------------|------------|---------|---------|
|        |        | $C_p^*$                                                   | $S^* - [G^\circ - HF(T)]/T$ | $H^\circ - H^\circ(T)/T$ | $\Delta_f H^\circ$ |            | $\Delta_f G^\circ$                              | $\log K_r$ |         |         |
| 0      | 0      | 0.00                                                      | 0.00                        | -9.03                    | 127.934            | INFINITE   | -9.03                                           | 127.934    | 127.934 | 127.934 |
| 50     | 29.104 | 186.214                                                   | -7.535                      | 128.200                  | 123.526            | 129.047    | -7.535                                          | 128.200    | 123.526 | 129.047 |
| 100    | 29.157 | 206.394                                                   | -6.099                      | 127.880                  | 118.056            | 127.136    | -6.099                                          | 127.880    | 118.056 | 127.136 |
| 150    | 29.263 | 218.290                                                   | -4.631                      | 127.421                  | 114.590            | 129.904    | -4.631                                          | 127.421    | 114.590 | 129.904 |
| 200    | 30.696 | 226.937                                                   | -3.124                      | 126.934                  | 103.387            | 128.830    | -3.124                                          | 126.934    | 103.387 | 128.830 |
| 250    | 31.865 | 231.933                                                   | -1.560                      | 126.455                  | 106.303            | 122.211    | -1.560                                          | 126.455    | 106.303 | 122.211 |
| 298.15 | 32.900 | 239.636                                                   | .000                        | 126.016                  | 102.465            | 127.951    | .000                                            | 126.016    | 102.465 | 127.951 |
| 300    | 32.938 | 239.839                                                   | .061                        | 125.999                  | 102.319            | 127.815    | .061                                            | 125.999    | 102.319 | 127.815 |
| 400    | 34.700 | 249.567                                                   | .346                        | 117.080                  | -12.385            | 94.840     | .346                                            | 117.080    | -12.385 | 94.840  |
| 500    | 36.155 | 257.470                                                   | .691                        | 94.997                   | 91.415             | 95.550     | .691                                            | 94.997     | 91.415  | 95.550  |
| 600    | 37.433 | 264.177                                                   | 1.067                       | 95.221                   | 90.680             | 97.894     | 1.067                                           | 95.221     | 90.680  | 97.894  |
| 700    | 38.533 | 270.032                                                   | 1.437                       | 95.510                   | 89.901             | 96.708     | 1.437                                           | 95.510     | 89.901  | 96.708  |
| 800    | 39.430 | 275.239                                                   | 1.837                       | 95.831                   | 88.075             | 97.816     | 1.837                                           | 95.831     | 88.075  | 97.816  |
| 900    | 39.792 | 255.091                                                   | 2.2351                      | 96.233                   | 85.207             | 98.207     | 2.2351                                          | 96.233     | 85.207  | 98.207  |
| 1000   | 40.624 | 284.180                                                   | 2.6389                      | 96.639                   | 87.292             | 98.650     | 2.6389                                          | 96.639     | 87.292  | 98.650  |
| 1100   | 40.968 | 288.069                                                   | 3.0470                      | 97.058                   | 86.338             | 98.400     | 3.0470                                          | 97.058     | 86.338  | 98.400  |
| 1200   | 41.187 | 294.644                                                   | 3.4277                      | 97.476                   | 83.345             | 97.715     | 3.4277                                          | 97.476     | 83.345  | 97.715  |
| 1300   | 41.311 | 294.946                                                   | 3.8704                      | 97.832                   | 84.317             | 98.338     | 3.8704                                          | 97.832     | 84.317  | 98.338  |
| 1400   | 41.366 | 298.010                                                   | 4.2839                      | 98.267                   | 83.259             | 98.106     | 4.2839                                          | 98.267     | 83.259  | 98.106  |
| 1500   | 41.371 | 300.864                                                   | 4.6976                      | 98.619                   | 82.175             | 98.262     | 4.6976                                          | 98.619     | 82.175  | 98.262  |
| 1600   | 41.344 | 303.533                                                   | 5.1112                      | 98.933                   | 81.069             | 98.647     | 5.1112                                          | 98.933     | 81.069  | 98.647  |
| 1700   | 41.294 | 306.038                                                   | 5.5244                      | 99.202                   | 79.944             | 98.456     | 5.5244                                          | 99.202     | 79.944  | 98.456  |
| 1800   | 41.229 | 308.397                                                   | 5.9370                      | 99.419                   | 78.803             | 98.287     | 5.9370                                          | 99.419     | 78.803  | 98.287  |
| 1900   | 41.154 | 310.624                                                   | 6.3490                      | 99.584                   | 78.693             | 98.187     | 6.3490                                          | 99.584     | 78.693  | 98.187  |
| 2000   | 41.071 | 312.733                                                   | 6.7602                      | 99.704                   | 78.593             | 98.087     | 6.7602                                          | 99.704     | 78.593  | 98.087  |
| 2100   | 40.980 | 314.735                                                   | 7.0703                      | 99.749                   | 78.496             | 98.000     | 7.0703                                          | 99.749     | 78.496  | 98.000  |
| 2200   | 40.882 | 316.639                                                   | 7.3797                      | 99.789                   | 78.395             | 97.908     | 7.3797                                          | 99.789     | 78.395  | 97.908  |
| 2300   | 40.774 | 318.454                                                   | 7.6879                      | 99.827                   | 78.295             | 97.827     | 7.6879                                          | 99.827     | 78.295  | 97.827  |
| 2400   | 40.655 | 320.186                                                   | 8.0057                      | 99.866                   | 78.195             | 97.748     | 8.0057                                          | 99.866     | 78.195  | 97.748  |
| 2500   | 40.524 | 321.844                                                   | 8.3235                      | 99.905                   | 78.095             | 97.654     | 8.3235                                          | 99.905     | 78.095  | 97.654  |
| 2600   | 40.380 | 323.430                                                   | 8.6424                      | 99.944                   | 77.995             | 97.557     | 8.6424                                          | 99.944     | 77.995  | 97.557  |
| 2700   | 40.221 | 324.951                                                   | 8.9616                      | 99.983                   | 77.895             | 97.457     | 8.9616                                          | 99.983     | 77.895  | 97.457  |
| 2800   | 40.048 | 326.411                                                   | 9.2772                      | 99.999                   | 77.795             | 97.357     | 9.2772                                          | 99.999     | 77.795  | 97.357  |
| 2900   | 39.859 | 327.813                                                   | 9.5871                      | 100.005                  | 77.695             | 97.255     | 9.5871                                          | 100.005    | 77.695  | 97.255  |
| 3000   | 39.655 | 329.161                                                   | 9.8970                      | 100.026                  | 77.595             | 97.152     | 9.8970                                          | 100.026    | 77.595  | 97.152  |
| 3100   | 39.438 | 330.438                                                   | 10.2025                     | 98.112                   | 63.922             | 107.077    | 10.2025                                         | 98.112     | 63.922  | 107.077 |
| 3200   | 39.208 | 331.706                                                   | 10.5171                     | 98.469                   | 62.826             | 107.026    | 10.5171                                         | 98.469     | 62.826  | 107.026 |
| 3300   | 38.966 | 332.969                                                   | 10.8221                     | 98.867                   | 61.736             | 107.000    | 10.8221                                         | 98.867     | 61.736  | 107.000 |
| 3400   | 38.713 | 334.068                                                   | 11.1271                     | 99.204                   | 60.659             | 106.992    | 11.1271                                         | 99.204     | 60.659  | 106.992 |
| 3500   | 38.452 | 335.187                                                   | 11.4321                     | 99.586                   | 59.586             | 106.903    | 11.4321                                         | 99.586     | 59.586  | 106.903 |
| 3600   | 38.184 | 336.266                                                   | 11.7355                     | 99.827                   | 58.527             | 106.819    | 11.7355                                         | 99.827     | 58.527  | 106.819 |
| 3700   | 37.912 | 337.309                                                   | 12.0396                     | 100.095                  | 57.346             | 106.735    | 12.0396                                         | 100.095    | 57.346  | 106.735 |
| 3800   | 37.653 | 338.316                                                   | 12.3436                     | 100.374                  | 56.143             | 106.643    | 12.3436                                         | 100.374    | 56.143  | 106.643 |
| 3900   | 37.358 | 339.290                                                   | 12.6476                     | 100.653                  | 55.044             | 106.551    | 12.6476                                         | 100.653    | 55.044  | 106.551 |
| 4000   | 37.080 | 340.233                                                   | 12.9516                     | 100.932                  | 54.044             | 106.453    | 12.9516                                         | 100.932    | 54.044  | 106.453 |
| 4100   | 36.803 | 341.145                                                   | 13.2556                     | 101.211                  | 53.044             | 106.352    | 13.2556                                         | 101.211    | 53.044  | 106.352 |
| 4200   | 36.529 | 342.058                                                   | 13.5595                     | 101.489                  | 52.044             | 106.254    | 13.5595                                         | 101.489    | 52.044  | 106.254 |
| 4300   | 36.259 | 342.895                                                   | 13.8635                     | 101.768                  | 51.044             | 106.156    | 13.8635                                         | 101.768    | 51.044  | 106.156 |
| 4400   | 35.993 | 343.715                                                   | 14.1717                     | 102.047                  | 50.044             | 106.056    | 14.1717                                         | 102.047    | 50.044  | 106.056 |
| 4500   | 35.734 | 344.521                                                   | 14.4763                     | 102.326                  | 49.044             | 105.959    | 14.4763                                         | 102.326    | 49.044  | 105.959 |
| 4600   | 35.480 | 345.304                                                   | 14.7803                     | 102.607                  | 48.044             | 105.859    | 14.7803                                         | 102.607    | 48.044  | 105.859 |
| 4700   | 35.234 | 346.054                                                   | 15.0843                     | 102.887                  | 47.044             | 105.759    | 15.0843                                         | 102.887    | 47.044  | 105.759 |
| 4800   | 34.996 | 346.803                                                   | 15.3883                     | 103.167                  | 46.044             | 105.659    | 15.3883                                         | 103.167    | 46.044  | 105.659 |
| 4900   | 34.765 | 347.523                                                   | 15.6823                     | 103.447                  | 45.044             | 105.559    | 15.6823                                         | 103.447    | 45.044  | 105.559 |
| 5000   | 34.543 | 348.223                                                   | 15.9863                     | 103.727                  | 44.044             | 105.459    | 15.9863                                         | 103.727    | 44.044  | 105.459 |
| 5100   | 34.328 | 348.905                                                   | 16.2803                     | 104.007                  | 43.044             | 105.359    | 16.2803                                         | 104.007    | 43.044  |         |

### Iodine oxide ( $\text{IO}$ )

$$\Delta_{ss}H^\circ(0\text{ K}) = [438 \pm 25]\text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta^\circ S(298.15\text{ K}) = [281.5 \pm 4]\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

Ideal Gas

$$M_r = 158.90327 \text{ Iodine oxide (OIO)}$$

$$\Delta H^\circ(0 \text{ K}) = [162.7 \pm 25] \text{ kJ/mol}^{-1}$$

$$\Delta H^\circ(298.15 \text{ K}) = [159.3 \pm 25] \text{ kJ/mol}^{-1}$$

Enthalpy Reference Temperature =  $T_r = 298.15 \text{ K}$

Standard State Pressure =  $p^\circ = 0.1 \text{ MPa}$   
 $\text{kJ}\cdot\text{mol}^{-1}$

| Electronic Level and Quantum Weight |                                 | v, cm <sup>-1</sup> | vibrational Frequencies and Degeneracies |
|-------------------------------------|---------------------------------|---------------------|------------------------------------------|
| state                               | $\epsilon_0$ , cm <sup>-1</sup> |                     |                                          |
| X <sup>2</sup> B <sub>1</sub>       | 0.0                             | 2                   |                                          |
|                                     |                                 | 765(1)<br>192(1)    | degeneracy                               |

Final Group: G<sub>2</sub>

Bond Distance: I-O = [1.8] Å  
 Bond Angle: O-I-O = [120]°  
 Product of the Moments of Inertia:  $I_{A\beta/C} = 725.5989 \times 10^{-117}$  g<sup>3</sup>·cm<sup>6</sup>

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**Heat Capacity and Entropy**

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 O<sub>2</sub>(E) family<sup>2</sup> and assuming  $\nu_3 > \nu_1$ .

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COSTANTINI, B.-ANAF Thermochemical Tables: OFO(g); (September 1995); OCIO(g); (March 1996); ORBogr (March 1996).

| T/K    | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$                      |                                         |                          | Standard State Pressure = $p^* = 0.1\text{ MPa}$                                   |                    |            |
|--------|-------------------------------------------------------------------------------|-----------------------------------------|--------------------------|------------------------------------------------------------------------------------|--------------------|------------|
|        | $\Delta_f H^\circ(0\text{ K}) = [162.7 \pm 25]\text{ kJ}\cdot\text{mol}^{-1}$ |                                         |                          | $\Delta_f H^\circ(298.15\text{ K}) = [159.3 \pm 25]\text{ kJ}\cdot\text{mol}^{-1}$ |                    |            |
|        | $C_p^\circ$                                                                   | $S^\circ = -[G^\circ - H^\circ(T_r)]/T$ | $H^\circ - H^\circ(T_r)$ | $\Delta_f H^\circ$                                                                 | $\Delta_f G^\circ$ | $\log K_r$ |
| 0      | .000                                                                          | .000 INFINITE                           | -11.861                  | 162.744                                                                            | 162.744            | INFINITE   |
| 50     | 34.278                                                                        | 211.198                                 | -10.189                  | 162.490                                                                            | 160.395            | -167.564   |
| 100    | 37.850                                                                        | 236.126                                 | -8.380                   | 161.795                                                                            | 158.563            | -82.825    |
| 150    | 40.093                                                                        | 251.918                                 | -6.429                   | 161.091                                                                            | 157.100            | -54.707    |
| 200    | 42.280                                                                        | 263.746                                 | 285.600                  | -4.371                                                                             | 160.427            | -40.709    |
| 250    | 44.599                                                                        | 273.429                                 | 282.252                  | -2.199                                                                             | 159.828            | -32.344    |
| 298.15 | 46.697                                                                        | 281.468                                 | 281.468                  | .000                                                                               | 153.882            | -26.959    |
| 300    | 46.772                                                                        | 281.757                                 | 281.468                  | .086                                                                               | 153.848            | -26.787    |
| 400    | 50.184                                                                        | 295.711                                 | 283.348                  | 4.945                                                                              | 150.373            | -19.908    |
| 500    | 52.445                                                                        | 307.170                                 | 287.000                  | 10.085                                                                             | 128.355            | -16.203    |
| 600    | 53.929                                                                        | 316.872                                 | 291.191                  | 15.408                                                                             | 128.642            | -13.966    |
| 700    | 54.929                                                                        | 325.265                                 | 295.473                  | 20.854                                                                             | 128.950            | -12.364    |
| 800    | 55.626                                                                        | 332.648                                 | 299.688                  | 26.384                                                                             | 129.253            | -11.160    |
| 900    | 56.127                                                                        | 339.230                                 | 303.705                  | 31.975                                                                             | 129.542            | -10.221    |
| 1000   | 56.498                                                                        | 345.164                                 | 307.559                  | 37.1605                                                                            | 129.811            | -9.469     |
| 1100   | 56.779                                                                        | 349.562                                 | 311.226                  | 43.270                                                                             | 130.059            | -8.852     |
| 1200   | 56.997                                                                        | 355.513                                 | 314.714                  | 48.959                                                                             | 130.283            | -8.336     |
| 1300   | 57.168                                                                        | 360.082                                 | 318.030                  | 54.668                                                                             | 130.480            | -7.900     |
| 1400   | 57.306                                                                        | 364.324                                 | 321.187                  | 60.391                                                                             | 130.647            | -7.525     |
| 1500   | 57.419                                                                        | 368.281                                 | 324.166                  | 66.128                                                                             | 130.779            | -7.200     |
| 1600   | 57.511                                                                        | 371.990                                 | 327.069                  | 71.875                                                                             | 130.870            | -6.915     |
| 1700   | 57.588                                                                        | 375.479                                 | 329.976                  | 77.630                                                                             | 130.915            | -6.664     |
| 1800   | 57.653                                                                        | 378.773                                 | 332.444                  | 83.392                                                                             | 130.915            | -6.440     |
| 1900   | 57.709                                                                        | 381.891                                 | 334.965                  | 89.160                                                                             | 130.855            | -6.240     |
| 2000   | 57.756                                                                        | 384.853                                 | 337.356                  | 94.933                                                                             | 130.745            | -6.061     |
| 2100   | 57.797                                                                        | 387.672                                 | 339.714                  | 100.711                                                                            | 130.583            | -5.898     |
| 2200   | 57.832                                                                        | 390.361                                 | 341.935                  | 106.492                                                                            | 130.371            | -5.751     |
| 2300   | 57.863                                                                        | 392.933                                 | 344.116                  | 112.277                                                                            | 130.113            | -5.616     |
| 2400   | 57.891                                                                        | 395.306                                 | 346.202                  | 118.065                                                                            | 129.813            | -5.493     |
| 2500   | 57.915                                                                        | 397.760                                 | 348.217                  | 123.855                                                                            | 129.476            | -5.380     |
| 2600   | 57.936                                                                        | 400.218                                 | 350.167                  | 129.648                                                                            | 126.636            | -5.276     |
| 2700   | 57.953                                                                        | 402.618                                 | 352.034                  | 135.442                                                                            | 128.718            | -5.181     |
| 2800   | 57.972                                                                        | 404.326                                 | 353.884                  | 141.239                                                                            | 128.309            | -5.092     |
| 2900   | 57.988                                                                        | 406.361                                 | 355.631                  | 147.037                                                                            | 127.837            | -5.009     |
| 3000   | 58.002                                                                        | 408.327                                 | 357.382                  | 152.836                                                                            | 127.458            | -4.933     |
| 3100   | 58.014                                                                        | 410.229                                 | 359.036                  | 158.637                                                                            | 127.026            | -4.861     |
| 3200   | 58.026                                                                        | 412.071                                 | 360.684                  | 164.439                                                                            | 126.596            | -4.794     |
| 3300   | 58.036                                                                        | 413.837                                 | 362.268                  | 170.242                                                                            | 126.172            | -4.732     |
| 3400   | 58.046                                                                        | 415.590                                 | 363.811                  | 176.046                                                                            | 125.756            | -4.673     |
| 3500   | 58.055                                                                        | 417.272                                 | 365.315                  | 181.851                                                                            | 125.351            | -4.618     |
| 3600   | 58.063                                                                        | 418.908                                 | 367.781                  | 187.657                                                                            | 124.959            | -4.566     |
| 3700   | 58.070                                                                        | 420.499                                 | 368.211                  | 193.464                                                                            | 124.581            | -4.517     |
| 3800   | 58.077                                                                        | 422.048                                 | 369.608                  | 199.271                                                                            | 124.219            | -4.471     |
| 3900   | 58.083                                                                        | 423.556                                 | 370.972                  | 205.079                                                                            | 123.874            | -4.427     |
| 4000   | 58.089                                                                        | 425.027                                 | 372.305                  | 210.888                                                                            | 123.546            | -4.386     |
| 4100   | 58.094                                                                        | 426.461                                 | 373.608                  | 216.697                                                                            | 123.234            | -4.347     |
| 4200   | 58.099                                                                        | 427.861                                 | 374.883                  | 222.507                                                                            | 122.940            | -4.309     |
| 4300   | 58.104                                                                        | 429.261                                 | 376.131                  | 228.317                                                                            | 122.663            | -4.274     |
| 4400   | 58.108                                                                        | 430.564                                 | 377.335                  | 234.128                                                                            | 122.402            | -4.240     |
| 4500   | 58.112                                                                        | 431.870                                 | 378.530                  | 239.939                                                                            | 122.136            | -4.208     |
| 4600   | 58.116                                                                        | 433.147                                 | 379.724                  | 245.750                                                                            | 121.926            | -4.177     |
| 4700   | 58.120                                                                        | 434.397                                 | 380.874                  | 251.562                                                                            | 121.709            | -4.147     |
| 4800   | 58.123                                                                        | 435.621                                 | 382.001                  | 257.374                                                                            | 121.505            | -4.119     |
| 4900   | 58.126                                                                        | 436.819                                 | 383.188                  | 263.186                                                                            | 121.313            | -4.092     |
| 5000   | 58.129                                                                        | 437.994                                 | 384.194                  | 268.999                                                                            | 121.132            | -4.067     |
| 5100   | 58.132                                                                        | 439.145                                 | 385.260                  | 274.812                                                                            | 120.939            | -4.042     |
| 5200   | 58.135                                                                        | 440.274                                 | 386.307                  | 280.616                                                                            | 120.795            | -4.018     |
| 5300   | 58.137                                                                        | 441.381                                 | 387.336                  | 286.439                                                                            | 120.636            | -3.995     |
| 5400   | 58.140                                                                        | 442.468                                 | 388.347                  | 292.253                                                                            | 120.483            | -3.973     |
| 5500   | 58.142                                                                        | 443.535                                 | 389.341                  | 298.067                                                                            | 120.333            | -3.952     |
| 5600   | 58.144                                                                        | 444.582                                 | 390.318                  | 303.882                                                                            | 120.184            | -3.931     |
| 5700   | 58.146                                                                        | 445.612                                 | 391.279                  | 309.696                                                                            | 120.036            | -3.912     |
| 5800   | 58.148                                                                        | 446.623                                 | 392.224                  | 315.511                                                                            | 119.886            | -3.893     |
| 5900   | 58.150                                                                        | 447.617                                 | 393.155                  | 321.326                                                                            | 119.733            | -3.875     |
| 6000   | 58.151                                                                        | 448.594                                 | 394.071                  | 327.141                                                                            | 119.575            | -3.857     |

1

## Iodine oxide (IO)

## Ideal Gas

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

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

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

| Electronic Level and Quantum Weight state | $\epsilon_{\nu}$ , cm <sup>-1</sup> | $\sigma$ = 1 |
|-------------------------------------------|-------------------------------------|--------------|
| [1500](1)                                 | 0.0                                 | [2]          |
| [150](1)                                  |                                     |              |
| [275](1)                                  |                                     |              |

Point Group: C<sub>1</sub>  
 Bond Distances: I-O = [2.4] Å; O=O = [1.25] Å  
 Bond Angle: I-O-O = [120]°  
 Product of the Moments of Inertia:  $I_A I_B I_C = [1314.2931 \times 10^{-11}] \text{ g} \cdot \text{cm}^6$

## Enthalpy of Formation

Following trends in the reaction  $XOO(g) \rightarrow X(g) + 2O(g)$ , a reasonable estimate for the iodine reaction would be 470 kJ mol which yields  $\Delta_f H^{\circ}(0 \text{ K}) = -91.25 \text{ kJ mol}^{-1}$ . 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 kJ mol<sup>-1</sup> which leads to a  $\Delta_f H^{\circ}(0 \text{ K}) = 119 \text{ kJ mol}^{-1}$ . 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 g·cm<sup>2</sup> are:  $I_A = 1.1391 \times 10^{-39}$ ,  $I_B = 33.4021 \times 10^{-39}$ , and  $I_C = 34.3412 \times 10^{-39}$ .

## References

NIST-JANAF Thermochemical Tables: FOO(g); Sept. 1995; ClOO(g); March 1996; BrOO(g); (March 1996).

| T/K    | $C_p^*$ | Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K |                                   |                                  | Standard State Pressure = p' = 0.1 MPa |                    |                    |
|--------|---------|------------------------------------------------------------|-----------------------------------|----------------------------------|----------------------------------------|--------------------|--------------------|
|        |         | S°                                                         | $-(G^{\circ} - H^{\circ}(T)) / T$ | $H^{\circ} - H^{\circ}(T_r) / T$ | $k_J \cdot \text{mol}^{-1}$            | $\Delta H^{\circ}$ | $\Delta G^{\circ}$ |
| 0      | 0.000   | 0.000                                                      | INFINITE                          | -12.806                          | 119.000                                | 119.000            | INFINITE           |
| 50     | 35.573  | 219.838                                                    | 442.181                           | -11.117                          | 118.762                                | 116.235            | -121.430           |
| 100    | 41.565  | 246.433                                                    | 338.245                           | -9.181                           | 118.195                                | 113.932            | -59.512            |
| 150    | 45.076  | 264.029                                                    | 310.132                           | -7.005                           | 117.715                                | 111.707            | -38.970            |
| 200    | 46.892  | 277.212                                                    | 300.780                           | -4.702                           | 117.297                                | 110.035            | -28.738            |
| 250    | 47.962  | 287.259                                                    | 297.172                           | -2.328                           | 116.599                                | 108.266            | -22.621            |
| 298.15 | 48.727  | 296.374                                                    | 296.374                           | .000                             | 116.523                                | 106.638            | -18.682            |
| 300    | 48.754  | 296.676                                                    | 296.375                           | .090                             | 116.509                                | 106.576            | -18.557            |
| 400    | 50.151  | 310.929                                                    | 298.305                           | 5.036                            | 107.564                                | 103.667            | -13.538            |
| 500    | 51.463  | 322.229                                                    | 301.993                           | 10.118                           | 85.389                                 | 104.801            | -10.948            |
| 600    | 52.620  | 331.717                                                    | 306.178                           | 15.323                           | 85.758                                 | 108.628            | -9.457             |
| 700    | 53.581  | 339.903                                                    | 310.424                           | 20.635                           | 85.931                                 | 112.426            | -8.389             |
| 800    | 54.355  | 347.110                                                    | 314.568                           | 26.033                           | 86.103                                 | 116.199            | -5.387             |
| 900    | 54.973  | 353.349                                                    | 318.548                           | 31.501                           | 86.270                                 | 119.950            | -5.962             |
| 1000   | 55.467  | 359.568                                                    | 322.344                           | 37.024                           | 86.430                                 | 123.684            | -6.461             |
| 1100   | 55.863  | 364.674                                                    | 325.954                           | 42.591                           | 86.580                                 | 127.402            | -6.050             |
| 1200   | 56.184  | 366.548                                                    | 329.387                           | 48.194                           | 86.718                                 | 131.107            | -5.707             |
| 1300   | 56.446  | 370.056                                                    | 332.652                           | 53.326                           | 86.859                                 | 134.801            | -5.416             |
| 1400   | 56.662  | 372.248                                                    | 337.761                           | 59.482                           | 86.938                                 | 138.487            | -5.167             |
| 1500   | 56.842  | 382.163                                                    | 338.725                           | 65.157                           | 87.009                                 | 142.166            | -4.951             |
| 1600   | 56.993  | 388.837                                                    | 341.556                           | 92.481                           | 85.554                                 | 164.254            | -4.086             |
| 1700   | 57.121  | 389.296                                                    | 344.253                           | 105.232                          | 85.045                                 | 145.842            | -4.761             |
| 1800   | 57.230  | 392.564                                                    | 346.857                           | 82.273                           | 86.992                                 | 153.192            | -4.594             |
| 1900   | 57.324  | 393.661                                                    | 349.345                           | 88.001                           | 86.895                                 | 156.873            | -4.446             |
| 2000   | 57.405  | 396.603                                                    | 351.735                           | 93.737                           | 86.749                                 | 160.559            | -4.313             |
| 2100   | 57.475  | 401.406                                                    | 354.034                           | 99.248                           | 86.621                                 | 164.254            | -4.193             |
| 2200   | 57.537  | 404.081                                                    | 356.248                           | 105.232                          | 86.554                                 | 164.254            | -4.086             |
| 2300   | 57.591  | 406.640                                                    | 358.384                           | 110.988                          | 86.024                                 | 167.961            | -3.988             |
| 2400   | 57.639  | 409.092                                                    | 360.446                           | 116.728                          | 86.698                                 | 171.678            | -3.899             |
| 2500   | 57.681  | 411.446                                                    | 362.439                           | 122.516                          | 86.750                                 | 175.408            | -3.818             |
| 2600   | 57.719  | 413.709                                                    | 364.368                           | 128.286                          | 84.948                                 | 182.914            | -3.675             |
| 2700   | 57.753  | 415.888                                                    | 366.236                           | 134.059                          | 84.536                                 | 186.690            | -3.612             |
| 2800   | 57.784  | 417.988                                                    | 368.047                           | 139.836                          | 84.107                                 | 190.481            | -3.551             |
| 2900   | 57.812  | 420.017                                                    | 369.804                           | 145.616                          | 83.667                                 | 194.288            | -3.499             |
| 3000   | 57.836  | 421.577                                                    | 371.511                           | 151.399                          | 83.220                                 | 198.110            | -3.449             |
| 3100   | 57.859  | 423.374                                                    | 373.170                           | 157.183                          | 82.773                                 | 201.948            | -3.403             |
| 3200   | 57.880  | 425.711                                                    | 374.783                           | 162.570                          | 82.328                                 | 205.798            | -3.359             |
| 3300   | 57.899  | 427.492                                                    | 376.333                           | 168.759                          | 81.889                                 | 209.663            | -3.319             |
| 3400   | 57.916  | 429.221                                                    | 377.883                           | 174.550                          | 81.450                                 | 213.542            | -3.281             |
| 3500   | 57.932  | 430.900                                                    | 379.374                           | 180.242                          | 81.042                                 | 217.433            | -3.245             |
| 3600   | 57.946  | 432.532                                                    | 380.828                           | 186.136                          | 80.638                                 | 221.136            | -3.211             |
| 3700   | 57.960  | 434.120                                                    | 382.247                           | 191.932                          | 80.249                                 | 226.727            | -3.180             |
| 3800   | 57.973  | 435.666                                                    | 383.632                           | 197.728                          | 79.876                                 | 229.174            | -3.150             |
| 3900   | 57.983  | 437.172                                                    | 384.996                           | 203.526                          | 79.521                                 | 231.108            | -3.122             |
| 4000   | 57.994  | 438.640                                                    | 386.369                           | 209.325                          | 79.183                                 | 237.049            | -3.096             |
| 4100   | 58.004  | 440.072                                                    | 387.603                           | 215.125                          | 78.867                                 | 241.000            | -3.070             |
| 4200   | 58.013  | 441.470                                                    | 388.869                           | 220.926                          | 78.559                                 | 244.837            | -2.926             |
| 4300   | 58.022  | 442.835                                                    | 390.108                           | 226.727                          | 78.234                                 | 248.924            | -3.047             |
| 4400   | 58.030  | 444.169                                                    | 391.322                           | 232.530                          | 78.004                                 | 252.835            | -3.024             |
| 4500   | 58.037  | 445.474                                                    | 392.511                           | 238.333                          | 77.751                                 | 256.873            | -2.982             |
| 4600   | 58.044  | 446.749                                                    | 393.676                           | 244.137                          | 77.513                                 | 260.855            | -2.962             |
| 4700   | 58.051  | 447.998                                                    | 394.819                           | 249.942                          | 77.290                                 | 264.844            | -2.943             |
| 4800   | 58.057  | 449.220                                                    | 395.939                           | 255.747                          | 77.079                                 | 268.837            | -2.833             |
| 4900   | 58.063  | 450.417                                                    | 397.039                           | 261.553                          | 76.880                                 | 272.834            | -2.810             |
| 5000   | 58.068  | 451.590                                                    | 398.118                           | 267.360                          | 76.693                                 | 276.835            | -2.892             |
| 5100   | 58.073  | 452.740                                                    | 399.178                           | 273.167                          | 76.514                                 | 280.840            | -2.876             |
| 5200   | 58.078  | 453.840                                                    | 400.219                           | 278.974                          | 76.344                                 | 284.847            | -2.861             |
| 5300   | 58.083  | 454.974                                                    | 401.242                           | 284.783                          | 76.180                                 | 288.859            | -2.847             |
| 5400   | 58.087  | 456.050                                                    | 402.247                           | 290.591                          | 76.021                                 | 292.873            | -2.813             |
| 5500   | 58.091  | 457.126                                                    | 403.235                           | 296.400                          | 75.866                                 | 296.890            | -2.810             |
| 5600   | 58.095  | 458.172                                                    | 404.207                           | 302.209                          | 75.712                                 | 300.911            | -2.807             |
| 5700   | 58.099  | 459.201                                                    | 405.162                           | 308.019                          | 75.559                                 | 304.933            | -2.794             |
| 5800   | 58.102  | 460.211                                                    | 406.103                           | 303.829                          | 75.405                                 | 308.959            | -2.782             |
| 5900   | 58.105  | 461.204                                                    | 407.028                           | 319.639                          | 75.247                                 | 312.986            | -2.771             |
| 6000   | 58.109  | 462.181                                                    | 407.939                           | 325.450                          | 75.085                                 | 317.018            | -2.760             |

CURRENT: March 1996 (1 bar)  
 PREVIOUS:

I<sub>1</sub>O<sub>2</sub>(g)  
 Iodine oxide (IOO)

## NIST-JANAF THERMOCHEMICAL TABLES

 $I_1O_3(g)$  $M_r = 174.90267$  Iodine oxide ( $I_1O_3$ )

| $\Delta_f H^\circ(0\text{ K}) = [248 \pm 50] \text{ kJ}\cdot\text{mol}^{-1}$ |                              | $\Delta_f H^\circ(298.15\text{ K}) = [241.9 \pm 50] \text{ kJ}\cdot\text{mol}^{-1}$ |        | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                                  | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                                 |
|------------------------------------------------------------------------------|------------------------------|-------------------------------------------------------------------------------------|--------|----------------------------------------------------------|--------------------------------------------------|-------------------------------------------------------|---------------------------------|
|                                                                              |                              | $T/K$                                                                               |        | $C_p^\circ$                                              | $S^\circ - [G^\circ - H^\circ(T_r)]/T$           | $H^\circ - H^\circ(T_r)$                              | $\Delta_f H^\circ$              |
|                                                                              |                              |                                                                                     |        | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$         | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $\text{kJ}\cdot\text{mol}^{-1}$                       | $\text{kJ}\cdot\text{mol}^{-1}$ |
| Electronic Level and Quantum Weight state                                    | $\epsilon_n, \text{cm}^{-1}$ | 0                                                                                   | 0      | 0.000                                                    | 0.000                                            | -13.505                                               | 248.000                         |
| state                                                                        | $g_s$                        | 50                                                                                  | 33.412 | 215.531                                                  | 452.355                                          | -11.841                                               | 248.530                         |
| $[2A_1]$                                                                     |                              | 100                                                                                 | 38.019 | 239.747                                                  | 340.560                                          | -10.881                                               | -259.637                        |
|                                                                              |                              | 150                                                                                 | 45.140 | 265.517                                                  | 309.838                                          | -8.001                                                | -150.907                        |
|                                                                              |                              | 200                                                                                 | 51.557 | 270.403                                                  | 298.303                                          | -5.580                                                | -88.256                         |
|                                                                              |                              | 250                                                                                 | 57.096 | 282.519                                                  | 293.959                                          | -2.860                                                | -67.036                         |
|                                                                              |                              | 289.15                                                                              | 61.560 | 292.970                                                  | 292.970                                          | .000                                                  | 260.131                         |
|                                                                              |                              | 300                                                                                 | 61.714 | 293.351                                                  | 292.971                                          | .114                                                  | -46.180                         |
|                                                                              |                              | 400                                                                                 | 68.430 | 312.098                                                  | 295.481                                          | 6.647                                                 | 263.727                         |
|                                                                              |                              | 500                                                                                 | 72.681 | 327.860                                                  | 300.474                                          | 13.718                                                | -35.443                         |
|                                                                              |                              | 600                                                                                 | 75.418 | 341.371                                                  | 306.149                                          | 21.133                                                | -29.573                         |
|                                                                              |                              | 700                                                                                 | 77.245 | 353.143                                                  | 312.040                                          | 28.772                                                | 297.316                         |
|                                                                              |                              | 800                                                                                 | 78.511 | 363.545                                                  | 317.841                                          | 36.563                                                | -23.238                         |
|                                                                              |                              | 900                                                                                 | 79.417 | 372.847                                                  | 323.445                                          | 44.052                                                | -21.246                         |
|                                                                              |                              | 1000                                                                                | 80.086 | 381.251                                                  | 328.812                                          | 52.439                                                | 19.690                          |
|                                                                              |                              | 1100                                                                                | 80.592 | 388.909                                                  | 333.933                                          | 60.474                                                | -18.439                         |
|                                                                              |                              | 1200                                                                                | 80.984 | 395.939                                                  | 338.811                                          | 68.553                                                | 33.011                          |
|                                                                              |                              | 1300                                                                                | 81.293 | 402.434                                                  | 343.458                                          | 76.668                                                | 18.367                          |
|                                                                              |                              | 1400                                                                                | 81.541 | 408.467                                                  | 347.889                                          | 84.810                                                | 19.145                          |
|                                                                              |                              | 1500                                                                                | 81.742 | 414.100                                                  | 352.117                                          | 92.975                                                | 20.884                          |
|                                                                              |                              | 1600                                                                                | 81.908 | 419.381                                                  | 356.158                                          | 101.157                                               | 420.687                         |
|                                                                              |                              | 1700                                                                                | 82.047 | 424.351                                                  | 360.025                                          | 109.355                                               | -14.650                         |
|                                                                              |                              | 1800                                                                                | 82.163 | 429.044                                                  | 363.750                                          | 117.566                                               | 427.373                         |
|                                                                              |                              | 1900                                                                                | 82.262 | 433.489                                                  | 367.286                                          | 125.787                                               | -13.746                         |
|                                                                              |                              | 2000                                                                                | 82.347 | 437.711                                                  | 370.702                                          | 134.018                                               | 427.312                         |
|                                                                              |                              | 2100                                                                                | 82.420 | 441.731                                                  | 373.989                                          | 142.256                                               | -12.723                         |
|                                                                              |                              | 2200                                                                                | 82.484 | 445.566                                                  | 377.156                                          | 150.502                                               | 427.299                         |
|                                                                              |                              | 2300                                                                                | 82.540 | 449.234                                                  | 380.211                                          | 158.753                                               | -11.962                         |
|                                                                              |                              | 2400                                                                                | 82.589 | 452.748                                                  | 383.161                                          | 167.010                                               | 539.875                         |
|                                                                              |                              | 2500                                                                                | 82.632 | 456.120                                                  | 386.012                                          | 175.271                                               | 224.089                         |
|                                                                              |                              | 2600                                                                                | 82.670 | 459.362                                                  | 388.771                                          | 183.536                                               | 553.028                         |
|                                                                              |                              | 2700                                                                                | 82.704 | 462.483                                                  | 391.444                                          | 191.804                                               | -11.555                         |
|                                                                              |                              | 2800                                                                                | 82.735 | 465.491                                                  | 394.035                                          | 200.076                                               | 566.175                         |
|                                                                              |                              | 2900                                                                                | 82.763 | 468.395                                                  | 396.550                                          | 208.351                                               | -11.375                         |
|                                                                              |                              | 3000                                                                                | 82.788 | 471.201                                                  | 398.991                                          | 216.629                                               | 592.454                         |
|                                                                              |                              | 3100                                                                                | 82.810 | 473.916                                                  | 401.365                                          | 224.802                                               | -10.932                         |
|                                                                              |                              | 3200                                                                                | 82.841 | 476.545                                                  | 403.673                                          | 224.852                                               | 592.586                         |
|                                                                              |                              | 3300                                                                                | 82.849 | 479.095                                                  | 405.920                                          | 233.191                                               | -10.417                         |
|                                                                              |                              | 3400                                                                                | 82.866 | 481.568                                                  | 408.109                                          | 241.475                                               | 658.103                         |
|                                                                              |                              | 3500                                                                                | 82.882 | 483.970                                                  | 410.247                                          | 249.761                                               | 671.229                         |
|                                                                              |                              | 3600                                                                                | 82.896 | 486.306                                                  | 412.323                                          | 256.337                                               | -10.213                         |
|                                                                              |                              | 3700                                                                                | 82.910 | 488.577                                                  | 414.533                                          | 274.627                                               | 697.476                         |
|                                                                              |                              | 3800                                                                                | 82.922 | 490.788                                                  | 416.636                                          | 282.919                                               | -10.120                         |
|                                                                              |                              | 3900                                                                                | 82.933 | 492.942                                                  | 418.273                                          | 291.212                                               | 723.718                         |
|                                                                              |                              | 4000                                                                                | 82.943 | 495.042                                                  | 420.166                                          | 299.506                                               | -9.793                          |
|                                                                              |                              | 4100                                                                                | 82.953 | 497.090                                                  | 422.017                                          | 307.800                                               | 733.065                         |
|                                                                              |                              | 4200                                                                                | 82.962 | 499.089                                                  | 423.828                                          | 316.096                                               | -9.722                          |
|                                                                              |                              | 4300                                                                                | 83.011 | 501.042                                                  | 425.601                                          | 324.933                                               | 776.175                         |
|                                                                              |                              | 4400                                                                                | 83.016 | 502.978                                                  | 427.338                                          | 332.690                                               | -9.633                          |
|                                                                              |                              | 4500                                                                                | 83.026 | 504.986                                                  | 429.039                                          | 340.988                                               | -9.526                          |
|                                                                              |                              | 4600                                                                                | 83.036 | 506.638                                                  | 430.706                                          | 349.287                                               | -9.466                          |
|                                                                              |                              | 4700                                                                                | 83.046 | 508.423                                                  | 432.341                                          | 357.587                                               | -9.409                          |
|                                                                              |                              | 4800                                                                                | 83.056 | 510.170                                                  | 433.944                                          | 365.897                                               | -9.354                          |
|                                                                              |                              | 4900                                                                                | 83.058 | 511.852                                                  | 435.517                                          | 374.188                                               | -9.302                          |
|                                                                              |                              | 5000                                                                                | 83.059 | 513.539                                                  | 437.061                                          | 382.489                                               | -9.203                          |
|                                                                              |                              | 5100                                                                                | 83.021 | 515.203                                                  | 438.577                                          | 390.791                                               | 880.949                         |
|                                                                              |                              | 5200                                                                                | 83.026 | 516.815                                                  | 440.066                                          | 399.993                                               | 894.031                         |
|                                                                              |                              | 5300                                                                                | 83.030 | 518.530                                                  | 441.530                                          | 407.996                                               | 907.107                         |
|                                                                              |                              | 5400                                                                                | 83.034 | 519.949                                                  | 442.967                                          | 413.699                                               | 920.182                         |
|                                                                              |                              | 5500                                                                                | 83.038 | 521.472                                                  | 444.381                                          | 227.344                                               | -9.069                          |
|                                                                              |                              | 5600                                                                                | 83.042 | 522.969                                                  | 445.771                                          | 432.207                                               | 922.858                         |
|                                                                              |                              | 5700                                                                                | 83.046 | 524.459                                                  | 447.138                                          | 440.611                                               | 972.445                         |
|                                                                              |                              | 5800                                                                                | 83.049 | 525.883                                                  | 448.484                                          | 448.916                                               | 887.505                         |
|                                                                              |                              | 5900                                                                                | 83.052 | 527.303                                                  | 449.807                                          | 457.221                                               | 998.559                         |
|                                                                              |                              | 6000                                                                                | 83.055 | 528.698                                                  | 451.111                                          | 465.527                                               | -8.807                          |

PREVIOUS.

CURRENT March 1996 (1 bar)

Iodine oxide ( $I_1O_3$ )

Ideal Gas

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

 $I_1O_3(g)$  $\Delta_f H^\circ(298.15\text{ K}) = [241.9 \pm 50] \text{ kJ}\cdot\text{mol}^{-1}$  $\Delta_f G^\circ$  $\log K_1$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ$  $\Delta_f S^\circ$  $\Delta_f A^\circ$  $\Delta_f H^\circ$  $\Delta_f C_p^\circ$  $\Delta_f U^\circ</math$

## IDEAL GAS

 $\text{PbI}_2(\text{g})$ 

$$\Delta H^\circ(0 \text{ K}) = 280.094 \pm 0.21 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

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

 $\text{M}_r = 334.1045$  Lead Iodide (PbI)

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |             |           |                               | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                                   |                    |                    |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------|-------------|-----------|-------------------------------|-------------------------------------------------------|-----------------------------------|--------------------|--------------------|
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | $T/K$                                                     | $C_p^\circ$ | $S^\circ$ | $-[G^\circ - H^\circ(T_r)]/T$ | $H^\circ - H^\circ(T_r)/T$                            | $k\text{J} \cdot \text{mol}^{-1}$ | $\Delta_f H^\circ$ | $\Delta_f G^\circ$ |
| Electronic Levels and Quantum Weights                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                           |             |           |                               |                                                       |                                   |                    |                    |
| State                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | $\epsilon, \text{cm}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                           |             |           |                               |                                                       |                                   |                    |                    |
| $X^2\Pi_{1/2}^0$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | 0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 2                                                         |             |           |                               |                                                       |                                   |                    |                    |
| $2\Pi_{1/2}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | [8300]                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | 2                                                         |             |           |                               |                                                       |                                   |                    |                    |
| $A^2\Pi_{1/2}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 20528.5                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | [4]                                                       |             |           |                               |                                                       |                                   |                    |                    |
| $B^2\Pi_{1/2}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 33488                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | [2]                                                       |             |           |                               |                                                       |                                   |                    |                    |
| $\omega_e = 160.5 \text{ cm}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | $\omega_e \epsilon_e = 0.25 \text{ cm}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | $\sigma_e = 1$                                            |             |           |                               |                                                       |                                   |                    |                    |
| $B_e = [0.02861] \text{ cm}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | $\alpha_e = [0.00006] \text{ cm}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | $r_e = [2.736] \text{ \AA}$                               |             |           |                               |                                                       |                                   |                    |                    |
| Enthalpy of Formation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                           |             |           |                               |                                                       |                                   |                    |                    |
| $\Delta_f H^\circ(\text{PbI}, \text{g}, 0 \text{ K}) = 26500 \pm 9 \text{ kcal/mol}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | with $\Delta H^\circ(\text{Pb, g}) = 46.91 \pm 0.13 \text{ kcal/mol}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | and                                                       |             |           |                               |                                                       |                                   |                    |                    |
| $\Delta H^\circ(\text{I, g}, 0 \text{ K}) = 25633 \text{ kcal/mol}^{-1}$                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 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>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 Brügel-Sponer extrapolation of the adopted ground state vibrational constants, derived from emission and absorption spectra ( $\nu = 0.36 \text{ eV}$ ) gives a dissociation energy of 3.18 eV. Correction for the ionic character of PbI as suggested by Hildenbrand <sup>6</sup> gives $D_0^\circ = 2.7 \text{ eV} (62.3 \text{ kcal/mol}^{-1})$ . 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>+</sup> mercury <sup>2+</sup> and potassium <sup>+</sup> halides suggests a $D_0^\circ$ value near 45 kcal/mol <sup>-1</sup> . The rounded value $D_0^\circ = 2.0 \pm 0.4 \text{ eV} (46 \pm 9 \text{ kcal/mol}^{-1})$ listed by Gaydon <sup>7</sup> is adopted. $\Delta_f H^\circ(\text{PbI, g}, 298.15 \text{ K}) = 2575 \pm 9 \text{ kcal/mol}^{-1}$ is calculated from the selected $\Delta H^\circ(\text{PbI, g, 0 K}) = 265 \pm 9 \text{ kcal/mol}^{-1}$ . |                                                           |             |           |                               |                                                       |                                   |                    |                    |
| 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 $^2\Pi_{1/2}$ state at 8300 cm <sup>-1</sup> is added in analogy to PbCl <sup>8</sup> and PbBr <sup>9</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>10</sup> $B_4$ is calculated from the adopted $r_e$ . The value for $\alpha$ 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; KB(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, "Dissociation 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).                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                           |             |           |                               |                                                       |                                   |                    |                    |
| <sup>7</sup> J. Ph. Chem. Ref. Data, Monograph 9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                           |             |           |                               |                                                       |                                   |                    |                    |

Lead Iodide (PbI)

 $\text{PbI}_2(\text{g})$ 

PREVIOUS December 1973 (1 atm)

CURRENT December 1973 (1 bar)

## NIST-JANAF THERMOCHEMICAL TABLES

DEAL GAS

$$M_r = 154.9900 \text{ lodosilylidyne (SII)}$$

$$S^\circ(298.15\text{ K}) = 253.854 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^{\circ}(298) = -313.51 \pm 41.8 \text{ kJ/mol}$$

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

$$\Delta H^\circ(298.15\text{ K}) = 313.63 \pm 41.8 \text{ kJ}\cdot\text{mol}^{-1}$$

| $T/K$ | $C_p^{\circ}$ | $S^{\circ}$ | $-[G^{\circ}-H^{\circ}(T_i)]T$ | $H^{\circ}-H^{\circ}(T_i)$ | $\Delta_e H^{\circ}$ | $\Delta_e G^{\circ}$ | $\log K_t$ |
|-------|---------------|-------------|--------------------------------|----------------------------|----------------------|----------------------|------------|
|-------|---------------|-------------|--------------------------------|----------------------------|----------------------|----------------------|------------|

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| State            | $\epsilon, \text{ cm}^{-1}$ | Electronic Levels and Molecular Constants ( $\sigma = 1$ ) |                             |                                 |                        |                             | $r_e, \text{ \AA}$ | Source |
|------------------|-----------------------------|------------------------------------------------------------|-----------------------------|---------------------------------|------------------------|-----------------------------|--------------------|--------|
|                  |                             | $g_s$                                                      | $\omega_e, \text{ cm}^{-1}$ | $\omega_{e,e}, \text{ cm}^{-1}$ | $B_e, \text{ cm}^{-1}$ | $\alpha_e, \text{ cm}^{-1}$ |                    |        |
| $^2\Pi_{3/2}$    | 0                           | 2                                                          | 363.2                       | 1.25                            | 0.123                  | [0.001]                     | 2.45               | 1      |
| $^2\Pi_{1/2}$    | 650                         | 2                                                          | 358.5                       | 1.1                             | 0.123                  | [0.001]                     | 2.45               | 1, 6   |
| $^4\Sigma_{1/2}$ | 20939.1                     | 4                                                          | 275.3                       | 5.6                             | 0.118                  | [0.001]                     | 2.50               | 1      |
| $^4\Sigma_{3/2}$ | 21204.9                     | 2                                                          | 208.3                       | 1.66                            | 0.085                  | [0.001]                     | 2.45               | 1      |
| $^2\Sigma^+$     | 32180.3                     | 2                                                          | 471.0                       | 0.9                             | [0.123]                | [0.001]                     | [2.45]             | 1      |
| $^2\Sigma^+$     | 42710                       | 4                                                          | 485                         | 3.5                             | [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  $\text{A}^{\infty}\Sigma$  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  $D_0^\infty = 57.3 \text{ kcal}\cdot\text{mol}^{-1}$ , 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 the approximate nature of Birge-Sponer extrapolation based on data from the first few vibrational levels only. The adopted value of  $D_0^\infty = 57.3 \pm 8 \text{ kcal}\cdot\text{mol}^{-1}$  is in good agreement with  $D_0^\infty = 56.9$  and  $61.8 \text{ kcal}\cdot\text{mol}^{-1}$  obtained in a similar manner from the  $\text{A}^{\infty}\Sigma$  state and ground state data, respectively.<sup>4-6</sup> The value is also in reasonable agreement with  $D_0^\infty = 72.4$  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  $D_0^\infty = 4.0 \text{ ev}$  ( $92.7 \text{ kcal}\cdot\text{mol}^{-1}$ ) is based on the observed predissociation of the  $\text{B}^{\infty}\Sigma$  state.<sup>1</sup> The adopted value of  $D_0^\infty$  is also in good agreement with the average (per bond) heat of atomization of  $\text{Si}_4(\text{g})$ .

Heat Capacity and Entropy

**Heat capacity and Entropy**

Electron 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 cm<sup>-1</sup> 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 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'Σ<sup>-</sup> state. Billingsley<sup>1</sup> interprets the observed A-X emission spectrum as terminating at the upper level of the split ground state and calculates the ground state splitting of 646.4 cm<sup>-1</sup> from the observation of one absorption line. Lakshminarayana and Haranath<sup>8</sup> observe a second emission series 650.3 cm<sup>-1</sup> to the red of that observed by Billingsley, and although the ground state splittings are in agreement, this would place the A' state approximately 650 cm<sup>-1</sup> lower than reported. We favor Billingsley's interpretation while recognizing the need for additional work to resolve this paradox. In addition the B'Δ state observed for the other silicon monohalides<sup>9</sup> is not observed for Si. 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 ±0.1 cal K<sup>-1</sup> mol<sup>-1</sup> to S<sup>T</sup>(298.15 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<sub>1</sub> = 123 cm<sup>-1</sup> 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<sup>T</sup>(298.15 K) should account for this also. All molecular constants have been corrected to reflect the natural abundance of Si.

## References

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## Strontium Iodide (SrI)

## IDEAL GAS

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

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

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

| Electronic Levels and Quantum Weights |                            |       |
|---------------------------------------|----------------------------|-------|
| State                                 | $\epsilon, \text{cm}^{-1}$ | $\xi$ |
| X $\Sigma^+$                          | 0                          | 2     |
| A $\Pi$                               | 14422.7                    | 2     |
| B $\Sigma$                            | 14748.8                    | 2     |
| C $\Pi$                               | 22666.1                    | 2     |
| D $\Sigma$                            | 23223.4                    | 2     |
|                                       | 28928.3                    | 2     |

$$\omega_{\text{e}} = 173.9 \text{ cm}^{-1}$$

$$B_e = [0.0354] \text{ cm}^{-1}$$

$$\omega_{\text{e}} = 0.42 \text{ cm}^{-1}$$

$$\alpha_e = [0.00011] \text{ cm}^{-1}$$

$$r_e = [3.03] \text{ \AA}$$

## Enthalpy of Formation

The adopted  $\Delta_f H^\circ(0 \text{ K}) = -6.65 \pm 20 \text{ kcal} \cdot \text{mol}^{-1}$  is obtained from  $D_0^\circ = 71.5 \text{ kcal} \cdot \text{mol}^{-1}$  calculated from the ratio  $D_0^\circ(\text{SrI})/D_0^\circ(\text{Sr}) = 0.46$ . This value for the ratio was found for a series of mono and difluorides,<sup>1</sup> and for other alkaline earth halide systems.<sup>2</sup> Other values for  $D_0^\circ$  in  $\text{kcal} \cdot \text{mol}^{-1}$  are 54.6 obtained from a linear Birge-Sponer extrapolation of  $\omega_{\text{e}}$  and  $\omega_{\text{e}} \cdot \epsilon_{\text{e}}$  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.  $\Delta_f H^\circ(298.15 \text{ K}) = -7.29 \pm 20 \text{ kcal} \cdot \text{mol}^{-1}$  from the adopted  $\Delta_f H^\circ(0 \text{ K}) = -6.65 \text{ kcal} \cdot \text{mol}^{-1}$ .

## 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 SrI<sub>2</sub>.  $B_e$  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>8,9</sup> and Reddy et al.<sup>10</sup> The data are similar to the values in Rosen,<sup>2</sup> but are more complete. The D<sup>2</sup> level is confirmed by Shah et al.<sup>11</sup>

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

|   |            | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                                      |                            |                    |                    |
|---|------------|-------------------------------------------------------|--------------------------------------|----------------------------|--------------------|--------------------|
|   |            | $T/K$                                                 |                                      | $H^\circ - H^\circ(T) / T$ |                    | $\Delta_f G^\circ$ |
|   |            | $C_p^\circ$                                           | $S^\circ - [G^\circ - H^\circ(T)]/T$ | $\Delta_f H^\circ$         | $\Delta_f S^\circ$ | $\log K_T$         |
|   |            | 0                                                     | 0                                    | -10.287                    | -27.614            | INFINITE           |
|   |            | 100                                                   | 34.228                               | 232.849                    | -27.540            | -44.971            |
| X | $\Sigma^+$ | 200                                                   | 36.539                               | 257.493                    | -1.620             | 23.490             |
|   |            | 250                                                   | 36.915                               | 265.651                    | -1.783             | 16.163             |
|   |            | 298.15                                                | 37.135                               | 272.213                    | 0.                 | -29.705            |
|   |            | 300                                                   | 37.141                               | 272.443                    | -30.494            | -77.736            |
|   |            | 350                                                   | 37.294                               | 278.181                    | 0.69               | 13.619             |
|   |            | 400                                                   | 37.403                               | 283.168                    | -31.423            | 13.586             |
|   |            | 450                                                   | 37.492                               | 287.579                    | -40.345            | -78.029            |
|   |            | 500                                                   | 37.563                               | 291.533                    | -41.891            | -93.318            |
|   |            | 600                                                   | 37.679                               | 298.392                    | -56.70             | -115.950           |
|   |            | 700                                                   | 37.774                               | 304.208                    | -63.522            | -104.304           |
|   |            | 800                                                   | 37.859                               | 309.257                    | -64.567            | -112.364           |
|   |            | 900                                                   | 37.936                               | 313.721                    | -65.712            | -120.241           |
|   |            | 1000                                                  | 38.010                               | 317.722                    | -66.959            | -127.946           |
|   |            | 1100                                                  | 38.082                               | 321.348                    | -68.919            | -135.518           |
|   |            | 1200                                                  | 38.152                               | 324.664                    | -70.076            | -142.744           |
|   |            | 1300                                                  | 38.229                               | 327.721                    | -70.450            | -74.866            |
|   |            | 1400                                                  | 38.358                               | 330.556                    | -71.711            | -149.590           |
|   |            | 1500                                                  | 38.358                               | 333.200                    | -73.885            | -159.506           |
|   |            | 1600                                                  | 38.428                               | 334.678                    | -74.382            | -162.051           |
|   |            | 1700                                                  | 38.502                               | 338.010                    | -75.699            | -168.038           |
|   |            | 1800                                                  | 38.580                               | 340.211                    | -76.886            | -173.876           |
|   |            | 1900                                                  | 38.663                               | 342.301                    | -78.083            | -181.336           |
|   |            | 2000                                                  | 38.755                               | 344.286                    | -79.945            | -187.692           |
|   |            | 2100                                                  | 38.857                               | 347.179                    | -81.817            | -195.437           |
|   |            | 2200                                                  | 38.970                               | 347.989                    | -82.606            | -229.822           |
|   |            | 2300                                                  | 39.097                               | 349.775                    | -72.587            | -230.244           |
|   |            | 2400                                                  | 39.238                               | 351.391                    | -76.491            | -167.652           |
|   |            | 2500                                                  | 39.395                               | 352.996                    | -80.407            | -167.934           |
|   |            | 2600                                                  | 39.570                               | 354.545                    | -84.339            | -163.433           |
|   |            | 2700                                                  | 39.762                               | 356.042                    | -88.287            | -231.737           |
|   |            | 2800                                                  | 39.972                               | 357.491                    | -92.253            | -232.312           |
|   |            | 2900                                                  | 40.200                               | 358.939                    | -96.240            | -233.585           |
|   |            | 3100                                                  | 40.447                               | 360.265                    | -104.288           | -151.159           |
|   |            | 3200                                                  | 40.711                               | 361.596                    | -108.338           | -148.280           |
|   |            | 3300                                                  | 40.992                               | 362.992                    | -112.423           | -145.375           |
|   |            | 3400                                                  | 41.289                               | 364.398                    | -116.537           | -142.443           |
|   |            | 3500                                                  | 41.601                               | 365.596                    | -120.682           | -126.769           |
|   |            | 3600                                                  | 41.928                               | 366.932                    | -124.838           | -139.483           |
|   |            | 3700                                                  | 42.267                               | 367.792                    | -131.940           | -156.843           |
|   |            | 3800                                                  | 42.618                               | 368.955                    | -132.925           | -163.194           |
|   |            | 3900                                                  | 42.980                               | 370.198                    | -137.592           | -162.433           |
|   |            | 4000                                                  | 43.350                               | 371.217                    | -141.908           | -171.782           |
|   |            | 4100                                                  | 44.110                               | 373.404                    | -146.262           | -177.822           |
|   |            | 4200                                                  | 44.986                               | 374.472                    | -150.654           | -183.475           |
|   |            | 4300                                                  | 45.856                               | 375.523                    | -154.084           | -190.824           |
|   |            | 4400                                                  | 46.728                               | 376.560                    | -158.595           | -197.132           |
|   |            | 4500                                                  | 47.597                               | 383.440                    | -164.062           | -203.045           |
|   |            | 5200                                                  | 48.330                               | 384.373                    | -169.609           | -243.030           |
|   |            | 5300                                                  | 48.684                               | 385.299                    | -174.621           | -243.885           |
|   |            | 5400                                                  | 49.030                               | 386.213                    | -179.090           | -254.985           |
|   |            | 5500                                                  | 49.367                               | 387.115                    | -182.487           | -261.141           |
|   |            | 5600                                                  | 49.693                               | 388.008                    | -187.190           | -263.345           |
|   |            | 5700                                                  | 50.010                               | 388.990                    | -191.931           | -265.601           |
|   |            | 5800                                                  | 50.316                               | 389.973                    | -196.709           | -267.890           |
|   |            | 5900                                                  | 50.611                               | 390.955                    | -201.524           | -270.242           |
|   |            | 6000                                                  | 50.894                               | 391.478                    | -211.265           | -272.630           |

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

## Strontium Iodide (SrI)

## IDEAL GAS

 $Ti_3Ti_4(g)$ 

$$S^\circ(298.15\text{ K}) = 268.827 \pm 8.4\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_fH^\circ(0\text{ K}) = [275.34 \pm 41.8]\text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_fH^\circ(298.15\text{ K}) = [274.05 \pm 41.8]\text{ kJ}\cdot\text{mol}^{-1}$$

| Electronic Levels and Quantum Weights<br>State<br>$\epsilon,$ cm $^{-1}$<br>$[r\Sigma]$ |     | $C_p^*$ | $S^\circ - (C^\circ - H^\circ(T))/T$ | $H^\circ - H^\circ(T)$ | $\Delta_fG^\circ$ | $\log K_r$ |
|-----------------------------------------------------------------------------------------|-----|---------|--------------------------------------|------------------------|-------------------|------------|
| 0                                                                                       | [4] | 0       | 0                                    | INFINITE               | -10.138           | 275.343    |
| 100                                                                                     | [4] | 32.578  | 230.074                              | 301.372                | -7.130            | 276.266    |
| 200                                                                                     | [4] | 36.180  | 253.948                              | 272.273                | -3.665            | 238.299    |
| 250                                                                                     | [4] | 37.373  | 262.151                              | 269.455                | -1.826            | 274.347    |
| 288.15                                                                                  | [4] | 38.459  | 268.827                              | 268.827                | 0.                | 274.052    |
| 300                                                                                     | [4] | 38.500  | 269.065                              | 268.828                | 0.071             | 274.026    |
| 350                                                                                     | [4] | 39.542  | 275.080                              | 269.301                | 2.023             | 273.284    |
| 450                                                                                     | [4] | 40.165  | 280.421                              | 270.263                | 4.023             | 264.546    |
| 450                                                                                     | [4] | 41.251  | 285.234                              | 271.152                | 6.067             | 263.215    |
| 500                                                                                     | [4] | 41.902  | 289.615                              | 273.523                | 8.146             | 241.830    |
| 600                                                                                     | [4] | 42.842  | 297.345                              | 276.700                | 12.387            | 241.368    |
| 700                                                                                     | [4] | 43.407  | 303.995                              | 280.135                | 16.702            | 178.800    |
| 800                                                                                     | [4] | 43.728  | 309.915                              | 283.489                | 21.060            | 168.469    |
| 900                                                                                     | [4] | 43.903  | 43.976                               | 286.706                | 25.443            | 147.815    |
| 1000                                                                                    | [4] | 44.002  | 319.607                              | 289.769                | 29.838            | 137.609    |
| 1100                                                                                    | [4] | 44.066  | 323.804                              | 292.675                | 34.242            | 127.476    |
| 1200                                                                                    | [4] | 44.119  | 327.641                              | 293.431                | 38.651            | 117.545    |
| 1300                                                                                    | [4] | 44.175  | 331.174                              | 298.047                | 43.066            | 103.011    |
| 1400                                                                                    | [4] | 44.238  | 334.450                              | 300.531                | 47.487            | 232.429    |
| 1500                                                                                    | [4] | 44.312  | 337.505                              | 302.896                | 51.914            | 231.743    |
| 1600                                                                                    | [4] | 44.395  | 340.657                              | 305.149                | 56.349            | 230.934    |
| 1700                                                                                    | [4] | 44.487  | 343.062                              | 307.301                | 60.793            | 229.988    |
| 1800                                                                                    | [4] | 44.585  | 345.607                              | 309.359                | 65.247            | 228.887    |
| 1900                                                                                    | [4] | 44.687  | 348.020                              | 311.331                | 69.710            | 227.618    |
| 2000                                                                                    | [4] | 44.791  | 350.315                              | 313.223                | 74.184            | 211.480    |
| 2100                                                                                    | [4] | 44.896  | 352.503                              | 315.042                | 78.669            | 209.086    |
| 2200                                                                                    | [4] | 45.001  | 354.594                              | 316.792                | 83.163            | 206.672    |
| 2300                                                                                    | [4] | 45.103  | 356.597                              | 318.480                | 87.669            | 204.241    |
| 2400                                                                                    | [4] | 45.203  | 358.318                              | 320.108                | 92.184            | 201.797    |
| 2500                                                                                    | [4] | 45.299  | 360.365                              | 321.682                | 96.709            | 199.347    |
| 2600                                                                                    | [4] | 45.391  | 362.144                              | 323.204                | 101.244           | 196.895    |
| 2700                                                                                    | [4] | 45.479  | 363.859                              | 324.678                | 105.787           | 194.446    |
| 2800                                                                                    | [4] | 45.562  | 365.314                              | 326.107                | 110.339           | 192.006    |
| 2900                                                                                    | [4] | 45.641  | 367.115                              | 327.494                | 114.900           | 189.581    |
| 3000                                                                                    | [4] | 45.716  | 368.663                              | 328.841                | 119.668           | 187.173    |
| 3100                                                                                    | [4] | 45.787  | 370.163                              | 330.150                | 124.043           | 184.788    |
| 3200                                                                                    | [4] | 45.854  | 371.618                              | 331.423                | 128.625           | 182.428    |
| 3300                                                                                    | [4] | 45.917  | 372.030                              | 332.662                | 133.213           | 180.096    |
| 3400                                                                                    | [4] | 45.977  | 374.402                              | 333.370                | 137.808           | 177.795    |
| 3500                                                                                    | [4] | 46.034  | 375.735                              | 333.047                | 142.409           | 175.525    |
| 3600                                                                                    | [4] | 46.089  | 377.033                              | 336.195                | 147.015           | 174.757    |
| 3700                                                                                    | [4] | 46.141  | 378.295                              | 337.316                | 151.626           | 173.289    |
| 3800                                                                                    | [4] | 46.191  | 379.528                              | 338.411                | 156.243           | 172.870    |
| 3900                                                                                    | [4] | 46.240  | 380.728                              | 339.481                | 160.864           | 173.945    |
| 4000                                                                                    | [4] | 46.287  | 381.899                              | 340.527                | 165.491           | 170.898    |
| 4100                                                                                    | [4] | 46.333  | 382.103                              | 341.550                | 170.122           | 167.575    |
| 4200                                                                                    | [4] | 46.378  | 384.160                              | 342.551                | 174.757           | 167.550    |
| 4300                                                                                    | [4] | 46.422  | 385.251                              | 343.531                | 179.397           | 163.901    |
| 4400                                                                                    | [4] | 46.466  | 386.319                              | 344.492                | 184.032           | 164.941    |
| 4500                                                                                    | [4] | 46.510  | 387.364                              | 345.433                | 188.691           | 165.992    |
| 4600                                                                                    | [4] | 46.554  | 388.387                              | 346.356                | 193.344           | 167.063    |
| 4700                                                                                    | [4] | 46.597  | 389.388                              | 347.261                | 198.001           | 167.469    |
| 4800                                                                                    | [4] | 46.641  | 390.370                              | 348.148                | 202.663           | 162.575    |
| 4900                                                                                    | [4] | 46.686  | 391.332                              | 349.020                | 207.330           | 162.255    |
| 5000                                                                                    | [4] | 46.731  | 392.276                              | 349.876                | 212.000           | 161.435    |
| 5100                                                                                    | [4] | 46.776  | 393.202                              | 350.716                | 216.676           | 162.588    |
| 5200                                                                                    | [4] | 46.823  | 394.110                              | 351.542                | 221.336           | 163.667    |
| 5300                                                                                    | [4] | 46.869  | 395.003                              | 352.354                | 226.040           | 164.409    |
| 5400                                                                                    | [4] | 46.917  | 395.379                              | 353.152                | 230.730           | 165.915    |
| 5500                                                                                    | [4] | 46.966  | 396.741                              | 353.936                | 235.424           | 167.575    |
| 5600                                                                                    | [4] | 47.015  | 397.187                              | 354.708                | 240.123           | 168.190    |
| 5700                                                                                    | [4] | 47.065  | 398.420                              | 355.468                | 244.827           | 169.830    |
| 5800                                                                                    | [4] | 47.117  | 399.239                              | 356.215                | 249.536           | 170.477    |
| 5900                                                                                    | [4] | 47.170  | 400.045                              | 356.951                | 254.220           | 171.551    |
| 6000                                                                                    | [4] | 47.223  | 400.338                              | 357.576                | 258.970           | 172.672    |

## TITANIUM IODIDE (TII)

 $Ti_3Ti_4(g)$  $M_r = 174.7845$  Titanium Iodide (TII)

| $T/K$  | $C_p^*$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                                  | Standard State Pressure = $p^\circ = 0.1\text{ MPa}$ |                   |
|--------|---------|----------------------------------------------------------|--------------------------------------------------|------------------------------------------------------|-------------------|
|        |         | $J\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$                | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $H^\circ - H^\circ(T_r)$                             | $\Delta_fH^\circ$ |
| 0      | 0       | 0                                                        | 0                                                | -10.138                                              | 275.343           |
| 100    | 32.578  | 230.074                                                  | 301.372                                          | -7.130                                               | 276.266           |
| 200    | 36.180  | 253.948                                                  | 272.273                                          | -3.665                                               | 238.299           |
| 250    | 37.373  | 262.151                                                  | 269.455                                          | -1.826                                               | 274.347           |
| 288.15 | 38.459  | 268.827                                                  | 268.827                                          | 0.                                                   | 274.052           |
| 300    | 38.500  | 269.065                                                  | 268.828                                          | 0.071                                                | 274.026           |
| 350    | 39.542  | 275.080                                                  | 269.301                                          | 2.023                                                | 273.284           |
| 450    | 40.165  | 280.421                                                  | 270.263                                          | 4.023                                                | 264.546           |
| 450    | 41.251  | 285.234                                                  | 271.152                                          | 6.067                                                | 263.215           |
| 500    | 41.902  | 289.615                                                  | 273.523                                          | 8.146                                                | 241.830           |
| 600    | 42.842  | 297.345                                                  | 276.700                                          | 12.387                                               | 241.368           |
| 700    | 43.407  | 303.995                                                  | 280.135                                          | 16.702                                               | 178.800           |
| 800    | 43.728  | 309.915                                                  | 283.489                                          | 21.060                                               | 168.469           |
| 900    | 43.903  | 43.976                                                   | 286.706                                          | 25.443                                               | 147.815           |
| 1000   | 44.002  | 319.607                                                  | 289.769                                          | 29.838                                               | 137.609           |
| 1100   | 44.066  | 323.804                                                  | 292.675                                          | 34.242                                               | 127.476           |
| 1200   | 44.119  | 327.641                                                  | 293.431                                          | 38.651                                               | 117.545           |
| 1300   | 44.175  | 331.174                                                  | 298.047                                          | 43.066                                               | 103.011           |
| 1400   | 44.238  | 334.450                                                  | 300.531                                          | 47.487                                               | 98.299            |
| 1500   | 44.312  | 337.505                                                  | 302.896                                          | 51.914                                               | 88.742            |
| 1600   | 44.395  | 340.657                                                  | 305.149                                          | 56.349                                               | 79.234            |
| 1700   | 44.487  | 343.062                                                  | 307.301                                          | 60.793                                               | 69.781            |
| 1800   | 44.585  | 345.607                                                  | 309.359                                          | 65.247                                               | 60.388            |
| 1900   | 44.687  | 348.020                                                  | 311.331                                          | 69.710                                               | 51.061            |
| 2000   | 44.791  | 350.315                                                  | 313.223                                          | 74.184                                               | 42.258            |
| 2100   | 44.896  | 352.503                                                  | 315.042                                          | 78.669                                               | 33.836            |
| 2200   | 45.001  | 354.594                                                  | 316.792                                          | 83.163                                               | 32.533            |
| 2300   | 45.103  | 356.597                                                  | 318.480                                          | 87.669                                               | 32.035            |
| 2400   | 45.203  | 358.318                                                  | 320.108                                          | 92.184                                               | 31.391            |
| 2500   | 45.299  | 360.365                                                  | 321.682                                          | 96.709                                               | 31.349            |
| 2600   | 45.391  | 362.144                                                  | 323.204                                          | 101.244                                              | 29.937            |
| 2700   | 45.479  | 363.859                                                  | 324.678                                          | 105.787                                              | 29.090            |
| 2800   | 45.562  | 365.314                                                  | 326.107                                          | 110.339                                              | 28.583            |
| 2900   | 45.641  | 367.115                                                  | 327.494                                          | 114.900                                              | 28.186            |
| 3000   | 45.716  | 368.663                                                  | 328.841                                          | 119.668                                              | 27.781            |
| 3100   | 45.787  | 370.163                                                  | 330.150                                          | 124.043                                              | 27.388            |
| 3200   | 45.854  | 371.618                                                  | 331.423                                          | 128.625                                              | 26.985            |
| 3300   | 45.917  | 372.030                                                  | 332.662                                          | 133.213                                              | 26.582            |
| 3400   | 45.977  | 374.402                                                  | 333.370                                          | 137.808                                              | 26.184            |
| 3500   | 46.034  | 375.735                                                  | 333.047                                          | 142.409                                              | 25.785            |
| 3600   | 46.089  | 377.033                                                  | 336.195                                          | 147.015                                              | 25.389            |
| 3700   | 46.141  | 378.295                                                  | 337.316                                          | 151.626                                              | 25.089            |
| 3800   | 46.191  | 379.528                                                  | 338.411                                          | 156.243                                              | 24.785            |
| 3900   | 46.240  | 380.728                                                  | 339.481                                          | 160.864                                              | 24.480            |
| 4000   | 46.287  | 381.899                                                  | 340.527                                          | 165.491                                              | 24.084            |
| 4100   | 46.333  | 382.103                                                  | 341.550                                          | 170.122                                              | 24.086            |
| 4200   | 46.378  | 384.160                                                  | 342.551                                          | 174.757                                              | 23.686            |
| 4300   | 46.422  | 385.251                                                  | 343.531                                          | 179.397                                              | 23.386            |
| 4400   | 46.466  | 386.319                                                  | 344.492                                          | 184.032                                              | 23.086            |
| 4500   | 46.510  | 387.364                                                  | 345.433                                          | 188.691                                              | 22.781            |
| 4600   | 46.554  | 388.387                                                  | 346.356                                          | 193.344                                              | 22.480            |
| 4700   | 46.597  | 389.388                                                  | 347.261                                          | 198.001                                              | 22.179            |
| 4800   | 46.641  | 390.370                                                  | 348.148                                          | 202.663                                              | 21.878            |
| 4900   | 46.686  | 391.332                                                  | 349.020                                          | 207.330                                              | 21.578            |
| 5000   | 46.731  | 392.276                                                  | 349.876                                          | 212.000                                              | 21.275            |
| 5100   | 46.776  | 393.202                                                  | 350.716                                          | 216.676                                              | 20.972            |
| 5200   | 46.823  | 394.110                                                  | 351.542                                          | 221.336                                              | 20.671            |
| 5300   | 46.869  | 395.003                                                  | 352.354                                          | 226.040                                              | 20.374            |
| 5400   | 46.917  | 395.379                                                  | 353.152                                          | 230.730                                              | 20.073            |
| 5500   | 46.966  | 396.741                                                  | 353.936                                          | 235.424                                              | 19.774            |
| 5600   | 47.015  | 397.387                                                  | 354.708                                          | 240.123                                              | 19.472            |
| 5700   | 47.065  | 398.420                                                  | 355.468                                          | 244.827                                              | 19.171            |
| 5800   | 47.117  | 399.239                                                  | 356.215                                          | 249.536                                              | 18.869            |
| 5900   | 47.170  | 400.045                                                  | 356.951                                          | 254.220                                              | 18.565            |
| 6000   | 47.223  | 400.338                                                  | 357.576                                          | 258.970                                              | 18.263            |

PREVIOUS: December 1968 (a atm)

CURRENT: December 1968 (1 bar)

 $Ti_3Ti_4(g)$  $Ti_3Ti_4(g)$  $Ti_3Ti_4(g)$ 

$$\Delta_fH^\circ(0\text{ K}) = [275$$

## Zirconium Iodide (ZrI)

## IDEAL GAS

$$S^*(298.15\text{ K}) = [275.805] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^*(0\text{ K}) = [593.20 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^*(298.15\text{ K}) = [591.20 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$$

| $\Sigma$ | $\omega_c = [223] \text{ cm}^{-1}$ | $\omega_c \epsilon_c = [1.2] \text{ cm}^{-1}$ | $\sigma = 1$ | $r_e = [2.9] \text{ \AA}$ |
|----------|------------------------------------|-----------------------------------------------|--------------|---------------------------|
|          | $B_c = [0.03789] \text{ cm}^{-1}$  | $\alpha_c = [0.00020] \text{ cm}^{-1}$        |              |                           |

## 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  $\Delta H^*(298.15\text{ K})$ .

## Heat Capacity and Entropy

The vibrational frequency was estimated from those of TiI(g), TiCl(g), ZrCl(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 interatomic distance was estimated from those of TiBr(g), TiI(g) and ZrI<sub>4</sub>(g).

## Reference

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

| $T/K$  | $C_p^*$ | $S^* - [G^* - H^*(T)]/T$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |              |                                 |
|--------|---------|--------------------------|----------------------------------------------------------|--------------|---------------------------------|
|        |         |                          | $H^* - H^*(T_r)/T$                                       | $\Delta H^*$ | $\text{kJ}\cdot\text{mol}^{-1}$ |
| 0      | 0       | 0                        | 0                                                        | 0            | 0                               |
| 100    | 32.964  | 237.198                  | -10.097                                                  | 593.198      | 593.198                         |
| 200    | 36.028  | 279.160                  | -7.071                                                   | 593.813      | 574.549                         |
| 250    | 36.593  | 269.329                  | -3.587                                                   | 592.637      | -145.134                        |
| 298.15 | 36.931  | 275.805                  | -1.771                                                   | 591.925      | 546.545                         |
| 300    | 36.941  | 276.033                  | 0                                                        | 591.199      | -14.194                         |
| 350    | 37.177  | 281.747                  | 0.068                                                    | 537.740      | -94.233                         |
| 400    | 37.349  | 286.723                  | 276.256                                                  | 590.347      | 528.665                         |
| 450    | 37.483  | 291.130                  | 277.260                                                  | 581.508      | 520.185                         |
| 500    | 37.592  | 295.085                  | 278.561                                                  | 580.038      | 512.607                         |
| 600    | 37.767  | 301.925                  | 283.120                                                  | 558.533      | 507.090                         |
| 700    | 37.910  | 307.788                  | 286.237                                                  | 515.085      | 507.090                         |
| 800    | 38.034  | 312.838                  | 289.255                                                  | 18.892       | 555.925                         |
| 900    | 38.148  | 317.345                  | 292.132                                                  | 22.692       | 476.653                         |
| 1000   | 38.256  | 321.370                  | 294.838                                                  | 26.512       | 533.755                         |
| 1100   | 38.360  | 325.021                  | 297.436                                                  | 30.343       | 552.507                         |
| 1200   | 38.460  | 328.363                  | 299.876                                                  | 34.184       | 496.875                         |
| 1300   | 38.559  | 331.445                  | 302.188                                                  | 38.035       | -19.088                         |
| 1400   | 38.636  | 334.306                  | 304.381                                                  | 41.895       | 420.498                         |
| 1500   | 38.751  | 336.976                  | 306.466                                                  | 45.766       | -14.133                         |
| 1600   | 38.847  | 339.480                  | 308.452                                                  | 49.646       | -21.106                         |
| 1700   | 38.941  | 341.838                  | 310.347                                                  | 53.533       | -23.888                         |
| 1800   | 39.035  | 344.067                  | 312.159                                                  | 57.434       | -21.262                         |
| 1900   | 39.128  | 346.180                  | 313.894                                                  | 61.342       | -10.338                         |
| 2000   | 39.221  | 348.189                  | 315.559                                                  | 63.260       | 537.685                         |
| 2100   | 39.314  | 350.105                  | 317.159                                                  | 69.186       | 535.954                         |
| 2200   | 39.407  | 351.936                  | 318.699                                                  | 73.122       | 552.244                         |
| 2300   | 39.499  | 353.690                  | 320.182                                                  | 77.068       | 510.300                         |
| 2400   | 39.592  | 355.373                  | 321.613                                                  | 81.022       | 337.826                         |
| 2500   | 39.684  | 356.991                  | 322.996                                                  | 84.986       | 505.364                         |
| 2600   | 39.776  | 358.549                  | 324.334                                                  | 88.959       | 502.889                         |
| 2700   | 39.868  | 360.052                  | 325.629                                                  | 92.949       | 321.906                         |
| 2800   | 39.960  | 361.503                  | 326.885                                                  | 96.933       | -6.507                          |
| 2900   | 40.052  | 362.907                  | 328.103                                                  | 100.933      | 317.069                         |
| 3000   | 40.143  | 364.267                  | 329.286                                                  | 104.943      | 493.087                         |
| 3100   | 40.235  | 365.584                  | 330.435                                                  | 108.962      | 490.685                         |
| 3200   | 40.327  | 366.863                  | 331.554                                                  | 112.990      | 338.311                         |
| 3300   | 40.418  | 368.106                  | 332.643                                                  | 117.027      | 485.968                         |
| 3400   | 40.510  | 369.314                  | 333.704                                                  | 121.074      | 277.838                         |
| 3500   | 40.602  | 370.489                  | 334.738                                                  | 125.129      | 497.939                         |
| 3600   | 40.693  | 371.634                  | 335.747                                                  | 129.194      | 310.323                         |
| 3700   | 40.785  | 372.751                  | 336.732                                                  | 133.268      | 503.665                         |
| 3800   | 40.876  | 373.839                  | 337.694                                                  | 137.351      | 476.945                         |
| 3900   | 40.968  | 374.902                  | 338.631                                                  | 141.443      | 241.159                         |
| 4000   | 41.059  | 375.941                  | 339.555                                                  | 145.544      | 470.576                         |
| 4100   | 41.150  | 376.956                  | 340.454                                                  | 149.655      | 468.531                         |
| 4200   | 41.242  | 377.948                  | 345.483                                                  | 153.774      | 229.392                         |
| 4300   | 41.333  | 378.920                  | 342.198                                                  | 157.903      | 464.555                         |
| 4400   | 41.425  | 379.871                  | 343.044                                                  | 162.041      | 462.623                         |
| 4500   | 41.516  | 380.803                  | 349.260                                                  | 166.188      | 460.728                         |
| 4600   | 41.607  | 381.717                  | 344.685                                                  | 170.344      | 438.858                         |
| 4700   | 41.699  | 382.612                  | 345.483                                                  | 174.510      | 457.043                         |
| 4800   | 41.790  | 383.491                  | 346.265                                                  | 178.684      | 195.215                         |
| 4900   | 41.881  | 384.354                  | 347.034                                                  | 182.868      | -2.170                          |
| 5000   | 41.973  | 385.201                  | 347.789                                                  | 187.060      | 207.090                         |
| 5100   | 42.064  | 386.033                  | 348.531                                                  | 191.262      | 214.128                         |
| 5200   | 42.155  | 386.851                  | 349.260                                                  | 195.473      | 212.107                         |
| 5300   | 42.247  | 387.655                  | 349.977                                                  | 199.693      | 211.225                         |
| 5400   | 42.338  | 388.445                  | 350.682                                                  | 203.923      | -113.897                        |
| 5500   | 42.429  | 389.223                  | 351.375                                                  | 208.161      | -115.206                        |
| 5600   | 42.521  | 389.988                  | 352.058                                                  | 212.408      | -116.496                        |
| 5700   | 42.612  | 390.742                  | 352.720                                                  | 216.665      | -117.768                        |
| 5800   | 42.703  | 391.483                  | 353.392                                                  | 220.931      | -119.020                        |
| 5900   | 42.795  | 392.214                  | 354.044                                                  | 225.206      | -120.252                        |
| 6000   | 42.886  | 392.934                  | 354.686                                                  | 229.490      | -121.463                        |

| $T/K$  | $C_p^*$ | $S^* - [G^* - H^*(T)]/T$ | $H^* - H^*(T_r)/T$ | $\Delta H^*$ | $\text{kJ}\cdot\text{mol}^{-1}$ |
|--------|---------|--------------------------|--------------------|--------------|---------------------------------|
| 0      | 0       | 0                        | 0                  | 0            | 0                               |
| 100    | 32.964  | 237.198                  | -10.097            | 593.198      | 593.198                         |
| 200    | 36.028  | 279.160                  | -7.071             | 593.813      | 574.549                         |
| 250    | 36.593  | 269.329                  | -3.587             | 592.637      | -145.134                        |
| 298.15 | 36.931  | 275.805                  | 0                  | 591.199      | -14.194                         |
| 300    | 36.941  | 276.033                  | 0.068              | 591.171      | -93.594                         |
| 350    | 37.177  | 281.747                  | 276.256            | 1.922        | -78.899                         |
| 400    | 37.349  | 286.723                  | 277.260            | 3.785        | 520.185                         |
| 450    | 37.483  | 291.130                  | 278.561            | 5.655        | 512.607                         |
| 500    | 37.592  | 295.085                  | 280.019            | 7.533        | 507.090                         |
| 550    | 37.767  | 301.925                  | 283.120            | 11.301       | 537.731                         |
| 600    | 37.910  | 307.788                  | 286.237            | 15.085       | 556.857                         |
| 700    | 37.910  | 307.788                  | 286.237            | 15.085       | 486.800                         |
| 800    | 38.034  | 312.838                  | 289.255            | 18.892       | 555.925                         |
| 900    | 38.148  | 317.345                  | 292.132            | 22.692       | 476.653                         |
| 1000   | 38.256  | 321.370                  | 294.838            | 26.512       | 533.755                         |
| 1100   | 38.360  | 325.021                  | 297.436            | 30.343       | 552.507                         |
| 1200   | 38.460  | 328.363                  | 299.876            | 34.184       | 496.875                         |
| 1300   | 38.559  | 331.445                  | 302.188            | 38.035       | -19.088                         |
| 1400   | 38.636  | 334.306                  | 304.381            | 41.895       | 420.498                         |
| 1500   | 38.751  | 336.976                  | 306.466            | 45.766       | -14.133                         |
| 1600   | 38.847  | 339.480                  | 308.452            | 49.646       | -21.106                         |
| 1700   | 38.941  | 341.838                  | 310.347            | 53.533       | -23.888                         |
| 1800   | 39.035  | 344.067                  | 312.159            | 57.434       | -21.262                         |
| 1900   | 39.128  | 346.180                  | 313.894            | 61.342       | -10.338                         |
| 2000   | 39.221  | 348.189                  | 315.559            | 63.260       | 537.685                         |
| 2100   | 39.314  | 350.105                  | 317.159            | 69.186       | 535.954                         |
| 2200   | 39.407  | 351.936                  | 318.699            | 73.122       | 552.244                         |
| 2300   | 39.499  | 353.690                  | 320.182            | 77.068       | 510.300                         |
| 2400   | 39.592  | 355.373                  | 321.613            | 81.022       | 337.826                         |
| 2500   | 39.684  | 356.991                  | 322.996            | 84.986       | 505.364                         |
| 2600   | 39.776  | 358.549                  | 324.334            | 88.959       | 502.889                         |
| 2700   | 39.868  | 360.052                  | 325.629            | 92.949       | -6.507                          |
| 2800   | 39.960  | 361.503                  | 326.885            | 96.933       | 317.069                         |
| 2900   | 40.052  | 362.907                  | 328.103            | 100.933      | 493.087                         |
| 3000   | 40.143  | 364.267                  | 329.286            | 104.943      | -12.107                         |
| 3100   | 40.235  | 365.584                  | 330.435            | 108.962      | -7.354                          |
| 3200   | 40.327  | 366.863                  | 331.554            | 112.990      | -6.912                          |
| 3300   | 40.418  | 368.106                  | 332.643            | 117.027      | -4.639                          |
| 3400   | 40.510  | 369.314                  | 333.704            | 121.074      | -4.398                          |
| 3500   | 40.602  | 370.489                  | 334.738            | 125.129      | -5.789                          |
| 3600   | 40.693  | 371.634                  | 335.747            | 129.194      | -3.761                          |
| 3700   | 40.785  | 372.751                  | 336.732            | 133.268      | -3.574                          |
| 3800   | 40.876  | 373.839                  | 337.694            | 137.351      | 474.783                         |
| 3900   | 40.968  | 374.902                  | 338.631            | 141.443      | 241.159                         |
| 4000   | 41.059  | 375.941                  | 339.555            | 145.544      | 470.576                         |
| 4100   | 41.150  | 376.956                  | 340.454            | 149.655      | 468.531                         |
| 4200   | 41.242  | 377.948                  | 341.335            | 153.774      | 229.392                         |
| 4300   | 41.333  | 378.920                  | 342.198            | 157.903      | 464.555                         |
| 4400   | 41.425  | 379.871                  | 343.044            | 162.041      | 462.623                         |
| 4500   | 41.516  | 380.803                  | 343.872            | 166.188      | 460.728                         |
| 4600   | 41.607  | 381.717                  | 344.685            | 170.344      | 203.805                         |
| 4700   | 41.699  | 382.612                  | 345.483            | 174.510      | 195.215                         |
| 4800   | 41.790  | 383.491                  | 346.265            | 178.684      | -2.922                          |
| 4900   | 41.881  | 384.354                  | 347.034            | 182.868      | -2.781                          |
| 5000   | 41.973  | 385.201                  | 347.789            | 187.060      | -2.646                          |
| 5100   | 42.064  | 386.033                  | 348.531            | 191.262      | -2.237                          |
| 5200   | 42.155  | 386.851                  | 349.260            | 195.473      | -2.518                          |
| 5300   | 42.247  | 387.655                  | 349.977            | 199.693      | -2.281                          |
| 5400   | 42.338  | 388.445                  | 350.682            | 203.923      | -2.302                          |
| 5500   | 42.429  | 389.223                  | 351.375            | 208.161      | -2.170                          |
| 5600   | 42.521  | 389.988                  | 352.058            | 212.408      | -2.343                          |
| 5700   | 42.612  | 390.742                  | 352.720            | 216.665      | -2.646                          |
| 5800   | 42.703  | 391.483                  | 353.392            | 220.931      | -2.382                          |
| 5900   | 42.795  | 392.214                  | 354.044            | 225.206      | -2.401                          |
| 6000   | 42.886  | 392.934                  | 354.686            | 229.490      | -2.437                          |

CURRENT September 1964 (1 atm)</p

REFERENCE STATE  
Iodine ( $I_2$ ) $M_r = 253.8090$  Iodine ( $I_2$ ) $I_2$ (ref)

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.

| T/K     | $C_p^*$ | Enthalpy Reference Temperature = $T_r = 298.15$ K |                  | Standard State Pressure = $p^* = 0.1$ MPa |                           |
|---------|---------|---------------------------------------------------|------------------|-------------------------------------------|---------------------------|
|         |         | $S^* - [G^* - H^*(T_r)]/T$                        | $H^* - H^*(T_r)$ | $\Delta_f G^*$                            | $\log K_r$                |
| 0       | 0       | 0                                                 | -13.198          | 0                                         | 0                         |
| 100     | 45.650  | 60.992                                            | -10.148          | 0                                         | 0                         |
| 200     | 51.566  | 94.938                                            | -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                                           | 117.859          | 20.670                                    |                           |
| 400     | 80.669  | 174.062                                           | 119.714          | 21.739                                    | 0                         |
| 457.666 | 80.669  | 184.926                                           | 127.262          | 26.391                                    | — LIQUID <--> IDEAL GAS — |
| 457.666 | 37.386  | 216.609                                           | 127.262          | 68.351                                    | FUGACITY = 1 bar          |
| 500     | 37.464  | 279.920                                           | 140.049          | 69.935                                    | 0                         |
| 600     | 37.612  | 286.764                                           | 163.948          | 73.690                                    | 0                         |
| 700     | 37.735  | 292.571                                           | 181.918          | 77.457                                    | 0                         |
| 800     | 37.847  | 297.618                                           | 196.072          | 81.236                                    | 0                         |
| 900     | 37.959  | 302.082                                           | 207.608          | 85.027                                    | 0                         |
| 1000    | 38.081  | 306.087                                           | 217.259          | 88.828                                    | 0                         |
| 1100    | 38.232  | 309.724                                           | 225.502          | 92.644                                    | 0                         |
| 1200    | 38.431  | 313.058                                           | 232.661          | 96.476                                    | 0                         |
| 1300    | 38.699  | 316.144                                           | 238.966          | 100.332                                   | 0                         |
| 1400    | 39.055  | 319.025                                           | 244.383          | 104.219                                   | 0                         |
| 1500    | 39.507  | 321.734                                           | 249.637          | 108.146                                   | 0                         |
| 1600    | 40.051  | 324.301                                           | 254.224          | 112.124                                   | 0                         |
| 1700    | 40.674  | 326.747                                           | 258.418          | 116.159                                   | 0                         |
| 1800    | 41.352  | 329.091                                           | 262.280          | 120.260                                   | 0                         |
| 1900    | 42.054  | 331.346                                           | 265.856          | 124.431                                   | 0                         |
| 2000    | 42.748  | 333.521                                           | 269.185          | 128.671                                   | 0                         |
| 2100    | 43.404  | 335.622                                           | 272.299          | 132.979                                   | 0                         |
| 2200    | 43.994  | 337.655                                           | 275.224          | 137.399                                   | 0                         |
| 2300    | 44.994  | 339.622                                           | 277.981          | 141.775                                   | 0                         |
| 2400    | 44.890  | 341.525                                           | 280.389          | 146.245                                   | 0                         |
| 2500    | 45.171  | 343.363                                           | 283.064          | 150.749                                   | 0                         |
| 2600    | 45.335  | 345.139                                           | 285.417          | 155.275                                   | 0                         |
| 2700    | 45.392  | 346.851                                           | 287.861          | 159.812                                   | 0                         |
| 2800    | 45.319  | 348.500                                           | 289.805          | 164.348                                   | 0                         |
| 2900    | 45.154  | 350.088                                           | 291.856          | 168.872                                   | 0                         |
| 3000    | 44.897  | 351.615                                           | 293.823          | 173.376                                   | 0                         |
| 3100    | 44.561  | 353.082                                           | 295.711          | 177.849                                   | 0                         |
| 3200    | 44.157  | 354.490                                           | 297.526          | 182.296                                   | 0                         |
| 3300    | 43.697  | 355.842                                           | 299.273          | 186.679                                   | 0                         |
| 3400    | 43.193  | 357.139                                           | 300.956          | 191.024                                   | 0                         |
| 3500    | 42.634  | 358.384                                           | 302.579          | 195.316                                   | 0                         |
| 3600    | 42.091  | 359.577                                           | 304.146          | 199.554                                   | 0                         |
| 3700    | 41.510  | 360.723                                           | 305.660          | 203.734                                   | 0                         |
| 3800    | 40.919  | 361.822                                           | 307.123          | 207.855                                   | 0                         |
| 3900    | 40.325  | 362.877                                           | 308.359          | 211.917                                   | 0                         |
| 4000    | 39.731  | 363.891                                           | 309.911          | 215.920                                   | 0                         |
| 4100    | 39.143  | 364.864                                           | 311.239          | 218.864                                   | 0                         |
| 4200    | 38.563  | 365.801                                           | 312.527          | 223.749                                   | 0                         |
| 4300    | 37.995  | 366.701                                           | 313.777          | 227.578                                   | 0                         |
| 4400    | 37.319  | 367.568                                           | 314.989          | 231.388                                   | 0                         |
| 4500    | 36.839  | 368.404                                           | 316.167          | 235.065                                   | 0                         |
| 4600    | 36.374  | 369.209                                           | 317.311          | 238.729                                   | 0                         |
| 4700    | 35.966  | 369.986                                           | 318.424          | 242.341                                   | 0                         |
| 4800    | 35.575  | 370.736                                           | 319.506          | 245.903                                   | 0                         |
| 4900    | 34.901  | 371.460                                           | 320.559          | 249.416                                   | 0                         |
| 5000    | 34.444  | 372.161                                           | 321.384          | 252.833                                   | 0                         |
| 5100    | 34.005  | 372.838                                           | 322.382          | 256.306                                   | 0                         |
| 5200    | 33.582  | 373.495                                           | 323.555          | 259.685                                   | 0                         |
| 5300    | 33.176  | 374.130                                           | 324.503          | 263.073                                   | 0                         |
| 5400    | 32.785  | 374.747                                           | 325.528          | 266.321                                   | 0                         |
| 5500    | 32.410  | 375.345                                           | 326.530          | 269.580                                   | 0                         |
| 5600    | 32.051  | 375.926                                           | 327.211          | 272.803                                   | 0                         |
| 5700    | 31.705  | 376.490                                           | 328.071          | 275.991                                   | 0                         |
| 5800    | 31.374  | 377.038                                           | 328.910          | 279.145                                   | 0                         |
| 5900    | 31.056  | 377.572                                           | 329.730          | 282.266                                   | 0                         |
| 6000    | 30.751  | 378.091                                           | 330.532          | 285.356                                   | 0                         |

Iodine ( $I_2$ )

PREVIOUS: September 1961 (1 atm)

CURRENT: June 1982 (1 bar)

**Iodine ( $I_2$ )****CRYSTAL** **$I_2(\text{cr})$** 

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= 116.142 \pm 0.080 \text{ J K}^{-1} \cdot \text{mol}^{-1} \\ T_{\text{fus}} &= 386.75 \pm 0.3 \text{ K} \\ \Delta_f H^\circ(298.15 \text{ K}) &= 0 \text{ kJ mol}^{-1} \\ \Delta_{\text{fs}} H^\circ &= 15.517 \pm 0.16 \text{ kJ mol}^{-1} \end{aligned}$$

**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.<sup>5</sup> The results are corrected by a factor which varies from 0 at 300 K to 0.995 at 400 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  $I_2(\text{cr})$ :  $H^\circ(T) - H^\circ(298.15 \text{ K}) = -50.6457 + 0.123457^2 - 27.97 \times 10^5 T^1 + 13508.7$ . 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**

$T_{\text{fus}} = 113.6 \text{ }^\circ\text{C}$  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  $I_2(g)$  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: *Curr.*, 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).

| $T/K$   | $C_p^\circ$ | $S^\circ - (G^\circ - H^\circ(T))/T$ | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                    | Standard State Pressure = $P^\circ = 0.1 \text{ kPa}$ |            |
|---------|-------------|--------------------------------------|-----------------------------------------------------------|--------------------|-------------------------------------------------------|------------|
|         |             |                                      | $H^\circ - H^\circ(T_r)/T$                                | $\Delta_f H^\circ$ | $\Delta_f G^\circ$                                    | $\log K_r$ |
| 0       | 0           | 0                                    | 0                                                         | 0                  | 0                                                     | 0          |
| 100     | 45.650      | 60.992                               | 162.472                                                   | -10.148            | 0                                                     | 0          |
| 200     | 51.566      | 94.958                               | 121.036                                                   | -5.216             | 0                                                     | 0          |
| 250     | 53.244      | 106.678                              | 117.030                                                   | -2.388             | 0                                                     | 0          |
| 298.15  | 54.436      | 116.142                              | 0                                                         | 0                  | 0                                                     | 0          |
| 300     | 54.506      | 116.479                              | 116.143                                                   | 0.101              | 0                                                     | 0          |
| 350     | 58.605      | 125.140                              | 116.818                                                   | 2.913              | 0                                                     | 0          |
| 386.750 | 63.545      | 131.224                              | 117.899                                                   | 5.153              | — CRYSTAL. —> LIQUID. —>                              | —          |
| 400     | 65.598      | 133.398                              | 118.376                                                   | 6.009              | -15.730                                               | 0.535      |
| 450     | 73.402      | 141.515                              | 120.500                                                   | 9.484              | -16.288                                               | -0.070     |
| 500     | 81.207      | 149.713                              | 123.015                                                   | 13.349             | -56.386                                               | -0.303     |
| 600     | 96.816      | 165.898                              | 128.815                                                   | 22.250             | -51.439                                               | -0.590     |
| 700     | 112.425     | 181.995                              | 135.263                                                   | 32.712             | -44.745                                               | -1.835     |
|         |             |                                      |                                                           |                    | 32.659                                                | -2.437     |

PREVIOUS

CURRENT: June 1982

**I<sub>2</sub>(l)****Iodine (I<sub>2</sub>)****Liquid**

| <b>M<sub>r</sub> = 253.8090 Iodine (I<sub>2</sub>)</b>                                                                                                                                                                                                                                                                     |  | Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K |                                                      |                                         |                                             |                                             |                                        | Standard State Pressure = p° = 0.1 MPa |                    |  |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|------------------------------------------------------------|------------------------------------------------------|-----------------------------------------|---------------------------------------------|---------------------------------------------|----------------------------------------|----------------------------------------|--------------------|--|
|                                                                                                                                                                                                                                                                                                                            |  | T/K                                                        | C <sub>p</sub> /J·K <sup>-1</sup> ·mol <sup>-1</sup> | S°/J·K <sup>-1</sup> ·mol <sup>-1</sup> | H°-H°(T <sub>r</sub> )/kJ·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> | Δ <sub>f</sub> G°/kJ·mol <sup>-1</sup> | log K <sub>t</sub> |  |
| Δ <sub>f</sub> H°(298.15 K) = [13.523] kJ·mol <sup>-1</sup>                                                                                                                                                                                                                                                                |  |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| Δ <sub>us</sub> H° = 15.517 ± 0.16 kJ·mol <sup>-1</sup>                                                                                                                                                                                                                                                                    |  |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| Enthalpy of Formation                                                                                                                                                                                                                                                                                                      |  |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| Δ <sub>f</sub> H°(I <sub>2</sub> , l, 298.15 K), is calculated from that of the crystal by adding Δ <sub>fw</sub> H° and the difference in enthalpy, H°(386.75 K)-H°(298.15 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 J·K <sup>-1</sup> ·mol <sup>-1</sup> , based on the data of Frederick and Hidebrand. <sup>1</sup> Their enthalpy data was corrected as discussed in the I <sub>2</sub> (cr) table. The enthalpy equation is H°(T)-H°(298.15 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                                                                                                                                                                                                                                                                                                                 |  |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| K. J. Frederick and J. H. Hidebrand, J. Am. Chem. Soc. 60, 1436 (1938).                                                                                                                                                                                                                                                    |  |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |

| <b>I<sub>2</sub>(l)</b>                                     |        | Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K |                                                      |                                         |                                             |                                             |                                        | Standard State Pressure = p° = 0.1 MPa |                    |  |
|-------------------------------------------------------------|--------|------------------------------------------------------------|------------------------------------------------------|-----------------------------------------|---------------------------------------------|---------------------------------------------|----------------------------------------|----------------------------------------|--------------------|--|
|                                                             |        | T/K                                                        | C <sub>p</sub> /J·K <sup>-1</sup> ·mol <sup>-1</sup> | S°/J·K <sup>-1</sup> ·mol <sup>-1</sup> | H°-H°(T <sub>r</sub> )/kJ·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> | Δ <sub>f</sub> G°/kJ·mol <sup>-1</sup> | log K <sub>t</sub> |  |
| Δ <sub>f</sub> H°(298.15 K) = [13.523] kJ·mol <sup>-1</sup> |        |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| T <sub>us</sub> = 386.75 ± 0.03 K                           |        |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| 0                                                           |        |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| 100                                                         |        |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| 200                                                         |        |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| 250                                                         |        |                                                            |                                                      |                                         |                                             |                                             |                                        |                                        |                    |  |
| 298.15                                                      | 80.669 | 150.356                                                    | 0                                                    | 13.523                                  | 3.322                                       | -0.582                                      |                                        |                                        |                    |  |
| 300                                                         | 80.669 | 150.357                                                    | 0.149                                                | 13.571                                  | 3.259                                       | -0.567                                      |                                        |                                        |                    |  |
| 350                                                         | 80.669 | 151.339                                                    | 4.183                                                | 14.793                                  | 1.440                                       | -0.215                                      |                                        |                                        |                    |  |
| 386.750                                                     | 80.669 | 152.864                                                    | 7.147                                                | —                                       | CRYSTAL ↔ LIQUID                            | —                                           |                                        |                                        |                    |  |
| 400                                                         | 80.669 | 153.521                                                    | 8.216                                                | 0.                                      | 0.                                          | 0.                                          |                                        |                                        |                    |  |
| 450                                                         | 80.669 | 156.342                                                    | 12.250                                               | 0.                                      | 0.                                          | 0.                                          |                                        |                                        |                    |  |
| 457.666                                                     | 80.669 | 156.809                                                    | 12.868                                               | —                                       | FUGACITY = 1 bar                            | —                                           |                                        |                                        |                    |  |
| 500                                                         | 80.669 | 192.062                                                    | 159.496                                              | 16.283                                  | -40.130                                     | 3.799                                       | -0.397                                 |                                        |                    |  |
| 600                                                         | 80.669 | 206.770                                                    | 166.187                                              | 24.350                                  | -35.817                                     | 12.179                                      | -1.060                                 |                                        |                    |  |
| 700                                                         | 80.669 | 219.205                                                    | 172.895                                              | 32.417                                  | -31.518                                     | 19.839                                      | -1.480                                 |                                        |                    |  |
| 800                                                         | 80.669 | 229.977                                                    | 179.372                                              | 40.384                                  | -27.230                                     | 26.883                                      | -1.755                                 |                                        |                    |  |
| 900                                                         | 80.669 | 239.478                                                    | 185.533                                              | 48.550                                  | -22.933                                     | 33.390                                      | -1.938                                 |                                        |                    |  |
| 1000                                                        | 80.669 | 247.978                                                    | 191.360                                              | 56.617                                  | -18.688                                     | 39.421                                      | -2.039                                 |                                        |                    |  |

## CRYSTAL-LIQUID

 $I_2$  = 253.8090 Iodine ( $I_2$ ) $I_2$ (cr.)

0 to 386.75 K crystal  
above 386.75 K liquid

Refer to the individual tables for details.

| T/K     | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                                  |         | Standard State Pressure = $p^* = 0.1\text{ MPa}$ |                                      |                                 |              |                                 |              |                                 |            |
|---------|----------------------------------------------------------|--------------------------------------------------|---------|--------------------------------------------------|--------------------------------------|---------------------------------|--------------|---------------------------------|--------------|---------------------------------|------------|
|         | $C_p^*$                                                  | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $S^*$   | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $H^*-H^*(T_r)$                       | $\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta H^*$ | $\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta G^*$ | $\text{kJ}\cdot\text{mol}^{-1}$ | $\log K_r$ |
| 0       | 0                                                        | 0                                                | 0       | 0                                                | INFINITE                             | -13.198                         | 0            | 0                               | 0            | 0                               | 0          |
| 100     | 45.650                                                   | 60.992                                           | 162.472 | -10.148                                          | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 200     | 51.566                                                   | 94.958                                           | 121.036 | -5.216                                           | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 250     | 53.244                                                   | 106.678                                          | 117.030 | -2.588                                           | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 298.15  | 54.436                                                   | 116.142                                          | 116.142 | 0                                                | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 300     | 54.506                                                   | 116.379                                          | 116.143 | 0.101                                            | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 350     | 58.605                                                   | 125.140                                          | 116.818 | 2.913                                            | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 386.750 | 63.545                                                   | 131.224                                          | 117.899 | 5.153                                            | — CRYSTAL <--> LIQUID — TRANSITION — |                                 |              |                                 |              |                                 |            |
| 386.750 | 80.669                                                   | 171.344                                          | 117.899 | 20.670                                           |                                      |                                 |              |                                 |              |                                 |            |
| 400     | 80.669                                                   | 174.062                                          | 119.714 | 21.739                                           | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 450     | 80.669                                                   | 183.663                                          | 126.291 | 25.772                                           | 0                                    | 0                               | 0            | 0                               | 0            | 0                               | 0          |
| 457.666 | 80.669                                                   | 184.926                                          | 121.262 | 26.391                                           | — FUGACITY = 1 bar —                 |                                 |              |                                 |              |                                 |            |
| 500     | 80.669                                                   | 192.062                                          | 132.451 | 29.806                                           | -40.130                              | 3.799                           | -0.397       |                                 |              |                                 |            |
| 600     | 80.669                                                   | 205.770                                          | 143.649 | 37.873                                           | -35.817                              | 12.179                          | -1.060       |                                 |              |                                 |            |
| 700     | 80.669                                                   | 219.205                                          | 153.577 | 45.940                                           | -31.518                              | 19.839                          | -1.480       |                                 |              |                                 |            |
| 800     | 80.669                                                   | 229.977                                          | 162.469 | 54.006                                           | -27.230                              | 26.883                          | -1.755       |                                 |              |                                 |            |
| 900     | 80.669                                                   | 239.478                                          | 170.508 | 62.073                                           | -22.953                              | 33.390                          | -1.938       |                                 |              |                                 |            |
| 1000    | 80.669                                                   | 247.978                                          | 177.837 | 70.140                                           | -18.688                              | 39.421                          | -2.059       |                                 |              |                                 |            |

Iodine ( $I_2$ )

## IDEAL GAS

$$D_0^{\circ} = 148.816 \pm 0.001 \text{ kJ/mol}^{-1}$$

$$S^{\circ}(298.15 \text{ K}) = 260.685 \pm 0.062 \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta_H^{\circ}(298.15 \text{ K}) = 65.504 \pm 0.092 \text{ kJ mol}^{-1}$$

$$\Delta_H^{\circ}(298.15 \text{ K}) = 62.421 \pm 0.079 \text{ kJ mol}^{-1}$$

Iodine ( $I_2$ )M<sub>r</sub> = 253.8090 Iodine ( $I_2$ )

| State              | $T_e$    | $D^{\circ}$ | $\omega_e$ | $\omega_{e\cdot e}$ | $B_e$    | $10^6 D_e$          | $r_e \text{ \AA}$    | References | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                                              | Standard State Pressure = $p^{\circ} = 0.1 \text{ MPa}$ |                     |
|--------------------|----------|-------------|------------|---------------------|----------|---------------------|----------------------|------------|-----------------------------------------------------------|----------------------------------------------|---------------------------------------------------------|---------------------|
|                    |          |             |            |                     |          |                     |                      |            | $C_p^{\circ}$                                             | $S^{\circ} - [G^{\circ} - H^{\circ}(T_r)]/T$ | $H^{\circ} - H^{\circ}(T_r)$                            | $kJ \cdot mol^{-1}$ |
| ${}^1\Sigma^+$     | 0        | 12440       | 214.5481   | 0.616759(a)         | 0.037395 | 0.12435(b)          | 0.00454(c)           | 2.6657     | ${}^1D_6'$                                                | 0                                            | -10.116                                                 | 65.504              |
| ${}^3\Pi_{u}$      | 10200    | 12440       | 110.366    | 1.3927 <sup>a</sup> | 0.028    | 0.1                 | 0.04                 | 3.104      | ${}^2$                                                    | 100                                          | 222.004                                                 | 292.808             |
| ${}^3\Pi_{g}$      | 11059    | 12440       | 90.6       | 2.57 <sup>a</sup>   | 0.02763  | 0.542 <sup>a</sup>  | 0.03                 | 3.101      | ${}^3$                                                    | 200                                          | 246.105                                                 | 264.038             |
| ${}^3\Pi_{u\star}$ | 15769.01 | 20043.15    | 125.697    | 0.7642 <sup>a</sup> | 0.029039 | 0.1582 <sup>a</sup> | 0.00543 <sup>a</sup> | 3.0247     | ${}^4$                                                    | 250                                          | 265.82                                                  | 254.213             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 300                                          | 266.897                                                 | 260.685             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 350                                          | 271.015                                                 | 262.138             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 400                                          | 271.256                                                 | 271.582             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 450                                          | 273.977                                                 | 263.436             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 457.666                                      | 31.386                                                  | 276.609             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 500                                          | 279.920                                                 | 264.891             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 500                                          | 37.464                                                  | 286.764             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 600                                          | 267.261                                                 | 267.983             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 700                                          | 271.091                                                 | 15.016              |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 800                                          | 37.847                                                  | 297.618             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 900                                          | 307.959                                                 | 274.098             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1000                                         | 363.081                                                 | 276.964             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1100                                         | 38.232                                                  | 264.407             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1200                                         | 313.724                                                 | 282.248             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1300                                         | 313.058                                                 | 284.679             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1400                                         | 316.144                                                 | 286.982             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1500                                         | 319.055                                                 | 289.169             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1600                                         | 319.507                                                 | 221.734             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1700                                         | 40.674                                                  | 326.747             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1800                                         | 42.430                                                  | 293.237             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 1900                                         | 41.352                                                  | 293.237             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2000                                         | 42.748                                                  | 329.091             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2100                                         | 43.404                                                  | 320.023             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2200                                         | 43.994                                                  | 337.655             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2300                                         | 44.494                                                  | 305.622             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2400                                         | 44.890                                                  | 341.525             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2500                                         | 45.171                                                  | 343.163             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2600                                         | 45.335                                                  | 345.139             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2700                                         | 45.382                                                  | 346.851             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2800                                         | 314.519                                                 | 310.551             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 2900                                         | 43.850                                                  | 348.500             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3000                                         | 45.154                                                  | 350.088             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3100                                         | 44.897                                                  | 351.615             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3200                                         | 44.157                                                  | 353.842             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3300                                         | 44.561                                                  | 355.842             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3400                                         | 43.697                                                  | 357.139             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3500                                         | 42.654                                                  | 358.384             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3600                                         | 42.091                                                  | 359.577             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3700                                         | 41.510                                                  | 360.723             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3800                                         | 40.919                                                  | 361.822             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 3900                                         | 40.325                                                  | 362.877             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4000                                         | 36.383                                                  | 363.891             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4100                                         | 39.143                                                  | 364.864             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4200                                         | 38.583                                                  | 365.801             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4300                                         | 39.955                                                  | 366.701             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4400                                         | 37.439                                                  | 367.568             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4500                                         | 36.899                                                  | 368.404             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4600                                         | 36.374                                                  | 369.209             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4700                                         | 35.866                                                  | 369.966             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4800                                         | 35.373                                                  | 370.736             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 4900                                         | 34.444                                                  | 371.460             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 5000                                         | 34.005                                                  | 372.161             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 5200                                         | 33.582                                                  | 372.838             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 5500                                         | 33.176                                                  | 373.495             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 5600                                         | 32.051                                                  | 375.926             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 5700                                         | 31.705                                                  | 376.490             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 5800                                         | 31.374                                                  | 377.038             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 5900                                         | 31.056                                                  | 377.572             |
|                    |          |             |            |                     |          |                     |                      |            |                                                           | 6000                                         | 30.751                                                  | 340.936             |

CURRENT: June 1982 (1 bar)

PREVIOUS: September 1961 (1 atm)

Iodine ( $I_2$ )

## Enthalpy of Formation

We adopt the enthalpy of formation values of CODATA<sup>5</sup> as follows:  $\Delta_H^{\circ}(298.15 \text{ K}) = 62.421 \pm 0.079 \text{ kJ mol}^{-1}$  and  $\Delta_H^{\circ}(0 \text{ K}) = 65.500 \pm 0.092 \text{ kJ mol}^{-1}$ . These values are based on the heat capacity study of Shirley and Giauque<sup>6</sup>, and the vapor pressure data of Baxter *et al.*<sup>7</sup>, Baxter and Gross<sup>8</sup>, Gillespie and Fraser<sup>9</sup>, and Stern.<sup>10</sup> Note that the latter value of  $\Delta_H^{\circ}$  is deduced from the former using the CODATA values of  $H^{\circ}(298.15 \text{ K}) - H^{\circ}(0 \text{ K})$  for  $I_2(g)$  and  $I_2(c)$ . Our calculated value of  $H^{\circ}(298.15 \text{ K}) - H^{\circ}(0 \text{ K})$  for  $I_2(g)$  is only  $1.5 \text{ J mol}^{-1}$  smaller than that recommended by CODATA. We adopted the dissociation energy for the  ${}^3\Sigma^+$ ,  ${}^1\Pi_g$ , and  ${}^3\Pi_u$  states as given by Huber *et al.*<sup>4</sup>. The  $D_0^{\circ}$  value for the  ${}^3\Pi_u$  state was deduced from the dissociation state energies given by Gurvich *et al.*<sup>11</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>12</sup> however, we truncate the  $B_e$  expression at the  $(v+1/2)^3$  term. The  ${}^3\Pi_u$  constants were taken from Gurvich *et al.*<sup>12</sup>. We adopt the spectroscopic constants of Ashby<sup>13</sup> for the  ${}^1\Pi_u$  state and the CODATA values of  $H^{\circ}(298.15 \text{ K}) - H^{\circ}(0 \text{ K})$  for  $I_2(g)$  and  $I_2(c)$ . The rotational levels above the dissociation limit (see CIE(g) table). The values of  $J_{lim}$  and  $v_{max}$  for the ground state are those given by Gurvich *et al.*<sup>12</sup>. The corresponding values for the  ${}^3\Pi_u$  state were estimated as  $J_{lim} = 500$  and  $v_{max} = 69$  based on the spectroscopic constants given by Gurvich<sup>12</sup> and CODATA.<sup>5</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 Kachatkurov<sup>14</sup> who proposed a simpler form of Wooley's method.<sup>15</sup> Our calculated value of  $S^{\circ}$  at  $298.15 \text{ K}$  is only  $0.112 \text{ J K}^{-1} \text{ mol}^{-1}$  larger than that given by Gurvich<sup>12</sup> and CODATA.<sup>5</sup>

## References

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

## IDEAL GAS

$$S^{\circ}(298.15 \text{ K}) = [395.773] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_H^{\circ}(298.15 \text{ K}) = -416.48 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_H^{\circ}(298.15 \text{ K}) = -422.17 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$$

| Vibrational Frequencies and Degeneracies |                     |
|------------------------------------------|---------------------|
| $\nu, \text{cm}^{-1}$                    | $v, \text{cm}^{-1}$ |
| [20](1)                                  | [80](1)             |
| [60](1)                                  | [103](1)            |
| [110](1)                                 | [120](1)            |

Ground State Quantum Weight: [1]

 $\sigma = [4]$ Point Group: [D<sub>2h</sub>]

Bond Distances: K-K = [3.29] Å

K-I = [105]<sup>o</sup>Bond Angles: K-I-K = [75]<sup>o</sup>Product of the Moments of Inertia:  $I_A I_B I_C = [5.073451] \times 10^{11} \text{ g}^3 \cdot \text{cm}^6$ 

## Enthalpy of Formation

The chemical equilibrium for the reaction K-I(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  $\Delta_H^{\circ}(K_2\text{I}_2, g, 298.15 \text{ K})$  is adopted as  $-100.9 \pm 1 \text{ kcal}\cdot\text{mol}^{-1}$ .

| Source                    | T/K       | Data Points | $\Delta_H^{\circ}(298.15 \text{ K}), \text{kcal}\cdot\text{mol}^{-1}$ |         | Drift, cal·K <sup>-1</sup> ·mol <sup>-1</sup> | $\Delta_H^{\circ}(298.15 \text{ K}), \text{kcal}\cdot\text{mol}^{-1}$ |
|---------------------------|-----------|-------------|-----------------------------------------------------------------------|---------|-----------------------------------------------|-----------------------------------------------------------------------|
|                           |           |             | 2nd law                                                               | 3rd law |                                               |                                                                       |
| 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:  $I_A = 52.0871 \times 10^{-39}$ ,  $I_B = 287.1362 \times 10^{-39}$ , and  $I_C = 339.2233 \times 10^{-39}$  g·cm<sup>2</sup>.

## References

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Potassium Iodide (KI)<sub>2</sub>M<sub>r</sub> = 332.0056

## Potassium Iodide (KI)

| T/K    | Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K |                | Standard State Pressure = p <sup>°</sup> = 0.1 MPa                  |                                                   |
|--------|------------------------------------------------------------|----------------|---------------------------------------------------------------------|---------------------------------------------------|
|        | C <sub>p</sub> <sup>r</sup>                                | S <sup>r</sup> | -[C <sup>°</sup> - H <sup>°</sup> (T <sub>r</sub> )]/T <sub>r</sub> | H <sup>°</sup> - H <sup>°</sup> (T <sub>r</sub> ) |
| 0      | 0                                                          | 0              | INFINITE                                                            | -21.676                                           |
| 100    | 75.971                                                     | 308.279        | -15.972                                                             | -416.480                                          |
| 200    | 81.203                                                     | 363.113        | -403.271                                                            | -417.290                                          |
| 250    | 81.890                                                     | 381.315        | -397.125                                                            | -419.471                                          |
| 298.15 | 82.258                                                     | 395.772        | 0                                                                   | -3.933                                            |
| 300    | 82.368                                                     | 396.281        | 0                                                                   | -422.166                                          |
| 350    | 82.499                                                     | 408.982        | 396.777                                                             | 4.272                                             |
| 400    | 82.649                                                     | 420.008        | 399.007                                                             | 8.401                                             |
| 450    | 82.752                                                     | 429.749        | 401.892                                                             | 12.536                                            |
| 500    | 82.826                                                     | 438.472        | 405.121                                                             | 16.675                                            |
| 600    | 82.923                                                     | 453.383        | 411.977                                                             | 20.963                                            |
| 700    | 82.982                                                     | 465.370        | 418.857                                                             | 23.259                                            |
| 800    | 83.020                                                     | 477.453        | 425.504                                                             | 24.559                                            |
| 900    | 83.046                                                     | 487.233        | 431.831                                                             | 24.861                                            |
| 1000   | 83.064                                                     | 493.584        | 437.816                                                             | 25.168                                            |
| 1010   | 83.078                                                     | 501.901        | 443.470                                                             | 66.475                                            |
| 1200   | 83.089                                                     | 511.131        | 448.811                                                             | 74.783                                            |
| 1300   | 83.097                                                     | 517.782        | 453.864                                                             | 83.993                                            |
| 1400   | 83.103                                                     | 522.940        | 458.652                                                             | 85.054                                            |
| 1500   | 83.109                                                     | 529.674        | 461.198                                                             | 91.403                                            |
| 1600   | 83.113                                                     | 535.038        | 467.522                                                             | 99.713                                            |
| 1700   | 83.116                                                     | 540.076        | 471.644                                                             | 108.025                                           |
| 1800   | 83.119                                                     | 544.927        | 475.579                                                             | 116.336                                           |
| 1900   | 83.124                                                     | 549.741        | 480.343                                                             | 124.648                                           |
| 2000   | 83.124                                                     | 553.585        | 482.949                                                             | 141.276                                           |
| 2100   | 83.126                                                     | 567.641        | 486.410                                                             | 149.585                                           |
| 2200   | 83.128                                                     | 561.508        | 489.736                                                             | 157.597                                           |
| 2300   | 83.129                                                     | 562.203        | 492.938                                                             | 166.210                                           |
| 2400   | 83.130                                                     | 568.741        | 496.023                                                             | 174.523                                           |
| 2500   | 83.131                                                     | 572.135        | 499.020                                                             | 182.336                                           |
| 2600   | 83.132                                                     | 575.395        | 501.876                                                             | 191.149                                           |
| 2700   | 83.133                                                     | 578.533        | 504.657                                                             | 199.463                                           |
| 2800   | 83.134                                                     | 581.536        | 507.350                                                             | 207.776                                           |
| 2900   | 83.135                                                     | 584.473        | 509.960                                                             | 216.089                                           |
| 3000   | 83.135                                                     | 587.292        | 512.491                                                             | 224.403                                           |
| 3200   | 83.136                                                     | 590.018        | 514.948                                                             | 232.717                                           |
| 3300   | 83.137                                                     | 592.657        | 517.335                                                             | 241.034                                           |
| 3400   | 83.137                                                     | 593.215        | 519.657                                                             | 249.344                                           |
| 3500   | 83.138                                                     | 594.797        | 521.916                                                             | 257.657                                           |
| 3700   | 83.138                                                     | 602.449        | 526.239                                                             | 274.285                                           |
| 3800   | 83.139                                                     | 606.944        | 530.388                                                             | 282.599                                           |
| 3900   | 83.139                                                     | 609.104        | 532.379                                                             | 290.913                                           |
| 4000   | 83.139                                                     | 611.209        | 534.324                                                             | 307.540                                           |
| 4100   | 83.139                                                     | 613.262        | 536.224                                                             | 315.854                                           |
| 4200   | 83.140                                                     | 615.265        | 538.082                                                             | 324.168                                           |
| 4300   | 83.140                                                     | 617.221        | 539.900                                                             | 332.687                                           |
| 4400   | 83.140                                                     | 620.176        | 541.679                                                             | 340.976                                           |
| 4500   | 83.140                                                     | 621.001        | 543.421                                                             | 349.110                                           |
| 4600   | 83.140                                                     | 622.829        | 545.128                                                             | 357.424                                           |
| 5100   | 83.141                                                     | 631.407        | 553.173                                                             | 381.995                                           |
| 5200   | 83.141                                                     | 631.022        | 554.693                                                             | 407.309                                           |
| 5300   | 83.141                                                     | 634.635        | 556.186                                                             | 415.623                                           |
| 5400   | 83.141                                                     | 636.160        | 557.653                                                             | 423.937                                           |
| 5500   | 83.141                                                     | 637.683        | 559.094                                                             | 432.251                                           |
| 5600   | 83.142                                                     | 639.183        | 560.047                                                             | 440.565                                           |
| 5700   | 83.142                                                     | 640.655        | 561.904                                                             | 448.879                                           |
| 5800   | 83.142                                                     | 642.101        | 563.274                                                             | 457.194                                           |
| 5900   | 83.142                                                     | 643.622        | 564.522                                                             | 463.454                                           |
| 6000   | 83.142                                                     | 644.919        | 565.949                                                             | 473.822                                           |

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)

## NIST-JANAF THERMOCHEMICAL TABLES

 $\text{Li}_2\text{LiI}_2(\text{g})$  $M_r = 267.6910$  Lithium Iodide ( $(\text{LiI})_2$ )

## IDEAL GAS

$$\text{S}^*(298.15 \text{ K}) = [330.628] \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta H^*(0 \text{ K}) = -356.74 \pm 16.7 \text{ kJ mol}^{-1}$$

$$\Delta H^*(298.15 \text{ K}) = -361.92 \pm 16.7 \text{ kJ mol}^{-1}$$

| Vibrational Frequencies and Degeneracies |                      |
|------------------------------------------|----------------------|
| $\nu, \text{ cm}^{-1}$                   | $v, \text{ cm}^{-1}$ |
| 1166(1)                                  | [310](1)             |
| 1160(1)                                  | 248 (1)              |
| 1383(1)                                  | 375 (1)              |

$\sigma = 4$   
 Ground State Quantum Weight: 1  
 Point Group:  $D_{2h}$   
 Bond Distances:  $\text{Li-Li} = 2.54 \text{ \AA}$ ;  $\text{Li-Li} = 2.71 \text{ \AA}$   
 Bond Angles:  $\text{L-L-L} = 116^\circ \pm 4^\circ$ ;  $\text{Li-L-L} = 64^\circ$   
 Product of the Moments of Inertia:  $I_{A,B,C} = 1.631229 \times 10^{-12} \text{ g}^3 \cdot \text{cm}^6$

## 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  $\text{LiI(g)}$  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.*<sup>2</sup> The selected bond distances and angle were obtained from the electron diffraction studies of monomer dimer vapor by Akischin and Rambidi.<sup>3</sup> The bond distances,  $r(\text{Li-Li}) = 2.712 \text{ \AA}$  and  $\tau(\text{L-L}) = 4.520 \text{ \AA}$ , calculated by Berkowitz are in good agreement with those from Akischin and Rambidi.<sup>3</sup> The principal moments of inertia are:  $I_A = 4.1763 \times 10^{-39}$ ,  $I_B = 195.5561 \times 10^{-39}$  and  $I_C = 199.7324 \times 10^{-39} \text{ g cm}^2$ .<sup>2</sup> Bauer *et al.* have estimated six vibrational frequencies (501, 501, 148, 200, 294, 360  $\text{cm}^{-1}$ ) for  $\text{Li}_2\text{LiI(g)}$  in the electron diffraction studies of the  $\text{Li}_2\text{Cl}_2\text{Li(g)}$ . Klemperer and Norris have observed two fundamental vibrational frequencies (248 and 375  $\text{cm}^{-1}$ ) in the infrared spectrum and tentatively assigned them as  $B_{2u}$  and  $B_{3u}$  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

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- <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).

| $T/\text{K}$ | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |         | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |              |
|--------------|-----------------------------------------------------------|---------|---------------------------------------------------|--------------|
|              | $C_p^*$                                                   | $S^*$   | $H^*-H^*(T_r)/T$                                  | $\Delta H^*$ |
| 0            | 0                                                         | 0       | -INFINITE                                         | -356.740     |
| 100          | 51.234                                                    | 259.423 | -17.267                                           | -356.740     |
| 200          | 69.270                                                    | 301.482 | -33.359                                           | -356.873     |
| 250          | 73.525                                                    | 317.446 | -7.186                                            | -352.639     |
| 298.15       | 76.044                                                    | 331.867 | -3.605                                            | -400.883     |
| 300          | 76.121                                                    | 330.628 | 0.                                                | -408.522     |
| 350          | 77.820                                                    | 331.098 | 0.141                                             | -361.967     |
| 400          | 78.982                                                    | 332.969 | 3.992                                             | -408.811     |
| 450          | 79.808                                                    | 333.441 | 7.914                                             | -416.504     |
| 500          | 80.414                                                    | 371.235 | 11.885                                            | -423.426     |
| 600          | 81.222                                                    | 385.974 | 15.891                                            | -428.942     |
| 700          | 81.720                                                    | 398.535 | 346.014                                           | -434.754     |
| 800          | 82.048                                                    | 409.470 | 352.642                                           | -436.223     |
| 900          | 82.275                                                    | 419.147 | 365.224                                           | -431.605     |
| 1000         | 82.438                                                    | 427.835 | 371.057                                           | -440.299     |
| 1100         | 82.559                                                    | 435.688 | 376.381                                           | -451.626     |
| 1200         | 82.652                                                    | 442.876 | 381.810                                           | -452.950     |
| 1300         | 82.724                                                    | 449.494 | 386.766                                           | -454.281     |
| 1400         | 82.782                                                    | 455.627 | 391.468                                           | -455.625     |
| 1500         | 82.828                                                    | 461.340 | 395.938                                           | -465.987     |
| 1600         | 82.866                                                    | 466.687 | 400.194                                           | -468.378     |
| 1700         | 82.898                                                    | 471.712 | 404.255                                           | -470.280     |
| 1800         | 82.924                                                    | 476.451 | 408.135                                           | -472.958     |
| 1900         | 82.947                                                    | 480.935 | 411.850                                           | -474.291     |
| 2000         | 82.966                                                    | 485.190 | 415.412                                           | -479.403     |
| 2100         | 82.983                                                    | 489.238 | 418.832                                           | -487.854     |
| 2200         | 82.997                                                    | 493.099 | 422.120                                           | -492.587     |
| 2300         | 83.009                                                    | 496.789 | 425.287                                           | -496.839     |
| 2400         | 83.020                                                    | 500.522 | 428.340                                           | -502.155     |
| 2500         | 83.030                                                    | 503.711 | 431.288                                           | -501.058     |
| 2600         | 83.039                                                    | 506.968 | 434.136                                           | -509.837     |
| 2700         | 83.046                                                    | 510.102 | 436.892                                           | -512.893     |
| 2800         | 83.053                                                    | 513.122 | 439.561                                           | -515.889     |
| 2900         | 83.059                                                    | 516.037 | 442.148                                           | -519.936     |
| 3000         | 83.065                                                    | 518.832 | 444.638                                           | -522.582     |
| 3100         | 83.070                                                    | 521.576 | 447.096                                           | -529.889     |
| 3200         | 83.074                                                    | 524.214 | 449.465                                           | -539.508     |
| 3300         | 83.079                                                    | 526.770 | 451.769                                           | -541.504     |
| 3400         | 83.082                                                    | 529.250 | 454.012                                           | -545.812     |
| 3500         | 83.086                                                    | 531.639 | 456.196                                           | -564.120     |
| 3600         | 83.089                                                    | 533.999 | 458.325                                           | -574.705     |
| 3700         | 83.092                                                    | 536.276 | 460.401                                           | -587.738     |
| 3800         | 83.095                                                    | 538.492 | 462.427                                           | -593.047     |
| 3900         | 83.097                                                    | 540.630 | 464.405                                           | -597.357     |
| 4000         | 83.099                                                    | 542.754 | 466.338                                           | -603.667     |
| 4100         | 83.102                                                    | 544.806 | 468.226                                           | -611.977     |
| 4200         | 83.104                                                    | 546.809 | 470.074                                           | -622.287     |
| 4300         | 83.105                                                    | 548.764 | 471.881                                           | -630.597     |
| 4400         | 83.107                                                    | 550.675 | 473.650                                           | -638.775     |
| 4500         | 83.109                                                    | 552.542 | 475.383                                           | -647.219     |
| 4600         | 83.110                                                    | 554.369 | 477.080                                           | -655.530     |
| 5300         | 83.112                                                    | 556.157 | 478.744                                           | -753.139     |
| 4800         | 83.113                                                    | 557.906 | 480.375                                           | -762.152     |
| 4900         | 83.114                                                    | 559.620 | 481.974                                           | -765.146     |
| 5000         | 83.115                                                    | 561.299 | 483.544                                           | -768.775     |
| 5100         | 83.117                                                    | 562.945 | 485.085                                           | -769.087     |
| 5200         | 83.118                                                    | 564.559 | 486.598                                           | -770.427     |
| 5300         | 83.119                                                    | 566.142 | 488.084                                           | -772.839     |
| 5400         | 83.120                                                    | 567.696 | 489.544                                           | -775.377     |
| 5500         | 83.120                                                    | 569.221 | 490.979                                           | -780.922     |
| 5600         | 83.121                                                    | 570.719 | 492.389                                           | -788.546     |
| 5700         | 83.122                                                    | 572.190 | 493.776                                           | -796.020     |
| 5800         | 83.123                                                    | 573.636 | 495.141                                           | -803.917     |
| 5900         | 83.124                                                    | 575.057 | 496.483                                           | -812.558     |
| 6000         | 83.124                                                    | 576.454 | 497.805                                           | -816.738     |

Lithium Iodide ( $(\text{LiI})_2$ )

PREVIOUS June 1966 (1 atm)

Lithium Iodide ( $(\text{LiI})_2$ )

CURRENT June 1966 (1 bar)

Magnesium Iodide ( $MgI_2$ )

## CRYSTAL

$$S(298.15 \text{ K}) = [129.704 \pm 4.2] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 907 \pm 15 \text{ K}$$

## Enthalpy of Formation

Finch *et al.*<sup>1</sup> measured the enthalpy of solution of  $MgO(\text{cr})$  in aqueous  $H_1$  and of  $MgI_2(\text{cr})$  in the same solvent. Combining and correcting for a concentration change gives  $\Delta_fH^\circ(298.15 \text{ K}) = 14.53 \text{ kcal} \cdot \text{mol}^{-1}$  for the process  $MgO(\text{cr}) + 2 H_1(0.5 \text{ M}) = MgI_2(\text{cr}) + H_2O$  from which  $\Delta_{\text{iss}}H^\circ = 29.288 \pm 8.4 \text{ kJ mol}^{-1}$  is calculated. The auxiliary data used are  $\Delta_fH^\circ(MgO, \text{cr}) = -143.7 \text{ kcal} \cdot \text{mol}^{-1}$ ,<sup>2</sup>  $\Delta_fH^\circ(H_1, \text{H}_2O, 1, 298.15 \text{ K}) = -87.70 \pm 1.5 \text{ kcal mol}^{-1}$ , and  $\Delta_fH^\circ(H_1, 0.5 \text{ M}, 298.15 \text{ K}) = -13.42 \text{ kcal mol}^{-1}$ . This last value was calculated from the CODATA value of  $-13.60$  for  $\Delta_fH^\circ(H_1, \text{aq, std. state}, 298.15 \text{ K})$  and the enthalpy of dilution of  $H_1$ .<sup>4</sup>

Combination of  $\Delta_fH^\circ(Mg^{+2}, \text{aq, std. state}, 298.15 \text{ K}) = -111.58 \text{ kcal} \cdot \text{mol}^{-1}$  selected by Parker<sup>5</sup> with the CODATA value of  $\Delta_fH^\circ(I^-, \text{aq, std. state}, 298.15 \text{ K}) = -138.78 \text{ kcal} \cdot \text{mol}^{-1}$ . Further combination with the enthalpy of solution,  $-50.96 \text{ kcal} \cdot \text{mol}^{-1}$ , gives  $\Delta_fH^\circ(MgI_2, \text{aq, std. state}, 298.15 \text{ K}) = -87.82 \text{ kcal} \cdot \text{mol}^{-1}$ . We adopt  $\Delta_fH^\circ(MgI_2, \text{cr}, 298.15 \text{ K}) = -87.7 \pm 1.5 \text{ kcal} \cdot \text{mol}^{-1}$  to retain internal consistency.

## Heat Capacity and Entropy

$C_p^\circ(298.15 \text{ K}) = 17.88 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  is calculated from the reaction  $MgCl_2(\text{cr}) + 2 NaI(\text{cr}) = MgI_2(\text{cr}) + 2 NaCl(\text{cr})$  assuming no net change in heat capacity.  $C_p^\circ = 21.0 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  at  $T_{\text{fus}} = 907 \text{ K}$  estimated from a Kopf's rule value of  $7.0 \text{ cal} \cdot \text{K}^{-1} \cdot \text{g atom}$  appears reasonable in comparison with a  $C_p^\circ$  vs.  $T$  plot for  $MgBr(\text{cr})$ ,  $MgCl(\text{cr})$  and  $CaI(\text{cr})$ .<sup>2</sup> Values of  $C_p^\circ$  between 298.15 and 907 K are read from the graphical comparison curve. The adopted values lead to  $H^\circ(500 \text{ K}) - H^\circ(298.15 \text{ K}) = 3.77 \text{ kcal} \cdot \text{mol}^{-1}$ , in reasonable agreement with the estimate of 4.0 by Brewer *et al.*<sup>6</sup>

$S^\circ(298.15 \text{ K}) = 31.0 \pm 1.0 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  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  $MgI_2$  to be molten at 910 K; a graph in the same paper infers that a  $T_{\text{fus}} = 907 \text{ K}$  was chosen. We adopt  $T_{\text{fus}} = 907 \pm 15 \text{ K}$ .

From the  $KI/MgI_2$  phase diagram by Klemm *et al.*<sup>10</sup> values of  $\Delta_{\text{iss}}H^\circ(MgI_2)$  ranging from 7 to 9  $\text{kcal} \cdot \text{mol}^{-1}$  are calculated. Brewer<sup>11</sup> earlier estimated 5.3  $\text{kcal} \cdot \text{mol}^{-1}$ . We adopt  $7.0 \pm 2.0 \text{ kcal} \cdot \text{mol}^{-1}$ .

## Sublimation Data

By a mass spectrometric-Knudsen cell technique, Berkowitz and Marguari<sup>12</sup> found the sublimation pressure of  $MgI_2(\text{cr})$  to be  $5.18 \times 10^{-6}$  atm at 734 K and  $2.02 \times 10^{-5}$  atm at 757 K. A 3rd law analysis of these two points gives  $\Delta_{\text{ss}}H^\circ(298.15 \text{ K}) = 49.4 \pm 0.8 \text{ kcal} \cdot \text{mol}^{-1}$ . The 2nd law analysis of these two points gives 57.5  $\text{kcal} \cdot \text{mol}^{-1}$  but other data covering an approximate range of 550 to 750 K are shown graphically by Berkowitz and Marguari,<sup>13</sup> from which they calculate  $\Delta_{\text{ss}}H^\circ(350-750 \text{ K}) = 45 \text{ kcal} \cdot \text{mol}^{-1}$ . We adopt  $\Delta_{\text{ss}}H^\circ(298.15 \text{ K}) = 49.4 \pm 0.8 \text{ kcal} \cdot \text{mol}^{-1}$ .

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| $M_f = 278.1140$                                       |                                   | $MgI_2(\text{cr})$                                        |                                                         | $MgI_2(\text{liq})$                                  |                                                         |
|--------------------------------------------------------|-----------------------------------|-----------------------------------------------------------|---------------------------------------------------------|------------------------------------------------------|---------------------------------------------------------|
| $\Delta_fH^\circ(0 \text{ K})$                         | $\Delta_fH^\circ(\text{Unknown})$ | $\Delta_fH^\circ(298.15 \text{ K})$                       | $\Delta_fH^\circ = -366.94 \pm 6.3 \text{ kJ mol}^{-1}$ | $\Delta_fH^\circ(298.15 \text{ K})$                  | $\Delta_fH^\circ = -366.94 \pm 8.4 \text{ kJ mol}^{-1}$ |
| $\Delta_fH^\circ = 29.288 \pm 8.4 \text{ kJ mol}^{-1}$ |                                   |                                                           |                                                         |                                                      |                                                         |
|                                                        |                                   |                                                           |                                                         |                                                      |                                                         |
| Enthalpy of Formation                                  |                                   | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                                                         | Standard State Pressure = $p = 0.1 \text{ MPa}$      |                                                         |
|                                                        |                                   | $T/K$                                                     | $C_p^\circ$                                             | $S^\circ$                                            | $G^\circ - H^\circ(T_r)/T$                              |
|                                                        |                                   |                                                           | $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$    | $\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ | $\text{kJ} \cdot \text{mol}^{-1}$                       |
|                                                        |                                   |                                                           |                                                         |                                                      | $\Delta_fG^\circ$                                       |
|                                                        |                                   |                                                           |                                                         |                                                      | $\log K_1$                                              |
| 0                                                      |                                   | 100                                                       | 74.810                                                  | 129.704                                              | 0.                                                      |
|                                                        |                                   | 200                                                       | 74.977                                                  | 130.167                                              | -366.937                                                |
|                                                        |                                   | 300                                                       | 74.408                                                  | 132.650                                              | -361.240                                                |
|                                                        |                                   | 400                                                       | 74.011                                                  | 138.432                                              | -361.204                                                |
|                                                        |                                   | 500                                                       | 73.624                                                  | 144.971                                              | -383.467                                                |
|                                                        |                                   | 600                                                       | 73.237                                                  | 151.626                                              | -348.555                                                |
|                                                        |                                   | 700                                                       | 72.850                                                  | 158.134                                              | -424.677                                                |
|                                                        |                                   | 800                                                       | 72.463                                                  | 164.925                                              | -422.928                                                |
|                                                        |                                   | 900                                                       | 72.076                                                  | 170.502                                              | -421.144                                                |
|                                                        |                                   | 907.000                                                   | 87.864                                                  | 164.395                                              | -288.143                                                |
|                                                        |                                   | 1000                                                      | 88.994                                                  | 220.182                                              | 50.210                                                  |
|                                                        |                                   | 1100                                                      | 90.249                                                  | 228.812                                              | 58.434                                                  |
|                                                        |                                   | 1200                                                      | 91.462                                                  | 237.354                                              | -426.201                                                |
|                                                        |                                   | 1300                                                      | 92.634                                                  | 245.259                                              | -277.943                                                |
|                                                        |                                   | 1400                                                      | 93.763                                                  | 252.626                                              | -257.700                                                |
|                                                        |                                   | 1500                                                      | 94.851                                                  | 259.532                                              | -242.663                                                |
|                                                        |                                   |                                                           |                                                         | 196.413                                              | -242.726                                                |
|                                                        |                                   |                                                           |                                                         |                                                      | 14.257                                                  |
|                                                        |                                   |                                                           |                                                         |                                                      | 12.237                                                  |
|                                                        |                                   |                                                           |                                                         |                                                      | 10.561                                                  |
|                                                        |                                   |                                                           |                                                         |                                                      | 9.149                                                   |
|                                                        |                                   |                                                           |                                                         |                                                      | 7.826                                                   |
|                                                        |                                   |                                                           |                                                         |                                                      | 6.471                                                   |

PREVIOUS

| $MgI_2(\text{cr})$                                     |                                                         |
|--------------------------------------------------------|---------------------------------------------------------|
| $\Delta_fH^\circ(0 \text{ K})$                         | $\Delta_fH^\circ(298.15 \text{ K})$                     |
| $\Delta_fH^\circ = 29.288 \pm 8.4 \text{ kJ mol}^{-1}$ | $\Delta_fH^\circ = -366.94 \pm 8.4 \text{ kJ mol}^{-1}$ |
|                                                        |                                                         |
| $\Delta_fG^\circ$                                      | $\Delta_fG^\circ$                                       |
| $\log K_1$                                             | $\log K_1$                                              |

Magnesium Iodide ( $MgI_2$ )

CURRENT December 1974

| Magnesium Iodide ( $Mg_2I$ )                                                                                                                                                                                                                                                                                                    |         | $M_r = 278.1140$ Magnesium Iodide ( $Mg_2I$ )                                   |                                                                       | $I_2Mg_1(I)$ |                                           |             |                                 |                                |                     |                    |            |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------|---------------------------------------------------------------------------------|-----------------------------------------------------------------------|--------------|-------------------------------------------|-------------|---------------------------------|--------------------------------|---------------------|--------------------|------------|
| Liquid                                                                                                                                                                                                                                                                                                                          | Solid   | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$                        | Standard State Pressure = $p^{\circ} = 0.1\text{ MPa}$                |              |                                           |             |                                 |                                |                     |                    |            |
|                                                                                                                                                                                                                                                                                                                                 |         | $\Delta_fH^{\circ}(298.15\text{ K}) = [-342.252]\text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_{us}H^{\circ} = 29.288 \pm 8.4\text{ kJ}\cdot\text{mol}^{-1}$ | $T/K$        | $C_p^{\circ}$                             | $S^{\circ}$ | $-[G^{\circ} - H^{\circ}(T)]/T$ | $H^{\circ} - H^{\circ}(T_r)/T$ | $\Delta_fH^{\circ}$ | $\Delta G^{\circ}$ | $\log K_r$ |
| Enthalpy of Formation<br>$\Delta_fH^{\circ}(Mg_2I, l, 298.15\text{ K})$ is calculated from $\Delta_fH^{\circ}(MgI_2, cr, 298.15\text{ K})$ by adding the enthalpy of fusion, $\Delta_{us}H^{\circ}$ , and the difference in enthalpy, $H^{\circ}(907\text{ K})H^{\circ}(298.15\text{ K})$ , between the crystal and the liquid. |         |                                                                                 |                                                                       |              |                                           |             |                                 |                                |                     |                    |            |
| 0                                                                                                                                                                                                                                                                                                                               | 100     | 298.15                                                                          | 74.810                                                                | 155.737      | 155.737                                   | 0.          | 0.139                           | -342.252                       | -344.316            | 60.323             |            |
| 200                                                                                                                                                                                                                                                                                                                             | 298.15  | 74.977                                                                          | 156.200                                                               | 155.738      | 7.815                                     | 0.139       | -342.260                        | -344.329                       | 59.953              |                    |            |
| 300                                                                                                                                                                                                                                                                                                                             | 400     | 78.408                                                                          | 158.723                                                               | 158.723      | 0.139                                     | -358.776    | -344.389                        | 44.973                         |                     |                    |            |
| 500                                                                                                                                                                                                                                                                                                                             | 80.919  | 196.035                                                                         | 164.464                                                               | 15.785       | -401.669                                  | -336.671    | 35.172                          |                                |                     |                    |            |
| 600                                                                                                                                                                                                                                                                                                                             | 83.011  | 210.980                                                                         | 171.004                                                               | 23.985       | -399.991                                  | -323.827    | 28.192                          |                                |                     |                    |            |
| 600.000                                                                                                                                                                                                                                                                                                                         | 83.011  | 210.980                                                                         | 171.004                                                               | 23.985       | GLASS $\leftrightarrow$ LIQUID TRANSITION |             |                                 |                                |                     |                    |            |
| 600.000                                                                                                                                                                                                                                                                                                                         | 100.416 | 210.980                                                                         | 171.004                                                               | 23.985       | 34.027                                    | -306.589    | -311.403                        | 23.237                         |                     |                    |            |
| 700                                                                                                                                                                                                                                                                                                                             | 100.416 | 226.459                                                                         | 177.849                                                               | 184.782      | 44.068                                    | -393.315    | -299.459                        | 19.553                         |                     |                    |            |
| 800                                                                                                                                                                                                                                                                                                                             | 100.416 | 239.867                                                                         | 191.572                                                               | 54.110       | -390.182                                  | -287.917    | 16.710                          |                                |                     |                    |            |
| 900                                                                                                                                                                                                                                                                                                                             | 100.416 | 251.695                                                                         | 191.572                                                               | 54.813       | CRYSTAL $\leftrightarrow$ LIQUID          |             |                                 |                                |                     |                    |            |
| 907.000                                                                                                                                                                                                                                                                                                                         | 100.416 | 252.473                                                                         | 192.040                                                               | 64.152       | -395.798                                  | -276.003    | -14.417                         |                                |                     |                    |            |
| 1000                                                                                                                                                                                                                                                                                                                            | 100.416 | 262.275                                                                         | 198.123                                                               | 204.397      | 74.193                                    | -393.003    | -264.159                        | 12.544                         |                     |                    |            |
| 1100                                                                                                                                                                                                                                                                                                                            | 100.416 | 271.845                                                                         | 210.387                                                               | 83.235       | -390.225                                  | -252.568    | 10.994                          |                                |                     |                    |            |
| 1200                                                                                                                                                                                                                                                                                                                            | 100.416 | 280.583                                                                         | 216.100                                                               | 94.276       | -387.470                                  | -241.269    | 9.692                           |                                |                     |                    |            |
| 1300                                                                                                                                                                                                                                                                                                                            | 100.416 | 288.620                                                                         | 221.549                                                               | 104.318      | -512.156                                  | -226.893    | 8.465                           |                                |                     |                    |            |
| 1400                                                                                                                                                                                                                                                                                                                            | 100.416 | 296.062                                                                         | 226.750                                                               | 114.360      | -508.120                                  | -206.658    | 7.196                           |                                |                     |                    |            |
| 1500                                                                                                                                                                                                                                                                                                                            | 100.416 | 302.990                                                                         | 231.720                                                               | 124.401      | -504.134                                  | -186.691    | 6.095                           |                                |                     |                    |            |
| 1600                                                                                                                                                                                                                                                                                                                            | 100.416 | 309.471                                                                         | 236.474                                                               | 134.443      | -500.207                                  | -166.972    | 5.130                           |                                |                     |                    |            |
| 1700                                                                                                                                                                                                                                                                                                                            | 100.416 | 315.538                                                                         | 321.298                                                               | 144.484      | -496.345                                  | -147.481    | 4.280                           |                                |                     |                    |            |
| 1800                                                                                                                                                                                                                                                                                                                            | 100.416 | 321.298                                                                         | 241.029                                                               | 154.526      | -492.552                                  | -128.204    | 3.525                           |                                |                     |                    |            |
| 1900                                                                                                                                                                                                                                                                                                                            | 100.416 | 326.727                                                                         | 245.398                                                               | 331.878      | -488.830                                  | -109.124    | 2.850                           |                                |                     |                    |            |
| 2000                                                                                                                                                                                                                                                                                                                            | 100.416 | 329.594                                                                         | 249.568                                                               |              |                                           |             |                                 |                                |                     |                    |            |

## Vaporization Data

$T_{vap} = 1255\text{ K}$  is calculated as the temperature at which the fugacity is 1 atm for the reaction  $Mg_2I(l) \rightleftharpoons MgI_2(g)$ .  $\Delta_{vap}H^{\circ} = 36.126\text{ kcal}\cdot\text{mol}^{-1}$  is the calculated difference between the enthalpies of formation of the ideal gas and the liquid at  $T_{vap}$ .

Fusion Data  
Refer to the crystal table for details.

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

## CRYSTAL-LIQUID

0 to 907 K crystal  
above 907 K liquid

Refer to the individual tables for details.

| $T/K$   | $C_p^*$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                          | Standard State Pressure = $P = 0.1\text{ MPa}$ |                                                |
|---------|---------|----------------------------------------------------------|--------------------------|------------------------------------------------|------------------------------------------------|
|         |         | $S^\circ - [G^\circ - H^\circ(T_r)]/T$                   | $H^\circ - H^\circ(T_r)$ | $\Delta_iH^\circ$                              | $\Delta_iG^\circ$                              |
| 0       |         |                                                          |                          |                                                | $\log K_r$                                     |
| 100     |         |                                                          |                          |                                                |                                                |
| 200     | 74.810  | 129.704                                                  | 129.704                  | 0.                                             | -366.937                                       |
| 300     | 74.977  | 130.167                                                  | 129.705                  | 0.139                                          | -366.945                                       |
| 400     | 78.408  | 152.229                                                  | 132.680                  | 7.815                                          | -383.462                                       |
| 500     | 80.919  | 170.002                                                  | 138.432                  | 15.785                                         | -426.355                                       |
| 600     | 83.011  | 184.946                                                  | 144.971                  | 23.985                                         | -424.677                                       |
| 700     | 84.726  | 197.873                                                  | 151.626                  | 32.373                                         | -422.928                                       |
| 800     | 86.274  | 209.290                                                  | 158.134                  | 40.923                                         | -421.144                                       |
| 900     | 87.655  | 219.502                                                  | 164.395                  | 49.596                                         | -419.381                                       |
| 907.000 | 87.864  | 220.182                                                  | 164.823                  | 50.210                                         | <u>CRYSTAL</u> $\leftarrow \rightarrow$ LIQUID |
| 907.000 | 100.416 | 252.471                                                  | 164.823                  | 79.498                                         | <u>TRANSITION</u>                              |
| 1000    | 100.416 | 262.275                                                  | 173.438                  | 88.837                                         | -395.798                                       |
| 1100    | 100.416 | 271.845                                                  | 181.956                  | 98.879                                         | -393.003                                       |
| 1200    | 100.416 | 280.583                                                  | 189.816                  | 108.920                                        | -390.225                                       |
| 1300    | 100.416 | 288.620                                                  | 197.111                  | 118.962                                        | -387.470                                       |
| 1400    | 100.416 | 296.082                                                  | 203.917                  | 129.003                                        | -512.156                                       |
| 1500    | 100.416 | 302.990                                                  | 210.293                  | 139.045                                        | -226.893                                       |
| 1600    | 100.416 | 309.471                                                  | 216.291                  | 149.087                                        | 8.465                                          |
| 1700    | 100.416 | 315.558                                                  | 221.933                  | 159.128                                        | -206.658                                       |
| 1800    | 100.416 | 321.298                                                  | 227.315                  | 169.170                                        | -241.209                                       |
| 1900    | 100.416 | 326.727                                                  | 232.405                  | 179.211                                        | -226.893                                       |
| 2000    | 100.416 | 331.878                                                  | 237.251                  | 189.253                                        | -109.124                                       |

 $I_2Mg_1(\text{cr},l)$ 

PREVIOUS.

CURRENT December 1974

 $MgI_2$

## NIST-JANAF THERMOCHEMICAL TABLES

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

| $\Delta H^\circ(0\text{ K}) = -157.56 \pm 10.5 \text{ kJ}\cdot\text{mol}^{-1}$ |             | $\Delta H^\circ(298.15\text{ K}) = -160.25 \pm 10.5 \text{ kJ}\cdot\text{mol}^{-1}$ |                               | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                  | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |            |
|--------------------------------------------------------------------------------|-------------|-------------------------------------------------------------------------------------|-------------------------------|----------------------------------------------------------|------------------|-------------------------------------------------------|------------|
| $T/K$                                                                          | $C_p^\circ$ | $S^\circ$                                                                           | $-[G^\circ - H^\circ(T_r)]/T$ | $H^\circ - H^\circ(T_r)$                                 | $\Delta H^\circ$ | $\Delta G^\circ$                                      | $\log K_r$ |
| Vibrational Frequencies and Degeneracies                                       |             |                                                                                     |                               |                                                          |                  |                                                       |            |
| $\nu, \text{ cm}^{-1}$                                                         |             |                                                                                     |                               |                                                          |                  |                                                       |            |
| 0                                                                              | 0           | 0                                                                                   | 0                             | -15.512                                                  | -157.563         | -157.563                                              | INFINITE   |
| 100                                                                            | 51.832      | 256.256                                                                             | 368.725                       | -112.47                                                  | -156.990         | -75.566                                               | 90.706     |
| 200                                                                            | 57.298      | 294.115                                                                             | 322.882                       | -57.53                                                   | -158.436         | -91.639                                               | 50.573     |
| 250                                                                            | 58.718      | 307.064                                                                             | 318.466                       | -28.90                                                   | -159.332         | -202.337                                              | 42.276     |
| 298.15                                                                         | 59.623      | 317.489                                                                             | 317.489                       | 0.                                                       | -160.247         | -210.538                                              | 36.885     |
| 300                                                                            | 59.551      | 317.488                                                                             | 317.489                       | 0.110                                                    | -160.284         | -210.850                                              | 36.712     |
| 350                                                                            | 60.281      | 327.104                                                                             | 318.219                       | 3.110                                                    | -161.339         | -219.196                                              | 32.713     |
| 400                                                                            | 60.721      | 335.183                                                                             | 319.845                       | 6.135                                                    | -178.452         | -226.834                                              | 29.621     |
| 450                                                                            | 61.038      | 342.255                                                                             | 321.955                       | 9.180                                                    | -180.762         | -232.743                                              | 27.016     |
| 500                                                                            | 61.273      | 348.798                                                                             | 324.223                       | 12.238                                                   | -223.213         | -234.595                                              | 24.508     |
| 600                                                                            | 61.590      | 360.000                                                                             | 329.363                       | 18.382                                                   | -223.590         | -236.838                                              | 20.619     |
| 700                                                                            | 61.787      | 369.310                                                                             | 334.436                       | 24.532                                                   | -224.060         | -239.010                                              | 17.835     |
| 800                                                                            | 61.917      | 377.770                                                                             | 339.348                       | 36.021                                                   | -224.641         | -241.108                                              | 15.743     |
| 900                                                                            | 62.008      | 383.068                                                                             | 344.030                       | 36.934                                                   | -225.354         | -243.125                                              | 14.111     |
| 1000                                                                           | 62.073      | 391.605                                                                             | 348.467                       | 43.138                                                   | -234.808         | -244.342                                              | 12.763     |
| 1100                                                                           | 62.122      | 397.523                                                                             | 352.662                       | 49.348                                                   | -235.844         | -245.245                                              | 11.646     |
| 1200                                                                           | 62.159      | 402.930                                                                             | 356.629                       | 55.562                                                   | -236.893         | -246.054                                              | 10.719     |
| 1300                                                                           | 62.189      | 407.907                                                                             | 360.384                       | 61.780                                                   | -237.962         | -247.774                                              | 9.916      |
| 1400                                                                           | 62.212      | 412.517                                                                             | 363.945                       | 68.000                                                   | -366.470         | -244.244                                              | 9.113      |
| 1500                                                                           | 62.230      | 416.809                                                                             | 367.328                       | 74.222                                                   | -366.253         | -235.521                                              | 8.202      |
| 1600                                                                           | 62.246      | 420.526                                                                             | 370.548                       | 80.446                                                   | -366.085         | -366.812                                              | 7.405      |
| 1700                                                                           | 62.259      | 424.600                                                                             | 373.617                       | 86.671                                                   | -365.974         | -218.111                                              | 6.702      |
| 1800                                                                           | 62.269      | 428.159                                                                             | 375.550                       | 92.897                                                   | -365.928         | -209.414                                              | 6.077      |
| 1900                                                                           | 62.278      | 431.526                                                                             | 379.355                       | 99.125                                                   | -365.949         | -200.719                                              | 5.518      |
| 2000                                                                           | 62.286      | 434.721                                                                             | 382.044                       | 105.353                                                  | -366.040         | -192.021                                              | 5.015      |
| 2100                                                                           | 62.293      | 440.658                                                                             | 384.626                       | 111.582                                                  | -366.198         | -183.316                                              | 4.560      |
| 2200                                                                           | 62.304      | 443.427                                                                             | 389.496                       | 124.042                                                  | -366.693         | -165.578                                              | 3.767      |
| 2300                                                                           | 62.304      | 443.427                                                                             | 391.799                       | 130.272                                                  | -367.014         | -157.140                                              | 3.420      |
| 2400                                                                           | 62.308      | 446.679                                                                             | 394.623                       | 136.503                                                  | -367.388         | -148.388                                              | 3.100      |
| 2500                                                                           | 62.312      | 448.623                                                                             | 394.021                       | 142.734                                                  | -367.747         | -139.621                                              | 2.805      |
| 2600                                                                           | 62.315      | 451.067                                                                             | 396.169                       | 148.966                                                  | -368.138         | -130.840                                              | 2.277      |
| 2700                                                                           | 62.318      | 453.418                                                                             | 402.257                       | 153.198                                                  | -368.531         | -122.044                                              | 2.040      |
| 2800                                                                           | 62.321      | 455.585                                                                             | 407.872                       | 161.430                                                  | -368.916         | -113.234                                              | 1.818      |
| 3000                                                                           | 62.324      | 459.985                                                                             | 404.697                       | 167.663                                                  | -369.285         | -104.411                                              |            |
| 3100                                                                           | 62.328      | 462.028                                                                             | 405.933                       | 173.896                                                  | -369.631         | -95.776                                               |            |
| 3200                                                                           | 62.330      | 464.007                                                                             | 407.717                       | 180.128                                                  | -369.947         | -86.730                                               |            |
| 3300                                                                           | 62.332      | 465.525                                                                             | 409.452                       | 186.362                                                  | -370.230         | -77.375                                               |            |
| 3400                                                                           | 62.333      | 467.786                                                                             | 411.141                       | 192.593                                                  | -370.475         | -69.012                                               |            |
| 3500                                                                           | 62.334      | 469.593                                                                             | 412.785                       | 198.828                                                  | -370.680         | -60.142                                               |            |
| 3600                                                                           | 62.336      | 471.349                                                                             | 414.387                       | 211.950                                                  | -370.846         | -51.268                                               |            |
| 3700                                                                           | 62.337      | 474.677                                                                             | 415.950                       | 211.295                                                  | -370.971         | -42.386                                               |            |
| 3800                                                                           | 62.338      | 474.719                                                                             | 417.475                       | 217.529                                                  | -371.057         | -33.507                                               |            |
| 3900                                                                           | 62.339      | 476.339                                                                             | 418.964                       | 223.763                                                  | -371.104         | -24.623                                               |            |
| 4000                                                                           | 62.340      | 477.917                                                                             | 420.418                       | 229.997                                                  | -371.117         | -15.233                                               |            |
| 4100                                                                           | 62.341      | 479.456                                                                             | 421.839                       | 236.231                                                  | -371.095         | -55.281                                               |            |
| 4200                                                                           | 62.342      | 480.593                                                                             | 423.229                       | 242.465                                                  | -371.044         | -0.087                                                |            |
| 4300                                                                           | 62.342      | 482.426                                                                             | 424.589                       | 248.699                                                  | -370.966         | -10.911                                               |            |
| 4400                                                                           | 62.343      | 483.859                                                                             | 425.919                       | 254.934                                                  | -370.865         | 19.790                                                |            |
| 4500                                                                           | 62.344      | 485.260                                                                             | 427.223                       | 261.168                                                  | -370.744         | 28.568                                                |            |
| 5000                                                                           | 62.347      | 493.063                                                                             | 434.519                       | 286.575                                                  | -369.819         | 81.865                                                |            |
| 5100                                                                           | 62.347      | 494.274                                                                             | 435.637                       | 304.810                                                  | -369.665         | 90.721                                                |            |
| 5200                                                                           | 62.348      | 495.461                                                                             | 436.774                       | 311.045                                                  | -369.521         | 99.572                                                |            |
| 5300                                                                           | 62.348      | 496.621                                                                             | 437.871                       | 317.637                                                  | -369.390         | 108.422                                               |            |
| 5400                                                                           | 62.348      | 496.627                                                                             | 438.950                       | 323.514                                                  | -369.275         | 117.269                                               |            |
| 5500                                                                           | 62.349      | 497.771                                                                             | 439.059                       | 329.341                                                  | -369.179         | 126.115                                               |            |
| 5600                                                                           | 62.349      | 498.894                                                                             | 440.011                       | 339.749                                                  | -369.078         | -0.133                                                |            |
| 5700                                                                           | 62.349      | 499.998                                                                             | 441.053                       | 340.524                                                  | -369.055         | -1.237                                                |            |
| 5800                                                                           | 62.349      | 501.082                                                                             | 442.079                       | 342.219                                                  | -369.032         | -1.295                                                |            |
| 5900                                                                           | 62.350      | 502.148                                                                             | 443.058                       | 348.454                                                  | -369.032         | -1.351                                                |            |
| 6000                                                                           | 62.350      | 503.196                                                                             | 444.081                       | 349.589                                                  | -369.039         | -1.406                                                |            |

CURRENT: December 1974 (1 bar)

Magnesium Iodide ( $MgI_2$ )

## IDEAL GAS

 $S^\circ(298.15\text{ K}) = 317.5 \pm 2 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ 

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

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

$$\Delta H^\circ = -[G^\circ - H^\circ(T_r)]/T$$

## Vibrational Frequencies and Degeneracies

$$\sigma = 2$$

cm<sup>-1</sup>Point Group: D<sub>oh</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>

## 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 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 model for MgI<sub>2</sub> is calculated, using the valence force constant of the ground state vibrational frequency given by Rosen.<sup>4</sup> The adopted vibrational frequencies has been indicated as a reasonable assumption.<sup>4</sup> The stretching force constant for MgI<sub>2</sub> is taken as 0.01 of the stretching force constant. The ground state vibrational frequency of 0.01 for MgI<sub>3</sub>; however, a factor of 0.01 appears more reasonable.<sup>7</sup> The adopted vibrational frequencies constant. Brewer *et al.*<sup>4</sup> used a factor of 0.1 for MgI<sub>3</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 ν<sub>1</sub>, ν<sub>2</sub>, and ν<sub>3</sub> are 132, 199, 446,<sup>8</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

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- P. A. Akishin and V. P. Spiridonov, *Zhur. Fiz. Khim.*, **32**, 1682 (1958).
- J. A. Buechler, J. L. Stauffer and W. Klempner, *J. Amer. Chem. Soc.*, **86**, 4544 (1964).
- L. Brewer, G. R. Somayajulu, and E. Brackett, *Chem. Rev.*, **63**, 111 (1963).
- JANAF Thermochemical Tables: BeF<sub>3</sub>(g), 6-30-74; BaF<sub>2</sub>(g), 12-31-72; SrF<sub>2</sub>(g), 12-31-68; SrF<sub>4</sub>(g), 12-31-72; CaF<sub>2</sub>(g), 6-30-74; SrI<sub>2</sub>(g), 6-30-74; BaI<sub>2</sub>(g), 6-30-74.
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- K. S. Krasnov and V. I. Svetsov, Izv. Vysshikh Uchebn. Zavedenii, Khim. i Khim. Tekhnol. **6**, 167 (1963).

**Molybdenum Iodide ( $\alpha$ -MoI<sub>2</sub>)****CRYSTAL( $\alpha$ )**

$$S^{\circ}(298.15 \text{ K}) = [149.662 \pm 16.7] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{d_{\text{cr}}} = 1305 \text{ K} \quad (\text{total } p = 1 \text{ atm})$$

**Enthalpy of Formation**

Barnes *et al.*<sup>1</sup> have measured calorimetrically the enthalpy of formation of MoI<sub>2</sub> by reacting iodine vapor with Mo(CO)<sub>6</sub> at 539 K. The products were shown to consist of MoI<sub>2</sub>, MoI, and Mo by chemical analysis. Assuming a difference in the enthalpies of formation of MoI<sub>3</sub> and MoI<sub>2</sub> of  $\sim 1.5 \text{ kcal/mol}^{-1}$ , 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  $\sim 5 \text{ kcal/mol}^{-1}$ , and he reanalyzed the enthalpy of iodination data with the result  $\Delta_f H^{\circ}(\text{MoI}_2, \text{cr}, 298.15 \text{ K})/R = -12500 \pm 1500 \text{ K}$  which is adopted in the assigned uncertainty ( $\pm 3 \text{ kcal/mol}^{-1}$ ) is determined from the product 1500 K R 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  $S^{\circ}(298.15 \text{ K})/R$  in a manner similar to that for the heat of formation.

**Phase Data**

The crystal structure<sup>2</sup> of  $\alpha$ -MoI<sub>2</sub> in the Pearson classification system of  $\text{oC72}$ , 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**

$T_{d_{\text{cr}}}$  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  $T_{d_{\text{cr}}} = 1305 \text{ K}$ , we calculate the vapor composition to consist of 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**

- D. S. Barnes, G. Pilcher, D. A. Pittam, H. A. Skinner, D. Todd, and Y. Virmani, *J. Less Common Met.* **6**, 177 (1974).
- 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. D. Glicksman and R. A. Walton, *Inorg. Chem.* **7**, 200 (1978).
- D. V. Drobot, L. G. Mikhailova, K. A. Bol'shakov, and V. L. Shnitnev, *Russ. J. Inorg. Chem.* **3**, 643 (1978).

| <b>I<sub>2</sub>Mo<sub>2</sub>(cr)</b> |                                        | <b>Molybdenum Iodide, Alpha (MoI<sub>2</sub>)</b>       |                                                                             |                              |                      |
|----------------------------------------|----------------------------------------|---------------------------------------------------------|-----------------------------------------------------------------------------|------------------------------|----------------------|
|                                        |                                        | M <sub>f</sub> = 349.7490                               |                                                                             |                              |                      |
|                                        |                                        | Standard State Pressure = $p^{\circ} = 0.1 \text{ MPa}$ |                                                                             |                              |                      |
| Enthalpy Reference                     | Temperature = $T_f = 298.15 \text{ K}$ | $\Delta H^{\circ}(0 \text{ K}) = \text{Unknown}$        | $\Delta H^{\circ}(298.15 \text{ K}) = -103.93 \pm 12.6 \text{ kJ mol}^{-1}$ |                              |                      |
| $T/K$                                  |                                        | $J \cdot K^{-1} \cdot \text{mol}^{-1}$                  | $J \cdot K^{-1} \cdot \text{mol}^{-1}$                                      | $\text{kJ mol}^{-1}$         | $\text{kJ mol}^{-1}$ |
|                                        |                                        | $C_p^{\circ}$                                           | $S^{\circ}$                                                                 | $H^{\circ} - H^{\circ}(T_f)$ | $\Delta H^{\circ}$   |
| 0                                      |                                        |                                                         |                                                                             |                              |                      |
| 100                                    |                                        |                                                         |                                                                             |                              |                      |
| 200                                    | 82.705                                 | 149.662                                                 | 0                                                                           | -103.93                      | -103.396             |
| 298.15                                 |                                        |                                                         |                                                                             |                              |                      |
| 300                                    | 82.730                                 | 149.663                                                 | 0.153                                                                       | -103.923                     | -105.405             |
| 400                                    | 83.977                                 | 174.144                                                 | 8.488                                                                       | -119.681                     | -103.353             |
| 500                                    | 85.224                                 | 193.017                                                 | 16.948                                                                      | -161.966                     | -13.763              |
| 600                                    | 86.471                                 | 208.865                                                 | 25.533                                                                      | -159.752                     | 10.214               |
| 700                                    | 87.718                                 | 222.089                                                 | 34.243                                                                      | -157.483                     | 5.438                |
| 800                                    | 88.964                                 | 233.983                                                 | 43.077                                                                      | -155.149                     | -60.950              |
| 900                                    | 90.211                                 | 244.433                                                 | 52.035                                                                      | -152.747                     | -49.318              |
| 1000                                   | 91.458                                 | 254.003                                                 | 61.119                                                                      | -150.278                     | -21.622              |
| 1100                                   | 92.705                                 | 262.778                                                 | 70.327                                                                      | -147.778                     | -37.958              |
| 1200                                   | 93.952                                 | 270.598                                                 | 79.660                                                                      | -145.166                     | -26.848              |
| 1300                                   | 95.199                                 | 278.467                                                 | 89.117                                                                      | -143.546                     | -12.755              |
| 1400                                   | 96.445                                 | 285.568                                                 | 98.700                                                                      | -139.900                     | -5.310               |
| 1500                                   | 97.696                                 | 292.264                                                 | 108.407                                                                     | -137.246                     | -0.192               |

PREVIOUS:

CURRENT: September 1978

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

## NIST-JANAF THERMOCHEMICAL TABLES

Molybdenum Iodide ( $\text{MoI}_2$ ) $M_r = 349.7490$  Molybdenum Iodide ( $\text{MoI}_2$ ) $\text{I}_2\text{MoI}_2(\text{g})$ 

| $\Delta H^\circ(0 \text{ K}) = [257.38 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$ |             |           |                             |                          |                                 |        |             |           |                             | $\Delta H^\circ(298.15 \text{ K}) = [257.73 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$ |                                 |        |             |           |                             |                          |                                 |                  |            |
|----------------------------------------------------------------------------------|-------------|-----------|-----------------------------|--------------------------|---------------------------------|--------|-------------|-----------|-----------------------------|---------------------------------------------------------------------------------------|---------------------------------|--------|-------------|-----------|-----------------------------|--------------------------|---------------------------------|------------------|------------|
| IDEAL GAS                                                                        |             |           |                             |                          |                                 |        |             |           |                             | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$                             |                                 |        |             |           |                             |                          |                                 |                  |            |
|                                                                                  |             |           |                             |                          |                                 |        |             |           |                             | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$                                 |                                 |        |             |           |                             |                          |                                 |                  |            |
|                                                                                  |             |           |                             |                          |                                 |        |             |           |                             |                                                                                       |                                 |        |             |           |                             |                          |                                 |                  |            |
|                                                                                  |             |           |                             |                          |                                 |        |             |           |                             |                                                                                       |                                 |        |             |           |                             |                          |                                 |                  |            |
| $T/K$                                                                            | $C_p^\circ$ | $S^\circ$ | $-G^\circ - H^\circ(T) / T$ | $H^\circ - H^\circ(T_r)$ | $k\text{J}\cdot\text{mol}^{-1}$ | $T/K$  | $C_p^\circ$ | $S^\circ$ | $-G^\circ - H^\circ(T) / T$ | $H^\circ - H^\circ(T_r)$                                                              | $k\text{J}\cdot\text{mol}^{-1}$ | $T/K$  | $C_p^\circ$ | $S^\circ$ | $-G^\circ - H^\circ(T) / T$ | $H^\circ - H^\circ(T_r)$ | $k\text{J}\cdot\text{mol}^{-1}$ | $\Delta G^\circ$ | $\log K_r$ |
| 0                                                                                | 0           | 0         | 0                           | 0                        | 0                               | 100    | 265.272     | 406.919   | -18.140                     | 257.377                                                                               | 257.377                         | 100    | 265.272     | 406.919   | -18.140                     | 257.377                  | 257.377                         | 0                | INFINITE   |
| 200                                                                              | 69.265      | 311.318   | 345.722                     | -6.981                   | 258.411                         | 200    | 69.265      | 311.318   | -6.981                      | 258.321                                                                               | 258.321                         | 200    | 69.265      | 311.318   | -6.981                      | 258.321                  | 258.321                         | -57.182          | -124.677   |
| 250                                                                              | 70.171      | 326.880   | 340.452                     | -3.393                   | 258.063                         | 250    | 70.171      | 326.880   | 340.452                     | 257.734                                                                               | 257.734                         | 250    | 70.171      | 326.880   | 340.452                     | 257.734                  | 257.734                         | -43.695          | -124.677   |
| 298.15                                                                           | 70.717      | 339.290   | 339.290                     | 0.                       | 199.731                         | 298.15 | 70.717      | 339.290   | 339.290                     | 199.731                                                                               | 199.731                         | 298.15 | 70.717      | 339.290   | 339.290                     | 199.731                  | 199.731                         | -34.992          | -124.677   |
| 300                                                                              | 70.733      | 339.728   | 339.290                     | 0.131                    | 257.724                         | 298.15 | 70.733      | 339.728   | 339.290                     | 257.724                                                                               | 257.724                         | 298.15 | 70.733      | 339.728   | 339.290                     | 257.724                  | 257.724                         | -28.308          | -124.677   |
| 350                                                                              | 71.082      | 350.660   | 340.154                     | 3.677                    | 189.682                         | 350    | 71.082      | 350.660   | 340.154                     | 189.682                                                                               | 189.682                         | 350    | 71.082      | 350.660   | 340.154                     | 189.682                  | 189.682                         | -9.983           | -124.677   |
| 400                                                                              | 71.254      | 360.164   | 342.074                     | 7.236                    | 180.614                         | 360    | 71.254      | 360.164   | 342.074                     | 180.614                                                                               | 180.614                         | 360    | 71.254      | 360.164   | 342.074                     | 180.614                  | 180.614                         | -23.586          | -124.677   |
| 450                                                                              | 71.268      | 368.559   | 344.560                     | 10.800                   | 238.997                         | 368    | 71.268      | 368.559   | 344.560                     | 238.997                                                                               | 238.997                         | 368    | 71.268      | 368.559   | 344.560                     | 238.997                  | 238.997                         | -20.105          | -124.677   |
| 500                                                                              | 71.146      | 376.063   | 347.342                     | 14.361                   | 197.111                         | 376    | 71.146      | 376.063   | 347.342                     | 197.111                                                                               | 197.111                         | 376    | 71.146      | 376.063   | 347.342                     | 197.111                  | 197.111                         | -17.737          | -124.677   |
| 600                                                                              | 70.599      | 388.591   | 353.240                     | 21.451                   | 197.830                         | 70     | 70.599      | 388.591   | 353.240                     | 197.830                                                                               | 197.830                         | 70     | 70.599      | 388.591   | 353.240                     | 197.830                  | 197.830                         | -14.299          | -124.677   |
| 700                                                                              | 68.827      | 399.818   | 359.142                     | 28.473                   | 198.412                         | 68     | 68.827      | 399.818   | 359.142                     | 198.412                                                                               | 198.412                         | 68     | 68.827      | 399.818   | 359.142                     | 198.412                  | 198.412                         | -11.835          | -124.677   |
| 800                                                                              | 68.995      | 409.087   | 364.820                     | 35.414                   | 152.889                         | 68     | 68.995      | 409.087   | 364.820                     | 152.889                                                                               | 152.889                         | 68     | 68.995      | 409.087   | 364.820                     | 152.889                  | 152.889                         | -9.983           | -124.677   |
| 900                                                                              | 68.198      | 417.167   | 370.197                     | 42.273                   | 199.156                         | 68     | 68.198      | 417.167   | 370.197                     | 199.156                                                                               | 199.156                         | 68     | 68.198      | 417.167   | 370.197                     | 199.156                  | 199.156                         | -8.539           | -124.677   |
| 1000                                                                             | 67.478      | 424.314   | 375.258                     | 49.056                   | 141.332                         | 67     | 67.478      | 424.314   | 375.258                     | 141.332                                                                               | 141.332                         | 67     | 67.478      | 424.314   | 375.258                     | 141.332                  | 141.332                         | -7.382           | -124.677   |
| 1100                                                                             | 66.347      | 430.715   | 380.014                     | 55.772                   | 133.530                         | 66     | 66.347      | 430.715   | 380.014                     | 133.530                                                                               | 133.530                         | 66     | 66.347      | 430.715   | 380.014                     | 133.530                  | 133.530                         | -6.436           | -124.677   |
| 1200                                                                             | 66.305      | 436.508   | 384.484                     | 62.429                   | 129.731                         | 66     | 66.305      | 436.508   | 384.484                     | 129.731                                                                               | 129.731                         | 66     | 66.305      | 436.508   | 384.484                     | 129.731                  | 129.731                         | -5.647           | -124.677   |
| 1300                                                                             | 65.842      | 441.796   | 388.692                     | 69.035                   | 123.944                         | 65     | 65.842      | 441.796   | 388.692                     | 123.944                                                                               | 123.944                         | 65     | 65.842      | 441.796   | 388.692                     | 123.944                  | 123.944                         | -4.980           | -124.677   |
| 1400                                                                             | 65.449      | 446.651   | 392.662                     | 75.599                   | 120.664                         | 64     | 65.449      | 446.651   | 392.662                     | 120.664                                                                               | 120.664                         | 64     | 65.449      | 446.651   | 392.662                     | 120.664                  | 120.664                         | -4.409           | -124.677   |
| 1500                                                                             | 65.118      | 451.165   | 396.414                     | 82.127                   | 118.181                         | 63     | 65.118      | 451.165   | 396.414                     | 118.181                                                                               | 118.181                         | 63     | 65.118      | 451.165   | 396.414                     | 118.181                  | 118.181                         | -3.916           | -124.677   |
| 1600                                                                             | 64.840      | 455.358   | 399.968                     | 88.625                   | 117.453                         | 62     | 64.840      | 455.358   | 399.968                     | 117.453                                                                               | 117.453                         | 62     | 64.840      | 455.358   | 399.968                     | 117.453                  | 117.453                         | -3.485           | -124.677   |
| 1700                                                                             | 64.609      | 459.282   | 403.134                     | 95.097                   | 106.758                         | 60     | 64.609      | 459.282   | 403.134                     | 106.758                                                                               | 106.758                         | 60     | 64.609      | 459.282   | 403.134                     | 106.758                  | 106.758                         | -3.107           | -124.677   |
| 1800                                                                             | 64.422      | 462.970   | 406.554                     | 101.548                  | 95.553                          | 58     | 64.422      | 462.970   | 406.554                     | 95.553                                                                                | 95.553                          | 58     | 64.422      | 462.970   | 406.554                     | 95.553                   | 95.553                          | -2.772           | -124.677   |
| 1900                                                                             | 64.272      | 465.499   | 409.016                     | 107.982                  | 90.004                          | 56     | 64.272      | 465.499   | 409.016                     | 107.982                                                                               | 107.982                         | 56     | 64.272      | 465.499   | 409.016                     | 107.982                  | 107.982                         | -2.474           | -124.677   |
| 2000                                                                             | 64.157      | 468.742   | 412.540                     | 114.403                  | 92.897                          | 54     | 64.157      | 468.742   | 412.540                     | 114.403                                                                               | 114.403                         | 54     | 64.157      | 468.742   | 412.540                     | 114.403                  | 114.403                         | -2.208           | -124.677   |
| 2100                                                                             | 64.075      | 472.870   | 415.339                     | 120.815                  | 91.875                          | 52     | 64.075      | 472.870   | 415.339                     | 120.815                                                                               | 120.815                         | 52     | 64.075      | 472.870   | 415.339                     | 120.815                  | 120.815                         | -1.969           | -124.677   |
| 2200                                                                             | 64.022      | 475.850   | 418.023                     | 127.179                  | 89.452                          | 50     | 64.022      | 475.850   | 418.023                     | 127.179                                                                               | 127.179                         | 50     | 64.022      | 475.850   | 418.023                     | 127.179                  | 127.179                         | -1.754           | -124.677   |
| 2300                                                                             | 63.996      | 478.695   | 420.599                     | 133.620                  | 87.433                          | 48     | 63.996      | 478.695   | 420.599                     | 133.620                                                                               | 133.620                         | 48     | 63.996      | 478.695   | 420.599                     | 133.620                  | 133.620                         | -1.559           | -124.677   |
| 2400                                                                             | 63.995      | 481.419   | 423.463                     | 140.019                  | 85.219                          | 46     | 63.995      | 481.419   | 423.463                     | 140.019                                                                               | 140.019                         | 46     | 63.995      | 481.419   | 423.463                     | 140.019                  | 140.019                         | -1.383           | -124.677   |
| 2500                                                                             | 63.917      | 484.031   | 425.463                     | 146.420                  | 82.528                          | 44     | 63.917      | 484.031   | 425.463                     | 146.420                                                                               | 146.420                         | 44     | 63.917      | 484.031   | 425.463                     | 146.420                  | 146.420                         | -1.223           | -124.677   |
| 2600                                                                             | 63.059      | 486.543   | 427.765                     | 152.823                  | 80.204                          | 42     | 63.059      | 486.543   | 427.765                     | 152.823                                                                               | 152.823                         | 42     | 63.059      | 486.543   | 427.765                     | 152.823                  | 152.823                         | -1.077           | -124.677   |
| 2700                                                                             | 63.120      | 488.962   | 429.987                     | 159.232                  | 77.369                          | 40     | 63.120      | 488.962   | 429.987                     | 159.232                                                                               | 159.232                         | 40     | 63.120      | 488.962   | 429.987                     | 159.232                  | 159.232                         | -0.944           | -124.677   |
| 2800                                                                             | 64.198      | 491.295   | 432.135                     | 165.648                  | 74.257                          | 38     | 64.198      | 491.295   | 432.135                     | 165.648                                                                               | 165.648                         | 38     | 64.198      | 491.295   | 432.135                     | 165.648                  | 165.648                         | -0.822           | -124.677   |
| 2900                                                                             | 64.289      | 493.349   | 434.214                     | 172.072                  | 71.917                          | 36     | 64.289      | 493.349   | 434.214                     | 172.072                                                                               | 172.072                         | 36     | 64.289      | 493.349   | 434.214                     | 172.072                  | 172.072                         | -0.712           | -124.677   |
| 3000                                                                             | 63.939      | 496.700   | 436.228                     | 178.506                  | 63.332                          | 34     | 63.939      | 496.700   | 436.228                     | 178.506                                                                               | 178.506                         | 34     | 63.939      | 496.700   | 436.228                     | 178.506                  | 178.506                         | -0.632           | -124.677   |
| 3100                                                                             | 64.507      | 497.844   | 438.182                     | 184.951                  | 60.287                          | 32     | 64.507      | 497.844   | 438.182                     | 184.951                                                                               | 184.951                         | 32     | 64.507      | 497.844   | 438.182                     | 184.951                  | 184.951                         | -0.558           | -124.677   |
| 3200                                                                             | 64.630      | 499.894   | 440.079                     | 191.488                  | 57.921                          | 30     | 64.630      | 499.894   | 440.079                     | 191.488                                                                               | 191.488                         | 30     | 64.630      | 499.894   | 440.079                     | 191.488                  | 191.488                         | -0.489           | -124.677   |
| 3300                                                                             | 64.760      | 501.884   | 441.933                     | 197.878                  | 55.721                          | 28     | 64.760      | 501.884   | 441.933                     | 197.878                                                                               | 197.878                         | 28     | 64.760      | 501.884   | 441.933                     | 197.878                  | 197.878                         | -0.425           | -124.677   |
| 3400                                                                             | 65.873      | 516.058   | 455.050                     | 204.360                  | 52.857                          | 26     | 65.873      | 516.058   | 455.050                     | 204.360                                                                               | 204.360                         | 26     | 65.873      | 516.058   | 455.050                     | 204.360                  | 204.360                         | -0.366           | -124.677   |
| 3500                                                                             | 65.034      | 503.703   | 443.458                     | 210.857                  | 50.857                          | 24     | 65.034      | 503.703   | 443.458                     | 210.857                                                                               | 210.857                         | 24     | 65.034      | 503.703   | 443.458                     | 210.857                  | 210.857                         | -0.311           | -124.677   |
| 3600                                                                             | 65.175      | 507.537   | 447.157                     | 217.367                  | 47.157                          | 22     | 65.175      | 507.537   | 447.157                     | 217.367                                                                               | 217.367                         | 22     | 65.175      | 507.537   | 447.157                     | 217.367                  | 217.367                         | -0.260           | -124.677   |
| 3700                                                                             | 65.317      | 509.524   | 451.068                     | 223.892                  | 43.751                          | 20     | 65.317      | 509.524   | 451.068                     | 223.892                                                                               | 223.892                         | 20     | 65.317      | 509.524   | 451.068                     | 223.892                  | 223.892                         | -0.212           | -124.677   |
| 3800                                                                             | 65.458      | 511.524   | 452.005                     | 230.430                  | 40.430                          | 18     | 65.458      | 511.524   | 452.005                     | 230.430                                                                               | 230.430                         | 18     | 65.458      | 511.524   | 452.005                     | 230.430                  | 230.430                         | -0.167           | -124.677   |
| 3900                                                                             | 65.599      | 512.770   | 452.214                     | 236.983                  | 39.521                          | 16     | 65.599      | 512.77    |                             |                                                                                       |                                 |        |             |           |                             |                          |                                 |                  |            |

## Iodine Oxide (IO)

## IDEAL GAS

$$\Delta_f H^\circ(0\text{ K}) = 348 \pm 25 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15\text{ K}) = [308.1 \pm 4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(0\text{ K}) = [124 \pm 25] \text{ J}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15\text{ K}) = [119.5 \pm 25] \text{ J}\cdot\text{mol}^{-1}$$

|  | $M_r = 269.80834$ | Iodine Oxide (IO)                                |                                                  | $I_2O(g)$                                        |                                 |
|--|-------------------|--------------------------------------------------|--------------------------------------------------|--------------------------------------------------|---------------------------------|
|  |                   | $\Delta_f H^\circ(0\text{ K})$                   | $\Delta_f H^\circ(298.15\text{ K})$              | $S^\circ$                                        | $H^\circ - H^\circ(T)/T$        |
|  |                   | $[124 \pm 25]$ $\text{kJ}\cdot\text{mol}^{-1}$   | $[119.5 \pm 25]$ $\text{kJ}\cdot\text{mol}^{-1}$ | $-G^\circ - H^\circ(T)/T$                        | $\Delta_f H^\circ$              |
|  |                   | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $\text{kJ}\cdot\text{mol}^{-1}$ |
|  |                   |                                                  |                                                  |                                                  | $\Delta_f G^\circ$              |
|  |                   |                                                  |                                                  |                                                  | $\log K_r$                      |
|  |                   |                                                  |                                                  |                                                  | INFINITE                        |
|  |                   |                                                  |                                                  |                                                  | -13.925                         |
|  |                   |                                                  |                                                  |                                                  | 124.000                         |
|  |                   |                                                  |                                                  |                                                  | 124.056                         |
|  |                   |                                                  |                                                  |                                                  | 117.968                         |
|  |                   |                                                  |                                                  |                                                  | -123.241                        |
|  |                   |                                                  |                                                  |                                                  | -58.598                         |
|  |                   |                                                  |                                                  |                                                  | 112.182                         |
|  |                   |                                                  |                                                  |                                                  | -122.204                        |
|  |                   |                                                  |                                                  |                                                  | 106.886                         |
|  |                   |                                                  |                                                  |                                                  | -37.221                         |
|  |                   |                                                  |                                                  |                                                  | 101.928                         |
|  |                   |                                                  |                                                  |                                                  | -26.621                         |
|  |                   |                                                  |                                                  |                                                  | 102.310                         |
|  |                   |                                                  |                                                  |                                                  | 97.207                          |
|  |                   |                                                  |                                                  |                                                  | -20.310                         |
|  |                   |                                                  |                                                  |                                                  | 120.322                         |
|  |                   |                                                  |                                                  |                                                  | -16.264                         |
|  |                   |                                                  |                                                  |                                                  | 92.832                          |
|  |                   |                                                  |                                                  |                                                  | -16.264                         |
|  |                   |                                                  |                                                  |                                                  | 124.000                         |
|  |                   |                                                  |                                                  |                                                  | 124.056                         |
|  |                   |                                                  |                                                  |                                                  | 117.968                         |
|  |                   |                                                  |                                                  |                                                  | -123.241                        |
|  |                   |                                                  |                                                  |                                                  | -58.598                         |
|  |                   |                                                  |                                                  |                                                  | 112.182                         |
|  |                   |                                                  |                                                  |                                                  | -122.204                        |
|  |                   |                                                  |                                                  |                                                  | 106.886                         |
|  |                   |                                                  |                                                  |                                                  | -37.221                         |
|  |                   |                                                  |                                                  |                                                  | 101.928                         |
|  |                   |                                                  |                                                  |                                                  | -26.621                         |
|  |                   |                                                  |                                                  |                                                  | 102.310                         |
|  |                   |                                                  |                                                  |                                                  | 97.207                          |
|  |                   |                                                  |                                                  |                                                  | -20.310                         |
|  |                   |                                                  |                                                  |                                                  | 120.322                         |
|  |                   |                                                  |                                                  |                                                  | -16.264                         |
|  |                   |                                                  |                                                  |                                                  | 92.832                          |
|  |                   |                                                  |                                                  |                                                  | -16.264                         |
|  |                   |                                                  |                                                  |                                                  | 124.000                         |
|  |                   |                                                  |                                                  |                                                  | 124.056                         |
|  |                   |                                                  |                                                  |                                                  | 117.968                         |
|  |                   |                                                  |                                                  |                                                  | -123.241                        |
|  |                   |                                                  |                                                  |                                                  | -58.598                         |
|  |                   |                                                  |                                                  |                                                  | 112.182                         |
|  |                   |                                                  |                                                  |                                                  | -122.204                        |
|  |                   |                                                  |                                                  |                                                  | 106.886                         |
|  |                   |                                                  |                                                  |                                                  | -37.221                         |
|  |                   |                                                  |                                                  |                                                  | 101.928                         |
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|  |                   |                                                  |                                                  |                                                  | 102.310                         |
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|  |                   |                                                  |                                                  |                                                  | 92.832                          |
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|  |                   |                                                  |                                                  |                                                  | 101.928                         |
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|  |                   |                                                  |                                                  |                                                  | -26.621                         |
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|  |                   |                                                  |                                                  |                                                  | 120.322                         |
|  |                   |                                                  |                                                  |                                                  | -16.264                         |
|  |                   |                                                  |                                                  |                                                  | 92.832                          |
|  |                   |                                                  |                                                  |                                                  | -16.264                         |



Lead Iodide ( $\text{PbI}_2$ )

## CRYSTAL

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= 174.836 \pm 0.21 \text{ J K}^{-1} \text{ mol}^{-1} \\ T_{\text{fus}} &= 683 \pm 2 \text{ K} \end{aligned}$$

## Enthalpy of Formation

Koref and Braune<sup>1</sup> determined  $\Delta H^\circ(\text{PbI}_2, \text{cr}, 298.15 \text{ K}) = -41.850 \text{ kcal mol}^{-1}$  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  $\Delta H^\circ(\text{PbI}_2, \text{cr}, 298.15 \text{ K}) = -41.923$  and  $-41.925 \text{ kcal mol}^{-1}$ , respectively.  $\Delta H^\circ(\text{PbI}_2, \text{cr}, 298.15 \text{ K}) = -41.92 \pm 0.10 \text{ kcal mol}^{-1}$  is adopted.

## Heat Capacity and Entropy

McBride<sup>4</sup> measured the low temperature heat capacity (4.52–29.100 K) of  $\text{PbI}_2$ . Enthalpies have been measured by Ehrhardt<sup>5</sup> (448–776 K), Magnus<sup>6</sup> (373–523 K), and Linsey<sup>7</sup> (323–877 K). The enthalpy data of Linsey<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>  $S^\circ(10 \text{ K}) = 0.662 \text{ cal K}^{-1} \text{ mol}^{-1}$  is adopted from McBride.<sup>4</sup> The data of Linsey<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  $\text{PbI}_2$  to exist in two crystalline forms with the  $\alpha$ – $\beta$  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  $\beta$ – $\alpha$  transition. Modestova and Sumarokova<sup>13</sup> observed the  $\beta$  form to melt at 669 K. Ehrhardt<sup>5</sup>'s 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  $\beta$ -phase. The observation by Novoselova *et al.*<sup>14</sup> that only the  $\alpha$  form crystallizes on cooling melts of the  $\text{PbI}_2$  rich region of the  $\text{PbI}_2$ – $\text{PbSe}$  system is consistent with the interpretation that the reference state for Ehrhardt's work is  $\alpha$ - $\text{PbI}_2$ . The enthalpy measurements by Linsey<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,  $\Delta_{\text{fus}}H^\circ = 5.43 \text{ kcal mol}^{-1}$  at 683 K is obtained. Kelley<sup>15</sup> derived 5.57, 5.67, and 5.80  $\text{kcal mol}^{-1}$  from phase diagram information and also gives  $6.01 \text{ kcal mol}^{-1}$ . Another analysis<sup>16</sup> has resulted in  $\Delta_{\text{fus}}H^\circ = 5.20 \text{ kcal mol}^{-1}$ . Blanc and Petit<sup>11</sup>'s value of 3.87  $\text{kcal mol}^{-1}$  is too low. The enthalpy data of Linsey<sup>7</sup> was analyzed to yield  $\Delta_{\text{fus}}H^\circ = 5.6 \text{ kcal mol}^{-1}$ .  $\Delta_{\text{fus}}H^\circ = 5.6 \pm 0.2 \text{ kcal mol}^{-1}$  is adopted.

## Sublimation Data

$\Delta_{\text{sub}}H^\circ(298.15 \text{ K})$  is calculated from the difference between the adopted values for  $\Delta_H^\circ(298.15 \text{ K})$  of the gas and crystal. Refer to  $\text{PbI}_2(\text{g})$  table.

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PREVIOUS: March 1962

CURRENT: December 1973

 $\text{I}_2\text{Pb}_1(\text{cr})$ 

| $T/\text{K}$ | $\frac{\text{Enthalpy Reference Temperature} = T = 298.15 \text{ K}}{\text{Standard State Pressure} = p^\circ = 0.1 \text{ MPa}}$ |                                                                               |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
|              | $\frac{\text{J K}^{-1} \text{ mol}^{-1}}{C_p^*}$                                                                                  | $\frac{\text{J K}^{-1} \text{ mol}^{-1}}{S^\circ - [G^\circ - H^\circ(T)]/T}$ |
| 100          | 0                                                                                                                                 | 0                                                                             |
| 200          | 69.789                                                                                                                            | 93.717                                                                        |
| 298.15       | 75.396                                                                                                                            | 144.332                                                                       |
| 300          | 75.573                                                                                                                            | 174.836                                                                       |
| 400          | 77.613                                                                                                                            | 175.316                                                                       |
| 500          | 80.391                                                                                                                            | 177.901                                                                       |
| 600          | 83.713                                                                                                                            | 190.305                                                                       |
| 683.000      | 87.780                                                                                                                            | 241.591                                                                       |
| 700          | 88.743                                                                                                                            | 243.761                                                                       |
| 800          | 95.102                                                                                                                            | 256.015                                                                       |
| 900          | 102.428                                                                                                                           | 267.537                                                                       |
| 1000         | 110.064                                                                                                                           | 278.821                                                                       |
|              | 15.925                                                                                                                            | 234.996                                                                       |
|              | 15.754                                                                                                                            | 191.933                                                                       |
|              | 15.723                                                                                                                            | 172.328                                                                       |
|              | 15.725                                                                                                                            | 163.287                                                                       |
|              | 15.925                                                                                                                            | 174.817                                                                       |
|              | 14.839                                                                                                                            | 174.972                                                                       |
|              | 7.506                                                                                                                             | 175.096                                                                       |
|              | 0.                                                                                                                                | 175.393                                                                       |
|              | 0.                                                                                                                                | 175.577                                                                       |
|              | 0.144                                                                                                                             | 175.400                                                                       |
|              | 0.144                                                                                                                             | 173.566                                                                       |
|              | 0.144                                                                                                                             | 22.504                                                                        |
|              | 0.                                                                                                                                | 91.182                                                                        |
|              | 0.                                                                                                                                | 45.474                                                                        |
|              | 0.                                                                                                                                | 30.416                                                                        |
|              | 0.                                                                                                                                | 10.027                                                                        |
|              | 0.                                                                                                                                | 7.832                                                                         |
|              | 0.                                                                                                                                | 6.144                                                                         |
|              | 0.                                                                                                                                | 4.814                                                                         |
|              | 0.                                                                                                                                | 227.076                                                                       |
|              | 0.                                                                                                                                | 92.166                                                                        |

LIQUID Lead Iodide ( $\text{PbI}_2$ ) $M_r = 461.0090$  Lead Iodide ( $\text{PbI}_2$ )

$$S^\circ(298.15 \text{ K}) = [1198.902] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{ins}} = 683 \pm 2 \text{ K}$$

| $\Delta_f H^\circ(298.15 \text{ K}) = [ -157.679 ] \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_{\text{ins}} H^\circ = 23.430 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$ | $T/K$   | $C_p^\circ$ | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ | Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$ |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|---------|-------------|-----------------------------------------------------------|-------------------------------------------------------|
|                                                                                    |                                                                               |         |             | $H^\circ - H^\circ(T_r)/T$                                | $H^\circ - H^\circ(T_r)$                              |
|                                                                                    |                                                                               |         |             | $S^\circ - [G^\circ - H^\circ(T_r)]/T$                    | $\Delta_f G^\circ$                                    |
| 0                                                                                  |                                                                               |         |             |                                                           |                                                       |
| 100                                                                                |                                                                               |         |             |                                                           |                                                       |
| 200                                                                                |                                                                               | 298.15  | 77.571      | 198.902                                                   | 0.                                                    |
|                                                                                    |                                                                               |         |             |                                                           | -157.679                                              |
|                                                                                    |                                                                               |         |             |                                                           | -163.038                                              |
| 300                                                                                |                                                                               | 77.613  | 199.382     | 198.904                                                   | 0.144                                                 |
|                                                                                    |                                                                               |         |             |                                                           | -157.686                                              |
| 400                                                                                |                                                                               | 78.836  | 221.912     | 201.967                                                   | 0.798                                                 |
|                                                                                    |                                                                               |         |             |                                                           | -174.219                                              |
| 450                                                                                | 0.000                                                                         | 79.592  | 232.980     | 205.306                                                   | 12.730                                                |
|                                                                                    |                                                                               |         |             |                                                           | GLASS $\leftrightarrow$ LIQUID                        |
| 460                                                                                | 0.000                                                                         | 108.575 | 232.980     | 205.306                                                   | 12.730                                                |
|                                                                                    |                                                                               |         |             |                                                           | TRANSITION                                            |
| 500                                                                                |                                                                               | 108.575 | 242.033     | 207.867                                                   | 17.073                                                |
|                                                                                    |                                                                               |         |             |                                                           | -157.655                                              |
| 600                                                                                |                                                                               | 108.575 | 261.829     | 215.278                                                   | 27.930                                                |
|                                                                                    |                                                                               |         |             |                                                           | -146.357                                              |
| 683                                                                                | 0.000                                                                         | 108.575 | 275.896     | 221.808                                                   | 36.942                                                |
|                                                                                    |                                                                               |         |             |                                                           | -146.357                                              |
| 700                                                                                |                                                                               | 108.575 | 278.565     | 223.154                                                   | 38.788                                                |
|                                                                                    |                                                                               |         |             |                                                           | -134.959                                              |
| 800                                                                                |                                                                               | 108.575 | 293.064     | 231.007                                                   | 49.645                                                |
|                                                                                    |                                                                               |         |             |                                                           | -124.137                                              |
| 900                                                                                |                                                                               | 108.575 | 305.852     | 238.627                                                   | 60.503                                                |
|                                                                                    |                                                                               |         |             |                                                           | -113.825                                              |
| 1000                                                                               |                                                                               | 108.575 | 317.291     | 245.931                                                   | 71.360                                                |
|                                                                                    |                                                                               |         |             |                                                           | -103.468                                              |
| 1100                                                                               |                                                                               | 108.575 | 327.640     | 252.896                                                   | 82.218                                                |
|                                                                                    |                                                                               |         |             |                                                           | -96.290                                               |
| 1200                                                                               |                                                                               | 108.575 | 337.087     | 259.524                                                   | 93.075                                                |
|                                                                                    |                                                                               |         |             |                                                           | -85.455                                               |
| 1300                                                                               |                                                                               | 108.575 | 345.778     | 265.829                                                   | 103.933                                               |
|                                                                                    |                                                                               |         |             |                                                           | -76.730                                               |
| 1400                                                                               |                                                                               | 108.575 | 353.824     | 271.831                                                   | 114.790                                               |
|                                                                                    |                                                                               |         |             |                                                           | -68.322                                               |
| 1500                                                                               |                                                                               | 108.575 | 361.151     | 277.550                                                   | 125.648                                               |
|                                                                                    |                                                                               |         |             |                                                           | -179.855                                              |

## Enthalpy of Formation

$\Delta_f H^\circ(\text{PbI}_3, l, 298.15 \text{ K})$  is calculated from  $\Delta_f H^\circ(\text{PbI}_2, cr, 298.15 \text{ K})$  by adding  $\Delta_{\text{ins}} H^\circ$  and the difference in the enthalpy,  $H^\circ(683 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and the liquid.  $\Delta_f H^\circ(l) = \text{PbI}_2(l) + \text{I}(g) = \text{PbI}_3(l)$  as reported by Murgulescu *et al.*<sup>1</sup> can also be obtained from a 2nd and 3rd law analysis of emf data for the cell reaction  $\text{Pb}(l) + \text{I}(g) = \text{PbI}_3(l)$  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  $\Delta_f H^\circ(\text{Pb}, l, 298.15 \text{ K}) = 1.025 \text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta_f H^\circ(\text{I}_2, g, 298.15 \text{ K}) = 41.70 \text{ kcal}\cdot\text{mol}^{-1}$  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 Elhardt<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 Elhardt 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.

$S^\circ(\text{PbI}_2, l, 298.15 \text{ K})$  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  $\text{PbI}_2(cr) = \text{PbI}_2(g)$ .  $\Delta_{\text{vap}} H^\circ = 28.34 \text{ kcal}\cdot\text{mol}^{-1}$  is calculated as the difference between  $\Delta_f H^\circ$  at  $T_{\text{vap}}$  for the gas and the liquid.

## References

- Murgulescu, S., Sternberg, and M. Terzi, *Electrochim. Acta* **12**, 1121 (1967).
- JANAF Thermochemical Tables:  $\text{PbI}_2$ , 3–31–62,  $\text{I}(g)$ , 9–30–61.
- O. Elhardt, *Wied. Ann.* **24**, 215 (1885).
- C. W. Linsey, Ph.D. Dissertation, North Texas State University, (1970).

 $\text{I}_2\text{Pb}_1(l)$  $M_r = 461.0090$  Lead Iodide ( $\text{PbI}_2$ )

| $\Delta_f H^\circ(298.15 \text{ K}) = [ -157.679 ] \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_{\text{ins}} H^\circ = 23.430 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$ | $T/K$   | $C_p^\circ$ | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ | Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$ |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|---------|-------------|-----------------------------------------------------------|-------------------------------------------------------|
|                                                                                    |                                                                               |         |             | $H^\circ - H^\circ(T_r)/T$                                | $H^\circ - H^\circ(T_r)$                              |
|                                                                                    |                                                                               |         |             | $S^\circ - [G^\circ - H^\circ(T_r)]/T$                    | $\Delta_f G^\circ$                                    |
| 0                                                                                  |                                                                               |         |             |                                                           |                                                       |
| 100                                                                                |                                                                               | 298.15  | 77.571      | 198.902                                                   | 0.                                                    |
| 200                                                                                |                                                                               |         |             |                                                           | -157.679                                              |
|                                                                                    |                                                                               |         |             |                                                           | -163.038                                              |
| 300                                                                                |                                                                               | 77.613  | 199.382     | 198.904                                                   | 0.144                                                 |
|                                                                                    |                                                                               |         |             |                                                           | -157.686                                              |
| 400                                                                                |                                                                               | 78.836  | 221.912     | 201.967                                                   | 0.798                                                 |
|                                                                                    |                                                                               |         |             |                                                           | -174.219                                              |
| 450                                                                                | 0.000                                                                         | 79.592  | 232.980     | 205.306                                                   | 12.730                                                |
|                                                                                    |                                                                               |         |             |                                                           | GLASS $\leftrightarrow$ LIQUID                        |
| 460                                                                                | 0.000                                                                         | 108.575 | 232.980     | 205.306                                                   | 12.730                                                |
|                                                                                    |                                                                               |         |             |                                                           | TRANSITION                                            |
| 500                                                                                |                                                                               | 108.575 | 242.033     | 207.867                                                   | 17.073                                                |
|                                                                                    |                                                                               |         |             |                                                           | -157.655                                              |
| 600                                                                                |                                                                               | 108.575 | 261.829     | 215.278                                                   | 27.930                                                |
|                                                                                    |                                                                               |         |             |                                                           | -146.357                                              |
| 683                                                                                | 0.000                                                                         | 108.575 | 275.896     | 221.808                                                   | 36.942                                                |
|                                                                                    |                                                                               |         |             |                                                           | -146.357                                              |
| 700                                                                                |                                                                               | 108.575 | 278.565     | 223.154                                                   | 38.788                                                |
|                                                                                    |                                                                               |         |             |                                                           | -134.959                                              |
| 800                                                                                |                                                                               | 108.575 | 293.064     | 231.007                                                   | 49.645                                                |
|                                                                                    |                                                                               |         |             |                                                           | -124.137                                              |
| 900                                                                                |                                                                               | 108.575 | 305.852     | 238.627                                                   | 60.503                                                |
|                                                                                    |                                                                               |         |             |                                                           | -113.825                                              |
| 1000                                                                               |                                                                               | 108.575 | 317.291     | 245.931                                                   | 71.360                                                |
|                                                                                    |                                                                               |         |             |                                                           | -103.468                                              |
| 1100                                                                               |                                                                               | 108.575 | 327.640     | 252.896                                                   | 82.218                                                |
|                                                                                    |                                                                               |         |             |                                                           | -96.290                                               |
| 1200                                                                               |                                                                               | 108.575 | 337.087     | 259.524                                                   | 93.075                                                |
|                                                                                    |                                                                               |         |             |                                                           | -85.455                                               |
| 1300                                                                               |                                                                               | 108.575 | 345.778     | 265.829                                                   | 103.933                                               |
|                                                                                    |                                                                               |         |             |                                                           | -76.730                                               |
| 1400                                                                               |                                                                               | 108.575 | 353.824     | 271.831                                                   | 114.790                                               |
|                                                                                    |                                                                               |         |             |                                                           | -68.322                                               |
| 1500                                                                               |                                                                               | 108.575 | 361.151     | 277.550                                                   | 125.648                                               |
|                                                                                    |                                                                               |         |             |                                                           | -179.855                                              |

 $\text{I}_2\text{Pb}_1(l)$  $M_r = 461.0090$  Lead Iodide ( $\text{PbI}_2$ ) $T_{\text{ins}} = 683 \pm 2 \text{ K}$ 

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## CRYSTAL-LIQUID

Lead Iodide ( $\text{PbI}_2$ ) $M_r = 461.0090$  Lead Iodide ( $\text{PbI}_2$ )

0 to 683 K crystal  
above 683 K liquid

Refer to the individual tables for details.

| T/K     | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$    |                                                           |             | Standard State Pressure = $p' = 0.1\text{ MPa}$ |                                                 |                                                 |
|---------|-------------------------------------------------------------|-----------------------------------------------------------|-------------|-------------------------------------------------|-------------------------------------------------|-------------------------------------------------|
|         | $C_p^*$<br>$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $S^*$<br>$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $-G^*(T)/T$ | $H^*(T)/T$                                      | $\Delta_H^*$<br>$\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta_G^*$<br>$\text{kJ}\cdot\text{mol}^{-1}$ |
| 0       | 0                                                           | 0                                                         | INFINITE    | -19.501                                         | -174.817                                        | INFINITE                                        |
| 100     | 69.789                                                      | 93.717                                                    | 242.169     | -14.839                                         | -174.972                                        | 91.182                                          |
| 200     | 75.396                                                      | 144.332                                                   | 181.860     | -7.506                                          | -175.096                                        | 45.474                                          |
| 298.15  | 77.573                                                      | 174.836                                                   | 174.836     | 0                                               | -175.393                                        | -174.116                                        |
| 300     | 77.613                                                      | 175.316                                                   | 174.838     | 0.144                                           | -175.400                                        | -173.577                                        |
| 400     | 78.856                                                      | 197.846                                                   | 177.901     | 7.978                                           | -191.933                                        | -173.566                                        |
| 500     | 80.391                                                      | 215.574                                                   | 183.723     | 15.925                                          | -234.996                                        | -172.328                                        |
| 600     | 83.713                                                      | 230.498                                                   | 190.305     | 24.116                                          | -163.287                                        | 22.504                                          |
| 683.000 | 87.780                                                      | 241.591                                                   | 195.872     | 233.448                                         | -149.087                                        | 17.059                                          |
| 683.000 | 108.575                                                     | 275.896                                                   | 195.872     | 312.226                                         | —                                               | 12979                                           |
| 700     | 108.575                                                     | 278.565                                                   | 197.848     | 56.502                                          | -212.652                                        | -134.959                                        |
| 800     | 108.575                                                     | 293.064                                                   | 208.864     | 67.359                                          | -124.137                                        | 8.105                                           |
| 900     | 108.575                                                     | 305.852                                                   | 218.944     | 78.217                                          | -208.591                                        | -113.825                                        |
| 1000    | 108.575                                                     | 317.291                                                   | 228.217     | 89.074                                          | -204.509                                        | 6.606                                           |
| 1100    | 108.575                                                     | 327.640                                                   | 236.792     | -203.468                                        | -103.969                                        | 5.311                                           |
| 1200    | 108.575                                                     | 337.087                                                   | 244.762     | 99.932                                          | -196.290                                        | 4.489                                           |
| 1300    | 108.575                                                     | 345.778                                                   | 252.203     | 110.789                                         | -192.159                                        | -85.455                                         |
| 1400    | 108.575                                                     | 353.824                                                   | 259.178     | 121.647                                         | -188.028                                        | 3.720                                           |
| 1500    | 108.575                                                     | 361.315                                                   | 265.740     | 132.504                                         | -183.970                                        | 3.083                                           |

PREVIOUS

CURRENT: December 1973

Lead Iodide ( $\text{PbI}_2$ ) $I_2\text{PbI}_3(\text{cr},l)$

## NIST-JANAF THERMOCHEMICAL TABLES

 $I_2Pb_2(g)$  $M_f = 461.0090$  Lead Iodide ( $PbI_2$ )

|  |  | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$                                                |           |                                                                                   |                                 | Standard State Pressure = $p^* = 0.1\text{ MPa}$                                   |                                 |                                                |            |
|--|--|---------------------------------------------------------------------------------------------------------|-----------|-----------------------------------------------------------------------------------|---------------------------------|------------------------------------------------------------------------------------|---------------------------------|------------------------------------------------|------------|
|  |  | $\Delta_f H^\circ(298.15\text{ K}) = [359.532 \pm 8.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ |           | $\Delta_f H^\circ(298.15\text{ K}) = 1.16 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$ |                                 | $\Delta_f H^\circ(298.15\text{ K}) = -3.18 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$ |                                 | $\Delta_f G^\circ = -G^\circ - H^\circ(T_r)/T$ |            |
|  |  | $T/K$                                                                                                   | $C^\circ$ | $S^\circ - (G^\circ - H^\circ(T_r))/T$                                            | $\text{kJ}\cdot\text{mol}^{-1}$ | $H^\circ - H^\circ(T)$                                                             | $\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta_f G^\circ$                             | $\log K_r$ |
|  |  | 0                                                                                                       | 0.        | 0.                                                                                | INFINITE                        | -15.736                                                                            | 1.161                           | 1.161                                          | INFINITE   |
|  |  | 100                                                                                                     | 53.807    | 298.094                                                                           | 410.195                         | 0.070                                                                              | -19.157                         | -19.157                                        | 10.007     |
|  |  | 200                                                                                                     | 56.934    | 336.667                                                                           | 364.806                         | -5.628                                                                             | -38.492                         | -38.492                                        | 10.053     |
|  |  | 250                                                                                                     | 57.375    | 349.424                                                                           | 360.499                         | -2.769                                                                             | -47.741                         | -47.741                                        | 9.975      |
|  |  | 298.15                                                                                                  | 57.615    | 359.552                                                                           | 359.552                         | 0.                                                                                 | -3.180                          | -56.437                                        | 9.888      |
|  |  | 300                                                                                                     | 57.622    | 359.908                                                                           | 359.553                         | 0.107                                                                              | -3.224                          | -56.767                                        | 9.884      |
|  |  | 350                                                                                                     | 57.773    | 368.803                                                                           | 360.255                         | 2.992                                                                              | -4.504                          | -65.593                                        | 9.789      |
|  |  | 400                                                                                                     | 57.872    | 376.524                                                                           | 361.817                         | 5.883                                                                              | -21.814                         | -13.681                                        | 9.622      |
|  |  | 450                                                                                                     | 57.940    | 383.345                                                                           | 363.837                         | 8.778                                                                              | -24.349                         | -80.012                                        | 9.288      |
|  |  | 500                                                                                                     | 57.989    | 389.452                                                                           | 366.099                         | 11.677                                                                             | -67.031                         | -82.262                                        | 8.594      |
|  |  | 600                                                                                                     | 58.054    | 400.031                                                                           | 370.899                         | 17.479                                                                             | -67.872                         | -85.230                                        | 7.420      |
|  |  | 700                                                                                                     | 58.092    | 408.983                                                                           | 375.717                         | 23.387                                                                             | -73.654                         | -87.253                                        | 6.511      |
|  |  | 800                                                                                                     | 58.118    | 416.742                                                                           | 380.371                         | 29.097                                                                             | -74.639                         | -89.128                                        | 5.819      |
|  |  | 900                                                                                                     | 58.135    | 423.588                                                                           | 384.800                         | 34.910                                                                             | -75.602                         | -90.882                                        | 5.275      |
|  |  | 1000                                                                                                    | 58.148    | 429.714                                                                           | 388.790                         | 40.724                                                                             | -76.545                         | -92.529                                        | 4.833      |
|  |  | 1100                                                                                                    | 58.157    | 435.257                                                                           | 392.948                         | 46.539                                                                             | -77.469                         | -94.082                                        | 4.468      |
|  |  | 1200                                                                                                    | 58.164    | 440.317                                                                           | 396.688                         | 52.355                                                                             | -78.380                         | -95.552                                        | 4.159      |
|  |  | 1300                                                                                                    | 58.169    | 444.973                                                                           | 400.226                         | 58.172                                                                             | -79.250                         | -96.946                                        | 3.895      |
|  |  | 1400                                                                                                    | 58.174    | 449.284                                                                           | 403.578                         | 63.989                                                                             | -80.222                         | -98.270                                        | 3.666      |
|  |  | 1500                                                                                                    | 58.177    | 453.298                                                                           | 406.760                         | 69.807                                                                             | -81.196                         | -99.525                                        | 3.466      |
|  |  | 1600                                                                                                    | 58.180    | 459.053                                                                           | 409.787                         | 75.625                                                                             | -82.228                         | -100.714                                       | 3.288      |
|  |  | 1700                                                                                                    | 58.182    | 460.580                                                                           | 412.672                         | 81.443                                                                             | -83.331                         | -101.836                                       | 3.129      |
|  |  | 1800                                                                                                    | 58.184    | 463.906                                                                           | 415.427                         | 87.261                                                                             | -84.515                         | -102.890                                       | 2.986      |
|  |  | 1900                                                                                                    | 58.186    | 467.052                                                                           | 418.062                         | 93.080                                                                             | -85.787                         | -103.877                                       | 2.856      |
|  |  | 2000                                                                                                    | 58.188    | 470.036                                                                           | 420.587                         | 98.898                                                                             | -87.149                         | -104.794                                       | 2.737      |
|  |  | 2100                                                                                                    | 58.189    | 472.875                                                                           | 423.010                         | 104.717                                                                            | -265.820                        | -98.526                                        | 2.451      |
|  |  | 2200                                                                                                    | 58.190    | 475.822                                                                           | 425.338                         | 110.536                                                                            | -266.964                        | -90.534                                        | 2.150      |
|  |  | 2300                                                                                                    | 58.191    | 480.645                                                                           | 427.580                         | 116.355                                                                            | -268.251                        | -82.486                                        | 1.873      |
|  |  | 2400                                                                                                    | 58.192    | 482.169                                                                           | 429.739                         | 122.174                                                                            | -269.674                        | -74.379                                        | 1.619      |
|  |  | 2500                                                                                                    | 58.192    | 483.021                                                                           | 431.823                         | 127.993                                                                            | -271.222                        | -66.210                                        | 1.383      |
|  |  | 2600                                                                                                    | 58.193    | 483.837                                                                           | 433.837                         | 133.813                                                                            | -272.882                        | -57.977                                        | 1.165      |
|  |  | 2700                                                                                                    | 58.194    | 487.499                                                                           | 435.784                         | 139.632                                                                            | -274.641                        | -49.678                                        | 0.961      |
|  |  | 2800                                                                                                    | 58.194    | 489.616                                                                           | 437.669                         | 145.451                                                                            | -276.484                        | -41.313                                        | 0.771      |
|  |  | 2900                                                                                                    | 58.195    | 491.658                                                                           | 439.496                         | 151.271                                                                            | -278.395                        | -32.881                                        | 0.592      |
|  |  | 3000                                                                                                    | 58.195    | 493.631                                                                           | 441.267                         | 157.990                                                                            | -280.359                        | -24.381                                        | 0.425      |
|  |  | 3100                                                                                                    | 58.195    | 497.539                                                                           | 442.987                         | 162.910                                                                            | -292.362                        | -16.816                                        | 0.266      |
|  |  | 3200                                                                                                    | 58.196    | 497.387                                                                           | 444.659                         | 168.729                                                                            | -284.390                        | -7.185                                         | 0.117      |
|  |  | 3300                                                                                                    | 58.196    | 499.177                                                                           | 446.284                         | 174.549                                                                            | -286.430                        | 1.509                                          | 0.024      |
|  |  | 3400                                                                                                    | 58.196    | 500.915                                                                           | 447.865                         | 180.368                                                                            | -288.470                        | 1.265                                          | 0.024      |
|  |  | 3500                                                                                                    | 58.197    | 502.602                                                                           | 449.403                         | 186.188                                                                            | -290.498                        | 19.081                                         | 0.285      |
|  |  | 3600                                                                                                    | 58.197    | 504.256                                                                           | 450.906                         | 192.008                                                                            | -292.506                        | 27.954                                         | 0.406      |
|  |  | 3700                                                                                                    | 58.197    | 505.836                                                                           | 452.369                         | 197.827                                                                            | -294.484                        | 36.884                                         | 0.521      |
|  |  | 3800                                                                                                    | 58.197    | 507.388                                                                           | 453.796                         | 203.647                                                                            | -296.425                        | 45.866                                         | 0.630      |
|  |  | 3900                                                                                                    | 58.197    | 508.999                                                                           | 455.190                         | 209.467                                                                            | -298.323                        | 54.898                                         | 0.725      |
|  |  | 4000                                                                                                    | 58.198    | 510.973                                                                           | 456.551                         | 215.287                                                                            | -300.172                        | 63.979                                         | 0.835      |
|  |  | 4100                                                                                                    | 58.198    | 511.810                                                                           | 457.882                         | 221.106                                                                            | -301.969                        | 73.105                                         | 0.931      |
|  |  | 4200                                                                                                    | 58.198    | 513.264                                                                           | 459.182                         | 226.926                                                                            | -303.708                        | 82.274                                         | 1.023      |
|  |  | 4300                                                                                                    | 58.198    | 514.382                                                                           | 460.455                         | 232.746                                                                            | -305.387                        | 91.484                                         | 1.111      |
|  |  | 4400                                                                                                    | 58.198    | 515.320                                                                           | 461.700                         | 238.566                                                                            | -307.805                        | 100.732                                        | 1.196      |
|  |  | 5100                                                                                                    | 58.199    | 524.512                                                                           | 469.746                         | 279.305                                                                            | -316.525                        | 166.362                                        | 1.074      |
|  |  | 4500                                                                                                    | 58.198    | 518.98                                                                            | 517.728                         | 345.807                                                                            | -348.359                        | 110.539                                        | 1.277      |
|  |  | 4700                                                                                                    | 58.198    | 526.551                                                                           | 471.835                         | 425.193                                                                            | -311.048                        | 129.335                                        | 1.335      |
|  |  | 4800                                                                                                    | 58.199    | 519.758                                                                           | 465.285                         | 250.205                                                                            | -316.025                        | 128.637                                        | 1.430      |
|  |  | 5000                                                                                                    | 58.199    | 520.984                                                                           | 466.433                         | 261.845                                                                            | -317.655                        | 138.065                                        | 1.502      |
|  |  | 5200                                                                                                    | 58.199    | 522.184                                                                           | 467.538                         | 267.665                                                                            | -314.127                        | 147.472                                        | 1.572      |
|  |  | 5300                                                                                                    | 58.199    | 523.359                                                                           | 468.662                         | 273.483                                                                            | -315.357                        | 156.904                                        | 1.639      |
|  |  | 5400                                                                                                    | 58.199    | 524.520                                                                           | 469.792                         | 285.566                                                                            | -307.805                        | 100.732                                        | 1.196      |
|  |  | 5500                                                                                                    | 58.199    | 525.682                                                                           | 471.920                         | 284.386                                                                            | -308.559                        | 110.539                                        | 1.277      |
|  |  | 5700                                                                                                    | 58.199    | 530.985                                                                           | 475.838                         | 279.305                                                                            | -316.525                        | 166.362                                        | 1.074      |
|  |  | 5800                                                                                                    | 58.199    | 531.997                                                                           | 476.817                         | 320.044                                                                            | -322.284                        | 222.518                                        | 20.48      |
|  |  | 5900                                                                                                    | 58.199    | 532.992                                                                           | 477.761                         | 323.100                                                                            | -323.052                        | 233.100                                        | -2.099     |
|  |  | 6000                                                                                                    | 58.199    | 533.970                                                                           | 478.690                         | 331.684                                                                            | -324.442                        | 242.695                                        | -2.149     |
|  |  |                                                                                                         |           |                                                                                   |                                 |                                                                                    |                                 | 252.302                                        | -2.196     |

CURRENT December 1973 (1 atm)

 $I_2Pb_2(g)$ Lead Iodide ( $PbI_2$ ) $I_2Pb_2(g)$ 

| Source                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     | Reaction | Data Points | $T/K$    | $\Delta_f H^\circ$ , kcal·mol <sup>-1</sup> | Drift, kcal·mol <sup>-1</sup> | $\Delta_f H^\circ(PbI_2, g, 298.15\text{ K})$ , kcal·mol <sup>-1</sup> |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------|-------------|----------|---------------------------------------------|-------------------------------|------------------------------------------------------------------------|
| Niwa <i>et al.</i> <sup>1</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | A        | 7           | 579.650  | 39.77 ± 0.37                                | 2.9 ± 0.60                    | 0.38                                                                   |
| Duncan and Thomas <sup>2</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | A        | 13          | 563.613  | 39.44 ± 0.40                                | 40.24 ± 0.09                  | 1.4 ± 0.7                                                              |
| Jellinek and Ruder <sup>3</sup>                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | B        | 4           | 923.1073 | 35.19 ± 0.52                                | 37.49 ± 0.32                  | 2.3 ± 0.6                                                              |
| Product of the moments of inertia are: $I_A = 67.3005 \times 10^{-39}$ , $I_B = 178.3336 \times 10^{-39}$ and $I_C = 245.6341 \times 10^{-39}$ g·cm <sup>2</sup> .                                                                                                                                                                                                                                                                                                                                         |          |             |          |                                             |                               |                                                                        |
| *Reactions: (A) $PbI_4(\text{cr}) = PbI_2(\text{g}) + PbI_2(\text{g})$ (B) $PbI_4(\text{g}) = PbI_2(\text{g})$                                                                                                                                                                                                                                                                                                                                                                                             |          |             |          |                                             |                               |                                                                        |
| <b>Heat Capacity and Entropy</b><br>Molecular dimensions are those given by Sutton. <sup>5</sup> Vibrational frequencies are estimated by comparison with the corresponding values for $HgI_2(g)$ and with the lead dihalide series. The electronic ground state is assumed to be $A_1$ based on analogy with $PbCl_2(g)$ . <sup>6</sup> The principal moments of inertia are: $I_A = 67.3005 \times 10^{-39}$ , $I_B = 178.3336 \times 10^{-39}$ and $I_C = 245.6341 \times 10^{-39}$ g·cm <sup>2</sup> . |          |             |          |                                             |                               |                                                                        |
| <b>References</b><br><sup>1</sup> K. Niva, M. Sato, and M. Yoshiyama, <i>J. Chem. Soc. Japan</i> <b>60</b> , 918 (1939).<br><sup>2</sup> J. F. Duncan and F. G. Thomas, <i>J. Chem. Soc.</i> <b>1964</b> , 360 (1964).<br><sup>3</sup> K. Jellinek and A. Ruder, <i>Z. physik. Chem.</i> <b>143</b> , 55 (1929).<br><sup>4</sup> JANAF Thermochemical Tables: $PbI_2(\text{cr})$ , 12-31-73; $PbF_4(\text{g})$ , 3-31-62; $Pb_6Cl_6(\text{g})$ , 6-30-73;<br>$PbBr_4(\text{g})$ , 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).                                                                                                                                                                                                                                                                                                                                                           |          |             |          |                                             |                               |                                                                        |
| <sup>6</sup> L. E. Sutton, Ed., "Tables of Interatomic Distances and Configuration in Molecules and Ions," The Chemical Society, London, (1958).                                                                                                                                                                                                                                                                                                                                                           |          |             |          |                                             |                               |                                                                        |

## IDEAL GAS

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

$$\Delta H^{\circ}(0 \text{ K}) = 95.09 \pm 8.4 \text{ kJ mol}^{-1}$$

$$\Delta H^{\circ}(298.15 \text{ K}) = [320.972 \pm 4.2] \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta H^{\circ}(0 \text{ K}) = 95.09 \pm 8.4 \text{ kJ mol}^{-1}$$

|  | $\Delta H^{\circ}$ (0 K) | $\Delta H^{\circ}$ (298.15 K) | $\Delta H^{\circ}$ (T) | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |
|--|--------------------------|-------------------------------|------------------------|-----------------------------------------------------------|---------------------------------------------------|
|  | $\Delta H^{\circ}$ (0 K) | $\Delta H^{\circ}$ (298.15 K) | $\Delta H^{\circ}$ (T) | $\Delta H^{\circ}$ (T)                                    | $\Delta H^{\circ}$ (T)                            |

| Electronic Levels and Quantum Weights    |                            |
|------------------------------------------|----------------------------|
| State                                    | $\epsilon, \text{cm}^{-1}$ |
| [A <sub>1</sub> ]                        | 0                          |
| [B <sub>1</sub> ]                        | [20000]                    |
|                                          | [3]                        |
| Vibrational Frequencies and Degeneracies |                            |
| v, 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]<sup>o</sup>Product of the Moments of Inertia  $I_A I_B I_C = [2.419819 \times 10^{-121}] \text{ g}^3 \cdot \text{cm}^6$ 

## 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 SiCH<sub>3</sub>(g) and SiBr<sub>2</sub>(g),<sup>3</sup> there is acceptable agreement between the 3rd law results of these two studies. Using the mean  $\Delta H^{\circ}(298.15 \text{ K})$ , we calculate and adopt  $\Delta H^{\circ}(\text{SiI}_2, \text{g}, 298.15 \text{ K}) = 20.84 \text{ kcal mol}^{-1}$  and an average bond energy of 67.6 kcal mol<sup>-1</sup>. This corresponds to  $\Delta_a H^{\circ} = 135.2 \text{ kcal mol}^{-1}$  and an average bond energy of 67.6 kcal mol<sup>-1</sup>. In comparison, the average bond energy of SiI(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.

Source Reaction  $\Delta H^{\circ}(298.15 \text{ K}), \text{ kcal mol}^{-1}$  Drift  $\Delta H^{\circ}(\text{SiI}_2, 298.15 \text{ K})^*$

| Source | Reaction                                           | T/K       | 2nd law | 3rd law | Drift  | $\Delta H^{\circ}(\text{SiI}_2, 298.15 \text{ K})^*$ |
|--------|----------------------------------------------------|-----------|---------|---------|--------|------------------------------------------------------|
| 1      | SiI(g) + SiI(g) + 2I(g)                            | 1361-1526 | 98.92   | 101.04  | 1.46   | 23.60                                                |
| 2      | Si(cr) + I <sub>2</sub> (g) = SiI <sub>2</sub> (g) | 1300-1470 | 3.21    | 5.14    | 1.38   | 20.50                                                |
| 4      | SiI(g) + Si(cr) = 2SiI <sub>2</sub> (g)            | 1173-1373 | 83.90   | 68.09   | -12.42 | 20.84                                                |

\*Based on 3rd law  $\Delta H^{\circ}(298.15 \text{ K})$  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  $\Delta H^{\circ}(\text{SiI}_2, \text{g}, 298.15 \text{ K}) = 20.84 \text{ kcal mol}^{-1}$  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>3</sub>I<sub>3</sub>.<sup>5</sup> The bond angle is estimated to be 113° based on the trend observed in SiF<sub>2</sub>, SiCl<sub>3</sub>, and SiBr<sub>2</sub>.<sup>3</sup> C<sub>2v</sub> symmetry is also assumed to be consistent with the other three silicon dihalides. The principal moments of inertia are  $I_A = 7.6158 \times 10^{-39}$ ,  $I_B = 174.4841 \times 10^{-39}$ , and  $I_C = 182.0999 \times 10^{-39}$ . The vibrational frequencies are estimated based on trends observed in the SiX<sub>2</sub> and SiH<sub>2</sub>X<sub>3</sub> species, where X = F, Cl, Br, and I. As suggested by SiF<sub>2</sub> and SiCl<sub>3</sub>, an electronic excited state is included at 20000 cm<sup>-1</sup>.

## References

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

PREVIOUS December 1977 (1 atm)

CURRENT December 1977 (1 bar)

|  | T/K    | C <sub>p</sub> | S <sup>o</sup> | -[G <sup>o</sup> - H <sup>o</sup> (T)]/T | H <sup>o</sup> - H <sup>o</sup> (T) | $\Delta H^{\circ}$ | $\Delta G^{\circ}$ | log K <sub>r</sub> |
|--|--------|----------------|----------------|------------------------------------------|-------------------------------------|--------------------|--------------------|--------------------|
|  | 0      | 0              | 0              | 0                                        | 0                                   | -13.792            | 95.090             | INFINITE           |
|  | 100    | 43.279         | 266.948        | 367.003                                  | -10.006                             | 93.561             | 75.348             | -39.358            |
|  | 200    | 51.344         | 299.763        | 325.833                                  | -5.224                              | 92.231             | 55.603             | -14.522            |
|  | 250    | 53.375         | 311.456        | 321.865                                  | -2.602                              | 93.375             | 46.042             | -9.620             |
|  | 298.15 | 54.624         | 320.972        | 320.972                                  | 0                                   | 92.466             | 37.008             | -6.484             |
|  | 300    | 54.663         | 321.310        | 321.973                                  | 0.101                               | 92.430             | 36.664             | -6.384             |
|  | 350    | 55.512         | 329.804        | 321.641                                  | 2.857                               | 91.339             | 27.452             | -4.097             |
|  | 400    | 56.096         | 337.257        | 323.137                                  | 5.648                               | 74.217             | 18.952             | -2.475             |
|  | 450    | 56.512         | 343.889        | 325.081                                  | 8.464                               | 71.875             | 12.184             | -1.414             |
|  | 500    | 56.817         | 349.860        | 327.666                                  | 11.297                              | 29.392             | 9.477              | -0.950             |
|  | 600    | 57.226         | 360.259        | 331.923                                  | 17.001                              | 28.966             | 5.533              | -0.482             |
|  | 700    | 57.478         | 369.100        | 336.618                                  | 22.737                              | 28.486             | 1.665              | -0.124             |
|  | 800    | 57.644         | 341.170        | 328.494                                  | 34.171                              | 27.955             | -2.131             | 0.139              |
|  | 900    | 57.759         | 383.584        | 345.512                                  | 34.265                              | 27.373             | -5.858             | 0.340              |
|  | 1000   | 57.842         | 369.674        | 349.629                                  | 40.045                              | 26.741             | -9.517             | 0.497              |
|  | 1100   | 57.904         | 395.190        | 353.524                                  | 45.832                              | 26.057             | -13.110            | 0.623              |
|  | 1200   | 57.951         | 400.120        | 357.209                                  | 51.625                              | 25.318             | -16.638            | 0.724              |
|  | 1300   | 57.988         | 404.870        | 360.699                                  | 57.422                              | 24.519             | -20.103            | 0.828              |
|  | 1400   | 58.017         | 409.169        | 364.010                                  | 63.222                              | 23.650             | -23.503            | 0.935              |
|  | 1500   | 58.040         | 413.170        | 367.155                                  | 69.025                              | 22.701             | -26.838            | 0.935              |
|  | 1600   | 58.060         | 416.919        | 370.150                                  | 74.830                              | 21.663             | -30.108            | 0.983              |
|  | 1700   | 58.076         | 420.439        | 373.005                                  | 80.637                              | 20.651             | -32.862            | 1.010              |
|  | 1800   | 58.090         | 423.759        | 375.734                                  | 86.445                              | 20.063             | -33.022            | 0.938              |
|  | 1900   | 58.104         | 426.900        | 378.345                                  | 92.255                              | 19.173             | -33.124            | 0.911              |
|  | 2000   | 58.113         | 429.881        | 380.848                                  | 98.066                              | 18.892             | -33.167            | 0.866              |
|  | 2100   | 58.124         | 432.716        | 383.251                                  | 103.878                             | 17.730             | -34.108            | 0.825              |
|  | 2200   | 58.135         | 435.470        | 385.561                                  | 109.697                             | 15.595             | -35.385            | 0.785              |
|  | 2300   | 58.147         | 438.005        | 387.785                                  | 115.505                             | 13.716             | -36.716            | 0.748              |
|  | 2400   | 58.160         | 440.480        | 389.920                                  | 121.320                             | 13.090             | -32.942            | 0.713              |
|  | 2500   | 58.176         | 442.854        | 392.000                                  | 127.137                             | 12.497             | -32.497            | 0.679              |
|  | 2600   | 58.195         | 445.156        | 394.000                                  | 132.955                             | 12.925             | -32.189            | 0.647              |
|  | 2700   | 58.218         | 447.333        | 395.935                                  | 138.776                             | 12.560             | -31.825            | 0.616              |
|  | 2800   | 58.245         | 449.451        | 397.808                                  | 144.599                             | 12.196             | -31.409            | 0.586              |
|  | 2900   | 58.278         | 451.495        | 399.625                                  | 150.423                             | 12.047             | -30.942            | 0.557              |
|  | 3000   | 58.317         | 453.472        | 401.387                                  | 156.255                             | 16.604             | -30.426            | 0.530              |
|  | 3100   | 58.363         | 455.385        | 403.098                                  | 162.089                             | 15.937             | -30.046            | 0.503              |
|  | 3200   | 58.416         | 457.238        | 406.379                                  | 167.928                             | 15.231             | -29.864            | 0.478              |
|  | 3300   | 58.477         | 459.037        | 406.379                                  | 173.779                             | 15.048             | -28.614            | 0.453              |
|  | 3400   | 58.540         | 460.784        | 407.933                                  | 179.623                             | 15.762             | -27.931            | 0.429              |
|  | 3500   | 58.624         | 462.482        | 409.487                                  | 185.482                             | 15.216             | -27.213            | 0.406              |
|  | 3600   | 58.710         | 464.114        | 410.982                                  | 191.349                             | -43.158            | -16.002            | 0.232              |
|  | 3700   | 58.805         | 465.744        | 412.440                                  | 197.224                             | -43.768            | -4.267             | 0.050              |
|  | 3800   | 58.909         | 467.314        | 413.864                                  | 193.311                             | -43.942            | -4.410             | -0.103             |
|  | 3900   | 59.020         | 467.890        | 414.761                                  | 193.314                             | -43.979            | -4.410             | -0.145             |
|  | 4000   | 59.143         | 470.341        | 416.613                                  | 214.915                             | -40.190            | 31.023             | -1.156             |
|  | 4100   | 59.273         | 471.803        | 417.941                                  | 220.835                             | -40.523            | 42.808             | -1.263             |
|  | 4200   | 59.411         | 473.233        | 419.241                                  | 226.745                             | -40.785            | 46.600             | -1.679             |
|  | 4300   | 59.557         | 474.633        | 420.513                                  | 232.718                             | -40.976            | 46.397             | -0.807             |
|  | 4400   | 59.710         | 475.979        | 421.758                                  | 238.681                             | -41.166            | 47.000             | -0.928             |
|  | 4500   | 59.870         | 477.348        | 422.979                                  | 244.660                             | -41.415            | 49.001             | -1.045             |
|  | 4600   | 60.036         | 478.665        | 424.175                                  | 250.655                             | -41.124            | 50.804             | -1.156             |
|  | 4700   | 60.208         | 480.938        | 425.348                                  | 256.667                             | -44.034            | 51.024             | -1.263             |
|  | 4800   | 60.385         | 481.228        | 426.533                                  | 262.657                             | -44.877            | 51.606             | -1.365             |
|  | 4900   | 60.567         | 482.475        | 427.459                                  | 268.745                             | -45.607            | 52.201             | -1.463             |
|  | 5000   | 60.753         | 483.700        | 428.738                                  | 274.811                             | -46.363            | 53.566             | -1.556             |
|  | 5100   | 60.943         | 484.905        | 429.827                                  | 280.896                             | -46.010            | 54.774             | -1.647             |
|  | 5200   | 61.135         | 486.090        | 430.898                                  | 286.999                             | -46.744            | 56.774             | -1.733             |
|  | 5300   | 61.330         | 487.257        | 431.950                                  | 293.123                             | -47.417            | 58.117             | -1.817             |
|  | 5400   | 61.526         | 488.403        | 432.985                                  | 299.365                             | -48.871            | 59.594             | -1.897             |
|  | 5500   | 61.723         | 489.536        | 434.003                                  | 305.428                             | -49.876            | 60.774             | -1.974             |
|  | 5600   | 61.920         | 490.650        | 435.005                                  | 311.610                             | -43.735            | 219.560            | -2.048             |
|  | 5700   | 62.118         | 491.747        | 435.991                                  | 317.812                             | -43.630            | 231.824            | -2.119             |
|  | 5800   | 62.315         | 492.820        | 436.961                                  | 324.034                             | -43.587            | 242.995            | -2.188             |
|  | 5900   | 62.511         | 493.896        | 437.917                                  | 330.275                             | -43.504            | 254.693            | -2.255             |
|  | 6000   | 62.705         | 494.948        | 438.859                                  | 336.536                             | -43.426            | 266.376            | -2.319             |

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

## NIST-JANAF THERMOCHEMICAL TABLES

Strontium Iodide ( $\text{SrI}_2$ )

## CRYSTAL

 $\text{I}_2\text{SrI}_2(\text{cr})$  $M_r = 341.4290$  Strontium Iodide ( $\text{SrI}_2$ )

|        | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$                        |                                                                                       |                                                                                |                                                                                          | Standard State Pressure = $P^* = 0.1 \text{ MPa}$                                |                                                                                       |                                                                                |                                                                                          |
|--------|----------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|--------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|--------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
|        | $\Delta_f H^\circ(0 \text{ K}) = -560.65 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_f H^\circ(298.15 \text{ K}) = -561.49 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_{\text{fus}} H^\circ = 19.665 \pm 0.38 \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_{\text{sub}} H^\circ(298.15 \text{ K}) = 286.604 \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_f H^\circ(0 \text{ K}) = -560.65 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_f H^\circ(298.15 \text{ K}) = -561.49 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_{\text{fus}} H^\circ = 19.665 \pm 0.38 \text{ kJ}\cdot\text{mol}^{-1}$ | $\Delta_{\text{sub}} H^\circ(298.15 \text{ K}) = 286.604 \text{ kJ}\cdot\text{mol}^{-1}$ |
|        | $T/K$                                                                            | $C_p^\circ$                                                                           | $S^\circ$                                                                      | $-G^\circ - H^\circ(T)/T$                                                                | $H^\circ - H^\circ(T)$                                                           | $k\text{J}\cdot\text{mol}^{-1}$                                                       | $\Delta G^\circ$                                                               |                                                                                          |
| 298.15 | 100                                                                              | 0                                                                                     | 0                                                                              | INFINITE                                                                                 | -18.919                                                                          | -560.645                                                                              | -560.645                                                                       |                                                                                          |
|        | 200                                                                              | 67.404                                                                                | 78.914                                                                         | 226.165                                                                                  | -14.725                                                                          | -561.001                                                                              | -559.988                                                                       |                                                                                          |
|        |                                                                                  | 75.019                                                                                | 128.568                                                                        | 166.164                                                                                  | -7.519                                                                           | -561.216                                                                              | -558.896                                                                       |                                                                                          |
|        | 300                                                                              | 100                                                                                   | 0                                                                              | INFINITE                                                                                 | 0                                                                                | 0                                                                                     | 145.969                                                                        |                                                                                          |
|        |                                                                                  | 75.948                                                                                | 159.120                                                                        | 159.120                                                                                  | 0                                                                                | -561.493                                                                              | -557.702                                                                       |                                                                                          |
|        | 400                                                                              | 130.032                                                                               | 159.603                                                                        | 159.122                                                                                  | 0.144                                                                            | -561.499                                                                              | 97.707                                                                         |                                                                                          |
|        |                                                                                  | 80.751                                                                                | 182.921                                                                        | 162.214                                                                                  | 8.083                                                                            | -557.678                                                                              | 97.100                                                                         |                                                                                          |
|        | 500                                                                              | 150.033                                                                               | 200.737                                                                        | 168.145                                                                                  | 16.296                                                                           | -557.928                                                                              | 72.579                                                                         |                                                                                          |
|        |                                                                                  | 83.513                                                                                | 200.737                                                                        | 216.207                                                                                  | 174.898                                                                          | -620.739                                                                              | -546.142                                                                       |                                                                                          |
|        | 600                                                                              | 160.034                                                                               | 208.994                                                                        | 229.710                                                                                  | 181.784                                                                          | 24.785                                                                                | 57.055                                                                         |                                                                                          |
|        |                                                                                  | 90.994                                                                                | 241.776                                                                        | 188.542                                                                                  | 42.587                                                                           | -616.972                                                                              | 46.262                                                                         |                                                                                          |
|        | 700                                                                              | 170.035                                                                               | 211.755                                                                        | 241.776                                                                                  | 42.587                                                                           | -614.832                                                                              | -502.807                                                                       |                                                                                          |
|        |                                                                                  | 91.755                                                                                | 241.776                                                                        | 188.542                                                                                  | 42.587                                                                           | -614.832                                                                              | 32.830                                                                         |                                                                                          |
|        | 800                                                                              | 180.036                                                                               | 211.755                                                                        | 241.776                                                                                  | 42.587                                                                           | -613.204                                                                              | -488.864                                                                       |                                                                                          |
|        |                                                                                  | 92.048                                                                                | 243.031                                                                        | 189.272                                                                                  | 43.598                                                                           | -610.453                                                                              | 28.373                                                                         |                                                                                          |
|        | 900                                                                              | 190.037                                                                               | 214.492                                                                        | 252.741                                                                                  | 193.5075                                                                         | -610.453                                                                              | -475.194                                                                       |                                                                                          |
|        |                                                                                  | 94.492                                                                                | 252.741                                                                        | 193.5075                                                                                 | 51.899                                                                           | -615.344                                                                              | 24.822                                                                         |                                                                                          |
|        | 1000                                                                             | 200.038                                                                               | 262.339                                                                        | 201.353                                                                                  | 61.486                                                                           | -615.344                                                                              | 21.912                                                                         |                                                                                          |
|        |                                                                                  | 97.236                                                                                | 272.234                                                                        | 207.374                                                                                  | 71.346                                                                           | -612.989                                                                              | -447.557                                                                       |                                                                                          |
|        | 1100                                                                             | 210.039                                                                               | 99.971                                                                         | 281.051                                                                                  | 213.150                                                                          | 81.480                                                                                | 19.482                                                                         |                                                                                          |
|        |                                                                                  | 102.717                                                                               | 281.051                                                                        | 213.150                                                                                  | 218.697                                                                          | 91.891                                                                                | 17.433                                                                         |                                                                                          |
|        | 1200                                                                             | 220.040                                                                               | 102.717                                                                        | 289.382                                                                                  | 218.697                                                                          | -610.380                                                                              | -433.876                                                                       |                                                                                          |
|        |                                                                                  | 95.493                                                                                | 289.382                                                                        | 218.697                                                                                  | 102.578                                                                          | -607.527                                                                              | 15.685                                                                         |                                                                                          |
|        | 1300                                                                             | 230.041                                                                               | 105.493                                                                        | 297.301                                                                                  | 224.031                                                                          | -607.527                                                                              | -420.404                                                                       |                                                                                          |
|        |                                                                                  | 98.246                                                                                | 297.301                                                                        | 224.031                                                                                  | 113.538                                                                          | -604.440                                                                              | -407.144                                                                       |                                                                                          |
|        | 1400                                                                             | 240.042                                                                               | 108.246                                                                        | 304.461                                                                                  | 229.169                                                                          | -604.440                                                                              | 14.178                                                                         |                                                                                          |
|        | 1500                                                                             | 250.043                                                                               | 110.956                                                                        |                                                                                          |                                                                                  |                                                                                       |                                                                                |                                                                                          |

## Heat Capacity and Entropy

$C^\circ(13.9-300.9 \text{ K})$  has been measured by Paukov *et al.*<sup>7</sup> and smoothed values have been published. Starting values of entropy and enthalpy,  $S^\circ(14 \text{ K})$  and  $H^\circ(14 \text{ K})$ , were not given. Our  $T^\circ$  extrapolation leads to  $S^\circ(298.15 \text{ K}) = 0.148 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  and  $H^\circ(8 \text{ K})$  and  $H^\circ(80 \text{ K}) = 0.891 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , which, when combined with our  $C_p^\circ$  extrapolation from 14 K to 8 K and with the Paukov *et al.*<sup>7</sup> data, gives  $S^\circ(298.15 \text{ K}) = 38.03 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  and  $H^\circ(298.15 \text{ K})$ . In as much as our integration of their data gives  $S^\circ(298.15 \text{ K}) = 37.26 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , it appears unlikely that their published value for  $S^\circ(298.15 \text{ K})$  is correct. The low temperature heat capacity joins smoothly with a linear extrapolation from  $C_p^\circ = 18.45 \text{ at } 270 \text{ K}$  to  $C_p^\circ = 22.0 \text{ at the adopted } T_{\text{fus}}$  of 811 K. The linearly extrapolated heat capacity at 298 K is 0.6% higher than the published smoothed value. Dworkin and Bredig<sup>8</sup> determined the heat capacity of the crystal near the melting point to be  $22.9 \pm 5\%$ . The graphically selected  $C_p^\circ(811 \text{ K}) = 22.0$  is within the experimental error and gives  $H^\circ(811 \text{ K}) - H^\circ(298.15 \text{ K}) = 10.42 \text{ kcal}\cdot\text{mol}^{-1}$  in agreement with Dworkin and Bredig's measured value of  $10.4 \text{ kcal}\cdot\text{mol}^{-1}$ .

## Fusion Data

Emons and Loeffelholz<sup>2</sup> determined  $\Delta_{\text{fus}} H^\circ = 4.580 \text{ kcal}\cdot\text{mol}^{-1}$  ( $\pm 5\%$ ) by high temperature cryoscopy, in good agreement with the drop calorimetry  $\Delta_{\text{fus}} H^\circ = 4.70 \text{ kcal}\cdot\text{mol}^{-1}$  ( $\pm 2\%$ ) and  $T_{\text{fus}} = 811 \text{ K}$  by Dworkin and Bredig.<sup>8</sup> Hutchison<sup>10</sup> found  $T_{\text{fus}} = 793 \text{ K}$ , noting that his melting point data were only approximate. Because drop calorimetry is a more direct measure of the enthalpy of melting, we adopt  $\Delta_{\text{fus}} H^\circ = 4.70 \pm 0.09 \text{ kcal}\cdot\text{mol}^{-1}$  at  $T_{\text{fus}} = 811 \pm 10 \text{ K}$ .

## Sublimation Data

$\Delta_{\text{sub}} H^\circ(298.15 \text{ K})$  is derived as the difference between the enthalpies of formation of the ideal gas and the crystal state at 298.15 K.

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1<sub>2</sub>SrI<sub>2</sub>(cr)

CRYSTAL

Strontium Iodide ( $\text{SrI}_2$ )

PREVIOUS:

CURRENT June

NEXT:

LAST

**Strontium Iodide ( $\text{SrI}_2$ )** **$M_r = 341.4290$**  **$I_2\text{Sr}_1(\text{I})$** 

$$\Delta_f H^\circ(298.15 \text{ K}) = [172.440] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 811 \pm 10 \text{ K}$$

**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,  $\Delta_f H^\circ(\text{SrI}_2, \text{K}) - H^\circ(298.15 \text{ K})$ , between the crystal and the liquid.

**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.

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

**Vaporization Data**

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 Hutchinson have extrapolated Knudsen effusion cell measurements in the 1061–1303 K range to obtain a normal boiling point of 2046 K.  $\Delta_{\text{vap}} H^\circ = 45.35 \text{ kcal/mol}^{-1}$  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**

- <sup>1</sup>A. S. Dworkin and M. A. Bredig, J. Phys. Chem., **67**, 697 (1963).
- <sup>2</sup>D. T. Peterson and J. F. Hutchinson, J. Chem. Eng. Data, **15**, 320 (1970).

$$\Delta_f H^\circ(298.15 \text{ K}) = [-548.748] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_{\text{fus}} H^\circ = 19.665 \pm 0.38 \text{ kJ} \cdot \text{mol}^{-1}$$

$$S^\circ(298.15 \text{ K}) = [172.440] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 811 \pm 10 \text{ K}$$

$$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$$

$$C_p^* = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{T/K}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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

$$T/K = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{C_p^*}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

$$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$$

$$C_p^* = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{T/K}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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

$$T/K = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{C_p^*}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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$$C_p^* = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{T/K}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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$$T/K = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{C_p^*}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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

$$T/K = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{C_p^*}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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

$$T/K = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{C_p^*}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

$$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$$

$$C_p^* = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{T/K}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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

$$T/K = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{C_p^*}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

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$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

$$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$$

$$C_p^* = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{T/K}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

$$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$$

$$C_p^* = \frac{S^\circ - [G^\circ - H^\circ(T_r)/T]}{T/K}$$

$$H^\circ - H^\circ(T_r) = \frac{\Delta H^\circ}{k \cdot \text{mol}^{-1}}$$

$$\log K_r = \frac{\Delta G^\circ}{k \cdot \text{mol}^{-1}}$$

Strontium Iodide ( $\text{SrI}_2$ ) $M_r = 341.4290$  Strontium Iodide ( $\text{SrI}_2$ ) $\text{I}_2\text{Sr}_1(\text{cr},\text{l})$ 

0 to 811 K crystal  
above 811 K liquid

Refer to the individual tables for details.

$T/K$

$C_p^{\circ}$

$S^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} - H^{\circ}(T_0)/T$

$G^{\circ} - [G^{\circ} - H^{\circ}(T)]/T$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} - H^{\circ}(T_0)$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$H^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$G^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

$E^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$

PREVIOUS:

Strontium Iodide ( $\text{SrI}_2$ )

|         |         | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |         |               |                     | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |          |                                |          |
|---------|---------|-----------------------------------------------------------|---------|---------------|---------------------|---------------------------------------------------|----------|--------------------------------|----------|
|         |         | $T/K$                                                     |         | $C_p^{\circ}$ |                     | $S^{\circ} \text{ J K}^{-1} \text{ mol}^{-1}$     |          | $H^{\circ} - H^{\circ}(T_r)/T$ |          |
|         |         | 0                                                         |         | 0             |                     | 0                                                 |          | -1859.9                        |          |
|         |         | 0                                                         | 0       | 0             | 0                   | 0                                                 | 0        | -1859.9                        | -560.645 |
| 100     | 67.404  | 78.914                                                    | 226.165 | -14.725       | -561.001            | -559.988                                          | -558.986 | -558.986                       | INFINITE |
| 200     | 75.019  | 128.568                                                   | 166.164 | -7.119        | -561.216            | -557.702                                          | -557.702 | -557.702                       | 145.969  |
| 298.15  | 77.948  | 159.120                                                   | 0       | 0             | -561.493            | -557.678                                          | -557.678 | -557.678                       | 97.707   |
| 300     | 78.032  | 159.603                                                   | 159.122 | 0.144         | -561.499            | -557.700                                          | -557.700 | -557.700                       | 97.100   |
| 400     | 80.731  | 182.421                                                   | 162.214 | 8.083         | -577.928            | -546.142                                          | -546.142 | -546.142                       | 72.579   |
| 500     | 83.513  | 200.737                                                   | 168.145 | 16.296        | -620.739            | -510.055                                          | -510.055 | -510.055                       |          |
| 600     | 86.274  | 216.207                                                   | 174.836 | 24.785        | -618.933            | -511.390                                          | -511.390 | -511.390                       | 46.262   |
| 700     | 88.994  | 229.710                                                   | 181.784 | 33.548        | -616.972            | -516.933                                          | -516.933 | -516.933                       | 38.575   |
| 800     | 91.735  | 241.776                                                   | 188.542 | 42.387        | -614.852            | -502.807                                          | -502.807 | -502.807                       | 32.830   |
| 811.000 | 92.048  | 243.031                                                   | 189.272 | 43.598        | CRYSTAL <--> LIQUID |                                                   |          |                                |          |
| 811.000 | 110.039 | 267.279                                                   | 189.272 | 63.263        | TRANSITION          |                                                   |          |                                |          |
| 900     | 110.039 | 278.737                                                   | 197.563 | 79.047        | -491.103            | -491.103                                          | -491.103 | -491.103                       | 28.503   |
| 1000    | 110.039 | 290.330                                                   | 206.270 | 84.061        | -487.878            | -480.111                                          | -480.111 | -480.111                       | 25.078   |
| 1100    | 110.039 | 300.818                                                   | 214.396 | 95.064        | -591.626            | -469.170                                          | -469.170 | -469.170                       | 22.279   |
| 1200    | 110.039 | 310.393                                                   | 222.003 | 106.068       | -588.401            | -438.180                                          | -438.180 | -438.180                       | 19.944   |
| 1300    | 110.039 | 319.201                                                   | 229.145 | 117.072       | -585.199            | -447.459                                          | -447.459 | -447.459                       | 17.979   |
| 1400    | 110.039 | 327.326                                                   | 235.873 | 128.076       | -582.028            | -436.982                                          | -436.982 | -436.982                       | 16.304   |
| 1500    | 110.039 | 334.948                                                   | 242.227 | 139.980       | -578.898            | -426.731                                          | -426.731 | -426.731                       | 14.850   |
| 1600    | 110.039 | 342.049                                                   | 248.247 | 150.084       | -575.818            | -416.688                                          | -416.688 | -416.688                       | 13.603   |
| 1700    | 110.039 | 348.720                                                   | 253.963 | 161.088       | -709.710            | -405.655                                          | -405.655 | -405.655                       | 12.464   |
| 1800    | 110.039 | 355.010                                                   | 259.403 | 172.092       | -704.893            | -387.909                                          | -387.909 | -387.909                       | 11.257   |
| 1900    | 110.039 | 360.960                                                   | 264.593 | 183.096       | -700.151            | -370.429                                          | -370.429 | -370.429                       | 10.184   |
| 2000    | 110.039 | 366.604                                                   | 269.554 | 194.100       | -693.487            | -353.198                                          | -353.198 | -353.198                       | 9.225    |
| 2100    | 110.039 | 371.973                                                   | 274.304 | 203.104       | -690.902            | -336.194                                          | -336.194 | -336.194                       | 8.362    |
| 2200    | 110.039 | 377.052                                                   | 278.861 | 216.08        | -684.397            | -319.410                                          | -319.410 | -319.410                       | 7.584    |
| 2300    | 110.039 | 381.931                                                   | 283.219 | 227.111       | -681.966            | -302.828                                          | -302.828 | -302.828                       | 6.877    |
| 2400    | 110.039 | 386.666                                                   | 287.452 | 238.115       | -677.514            | -286.437                                          | -286.437 | -286.437                       | 6.234    |
| 2500    | 110.039 | 391.158                                                   | 291.511 | 249.119       | -673.330            | -270.226                                          | -270.226 | -270.226                       | 5.646    |
| 2600    | 110.039 | 395.474                                                   | 295.427 | 260.123       | -669.112            | -254.185                                          | -254.185 | -254.185                       | 5.107    |

CURRENT: June 1974

 $\text{I}_2\text{Sr}_1(\text{cr},\text{l})$

Strontium Iodide ( $\text{SrI}_2$ ) $M_r = 341.4290$  Strontium Iodide ( $\text{SrI}_2$ )

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

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

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

## IDEAL GAS

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

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

Ground State Quantum Weight: [1]

 $\sigma = 2$ Point Group:  $D_{\infty h}$ Bond Distance:  $\text{Sr}-\text{I} = 3.03 \pm 0.03 \text{ \AA}$ Bond Angle:  $\text{I}-\text{Sr}-\text{I} = [180]^\circ$ Rotational Constant:  $B_0 = 0.007234 \text{ cm}^{-1}$ 

## 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 1308 K to 1308 K. Our 2nd and 3rd law analyses of these data give  $\Delta_{vap}H^\circ(298.15 \text{ K}) = 65.72 \pm 1.48 \text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta_{vap}H^\circ(298.15 \text{ K}) / (3 \text{rd law}) = 65.48 \pm 0.68 \text{ kcal}\cdot\text{mol}^{-1}$  with a drift of  $-0.2 \pm 1.2 \text{ cal}\cdot\text{K}^{-1}\text{mol}^{-1}$ . We adopt  $\Delta_{vap}H^\circ(298.15 \text{ K}) = 65.5 \pm 0.7 \text{ kcal}\cdot\text{mol}^{-1}$  and combine this with the adopted enthalpy of formation of the liquid to obtain  $\Delta H^\circ(\text{SrI}_2, g, 298.15 \text{ K}) = -65.7 \pm 1.5 \text{ kcal}\cdot\text{mol}^{-1}$ .

## Heat Capacity and Entropy

The bond distance, as determined from an electron diffraction study, is taken from Krishnan *et al.*<sup>3</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,  $k$  (monohalide)/ $k$  (dihalide), has indicated that  $k(\text{SrI}_2)/k(\text{SrI}_2) = 1$  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  $v_1$ ,  $v_2$ , and  $v_3$  are 111, 49, and 220.<sup>7</sup>

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

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| $T/\text{K}$ | $C_p^*$ | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                            | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                  |
|--------------|---------|-----------------------------------------------------------|----------------------------|-------------------------------------------------------|------------------|
|              |         | $S^\circ - (G^\circ - H^\circ(T_r))/T$                    | $H^\circ - H^\circ(T_r)/T$ | $\Delta H^\circ$                                      | $\Delta G^\circ$ |
| 0            | 0       | 0                                                         | 0                          | -16.542                                               | -271.664         |
| 100          | 56.065  | 274.673                                                   | 393.256                    | -11.838                                               | -290.093         |
| 200          | 60.336  | 315.227                                                   | 345.144                    | -5.983                                                | -308.088         |
| 250          | 61.019  | 328.771                                                   | 340.263                    | -2.948                                                | -316.744         |
| 298.15       | 61.399  | 339.254                                                   | 339.554                    | 0.                                                    | -374.889         |
| 300          | 61.410  | 339.334                                                   | 339.555                    | 0.114                                                 | -374.926         |
| 350          | 61.653  | 349.420                                                   | 340.304                    | 3.191                                                 | -375.204         |
| 400          | 61.814  | 357.664                                                   | 341.970                    | 6.278                                                 | -376.013         |
| 450          | 61.926  | 364.470                                                   | 344.126                    | 9.371                                                 | -379.470         |
| 500          | 62.007  | 371.480                                                   | 346.341                    | 12.470                                                | -387.961         |
| 600          | 62.113  | 382.796                                                   | 351.669                    | 18.676                                                | -390.848         |
| 700          | 62.177  | 392.376                                                   | 356.817                    | 24.891                                                | -399.025         |
| 800          | 62.220  | 400.681                                                   | 361.793                    | 31.111                                                | -402.877         |
| 900          | 62.248  | 408.011                                                   | 366.529                    | 37.334                                                | -404.804         |
| 1000         | 62.269  | 414.571                                                   | 371.011                    | 43.560                                                | -406.569         |
| 1100         | 62.283  | 420.507                                                   | 378.245                    | 49.788                                                | -411.774         |
| 1200         | 62.296  | 422.927                                                   | 379.246                    | 56.017                                                | -415.288         |
| 1300         | 62.305  | 430.914                                                   | 383.031                    | 62.247                                                | -420.906         |
| 1400         | 62.313  | 435.531                                                   | 386.618                    | 68.478                                                | -425.485         |
| 1500         | 62.318  | 439.830                                                   | 390.024                    | 74.710                                                | -436.822         |
| 1600         | 62.323  | 443.853                                                   | 393.264                    | 80.942                                                | -458.356         |
| 1700         | 62.327  | 447.631                                                   | 396.152                    | 87.174                                                | -472.020         |
| 1800         | 62.331  | 451.194                                                   | 399.301                    | 93.407                                                | -486.974         |
| 1900         | 62.333  | 454.564                                                   | 402.121                    | 99.640                                                | -497.002         |
| 2000         | 62.336  | 457.161                                                   | 404.824                    | 105.374                                               | -497.108         |
| 2100         | 62.338  | 460.803                                                   | 407.418                    | 112.108                                               | -497.294         |
| 2200         | 62.340  | 463.703                                                   | 409.911                    | 118.341                                               | -497.559         |
| 2300         | 62.341  | 466.574                                                   | 412.210                    | 124.576                                               | -497.901         |
| 2400         | 62.343  | 469.127                                                   | 414.623                    | 130.810                                               | -503.044         |
| 2500         | 62.344  | 471.672                                                   | 416.854                    | 137.044                                               | -498.301         |
| 2600         | 62.345  | 474.117                                                   | 419.019                    | 143.278                                               | -499.353         |
| 2700         | 62.346  | 476.670                                                   | 421.095                    | 149.513                                               | -499.968         |
| 2800         | 62.347  | 478.337                                                   | 422.113                    | 155.738                                               | -500.646         |
| 2900         | 62.347  | 480.000                                                   | 423.133                    | 161.982                                               | -502.185         |
| 3000         | 62.348  | 483.039                                                   | 426.909                    | 167.217                                               | -502.325         |
| 3100         | 62.349  | 485.083                                                   | 428.808                    | 174.452                                               | -502.567         |
| 3200         | 62.349  | 487.963                                                   | 430.598                    | 180.687                                               | -503.979         |
| 3300         | 62.350  | 488.981                                                   | 432.338                    | 186.922                                               | -504.978         |
| 3400         | 62.350  | 490.843                                                   | 434.032                    | 193.157                                               | -506.051         |
| 3500         | 62.351  | 492.650                                                   | 435.681                    | 199.392                                               | -507.202         |
| 3600         | 62.351  | 494.407                                                   | 437.288                    | 205.627                                               | -508.436         |
| 3700         | 62.352  | 496.115                                                   | 441.515                    | 211.862                                               | -509.756         |
| 3800         | 62.352  | 497.778                                                   | 440.384                    | 218.097                                               | -511.167         |
| 3900         | 62.352  | 499.397                                                   | 441.876                    | 224.333                                               | -512.672         |
| 4000         | 62.352  | 500.976                                                   | 443.334                    | 230.568                                               | -514.275         |
| 4100         | 62.353  | 502.516                                                   | 444.759                    | 236.803                                               | -515.977         |
| 4200         | 62.353  | 504.018                                                   | 446.152                    | 243.038                                               | -517.776         |
| 4300         | 62.353  | 505.483                                                   | 447.515                    | 249.274                                               | -519.677         |
| 4400         | 62.353  | 506.919                                                   | 448.849                    | 250.509                                               | -520.844         |
| 5100         | 62.355  | 516.125                                                   | 457.466                    | 299.157                                               | -537.990         |
| 5200         | 62.355  | 517.335                                                   | 458.606                    | 305.392                                               | -540.611         |
| 5300         | 62.355  | 518.523                                                   | 459.725                    | 311.628                                               | -543.283         |
| 5400         | 62.355  | 519.689                                                   | 460.825                    | 317.863                                               | -546.001         |
| 5500         | 62.355  | 520.833                                                   | 461.906                    | 324.099                                               | -548.736         |
| 5600         | 62.355  | 521.956                                                   | 462.968                    | 330.334                                               | -552.952         |
| 5700         | 62.355  | 523.080                                                   | 464.013                    | 342.805                                               | -554.352         |
| 5800         | 62.355  | 524.145                                                   | 465.040                    | 349.041                                               | -557.179         |
| 5900         | 62.356  | 525.210                                                   | 465.605                    | 349.987                                               | -559.807         |
| 6000         | 62.356  | 526.259                                                   | 467.046                    | 355.276                                               | -562.618         |

PREVIOUS June 1974 (1 atm)

**Strontium Iodide ( $\text{SrI}_2$ )**  
CURRENT June 1974 (1 bar)

| TITANIUM IODIDE ( $TiI_2$ )                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                 | $M_r = 301.6890$ TITANIUM IODIDE ( $TiI_2$ )             |                                                                           | $I_2Ti_1(cr)$                                   |             |                                  |                      |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------|----------------------------------------------------------|---------------------------------------------------------------------------|-------------------------------------------------|-------------|----------------------------------|----------------------|
| CRYSTAL                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | $S^\circ(298.15\text{ K}) = [122.591 \pm 12.6] \text{ J K}^{-1}\text{mol}^{-1}$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                                                           | Standard State Pressure = $p = 0.1 \text{ mPa}$ |             |                                  |                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                                                                 | $\Delta_fH^\circ(0\text{ K}) = \text{Unknown}$           | $\Delta_fH^\circ(298.15\text{ K}) = -266.10 \pm 12.6 \text{ kJ mol}^{-1}$ | $T_K$                                           | $C_p^\circ$ | $J\text{-K}^{-1}\text{mol}^{-1}$ | $\text{kJ mol}^{-1}$ |
| Enthalpy of Formation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                                                                 | 0                                                        |                                                                           |                                                 |             |                                  |                      |
| The enthalpy of formation of $TiI_x(cr)$ is calculated from the enthalpy of reaction for the process $2TiI_2(cr) = Ti(cr) + TiI_3(g)$ , and the enthalpy of formation of $TiI_x(cr)$ . 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 $\Delta_fH^\circ(298.15\text{ K})$ of $60.5 \pm 0.8$ and $60.85 \text{ kcal mol}^{-1}$ , respectively, the 3rd law drift being $0.4 \pm 1.0 \text{ cal K}^{-1}\text{mol}^{-1}$ . The 3rd law $\Delta_fH^\circ(298.15\text{ K})$ is used to obtain the adopted value of $\Delta_fH^\circ(298.15\text{ K})$ . | 100                                                                             | 100                                                      | 122.591                                                                   | 0.                                              | -266.102    | -258.854                         |                      |
| Heat Capacity and Entropy                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                                 | 200                                                      |                                                                           |                                                 |             |                                  |                      |
| The estimated heat capacity is that reported by Kelley. <sup>2</sup> The value of $S^\circ(298.15\text{ K})$ is estimated from that of $TiCl_2(cr)$ and the difference between ionic entropy contributions of $Cl^-$ and $I^-$ .                                                                                                                                                                                                                                                                                                                                                                                                                                                          | 298.15                                                                          | 86.228                                                   | 122.591                                                                   | 0.160                                           | -266.090    | -258.810                         |                      |
| Sublimation Data                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                                 | 300                                                      |                                                                           |                                                 |             |                                  |                      |
| The enthalpy of sublimation of $TiI_x(cr)$ is taken as the difference in the enthalpies of formation of $TiI_x(cr)$ and $TiI_x(g)$ at the sublimation temperature. The sublimation temperature is taken as the point at which $\Delta_fG^\circ = 0$ for the reaction $TiI_x(cr) = TiI_x(g)$ .                                                                                                                                                                                                                                                                                                                                                                                             | 85.969                                                                          | 85.969                                                   | 122.593                                                                   | 0.8820                                          | -281.682    | -253.901                         |                      |
| References                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                 | 400                                                      |                                                                           |                                                 |             |                                  |                      |
| <sup>1</sup> A. Herzog and L. M. Pidgeon, Can. J. Chem., <b>34</b> , 1687 (1956).                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | 85.969                                                                          | 85.969                                                   | 123.594                                                                   | 0.8820                                          | -281.682    | -253.901                         |                      |
| <sup>2</sup> K. K. Kelley, U. S. Bur. Mines Bull. <b>584</b> , (1961).                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 500                                                                             | 87.697                                                   | 167.519                                                                   | 17.553                                          | -323.885    | -245.418                         |                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 600                                                                             | 88.125                                                   | 183.572                                                                   | 139.640                                         | 26.359      | -321.659                         | -229.934             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 700                                                                             | 89.153                                                   | 197.258                                                                   | 146.917                                         | 35.238      | -319.435                         | -214.822             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 800                                                                             | 89.881                                                   | 209.210                                                                   | 153.973                                         | 44.190      | -317.188                         | -200.030             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 900                                                                             | 90.609                                                   | 219.838                                                                   | 160.711                                         | 53.214      | -314.944                         | -185.521             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1000                                                                            | 91.337                                                   | 229.423                                                                   | 167.111                                         | 62.312      | -312.770                         | -171.258             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1100                                                                            | 92.065                                                   | 238.162                                                                   | 173.179                                         | 71.482      | -310.730                         | -157.207             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1200                                                                            | 92.793                                                   | 246.204                                                                   | 178.933                                         | 80.725      | -312.815                         | -143.215             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1300                                                                            | 93.521                                                   | 253.660                                                                   | 184.398                                         | 90.040      | -310.336                         | -129.182             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1400                                                                            | 94.249                                                   | 260.617                                                                   | 189.597                                         | 99.429      | -307.893                         | -115.339             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1500                                                                            | 94.977                                                   | 267.145                                                                   | 194.551                                         | 108.890     | -305.509                         | -101.669             |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1600                                                                            | 95.705                                                   | 273.298                                                                   | 199.282                                         | 118.424     | -303.207                         | -88.155              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1700                                                                            | 96.433                                                   | 279.121                                                                   | 203.809                                         | 128.031     | -301.008                         | -74.782              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1800                                                                            | 97.161                                                   | 284.654                                                                   | 208.148                                         | 137.711     | -298.933                         | -61.535              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1900                                                                            | 97.889                                                   | 289.977                                                                   | 212.315                                         | 147.463     | -296.999                         | -48.400              |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 2000                                                                            | 98.617                                                   | 294.966                                                                   | 216.522                                         | 157.288     | -309.906                         | -34.909              |

TITANIUM IODIDE ( $TiI_2$ )

$$S^\circ(298.15\text{ K}) = [122.591 \pm 12.6] \text{ J K}^{-1}\text{mol}^{-1}$$

Enthalpy of Formation

The enthalpy of formation of  $TiI_x(cr)$  is calculated from the enthalpy of reaction for the process  $2TiI_2(cr) = Ti(cr) + TiI_3(g)$ , and the enthalpy of formation of  $TiI_x(cr)$ . 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  $\Delta_fH^\circ(298.15\text{ K})$  of  $60.5 \pm 0.8$  and  $60.85 \text{ kcal mol}^{-1}$ , respectively, the 3rd law drift being  $0.4 \pm 1.0 \text{ cal K}^{-1}\text{mol}^{-1}$ . The 3rd law  $\Delta_fH^\circ(298.15\text{ K})$  is used to obtain the adopted value of  $\Delta_fH^\circ(298.15\text{ K})$ .

Heat Capacity and Entropy

The estimated heat capacity is that reported by Kelley.<sup>2</sup> The value of  $S^\circ(298.15\text{ K})$  is estimated from that of  $TiCl_2(cr)$  and the difference between ionic entropy contributions of  $Cl^-$  and  $I^-$ .

## Sublimation Data

The enthalpy of sublimation of  $TiI_x(cr)$  is taken as the difference in the enthalpies of formation of  $TiI_x(cr)$  and  $TiI_x(g)$  at the sublimation temperature. The sublimation temperature is taken as the point at which  $\Delta_fG^\circ = 0$  for the reaction  $TiI_x(cr) = TiI_x(g)$ .

## 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).

PREVIOUS June 1964

CURRENT: December 1968

TITANIUM IODIDE ( $TiI_2$ )

Titanium Iodide ( $\text{TiI}_2$ )

## IDEAL GAS

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

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

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

| Electronic Levels and Quantum Weights |      |
|---------------------------------------|------|
| $\epsilon, \text{ cm}^{-1}$           | g.   |
| 0                                     | [3]  |
| [7000]                                | [6]  |
| [17000]                               | [15] |
| [22000]                               |      |

| Vibrational Frequencies and Degeneracies |  |
|------------------------------------------|--|
| $\nu, \text{ cm}^{-1}$                   |  |
| [134](1)                                 |  |
| [192](2)                                 |  |
| [290](1)                                 |  |

Ground State Quantum Weight: [3]

Point Group: [D<sub>3d</sub>]

Bond Distance, Ti-I = [2.7] Å

Bond Angle, I-Ti-I = [180]°

Rotational Constant  $B_0 = [0.009111] \text{ cm}^{-1}$ 

## Enthalpy of Formation

The enthalpy of formation of  $\text{TiI}_2(\text{g})$  is calculated from that of  $\text{TiI}_2(\text{cr})$  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 2nd 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  $8.3 \pm 1.1 \text{ cal K}^{-1} \text{ mol}^{-1}$ , with one point rejected due to failure of a statistical test. The adopted value of  $\Delta H^\circ(298.15 \text{ K})$  is calculated from the 3rd law enthalpy of vaporization.

## Heat Capacity and Entropy

The interatomic distances are estimated from those of  $\text{TiCl}_4(\text{g})$ ,  $\text{TiBr}_4(\text{g})$ ,  $\text{TiI}_4(\text{g})$  and  $\text{TiI}_4(\text{g})$ . The vibrational frequencies are estimated from a valence force field model.<sup>2</sup> The force constant K is estimated as 1.0 millidynes/Å, and the constant  $K_3/\nu^2$  is assumed to be 0.05 millidynes/Å.<sup>3</sup>

The electronic levels of  $\text{TiCl}_4(\text{g})$  are estimated by assuming they correspond to the inverted states of  $\text{NiCl}_4(\text{g})$ .<sup>4</sup> The linear configuration is adopted, since experimental evidence indicates that other transition metal dihalides are linear.<sup>5</sup>

## References

- A. Herzog and L. M. Pidgeon, Can. J. Chem., **34**, 1687 (1956).
- C. W. DeKock and D. M. Gruen, J. Chem. Phys., **44**, 4387 (1966).
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- A. Buchler, J. L. Stauffer, and W. Klempner, J. Chem. Phys., **40**, 3471 (1964).

Titanium Iodide ( $\text{TiI}_2$ ) $\text{I}_2\text{TiI}_4(\text{g})$ 

| $T/K$  | $C_v^*$ | $S^*$   | Enthalpy Reference Temperature = $T_f = 298.15 \text{ K}$ |                  | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |                  |
|--------|---------|---------|-----------------------------------------------------------|------------------|---------------------------------------------------|------------------|
|        |         |         | $H^\circ - H^\circ(T_f)/T$                                | $\Delta H^\circ$ | $H^\circ - H^\circ(T_f)/T$                        | $\Delta H^\circ$ |
| 0      | 0       | 0       | -15.514                                                   | -17.151          | -17.151                                           | -17.151          |
| 100    | 51.937  | 0.0     | -11.479                                                   | -16.726          | -35.921                                           | 18.763           |
| 200    | 58.692  | 375.991 | -5.869                                                    | -17.965          | -54.693                                           | 14.284           |
| 250    | 59.887  | 329.167 | -2.901                                                    | -18.789          | -63.782                                           | 13.327           |
| 298.15 | 60.570  | 324.667 | 0.                                                        | -19.665          | -72.369                                           | 12.679           |
| 300    | 60.591  | 323.673 | 0.112                                                     | -19.700          | -72.595                                           | 12.658           |
| 350    | 61.036  | 324.498 | 3.154                                                     | -20.738          | -81.449                                           | 12.156           |
| 400    | 61.333  | 341.595 | 6.213                                                     | -37.851          | -89.495                                           | 11.687           |
| 450    | 61.542  | 348.832 | 9.285                                                     | -40.170          | -91.811                                           | 11.121           |
| 500    | 61.693  | 355.324 | 12.366                                                    | -82.634          | -98.070                                           | 10.245           |
| 600    | 61.893  | 366.591 | 18.547                                                    | -83.034          | -101.120                                          | 8.803            |
| 700    | 62.016  | 376.142 | 34.742                                                    | -83.493          | -104.099                                          | 7.688            |
| 800    | 62.103  | 384.429 | 345.743                                                   | -83.991          | -107.009                                          | 6.987            |
| 900    | 62.178  | 391.748 | 350.436                                                   | -84.538          | -109.853                                          | 6.376            |
| 1000   | 62.260  | 398.303 | 354.919                                                   | -84.384          | -85.260                                           | 5.883            |
| 1100   | 62.365  | 404.242 | 359.137                                                   | -49.615          | -86.159                                           | -115.323         |
| 1200   | 62.505  | 409.674 | 363.125                                                   | -91.243          | -117.807                                          | 5.476            |
| 1300   | 62.688  | 414.684 | 366.901                                                   | 62.118           | -91.820                                           | -119.998         |
| 1400   | 62.916  | 419.338 | 370.482                                                   | 68.320           | -92.486                                           | 4.822            |
| 1500   | 63.188  | 423.688 | 373.886                                                   | 74.703           | -93.256                                           | -122.141         |
| 1600   | 63.500  | 427.775 | 377.127                                                   | 81.037           | -94.157                                           | -126.769         |
| 1700   | 63.845  | 431.635 | 380.221                                                   | 87.404           | -95.198                                           | 4.122            |
| 1800   | 64.215  | 435.295 | 383.180                                                   | 93.806           | -96.400                                           | 3.940            |
| 1900   | 64.603  | 438.777 | 386.015                                                   | 100.247          | -97.777                                           | 3.777            |
| 2000   | 65.000  | 442.101 | 388.737                                                   | 106.727          | -114.029                                          | 3.629            |
| 2100   | 65.400  | 445.282 | 391.355                                                   | 113.247          | -131.302                                          | 3.481            |
| 2200   | 65.795  | 448.334 | 393.876                                                   | 119.807          | -134.541                                          | -134.204         |
| 2300   | 66.182  | 451.267 | 396.308                                                   | 126.406          | -121.626                                          | -133.657         |
| 2400   | 66.555  | 454.091 | 398.657                                                   | 133.043          | -124.183                                          | 3.081            |
| 2500   | 66.913  | 456.816 | 400.929                                                   | 139.717          | -126.737                                          | -136.205         |
| 2600   | 67.254  | 459.447 | 403.129                                                   | 146.425          | -129.278                                          | 2.964            |
| 2700   | 67.576  | 461.991 | 405.233                                                   | 153.167          | -131.797                                          | -136.555         |
| 2800   | 67.879  | 464.454 | 407.333                                                   | 159.940          | -134.284                                          | 2.655            |
| 2900   | 68.164  | 466.841 | 409.344                                                   | 166.742          | -137.475                                          | 2.363            |
| 3000   | 68.431  | 469.157 | 411.299                                                   | 173.572          | -139.127                                          | 2.393            |
| 3100   | 68.681  | 471.405 | 413.202                                                   | 180.428          | -141.469                                          | -137.366         |
| 3200   | 68.916  | 473.389 | 415.055                                                   | 187.308          | -143.749                                          | 2.315            |
| 3300   | 69.137  | 475.713 | 416.861                                                   | 194.211          | -145.963                                          | -137.197         |
| 3400   | 69.346  | 477.780 | 418.623                                                   | 201.135          | -148.107                                          | 2.240            |
| 3500   | 69.543  | 479.793 | 420.342                                                   | 208.079          | -150.179                                          | -137.251         |
| 3600   | 69.730  | 481.755 | 422.021                                                   | 215.043          | -152.176                                          | 2.068            |
| 3700   | 69.908  | 483.568 | 423.661                                                   | 222.025          | -153.197                                          | -135.876         |
| 3800   | 70.078  | 485.334 | 425.265                                                   | 229.074          | -153.197                                          | 2.024            |
| 3900   | 70.242  | 487.357 | 426.834                                                   | 236.040          | -154.399                                          | -135.876         |
| 4000   | 70.399  | 489.137 | 428.369                                                   | 243.007          | -156.969                                          | -137.251         |
| 4100   | 70.551  | 490.877 | 429.872                                                   | 250.120          | -156.516                                          | -138.285         |
| 4200   | 70.697  | 492.379 | 431.145                                                   | 257.182          | -155.042                                          | 2.074            |
| 4300   | 70.839  | 494.244 | 432.789                                                   | 264.229          | -156.544                                          | -138.285         |
| 4400   | 70.977  | 495.375 | 434.204                                                   | 271.350          | -157.024                                          | -144.822         |
| 4500   | 71.110  | 497.471 | 435.592                                                   | 278.455          | -157.481                                          | -144.306         |
| 4600   | 71.240  | 499.025 | 436.955                                                   | 285.572          | -156.791                                          | -144.306         |
| 4700   | 71.365  | 500.069 | 438.292                                                   | 292.702          | -158.238                                          | -145.998         |
| 4800   | 71.486  | 501.073 | 439.605                                                   | 299.845          | -159.817                                          | 2.034            |
| 4900   | 71.603  | 503.348 | 440.895                                                   | 306.999          | -160.084                                          | -146.338         |
| 5000   | 71.716  | 504.996 | 442.162                                                   | 314.165          | -162.554                                          | -147.277         |
| 5100   | 71.825  | 506.417 | 443.408                                                   | 321.343          | -163.751                                          | -148.477         |
| 5200   | 71.928  | 507.813 | 444.534                                                   | 328.530          | -164.751                                          | -149.522         |
| 5300   | 72.028  | 509.184 | 445.839                                                   | 335.728          | -165.730                                          | -150.406         |
| 5400   | 72.122  | 510.531 | 447.024                                                   | 342.936          | -167.500                                          | -151.387         |
| 5500   | 72.212  | 511.835 | 448.191                                                   | 350.152          | -168.717                                          | -152.269         |
| 5600   | 72.296  | 513.157 | 449.339                                                   | 357.378          | -170.035                                          | -153.624         |
| 5700   | 72.315  | 514.437 | 450.470                                                   | 364.611          | -171.228                                          | -154.173         |
| 5800   | 72.449  | 515.697 | 451.780                                                   | 371.833          | -172.400                                          | -154.889         |
| 5900   | 72.517  | 516.936 | 452.581                                                   | 379.101          | -173.550                                          | -155.437         |
| 6000   | 72.580  | 518.155 | 453.762                                                   | 386.356          | -174.681                                          | -156.998         |

CURRENT: December 1968 (1 atm)

PREVIOUS: December 1968 (1 atm)

 $\text{I}_2\text{TiI}_4(\text{g})$

**Zirconium Iodide (ZrI<sub>2</sub>)****CRYSTAL****I<sub>2</sub>ZrI<sub>4</sub>(cr)**

$$S^\circ(298.15\text{ K}) = [150.205] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{dis}} = [70.0] \text{ K}$$

$$\Delta_H^\circ(298.15\text{ K}) = [-259.408] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{dis}}H^\circ = [25.104] \text{ kJ}\cdot\text{mol}^{-1}$$

**Enthalpy of Formation**

Estimated from a consideration of  $\Delta_H^\circ(\text{ZrI}_4, \text{cr})$  and of the disproportionation data given by Roisten.<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**

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

**Reference**

- <sup>1</sup>R. F. Roisten, "Iodide Metals and Metal Iodides," John Wiley and Sons, Inc., New York, (1961).  
<sup>2</sup>L. Brewer, National Nuclear Energy Series, Div. IV, 19B, paper 7, McGraw-Hill Book Co., Inc., (1950).

**M<sub>f</sub> = 345.0290 Zirconium Iodide (ZrI<sub>2</sub>)**

| T/K     | $C_p^\circ$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                        | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                            |
|---------|-------------|----------------------------------------------------------|----------------------------------------|-------------------------------------------------------|----------------------------|
|         |             | $J\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$                | $S^\circ - [G^\circ - H^\circ(T_r)]/T$ | $k\text{J}\cdot\text{mol}^{-1}$                       | $H^\circ - H^\circ(T_r)/T$ |
| 100     | 0           |                                                          |                                        |                                                       |                            |
| 200     | 94.140      | 150.206                                                  | 150.206                                | 0.                                                    | -259.408                   |
| 300     | 94.349      | 150.789                                                  | 150.207                                | 0.174                                                 | -259.381                   |
| 400     | 95.019      | 178.019                                                  | 151.915                                | 9.641                                                 | -274.112                   |
| 500     | 95.855      | 199.313                                                  | 160.942                                | 19.186                                                | -315.389                   |
| 600     | 96.609      | 216.835                                                  | 168.841                                | 28.808                                                | -312.211                   |
| 700     | 97.445      | 231.809                                                  | 176.794                                | 38.510                                                | -309.043                   |
| 700,000 | 97.445      | 231.809                                                  | 176.794                                | 38.510                                                | -- CRYSTAL <--> LIQUID --- |
| 800     | 98.157      | 244.862                                                  | 184.504                                | 48.286                                                | -305.897                   |
| 900     | 99.621      | 256.520                                                  | 191.570                                | 58.185                                                | -302.735                   |
| 1000    | 99.830      | 267.022                                                  | 198.869                                | 68.153                                                | -299.625                   |
| 1100    | 100.383     | 276.571                                                  | 205.505                                | 78.173                                                | -296.592                   |
| 1200    | 101.420     | 285.359                                                  | 211.798                                | 88.274                                                | -297.376                   |
| 1300    | 102.215     | 293.509                                                  | 217.774                                | 98.455                                                | -293.868                   |
| 1400    | 103.010     | 301.113                                                  | 223.358                                | 108.717                                               | -290.405                   |
| 1500    | 103.805     | 308.247                                                  | 228.875                                | 119.057                                               | -286.935                   |
|         |             |                                                          |                                        |                                                       | 4.715                      |

PREVIOUS

CURRENT June 1962

**Zirconium Iodide (ZrI<sub>2</sub>)****I<sub>2</sub>ZrI<sub>4</sub>(cr)**

**Zirconium Iodide (ZrI<sub>2</sub>)**  
**Liquid**  
*M<sub>r</sub>* = 345.0290

| <i>T/K</i>                                           | $\Delta_{\text{fus}}H^\circ = [186.168] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$                                                                                                                                       | <b>Zirconium Iodide (ZrI<sub>2</sub>)</b> |                                                       |                                                                    | <b>I<sub>2</sub>Zr<sub>1</sub>(l)</b> |
|------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------|-------------------------------------------------------|--------------------------------------------------------------------|---------------------------------------|
|                                                      |                                                                                                                                                                                                                                | $S^\circ = [700] \text{ K}$               | $C_p^\circ = [25.104] \text{ kJ}\cdot\text{mol}^{-1}$ | $G^\circ - H^\circ(T) = [-234.239] \text{ kJ}\cdot\text{mol}^{-1}$ |                                       |
| <b>Enthalpy of Formation</b>                         |                                                                                                                                                                                                                                |                                           |                                                       |                                                                    |                                       |
| $H^\circ(700 \text{ K}) - H^\circ(298.15 \text{ K})$ | 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. |                                           |                                                       |                                                                    |                                       |
| <b>Heat Capacity and Entropy</b>                     | The liquid phase heat capacity is estimated. $S^\circ(\text{ZrI}_2, \text{l}, 298.15 \text{ K})$ is calculated in a manner analogous to that used for the enthalpy of formation.                                               |                                           |                                                       |                                                                    |                                       |
| <b>Fusion and Vaporization Data</b>                  | $\Delta_{\text{fus}}H^\circ$ was estimated. $T_{\text{fus}}$ , $T_{\text{vap}}$ and $\Delta_{\text{vap}}H^\circ$ from Brewer. <sup>1</sup>                                                                                     |                                           |                                                       |                                                                    |                                       |
| <b>Reference</b>                                     | L. Brewer, National Nuclear Energy Series, Div. IV, 19B, paper 7, McGraw Hill Book Co., Inc., (1950).                                                                                                                          |                                           |                                                       |                                                                    |                                       |

 $S^\circ \text{ K}^{-1} = [186.168] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = [700] \text{ K}$ 
**Enthalpy of Formation**
 $\Delta_{\text{fus}}H^\circ(\text{ZrI}_2, \text{l}, 298.15 \text{ K})$  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.  $S^\circ(\text{ZrI}_2, \text{l}, 298.15 \text{ K})$  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).

Zirconium Iodide ( $ZrI_2$ )

## CRYSTAL-LIQUID

0 to 700 K crystal  
above 700 K liquid

Refer to the individual tables for details.

 $I_2Zr_1(cr,I)$ 

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

| $T/K$   | $C_p^*$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                        | Standard State Pressure = $p^\circ = 0.1\text{ MPa}$ |                                                      |
|---------|---------|----------------------------------------------------------|----------------------------------------|------------------------------------------------------|------------------------------------------------------|
|         |         | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$         | $S^\circ - (G^\circ - H^\circ(T)) / T$ | $H^\circ - H^\circ(T_r)$                             | $k\text{J}\cdot\text{mol}^{-1}$                      |
| 0       |         |                                                          |                                        |                                                      |                                                      |
| 100     |         |                                                          |                                        |                                                      |                                                      |
| 200     | 94.140  | 150.206                                                  | 150.206                                | 0.                                                   | -259.408                                             |
| 298.15  | 94.349  | 150.789                                                  | 150.207                                | 0.174                                                | -259.381                                             |
| 300     | 94.349  | 150.789                                                  | 153.915                                | 9.641                                                | -257.966                                             |
| 400     | 95.0119 | 178.019                                                  | 153.913                                | 174.112                                              | -251.141                                             |
| 500     | 95.855  | 199.313                                                  | 160.942                                | 19.186                                               | -248.966                                             |
| 600     | 96.609  | 216.855                                                  | 168.841                                | 28.808                                               | -235.980                                             |
| 700     | 97.445  | 231.809                                                  | 176.194                                | 38.510                                               | -223.526                                             |
| 700.000 | 97.445  | 231.809                                                  | 176.794                                | 38.510                                               | 16.680                                               |
| 700.000 | 97.445  | 267.672                                                  | 176.794                                | 63.614                                               | — CRYSTAL $\rightleftharpoons$ LIQUID — TRANSITION — |
| 800     | 106.148 | 281.251                                                  | 189.009                                | 73.794                                               | -215.128                                             |
| 900     | 114.893 | 294.259                                                  | 199.986                                | 84.846                                               | -207.222                                             |
| 1000    | 123.595 | 306.815                                                  | 210.044                                | 96.770                                               | -199.836                                             |
| 1100    | 132.298 | 319.003                                                  | 219.398                                | 109.565                                              | -192.994                                             |
| 1200    | 141.001 | 330.887                                                  | 228.196                                | 123.230                                              | -186.492                                             |
| 1300    | 149.704 | 342.517                                                  | 236.344                                | 137.765                                              | -180.480                                             |
| 1400    | 158.448 | 353.931                                                  | 244.522                                | 153.173                                              | -175.099                                             |
| 1500    | 167.151 | 365.160                                                  | 252.191                                | 169.453                                              | -170.362                                             |
| 1600    | 175.854 | 376.225                                                  | 259.598                                | 186.603                                              | -166.275                                             |
| 1700    | 184.556 | 387.148                                                  | 266.781                                | 204.623                                              | -162.846                                             |
| 1800    | 193.259 | 397.943                                                  | 273.768                                | 223.514                                              | -160.078                                             |
| 1900    | 202.004 | 408.626                                                  | 280.585                                | 243.277                                              | -151.613                                             |
| 2000    | 210.706 | 419.209                                                  | 287.252                                | 263.913                                              | -156.538                                             |

 $I_2Zr_1(cr,I)$ 

| $T/K$   | $C_p^*$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                        | Standard State Pressure = $p^\circ = 0.1\text{ MPa}$ |                                                      |
|---------|---------|----------------------------------------------------------|----------------------------------------|------------------------------------------------------|------------------------------------------------------|
|         |         | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$         | $S^\circ - (G^\circ - H^\circ(T)) / T$ | $H^\circ - H^\circ(T_r)$                             | $k\text{J}\cdot\text{mol}^{-1}$                      |
| 0       |         |                                                          |                                        |                                                      |                                                      |
| 100     |         |                                                          |                                        |                                                      |                                                      |
| 200     | 94.140  | 150.206                                                  | 150.206                                | 0.                                                   | -259.408                                             |
| 298.15  | 94.349  | 150.789                                                  | 150.207                                | 0.174                                                | -259.381                                             |
| 300     | 94.349  | 150.789                                                  | 153.915                                | 9.641                                                | -257.966                                             |
| 400     | 95.0119 | 178.019                                                  | 153.913                                | 174.112                                              | -251.141                                             |
| 500     | 95.855  | 199.313                                                  | 160.942                                | 19.186                                               | -248.966                                             |
| 600     | 96.609  | 216.855                                                  | 168.841                                | 28.808                                               | -235.980                                             |
| 700     | 97.445  | 231.809                                                  | 176.194                                | 38.510                                               | -223.526                                             |
| 700.000 | 97.445  | 231.809                                                  | 176.794                                | 38.510                                               | 16.680                                               |
| 700.000 | 97.445  | 267.672                                                  | 176.794                                | 63.614                                               | — CRYSTAL $\rightleftharpoons$ LIQUID — TRANSITION — |
| 800     | 106.148 | 281.251                                                  | 189.009                                | 73.794                                               | -215.128                                             |
| 900     | 114.893 | 294.259                                                  | 199.986                                | 84.846                                               | -207.222                                             |
| 1000    | 123.595 | 306.815                                                  | 210.044                                | 96.770                                               | -199.836                                             |
| 1100    | 132.298 | 319.003                                                  | 219.398                                | 109.565                                              | -192.994                                             |
| 1200    | 141.001 | 330.887                                                  | 228.196                                | 123.230                                              | -186.492                                             |
| 1300    | 149.704 | 342.517                                                  | 236.344                                | 137.765                                              | -180.480                                             |
| 1400    | 158.448 | 353.931                                                  | 244.522                                | 153.173                                              | -175.099                                             |
| 1500    | 167.151 | 365.160                                                  | 252.191                                | 169.453                                              | -170.362                                             |
| 1600    | 175.854 | 376.225                                                  | 259.598                                | 186.603                                              | -166.275                                             |
| 1700    | 184.556 | 387.148                                                  | 266.781                                | 204.623                                              | -162.846                                             |
| 1800    | 193.259 | 397.943                                                  | 273.768                                | 223.514                                              | -160.078                                             |
| 1900    | 202.004 | 408.626                                                  | 280.585                                | 243.277                                              | -151.613                                             |
| 2000    | 210.706 | 419.209                                                  | 287.252                                | 263.913                                              | -156.538                                             |

 $I_2Zr_1(cr,I)$

## IDEAL GAS

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

$$S^\circ(298.15\text{ K}) = [344.782] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(0\text{ K}) = [-63.262] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = [-66.643] \text{ kJ}\cdot\text{mol}^{-1}$$

| Vibrational Frequencies and Degeneracies |              |
|------------------------------------------|--------------|
| $\nu, \text{ cm}^{-1}$                   | $\sigma = 2$ |
| [60](1)                                  |              |
| [120](1)                                 |              |
| [210](1)                                 |              |

Ground State Quantum Weight: [1]

Point Group:  $C_{2v}$ Bond Angle:  $Zr-I-Zr-I = 126^\circ$ Bond Angle:  $I-Zr-I = 120^\circ$ Product of the Moments of Inertia:  $I_A I_B / C = 1.072892 \times 10^{-111} \text{ g} \cdot \text{cm}^6$ 

**Enthalpy of Formation**  
Based upon the estimated value of the  $\Delta H^\circ$  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:  $I_A = 19.7106 \times 10^{-39}$ ,  $I_B = 223.6596 \times 10^{-39}$  and  $I_C = 243.3703 \times 10^{-39} \text{ g cm}^2$ .

**Enthalpy of Formation**  
Based upon the estimated value of the  $\Delta H^\circ$  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:  $I_A = 19.7106 \times 10^{-39}$ ,  $I_B = 223.6596 \times 10^{-39}$  and  $I_C = 243.3703 \times 10^{-39} \text{ g cm}^2$ .

| $T/K$  | $C_p^\circ$ | $S^\circ$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                             |                          | $\Delta G^\circ$ |
|--------|-------------|-----------|----------------------------------------------------------|-----------------------------|--------------------------|------------------|
|        |             |           | $J\text{K}^{-1}\text{mol}^{-1}$                          | $-G^\circ - H^\circ(T_r)/T$ | $H^\circ - H^\circ(T_r)$ |                  |
| 0      | 0           | 0         | 0                                                        | INFINITE                    | -15.315                  | -63.262          |
| 100    | 51.886      | 284.507   | 394.767                                                  | -11.026                     | -62.910                  | -83.856          |
| 200    | 56.159      | 322.118   | 349.992                                                  | -5.575                      | -64.584                  | -43.802          |
| 250    | 56.834      | 334.733   | 345.723                                                  | -2.748                      | -63.600                  | -27.216          |
| 298.15 | 57.238      | 344.782   | 344.782                                                  | 0.                          | -66.643                  | -13.996          |
| 300    | 57.436      | 345.136   | 345.783                                                  | 0.106                       | -66.684                  | -12.323          |
| 350    | 57.495      | 353.981   | 345.481                                                  | 2.975                       | -67.898                  | -12.574          |
| 400    | 57.656      | 361.670   | 347.035                                                  | 5.854                       | -65.134                  | -18.494          |
| 450    | 57.759      | 368.468   | 349.046                                                  | 8.740                       | -87.586                  | -48.338          |
| 500    | 57.830      | 374.558   | 351.298                                                  | 11.630                      | -130.179                 | -151.379         |
| 600    | 57.956      | 385.116   | 356.081                                                  | 17.421                      | -131.568                 | -155.539         |
| 700    | 58.020      | 394.035   | 360.883                                                  | 23.220                      | -131.911                 | -159.623         |
| 800    | 58.062      | 401.806   | 365.525                                                  | 29.024                      | -132.393                 | -163.576         |
| 900    | 58.091      | 408.646   | 369.944                                                  | 34.832                      | -133.323                 | -167.419         |
| 1000   | 58.112      | 414.768   | 374.125                                                  | 40.642                      | -134.371                 | -171.152         |
| 1100   | 58.127      | 420.307   | 378.076                                                  | 46.454                      | -135.545                 | -174.774         |
| 1200   | 58.139      | 425.366   | 381.809                                                  | 52.268                      | -140.566                 | -178.062         |
| 1300   | 58.148      | 430.020   | 385.241                                                  | 58.082                      | -141.476                 | -181.151         |
| 1400   | 58.156      | 434.349   | 388.688                                                  | 63.897                      | -142.459                 | -184.166         |
| 1500   | 58.161      | 438.342   | 391.866                                                  | 69.713                      | -143.534                 | -187.108         |
| 1600   | 58.166      | 442.095   | 394.889                                                  | 75.530                      | -144.721                 | -189.975         |
| 1700   | 58.170      | 445.632   | 397.771                                                  | 81.346                      | -146.041                 | -192.764         |
| 1800   | 58.173      | 448.597   | 400.523                                                  | 87.164                      | -147.510                 | -195.471         |
| 1900   | 58.176      | 452.029   | 403.155                                                  | 92.981                      | -149.144                 | -198.092         |
| 2000   | 58.179      | 455.076   | 405.677                                                  | 98.799                      | -150.953                 | -200.622         |
| 2100   | 58.181      | 457.915   | 408.097                                                  | 104.617                     | -152.947                 | -203.057         |
| 2200   | 58.182      | 460.621   | 410.424                                                  | 110.435                     | -156.452                 | -204.647         |
| 2300   | 58.184      | 463.208   | 412.663                                                  | 116.253                     | -179.243                 | -205.866         |
| 2400   | 58.185      | 465.684   | 414.821                                                  | 122.072                     | -182.079                 | -202.963         |
| 2500   | 58.187      | 468.039   | 416.903                                                  | 127.890                     | -184.948                 | -207.941         |
| 2600   | 58.188      | 470.342   | 418.915                                                  | 133.709                     | -187.840                 | -208.864         |
| 2700   | 58.189      | 472.538   | 420.861                                                  | 139.528                     | -190.542                 | -209.555         |
| 2800   | 58.190      | 474.634   | 422.744                                                  | 145.347                     | -193.643                 | -210.199         |
| 2900   | 58.191      | 476.656   | 424.570                                                  | 150.166                     | -196.532                 | -210.739         |
| 3000   | 58.191      | 478.668   | 426.340                                                  | 156.985                     | -199.401                 | -211.180         |
| 3100   | 58.192      | 480.577   | 428.059                                                  | 162.804                     | -202.239                 | -211.526         |
| 3200   | 58.192      | 482.424   | 429.729                                                  | 168.623                     | -203.040                 | -211.948         |
| 3300   | 58.193      | 484.215   | 431.353                                                  | 174.442                     | -207.798                 | -211.948         |
| 3400   | 58.193      | 485.932   | 432.934                                                  | 180.262                     | -210.508                 | -212.033         |
| 3500   | 58.194      | 487.639   | 434.473                                                  | 186.081                     | -213.165                 | -212.039         |
| 3600   | 58.194      | 497.656   | 442.570                                                  | 191.900                     | -215.767                 | -211.970         |
| 3700   | 58.194      | 498.668   | 443.455                                                  | 197.720                     | -218.312                 | -211.829         |
| 3800   | 58.195      | 500.926   | 448.862                                                  | 203.539                     | -220.798                 | -211.526         |
| 3900   | 58.195      | 503.916   | 440.255                                                  | 209.359                     | -223.225                 | -211.347         |
| 4000   | 58.195      | 505.410   | 441.615                                                  | 215.178                     | -225.592                 | -211.013         |
| 4100   | 58.196      | 496.847   | 442.945                                                  | 220.998                     | -227.900                 | -212.036         |
| 4200   | 58.196      | 498.249   | 444.245                                                  | 226.817                     | -230.150                 | -210.171         |
| 4300   | 58.196      | 499.618   | 445.517                                                  | 232.637                     | -232.342                 | -214.569         |
| 4400   | 58.196      | 500.926   | 446.762                                                  | 238.457                     | -234.478                 | -215.658         |
| 4500   | 58.196      | 502.264   | 447.981                                                  | 244.276                     | -236.559                 | -216.517         |
| 4600   | 58.197      | 503.543   | 449.175                                                  | 250.996                     | -238.587                 | -207.872         |
| 4700   | 58.197      | 504.795   | 450.345                                                  | 255.916                     | -240.563                 | -207.182         |
| 4800   | 58.197      | 506.070   | 451.497                                                  | 261.735                     | -246.817                 | -203.030         |
| 4900   | 58.197      | 507.220   | 452.617                                                  | 267.555                     | -252.347                 | -210.620         |
| 5000   | 58.197      | 508.396   | 453.721                                                  | 273.375                     | -260.456                 | -217.414         |
| 5100   | 58.197      | 509.548   | 454.804                                                  | 279.195                     | -267.927                 | -216.658         |
| 5200   | 58.198      | 510.678   | 455.868                                                  | 285.014                     | -280.369                 | -214.445         |
| 5300   | 58.198      | 511.797   | 456.913                                                  | 290.834                     | -281.782                 | -211.063         |
| 5400   | 58.198      | 512.875   | 457.939                                                  | 296.654                     | -282.168                 | -218.225         |
| 5500   | 58.198      | 513.943   | 458.947                                                  | 302.474                     | -283.525                 | -214.444         |
| 5600   | 58.198      | 514.991   | 459.939                                                  | 308.293                     | -284.855                 | -214.834         |
| 5700   | 58.198      | 516.021   | 460.914                                                  | 314.113                     | -286.474                 | -216.414         |
| 5800   | 58.198      | 517.034   | 461.873                                                  | 319.323                     | -287.562                 | -217.529         |
| 5900   | 58.198      | 518.028   | 462.816                                                  | 325.753                     | -288.680                 | -218.600         |
| 6000   | 58.198      | 519.007   | 463.744                                                  | 331.573                     | -289.501                 | -219.673         |

| $I_2Zr_1(g)$ | CURRENT June 1962 (1 atm) |
|--------------|---------------------------|
|              |                           |

Zirconium Iodide ( $ZrI_2$ )

PREVIOUS: June 1962 (1 atm)

CURRENT: June 1962 (1 bar)

**Molybdenum Iodide ( $\text{MoI}_3$ )****CRYSTAL** **$\text{I}_3\text{MoI}_3(\text{cr})$** 

$$\Delta H^\circ(0 \text{ K}) = [195.393 \pm 16.7] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

**Enthalpy of Formation**

Barnes *et al.*<sup>1</sup> have measured calorimetrically the enthalpy of formation of  $\text{MoI}_3$  by reacting iodine vapor with  $\text{Mo(CO)}_6$  at 539 K. The products were found to consist of  $\text{MoI}_3$ ,  $\text{MoI}_2$ , and Mo by chemical analysis. Assuming a difference in the enthalpies of formation of  $\text{MoI}_3$  and  $\text{MoI}_2$  of 1.5 kcal/mol<sup>-1</sup>, Barnes *et al.*<sup>1</sup> determined that the  $\Delta_f H^\circ(\text{MoI}_3, \text{cr}, 298.15 \text{ K}) = 26.2 \pm 2.0$  kcal/mol<sup>-1</sup>. 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 kcal/mol<sup>-1</sup> and reanalyzed the heat of iodination data with the result  $\Delta_f H^\circ(\text{MoI}_3, \text{cr}, 298.15 \text{ K}) = -15000 \pm 1000$  K which is adopted. We adopt the estimate of Brewer,<sup>2</sup> The assigned uncertainty ( $\pm 2.0$  kcal/mol<sup>-1</sup>) 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  $S^\circ(298.15 \text{ K})$  and  $C_p^\circ$  over the temperature range 298–1000 K are estimates reported by Brewer.<sup>2</sup> We treat the estimated entropy value given as  $S^\circ(298.15 \text{ K})$  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  $\text{MoI}_3$  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  $\text{I}/\text{Mo}$  varied from 3.00 to 2.5. The crystal structure of  $\text{MoI}_3$  is  $\text{OPI}6$  in the Pearson classification system.

**Decomposition Data**

$T_{\text{dec}}$  of 629.5 K is calculated as the decomposition temperature at which the fugacity of iodine is 1 atm for the dissociation reaction  $\text{MoI}_3(\text{cr}) = \text{MoI}(\text{cr}) + 0.5 \text{ I}_2(\text{g})$ . Saturated vapor pressure measurements by Drobot *et al.*<sup>3</sup> indicate that  $\text{MoI}_3(\text{cr})$  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. 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. Bor'chakov, and V. L. Sbitnev, *Russ. J. Inorg. Chem.* **23**, 5, 643 (1978).

|        |         | <b><math>\text{I}_3\text{MoI}_3</math> Molybdenum Iodide (<math>\text{MoI}_3</math>)</b> |             |                                                                          |                             |                                                     |                    |
|--------|---------|------------------------------------------------------------------------------------------|-------------|--------------------------------------------------------------------------|-----------------------------|-----------------------------------------------------|--------------------|
|        |         |                                                                                          |             |                                                                          |                             |                                                     |                    |
|        |         | $\Delta H^\circ(0 \text{ K}) = \text{Unknown}$                                           |             | $\Delta H^\circ(298.15 \text{ K}) = -124.68 \pm 8.4 \text{ kJ mol}^{-1}$ |                             | $\Delta H^\circ(298.15 \text{ K}) = \text{Unknown}$ |                    |
|        |         | $T/\text{K}$                                                                             | $C_p^\circ$ | $S^\circ$                                                                | $-(G^\circ - H^\circ(T))/T$ | $H^\circ - H^\circ(T_s)$                            | $\Delta_f G^\circ$ |
| 0      |         |                                                                                          |             |                                                                          |                             |                                                     |                    |
| 100    |         |                                                                                          |             |                                                                          |                             |                                                     |                    |
| 200    |         |                                                                                          |             |                                                                          |                             |                                                     |                    |
| 298.15 | 108.889 | 195.393                                                                                  | 195.393     | 0.                                                                       | -124.683                    | -122.469                                            | 21.456             |
| 300    | 108.918 | 196.066                                                                                  | 195.395     | 0.201                                                                    | -124.677                    | -122.456                                            | 21.321             |
| 400    | 108.933 | 227.628                                                                                  | 199.887     | 11.177                                                                   | -148.615                    | -120.905                                            | 15.789             |
| 500    | 112.244 | 252.483                                                                                  | 207.847     | 22.318                                                                   | -212.317                    | -107.872                                            | 11.269             |
| 600    | 113.909 | 273.094                                                                                  | 217.052     | 33.626                                                                   | -209.257                    | -87.269                                             | 7.597              |
| 700    | 115.570 | 290.778                                                                                  | 226.550     | 45.100                                                                   | -206.107                    | -67.185                                             | 3.105              |
| 800    | 117.231 | 306.319                                                                                  | 235.934     | 56.740                                                                   | -202.857                    | -47.539                                             | 3.105              |
| 900    | 118.897 | 320.223                                                                                  | 244.061     | 68.546                                                                   | -199.502                    | -28.347                                             | 1.645              |
| 1000   | 120.558 | 332.836                                                                                  | 252.317     | 80.519                                                                   | -196.045                    | -9.515                                              | 0.497              |

**Phase Data**

Drobot *et al.*<sup>3</sup> have studied the thermal decomposition of  $\text{MoI}_3$  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  $\text{I}/\text{Mo}$  varied from 3.00 to 2.5. The crystal structure of  $\text{MoI}_3$  is  $\text{OPI}6$  in the Pearson classification system.

**Decomposition Data**

$T_{\text{dec}}$  of 629.5 K is calculated as the decomposition temperature at which the fugacity of iodine is 1 atm for the dissociation reaction  $\text{MoI}_3(\text{cr}) = \text{MoI}(\text{cr}) + 0.5 \text{ I}_2(\text{g})$ . Saturated vapor pressure measurements by Drobot *et al.*<sup>3</sup> indicate that  $\text{MoI}_3(\text{cr})$  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. 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. Bor'chakov, and V. L. Sbitnev, *Russ. J. Inorg. Chem.* **23**, 5, 643 (1978).

PREVIOUS:

CURRENT: September 1978

 **$\text{I}_3\text{MoI}_3$  Molybdenum Iodide ( $\text{MoI}_3$ )**

## IDEAL GAS

Molybdenum Iodide ( $\text{MoI}_3$ ) $M_r = 476.6535$  Molybdenum Iodide ( $\text{MoI}_3$ )

$$S^\circ(298.15 \text{ K}) = [403.532 \pm 8.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(0 \text{ K}) = [186.15 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = [182.84 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$$

| Electronic Levels and Quantum Weights<br>$\epsilon_i$ , cm <sup>-1</sup><br>g, |   |
|--------------------------------------------------------------------------------|---|
| [0]                                                                            | 2 |
| [3505.4]                                                                       | 2 |
| [10861.0]                                                                      | 4 |
| [11062.0]                                                                      | 4 |

| Vibrational Frequencies and Degeneracies<br>$\nu$ , cm <sup>-1</sup> |  |
|----------------------------------------------------------------------|--|
| [110](1)                                                             |  |
| [75](1)                                                              |  |
| [200](2)                                                             |  |
| [60](2)                                                              |  |

Point Group: [D<sub>3d</sub>] $\sigma = [6]$ 

Bond Distance: Mo-I = [2.66] Å

Bond Angle: I-Mo-I = [112]°

Product of the Moments of Inertia:  $I_{ABIC} = [2.237654 \times 10^{-10}] \text{ g}\cdot\text{cm}^6$ 

## Enthalpy of Formation

The adopted value of  $\Delta_f H^\circ$  at 298.15 K is that estimated by Brewer.<sup>1</sup> A planar structure has been predicted for  $\text{MoI}_3$  by Drak and molybdenum in iodine vapor reported by Schafer *et al.*<sup>2</sup> The estimated value given by Brewer is  $\Delta_f H^\circ(298.15 \text{ K})R = 22000 \pm 3000 \text{ K}$ . The assigned uncertainty ( $\pm 10 \text{ kcal}\cdot\text{mol}^{-1}$ ) is determined from the product  $S^\circ \times R$  which has been rounded to the nearest  $\text{kcal}\cdot\text{mol}^{-1}$ . The value of  $\Delta_f H^\circ(0 \text{ K})$  combined with JANAF data for Mo(g) and I(g) gives  $\Delta_u H^\circ(0 \text{ K}) = 189 \pm 11 \text{ kcal}\cdot\text{mol}^{-1}$  and an average Mo-I bond energy of  $\Delta_u H^\circ(0 \text{ K})Y_3 = 63 \pm 4 \text{ kcal}\cdot\text{mol}^{-1}$ .

## 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  $\text{MoI}_3$  by Drak and Rosenblatt.<sup>3</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>4</sup> however, we only include four levels. The principal moments of inertia are:  $I_x = I_y = 223.6596 \times 10^{-39}$ , and  $I_z = 447.3193 \times 10^{-39} \text{ g}\cdot\text{cm}^2$ .

## References

- <sup>1</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>2</sup>H. Schafer, T. Grotz, and M. M. Trenkel, *J. Solid State Chem.* **8**, 14 (1973).
- <sup>3</sup>JANAF Thermochemical Tables: Mo(g), 3-31-78; I(g), 3-30-74; TaO(g), 12-31-73.
- <sup>4</sup>M. C. Drake and G. M. Rosenblatt, Paper 388, The Electrochemical Society, Atlanta, Georgia, (October 1977).

 $\text{I}_3\text{Mo}_1(\text{g})$ 

|        |        | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |             |                                          |                            | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                    |            |  |
|--------|--------|-----------------------------------------------------------|-------------|------------------------------------------|----------------------------|-------------------------------------------------------|--------------------|------------|--|
|        |        | $T/K$                                                     | $C_p^\circ$ | $S^\circ - [C^\circ - H^\circ(T_r)/T]/T$ | $H^\circ - H^\circ(T_r)/T$ | $\Delta_f H^\circ$                                    | $\Delta_f G^\circ$ | $\log K_r$ |  |
| 0      | 0      | 0                                                         | 0           | 0.0                                      | -INFINITE                  | -21,071                                               | 186,152            | INFINITE   |  |
| 100    | 71,920 | 318,351                                                   | 474,458     | -15,611                                  | 186,546                    | 164,562                                               | -85,958            |            |  |
| 200    | 79,674 | 371,309                                                   | 410,943     | -7,927                                   | 184,589                    | 143,110                                               | -57,777            |            |  |
| 250    | 80,859 | 389,229                                                   | 404,871     | -3,910                                   | 183,946                    | 132,758                                               | -27,738            |            |  |
| 298.15 | 81,513 | 403,532                                                   | 403,532     | 0                                        | 182,841                    | 122,998                                               | -21,549            |            |  |
| 300    | 81,532 | 404,036                                                   | 403,533     | 0.151                                    | 182,796                    | 122,627                                               | -21,352            |            |  |
| 350    | 81,949 | 416,638                                                   | 404,528     | 4,239                                    | 181,452                    | 112,797                                               | -16,820            |            |  |
| 400    | 82,227 | 427,600                                                   | 406,742     | 8,343                                    | 180,787                    | 103,797                                               | -13,554            |            |  |
| 450    | 82,427 | 437,297                                                   | 409,608     | 12,460                                   | 152,878                    | 97,454                                                | -11,312            |            |  |
| 500    | 82,585 | 445,990                                                   | 412,819     | 16,385                                   | 89,474                     | 97,166                                                | -10,151            |            |  |
| 600    | 82,861 | 471,072                                                   | 419,642     | 89,499                                   | 89,701                     | -8,593                                                |                    |            |  |
| 700    | 83,159 | 473,867                                                   | 426,497     | 33,159                                   | 89,476                     | 100,236                                               | -7,480             |            |  |
| 800    | 83,512 | 484,994                                                   | 433,129     | 41,492                                   | 89,419                     | 101,777                                               | -6,645             |            |  |
| 900    | 83,914 | 494,853                                                   | 439,450     | 49,953                                   | 89,338                     | 103,326                                               | -5,997             |            |  |
| 1000   | 84,342 | 503,716                                                   | 445,441     | 58,275                                   | 89,236                     | 104,886                                               | -5,479             |            |  |
| 1100   | 84,772 | 511,775                                                   | 451,110     | 66,731                                   | 89,106                     | 106,457                                               | -5,053             |            |  |
| 1200   | 85,183 | 519,169                                                   | 466,478     | 75,229                                   | 88,936                     | 108,041                                               | -4,703             |            |  |
| 1300   | 85,562 | 526,002                                                   | 461,566     | 83,767                                   | 88,709                     | 109,642                                               | -4,405             |            |  |
| 1400   | 85,906 | 532,356                                                   | 466,399     | 92,240                                   | 88,402                     | 111,264                                               | -4,151             |            |  |
| 1500   | 86,214 | 538,294                                                   | 470,996     | 100,347                                  | 87,992                     | 112,910                                               | -3,932             |            |  |
| 1600   | 86,492 | 543,867                                                   | 475,378     | 109,582                                  | 87,455                     | 114,588                                               | -3,741             |            |  |
| 1700   | 86,745 | 549,118                                                   | 479,563     | 118,244                                  | 86,768                     | 116,304                                               | -3,574             |            |  |
| 1800   | 86,980 | 554,083                                                   | 483,566     | 126,931                                  | 85,912                     | 118,065                                               | -3,426             |            |  |
| 1900   | 87,205 | 558,792                                                   | 487,402     | 135,540                                  | 84,879                     | 119,879                                               | -3,296             |            |  |
| 2000   | 87,425 | 563,270                                                   | 491,085     | 143,771                                  | 83,636                     | 121,753                                               | -3,180             |            |  |
| 2100   | 87,644 | 567,541                                                   | 494,625     | 153,125                                  | 82,201                     | 123,693                                               | -3,077             |            |  |
| 2200   | 87,865 | 571,674                                                   | 498,032     | 161,900                                  | 80,566                     | 125,706                                               | -2,985             |            |  |
| 2300   | 88,090 | 575,534                                                   | 501,318     | 170,698                                  | 78,730                     | 127,798                                               | -2,902             |            |  |
| 2400   | 88,318 | 579,288                                                   | 504,489     | 179,319                                  | 76,702                     | 129,974                                               | -2,829             |            |  |
| 2500   | 88,550 | 582,898                                                   | 507,533     | 188,362                                  | 74,486                     | 132,239                                               | -2,763             |            |  |
| 2600   | 88,784 | 586,376                                                   | 510,519     | 197,229                                  | 70,078                     | 134,596                                               | -2,704             |            |  |
| 2700   | 89,018 | 589,331                                                   | 513,391     | 206,119                                  | 69,455                     | 137,050                                               | -2,651             |            |  |
| 2800   | 89,250 | 592,972                                                   | 516,175     | 215,032                                  | 68,574                     | 139,605                                               | -2,604             |            |  |
| 2900   | 89,479 | 596,108                                                   | 518,878     | 223,969                                  | 21,483                     | 142,318                                               | -2,563             |            |  |
| 3000   | 89,702 | 599,146                                                   | 521,500     | 232,928                                  | 25,922                     | 146,302                                               | -2,547             |            |  |
| 3100   | 89,917 | 602,091                                                   | 524,055     | 241,909                                  | 24,427                     | 150,343                                               | -2,533             |            |  |
| 3200   | 90,122 | 604,948                                                   | 526,539     | 250,911                                  | 21,008                     | 154,427                                               | -2,521             |            |  |
| 3300   | 90,316 | 607,200                                                   | 528,937     | 259,933                                  | 21,675                     | 158,535                                               | -2,510             |            |  |
| 3400   | 90,498 | 610,424                                                   | 531,314     | 268,973                                  | 20,433                     | 162,721                                               | -2,500             |            |  |
| 3500   | 90,666 | 613,049                                                   | 533,612     | 278,032                                  | 19,287                     | 166,924                                               | -2,491             |            |  |
| 3600   | 90,819 | 615,606                                                   | 535,854     | 287,106                                  | 18,239                     | 171,157                                               | -2,483             |            |  |
| 3700   | 90,957 | 618,996                                                   | 538,043     | 296,195                                  | 17,293                     | 175,418                                               | -2,476             |            |  |
| 3800   | 91,081 | 620,523                                                   | 540,182     | 305,297                                  | 16,447                     | 179,703                                               | -2,470             |            |  |
| 3900   | 91,188 | 622,890                                                   | 542,277     | 314,411                                  | 15,055                     | 184,009                                               | -2,465             |            |  |
| 4000   | 91,294 | 625,200                                                   | 544,317     | 323,334                                  | 15,055                     | 188,333                                               | -2,459             |            |  |
| 4100   | 91,357 | 627,455                                                   | 546,317     | 332,666                                  | 14,506                     | 192,672                                               | -2,455             |            |  |
| 4200   | 91,418 | 629,658                                                   | 548,275     | 341,805                                  | 14,052                     | 197,023                                               | -2,450             |            |  |
| 4300   | 91,466 | 631,089                                                   | 550,193     | 350,949                                  | 13,689                     | 201,384                                               | -2,446             |            |  |
| 4400   | 91,499 | 633,912                                                   | 552,072     | 360,098                                  | 13,414                     | 205,752                                               | -2,443             |            |  |
| 4500   | 91,519 | 635,969                                                   | 553,914     | 369,249                                  | 13,224                     | 210,126                                               | -2,439             |            |  |
| 4600   | 91,527 | 637,980                                                   | 555,719     | 378,401                                  | 13,116                     | 214,503                                               | -2,436             |            |  |
| 4700   | 91,532 | 639,949                                                   | 557,491     | 387,754                                  | 13,085                     | 218,881                                               | -2,433             |            |  |
| 4800   | 91,507 | 641,876                                                   | 559,229     | 396,705                                  | 13,128                     | 223,260                                               | -2,430             |            |  |
| 4900   | 91,481 | 643,762                                                   | 560,935     | 405,855                                  | 13,241                     | 227,637                                               | -2,427             |            |  |
| 5000   | 91,446 | 645,610                                                   | 562,610     | 415,001                                  | 13,794                     | 237,741                                               | -2,484             |            |  |
| 5100   | 91,402 | 647,420                                                   | 564,255     | 424,144                                  | 13,427                     | 254,070                                               | -2,602             |            |  |
| 5200   | 91,349 | 649,195                                                   | 563,871     | 433,281                                  | 13,282                     | 270,427                                               | -2,716             |            |  |
| 5300   | 91,290 | 650,934                                                   | 567,460     | 442,413                                  | 13,166                     | 286,814                                               | -2,827             |            |  |
| 5400   | 91,223 | 652,640                                                   | 569,022     | 451,539                                  | 13,053                     | 303,233                                               | -2,933             |            |  |
| 5500   | 91,151 | 654,413                                                   | 570,557     | 460,658                                  | 13,036                     | 319,683                                               | -3,036             |            |  |
| 5600   | 91,073 | 655,955                                                   | 572,068     | 469,769                                  | 13,086                     | 336,168                                               | -3,136             |            |  |
| 5700   | 90,991 | 657,566                                                   | 573,554     | 478,872                                  | 13,086                     | 352,686                                               | -3,232             |            |  |
| 5800   | 90,904 | 659,148                                                   | 575,016     | 487,967                                  | 13,086                     | 369,240                                               | -3,325             |            |  |
| 5900   | 90,813 | 660,701                                                   | 576,455     | 497,053                                  | 13,086                     | 385,830                                               | -3,416             |            |  |
| 6000   | 90,720 | 662,227                                                   | 577,872     | 506,129                                  | 13,086                     | 402,457                                               | -3,504             |            |  |

CURRENT September 1978 (1 atm)

Molybdenum Iodide ( $\text{MoI}_3$ )

## NIST-JANAF THERMOCHEMICAL TABLES

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

## IDEAL GAS

$$S^o(298.15\text{ K}) = [378.305 \pm 8.4]\text{ J K}^{-1}\text{-mol}^{-1}$$

$$\Delta H^o(0\text{ K}) = [39.75 \pm 62.8]\text{ kJ-mol}^{-1}$$

$$\Delta H^o(298.15\text{ K}) = [35.31 \pm 62.8]\text{ kJ-mol}^{-1}$$

|                                                                                                       | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |         |                                       |         | Standard State Pressure = $p^* = 0.1\text{ MPa}$ |                   |                                 |              |
|-------------------------------------------------------------------------------------------------------|----------------------------------------------------------|---------|---------------------------------------|---------|--------------------------------------------------|-------------------|---------------------------------|--------------|
|                                                                                                       | $T/\text{K}$                                             | $C_p^*$ | $J\cdot\text{K}^{-1}\text{-mol}^{-1}$ | $S^o$   | $\text{J}\cdot\text{K}^{-1}\text{-mol}^{-1}$     | $H^o - H(T_r)/JT$ | $\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta G^o$ |
| Vibrational Frequencies and Degeneracies<br>$\nu, \text{cm}^{-1}$                                     | 0                                                        | 0       | 0                                     | 0       | INFINITE                                         | -18.578           | 39.751                          | 39.751       |
| [286](1)<br>[122](1)<br>[399](2)<br>[80](2)                                                           | 100                                                      | 58.786  | 303.097                               | 442.837 | -13.974                                          | 39.514            | 187.36                          | -9.787       |
|                                                                                                       | 200                                                      | 71.973  | 348.463                               | 385.228 | -7.353                                           | 37.557            | 5.315                           | 0.343        |
|                                                                                                       | 250                                                      | 75.152  | 364.381                               | 379.365 | -3.671                                           | 36.448            | -10.907                         | 2.279        |
|                                                                                                       | 298.15                                                   | 77.191  | 378.305                               | 378.305 | 0.                                               | 35.314            | -19.925                         | 3.491        |
|                                                                                                       | 300                                                      | 77.254  | 378.783                               | 378.305 | 0.143                                            | 35.268            | -20.688                         | 3.529        |
|                                                                                                       | 350                                                      | 78.652  | 390.803                               | 379.253 | 4.043                                            | 33.916            | -29.421                         | 4.391        |
|                                                                                                       | 400                                                      | 79.619  | 401.373                               | 381.276 | 8.001                                            | 38.548            | -37.551                         | 4.904        |
|                                                                                                       | 450                                                      | 80.310  | 410.793                               | 384.126 | 12.000                                           | 5.373             | -43.123                         | 5.006        |
|                                                                                                       | 500                                                      | 80.320  | 419.282                               | 387.224 | 16.029                                           | -57.997           | -42.643                         | 4.455        |
|                                                                                                       | 600                                                      | 81.503  | 434.083                               | 393.836 | 24.148                                           | -57.885           | -39.583                         | 3.446        |
|                                                                                                       | 700                                                      | 81.926  | 446.681                               | 400.508 | 32.321                                           | -57.811           | -36.539                         | 2.727        |
|                                                                                                       | 800                                                      | 82.206  | 457.640                               | 406.579 | 40.529                                           | -57.781           | -33.503                         | 2.188        |
|                                                                                                       | 900                                                      | 82.399  | 467.234                               | 415.157 | 48.759                                           | -57.758           | -30.467                         | 1.768        |
|                                                                                                       | 1000                                                     | 82.339  | 476.023                               | 419.917 | 57.007                                           | -57.864           | -27.428                         | 1.433        |
|                                                                                                       | 1100                                                     | 82.643  | 483.895                               | 424.563 | 65.266                                           | -57.984           | -24.379                         | 1.158        |
|                                                                                                       | 1200                                                     | 82.722  | 491.090                               | 429.811 | 73.534                                           | -58.163           | -21.316                         | 0.928        |
|                                                                                                       | 1300                                                     | 82.784  | 497.714                               | 434.783 | 81.810                                           | -58.412           | -18.236                         | 0.733        |
|                                                                                                       | 1400                                                     | 82.833  | 503.850                               | 439.500 | 90.091                                           | -58.744           | -15.134                         | 0.565        |
|                                                                                                       | 1500                                                     | 82.873  | 509.567                               | 443.983 | 98.376                                           | -59.174           | -12.004                         | 0.418        |
| Ground State Quantum Weight [2]                                                                       |                                                          |         |                                       |         |                                                  |                   |                                 |              |
| Point Group: [C <sub>3</sub> ]                                                                        |                                                          |         |                                       |         |                                                  |                   |                                 |              |
| Bond Distance: Si-I = [2.425] Å                                                                       |                                                          |         |                                       |         |                                                  |                   |                                 |              |
| Bond Angle: I-Si-I = [112] <sup>o</sup>                                                               |                                                          |         |                                       |         |                                                  |                   |                                 |              |
| Product of the Moments of Inertia: $I_A/I_B/I_C = [1.038908 \times 10^{-10}] \text{ g}^3\text{-cm}^6$ |                                                          |         |                                       |         |                                                  |                   |                                 |              |

**Enthalpy of Formation**  
The enthalpy of formation of SiI<sub>3</sub>(g) is based on an assumed average bond energy of 58 ± 5 kcal·mol<sup>-1</sup>. This average bond energy is that of Si(g), i.e.,  $\Delta_H^o(\text{SiI}_3\text{g}, 0\text{ K})$ . 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 SiHI<sub>3</sub>.<sup>1</sup> From this structure we estimate the following principal moments of inertia:  $I_A = I_B = 173.9077 \times 10^{-30}$ , and  $I_C = 343.5099 \times 10^{-30} \text{ g cm}^2$ . The vibrational frequencies are assumed to be those of the SiI<sub>3</sub> group in SiHI<sub>3</sub>(g).

## Reference

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

|                                                                                                       | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |         |                                       |         | Standard State Pressure = $p^* = 0.1\text{ MPa}$ |                   |                                 |              |            |
|-------------------------------------------------------------------------------------------------------|----------------------------------------------------------|---------|---------------------------------------|---------|--------------------------------------------------|-------------------|---------------------------------|--------------|------------|
|                                                                                                       | $T/\text{K}$                                             | $C_p^*$ | $J\cdot\text{K}^{-1}\text{-mol}^{-1}$ | $S^o$   | $\text{J}\cdot\text{K}^{-1}\text{-mol}^{-1}$     | $H^o - H(T_r)/JT$ | $\text{kJ}\cdot\text{mol}^{-1}$ | $\Delta G^o$ | $\log K_r$ |
| Vibrational Frequencies and Degeneracies<br>$\nu, \text{cm}^{-1}$                                     | 0                                                        | 0       | 0                                     | 0       | INFINITE                                         | -18.578           | 39.751                          | 39.751       | INFITE     |
| [286](1)<br>[122](1)<br>[399](2)<br>[80](2)                                                           | 100                                                      | 58.786  | 303.097                               | 442.837 | -13.974                                          | 39.514            | 187.36                          | -9.787       | -0.343     |
|                                                                                                       | 200                                                      | 71.973  | 348.463                               | 385.228 | -7.353                                           | 37.557            | 5.315                           | 0.343        | 0.343      |
|                                                                                                       | 250                                                      | 75.152  | 364.381                               | 379.365 | -3.671                                           | 36.448            | -10.907                         | 2.279        | 2.279      |
|                                                                                                       | 298.15                                                   | 77.191  | 378.305                               | 378.305 | 0.                                               | 35.314            | -19.925                         | 3.491        | 3.491      |
|                                                                                                       | 300                                                      | 77.254  | 378.783                               | 378.305 | 0.143                                            | 35.268            | -20.688                         | 3.529        | 3.529      |
|                                                                                                       | 350                                                      | 78.652  | 390.803                               | 379.253 | 4.043                                            | 33.916            | -29.421                         | 4.391        | 4.391      |
|                                                                                                       | 400                                                      | 79.619  | 401.373                               | 381.276 | 8.001                                            | 38.548            | -37.551                         | 4.904        | 4.904      |
|                                                                                                       | 450                                                      | 80.310  | 410.793                               | 384.126 | 12.000                                           | 5.373             | -43.123                         | 5.006        | 5.006      |
|                                                                                                       | 500                                                      | 80.320  | 419.282                               | 387.224 | 16.029                                           | -57.997           | -42.643                         | 4.455        | 4.455      |
|                                                                                                       | 600                                                      | 81.503  | 434.083                               | 393.836 | 24.148                                           | -57.885           | -39.583                         | 3.446        | 3.446      |
|                                                                                                       | 700                                                      | 81.926  | 446.681                               | 400.508 | 32.321                                           | -57.811           | -36.539                         | 2.727        | 2.727      |
|                                                                                                       | 800                                                      | 82.206  | 457.640                               | 406.579 | 40.529                                           | -57.781           | -33.503                         | 2.188        | 2.188      |
|                                                                                                       | 900                                                      | 82.399  | 467.234                               | 415.157 | 48.759                                           | -57.758           | -30.467                         | 1.768        | 1.768      |
|                                                                                                       | 1000                                                     | 82.339  | 476.023                               | 419.917 | 57.007                                           | -57.864           | -27.428                         | 1.433        | 1.433      |
|                                                                                                       | 1100                                                     | 82.643  | 483.895                               | 424.563 | 65.266                                           | -57.984           | -24.379                         | 1.158        | 1.158      |
|                                                                                                       | 1200                                                     | 82.722  | 491.090                               | 429.811 | 73.534                                           | -58.163           | -21.316                         | 0.928        | 0.928      |
|                                                                                                       | 1300                                                     | 82.784  | 497.714                               | 434.783 | 81.810                                           | -58.412           | -18.236                         | 0.733        | 0.733      |
|                                                                                                       | 1400                                                     | 82.833  | 503.850                               | 439.500 | 90.091                                           | -58.744           | -15.134                         | 0.565        | 0.565      |
|                                                                                                       | 1500                                                     | 82.873  | 509.567                               | 443.983 | 98.376                                           | -59.174           | -12.004                         | 0.418        | 0.418      |
| Ground State Quantum Weight [2]                                                                       |                                                          |         |                                       |         |                                                  |                   |                                 |              |            |
| Point Group: [C <sub>3</sub> ]                                                                        |                                                          |         |                                       |         |                                                  |                   |                                 |              |            |
| Bond Distance: Si-I = [2.425] Å                                                                       |                                                          |         |                                       |         |                                                  |                   |                                 |              |            |
| Bond Angle: I-Si-I = [112] <sup>o</sup>                                                               |                                                          |         |                                       |         |                                                  |                   |                                 |              |            |
| Product of the Moments of Inertia: $I_A/I_B/I_C = [1.038908 \times 10^{-10}] \text{ g}^3\text{-cm}^6$ |                                                          |         |                                       |         |                                                  |                   |                                 |              |            |

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

PREVIOUS: December 1977 (1 atm)

CURRENT: December 1977 (1 bar)

**Titanium Iodide ( $TiI_3$ )****CRYSTAL** **$Ti_3Ti_1(cr)$** 

$$\Delta_f^{\circ}H^{\circ}(298.15\text{ K}) = [192.464 \pm 8.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{abs}} = [1000] \text{ K}$$

**Enthalpy of Formation**

The enthalpy of formation of  $Ti_3(cr)$  is calculated from the free energy of formation at 623 K combined with the increment  $\Delta_f^{\circ}G^{\circ}(623\text{ K}) - \Delta_f^{\circ}G^{\circ}(298.15\text{ K})$  and the entropies,  $S^{\circ}(298.15\text{ K})$ , of  $Ti_3(cr)$ ,  $Ti_3(cr)$  and  $Ti_4(g)$ . The free energy of formation,  $\Delta_f^{\circ}G^{\circ}(623\text{ K})$ , is estimated such that  $\Delta_f^{\circ}G^{\circ}(623\text{ K}) = 0$  for the process  $2Ti_3(cr) = Ti_2(cr) + Ti_4(g)$ . This assumption is based on the observations of Hercog and Pidgeon<sup>1</sup> and Fast<sup>2</sup>.

**Heat Capacity and Entropy**

The heat capacities of  $Ti_3(cr)$  and the value of  $S^{\circ}(298.15\text{ K})$  estimated by Kelley<sup>3</sup> have been adopted.

**Sublimation Data**

The enthalpy of sublimation of  $Ti_3(cr)$  is taken as the difference in the enthalpies of formation of  $Ti_3(cr)$  and  $Ti_3(g)$  at the sublimation temperature. The sublimation temperature is estimated as the point at which  $\Delta_f^{\circ}G^{\circ} = 0$  for the process  $Ti_3(cr) = Ti_3(g)$ .

**References**

- <sup>1</sup>A. Hercog 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. Kelley, U. S. Bur. Mines Bull. 584, 232 pp. 1960; U. S. Bur. Mines Bull. 592, 149 pp. (1961).

 **$M_r = 428.5935$  Titanium Iodide ( $TiI_3$ )**

| $T/K$  | $C_p^{\circ}$ | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                                                                                   | Standard State Pressure = $p^{\circ} = 0.1 \text{ MPa}$ |                            |
|--------|---------------|----------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------|----------------------------|
|        |               | $\Delta_f^{\circ}H^{\circ}(0\text{ K}) = \text{Unknown}$ | $\Delta_f^{\circ}H^{\circ}(298.15\text{ K}) = [1-322.17 \pm 20.9] \text{ kJ}\cdot\text{mol}^{-1}$ | $S^{\circ} = -(G^{\circ}-H^{\circ}(T_r))/T$             | $H^{\circ}-H^{\circ}(T_r)$ |
| 100    | 0             |                                                          |                                                                                                   |                                                         |                            |
| 200    | 116.711       | 192.464                                                  | 192.464                                                                                           | 0                                                       | -322.168                   |
| 298.15 | 116.711       | 192.464                                                  | 192.464                                                                                           | 0                                                       | -322.168                   |
| 300    | 116.784       | 193.186                                                  | 192.466                                                                                           | 0.216                                                   | -322.150                   |
| 400    | 175.112       | 226.983                                                  | 197.056                                                                                           | 11.931                                                  | -345.506                   |
| 500    | 182.40        | 253.183                                                  | 205.746                                                                                           | 23.718                                                  | -408.753                   |
| 600    | 188.968       | 274.805                                                  | 215.507                                                                                           | 35.579                                                  | -405.350                   |
| 700    | 195.696       | 293.199                                                  | 223.324                                                                                           | 47.512                                                  | -401.156                   |
| 800    | 202.424       | 309.229                                                  | 234.832                                                                                           | 59.518                                                  | -398.543                   |
| 900    | 121.152       | 323.455                                                  | 243.903                                                                                           | 71.597                                                  | -395.141                   |
| 1000   | 121.880       | 336.257                                                  | 252.509                                                                                           | 83.748                                                  | -391.813                   |
| 1100   | 122.608       | 347.908                                                  | 260.660                                                                                           | 95.973                                                  | -388.627                   |
| 1200   | 123.336       | 358.607                                                  | 268.383                                                                                           | 108.270                                                 | -389.573                   |
| 1300   | 124.064       | 368.508                                                  | 275.708                                                                                           | 120.640                                                 | -385.968                   |
| 1400   | 124.792       | 377.729                                                  | 282.670                                                                                           | 133.083                                                 | -382.414                   |
| 1500   | 125.520       | 386.364                                                  | 289.298                                                                                           | 145.598                                                 | -378.940                   |

PREVIOUS June 1964

CURRENT December 1968

## NIST-JANAF THERMOCHEMICAL TABLES

TITANIUM IODIDE (TiI<sub>3</sub>)

## IDEAL GAS

$$S^{\circ}(298.15 \text{ K}) = [382.164 \pm 12.6] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

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

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

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

|                                       |        | Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K |         |                                                                        |         | Standard State Pressure = p <sup>o</sup> = 0.1 MPa  |          |                      |          |
|---------------------------------------|--------|------------------------------------------------------------|---------|------------------------------------------------------------------------|---------|-----------------------------------------------------|----------|----------------------|----------|
|                                       |        | T/K                                                        |         | C <sub>p</sub> , J·K <sup>-1</sup> ·mol <sup>-1</sup>                  |         | H <sup>°</sup> - H <sup>°</sup> (T <sub>r</sub> )/T |          | kJ·mol <sup>-1</sup> |          |
|                                       |        | T/K                                                        |         | S <sup>°</sup> - [G <sup>°</sup> - H <sup>°</sup> (T <sub>r</sub> )]/T |         | ΔH <sup>°</sup>                                     |          | ΔG <sup>°</sup>      |          |
| Electronic Levels and Quantum Weights |        | 0                                                          | 0       | 0                                                                      | 0       | 0                                                   | 0        | 0                    | 0        |
| ε, cm <sup>-1</sup>                   | g      | 100                                                        | 58.519  | 305.563                                                                | 448.602 | -14.304                                             | -144.511 | -144.511             | -144.511 |
| ε, cm <sup>-1</sup>                   | g      | 200                                                        | 73.632  | 351.232                                                                | 389.367 | -7.627                                              | -165.600 | 86.500               | 86.500   |
| ε, cm <sup>-1</sup>                   | g      | 250                                                        | 78.018  | 368.168                                                                | 383.480 | -3.828                                              | -185.170 | 48.362               | 48.362   |
| 298.15                                | 80.800 | 382.164                                                    | 382.164 | 0.                                                                     | 0.      | -194.397                                            | -194.397 | 40.617               | 40.617   |
| 300                                   | 80.886 | 382.164                                                    | 382.166 | 0.150                                                                  | 0.150   | -203.035                                            | -203.035 | 35.571               | 35.571   |
| 350                                   | 82.769 | 395.284                                                    | 383.158 | 4.244                                                                  | 4.244   | -203.363                                            | -203.363 | 35.409               | 35.409   |
| 400                                   | 84.024 | 406.424                                                    | 385.384 | 8.416                                                                  | 8.416   | -212.107                                            | -212.107 | 31.635               | 31.635   |
| 450                                   | 84.370 | 416.373                                                    | 388.284 | 12.640                                                                 | 12.640  | -219.822                                            | -219.822 | 28.706               | 28.706   |
| 500                                   | 85.440 | 425.346                                                    | 391.549 | 16.899                                                                 | 16.899  | -224.976                                            | -224.976 | 26.114               | 26.114   |
| 600                                   | 86.063 | 440.987                                                    | 398.523 | 25.478                                                                 | 25.478  | -23.409                                             | -23.409  | -224.077             | -224.077 |
| 700                                   | 86.063 | 454.275                                                    | 405.563 | 34.099                                                                 | 34.099  | -19.169                                             | -19.169  | -220.183             | -220.183 |
| 800                                   | 86.163 | 465.804                                                    | 412.388 | 51.369                                                                 | 51.369  | -16.141                                             | -16.141  | -216.305             | -216.305 |
| 900                                   | 86.344 | 475.976                                                    | 418.900 | 51.369                                                                 | 51.369  | -13.871                                             | -13.871  | -212.437             | -212.437 |
| 1000                                  | 86.297 | 485.071                                                    | 425.070 | 60.001                                                                 | 60.001  | -10.820                                             | -10.820  | -204.490             | -204.490 |
| 1100                                  | 86.242 | 493.293                                                    | 430.904 | 68.628                                                                 | 68.628  | -7.534                                              | -7.534   | -200.782             | -200.782 |
| 1200                                  | 86.187 | 500.795                                                    | 436.420 | 77.249                                                                 | 77.249  | -5.562                                              | -5.562   | -196.705             | -196.705 |
| 1300                                  | 86.133 | 507.691                                                    | 441.541 | 88.865                                                                 | 88.865  | -3.536                                              | -3.536   | -192.373             | -192.373 |
| 1400                                  | 86.083 | 514.073                                                    | 446.520 | 94.476                                                                 | 94.476  | -1.505                                              | -1.505   | -188.024             | -188.024 |
| 1500                                  | 86.034 | 520.010                                                    | 451.289 | 103.082                                                                | 103.082 | -0.494                                              | -0.494   | -183.651             | -183.651 |
| 1600                                  | 86.988 | 525.561                                                    | 455.759 | 111.683                                                                | 111.683 | -0.447                                              | -0.447   | -179.242             | -179.242 |
| 1700                                  | 85.943 | 530.773                                                    | 460.020 | 120.943                                                                | 120.943 | -5.371                                              | -5.371   | -174.788             | -174.788 |
| 1800                                  | 85.900 | 535.684                                                    | 464.088 | 128.871                                                                | 128.871 | -170.279                                            | -170.279 | -170.279             | -170.279 |
| 1900                                  | 85.862 | 540.327                                                    | 467.980 | 137.459                                                                | 137.459 | -165.104                                            | -165.104 | -165.104             | -165.104 |
| 2000                                  | 85.822 | 544.730                                                    | 471.708 | 146.044                                                                | 146.044 | -160.590                                            | -160.590 | -160.590             | -160.590 |
| 2100                                  | 85.787 | 548.917                                                    | 475.286 | 154.624                                                                | 154.624 | -152.195                                            | -152.195 | -151.086             | -151.086 |
| 2200                                  | 85.754 | 552.907                                                    | 478.724 | 163.201                                                                | 163.201 | -147.838                                            | -147.838 | -147.838             | -147.838 |
| 2300                                  | 85.723 | 556.718                                                    | 482.033 | 171.775                                                                | 171.775 | -142.447                                            | -142.447 | -142.447             | -142.447 |
| 2400                                  | 85.693 | 560.366                                                    | 485.221 | 180.346                                                                | 180.346 | -145.683                                            | -145.683 | -145.683             | -145.683 |
| 2500                                  | 85.669 | 563.863                                                    | 488.298 | 189.914                                                                | 189.914 | -157.795                                            | -157.795 | -157.795             | -157.795 |
| 2600                                  | 85.644 | 567.223                                                    | 491.269 | 197.479                                                                | 197.479 | -161.788                                            | -161.788 | -161.788             | -161.788 |
| 2700                                  | 85.622 | 570.455                                                    | 494.142 | 206.043                                                                | 206.043 | -165.402                                            | -165.402 | -165.402             | -165.402 |
| 2800                                  | 85.600 | 573.568                                                    | 496.924 | 214.604                                                                | 214.604 | -169.358                                            | -169.358 | -169.358             | -169.358 |
| 2900                                  | 85.580 | 576.917                                                    | 500.177 | 223.163                                                                | 223.163 | -173.335                                            | -173.335 | -173.335             | -173.335 |
| 3000                                  | 85.561 | 579.472                                                    | 509.619 | 231.720                                                                | 231.720 | -179.288                                            | -179.288 | -179.288             | -179.288 |
| 3100                                  | 85.543 | 582.278                                                    | 504.770 | 240.275                                                                | 240.275 | -184.086                                            | -184.086 | -184.086             | -184.086 |
| 3200                                  | 85.525 | 584.993                                                    | 507.234 | 248.829                                                                | 248.829 | -189.911                                            | -189.911 | -189.911             | -189.911 |
| 3300                                  | 85.507 | 587.625                                                    | 509.631 | 257.380                                                                | 257.380 | -195.733                                            | -195.733 | -195.733             | -195.733 |
| 3400                                  | 85.490 | 590.177                                                    | 511.962 | 265.930                                                                | 265.930 | -201.555                                            | -201.555 | -201.555             | -201.555 |
| 3500                                  | 85.473 | 592.655                                                    | 514.233 | 274.478                                                                | 274.478 | -207.378                                            | -207.378 | -207.378             | -207.378 |
| 3600                                  | 85.456 | 595.063                                                    | 516.445 | 283.025                                                                | 283.025 | -213.208                                            | -213.208 | -213.208             | -213.208 |
| 3700                                  | 85.439 | 597.404                                                    | 518.601 | 291.569                                                                | 291.569 | -219.040                                            | -219.040 | -219.040             | -219.040 |
| 3800                                  | 85.422 | 599.682                                                    | 520.705 | 300.112                                                                | 300.112 | -224.900                                            | -224.900 | -224.900             | -224.900 |
| 3900                                  | 85.404 | 601.901                                                    | 522.759 | 308.654                                                                | 308.654 | -230.760                                            | -230.760 | -230.760             | -230.760 |
| 4000                                  | 85.386 | 604.063                                                    | 524.764 | 317.193                                                                | 317.193 | -236.620                                            | -236.620 | -236.620             | -236.620 |
| 4100                                  | 85.369 | 606.171                                                    | 526.724 | 325.731                                                                | 325.731 | -242.478                                            | -242.478 | -242.478             | -242.478 |
| 4200                                  | 85.350 | 608.228                                                    | 528.641 | 334.267                                                                | 334.267 | -248.336                                            | -248.336 | -248.336             | -248.336 |
| 4300                                  | 85.332 | 610.236                                                    | 530.515 | 342.801                                                                | 342.801 | -254.194                                            | -254.194 | -254.194             | -254.194 |
| 4400                                  | 85.313 | 612.198                                                    | 532.349 | 351.333                                                                | 351.333 | -260.052                                            | -260.052 | -260.052             | -260.052 |
| 4500                                  | 85.294 | 614.115                                                    | 534.145 | 359.864                                                                | 359.864 | -265.916                                            | -265.916 | -265.916             | -265.916 |
| 4600                                  | 85.275 | 615.989                                                    | 535.904 | 368.392                                                                | 368.392 | -271.779                                            | -271.779 | -271.779             | -271.779 |
| 4700                                  | 85.255 | 617.823                                                    | 537.627 | 376.919                                                                | 376.919 | -277.644                                            | -277.644 | -277.644             | -277.644 |
| 4800                                  | 85.235 | 619.617                                                    | 539.317 | 385.443                                                                | 385.443 | -283.508                                            | -283.508 | -283.508             | -283.508 |
| 4900                                  | 85.215 | 621.375                                                    | 540.974 | 393.965                                                                | 393.965 | -289.367                                            | -289.367 | -289.367             | -289.367 |
| 5000                                  | 85.195 | 623.096                                                    | 542.599 | 402.486                                                                | 402.486 | -295.099                                            | -295.099 | -295.099             | -295.099 |
| 5100                                  | 85.174 | 624.783                                                    | 544.194 | 411.005                                                                | 411.005 | -300.793                                            | -300.793 | -300.793             | -300.793 |
| 5200                                  | 85.154 | 626.437                                                    | 545.760 | 419.521                                                                | 419.521 | -306.460                                            | -306.460 | -306.460             | -306.460 |
| 5300                                  | 85.133 | 628.939                                                    | 547.297 | 428.035                                                                | 428.035 | -312.129                                            | -312.129 | -312.129             | -312.129 |
| 5400                                  | 85.112 | 629.650                                                    | 548.808 | 435.548                                                                | 435.548 | -317.766                                            | -317.766 | -317.766             | -317.766 |
| 5500                                  | 85.091 | 631.211                                                    | 550.292 | 445.038                                                                | 445.038 | -323.386                                            | -323.386 | -323.386             | -323.386 |
| 5600                                  | 85.070 | 632.744                                                    | 551.750 | 453.566                                                                | 453.566 | -329.081                                            | -329.081 | -329.081             | -329.081 |
| 5700                                  | 85.049 | 634.250                                                    | 553.185 | 462.072                                                                | 462.072 | -334.790                                            | -334.790 | -334.790             | -334.790 |
| 5800                                  | 85.028 | 635.729                                                    | 554.595 | 470.576                                                                | 470.576 | -340.507                                            | -340.507 | -340.507             | -340.507 |
| 5900                                  | 85.007 | 637.182                                                    | 555.983 | 479.077                                                                | 479.077 | -346.248                                            | -346.248 | -346.248             | -346.248 |
| 6000                                  | 84.986 | 638.611                                                    | 557.348 | 487.577                                                                | 487.577 | -352.541                                            | -352.541 | -352.541             | -352.541 |

TITANIUM IODIDE (TiI<sub>3</sub>)

PREVIOUS: December 1968 (1 atm)

CURRENT: December 1988 (1 bar)

$I_3Zr_1(cr)$  $M_f = 471.9335$  Zirconium Iodide ( $ZrI_3$ )

## CRYSTAL

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= [204.585] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \\ T_{ab} &= [970] \text{ K} \end{aligned}$$

## Enthalpy of Formation

Larsen and Leddy<sup>1</sup> studied the reaction  $Zr(cr) + 3ZrI_4(g) = 4ZrI_3(cr)$  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  $\Delta_f H^\circ(298.15 \text{ K})$  accordingly calculated. These values and the enthalpy of formation of  $ZrI_4(g)$  [see  $ZrI_4$  table] were used to compute a series of values for the enthalpy of formation of  $ZrI_3(cr)$  at 298.15 K. The following table gives representative values at four temperatures.

| $T/K$ | $K_p$ | $\Delta_f H^\circ(298.15 \text{ K}), \text{ kcal}\cdot\text{mol}^{-1}$ | $\Delta_f H^\circ(298.15 \text{ K}), \text{ kcal}\cdot\text{mol}^{-1}$ |
|-------|-------|------------------------------------------------------------------------|------------------------------------------------------------------------|
| 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  $ZrI_4$ , 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  $ZrI_4$  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  $ZrI_3$  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  $ZrBr_4(cr)$  [refer to the  $ZrBr_4(cr)$  table]. The value  $\theta_0 = 60 \text{ K}$  and  $\theta_e = 115 \text{ K}$  were taken to be the same as those estimated for  $ZrI_4(cr)$ . The internal contribution was obtained from the estimated  $ZrI_3$  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  $ZrI_3$  molecules. However, Holze<sup>2</sup> came to the conclusion that crystalline  $ZrI_3$  is composed of a chain lattice of  $[ZrI_6]_n$  units. The results of an analysis for a crystalline lattice composed of  $ZrI_6$  units would probably not differ significantly from that for a crystalline lattice composed of  $ZrI_3$  units since both are approaching the classical harmonic heat capacity of  $12R$  calories per formula weight of  $ZrI_3$  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  $ZrI_3$ .

## Decomposition Data

As 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

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

PREVIOUS: June 1962

CURRENT: June 1964

 $I_3Zr_1(g)$  $I_3Zr_1(cr)$ 

|                                      |                                             | Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$     |             |                          |                               |                    |
|--------------------------------------|---------------------------------------------|-----------------------------------------------------------|-------------|--------------------------|-------------------------------|--------------------|
|                                      |                                             | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |             | $H^\circ - H^\circ(T_s)$ |                               | $\Delta_f G^\circ$ |
|                                      |                                             | $T/K$                                                     | $C_p^\circ$ | $S^\circ$                | $-[G^\circ - H^\circ(T_s)]/T$ | $\Delta_f H^\circ$ |
| $\Delta_f H^\circ(0 \text{ K})$      | $[-396.545] \text{ kJ}\cdot\text{mol}^{-1}$ | 0                                                         | 0           | 0                        | -24.359                       | -396.545           |
| $\Delta_f H^\circ(298.15 \text{ K})$ | $[-397.480] \text{ kJ}\cdot\text{mol}^{-1}$ | 100                                                       | 83.366      | 100.663                  | -19.196                       | -396.543           |
|                                      |                                             | 200                                                       | 98.328      | 164.189                  | -9.950                        | -395.728           |
|                                      |                                             | 298.15                                                    | 103.818     | 204.585                  | 0                             | -397.480           |
|                                      |                                             | 300                                                       | 103.897     | 205.227                  | 0.192                         | -397.486           |
|                                      |                                             | 400                                                       | 105.855     | 235.422                  | 208.690                       | -422.002           |
|                                      |                                             | 500                                                       | 106.274     | 259.088                  | 216.490                       | -421.344           |
|                                      |                                             | 1200                                                      | 107.692     | 316.966                  | 229.229                       | -397.800           |
|                                      |                                             | 1700                                                      | 106.901     | 294.966                  | 42.629                        | -483.287           |
|                                      |                                             | 200                                                       | 107.110     | 309.254                  | 242.593                       | -481.726           |
|                                      |                                             | 900                                                       | 107.320     | 321.883                  | 250.715                       | -479.544           |
|                                      |                                             | 1000                                                      | 107.445     | 333.197                  | 258.407                       | -477.454           |
|                                      |                                             | 1100                                                      | 107.529     | 343.442                  | 265.679                       | -475.474           |
|                                      |                                             | 1200                                                      | 107.612     | 357.802                  | 272.555                       | -473.620           |
|                                      |                                             | 1300                                                      | 107.696     | 361.419                  | 279.064                       | -471.952           |
|                                      |                                             | 1400                                                      | 107.738     | 365.401                  | 285.235                       | -471.583           |
|                                      |                                             | 1500                                                      | 107.780     | 376.836                  | 291.609                       | -469.348           |
|                                      |                                             | 1600                                                      | 107.822     | 383.793                  | 296.675                       | -467.761           |
|                                      |                                             | 1700                                                      | 107.864     | 390.331                  | 301.994                       | -465.131           |
|                                      |                                             | 1800                                                      | 107.905     | 396.498                  | 307.074                       | -463.679           |
|                                      |                                             | 1900                                                      | 107.947     | 402.333                  | 311.936                       | -462.423           |
|                                      |                                             | 2000                                                      | 107.989     | 407.871                  | 316.595                       | -462.373           |

## NIST-JANAF THERMOCHEMICAL TABLES

 $I_3ZrI(g)$  $M_r = 471.9335 \text{ Zirconium Iodide (ZrI}_3\text{)}$ 

IDEAL GAS

$$S^\circ(298.15 \text{ K}) = [397.776] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(0 \text{ K}) = [-216.860] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = [-221.752] \text{ kJ}\cdot\text{mol}^{-1}$$

|                                          | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |         |           |                            |                            |                  | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                  |            |
|------------------------------------------|-----------------------------------------------------------|---------|-----------|----------------------------|----------------------------|------------------|-------------------------------------------------------|------------------|------------|
|                                          | $T/K$                                                     | $C_p^*$ | $S^\circ$ | $-J_K^{-1}\text{mol}^{-1}$ | $H^\circ - H^\circ(T_r)/T$ | $\Delta H^\circ$ | $\text{kJ}\cdot\text{mol}^{-1}$                       | $\Delta G^\circ$ | $\log K_r$ |
| Vibrational Frequencies and Degeneracies |                                                           |         |           |                            |                            |                  |                                                       |                  |            |
| $\nu, \text{ cm}^{-1}$                   | 0                                                         | 0.      | 0.        | INFINITE                   | -20.403                    | -216.860         | -216.860                                              | INFINITE         |            |
|                                          | 100                                                       | 68.161  | 314.735   | 487.501                    | -15.277                    | -217.195         | -218.115                                              | -124.378         |            |
|                                          | 200                                                       | 78.257  | 365.960   | 405.106                    | -7.829                     | -219.340         | -238.234                                              | 67.444           |            |
|                                          | 250                                                       | 383.617 | 399.102   | 3.871                      | -267.539                   | -267.821         | 55.958                                                |                  |            |
|                                          | 298.15                                                    | 80.820  | 397.776   | 397.776                    | 0.                         | -221.752         | -276.819                                              | 48.497           |            |
|                                          | 300                                                       | 80.847  | 398.276   | 397.778                    | 0.150                      | -221.800         | -277.160                                              | 48.258           |            |
|                                          | 350                                                       | 81.436  | 410.761   | 398.764                    | 4.208                      | -226.278         | -42.725                                               |                  |            |
|                                          | 400                                                       | 81.826  | 421.688   | 400.963                    | 8.290                      | -248.677         | -294.361                                              | 38.440           |            |
|                                          | 450                                                       | 82.997  | 431.342   | 403.812                    | 12.388                     | -251.933         | -299.876                                              | 34.809           |            |
|                                          | 500                                                       | 82.292  | 440.002   | 407.006                    | 16.498                     | -315.388         | -329.330                                              | 31.271           |            |
|                                          | 600                                                       | 82.549  | 455.031   | 413.795                    | 24.741                     | -315.467         | -296.112                                              | 25.779           |            |
|                                          | 700                                                       | 82.706  | 467.768   | 420.619                    | 33.005                     | -321.749         | -292.875                                              | 21.855           |            |
|                                          | 800                                                       | 82.868  | 478.819   | 427.218                    | 41.281                     | -315.864         | -289.610                                              | 18.910           |            |
|                                          | 900                                                       | 82.878  | 488.577   | 433.504                    | 49.565                     | -316.212         | -286.309                                              | 16.617           |            |
|                                          | 1000                                                      | 82.928  | 497.312   | 439.436                    | 57.856                     | -316.681         | -282.962                                              | 14.780           |            |
|                                          | 1100                                                      | 82.966  | 505.218   | 445.081                    | 66.151                     | -317.280         | -279.563                                              | 13.275           |            |
|                                          | 1200                                                      | 82.994  | 512.438   | 450.397                    | 74.449                     | -321.733         | -275.881                                              | 12.009           |            |
|                                          | 1300                                                      | 83.016  | 519.082   | 455.428                    | 82.749                     | -322.085         | -272.046                                              | 10.931           |            |
|                                          | 1400                                                      | 83.034  | 525.235   | 460.198                    | 91.052                     | -322.523         | -268.181                                              | 10.006           |            |
|                                          | 1500                                                      | 83.048  | 530.964   | 464.727                    | 99.356                     | -323.074         | -264.281                                              | 9.203            |            |
|                                          | 1600                                                      | 83.060  | 536.324   | 469.036                    | 107.661                    | -324.161         | -260.340                                              |                  |            |
|                                          | 1700                                                      | 83.069  | 541.306   | 473.143                    | 115.968                    | -324.609         | -256.351                                              |                  |            |
|                                          | 1800                                                      | 83.077  | 546.108   | 477.066                    | 124.275                    | -325.638         | -252.307                                              |                  |            |
|                                          | 1900                                                      | 83.084  | 550.600   | 480.819                    | 132.583                    | -326.866         | -248.201                                              |                  |            |
|                                          | 2000                                                      | 83.090  | 554.802   | 484.416                    | 140.892                    | -328.305         | -244.024                                              |                  |            |
|                                          | 2100                                                      | 83.095  | 558.916   | 487.868                    | 149.201                    | -329.770         | -240.770                                              |                  |            |
|                                          | 2200                                                      | 83.099  | 562.782   | 491.186                    | 157.511                    | -335.961         | -234.687                                              |                  |            |
|                                          | 2300                                                      | 83.103  | 566.476   | 494.380                    | 163.821                    | -353.877         | -224.245                                              |                  |            |
|                                          | 2400                                                      | 83.107  | 570.013   | 497.438                    | 174.131                    | -358.251         | -223.694                                              |                  |            |
|                                          | 2500                                                      | 83.109  | 573.405   | 500.428                    | 182.442                    | -360.880         | -218.033                                              |                  |            |
|                                          | 2600                                                      | 83.112  | 576.665   | 503.298                    | 190.153                    | -363.542         | -212.267                                              |                  |            |
|                                          | 2700                                                      | 83.114  | 579.802   | 506.074                    | 199.065                    | -366.220         | -206.397                                              |                  |            |
|                                          | 2800                                                      | 83.116  | 582.824   | 508.761                    | 207.376                    | -368.897         | -200.429                                              |                  |            |
|                                          | 2900                                                      | 83.118  | 585.741   | 511.366                    | 215.688                    | -371.556         | -194.365                                              |                  |            |
|                                          | 3000                                                      | 83.120  | 588.559   | 513.892                    | 224.000                    | -374.183         | -188.211                                              |                  |            |
|                                          | 3100                                                      | 83.122  | 591.284   | 520.345                    | 232.210                    | -376.765         | -181.969                                              |                  |            |
|                                          | 3200                                                      | 83.123  | 593.923   | 518.728                    | 240.624                    | -379.291         | -175.645                                              |                  |            |
|                                          | 3300                                                      | 83.124  | 596.481   | 521.046                    | 248.337                    | -381.753         | -169.242                                              |                  |            |
|                                          | 3400                                                      | 83.125  | 598.963   | 523.301                    | 257.249                    | -384.141         | -162.767                                              |                  |            |
|                                          | 3500                                                      | 83.126  | 601.372   | 525.498                    | 265.562                    | -386.452         | -156.222                                              |                  |            |
|                                          | 3600                                                      | 83.127  | 603.714   | 527.638                    | 273.874                    | -388.679         | -149.612                                              |                  |            |
|                                          | 3700                                                      | 83.128  | 605.992   | 529.725                    | 282.187                    | -390.821         | -142.921                                              |                  |            |
|                                          | 3800                                                      | 83.129  | 608.209   | 531.761                    | 290.500                    | -392.874         | -136.214                                              |                  |            |
|                                          | 3900                                                      | 83.130  | 610.368   | 533.749                    | 298.813                    | -394.838         | -129.434                                              |                  |            |
|                                          | 4000                                                      | 83.131  | 612.473   | 535.691                    | 307.126                    | -396.714         | -122.605                                              |                  |            |
|                                          | 4100                                                      | 83.131  | 614.525   | 537.589                    | 315.439                    | -398.500         | -115.730                                              |                  |            |
|                                          | 4200                                                      | 83.132  | 616.529   | 539.445                    | 323.752                    | -400.199         | -108.813                                              |                  |            |
|                                          | 4300                                                      | 83.132  | 618.483   | 541.260                    | 332.065                    | -401.811         | -101.856                                              |                  |            |
|                                          | 4400                                                      | 83.133  | 620.396   | 543.037                    | 340.379                    | -403.339         | -94.862                                               |                  |            |
|                                          | 4500                                                      | 83.133  | 622.264   | 544.777                    | 348.692                    | -404.785         | -87.835                                               |                  |            |
|                                          | 5100                                                      | 83.136  | 624.091   | 546.482                    | 357.005                    | -406.151         | -80.777                                               |                  |            |
|                                          | 5200                                                      | 83.136  | 624.134   | 546.482                    | 365.319                    | -407.439         | -73.689                                               |                  |            |
|                                          | 5300                                                      | 83.136  | 625.879   | 548.152                    | 373.632                    | -409.589         | -54.957                                               |                  |            |
|                                          | 5400                                                      | 83.137  | 627.630   | 549.789                    | 381.946                    | -410.382         | -35.894                                               |                  |            |
|                                          | 5500                                                      | 83.137  | 629.344   | 551.396                    | 390.259                    | -411.122         | -16.816                                               |                  |            |
|                                          | 5600                                                      | 83.137  | 640.445   | 561.848                    | 448.445                    | -974.518         | 97.915                                                | -0.913           |            |
|                                          | 5700                                                      | 83.137  | 641.917   | 563.240                    | 448.455                    | -974.920         | 117.069                                               | -1.073           |            |
|                                          | 5800                                                      | 83.138  | 643.462   | 564.609                    | 456.769                    | -975.278         | 136.229                                               | -1.227           |            |
|                                          | 5900                                                      | 83.138  | 644.784   | 565.956                    | 465.082                    | -975.593         | 155.396                                               | -1.376           |            |
|                                          | 6000                                                      | 83.138  | 646.181   | 567.282                    | 473.396                    | -975.885         | 174.568                                               | -1.520           |            |

PREVIOUS June 1964 (1 atm)

CURRENT: June 1964 (1 bar)

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

## Heat Capacity and Entropy

The enthalpies of formation, from the gaseous atoms, of the 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 tri- and tetrachloride, it was found that the bond energy of the trichloride was around 7 kJ·mol<sup>-1</sup> greater than that for gaseous titanium tri- and tetrachloride. It was found that the bond energy of zirconium trichloride is 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 kJ·mol<sup>-1</sup> and from the elements in their standard state, -53 kJ·mol<sup>-1</sup>.

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:  $I_a = I_b = 185.2317 \times 10^{-39}$  and  $I_c = 363.6703 \times 10^{-39}$  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  $\nu_1 = 195$ ,  $\nu_2 = 90$ ,  $\nu_3 = 220$ , and  $\nu_4 = 65$  cm<sup>-1</sup> for the fluorides and chlorides of P, As, and Sb,  $\nu_1$  is greater than  $\nu_3$  but there appears to be a reversal as one goes to the bromides and iodides with  $\nu_3$  becoming greater than  $\nu_1$ . An empirical correlation procedure for ZrI<sub>3</sub> gave  $\nu_1 = 195$ ,  $\nu_2 = 90$ ,  $\nu_3 = 220$ , and  $\nu_4 = 65$  cm<sup>-1</sup> in which  $\nu_3 > \nu_1$  for P<sub>3</sub> and As<sub>3</sub>, the correlation value for  $\nu_3$  was used to represent this frequency in ZrI<sub>3</sub>.

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

**Molybdenum Iodide ( $\text{MoI}_4$ )****CRYSTAL** **$\text{I}_4\text{Mo}_4(\text{cr})$** 

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= [266.061 \pm 16.7] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \\ T_{\text{diss}} &= [293] \text{ K} \end{aligned}$$

**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  $\text{MoI}_4(\text{cr})$  is unstable with respect to  $\text{MoI}_3(\text{cr})$  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 ( $\pm 2 \text{ kcal mol}^{-1}$ ) is determined from the product  $1000 \times R$  which has been rounded to the nearest  $\text{kcal mol}^{-1}$ .

**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  $32.79 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  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  $\text{MoI}_4(\text{cr})$  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  $\text{MoI}_4$  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  $T_{\text{diss}}$  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  $T_{\text{diss}}$  appears to lie outside the temperature range selected for our  $\text{MoI}_4(\text{cr})$  phase table.

**References**

- <sup>1</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>2</sup>J. Lewis, D. J. Machin, R. S. Nyholm, P. Pauling, and P. W. Smith, *Chemistry and Industry*, 1960, 259 (1960).
- <sup>3</sup>M. Guichard, *Annales de Chimie et de Physique*, 23, 498 (1901).

$$\Delta_f H^\circ(0 \text{ K}) = \text{Unknown}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = [-123.010 \pm 8.4] \text{ kJ}\cdot\text{mol}^{-1}$$

| $T/K$  | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |           | Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$ |                    |
|--------|-----------------------------------------------------------|-----------|-------------------------------------------------------|--------------------|
|        | $C_p^\circ$                                               | $S^\circ$ | $H^\circ - H^\circ(T_r)$                              | $\Delta_f H^\circ$ |
| 0      |                                                           |           |                                                       |                    |
| 100    |                                                           |           |                                                       |                    |
| 200    | 137.193                                                   | 266.061   | 0.                                                    | -123.010           |
| 298.15 | 137.193                                                   | 266.061   | 0.                                                    | -124.552           |
| 300    | 137.193                                                   | 266.909   | 0.254                                                 | -123.002           |
| 400    | 137.193                                                   | 306.377   | 13.973                                                | -155.014           |
| 500    | 137.193                                                   | 336.991   | 281.606                                               | -240.237           |
| 600    | 137.193                                                   | 362.004   | 292.985                                               | 41.412             |
|        |                                                           |           |                                                       | -236.642           |
|        |                                                           |           |                                                       | -81.970            |
|        |                                                           |           |                                                       | 7.136              |

 **$\text{MoI}_4 = 603.5580 \text{ Molybdenum Iodide } (\text{MoI}_4)$** 

PREVIOUS.

CURRENT September 1978

**Molybdenum Iodide ( $\text{MoI}_4$ )** **$\text{I}_4\text{Mo}_4(\text{cr})$**

## NIST-JANAF THERMOCHEMICAL TABLES

**Molybdenum Iodide (Mo<sub>4</sub>)****IDEAL GAS**

$$S^o(298.15 \text{ K}) = [452.812 \pm 12.6] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_H^o(0 \text{ K}) = [(129.32 \pm 41.8) \text{ kJ}\cdot\text{mol}^{-1}]$$

$$\Delta_H^o(298.15 \text{ K}) = [(124.68 \pm 41.8) \text{ kJ}\cdot\text{mol}^{-1}]$$

**I<sub>4</sub>Mo<sub>1</sub>(g)*****M*<sub>t</sub> = 603.5580 Molybdenum Iodide (Mo<sub>4</sub>)**

|  |  | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                                                  |                            |                                                  | Standard State Pressure = $p^o = 0.1 \text{ MPa}$ |                |                                 |            |
|--|--|-----------------------------------------------------------|--------------------------------------------------|----------------------------|--------------------------------------------------|---------------------------------------------------|----------------|---------------------------------|------------|
|  |  | $C_p^o$                                                   |                                                  | $S^o - [G^o - H^o(T_r)]/T$ |                                                  | $H^o - H^o(T_r)$                                  |                | $\Delta_f G^o$                  |            |
|  |  | $T/K$                                                     | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $S^o$                      | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $\text{kJ}\cdot\text{mol}^{-1}$                   | $\Delta_f H^o$ | $\text{kJ}\cdot\text{mol}^{-1}$ | $\log K_f$ |
|  |  | 0                                                         | 0                                                | 0                          | 0                                                | -26.344                                           | 129.320        | INFINITE                        |            |
|  |  | 100                                                       | 88.195                                           | 345.225                    | 543.185                                          | -19.796                                           | 129.277        | 107.655                         | 107.320    |
|  |  | 200                                                       | 101.392                                          | 411.558                    | 462.319                                          | -10.152                                           | 127.214        | 86.781                          | 106.233    |
|  |  | 250                                                       | 103.615                                          | 434.446                    | 454.532                                          | -5.022                                            | 125.971        | 76.814                          | 102.665    |
|  |  | 298.15                                                    | 104.869                                          | 452.812                    | 452.812                                          | 0.                                                | 124.683        | 67.461                          | 111.819    |
|  |  | 300                                                       | 104.906                                          | 453.461                    | 452.814                                          | 0.194                                             | 124.631        | 67.106                          | 111.684    |
|  |  | 350                                                       | 105.716                                          | 469.698                    | 465.948                                          | 5.461                                             | 123.061        | 57.638                          | 108.602    |
|  |  | 400                                                       | 106.254                                          | 483.851                    | 460.647                                          | 10.761                                            | 89.467         | 49.499                          | 106.464    |
|  |  | 450                                                       | 106.629                                          | 496.389                    | 460.647                                          | 16.084                                            | 85.458         | 44.744                          | 105.194    |
|  |  | 500                                                       | 106.901                                          | 507.639                    | 464.794                                          | 21.422                                            | 11.186         | 43.034                          | 105.018    |
|  |  | 600                                                       | 107.258                                          | 527.163                    | 473.610                                          | 32.132                                            | 1.771          | 57.347                          | 4.993      |
|  |  | 700                                                       | 107.476                                          | 543.715                    | 482.473                                          | 48.869                                            | 53.625         | 66.567                          | 4.967      |
|  |  | 800                                                       | 107.618                                          | 558.076                    | 491.045                                          | 53.326                                            | 2.776          | 75.715                          | 4.944      |
|  |  | 900                                                       | 107.758                                          | 570.758                    | 499.212                                          | 64.392                                            | 3.196          | 84.807                          | 4.922      |
|  |  | 1000                                                      | 107.786                                          | 582.111                    | 506.944                                          | 75.167                                            | 3.555          | 93.855                          | 4.902      |
|  |  | 1100                                                      | 107.838                                          | 592.386                    | 514.252                                          | 85.948                                            | 3.843          | 102.870                         | 4.885      |
|  |  | 1200                                                      | 107.878                                          | 601.771                    | 521.159                                          | 96.734                                            | 4.045          | 111.863                         | 4.869      |
|  |  | 1300                                                      | 107.909                                          | 610.407                    | 527.697                                          | 107.524                                           | 4.412          | 120.843                         | 4.836      |
|  |  | 1400                                                      | 107.935                                          | 618.405                    | 533.894                                          | 118.316                                           | 4.110          | 129.820                         | 4.844      |
|  |  | 1500                                                      | 107.957                                          | 625.853                    | 539.779                                          | 129.110                                           | 3.925          | 138.805                         | 4.834      |
|  |  | 1600                                                      | 107.977                                          | 632.821                    | 545.379                                          | 139.907                                           | 3.560          | 147.808                         | 4.825      |
|  |  | 1700                                                      | 107.998                                          | 639.367                    | 550.717                                          | 150.706                                           | 2.992          | 156.840                         | 4.819      |
|  |  | 1800                                                      | 108.022                                          | 645.541                    | 555.815                                          | 161.507                                           | 2.200          | 165.911                         | 4.815      |
|  |  | 1900                                                      | 108.051                                          | 651.382                    | 560.593                                          | 172.310                                           | 1.169          | 175.033                         | 4.812      |
|  |  | 2000                                                      | 108.088                                          | 656.925                    | 565.367                                          | 183.117                                           | -0.111         | 184.216                         | 4.811      |
|  |  | 2100                                                      | 108.113                                          | 662.230                    | 569.853                                          | 193.928                                           | -1.643         | 193.469                         | 4.812      |
|  |  | 2200                                                      | 108.195                                          | 667.232                    | 574.166                                          | 204.745                                           | -3.424         | 202.800                         | 4.815      |
|  |  | 2300                                                      | 108.270                                          | 672.043                    | 578.318                                          | 215.568                                           | -5.445         | 212.219                         | 4.820      |
|  |  | 2400                                                      | 108.343                                          | 676.653                    | 582.220                                          | 225.399                                           | -7.697         | 221.730                         | 4.826      |
|  |  | 2500                                                      | 108.416                                          | 681.079                    | 586.182                                          | 237.241                                           | -10.167        | 231.339                         | 4.834      |
|  |  | 2700                                                      | 108.768                                          | 689.438                    | 593.525                                          | 258.964                                           | -15.763        | 250.872                         | 4.835      |
|  |  | 2800                                                      | 108.930                                          | 693.956                    | 597.022                                          | 269.850                                           | -18.940        | 260.805                         | 4.835      |
|  |  | 2900                                                      | 109.156                                          | 697.223                    | 600.411                                          | 280.755                                           | -38.325        | 270.905                         | 4.835      |
|  |  | 3000                                                      | 109.388                                          | 700.928                    | 603.700                                          | 291.682                                           | -60.170        | 282.290                         | 4.915      |
|  |  | 3100                                                      | 109.644                                          | 704.518                    | 606.895                                          | 302.633                                           | -61.931        | 293.735                         | 4.949      |
|  |  | 3200                                                      | 109.924                                          | 708.004                    | 610.000                                          | 313.611                                           | -63.591        | 305.234                         | 4.982      |
|  |  | 3300                                                      | 110.228                                          | 711.586                    | 613.022                                          | 324.619                                           | -65.136        | 316.784                         | 5.014      |
|  |  | 3400                                                      | 110.534                                          | 714.686                    | 615.964                                          | 335.658                                           | -66.552        | 328.379                         | 5.045      |
|  |  | 3500                                                      | 110.901                                          | 717.850                    | 618.830                                          | 346.730                                           | -67.830        | 340.014                         | 5.074      |
|  |  | 3600                                                      | 111.267                                          | 721.026                    | 621.626                                          | 357.838                                           | -68.963        | 351.683                         | 5.103      |
|  |  | 3700                                                      | 111.650                                          | 724.079                    | 624.334                                          | 368.984                                           | -69.943        | 363.382                         | 5.130      |
|  |  | 3800                                                      | 112.049                                          | 727.082                    | 627.017                                          | 380.169                                           | -70.167        | 375.105                         | 5.156      |
|  |  | 3900                                                      | 112.460                                          | 729.978                    | 629.620                                          | 391.394                                           | -71.431        | 386.847                         | 5.181      |
|  |  | 4000                                                      | 112.882                                          | 732.830                    | 632.165                                          | 402.661                                           | -71.935        | 398.604                         | 5.205      |
|  |  | 4100                                                      | 113.313                                          | 735.623                    | 634.654                                          | 413.974                                           | -72.279        | 410.372                         | 5.228      |
|  |  | 4200                                                      | 113.749                                          | 738.339                    | 637.091                                          | 423.524                                           | -72.462        | 422.147                         | 5.250      |
|  |  | 4300                                                      | 114.189                                          | 743.071                    | 641.816                                          | 436.721                                           | -72.486        | 433.924                         | 5.271      |
|  |  | 4400                                                      | 114.630                                          | 746.252                    | 644.108                                          | 448.162                                           | -72.354        | 445.699                         | 5.291      |
|  |  | 4500                                                      | 115.071                                          | 749.537                    | 650.647                                          | 459.647                                           | -72.068        | 457.470                         | 5.310      |
|  |  | 4600                                                      | 115.508                                          | 752.836                    | 646.336                                          | 471.176                                           | -71.632        | 469.233                         | 5.328      |
|  |  | 4700                                                      | 115.940                                          | 751.274                    | 648.562                                          | 482.748                                           | -71.048        | 480.985                         | 5.346      |
|  |  | 4800                                                      | 116.365                                          | 753.720                    | 652.364                                          | 494.364                                           | -70.323        | 492.724                         | 5.362      |
|  |  | 4900                                                      | 116.780                                          | 756.123                    | 652.834                                          | 506.021                                           | -69.458        | 504.445                         | 5.377      |
|  |  | 5000                                                      | 117.185                                          | 758.487                    | 654.943                                          | 517.719                                           | -69.845        | 512.878                         | 5.452      |
|  |  | 5100                                                      | 117.578                                          | 760.811                    | 656.996                                          | 529.458                                           | -66.329        | 545.519                         | 5.587      |
|  |  | 5200                                                      | 117.937                                          | 763.098                    | 659.014                                          | 541.234                                           | -66.039        | 569.170                         | 5.717      |
|  |  | 5300                                                      | 118.321                                          | 765.348                    | 661.000                                          | 552.048                                           | -66.156        | 592.831                         | 5.843      |
|  |  | 5400                                                      | 118.669                                          | 767.563                    | 662.953                                          | 564.898                                           | -66.219        | 616.505                         | 5.964      |
|  |  | 5500                                                      | 119.000                                          | 769.744                    | 664.874                                          | 576.782                                           | -66.283        | 640.190                         | 6.080      |
|  |  | 5600                                                      | 119.314                                          | 771.891                    | 666.766                                          | 588.697                                           | -66.329        | 663.885                         | 6.192      |
|  |  | 5700                                                      | 119.609                                          | 774.025                    | 668.629                                          | 600.644                                           | -66.248        | 687.599                         | 6.301      |
|  |  | 5800                                                      | 119.886                                          | 776.038                    | 670.464                                          | 612.619                                           | -66.103        | 708.321                         | 6.406      |
|  |  | 5900                                                      | 120.144                                          | 778.140                    | 672.272                                          | 624.520                                           | -66.579        | 735.058                         | 6.508      |
|  |  | 6000                                                      | 120.383                                          | 780.161                    | 674.053                                          | 636.647                                           | -66.625        | 758.828                         | 6.606      |

CURRENT - September 1978 (1 atm)

PREVIOUS - September 1978 (1 atm)

**Molybdenum Iodide (Mo<sub>4</sub>)**

Lead Iodide (PbI<sub>4</sub>)

## IDEAL GAS

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

$$\Delta dH^o(0\text{ K}) = [-218.82 \pm 83.7] \text{ J}\cdot\text{mol}^{-1}$$

$$\Delta dH^o(298.15\text{ K}) = [-224.47 \pm 83.7] \text{ J}\cdot\text{mol}^{-1}$$

| Vibrational Frequencies and Degeneracies<br>$\nu, \text{cm}^{-1}$ |         |
|-------------------------------------------------------------------|---------|
| 0                                                                 | 0       |
| 100                                                               | 95.214  |
| 200                                                               | 104.275 |
| 250                                                               | 105.593 |
| 298.15                                                            | 106.313 |
| 300                                                               | 106.334 |
| 350                                                               | 106.790 |
| 400                                                               | 107.089 |
| 450                                                               | 107.296 |
| 500                                                               | 107.445 |
| 600                                                               | 107.640 |
| 700                                                               | 107.758 |
| 800                                                               | 107.835 |
| 900                                                               | 107.888 |
| 1000                                                              | 107.926 |
| 1200                                                              | 107.975 |
| 1300                                                              | 107.991 |
| 1400                                                              | 108.005 |
| 1500                                                              | 108.015 |
| 1600                                                              | 108.024 |
| 1700                                                              | 108.031 |
| 1800                                                              | 108.037 |
| 1900                                                              | 108.042 |
| 2000                                                              | 108.047 |
| 2100                                                              | 108.051 |
| 2200                                                              | 108.054 |
| 2300                                                              | 108.057 |
| 2400                                                              | 108.059 |
| 2500                                                              | 108.061 |
| 2600                                                              | 108.063 |
| 2700                                                              | 108.065 |
| 2800                                                              | 108.067 |
| 2900                                                              | 108.068 |
| 3000                                                              | 108.069 |
| 3100                                                              | 108.070 |
| 3200                                                              | 108.071 |
| 3300                                                              | 108.072 |
| 3400                                                              | 108.073 |
| 3500                                                              | 108.074 |
| 3600                                                              | 108.075 |
| 3700                                                              | 108.075 |
| 3800                                                              | 108.076 |
| 3900                                                              | 108.077 |
| 4000                                                              | 108.077 |
| 4100                                                              | 108.078 |
| 4200                                                              | 108.078 |
| 4300                                                              | 108.079 |
| 4400                                                              | 108.079 |
| 4500                                                              | 108.079 |
| 4600                                                              | 108.080 |
| 4700                                                              | 108.080 |
| 4800                                                              | 108.081 |
| 4900                                                              | 108.081 |
| 5000                                                              | 108.081 |
| 5100                                                              | 108.081 |
| 5200                                                              | 108.081 |
| 5300                                                              | 108.082 |
| 5400                                                              | 108.082 |
| 5500                                                              | 108.082 |
| 5600                                                              | 108.082 |
| 5700                                                              | 108.082 |
| 5800                                                              | 108.083 |
| 5900                                                              | 108.083 |
| 6000                                                              | 108.083 |

$\Delta dH^o(0\text{ K}) = -32.3 \pm 20 \text{ kcal}\cdot\text{mol}^{-1}$  is derived from the atomization energy for the process  $\text{Pb}_4(\text{g}) \rightarrow \text{Pb}(\text{g}) + 4 \text{ I(g)}$ .  $\Delta dH^o(0\text{ K}) = 8.75 \text{ eV}$  is estimated from an intercomparison of the lead mono-, di-, and tetra-halides. This adopted value for  $\text{Pb}_4(\text{g})$  is greater than the  $\Delta dH^o(0\text{ K})$  value for  $\text{Pb}_3(\text{g})$  by a factor of 2.04. The auxiliary values  $\Delta H^o(\text{Pb}_4, 0\text{ K}) = 46.91 \text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta dH^o(\text{I}, 0\text{ K}) = 25.633 \text{ kcal}\cdot\text{mol}^{-1}$  are used.  $\Delta dH^o(\text{Pb}_4, \text{g}, 298.15\text{ K}) = -55.6 \pm 20 \text{ kcal}\cdot\text{mol}^{-1}$  is calculated from  $\Delta dH^o(0\text{ K})$ .

## Enthalpy of Formation

The adopted  $\Delta dH^o(0\text{ K}) = -32.3 \pm 20 \text{ kcal}\cdot\text{mol}^{-1}$  is derived from the atomization energy for the process  $\text{Pb}_4(\text{g}) \rightarrow \text{Pb}(\text{g}) + 4 \text{ I(g)}$ .  $\Delta dH^o(0\text{ K}) = 8.75 \text{ eV}$  is estimated from an intercomparison of the lead mono-, di-, and tetra-halides. This adopted value for  $\text{Pb}_4(\text{g})$  is greater than the  $\Delta dH^o(0\text{ K})$  value for  $\text{Pb}_3(\text{g})$  by a factor of 2.04. The auxiliary values  $\Delta H^o(\text{Pb}_4, 0\text{ K}) = 46.91 \text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta dH^o(\text{I}, 0\text{ K}) = 25.633 \text{ kcal}\cdot\text{mol}^{-1}$  are used.  $\Delta dH^o(\text{Pb}_4, \text{g}, 298.15\text{ K}) = -55.6 \pm 20 \text{ kcal}\cdot\text{mol}^{-1}$  is calculated from  $\Delta dH^o(0\text{ K})$ .

## 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:  $I_A = I_B = I_C = 431.1831 \times 10^{-39} \text{ g}\cdot\text{cm}^2$ .

## References

- JANAF Thermochemical Tables:  $\text{PbF}(\text{g}), \text{PbF}_2(\text{g}), \text{PbBr}(\text{g}), \text{PbBr}_2(\text{g}), \text{PbCl}(\text{g}), \text{PbCl}_2(\text{g}), \text{PbCl}_3(\text{g}), \text{PbCl}_4(\text{g})$ , 6-30-73,  $\text{Pb}(\text{g})$ , 3-31-62;  $(\text{g})$ , 12-31-73,  $\text{PbCl}(\text{g})$  and  $\text{PbCl}_4(\text{g})$ .
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|        |         | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                                  | Standard State Pressure = $P^o = 0.1 \text{ MPa}$ |                                 |
|--------|---------|----------------------------------------------------------|--------------------------------------------------|---------------------------------------------------|---------------------------------|
|        |         | $\frac{\partial H}{\partial T} \text{ at } T_r$          | $\frac{\partial S}{\partial T} \text{ at } T_r$  | $H^o - H^o(T_r)$                                  | $\Delta H^o$                    |
|        |         | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$         | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $\text{kJ}\cdot\text{mol}^{-1}$                   | $\text{kJ}\cdot\text{mol}^{-1}$ |
| 0      | 0       | 0                                                        | 0                                                | -INFINITE                                         | -INFINITE                       |
| 100    | 95.214  | 354.506                                                  | 559.058                                          | -218.820                                          | -218.820                        |
| 200    | 104.275 | 424.175                                                  | 475.941                                          | -245.455                                          | -245.455                        |
| 250    | 105.593 | 447.600                                                  | 468.013                                          | -10.533                                           | -10.533                         |
| 298.15 | 106.313 | 466.266                                                  | 466.268                                          | 0                                                 | 0                               |
| 300    | 106.334 | 466.324                                                  | 466.268                                          | 0.197                                             | 0.197                           |
| 350    | 106.790 | 483.352                                                  | 467.565                                          | 5.526                                             | 5.526                           |
| 400    | 107.089 | 497.633                                                  | 470.450                                          | 10.873                                            | 10.873                          |
| 450    | 107.296 | 510.559                                                  | 474.185                                          | 16.223                                            | 16.223                          |
| 500    | 107.445 | 521.572                                                  | 478.368                                          | 21.602                                            | 21.602                          |
| 600    | 107.640 | 541.180                                                  | 487.257                                          | 32.357                                            | 32.357                          |
| 700    | 107.758 | 557.782                                                  | 496.172                                          | 43.127                                            | 43.127                          |
| 800    | 107.835 | 572.777                                                  | 504.793                                          | 53.907                                            | 53.907                          |
| 900    | 107.888 | 584.481                                                  | 512.000                                          | 64.693                                            | 64.693                          |
| 1000   | 107.926 | 596.250                                                  | 520.166                                          | 75.484                                            | 75.484                          |
| 1200   | 107.975 | 615.932                                                  | 538.103                                          | 82.278                                            | 82.278                          |
| 1300   | 107.991 | 624.376                                                  | 541.596                                          | 107.373                                           | 107.373                         |
| 1400   | 108.005 | 632.779                                                  | 547.813                                          | 118.673                                           | 118.673                         |
| 1500   | 108.015 | 640.031                                                  | 553.713                                          | 129.474                                           | 129.474                         |
| 1600   | 108.024 | 647.002                                                  | 559.330                                          | 140.276                                           | 140.276                         |
| 1700   | 108.031 | 653.552                                                  | 564.682                                          | 151.079                                           | 151.079                         |
| 1800   | 108.037 | 659.727                                                  | 569.792                                          | 161.882                                           | 161.882                         |
| 1900   | 108.042 | 665.942                                                  | 574.681                                          | 172.636                                           | 172.636                         |
| 2000   | 108.047 | 671.110                                                  | 579.365                                          | 183.491                                           | 183.491                         |
| 2100   | 108.051 | 676.382                                                  | 582.960                                          | 194.295                                           | 194.295                         |
| 2200   | 108.054 | 681.408                                                  | 588.181                                          | 205.101                                           | 205.101                         |
| 2300   | 108.057 | 686.212                                                  | 592.339                                          | 215.906                                           | 215.906                         |
| 2400   | 108.059 | 690.810                                                  | 596.347                                          | 226.712                                           | 226.712                         |
| 2500   | 108.061 | 692.222                                                  | 600.215                                          | 237.518                                           | 237.518                         |
| 2600   | 108.063 | 699.460                                                  | 603.951                                          | 248.324                                           | 248.324                         |
| 2700   | 108.065 | 703.338                                                  | 607.564                                          | 259.131                                           | 259.131                         |
| 2800   | 108.067 | 707.468                                                  | 611.062                                          | 269.937                                           | 269.937                         |
| 2900   | 108.068 | 711.261                                                  | 614.452                                          | 280.744                                           | 280.744                         |
| 3000   | 108.069 | 714.924                                                  | 729.551                                          | 301.551                                           | 301.551                         |
| 3100   | 108.070 | 718.468                                                  | 730.333                                          | 302.358                                           | 302.358                         |
| 3200   | 108.071 | 721.399                                                  | 731.035                                          | 313.165                                           | 313.165                         |
| 3300   | 108.072 | 725.225                                                  | 727.051                                          | 323.972                                           | 323.972                         |
| 3400   | 108.073 | 728.451                                                  | 629.986                                          | 334.779                                           | 334.779                         |
| 3500   | 108.074 | 731.584                                                  | 632.845                                          | 345.587                                           | 345.587                         |
| 3600   | 108.075 | 734.528                                                  | 633.630                                          | 346.394                                           | 346.394                         |
| 3700   | 108.075 | 737.589                                                  | 638.346                                          | 367.202                                           | 367.202                         |
| 3800   | 108.076 | 740.472                                                  | 640.595                                          | 368.009                                           | 368.009                         |
| 3900   | 108.077 | 743.472                                                  | 643.520                                          | 388.817                                           | 388.817                         |
| 4000   | 108.077 | 746.015                                                  | 646.109                                          | 399.625                                           | 399.625                         |
| 4100   | 108.078 | 748.684                                                  | 648.577                                          | 410.432                                           | 410.432                         |
| 4200   | 108.078 | 751.528                                                  | 650.593                                          | 421.240                                           | 421.240                         |
| 4300   | 108.079 | 753.831                                                  | 653.355                                          | 432.048                                           | 432.048                         |
| 4400   | 108.079 | 756.316                                                  | 655.667                                          | 442.856                                           | 442.856                         |
| 4500   | 108.079 | 758.745                                                  | 657.931                                          | 453.664                                           | 453.664                         |
| 4600   | 108.080 | 761.120                                                  | 660.148                                          | 464.472                                           | 464.472                         |
| 4700   | 108.080 | 763.445                                                  | 662.322                                          | 475.280                                           | 475.280                         |
| 4800   | 108.082 | 765.720                                                  | 664.452                                          | 486.058                                           | 486.058                         |
| 4900   | 108.081 | 767.949                                                  | 666.342                                          | 496.896                                           | 496.896                         |
| 5000   | 108.081 | 770.132                                                  | 668.392                                          | 507.704                                           | 507.704                         |
| 5100   | 108.081 | 772.273                                                  | 670.604                                          | 518.512                                           | 518.512                         |
| 5200   | 108.081 | 774.371                                                  | 672.579                                          | 529.320                                           | 529.320                         |
| 5300   | 108.082 | 776.430                                                  | 674.119                                          | 540.128                                           | 540.128                         |
| 5400   | 108.082 | 778.450                                                  | 676.322                                          | 550.926                                           | 550.926                         |
| 5500   | 108.082 | 780.434                                                  | 678.298                                          | 561.745                                           | 561.745                         |
| 5600   | 108.082 | 782.381                                                  | 680.140                                          | 572.553                                           | 572.553                         |
| 5700   | 108.082 | 784.394                                                  | 681.950                                          | 583.361                                           | 583.361                         |
| 5800   | 108.083 | 786.174                                                  | 683.731                                          | 594.169                                           | 594.169                         |
| 5900   | 108.083 | 788.022                                                  | 685.483                                          | 604.978                                           | 604.978                         |
| 6000   | 108.083 | 789.338                                                  | 687.207                                          | 615.786                                           | 615.786                         |

PREVIOUS December 1973 (1 atm)

CURRENT December 1973 (1 bar)

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

## NIST-JANAF THERMOCHEMICAL TABLES

CRYSTAL  
Tetraiodosilane ( $\text{SiI}_4$ ) $M_r = 535.7035$  Tetralodosilane ( $\text{SiI}_4$ ) $\text{I}_4\text{Si}_1(\text{cr})$ 

|  | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |                                                  |                                                  |                                                                                   |                                            |             | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |                                        |                          |                    |                     |            |
|--|-----------------------------------------------------------|--------------------------------------------------|--------------------------------------------------|-----------------------------------------------------------------------------------|--------------------------------------------|-------------|---------------------------------------------------|----------------------------------------|--------------------------|--------------------|---------------------|------------|
|  | $\Delta_f H^\circ(0 \text{ K}) = \text{Unknown}$          | $\Delta_f J^\circ(0 \text{ K}) = \text{Unknown}$ | $\Delta_f K^\circ(0 \text{ K}) = \text{Unknown}$ | $S^\circ(298.15 \text{ K}) = [258.153 \pm 3.3] \text{ J K}^{-1} \text{ mol}^{-1}$ | $T_{\text{fs}} = 393.65 \pm 3.0 \text{ K}$ | $C_p^\circ$ | $C_v^\circ$                                       | $S^\circ - (G^\circ - H^\circ(T_r))/T$ | $H^\circ - H^\circ(T_r)$ | $\Delta_f H^\circ$ | $\Delta_f G^\circ$  | $\log K_r$ |
|  | 0                                                         | 0                                                | 0                                                | 0                                                                                 | 0                                          | 100         | 100                                               | 258.153                                | 258.153                  | 0                  | -189.535            | -191.637   |
|  | 298.15                                                    | 108.035                                          | 298.15                                           | 258.153                                                                           | 300                                        | 108.198     | 258.822                                           | 258.155                                | 0.200                    | -189.574           | -191.650            | 33.369     |
|  | 393.650                                                   | 116.388                                          | 393.650                                          | 289.279                                                                           | 500                                        | 125.687     | 262.503                                           | 262.056                                | 10.716                   | --                 | CRYSTAL <--> LIQUID | --         |
|  | 400                                                       | 116.943                                          | 400                                              | 291.146                                                                           | 500                                        | 318.180     | 271.003                                           | 271.003                                | 11.457                   | -223.715           | -190.911            | 24.930     |
|  |                                                           |                                                  |                                                  |                                                                                   |                                            |             |                                                   |                                        | 23.589                   | -310.254           | -174.369            | 18.216     |

## Enthalpy of Formation

Schafer and Heine<sup>1</sup> measured the enthalpies of solution of  $\text{Si}(\text{cr})$  and  $\text{SiI}_4(\text{cr})$  in an HF solution containing  $\text{AgF}$ . For the overall reaction  $\text{SiI}_4(\text{cr}) + 4\text{Ag}(\text{cr}) = \text{Si}(\text{cr}) + 4\text{AgI}(\text{cr})$ , they reported  $\Delta_f H^\circ(298.15 \text{ K}) = -13.80 \pm 0.44 \text{ kcal/mol}^{-1}$ . Using auxiliary data for  $\text{AgI}^\circ$  we calculate  $\Delta_f H^\circ = 19.665 \pm 2.1 \text{ kJ/mol}^{-1}$ . We adopt this value and assign an uncertainty of  $\pm 4.0 \text{ kcal/mol}^{-1}$  due to the overall inaccuracy in the  $\text{SiI}_4$  thermochimical data. Refer to the  $\text{SiI}_4(\text{g})$  table for more details.

Wolf<sup>2</sup> studied the enthalpies of solution of  $\text{SiI}_4(\text{cr})$  and  $\text{Na}_2\text{SiO}_3(\text{cr})$  in caustic solution. The net reaction of interest  $\text{SiI}_4(\text{cr}) + 6\text{NaOH}(\text{cr}) = \text{Na}_2\text{SiO}_3(\text{cr}) + 4\text{NaI}(\text{cr}) + 3\text{H}_2\text{O}(\text{l})$  yielded a enthalpy of reaction of  $\Delta_f H^\circ(298.15 \text{ K}) = -191.5 \pm 1.5 \text{ kcal/mol}^{-1}$  based on the appropriate combination of results from five solution studies. Using current auxiliary data,<sup>4,5</sup> we calculate  $\Delta_f H^\circ(298.15 \text{ K}) = -51.0 \text{ kcal/mol}^{-1}$  for  $\text{SiI}_4(\text{cr})$ . This data is suspect due to uncertainties in how Wolf converted his data from  $\text{Na}_2\text{SiO}_3(\text{calorimetric solution})$  to  $\text{Na}_2\text{SiO}_3(\text{cr})$ .

## 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 standard heat measurements and differential thermal analysis. Similar studies on  $\text{Cr}(\text{cr})$  and  $\text{Si}(\text{cr})$  would suggest uncertainties of the order of 3% near room temperature and 0.10% at 600–700 K. There is no low temperature heat capacity data for  $\text{SiI}_4$  at 298.15 K. The entropy at 298.15 K is chosen from a consideration of the sublimation and vaporization data. Refer to the  $\text{SiI}_4(\text{g})$  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  $\Delta_{\text{fs}} H^\circ = 4.7 \text{ kcal/mol}^{-1}$ , an average of eight measurements with a standard deviation of 0.08  $\text{kcal/mol}^{-1}$ . The same study reported  $T_{\text{fs}} = 120.5^\circ\text{C}$  as determined from the cooling curve. McCarty *et al.*<sup>7</sup> reported  $T_{\text{fs}} = 123.68 \pm 0.06^\circ\text{C}$  for 99.998% (mole) pure  $\text{SiI}_4$ . 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  $4.1 \pm 0.6 \text{ kcal/mol}^{-1}$ . 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  $\text{SiI}_4(\text{g})$  table, show poor agreement in the vicinity of  $T_{\text{fs}}$ . We adopt  $T_{\text{fs}} = 120.5^\circ\text{C}$  and  $\Delta_{\text{fs}} H^\circ = 4.7 \text{ kcal/mol}^{-1}$  as derived from Kurosawa *et al.*<sup>6</sup> We assign respective uncertainties of  $\pm 3.0 \text{ K}$  and  $0.5 \text{ kcal/mol}^{-1}$  due to the variances among the various studies.

## Sublimation Data

The enthalpy of sublimation,  $\Delta_{\text{sub}} H^\circ(298.15 \text{ K})$ , is the difference between the  $\Delta_f H^\circ(298.15 \text{ K})$  values for  $\text{SiI}_4(\text{g})$  and  $\text{SiI}_4(\text{cr})$ . Three sublimation studies are summarized in the  $\text{SiI}_4(\text{g})$  table.

## References

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- U. S. Natl. Bur. Stand. Tech. Note 270-4, 141 pp. (1969).
- E. Wolf, Z. Chem. 7, 283 (1967).
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- JANAF Thermochemical Tables:  $\text{Na}(\text{cr}), 9-30-63$ ;  $\text{Na}_2\text{SiO}_3(\text{cr}), 12-31-70$ ;  $\text{NaOH}(\text{cr}), 9-30-67$ ;  $\text{SiCl}(\text{g}), 12-31-70$ ;  $\text{Si}_4(\text{cr}), 6-30-76$ .
- T. Kurosawa, R. Haségawa, and T. Yagihashi, Trans. Japan Inst. Metals. 6, 229 (1965); Trans. Natl. Res. Inst. Metals. (Tokyo) 7, 222 (1965).
- L. V. McCarty, L. C. Landauer, and J. M. Binkowski, J. Chem. Eng. Data 5, 365–6 (1960).
- K. Bartsch and E. Wolf, Z. anorg. allg. Chem. 383, 66 (1971).

PREVIOUS

CURRENT: June 1976

Tetralodosilane ( $\text{SiI}_4$ ) $\text{I}_4\text{Si}_1(\text{cr})$

Tetraiodosilane ( $\text{SiI}_4$ )LIQUID  $M_r = 535.7035$ 

$$\Delta H^\circ(298.15 \text{ K}) = [294.309] \text{ J K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{m}} = 393.65 \pm 3.0 \text{ K}$$

## Enthalpy of Formation

$\Delta H^\circ(\text{SiI}_4, \text{l}, 298.15 \text{ K})$  is calculated from that of the crystal by adding the enthalpy of melting,  $\Delta_{\text{m}}H^\circ$ , 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

Kurosewa *et al.*<sup>1</sup> measured the heat capacity of  $\text{SiI}_4$  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  $\Delta_fH^\circ(298.15 \text{ K})$ .

## Vaporization Data

$T_{\text{vap}} = -576 \text{ K}$  is calculated as that temperature at which the fugacity is one atmosphere for the process  $\text{SiI}_4(\text{l}) = \text{SiI}_4(\text{g})$ .  $\Delta_{\text{vap}}H^\circ$  is calculated as the difference between the  $\Delta_fH^\circ$  values for the ideal gas and the liquid at  $T_{\text{vap}}$ . The vaporization studies near  $T_{\text{vap}}$  are discussed in the  $\text{SiI}_4(\text{g})$  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  $p = 760 \text{ mm Hg}$ .

## References

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

|  |  | $\text{I}_4\text{Si}_4(\text{l})$                         |         |                                               |                                      | $\text{I}_4\text{Si}_4(\text{l})$ Tetraiodosilane ( $\text{SiI}_4$ ) |                                   |                        |            |
|--|--|-----------------------------------------------------------|---------|-----------------------------------------------|--------------------------------------|----------------------------------------------------------------------|-----------------------------------|------------------------|------------|
|  |  | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |         |                                               |                                      | Standard State Pressure = $p^* = 0.1 \text{ MPa}$                    |                                   |                        |            |
|  |  | $T/K$                                                     | $C_p$   | $J \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ | $S^\circ - (G^\circ - H^\circ(T))/T$ | $H^\circ - H^\circ(T)$                                               | $\text{kJ} \cdot \text{mol}^{-1}$ | $\Delta_fG^\circ$      | $\log K_r$ |
|  |  | 0                                                         |         |                                               |                                      |                                                                      |                                   |                        |            |
|  |  | 100                                                       |         |                                               |                                      |                                                                      |                                   |                        |            |
|  |  | 200                                                       |         |                                               |                                      |                                                                      |                                   |                        |            |
|  |  | 298.15                                                    | 159.800 | 294.309                                       | 294.309                              | 0.                                                                   | -174.603                          | -187.485               | 32.847     |
|  |  | 300                                                       | 159.875 | 295.298                                       | 294.312                              | 0.296                                                                | -174.546                          | -187.565               | 32.638     |
|  |  | 393.650                                                   | 163.744 | 339.234                                       | 299.988                              | 15.449                                                               | --                                | -- CRYSTAL <--> LIQUID | --         |
|  |  | 400                                                       | 164.004 | 341.856                                       | 300.632                              | 16.490                                                               | -203.750                          | -191.230               | 24.972     |
|  |  | 500                                                       | 168.134 | 378.897                                       | 312.703                              | 33.097                                                               | -285.814                          | -180.287               | 18.834     |
|  |  | 600                                                       | 172.264 | 409.916                                       | 326.389                              | 50.117                                                               | -278.678                          | -159.847               | 13.916     |
|  |  | 700                                                       | 176.393 | 436.781                                       | 340.282                              | 67.549                                                               | -271.228                          | -140.627               | 10.494     |

14Si<sub>4</sub>(cr, l)

$$M_r = 535.7035 \text{ Tetraiodosilane (SiI}_4\text{)}$$

Refer to the individual tables for details.

Refer to the individual tables for details.

| T/K     | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |                                                                                   | Standard State Pressure = $p^* = 0.1\text{ MPa}$ |                |                                         |
|---------|----------------------------------------------------------|-----------------------------------------------------------------------------------|--------------------------------------------------|----------------|-----------------------------------------|
|         | $C_p^*$                                                  | $\frac{\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}}{S^* - [G^* - H^*(T_r)]/T}$ | $H^* - H^*(T_r)/T$                               | $\Delta_i H^*$ | $\Delta_i G^*$                          |
| 0       |                                                          |                                                                                   |                                                  |                | $\log K_r$                              |
| 100     |                                                          |                                                                                   |                                                  |                |                                         |
| 200     |                                                          |                                                                                   |                                                  |                |                                         |
| 298.15  | 108.035                                                  | 258.153                                                                           | 258.153                                          | 0.             | -189.535                                |
| 300     | 108.198                                                  | 258.822                                                                           | 258.155                                          | 0.200          | -189.574                                |
| 393.650 | 116.390                                                  | 229.279                                                                           | 262.056                                          | 10.716         | CRYSTAL $\leftarrow \rightarrow$ LIQUID |
| 393.650 | 163.744                                                  | 339.234                                                                           | 262.056                                          | 30.381         | TRANSITION                              |
| 400     | 164.004                                                  | 341.856                                                                           | 263.302                                          | 31.422         | -203.750                                |
| 500     | 168.134                                                  | 378.897                                                                           | 282.839                                          | 40.029         | -285.814                                |
| 600     | 172.264                                                  | 409.916                                                                           | 301.502                                          | 65.049         | -278.678                                |
| 700     | 176.393                                                  | 436.781                                                                           | 318.950                                          | 82.481         | -271.228                                |

PREVIOUS

CURRENT December 1977

### Tetraiodosilane ( $\text{SiI}_4$ )

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





**Titanium Iodide ( $\text{TiI}_4$ )****Liquid**

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

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

**Enthalpy of Formation**

$\Delta_fH^\circ(\text{TiI}_4, \text{l}, 298.15\text{ K})$  is calculated from  $\Delta_fH^\circ(\text{TiI}_4, \text{cr}, 298.15\text{ K})$  by adding the enthalpy of fusion,  $\Delta_fH^\circ$ , 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  $\text{TiI}_4(\text{l})$  above the melting temperature. The heat capacity derived from these data is constant.  $S^\circ(\text{TiI}_4, \text{l}, 298.15\text{ K})$  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,  $T_{\text{boil}}$ , is taken as the temperature at which the fugacity is 1 bar for the reaction  $\text{TiI}_4(\text{l}) = \text{TiI}_4(\text{g})$ . The enthalpy of vaporization is calculated as the difference between  $\Delta_fH^\circ$  of the liquid and gas at the boiling temperature. The vapor pressure data are discussed in the table for  $\text{TiI}_4(\text{g})$ .

**Reference**

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

|  |  | $\text{LiTi}_4(\text{l})$                                |  | $M_i = 555.4980$ Titanium iodide ( $\text{TiI}_4$ ) |  |  |  |
|--|--|----------------------------------------------------------|--|-----------------------------------------------------|--|--|--|
|  |  |                                                          |  |                                                     |  |  |  |
|  |  |                                                          |  |                                                     |  |  |  |
|  |  | Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ |  | Standard State Pressure = $p^* = 0.1\text{ MPa}$    |  |  |  |
|  |  | $T/K$                                                    |  | $T/K$                                               |  |  |  |
|  |  | $C_p^\circ$                                              |  | $C_p^\circ$                                         |  |  |  |
|  |  | $J\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$                |  | $J\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$           |  |  |  |
|  |  | $S^\circ$                                                |  | $S^\circ$                                           |  |  |  |
|  |  | $-[G^\circ - HF(T_r)]/T$                                 |  | $H^\circ - H^\circ(T_r)$                            |  |  |  |
|  |  | $\text{J}\cdot\text{mol}^{-1}$                           |  | $\text{J}\cdot\text{mol}^{-1}$                      |  |  |  |
|  |  | $\Delta_fH^\circ$                                        |  | $\Delta_fH^\circ$                                   |  |  |  |
|  |  | $\text{kJ}\cdot\text{mol}^{-1}$                          |  | $\text{kJ}\cdot\text{mol}^{-1}$                     |  |  |  |
|  |  | 0                                                        |  | 0                                                   |  |  |  |
|  |  | 100                                                      |  | 0                                                   |  |  |  |
|  |  | 200                                                      |  | 0                                                   |  |  |  |
|  |  | 298.15                                                   |  | 0                                                   |  |  |  |
|  |  | 300                                                      |  | 0                                                   |  |  |  |
|  |  | 400                                                      |  | 0                                                   |  |  |  |
|  |  | 428.000                                                  |  | 0                                                   |  |  |  |
|  |  | 500                                                      |  | 0                                                   |  |  |  |
|  |  | 600                                                      |  | 0                                                   |  |  |  |
|  |  | 700                                                      |  | 0                                                   |  |  |  |
|  |  | 800                                                      |  | 0                                                   |  |  |  |
|  |  | 900                                                      |  | 0                                                   |  |  |  |
|  |  | 1000                                                     |  | 0                                                   |  |  |  |
|  |  | 1100                                                     |  | 0                                                   |  |  |  |
|  |  | 1200                                                     |  | 0                                                   |  |  |  |
|  |  | 1300                                                     |  | 0                                                   |  |  |  |
|  |  | 1400                                                     |  | 0                                                   |  |  |  |
|  |  | 1500                                                     |  | 0                                                   |  |  |  |
|  |  | 200                                                      |  | 0                                                   |  |  |  |
|  |  | 300                                                      |  | 0                                                   |  |  |  |
|  |  | 400                                                      |  | 0                                                   |  |  |  |
|  |  | 428.000                                                  |  | 0                                                   |  |  |  |
|  |  | 500                                                      |  | 0                                                   |  |  |  |
|  |  | 600                                                      |  | 0                                                   |  |  |  |
|  |  | 700                                                      |  | 0                                                   |  |  |  |
|  |  | 800                                                      |  | 0                                                   |  |  |  |
|  |  | 900                                                      |  | 0                                                   |  |  |  |
|  |  | 1000                                                     |  | 0                                                   |  |  |  |
|  |  | 1100                                                     |  | 0                                                   |  |  |  |
|  |  | 1200                                                     |  | 0                                                   |  |  |  |
|  |  | 1300                                                     |  | 0                                                   |  |  |  |
|  |  | 1400                                                     |  | 0                                                   |  |  |  |
|  |  | 1500                                                     |  | 0                                                   |  |  |  |
|  |  | 200                                                      |  | 0                                                   |  |  |  |
|  |  | 300                                                      |  | 0                                                   |  |  |  |
|  |  | 400                                                      |  | 0                                                   |  |  |  |
|  |  | 428.000                                                  |  | 0                                                   |  |  |  |
|  |  | 500                                                      |  | 0                                                   |  |  |  |
|  |  | 600                                                      |  | 0                                                   |  |  |  |
|  |  | 700                                                      |  | 0                                                   |  |  |  |
|  |  | 800                                                      |  | 0                                                   |  |  |  |
|  |  | 900                                                      |  | 0                                                   |  |  |  |
|  |  | 1000                                                     |  | 0                                                   |  |  |  |
|  |  | 1100                                                     |  | 0                                                   |  |  |  |
|  |  | 1200                                                     |  | 0                                                   |  |  |  |
|  |  | 1300                                                     |  | 0                                                   |  |  |  |
|  |  | 1400                                                     |  | 0                                                   |  |  |  |
|  |  | 1500                                                     |  | 0                                                   |  |  |  |
|  |  | 200                                                      |  | 0                                                   |  |  |  |
|  |  | 300                                                      |  | 0                                                   |  |  |  |
|  |  | 400                                                      |  | 0                                                   |  |  |  |
|  |  | 428.000                                                  |  | 0                                                   |  |  |  |
|  |  | 500                                                      |  | 0                                                   |  |  |  |
|  |  | 600                                                      |  | 0                                                   |  |  |  |
|  |  | 700                                                      |  | 0                                                   |  |  |  |
|  |  | 800                                                      |  | 0                                                   |  |  |  |
|  |  | 900                                                      |  | 0                                                   |  |  |  |
|  |  | 1000                                                     |  | 0                                                   |  |  |  |
|  |  | 1100                                                     |  | 0                                                   |  |  |  |
|  |  | 1200                                                     |  | 0                                                   |  |  |  |
|  |  | 1300                                                     |  | 0                                                   |  |  |  |
|  |  | 1400                                                     |  | 0                                                   |  |  |  |
|  |  | 1500                                                     |  | 0                                                   |  |  |  |
|  |  | 200                                                      |  | 0                                                   |  |  |  |
|  |  | 300                                                      |  | 0                                                   |  |  |  |
|  |  | 400                                                      |  | 0                                                   |  |  |  |
|  |  | 428.000                                                  |  | 0                                                   |  |  |  |
|  |  | 500                                                      |  | 0                                                   |  |  |  |
|  |  | 600                                                      |  | 0                                                   |  |  |  |
|  |  | 700                                                      |  | 0                                                   |  |  |  |
|  |  | 800                                                      |  | 0                                                   |  |  |  |
|  |  | 900                                                      |  | 0                                                   |  |  |  |
|  |  | 1000                                                     |  | 0                                                   |  |  |  |
|  |  | 1100                                                     |  | 0                                                   |  |  |  |
|  |  | 1200                                                     |  | 0                                                   |  |  |  |
|  |  | 1300                                                     |  | 0                                                   |  |  |  |
|  |  | 1400                                                     |  | 0                                                   |  |  |  |
|  |  | 1500                                                     |  | 0                                                   |  |  |  |
|  |  | 200                                                      |  | 0                                                   |  |  |  |
|  |  | 300                                                      |  | 0                                                   |  |  |  |
|  |  | 400                                                      |  | 0                                                   |  |  |  |
|  |  | 428.000                                                  |  | 0                                                   |  |  |  |
|  |  | 500                                                      |  | 0                                                   |  |  |  |
|  |  | 600                                                      |  | 0                                                   |  |  |  |
|  |  | 700                                                      |  | 0                                                   |  |  |  |
|  |  | 800                                                      |  | 0                                                   |  |  |  |
|  |  | 900                                                      |  | 0                                                   |  |  |  |
|  |  | 1000                                                     |  | 0                                                   |  |  |  |
|  |  | 1100                                                     |  | 0                                                   |  |  |  |
|  |  |                                                          |  |                                                     |  |  |  |

TITANIUM IODIDE (TiI<sub>4</sub>)M<sub>r</sub> = 555.4980 Titanium Iodide (TiI<sub>4</sub>)

O to 379 K crystal, I  
379 to 428 K crystal, II  
above 428 K liquid

Refer to the individual tables for details.

I<sub>4</sub>Ti<sub>4</sub>(cr,I)

| T/K     | Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K |                                     | Standard State Pressure = p° = 0.1 MPa |                                                        |                                                   |                      |          |          |                    |  |
|---------|------------------------------------------------------------|-------------------------------------|----------------------------------------|--------------------------------------------------------|---------------------------------------------------|----------------------|----------|----------|--------------------|--|
|         | C <sub>p</sub> <sup>°</sup>                                | J·K <sup>-1</sup> mol <sup>-1</sup> | S <sup>°</sup>                         | -[G <sup>°</sup> - H <sup>°</sup> (T <sub>r</sub> )]/T | H <sup>°</sup> - H <sup>°</sup> (T <sub>r</sub> ) | kJ·mol <sup>-1</sup> | ΔH°      | ΔG°      | log K <sub>f</sub> |  |
| 0       | 0                                                          | 0                                   | 0                                      | INFINITE                                               | -29.141                                           | -29.141              | -373.638 | -373.638 | INFINITE           |  |
| 100     | 100.671                                                    | 120.059                             | 357.958                                | -23.290                                                | -374.448                                          | -374.448             | -373.429 | -373.429 | 195.059            |  |
| 200     | 193.349                                                    | 197.192                             | 257.466                                | -12.655                                                | -374.995                                          | -374.995             | -372.204 | -372.204 | 97.210             |  |
| 298.15  | 255.629                                                    | 246.150                             | 246.150                                | 0.                                                     | -375.723                                          | -375.723             | -370.687 | -370.687 | 64.943             |  |
| 300     | 255.947                                                    | 246.528                             | 246.153                                | 0.233                                                  | -375.739                                          | -375.739             | -370.655 | -370.655 | 64.537             |  |
| 379.000 | 339.603                                                    | 277.904                             | 249.613                                | 10.722                                                 | I ⇌ II                                            |                      |          |          | TRANSITION         |  |
| 379.000 | 348.114                                                    | 304.068                             | 249.613                                | 20.639                                                 | II ⇌ LIQUID                                       |                      |          |          | TRANSITION         |  |
| 400     | 48.114                                                     | 312.056                             | 252.883                                | 23.749                                                 | -398.112                                          | -398.112             | -368.316 | -368.316 | 48.097             |  |
| 428.000 | 481.114                                                    | 372.077                             | 256.899                                | 27.896                                                 | II ⇌ LIQUID                                       |                      |          |          | TRANSITION         |  |
| 428.000 | 156.482                                                    | 368.414                             | 256.899                                | 47.728                                                 | TRANSITION                                        |                      |          |          | TRANSITION         |  |
| 500     | 156.482                                                    | 392.744                             | 274.754                                | 58.995                                                 | -462.000                                          | -462.000             | -356.185 | -356.185 | 37.210             |  |
| 600     | 156.482                                                    | 421.274                             | 296.869                                | 74.643                                                 | -456.685                                          | -456.685             | -355.523 | -355.523 | 29.210             |  |
| 700     | 156.482                                                    | 445.396                             | 316.408                                | 90.291                                                 | -451.460                                          | -451.460             | -315.744 | -315.744 | 23.361             |  |
| 800     | 156.482                                                    | 466.291                             | 333.867                                | 105.939                                                | -446.295                                          | -446.295             | -296.709 | -296.709 | 19.373             |  |
| 900     | 156.482                                                    | 484.722                             | 349.625                                | 121.588                                                | -441.219                                          | -441.219             | -278.316 | -278.316 | 16.153             |  |
| 1000    | 156.482                                                    | 501.209                             | 363.973                                | 137.236                                                | -436.295                                          | -436.295             | -260.482 | -260.482 | 13.606             |  |
| 1100    | 156.482                                                    | 516.123                             | 377.138                                | 152.884                                                | -431.593                                          | -431.593             | -243.130 | -243.130 | 11.545             |  |
| 1200    | 156.482                                                    | 529.739                             | 389.296                                | 168.532                                                | -431.105                                          | -431.105             | -226.076 | -226.076 | 9.841              |  |
| 1300    | 156.482                                                    | 542.264                             | 400.587                                | 184.180                                                | -426.149                                          | -426.149             | -209.193 | -209.193 | 8.405              |  |
| 1400    | 156.482                                                    | 553.861                             | 411.126                                | 199.828                                                | -421.333                                          | -421.333             | -197.685 | -197.685 | 7.189              |  |
| 1500    | 156.482                                                    | 564.657                             | 421.006                                | 215.477                                                | -416.690                                          | -416.690             | -176.516 | -176.516 | 6.147              |  |

I<sub>4</sub>Ti<sub>4</sub>(cr,I)

## CRYSTAL (I-II)-LIQUID

O to 379 K crystal, I  
379 to 428 K crystal, II  
above 428 K liquid

Refer to the individual tables for details.

I<sub>4</sub>Ti<sub>4</sub>(cr,I)

## PREVIOUS

TITANIUM IODIDE (TiI<sub>4</sub>)

CURRENT: December 1983

## IDEAL GAS

 $M_r = 555.4980$  Titanium Iodide ( $Tl_4$ )

$$S^\circ(298.15\text{ K}) = 433.072 \pm 8.4 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(0\text{ K}) = -271.86 \pm 8.4 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15\text{ K}) = -277.27 \pm 8.4 \text{ kJ}\cdot\text{mol}^{-1}$$

Vibrational Frequencies and Degeneracies

| $\nu, \text{cm}^{-1}$ | $v, \text{cm}^{-1}$ | $\sigma = 12$ |
|-----------------------|---------------------|---------------|
| [175](1)              | [260](3)            |               |
| [55](2)               | [69](3)             |               |

Product of the Moments of Inertia:  $I_A/I_B/I_C = [4.332573 \times 10^{-10}] \text{ g}^3 \text{ cm}^6$ 

## Enthalpy of Formation

The enthalpy of formation of  $Tl_4(g)$  is calculated from that of  $Tl_4(l)$  and the enthalpy of vaporization of the liquid. Blocher and Campbell<sup>1</sup> reported vapor pressure data for  $Tl_4(l)$  over the temperature range 473 to 655 K. 2nd and 3rd law analyses of these data give values for  $\Delta_{vap}H^\circ(298.15\text{ K})$  of  $17.2 \pm 0.1$  and  $16.38 \text{ kcal}\cdot\text{mol}^{-1}$ , respectively, the 3rd law drift being  $-0.4 \pm 0.2 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . The adopted value of  $\Delta_f H^\circ(298.15\text{ K})$  is based on the 3rd law enthalpy of vaporization.

## Heat Capacity and Entropy

The interatomic distances are estimated from those of  $TlBr_4(cr)$ ,  $TlBr_4(g)$ , and  $Tl_4(cr)$ .<sup>2</sup> The tetrahedral model is assumed by analogy with  $TlCl_4(g)$  and  $TlBr_4(g)$ . The principal moments of inertia are:  $I_A = I_B = I_C = 351.2222 \times 10^{-39} \text{ g}\cdot\text{cm}^2$ .

The vibrational frequencies of  $Tl_4(g)$  have been estimated by Ushanova *et al.*<sup>3</sup> The given estimates are based on their predictions and valence force field calculations.

## References

<sup>1</sup>J. M. Blocher, Jr. and I. E. Campbell, J. Amer. Chem. Soc., **69**, 2100 (1947).
<sup>2</sup>O. Hasel and H. Kangstrand, Z. Phys. Chem., **1315**, 274 (1932).
<sup>3</sup>N. I. Ushanova, I. N. Godnev and I. V. Orlova, Opt. Spektrosk., **5**, 567 (1958). $I_4Tl_4(g)$ 

| $T/K$  | $C_p^\circ$ | Enthalpy Reference Temperature = $T_r = 293.15\text{ K}$ |                          |                    | Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$ |          |        |
|--------|-------------|----------------------------------------------------------|--------------------------|--------------------|-------------------------------------------------------|----------|--------|
|        |             | $S^\circ - (G^\circ - H^\circ(T_r))/T$                   | $H^\circ - H^\circ(T_r)$ | $\Delta_f H^\circ$ | $\Delta_f G^\circ$                                    |          |        |
| 0      | 0           | 0                                                        | -25.812                  | -271.860           | -271.850                                              | INFINITE |        |
| 100    | 83.757      | 327.171                                                  | -19.527                  | -272.236           | -291.928                                              | 152.488  |        |
| 200    | 100.193     | 392.170                                                  | 442.507                  | -10.068            | -274.558                                              | -310.763 | 81.163 |
| 250    | 102.779     | 414.832                                                  | 434.781                  | -4.987             | -275.896                                              | -319.662 | 66.790 |
| 298.15 | 104.254     | 433.072                                                  | 0                        | -277.274           | -327.968                                              | 57.459   |        |
| 300    | 104.298     | 433.711                                                  | 433.074                  | 0.193              | -277.329                                              | -328.282 | 57.159 |
| 350    | 103.256     | 449.877                                                  | 434.347                  | 5.433              | -278.999                                              | -336.648 | 50.242 |
| 400    | 103.895     | 463.971                                                  | 431.188                  | 10.713             | -282.699                                              | -343.668 | 44.878 |
| 450    | 103.342     | 476.471                                                  | 440.871                  | 16.020             | -316.816                                              | -347.292 | 40.313 |
| 500    | 106.666     | 487.693                                                  | 445.002                  | 21.345             | -401.200                                              | -342.859 | 35.818 |
| 600    | 107.093     | 507.181                                                  | 453.789                  | 32.035             | -403.844                                              | -331.226 | 28.836 |
| 700    | 107.354     | 523.711                                                  | 462.627                  | 42.759             | -405.543                                              | -319.647 | 23.852 |
| 800    | 107.524     | 538.058                                                  | 471.179                  | 53.503             | -402.282                                              | -308.109 | 20.117 |
| 900    | 107.641     | 550.730                                                  | 479.328                  | 64.262             | -400.095                                              | -296.600 | 17.214 |
| 1000   | 107.726     | 562.075                                                  | 487.045                  | 75.030             | -400.051                                              | -285.104 | 14.892 |
| 1100   | 107.788     | 572.346                                                  | 494.340                  | 85.806             | -400.221                                              | -273.603 | 12.992 |
| 1200   | 107.836     | 581.727                                                  | 501.237                  | 96.387             | -404.600                                              | -261.937 | 11.403 |
| 1300   | 107.873     | 590.360                                                  | 507.765                  | 107.373            | -404.507                                              | -250.074 | 10.048 |
| 1400   | 107.902     | 598.355                                                  | 513.954                  | 118.162            | -404.550                                              | -238.194 | 8.887  |
| 1500   | 107.926     | 605.800                                                  | 519.832                  | 128.933            | -404.764                                              | -226.505 | 7.881  |
| 1600   | 107.945     | 612.766                                                  | 525.425                  | 139.747            | -405.179                                              | -214.396 | 6.999  |
| 1700   | 107.962     | 619.311                                                  | 530.757                  | 150.542            | -405.828                                              | -202.453 | 6.221  |
| 1800   | 107.975     | 625.482                                                  | 535.850                  | 161.339            | -405.737                                              | -190.465 | 5.527  |
| 1900   | 107.987     | 631.320                                                  | 540.722                  | 172.137            | -407.407                                              | -178.419 | 4.905  |
| 2000   | 107.996     | 636.860                                                  | 545.392                  | 182.926            | -424.101                                              | -165.849 | 4.332  |
| 2100   | 108.005     | 642.129                                                  | 549.874                  | 193.736            | -426.640                                              | -152.874 | 3.803  |
| 2200   | 108.012     | 647.154                                                  | 554.182                  | 204.537            | -429.304                                              | -139.716 | 3.319  |
| 2300   | 108.019     | 651.955                                                  | 558.330                  | 215.339            | -432.077                                              | -126.554 | 2.874  |
| 2400   | 108.024     | 656.552                                                  | 562.327                  | 226.141            | -434.939                                              | -113.210 | 2.464  |
| 2500   | 108.029     | 660.962                                                  | 566.185                  | 236.943            | -437.688                                              | -99.744  | 2.084  |
| 2600   | 108.034     | 665.199                                                  | 569.912                  | 247.747            | -440.841                                              | -86.160  | 1.731  |
| 2700   | 108.037     | 669.277                                                  | 573.517                  | 258.550            | -443.835                                              | -72.462  | 1.402  |
| 2800   | 108.041     | 673.206                                                  | 573.206                  | 269.354            | -446.827                                              | -58.653  | 1.094  |
| 2900   | 108.044     | 676.997                                                  | 580.391                  | 280.158            | -449.795                                              | -44.737  | 0.806  |
| 3000   | 108.047     | 680.660                                                  | 583.672                  | 290.663            | -452.721                                              | -30.719  | 0.535  |
| 3100   | 108.049     | 684.203                                                  | 586.859                  | 301.768            | -455.387                                              | -16.605  | 0.280  |
| 3200   | 108.052     | 687.633                                                  | 589.934                  | 312.573            | -458.378                                              | -11.400  | -0.039 |
| 3300   | 108.054     | 690.938                                                  | 592.965                  | 323.378            | -461.083                                              | -11.891  | -0.188 |
| 3400   | 108.056     | 694.184                                                  | 595.895                  | 334.184            | -463.691                                              | -26.263  | -0.403 |
| 3500   | 108.058     | 697.316                                                  | 598.748                  | 344.989            | -466.194                                              | 40.711   | -0.608 |
| 3600   | 108.059     | 700.561                                                  | 601.529                  | 355.795            | -468.587                                              | 55.227   | -0.801 |
| 3700   | 108.061     | 703.321                                                  | 604.885                  | 366.601            | -479.963                                              | 77.598   | -1.093 |
| 3800   | 108.062     | 706.203                                                  | 606.845                  | 377.407            | -480.890                                              | 103.491  | -1.423 |
| 3900   | 108.063     | 709.010                                                  | 609.468                  | 388.213            | -482.752                                              | 129.407  | -1.733 |
| 4000   | 108.065     | 711.746                                                  | 611.991                  | 399.020            | -482.550                                              | 155.344  | -2.029 |
| 4100   | 108.066     | 714.414                                                  | 614.457                  | 409.826            | -483.283                                              | 181.301  | -2.310 |
| 4200   | 108.067     | 717.019                                                  | 616.868                  | 420.633            | -487.274                                              | 207.274  | -2.578 |
| 4300   | 108.068     | 719.561                                                  | 619.227                  | 431.440            | -488.549                                              | 233.263  | -2.834 |
| 4400   | 108.069     | 722.046                                                  | 621.535                  | 442.407            | -489.085                                              | 259.265  | -3.078 |
| 5100   | 108.073     | 738.001                                                  | 636.453                  | 517.896            | -487.112                                              | 441.513  | -4.322 |
| 5200   | 108.074     | 740.100                                                  | 638.426                  | 528.704            | -487.172                                              | 467.565  | -4.697 |
| 5300   | 108.074     | 742.158                                                  | 640.364                  | 539.511            | -488.965                                              | 493.617  | -4.865 |
| 5400   | 108.075     | 744.174                                                  | 628.181                  | 550.238            | -487.133                                              | 519.670  | -5.027 |
| 5500   | 108.075     | 746.162                                                  | 644.139                  | 485.475            | -486.599                                              | 563.372  | -5.183 |
| 5600   | 108.076     | 748.109                                                  | 647.578                  | 516.126            | -487.037                                              | 545.721  | -4.151 |
| 5700   | 108.076     | 750.022                                                  | 647.786                  | 517.934            | -486.592                                              | 571.770  | -5.333 |
| 5800   | 108.077     | 751.901                                                  | 649.565                  | 528.741            | -486.457                                              | 597.816  | -5.478 |
| 5900   | 108.077     | 753.149                                                  | 651.316                  | 539.549            | -486.457                                              | 623.838  | -5.618 |
| 6000   | 108.077     | 755.565                                                  | 653.038                  | 604.336            | -486.170                                              | 649.896  | -5.754 |

PREVIOUS: December 1968 (1 atm)

CURRENT: December 1968 (1 bar)

TITANIUM IODIDE ( $Tl_4$ )

## Zirconium Iodide ( $ZrI_4$ )

### CRYSTAL

### $I_4ZrI_4$ (cr)

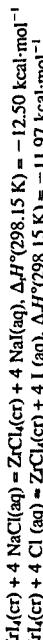
$$\Delta_fH^\circ(0\text{ K}) = [260.270 \pm 4.2] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{fus}} = 772 \pm 2 \text{ K}$$

$$T_{\text{sub}} = 705.6 \text{ K}$$

#### Enthalpy of Formation

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\*</sup> we calculate  $\Delta_fH^\circ(298.15 \text{ K}) = -116.52$  and  $-117.05 \text{ kcal}\cdot\text{mol}^{-1}$  for  $ZrI_4(\text{cr})$  from these two reactions. We adopt a mean of these two values,  $\Delta_fH^\circ(298.15 \text{ K}) = -116.8 \text{ kcal}\cdot\text{mol}^{-1}$ , and assign an uncertainty of  $\pm 1.5 \text{ kcal}\cdot\text{mol}^{-1}$ . The value suggested by NBS<sup>3</sup> is  $1.7 \text{ kcal}\cdot\text{mol}^{-1}$  more positive.

Baev and Shelton<sup>4</sup> reference an enthalpy of formation value for  $ZrI_4(\text{cr})$ . The reported  $\Delta_fH^\circ(298.15 \text{ K}) = 105.9 \text{ kcal}\cdot\text{mol}^{-1}$  as supposedly extracted from Karapetyants and Karapetyants.<sup>5</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  $ZrI_4(\text{cr})$ . The adopted heat capacity values are estimated such they parallel those adopted for  $ZrCl_4(\text{cr})$  and  $ZrBr_4(\text{cr})$ , and are consistent with the sublimation data.

The crystal data compilation of Donnay and Ondik<sup>6</sup> does not list the crystal structure of  $ZrI_4(\text{cr})$  but does tabulate both  $ZrCl_4$  and  $ZrBr_4$  as cubic structures. The literature data related to the crystal structure of  $ZrI_4(\text{cr})$  is not definitive. Assuming  $ZrI_4(\text{cr})$  also has a cubic structure, the adopted heat capacity values are estimated so as to parallel those for  $ZrCl_4$  and  $ZrBr_4$ . The values below 300 K are calculated in the same manner as for  $ZrBr_4(\text{cr})$ . The high temperature heat capacities are obtained graphically.

#### Fusion Data

The melting point was observed by Rahlfis and Fischer<sup>9</sup> to be  $772 \pm 2 \text{ K}$  and by Nisel'son<sup>10</sup> to be 773 K.

#### Sublimation Data

The sublimation data are treated in the  $ZrI_4(\text{g})$  table.<sup>2</sup> The sublimation temperature,  $T_{\text{sub}}$ , is calculated from the Gibbs energy crossover between the crystal and gas. Since  $T_{\text{sub}}$  is less than  $T_{\text{fus}}$ , the liquid phase is thermodynamically unstable at one atmosphere pressure.

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| $M_r = 598.8380$ Zirconium Iodide ( $ZrI_4$ )                                                   |         |                                                  |                                                   |                               |                   |
|-------------------------------------------------------------------------------------------------|---------|--------------------------------------------------|---------------------------------------------------|-------------------------------|-------------------|
| Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$                                       |         |                                                  |                                                   |                               |                   |
|                                                                                                 |         |                                                  | Standard State Pressure = $p^* = 0.1 \text{ MPa}$ |                               |                   |
|                                                                                                 |         |                                                  | $\text{kJ}\cdot\text{mol}^{-1}$                   |                               |                   |
| $\Delta_fH^\circ(0 \text{ K}) = [-487.24 \pm 8.4] \text{ kJ}\cdot\text{mol}^{-1}$               |         | $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ | $S^\circ$                                         | $-G^\circ - RT^\circ \ln T_r$ | $\Delta_fH^\circ$ |
| $\Delta_fH^\circ(298.15 \text{ K}) = -488.69 \pm 3 \text{ kJ}\cdot\text{mol}^{-1}$              |         | Unknown                                          |                                                   |                               |                   |
| $\Delta_{\text{sub}}H^\circ(298.15 \text{ K}) = 126.357 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$ |         |                                                  |                                                   |                               |                   |
| 0                                                                                               | 0       | 0                                                | 0                                                 | 0                             | 0                 |
| 100                                                                                             | 104.207 | 131.545                                          | 136.971                                           | -30.439                       | -487.236          |
| 200                                                                                             | 121.579 | 210.426                                          | 271.784                                           | -23.753                       | -487.087          |
| 298.15                                                                                          | 127.800 | 260.270                                          | 260.270                                           | -12.272                       | -486.406          |
| 300                                                                                             | 127.880 | 261.061                                          | 260.272                                           | 0                             | -488.691          |
| 400                                                                                             | 131.001 | 298.303                                          | 265.329                                           | 0.236                         | -488.703          |
| 500                                                                                             | 133.009 | 327.759                                          | 274.971                                           | -521.586                      | -483.104          |
| 600                                                                                             | 134.509 | 352.154                                          | 285.860                                           | -604.216                      | -483.240          |
| 700                                                                                             | 135.938 | 373.035                                          | 296.856                                           | -603.990                      | -409.509          |
| 800                                                                                             | 137.152 | 391.236                                          | 307.537                                           | -597.743                      | -382.376          |
| 900                                                                                             | 138.365 | 407.460                                          | 317.755                                           | 80.735                        | -394.896          |
| 1000                                                                                            | 139.578 | 422.101                                          | 327.469                                           | 94.632                        | -391.258          |

## Zirconium Iodide ( $ZrI_4$ )

PREVIOUS June 1964

CURRENT June 1975

## IDEAL GAS

 $I_{\text{Zr}}(\text{g})$ 

|                                          | $M_r = 598.8380 \text{ Zirconium Iodide (ZrI}_4)$         |         |         | Standard State Pressure = $P = 0.1 \text{ NPa}$ |                |              |
|------------------------------------------|-----------------------------------------------------------|---------|---------|-------------------------------------------------|----------------|--------------|
|                                          | Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$ |         |         | Standard State Pressure = $P = 0.1 \text{ NPa}$ |                |              |
|                                          | $T/K$                                                     | $C_v^*$ | $S^*$   | $-(G^* - H^*(T))/T$                             | $H^* - H^*(T)$ | $\Delta G^*$ |
| Vibrational Frequencies and Degeneracies |                                                           |         |         |                                                 |                |              |
| $v, \text{ cm}^{-1}$                     |                                                           |         |         |                                                 |                |              |
| 0                                        | 0                                                         | 0       | 0       | -INFINITE                                       | -26311         | -356.752     |
| 100                                      | 87.629                                                    | 39.627  | 536.514 | -19.689                                         | -357.116       | -377.473     |
| 200                                      | 100.873                                                   | 40.5465 | 456.038 | -10.115                                         | -359.600       | -396.900     |
| 250                                      | 103.241                                                   | 42.8254 | 448.278 | -5.006                                          | -360.962       | -406.059     |
| 298.15                                   | 104.589                                                   | 446.563 | 446.563 | 0.                                              | -362.334       | -414.633     |
| 300                                      | 104.629                                                   | 447.210 | 446.565 | 0.194                                           | -362.389       | -414.937     |
| 350                                      | 105.504                                                   | 463.409 | 447.843 | 5.448                                           | -364.029       | -423.584     |
| 400                                      | 106.088                                                   | 477.538 | 450.690 | 10.739                                          | -397.579       | -450.892     |
| 450                                      | 106.496                                                   | 490.058 | 454.382 | 21.387                                          | -401.136       | -434.800     |
| 500                                      | 106.791                                                   | 501.293 | 458.521 | 44.591                                          | -430.638       | -449.991     |
| 600                                      | 107.181                                                   | 520.803 | 457.374 | 32.087                                          | -485.549       | -419.628     |
| 700                                      | 107.418                                                   | 537.344 | 476.175 | 42.818                                          | -485.119       | -408.676     |
| 800                                      | 107.574                                                   | 551.698 | 484.738 | 53.368                                          | -484.542       | -397.780     |
| 900                                      | 107.681                                                   | 564.373 | 492.836 | 64.331                                          | -484.342       | -386.921     |
| 1000                                     | 107.738                                                   | 575.723 | 500.622 | 75.103                                          | -376.081       | 19.644       |
| 1100                                     | 107.814                                                   | 585.998 | 507.924 | 85.882                                          | -484.453       | -365.246     |
| 1200                                     | 107.858                                                   | 595.381 | 514.826 | 96.566                                          | -488.336       | -354.181     |
| 1300                                     | 107.892                                                   | 604.016 | 521.359 | 107.453                                         | -488.129       | -343.011     |
| 1400                                     | 107.919                                                   | 612.012 | 527.553 | 118.244                                         | -488.023       | -331.852     |
| 1500                                     | 107.940                                                   | 619.459 | 533.434 | 129.037                                         | -483.048       | -320.697     |
| 1600                                     | 107.958                                                   | 626.426 | 539.031 | 139.933                                         | -488.235       | -309.536     |
| 1700                                     | 107.973                                                   | 632.971 | 544.366 | 150.628                                         | -488.610       | -298.356     |
| 1800                                     | 107.985                                                   | 639.143 | 549.462 | 161.426                                         | -489.200       | -287.149     |
| 1900                                     | 107.996                                                   | 644.982 | 554.337 | 172.225                                         | -490.022       | -275.903     |
| 2000                                     | 108.005                                                   | 650.521 | 559.009 | 183.025                                         | -491.089       | -264.607     |
| 2100                                     | 108.012                                                   | 655.791 | 563.493 | 193.326                                         | -492.408       | -253.251     |
| 2200                                     | 108.019                                                   | 660.816 | 567.803 | 204.628                                         | -515.301       | -241.082     |
| 2300                                     | 108.025                                                   | 665.933 | 571.933 | 215.303                                         | -517.533       | -228.567     |
| 2400                                     | 108.030                                                   | 670.618 | 575.932 | 226.233                                         | -519.855       | -215.954     |
| 2500                                     | 108.034                                                   | 674.625 | 579.811 | 237.036                                         | -522.243       | -203.243     |
| 2600                                     | 108.038                                                   | 678.863 | 583.540 | 247.839                                         | -524.676       | -190.435     |
| 2700                                     | 108.042                                                   | 682.940 | 587.146 | 258.643                                         | -527.130       | -177.532     |
| 2800                                     | 108.045                                                   | 686.869 | 590.638 | 269.448                                         | -529.582       | -164.540     |
| 2900                                     | 108.048                                                   | 690.661 | 594.022 | 280.252                                         | -532.010       | -151.460     |
| 3000                                     | 108.050                                                   | 694.374 | 597.305 | 291.057                                         | -534.395       | -138.296     |
| 3100                                     | 108.053                                                   | 697.867 | 600.492 | 301.863                                         | -542.054       | -2.408       |
| 3200                                     | 108.055                                                   | 701.298 | 603.589 | 312.668                                         | -538.973       | -111.759     |
| 3300                                     | 108.057                                                   | 704.623 | 606.600 | 312.474                                         | -541.137       | 1.557        |
| 3400                                     | 108.059                                                   | 707.243 | 609.531 | 334.279                                         | -543.205       | -84.905      |
| 3500                                     | 108.060                                                   | 710.981 | 612.385 | 345.085                                         | -545.169       | -71.397      |
| 3600                                     | 108.062                                                   | 714.025 | 615.166 | 355.891                                         | -547.021       | -83.839      |
| 3700                                     | 108.063                                                   | 716.878 | 617.878 | 366.599                                         | -548.759       | -44.221      |
| 3800                                     | 108.064                                                   | 719.868 | 620.525 | 377.504                                         | -550.380       | -30.563      |
| 3900                                     | 108.066                                                   | 722.765 | 623.108 | 388.310                                         | -551.882       | -16.864      |
| 4000                                     | 108.067                                                   | 725.675 | 625.631 | 399.117                                         | -553.265       | -3.128       |
| 4100                                     | 108.068                                                   | 728.079 | 628.098 | 409.924                                         | -545.529       | 10.641       |
| 4200                                     | 108.069                                                   | 730.633 | 630.509 | 420.731                                         | -555.677       | 24.441       |
| 4300                                     | 108.070                                                   | 733.226 | 632.869 | 431.537                                         | -556.710       | 38.265       |
| 4400                                     | 108.070                                                   | 735.711 | 635.178 | 442.244                                         | -557.530       | 52.113       |
| 4500                                     | 108.071                                                   | 738.139 | 637.439 | 453.152                                         | -558.441       | 65.980       |
| 4600                                     | 108.072                                                   | 740.515 | 641.825 | 463.959                                         | -559.144       | 93.762       |
| 4700                                     | 108.072                                                   | 742.839 | 643.953 | 474.766                                         | -559.745       | 97.863       |
| 4800                                     | 108.073                                                   | 745.114 | 643.953 | 485.573                                         | -561.225       | 112.182      |
| 4900                                     | 108.074                                                   | 747.343 | 646.040 | 496.380                                         | -562.238       | 145.133      |
| 5000                                     | 108.074                                                   | 749.526 | 648.088 | 507.188                                         | -563.178       | 170.977      |
| 5100                                     | 108.075                                                   | 751.666 | 650.098 | 517.995                                         | -564.123       | 196.821      |
| 5200                                     | 108.075                                                   | 753.765 | 652.072 | 528.803                                         | -565.561       | 222.661      |
| 5300                                     | 108.076                                                   | 755.823 | 654.010 | 539.610                                         | -566.720       | 248.497      |
| 5400                                     | 108.076                                                   | 757.844 | 655.914 | 550.418                                         | -567.845       | 274.339      |
| 5500                                     | 108.076                                                   | 759.827 | 657.786 | 561.225                                         | -568.045       | 300.154      |
| 5600                                     | 108.077                                                   | 761.774 | 659.625 | 572.033                                         | -569.973       | 325.973      |
| 5700                                     | 108.077                                                   | 763.687 | 661.434 | 582.841                                         | -571.872       | 331.782      |
| 5800                                     | 108.077                                                   | 765.567 | 663.213 | 593.649                                         | -572.553       | 337.582      |
| 5900                                     | 108.078                                                   | 767.414 | 664.964 | 604.456                                         | -574.934       | 403.372      |
| 6000                                     | 108.078                                                   | 769.231 | 666.637 | 615.264                                         | -577.127       | 429.152      |

CURRENT: June 1975 (1 atm)

PREVIOUS: June 1975 (1 atm)

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Zirconium Iodide (ZrI<sub>4</sub>) $I_{\text{Zr}}(\text{g})$ 

\*One point rejected due to a statistical test  
\*\*Orifice area ( $\text{cm}^2$ ) A = 0.5364 B = 0.0935

## Heat Capacity and Entropy

The adopted vibrational frequencies are from the work of Clark *et al.*<sup>67</sup>, who recorded the Raman spectra of ZrI<sub>4</sub> in the vapor phase (380–420°C). These studies indicated that ZrI<sub>4</sub> 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>67</sup> for ZrI<sub>4</sub>(g). Rahlf and Fischer,<sup>2</sup> though vapor density measurements had earlier concluded that ZrI<sub>4</sub> was monomeric in the vapor phase.

An electron diffraction study of ZrI<sub>4</sub>(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 ± 0.005 Å. We adopt this value. Other interatomic distances reported in the literature estimates. The principal moments of inertia are:  $I_x = I_y = I_z = 397.6172 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ .

Much literature has been published on the interrelationships 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<sub>4</sub>(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 cal·K<sup>-1</sup>·mol<sup>-1</sup> in the range 100–1000 K.

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## Iodine

## Continuation of discussions of selected I species

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