

Thermodynamic Properties of Beryllium

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The thermodynamic properties of beryllium have been evaluated up to 2800 K. A further evaluation is justified by the inclusion of not only new specific heat measurements at low temperature but also new enthalpy measurements at high temperature which lead to a reassessment of the enthalpies and entropies of transition and fusion. Selected values include an enthalpy of sublimation of 324 ± 5 kJ/mol at 298.15 K and a boiling point at one atmosphere pressure of 2745 K.

Keywords beryllium, gas, liquid, solid, thermodynamic properties

1. Introduction

This work is one of a series of articles on thermodynamic properties of the elements to appear in the *Journal of Phase Equilibria and Diffusion*. The articles are expected to be especially useful to those who are updating thermodynamic databases for phase diagram prediction and for other applications as well. Each article in the series will list the properties of a single element, including Ag,^[1] Au,^[2] Be, Cr, Cu,^[3] Hf,^[4] Nb, Ta, V, or W. References are given for papers that have already been published. In addition, the series will also include two summary papers on selected values of the melting points and boiling points of the elements and on the enthalpies and entropies of fusion and transition of the elements.

Previous reviews on beryllium were by Hultgren et al.,^[5] Spencer,^[6] Alcock et al.,^[7] Gurvich et al.^[8] and by JANAF (Chase^[9]). The values given for the condensed phases by CODATA (Cox et al.^[10]) are the same as those of Gurvich et al. A further evaluation for this element is justified by new measurements of the specific heat below 110 K by Swenson^[11] and further determinations of the enthalpies of transition and fusion by Kleykamp.^[12] The close-packed hexagonal alpha phase transforms to the body-centred cubic beta phase at a selected temperature of 1543 ± 5 K whilst the melting point is selected as 1560 ± 5 K. The selection of these values are reviewed in Part 4.

Wherever possible, values have been corrected to the currently accepted atomic weight of 9.0121831 ± 0.0000005 ^[13] and to the ITS-90 temperature scale using correction factors of Douglas,^[14] Rusby,^[15] Rusby et al.,^[16] and Weir and Goldberg.^[17]

2. Alpha Phase

The superconducting temperature at 0.026 K^[18] is below the experimentally determined specific heat values and was therefore not included in the evaluation.

Low temperature specific heat is generally given in terms of the Debye equation where below 4.2 K only the first two terms are considered so that $C_p = \gamma T + AT^3$ where γ is the electronic coefficient and A is usually represented in terms of a limited Debye temperature, θ_D , where $\theta_D^3 = (12/5)\pi^4 R/A = 1943.770/A$ where R is the gas constant and A is given in units of J/(mol K⁴). Values determined for γ and θ_D are given in Table 1.

Although the values of Ahlers^[20] and Swenson^[11] agree closely, the latter measurements are selected since they are part of the equation given by Swenson to cover the range up to 108 K. In order to represent the thermodynamic properties up to 298.15 K values derived from this equation were combined with specific heat measurements of Hill and Smith^[21] (4–300 K) obtained at 150, 200, 250 and 300 K. It is noted that the measurements of Ahlers deviate up to 4% higher than the selected curve at 30 K whilst below 150 K the measurements of Hill and Smith are up to 67% higher at 20 K but rapidly falling to be only 1% higher at 120 K. Low temperature specific heat equations are given in Table 6 and low temperature thermodynamic properties are summarised in Table 12.

Above 298.15 K the sample 1 enthalpy measurements of Ginnings et al.^[22] (367–1170 K) were combined with the enthalpy measurements of Kantor et al.^[23] (600–1560 K). The latter were given only in the form of an equation and shown graphically. Based on the number of data points shown on the graph, values were evaluated at 80 K intervals from 600 to 1480 K together with the value at the transition temperature 1543 K. The temperature measurements of Ginnings et al. were corrected to ITS-90 but in view of the manner in which the measurements of Kantor et al. were reported a correction was not applied. Equation 1 represents the selected data over the range 298.15 to 1543 K:

$$H_T^\circ - H_{298.15}^\circ (\text{J/mol}) = 21.5390T + 2.47286 \times 10^{-3}T^2 + 4.52108 \times 10^{-7}T^3 + 594,083/T - 8646.22. \quad (\text{Eq 1})$$

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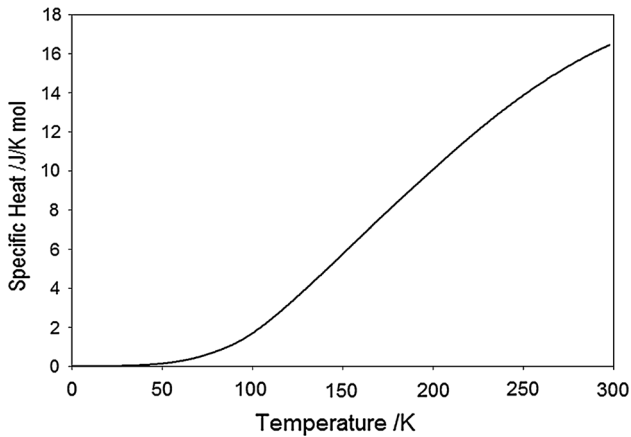


Fig. 1 Low temperature specific heat of solid beryllium, taken from Table 12

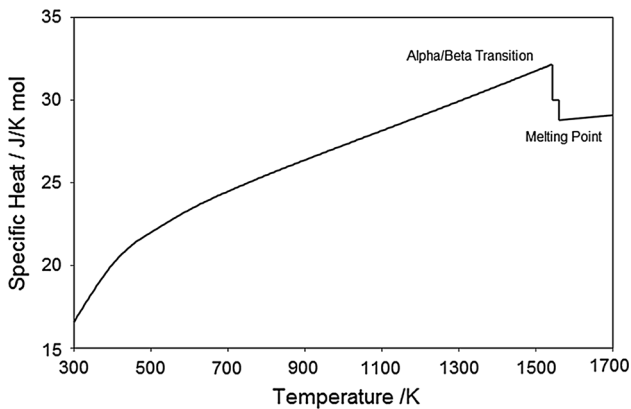


Fig. 2 Specific heat of beryllium for $300 < T < 1700$ K, taken from Table 13

The enthalpy sample 2 of Ginnings et al.^[22] (367-1170 K) averaged 0.7% lower than the selected values. The high temperature thermodynamic properties are given in Table 13 whilst derivations of other experimental specific heat and enthalpy measurements are compared with the selected values in Tables 10 and 11 respectively.

3. A Comparison of Selected Values at 298.15 K

The present values of enthalpy and entropy represent the inclusion of the newer low temperature measurements of Swenson^[11] which avoids the previous problems of having to try and reconcile the very different specific heat values given by Ahlers^[20] and Hill and Smith^[21] below 100 K. The comparison is given in Table 2.

4. Selected Values of the Transition Temperature and Melting Point

A comprehensive review of the published transition temperatures and melting points was carried out by Alcock et al.^[7] A transition temperature of 1543 ± 6 K was selected based on the measurements of Martin and Moore^[24] and Loasby and Dearden.^[25] A more recent determination by Kleykamp^[12] at 1542 ± 1 K is considered to be of equal merit but would not alter the selected value, although with more confidence placed on this value the uncertainty is lowered to ± 5 K.

For the melting point, Alcock et al. selected 1563 ± 4 K based on the values of Martin and Moore,^[24] Loasby and Dearden^[25] and Kantor et al.^[23] However Kleykamp^[12] obtained a notably lower value of 1556 ± 2 K and suggested that the higher melting point values obtained are in reality the liquidus temperature of oxygen contaminated material in the degenerate eutectic Be-BeO system. On these grounds, the melting point is chosen as a lower value of 1560 ± 5 K in agreement with Gurvich et al.^[8] and JANAF (Chase^[9]).

5. Beta Phase and the Enthalpies of Transition and Fusion

The specific heat of the beta phase has not been measured but in agreement with previous reviews was assumed to be 30 J/(mol K). The enthalpy of the alpha phase at the transition temperature is $H^{\circ}_{1543\text{K}} - H^{\circ}_{298.15\text{K}} = 32,522$ J/mol and for the liquid at the melting point $H^{\circ}_{1560\text{K}} - H^{\circ}_{298.15\text{K}} = 47,846$ J/mol. The difference is 15,324 J/mol, and if a value of 510 J/mol is subtracted to represent the enthalpy of the beta phase over the range of stability, then the combined enthalpies of transition and fusion are 14,814 J/mol. In the literature, vastly different values have been reported for both the transition enthalpy and the enthalpy of fusion. However, it was noted that for any set of measurements the ratio of the enthalpies of transition and fusion are very similar. On these grounds, reported values of the transition enthalpies have been normalised so that their sum is 14,814 J/mol as given in Table 3. This enthalpy ratio technique was also used by both Alcock et al.^[7] and JANAF (Chase^[9]). The discrepant measurements of Aldinger and Petzow^[27] were rejected and the remainder averaged to selected values of 6855 ± 500 and 7959 ± 500 J/mol for the enthalpies of transition and fusion respectively, where the assigned accuracies take into account the diversities of the original measurements. The enthalpy of the beta phase can then be represented by Eq 2:

$$H^{\circ}_{\text{T}} - H^{\circ}_{298.15}(\text{J/mol}) = 30.0000T - 6913.13. \quad (\text{Eq 2})$$

Derived thermodynamic properties are also given in Table 13.

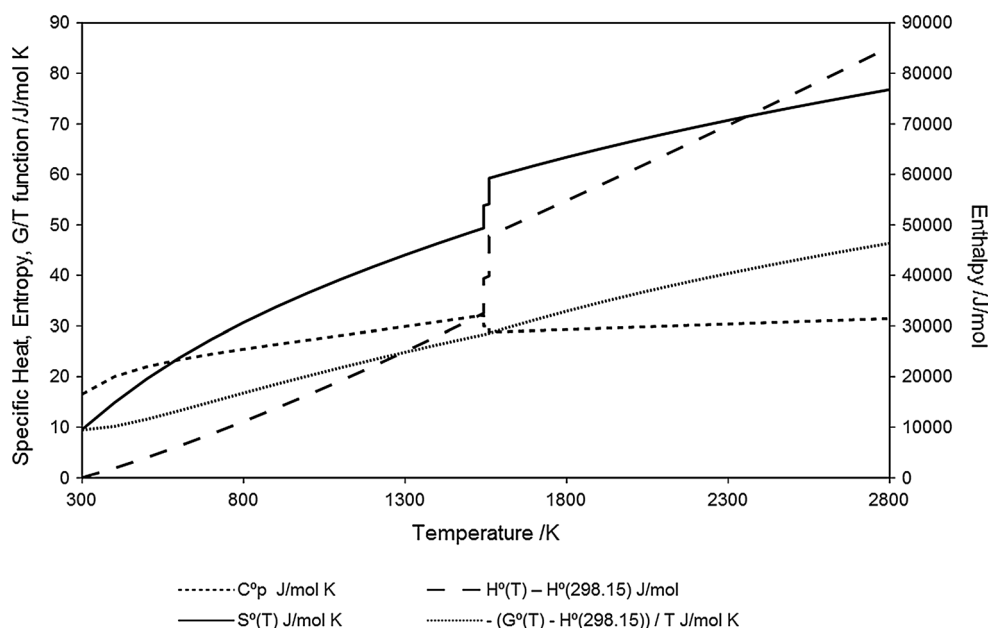


Fig. 3 High temperature thermodynamic properties of beryllium for $300 < T < 2800$ K, taken from Table 13

Table 1 Low temperature specific heat coefficients

Authors	Ref	Temperature range, K	γ , mJ/(mol K ²)	θ_D , K
Gmelin	19	1.2-4.4	0.182	1390
Ahlers	20	1.4-30	0.1714	1481
Swenson	11	4.6-108	0.1706	1485

Table 2 A comparison of specific heat, enthalpy and entropy values at 298.15 K

Authors	Ref	C°_p , J/(mol K)	$H^{\circ}_{298.15} - H^{\circ}_0$, J/mol	$S^{\circ}_{298.15}$, J/(mol K)
Hultgren et al.	5	16.44	1950	9.50
Alcock et al.	7	16.44	1942	9.503
Gurvich et al.	8	16.44	1950	9.50
JANAF	9	16.38	1932	9.440
This work	...	16.45	1948	9.466

Table 3 Values of the enthalpies of transition and fusion

Authors	Ref	Original values		Normalised values	
		$\Delta H_{\alpha, \beta}$, J/mol	$\Delta H_{s, l}$, J/mol	$\Delta H_{\alpha, \beta}$, J/mol	$\Delta H_{s, l}$, J/mol
Potard et al.	26	6736	7908	6814	8000
Loasby and Dearden	25	2113	2414	6914	7900
Aldinger and Petzow	27	6560	8220	6575	8239
Abey	28	7950	9205	6865	7949
Kleykamp	12	6149	7194	6827	7987
Selected				6855 ± 500	7959 ± 500

Table 4 Enthalpy of sublimation values at 298.15 K

Authors	Ref	Method	Temperature range, K	$\Delta H^\circ_{298.15\text{K}}$ (II), kJ/mol	$\Delta H^\circ_{298.15\text{K}}$ (III), kJ/mol	Notes
Baur and Brunner	33	BP	1850-2331	248 ± 6	332.1 ± 2.9	(a)
Schuman and Garrett	34	L	1174-1336	344 ± 19	337.3 ± 0.7	(a)
Magee et al.	35	L	1273-1373	294 ± 60	324.8 ± 1.6	(a)
Ansara and Bonnier	36	KE	1578-1671	287 ± 51	319.7 ± 0.8	(a)
Holden et al.	37	L, KE	1172-1552	344 ± 5	325.2 ± 0.5	(b)
Gulbransen and Andrew	38	L	1103-1229	340 ± 13	327.1 ± 0.4	(c)
Kovtun et al.	39	L, KE	1178-1373	343 ± 10	318.8 ± 0.5	(d)
Hildenbrand et al.	40	L	323.8 ± 2.1	(d)
Selected					324 ± 5	

Notes for Table 3. $\Delta H^\circ_{298.15\text{K}}$ (II) and $\Delta H^\circ_{298.15\text{K}}$ (III) are the second law and third law enthalpies of sublimation at 298.15 K. (a) Not included in the average. (b) Only values for vacuum cast sample were included. Results on a second sample were rejected by the authors. (c) Average of two samples. (d) Value given only at 298.15 K. Methods for Table 3. BP: boiling point; KE: Knudsen effusion; L: Langmuir

Table 5 Vapor pressure equations

Phase	Range, K	A	B	C	D	E
Alpha	750-1543	13.81239	0.28613	-38,992.8	-5.27429 × 10 ⁻⁴	-1.25015 × 10 ⁻⁹
Beta	1543-1560	14.02174	0	-37,334.9	0	0
Liquid	1560-2800	18.14516	-0.512217	-37,525.7	-1.54090 × 10 ⁻⁴	2.18352 × 10 ⁻⁹

Table 6 Specific heat equations of the solid below 298.15 K

0-89 K

$$C_p^\circ (\text{J/mol K}) = 1.70564 \times 10^{-4}$$

$$T + 5.93899 \times 10^{-7} T^3 + 1.43631 \times 10^{-10} T^6 + 8.84260 \times 10^{-15} T^7 - 2.17579 \times 10^{-18} T^9 + 8.26363 \times 10^{-23} T^{11}$$

89-200 K

$$C_p^\circ (\text{J/mol K}) = 0.154478T - 1.62236 \times 10^{-4} T^2 + 29582.3/T^2 - 15.10406$$

200-298.15 K

$$C_p^\circ (\text{J/mol K}) = 0.2323054T - 3.073849 \times 10^{-4} T^2 + 99078.95/T^2 - 26.60106$$

Table 7 Representative equations above 298.15 K

Alpha phase: 298.15-1543 K

$$C_p^\circ (\text{J/mol K}) = 21.5390 + 4.94572 \times 10^{-3} T + 1.356324 \times 10^{-6} T^2$$

594,083/T²

$$H_T^\circ - H_{298.15}^\circ (\text{J/mol}) = 21.5390T + 2.47286 \times 10^{-3} T^2 + 4.52108 \times 10^{-7} T^3$$

$$+ 594,083/T - 8646.22$$

$$S_T^\circ (\text{J/mol K}) = 21.5390 \ln(T) + 4.94572 \times 10^{-3} T + 6.78162 \times 10^{-7} T^2$$

$$+ 297,041.5/T^2 - 118.1306$$

Beta phase: 1543-1560 K

$$C_p^\circ (\text{J/mol K}) = 30.0000$$

$$H_T^\circ - H_{298.15}^\circ (\text{J/mol}) = 30.0000T - 6913.13$$

$$S_T^\circ (\text{J/mol K}) = 30.0000 \ln(T) - 166.4337$$

Liquid phase: 1560-2800 K

$$C_p^\circ (\text{J/mol K}) = 25.4345 + 2.15008 \times 10^{-3} T$$

$$H_T^\circ - H_{298.15}^\circ (\text{J/mol}) = 25.4345T + 1.07504 \times 10^{-3} T^2 + 5551.83$$

$$S_T^\circ (\text{J/mol K}) = 25.4735 \ln(T) + 2.15008 \times 10^{-3} T - 131.1183 \text{ J/(mol K)}$$

Table 8 Gibbs energy equations above 298.15 K

Alpha phase: 298.15-1543 K

$$G^{\circ}_T - H^{\circ}_{298.15} \text{ (J/mol)} = 139.6696T - 2.47286 \times 10^{-3} T^2 - 2.26054 \times 10^{-7} T^3 + 297,041.5/T - 21.5390T \ln(T) - 8646.22$$

Beta phase: 1543-1560 K

$$G^{\circ}_T - H^{\circ}_{298.15} \text{ (J/mol)} = 196.4337T - 30.0000T \ln(T) - 6913.13$$

Liquid: 1560-2800 K

$$G^{\circ}_T - H^{\circ}_{298.15} \text{ (J/mol)} = 156.5528T - 1.07504 \times 10^{-3} T^2 - 25.4345T \ln(T) + 5551.83$$

Table 9 Transition values involved with the Gibbs energy equations

Transition	Temperature, K	ΔH° , J/mol	ΔS° , J/(mol K)
Alpha-beta	1543	6855	4.4426
Fusion	1560	7959	5.1019

Table 10 Deviations of specific measurements

Authors	Ref	Temperature range, K	% deviations from the selected values
Simon and Ruhemann	41	71-80	Average bias 24.4 high
Lewis	42	98-463	Trend 5.1 low to 4.7 high
Vernotte and Jeufroy	43	286	5.9 low
Cristescu and Simon	44	10-300	Trends from initially 87 high to 102 high at 30 K to 12.0 low at 120 K to 8.2 high at 300 K
Losana	45	303-1073	Above 373 K trend 2.3 high to 8.2 low
Mit'kina	46	323-773	Scatter 4.3 low to 0.6 high
Walker et al.	47	303-1073	Trends from initially 1.3 low to 3.3 low at 673 K to 1.5 low at 1073 K
Smith et al.	48	324-973	Above 412 K initially scatters 0.9 low to 0.4 high but averages 2.0 low above 816 K
Tye and Brazel	49	323-623	Scatter 0.9 low to 1.8 high

Table 11 Deviations of enthalpy measurements

Authors	Ref	Temperature range, K	% deviations from the selected values
Tye and Brazel	49	532-1111	Scatter 1.5 low to 2.5 high
Magnus and Holzmann	50	525-1173	Trends from average of 6.7 low below 473 K to average 5.4 low above 1073 K
Jaeger and Rosenbaum	51	373-1338	Average bias 4.8 low
Fieldhouse et al.	52	434-1329	First sample scatters 2.9 low to 1.0 high and second sample scatters 4.3 low to 6.4 high
Boivineau et al.	53	525-1564 1564-2062	Solid trends 2.6 low to 0.5 high Liquid trends 9.0 low to 6.4 low

6. Liquid Phase

Kantor et al.^[23] represented the enthalpy of the liquid, 1560-2200 K, by means of a quadratic equation which is probably more representative of a possible scatter in the data. Rather than try to reduce this to a linear equation, which would tend to diminish the representation of the

actual data, in agreement with Alcock et al.^[7] the original equation is retained and can be represented by Eq 3:

$$H^{\circ}_T - H^{\circ}_{298.15} \text{ (J/mol)} = 25.4345T + 1.07504 \times 10^{-3} T^2 + 5551.83. \quad (\text{Eq 3})$$

Derived thermodynamic properties are also given in Table 13.

Table 12 Low temperature thermodynamic properties

Temperature, K	C_p° , J/(mol K)	$H_T^\circ - H_0^\circ$, J/mol	S_T° , J/(mol K)	$-(G_T^\circ - H_0^\circ)$, J/mol	$-(G_T^\circ - H_0^\circ)/T$, J/(mol K)
5	0.000928	0.00223	0.000878	0.00216	0.000433
10	0.00231	0.0100	0.00191	0.00903	0.000903
15	0.00467	0.0270	0.00325	0.0217	0.00145
20	0.00863	0.0594	0.00509	0.0423	0.00212
25	0.0150	0.117	0.00764	0.0738	0.00295
30	0.0248	0.215	0.0112	0.120	0.00401
40	0.0605	0.620	0.0226	0.284	0.00709
50	0.131	1.539	0.0428	0.601	0.0120
60	0.256	3.417	0.0767	1.185	0.0198
70	0.458	6.917	0.130	2.201	0.0314
80	0.753	12.89	0.210	3.876	0.0485
90	1.137	22.27	0.320	6.496	0.0722
100	1.680	36.20	0.466	10.39	0.104
110	2.370	56.35	0.657	15.97	0.145
120	3.151	83.90	0.897	23.70	0.197
130	3.987	119.6	1.182	34.05	0.262
140	4.852	163.7	1.509	47.47	0.339
150	5.732	216.7	1.873	64.35	0.429
160	6.615	278.4	2.271	85.05	0.532
170	7.492	348.9	2.699	109.9	0.646
180	8.359	428.2	3.152	139.1	0.773
190	9.209	516.1	3.626	173.0	0.910
200	10.042	612.3	4.120	211.7	1.059
210	10.874	716.9	4.630	255.4	1.216
220	11.676	829.7	5.155	304.4	1.383
230	12.441	950.3	5.691	358.6	1.559
240	13.167	1078.4	6.236	418.2	1.743
250	13.849	1213.5	6.787	483.3	1.933
260	14.485	1355.2	7.343	554.0	2.131
270	15.072	1503.0	7.901	630.2	2.334
280	15.609	1656.5	8.459	712.0	2.543
290	16.095	1815.1	9.015	799.4	2.756
298.15	16.451	1947.7	9.466	874.7	2.934

7. Monatomic Gas Phase

Values are based on one bar standard state pressure and are calculated from the fourteen energy levels below $61,000 \text{ cm}^{-1}$ selected by Kraminda and Martin^[29] Thermodynamic properties were calculated using the method of Kolsky et al.^[30] and the 2010 Fundamental Constants^[31,32] and are given in Table 14.

8. Diatomic Gas Phase

Based on very limited data, both Gurvich et al.^[8] and JANAF (Chase^[9]) estimated the thermodynamic values of the diatomic gas. However, both sets of estimates suggest that the contribution of the diatomic gas to the total

vapour pressure at the boiling point was only of the order of 2.7×10^{-5} bar (0.0027%). On these grounds, the diatomic gas was not considered further in the evaluation.

9. Enthalpy of Sublimation of the Monatomic Gas

Because of a lack of detail as to what temperature scales were being used then no attempt was made to correct values to ITS-90 from what would be contemporary scales. Values for the enthalpy of sublimation are derived in Table 4. The selected value of $324 \pm 5 \text{ kJ/mol}$ at 298.15 K was based on the last four sets of measurements and agrees with the value selected by CODATA (Cox et al.^[10]) which was also based on these measurements.

Table 13 High temperature thermodynamic properties

Temperature, K	C_p° , J/(mol K)	$H^\circ_T - H^\circ_{298.15}$, J/mol	S°_T , J/(mol K)	$-(G^\circ_T - H^\circ_{298.15})/T$, J/(mol K)
Alpha				
298.15	16.451	0	9.466	9.466
300	16.544	31	9.568	9.467
400	20.021	1879	14.863	10.165
500	21.975	3986	19.556	11.584
600	23.344	6255	23.690	13.264
700	24.453	8647	27.374	15.021
800	25.435	11,142	30.704	16.777
900	26.355	13,732	33.753	18.496
1000	27.247	16,412	36.576	20.165
1100	28.129	19,181	39.215	21.778
1200	29.014	22,038	41.700	23.335
1300	29.909	24,984	44.058	24.839
1400	30.818	28,020	46.308	26.294
1500	31.745	31,148	48.465	27.700
1543	32.150	32,522	49.368	28.291
Beta				
1543	30.000	39,377	53.811	28.291
1560	30.000	39,887	54.140	28.571
Liquid				
1560	28.789	47,846	59.241	28.571
1600	28.875	48,999	59.971	29.347
1700	29.090	51,897	61.728	31.201
1800	29.305	54,817	63.397	32.943
1900	29.520	57,758	64.987	34.588
2000	29.735	60,721	66.507	36.147
2100	29.950	63,705	67.963	37.627
2200	30.165	66,711	69.361	39.038
2300	30.380	69,738	70.707	40.386
2400	30.595	72,787	72.004	41.676
2500	30.810	75,857	73.258	42.915
2600	31.025	78,949	74.470	44.105
2700	31.240	82,062	75.645	45.252
2800	31.455	85,197	76.785	46.358

10. Vapor Pressure

As given in Table 5, vapor pressure equations for the alpha phase and the gas were evaluated at 25 K intervals from 750 to 1525 K and the transition temperature and for the liquid phase and the gas at the melting point and 50 K intervals from 1600 to 2800 K. Values for the beta phase were calculated from the vapor pressure values of the alpha phase at the transition temperature and for the liquid phase at the melting point. Values were fitted to the equation:

$$\ln(p, \text{bar}) = A + B \ln(T) + C/T + DT + ET^2.$$

11. Comments on Previous Reviews of the Thermodynamic Properties

Using similar enthalpy ratio values as used in the present review, Alcock et al.^[7] selected enthalpies of transition and fusion of 6700 and 8000 J/mol respectively whilst JANAF (Chase^[9]) selected 6849 and 7895 J/mol, with both sets of measurements showing satisfactory agreement with the presently accepted values as given in Part 5. However, extraordinarily Gurvich et al.^[8] accepted the very low original enthalpy of transition value of 2100 J/mol deter-

Table 14 Thermodynamic properties of the gas phase

Temperature, K	C_p° , J/(mol K)	$H^\circ_T - H^\circ_{298.15}$, J/mol	S°_T , J/(mol K)	$-(G^\circ_T - H^\circ_{298.15})/T$, J/(mol K)
298.15	20.786	0	136.275	136.275
300	20.786	38	136.404	136.276
400	20.786	2117	142.384	137.091
500	20.786	4196	147.022	138.631
600	20.786	6274	150.812	140.355
700	20.786	8353	154.016	142.083
800	20.786	10,432	156.792	143.752
900	20.786	12,510	159.240	145.340
1000	20.786	14,589	161.430	146.841
1100	20.786	16,667	163.411	148.259
1200	20.786	18,746	165.220	149.598
1300	20.786	20,825	166.883	150.864
1400	20.786	22,903	168.424	152.064
1500	20.786	24,982	169.858	153.203
1543	20.786	25,876	170.445	153.676
1560	20.786	26,229	170.673	153.860
1600	20.786	27,060	171.199	154.287
1700	20.786	29,139	172.460	155.319
1800	20.787	31,218	173.648	156.304
1900	20.787	33,296	174.772	157.247
2000	20.789	35,375	175.838	158.150
2100	20.791	37,454	176.852	159.017
2200	20.795	39,534	177.819	159.850
2300	20.801	41,613	178.744	160.651
2400	20.811	43,694	179.629	161.424
2500	20.825	45,776	180.479	162.169
2600	20.844	47,859	181.296	162.889
2700	20.870	49,945	182.083	163.585
2800	20.905	52,033	182.843	164.260

$$H^\circ_{298.15} - H^\circ_0 = 6197.4 \text{ J/mol}$$

mined by Loasby and Dearden^[25] but then ignored an enthalpy of fusion of 2400 J/mol determined by the same authors and instead selected a much higher value of 12,600 J/mol in complete contradiction to the experimental values given in Table 3.

12. Summary of Representative Equations

Low temperature specific heat equations are given in Table 6 and high temperature specific heat equations are given in Table 7. Gibbs energy equations are given in Table 8 and transition values involved with the Gibbs energy equations in Table 9.

13. Deviations from the Selected Values

Deviations of specific heat and enthalpy values in the solid range are given in Tables 10 and 11 respectively.

14. Thermodynamic Tables

Low temperature thermodynamic properties of the solid are given in Tables 12 (Fig. 1) and the high temperature thermodynamic properties of the condensed phases in Table 13 (Fig. 2, 3). Thermodynamic properties of the gas phase are given in Table 14 whilst the vapour pressure summary is given in Table 15.

Table 15 Vapor pressure

<i>T</i> , K	<i>p</i> , bar	ΔG_T , J/mol	ΔH_T , J/mol	<i>p</i> , bar	<i>T</i> , K
298.15	7.27×10^{-51}	286,192	324,000	10^{-15}	782
300	1.63×10^{-50}	285,957	324,008	10^{-14}	820
400	2.09×10^{-36}	273,230	324,238	10^{-13}	862
500	6.15×10^{-28}	260,477	324,210	10^{-12}	909
600	2.71×10^{-22}	247,746	324,019	10^{-11}	960
700	2.89×10^{-18}	235,057	323,706	10^{-10}	1019
800	3.00×10^{-15}	222,420	323,290	10^{-9}	1084
900	6.63×10^{-13}	209,841	322,779	10^{-8}	1159
1000	4.93×10^{-11}	197,324	322,177	10^{-7}	1245
1100	1.66×10^{-9}	184,871	321,487	10^{-6}	1346
1200	3.11×10^{-8}	172,485	320,708	10^{-5}	1464
1300	3.67×10^{-7}	160,168	319,841	10^{-4}	1608
1400	3.03×10^{-6}	147,920	318,883	10^{-3}	1791
1500	1.88×10^{-5}	135,745	317,834	10^{-2}	2023
1543	3.81×10^{-5}	130,532	317,354	10^{-1}	2326
1543	3.81×10^{-5}	130,532	310,499	1	2742.30
1560	4.96×10^{-5}	128,550	310,342	NBP	2745.13
1560	4.96×10^{-5}	128,550	302,383		
1600	8.89×10^{-5}	124,097	302,061		
1700	3.37×10^{-4}	112,999	301,242		
1800	1.10×10^{-3}	101,950	300,401		
1900	3.16×10^{-3}	90,948	299,538		
2000	8.14×10^{-3}	79,993	298,654		
2100	1.91×10^{-2}	69,082	297,749		
2200	4.15×10^{-2}	58,214	296,823		
2300	8.39×10^{-2}	47,390	295,875		
2400	0.160	36,607	294,907		
2500	0.288	25,864	293,919		
2600	0.496	15,162	292,910		
2700	0.818	4499	291,883		
2742.30	1.000	0	291,442		
2800	1.301	-6126	290,837		

NBP normal boiling point at 1 atmosphere pressure (1.01325 bar)
 Enthalpy of sublimation at 0 K: ΔH°_0 319,750 J/mol

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