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THE THERMODYNAMIC PROPERTIES OF GASEOUS Ge_2, GeF_4, GeF_2, AND GeF

by

P. A. G. O'Hare

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Chemical Engineering Division

December 1968

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ABSTRACT

The thermodynamic functions $(G^\circ - H_0^\circ)/T$, $(H^\circ - H_0^\circ)/T$, S°, C_p°, $H^\circ - H_{298}^\circ$, ΔHf, ΔGf, and log Kf have been calculated and are tabulated for Ge_2, GeF_4, GeF_2, and GeF in the ideal gas state at selected temperatures between 0 and 6000°K.

I. INTRODUCTION

This report deals with the molecules Ge_2, GeF_4, GeF_2, and GeF in the ideal gas state. Values for the thermodynamic functions*--S°, C_p°, $(H^\circ - H_0^\circ)/T$, $(G^\circ - H_0^\circ)/T$, and $H^\circ - H_{298}^\circ$--have been calculated by the formulas of statistical mechanics, and are tabulated at selected intervals between 0 and 6000°K and also at 273.15 and 298.15°K. The quantities ΔHf, ΔGf, and log Kf, based on literature values for $\Delta Hf_{298.15}$, are tabulated at the same temperatures.

II. CALCULATIONS

The thermodynamic functions were obtained by means of the rigid-rotator, harmonic-oscillator approximation. Formulas used to calculate the thermodynamic functions, together with the appropriate constants and their values, have been given elsewhere.[1,2] The atomic weights of germanium (72.59) and fluorine (18.9984) have been taken from the 1961 table of atomic weights.[3] All the ΔHf, ΔGf, and log Kf values given in the tabulations have been arbitrarily based on $Ge_2(g)$ and $F_2(g)$ as reference states.

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*Most of the symbols used in this report have been explained in Ref. 1.

THE THERMODYNAMIC PROPERTIES OF GASEOUS Ge_2, GeF_4, GeF_2, AND GeF

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P. A. G. O'Hare

ABSTRACT

The thermodynamic functions $(G^\circ - H_0^\circ)/T$, $(H^\circ - H_0^\circ)/T$, S°, C_p°, $H^\circ - H_0^\circ$, $\Delta H_f^\circ/RT$, and $\log Kf$ have been calculated and are tabulated for Ge_2, GeF_4, GeF_2, and GeF in the ideal gas state at selected temperatures between 0 and 6000°K.

I. INTRODUCTION

This report deals with the molecules Ge_2, GeF_4, GeF_2, and GeF in the ideal gas state. Values for the thermodynamic functions*—$-S_T^\circ$, C_p°, $(H^\circ - H_0^\circ)/T$, $(G^\circ - H_0^\circ)/T$, and $H^\circ - H_0^\circ$—have been calculated by the formulas of statistical mechanics, and are tabulated at selected intervals between 0 and 6000°K and also at 273.15 and 298.15°K. The quantities ΔH_f°, and $\log Kf$, based on literature values for $\Delta H_{298.15}^\circ$, are tabulated at the same temperatures.

II. CALCULATIONS

The thermodynamic functions were obtained by means of the rigid-rotator, harmonic-oscillator approximation. Formulas used to calculate the thermodynamic functions, together with the appropriate constants and their values, have been given elsewhere.[1,2] The atomic weights of germanium (72.59) and fluorine (18.998) have been taken from the 1961 table of atomic weights.[3] All the ΔH_f°, ΔGf°, and $\log Kf$ values given in the tabulations have been arbitrarily based on $Ge(g)$ and $F_2(g)$ as reference states.

---

*Most of the quantities used in this report have been explained in Ref. 1.

III. THERMODYNAMIC PROPERTIES

A. Diatomic Germanium (Ge_2,g)

The internuclear distance in Ge_2 was estimated to be 2.35 ± 0.05 Å by interpolating the bond-length data[4] for other homonuclear diatomic molecules in the same region of the periodic table. The calculated moment of inertia is 3.3282×10^{-38} g cm^2.

A value of 345 ± 20 cm^{-1} was estimated for ω_e by Guggenheimer's rule.[5] For the purposes of the estimate, it was assumed that the germanium atoms were joined by a double bond.[6] For Ge_2, the symmetry number (σ) and the quantum weight of the electronic state (g_i) were taken to be 2 and 3,[7] respectively.

Drowart and Honig[7] determined $D_0^\circ(Ge_2)$ to be 2.8 eV (64.6 kcal mol^{-1}) from a mass-spectrometric study. Enthalpy functions for Ge(g)[8a] and Ge_2(g) (this report) were used to adjust the data of Drowart and Honig to 298.15°K; in this way, $D_{298}^\circ(Ge_2)$ was calculated to be 65.8 kcal mol^{-1}. Kant and Strauss[9] have reported a corroborative value of 65 ± 5 kcal mol^{-1}. A mean value, 65.4 ± 5 kcal mol^{-1}, has been selected for $D_{298}^\circ(Ge_2)$. Therefore,

$$\Delta Hf^\circ(Ge_2,g) = \tfrac{1}{2}[2\Delta Hf^\circ(Ge,g) - D_{298}^\circ(Ge_2)] = 113.6 \pm 5.1 \text{ kcal mol}^{-1},$$

based on $\Delta Hf^\circ(Ge,g) = 89.5 \pm 0.5$ kcal mol^{-1}.[8a]

The thermodynamic properties of Ge_2(g) are given in Table I. Because of the estimates made, the thermodynamic data at 298.15°K are uncertain by about 2%.

B. Germanium Tetrafluoride (GeF_4,g)

An electron-diffraction study of GeF_4 by Caunt, Mackle, and Sutton[10] has shown the molecule to be tetrahedral with ℓ(Ge-F) = 1.67 ± 0.03 Å. The product of the three principal moments of inertia has been calculated to be 1.2914×10^{-113} g^3 cm^6.

Caunt, Short, and Woodward[11] and Woltz and Nielsen[12] have investigated the spectrum of GeF_4; the results of the two sets of observations are in excellent agreement. For the purposes of the present calculations, the following vibrational frequencies (cm^{-1}) and degeneracies have been selected: 738, 205(2), 800(3), 260(3). Values of 12 and 1 were taken for σ and g_i, respectively.

III. THERMODYNAMIC PROPERTIES

A. Diatomic Germanium (Ge_2, g)

The internuclear distance in Ge_2 was estimated to be 2.35 ± 0.05 Å by interpolating the bond-length data[4] for other homonuclear diatomic molecules in the same region of the periodic table. The calculated moment of inertia is 3.3282×10^{-38} g cm^2.

A value of 345 ± 20 cm^{-1} was estimated for ω_e by Guggenheimer's rule.[5] For the purposes of the estimate, it was assumed that the germanium atoms were joined by a double bond.[6] For Ge_2, the symmetry number, σ (c), and the quantum weight of the electronic state (g_1) were taken to be 2 and 3, respectively.

Drowart and Hoslig[7] determined $D_0^\circ(Ge_2)$ to be 2.8 ± 0.4 kcal mol^{-1} from a mass-spectrometric study. Enthalpy functions for Ge(g)[8] and Ge_2(g) (this report) were used to adjust the data of Drowart and Hoslig to 298.15 K; in this way, $D_{298}^\circ(Ge_2)$ was calculated to be 2.8 kcal mol^{-1}. Kant and Strauss[9] have reported a correlation value of 2.5 ± 5 kcal mol^{-1}. A mean value, 65.4 ± 5 kcal mol^{-1}, has been selected for $D_{298}^\circ(Ge_2)$. Therefore,

$$\Delta H_f^\circ(Ge_2,g) = \frac{1}{2}\Delta H_f^\circ(Ge,g) - D_{298}^\circ(Ge_2) = 114.6 \pm 5.1 \text{ kcal mol}^{-1},$$

based on $\Delta H_f^\circ(Ge,g) = 89 \pm 0.5$ kcal mol^{-1}.[8]

The thermodynamic properties of Ge_2(g) are given in Table 1. Because of the estimates made, the thermodynamic data at 298.15 K are uncertain by about 2%.

B. Germanium Tetrafluoride (GeF_4, g)

An electron-diffraction study of GeF_4 by Cossé, Vierkle, and Sutton[10] has shown the molecule to be tetrahedral with $d(Ge-F) = 1.67 \pm 0.02$ Å. The product of the three principal moments of inertia has been calculated to be 1.291×10^{-113} g^3 cm^6.

Cossé, Sheer, and Woodward[11] and Weir[12] and Dalziel[13] have investigated the spectrum of GeF_4; the results of the two sets of observations are in excellent agreement. For the purposes of the present calculations, the following vibrational frequencies (cm^{-1}) and degeneracies have been selected: 718, 205(2), 806(3), 260(3). Values of 12 and 1 were taken for σ and g_1, respectively.

TABLE I. Thermodynamic Properties of Diatomic Germanium Gas (M = 145.1800)

T (DEG.K.)	$-(G^\circ-H^\circ_0)/T$ (GIBBS/MOL)	$(H^\circ-H^\circ_0)/T$ (GIBBS/MOL)	S° (GIBBS/MOL)	C_p° (GIBBS/MOL)
0.00	0.000	0.0000	0.000	0.0000
100.00	44.602	7.0237	51.625	7.3020
200.00	49.582	7.4045	56.986	8.1733
273.15	51.928	7.6553	59.584	8.4751
298.15	52.602	7.7269	60.329	8.5405
300.00	52.650	7.7319	60.382	8.5448
400.00	54.907	7.9578	62.865	8.7057
500.00	56.701	8.1163	64.817	8.7868
600.00	58.191	8.2322	66.424	8.8327
700.00	59.467	8.3201	67.787	8.8610
800.00	60.583	8.3890	68.972	8.8797
900.00	61.574	8.4443	70.019	8.8926
1000.00	62.466	8.4896	70.956	8.9019
1100.00	63.277	8.5274	71.805	8.9089
1200.00	64.021	8.5594	72.580	8.9142
1300.00	64.707	8.5869	73.294	8.9183
1400.00	65.344	8.6107	73.955	8.9216
1500.00	65.939	8.6315	74.571	8.9242
1600.00	66.497	8.6499	75.147	8.9264
1700.00	67.022	8.6662	75.688	8.9282
1800.00	67.517	8.6808	76.198	8.9297
1900.00	67.987	8.6939	76.681	8.9310
2000.00	68.433	8.7058	77.139	8.9321
2200.00	69.264	8.7265	77.991	8.9338
2400.00	70.024	8.7438	78.768	8.9352
2600.00	70.725	8.7586	79.483	8.9362
2800.00	71.374	8.7713	80.145	8.9371
3000.00	71.980	8.7824	80.762	8.9377
3200.00	72.547	8.7921	81.339	8.9383
3400.00	73.080	8.8007	81.881	8.9387
3600.00	73.583	8.8084	82.392	8.9391
3800.00	74.060	8.8153	82.875	8.9394
4000.00	74.512	8.8215	83.334	8.9397
4200.00	74.943	8.8271	83.770	8.9399
4400.00	75.353	8.8322	84.186	8.9401
4600.00	75.746	8.8369	84.583	8.9403
4800.00	76.122	8.8413	84.964	8.9405
5000.00	76.483	8.8452	85.329	8.9406
5200.00	76.830	8.8489	85.679	8.9407
5400.00	77.164	8.8523	86.017	8.9409
5600.00	77.486	8.8555	86.342	8.9409
5800.00	77.797	8.8584	86.656	8.9410
6000.00	78.097	8.8612	86.959	8.9411

TABLE I. Thermodynamic Properties of
Diatomic Germanium Gas (M = 145.1500)

T	$-(G^{\circ}-H_0^{\circ})/T$	H°	C_p°
(DEG.K)	(CIBBS/MOL)	(KIBBS/MOL)	(CIBBS/MOL)
0.00	0.000	0.000	0.000
100.00	44.602	1.0127	7.3020
200.00	49.582	2.4065	8.1733
273.15	51.924	3.0553	8.4751
298.15	52.602	3.2649	8.5405
300.00	52.650	3.2819	8.5448
400.00	54.907	4.2958	8.7051
500.00	56.701	5.3143	8.7808
600.00	58.191	6.3322	8.8321
700.00	59.467	7.3491	8.8610
800.00	60.583	8.3670	8.8797
900.00	61.576	9.3843	8.8926
1000.00	62.469	10.4046	8.9018
1100.00	63.277	11.4209	8.9087
1200.00	64.021	12.4394	8.9142
1300.00	64.701	13.4597	8.9181
1400.00	65.344	14.4807	8.9216
1500.00	65.939	15.5015	8.9242
1600.00	66.497	16.5223	8.9264
1700.00	67.022	17.5435	8.9282
1800.00	67.512	18.5648	8.9297
1900.00	67.984	19.5861	8.9310
2000.00	68.419	20.6078	8.9321
2100.00	68.844	21.6295	8.9328
2200.00	69.244	22.6513	8.9332
2300.00	69.625	23.6734	8.9335
2400.00	70.025	24.6957	8.9335
2500.00	70.385	25.7181	8.9334
2600.00	70.734	26.7406	8.9332
2700.00	71.076	27.7633	8.9329
2800.00	71.416	28.7861	8.9327
2900.00	71.750	29.8090	8.9323
3000.00	72.083	30.8321	8.9319
3100.00	72.416	31.8553	8.9315
3200.00	72.749	32.8786	8.9311
3300.00	73.082	33.9021	8.9307
3400.00	73.415	34.9257	8.9303
3500.00	73.748	35.9494	8.9299
3600.00	74.080	36.9732	8.9294
3700.00	74.413	37.9971	8.9290
3800.00	74.746	39.0212	8.9286
3900.00	75.079	40.0453	8.9282
4000.00	75.412	41.0696	8.9278
4100.00	75.745	42.0940	8.9274
4200.00	76.078	43.1185	8.9270
4300.00	76.411	44.1431	8.9266
4400.00	76.744	45.1678	8.9262
4500.00	77.077	46.1926	8.9259
4600.00	77.410	47.2175	8.9255
4700.00	77.743	48.2425	8.9251
4800.00	78.076	49.2676	8.9248
4900.00	78.409	50.2928	8.9244
5000.00	78.742	51.3181	8.9241
5100.00	79.075	52.3435	8.9237
5200.00	79.408	53.3690	8.9234
5300.00	79.741	54.3946	8.9230
5400.00	80.074	55.4203	8.9227
5500.00	80.407	56.4461	8.9224
5600.00	80.740	57.4720	8.9220
5700.00	81.073	58.4980	8.9217
5800.00	81.406	59.5241	8.9214
5900.00	81.739	60.5503	8.9211
6000.00	82.072	61.5766	8.9208

TABLE I (Contd.)

T (DEG.K.)	$(H^\circ - H^\circ_{298})$ (KCAL/MOL)	$-\Delta Hf$ (KCAL/MOL)	$-\Delta Gf$ (KCAL/MOL)	LOG Kf
0.00	-2.3038	0.00	0.00	INF
100.00	-1.6014	0.00	0.00	0.00
200.00	-0.8229	0.00	0.00	0.00
273.15	-0.2127	0.00	0.00	0.00
298.15	0.0000	0.00	0.00	0.00
300.00	0.0158	0.00	0.00	0.00
400.00	0.8793	0.00	0.00	0.00
500.00	1.7544	0.00	0.00	0.00
600.00	2.6355	0.00	0.00	0.00
700.00	3.5203	0.00	0.00	0.00
800.00	4.4074	0.00	0.00	0.00
900.00	5.2961	0.00	0.00	0.00
1000.00	6.1858	0.00	0.00	0.00
1100.00	7.0764	0.00	0.00	0.00
1200.00	7.9676	0.00	0.00	0.00
1300.00	8.8592	0.00	0.00	0.00
1400.00	9.7512	0.00	0.00	0.00
1500.00	10.6435	0.00	0.00	0.00
1600.00	11.5360	0.00	0.00	0.00
1700.00	12.4287	0.00	0.00	0.00
1800.00	13.3216	0.00	0.00	0.00
1900.00	14.2147	0.00	0.00	0.00
2000.00	15.1078	0.00	0.00	0.00
2200.00	16.8944	0.00	0.00	0.00
2400.00	18.6813	0.00	0.00	0.00
2600.00	20.4685	0.00	0.00	0.00
2800.00	22.2558	0.00	0.00	0.00
3000.00	24.0433	0.00	0.00	0.00
3200.00	25.8309	0.00	0.00	0.00
3400.00	27.6186	0.00	0.00	0.00
3600.00	29.4064	0.00	0.00	0.00
3800.00	31.1942	0.00	0.00	0.00
4000.00	32.9821	0.00	0.00	0.00
4200.00	34.7701	0.00	0.00	0.00
4400.00	36.5581	0.00	0.00	0.00
4600.00	38.3462	0.00	0.00	0.00
4800.00	40.1342	0.00	0.00	0.00
5000.00	41.9224	0.00	0.00	0.00
5200.00	43.7105	0.00	0.00	0.00
5400.00	45.4986	0.00	0.00	0.00
5600.00	47.2868	0.00	0.00	0.00
5800.00	49.0750	0.00	0.00	0.00
6000.00	50.8632	0.00	0.00	0.00

A weighted mean value, -284.45 ± 0.12 kcal mol^{-1}, has been recommended[13] for $\Delta Hf°(GeF_4,g)$. The enthalpy of formation, based on the reaction

$$\tfrac{1}{2}Ge_2(g) + 2F_2(g) \rightarrow GeF_4(g), \qquad (1)$$

is calculated to be -341.25 kcal mol^{-1}.

The thermodynamic properties for GeF_4, listed in Table II, extend and update previous calculations by Voelz[14] and Kučírek and Papoušek.[15]

C. Germanium Difluoride (GeF_2,g)

The Ge-F bond length and the FGeF bond angle in GeF_2 have been estimated to be 1.72 ± 0.02 Å and 100 ± 3°, respectively, by comparison with CF_2,[16,17] SiF_2,[18] and PbF_2.[19] The product of the three principal moments of inertia has been calculated to be 8.8802 x 10^{-115} g^3 cm^6.

Spectroscopic data for $GeF_2(g)$ have been published recently,[20] and the vibrational frequencies were found to be 692, 663, and 263 cm^{-1}. By analogy with SiF_2,[21] g_i was taken to be unity; σ was taken to be 2.

Margrave and coworkers[22] have reported a value of 6.1 ± 1.5 kcal mol^{-1} for the enthalpy of the reaction

$$2GeF_2(g) \rightarrow Ge(g) + GeF_4(g). \qquad (2)$$

Enthalpies of formation given in the present report have been used to derive a value for $\Delta Hf°(GeF_2,g)$ from Eq. 2. Thus,

$$\Delta Hf°(GeF_2,g) = \tfrac{1}{2}[89.5 - 284.45 - 6.1] = -100.53 \text{ kcal mol}^{-1}.$$

For the reaction

$$\tfrac{1}{2}Ge_2(g) + F_2(g) \rightarrow GeF_2(g), \qquad (3)$$

$\Delta Hf(GeF_2,g)$ is calculated to be -157.33 kcal mol^{-1}.

The thermodynamic properties for GeF_2 are given in Table III.

D. Germanium Monofluoride (GeF,g)

Herzberg[23] has given 665.2 and 2.79 cm^{-1} for ω_e and $\omega_e x_e$, respectively. The above value for ω_e, in conjunction with Guggenheimer's rule,[5]

A weighted mean value, -286.45 ± 0.12 kcal mol^{-1}, has been recommended[11] for $\Delta H_f^\circ(GeF_4, g)$. The enthalpy of formation, based on the reaction

$$GeO_2(g) + 2F_2(g) \rightarrow GeF_4(g), \qquad (1)$$

is calculated to be -141.25 kcal mol^{-1}.

The thermodynamic properties for GeF_4, listed in Table II, extend and update previous calculations by Voele[4] and Hultgren and Dayhoff.[12]

C. Germanium Difluoride (GeF_2, g)

The Ge–F bond length and the FGeF bond angle in GeF_2 have been estimated to be 1.72 ± 0.02 Å and $100 \pm 5°$, respectively, by comparison with CF_2,[10,11] SiF_2,[10] and PbF_2.[9] The principal moment of inertia has been calculated to be 2.4804×10^{-39} g cm^2.

Spectroscopic data for $GeF_2(g)$ have been published recently,[9] and the vibrational frequencies were found to be 670, 301, and 275 cm^{-1}, by analogy with SiF_2.[11] ω_1 was taken to be unity, ω_2 taken to be 2.

Margrave and coworkers[13] have reported a value of -6.1 ± 1.5 kcal mol^{-1} for the enthalpy of the reaction

$$2GeF_2(g) \rightarrow Ge(g) + GeF_4(g). \qquad (2)$$

Enthalpies of formation given in the present report have been used to derive a value for $\Delta H_f^\circ(GeF_2, g)$ from Eq. 2. Thus,

$$\Delta H_f^\circ(GeF_2, g) = \tfrac{1}{2}[(89.9 + 286.45 - 6.1)] = -190.55 \text{ kcal mol}^{-1}.$$

For the reaction

$$GeO_2(g) + Ge(g) \rightarrow GeF_2(g),$$

$\Delta H_f^\circ(GeF_2, g)$ is calculated to be -127.22 kcal mol^{-1}.

The thermodynamic properties for GeF_2 are given in Table III.

D. Germanium Monofluoride (GeF, g)

Herzberg[14] has given 645.2 and 2.5 cm^{-1} for ω_e and $\omega_e x_e$, respectively. The above value for ω_e is in agreement with Cheng-Chuanhsu's value.

TABLE II. Thermodynamic Properties of Germanium Tetrafluoride (M = 145.5836)

T (DEG.K.)	$-(G^\circ-H^\circ_0)/T$ (GIBBS/MOL)	$(H^\circ-H^\circ_0)/T$ (GIBBS/MOL)	S° (GIBBS/MOL)	C_p° (GIBBS/MOL)
0.00	0.000	0.0000	0.000	0.0000
100.00	46.039	9.1398	55.178	12.0557
200.00	53.250	11.8800	65.130	16.6737
273.15	57.197	13.4780	70.675	18.9238
298.15	58.398	13.9619	72.360	19.5619
300.00	58.485	13.9965	72.481	19.6066
400.00	62.749	15.6603	78.409	21.5514
500.00	66.390	16.9713	83.361	22.7864
600.00	69.579	18.0115	87.591	23.5828
700.00	72.421	18.8478	91.269	24.1147
800.00	74.984	19.5305	94.514	24.4832
900.00	77.318	20.0963	97.414	24.7472
1000.00	79.461	20.5716	100.032	24.9421
1100.00	81.441	20.9759	102.417	25.0895
1200.00	83.281	21.3236	104.605	25.2037
1300.00	85.000	21.6257	106.626	25.2937
1400.00	86.613	21.8904	108.503	25.3658
1500.00	88.131	22.1241	110.255	25.4246
1600.00	89.566	22.3319	111.898	25.4729
1700.00	90.925	22.5179	113.443	25.5133
1800.00	92.217	22.6853	114.902	25.5472
1900.00	93.448	22.8367	116.284	25.5761
2000.00	94.623	22.9743	117.597	25.6008
2200.00	96.824	23.2150	120.039	25.6406
2400.00	98.853	23.4184	122.271	25.6711
2600.00	100.734	23.5927	124.327	25.6949
2800.00	102.489	23.7435	126.232	25.7138
3000.00	104.131	23.8754	128.007	25.7291
3200.00	105.676	23.9917	129.668	25.7416
3400.00	107.134	24.0949	131.228	25.7520
3600.00	108.513	24.1872	132.701	25.7607
3800.00	109.823	24.2702	134.094	25.7681
4000.00	111.070	24.3453	135.416	25.7745
4200.00	112.260	24.4135	136.673	25.7799
4400.00	113.397	24.4757	137.873	25.7846
4600.00	114.486	24.5327	139.019	25.7887
4800.00	115.531	24.5851	140.117	25.7924
5000.00	116.536	24.6335	141.169	25.7956
5200.00	117.503	24.6782	142.181	25.7984
5400.00	118.435	24.7198	143.155	25.8009
5600.00	119.335	24.7584	144.093	25.8032
5800.00	120.204	24.7945	144.999	25.8052
6000.00	121.045	24.8282	145.874	25.8070

TABLE II. Thermodynamic Properties of Germanium Tetrafluoride ($M = 145.3836$)

T (DEG. K.)	$-(G^\circ - H^\circ_0)/T$ (CAL/MOL)	$H^\circ - H^\circ_0$ (CAL/MOL)	S° (CAL/MOL)	C°_p (CAL/MOL)
0.00	0.000	0.000	0.000	0.0000
100.00	46.019	4.1398	55.178	12.0587
200.00	33.250	11.8800	65.130	16.6747
273.15	37.197	13.4780	70.675	18.9238
298.15	38.394	13.9619	72.360	19.5619
300.00	38.485	14.0095	72.481	19.6064
400.00	42.749	15.8603	78.409	21.8514
500.00	46.390	16.9713	83.321	22.7664
600.00	49.329	18.0115	87.347	23.5928
700.00	51.821	18.8478	91.269	24.1461
800.00	54.984	19.5395	94.518	24.4832
900.00	57.318	20.0993	97.414	24.7172
1000.00	59.401	20.5716	100.032	24.9621
1100.00	61.441	20.9750	102.419	25.0895
1200.00	63.328	21.3278	104.605	25.2027
1300.00	65.000	21.6297	106.626	25.2947
1400.00	66.413	21.8908	108.503	25.3658
1500.00	68.121	22.1251	110.255	25.4246
1600.00	69.568	22.3329	111.899	25.4729
1700.00	70.825	22.5170	113.443	25.5133
1800.00	72.117	22.6852	114.902	25.5472
1900.00	73.448	22.8367	116.298	25.5761
2000.00	74.623	22.9743	117.597	25.6008
2100.00	75.824	23.2150	120.039	25.6806
2200.00	76.853	23.4184	122.271	25.7211
2300.00	77.734	23.5927	124.327	25.6469
2400.00	78.489	23.7435	126.232	25.7138
2500.00	79.121	23.8756	128.007	25.7291
2600.00	79.656	23.9917	129.668	25.7416
2700.00	80.124	24.0949	131.228	25.7520
2800.00	80.513	24.1872	132.701	25.7607
2900.00	80.827	24.2702	134.094	25.7681
3000.00	81.070	24.3452	135.416	25.7745
3100.00	81.260	24.4135	136.673	25.7799
3200.00	81.397	24.4757	137.873	25.7846
3300.00	81.486	24.5327	139.019	25.7887
3400.00	81.531	24.5851	140.117	25.7924
3500.00	81.536	24.6332	141.169	25.7956
3600.00	81.507	24.6782	142.181	25.7984
3700.00	81.438	24.7198	143.155	25.8009
3800.00	81.375	24.7584	144.092	25.8032
3900.00	81.295	24.7945	144.998	25.8052
4000.00	81.216	24.8282	145.874	25.8070

TABLE II (Contd.)

T (DEG.K.)	$(H^\circ - H^\circ_{298})$ (KCAL/MOL)	$-\Delta Hf$ (KCAL/MOL)	$-\Delta Gf$ (KCAL/MOL)	LOG Kf
0.00	-4.1627	340.04	340.04	INF
100.00	-3.2488	340.87	335.67	733.60
200.00	-1.7867	341.20	330.31	360.94
273.15	-0.4812	341.26	326.37	261.13
298.15	0.0000	341.25	324.94	238.19
300.00	0.0362	341.25	324.84	236.65
400.00	2.1014	341.16	319.38	174.50
500.00	4.3229	340.99	313.96	137.23
600.00	6.6442	340.77	308.57	112.40
700.00	9.0307	340.53	303.22	94.67
800.00	11.4617	340.27	297.91	81.39
900.00	13.9239	340.01	292.63	71.06
1000.00	16.4088	339.74	287.38	62.81
1100.00	18.9107	339.46	282.16	56.06
1200.00	21.4256	339.19	276.96	50.44
1300.00	23.9507	338.91	271.79	45.69
1400.00	26.4838	338.64	266.64	41.62
1500.00	29.0234	338.37	261.50	38.10
1600.00	31.5684	338.10	256.39	35.02
1700.00	34.1177	337.83	251.29	32.31
1800.00	36.6708	337.57	246.21	29.89
1900.00	39.2270	337.31	241.14	27.74
2000.00	41.7859	337.05	236.08	25.80
2200.00	46.9102	336.55	226.01	22.45
2400.00	52.0415	336.06	215.98	19.67
2600.00	57.1782	335.58	206.00	17.32
2800.00	62.3191	335.12	196.05	15.30
3000.00	67.4634	334.67	186.13	13.56
3200.00	72.6105	334.24	176.24	12.04
3400.00	77.7599	333.83	166.38	10.69
3600.00	82.9112	333.43	156.53	9.50
3800.00	88.0641	333.04	146.71	8.44
4000.00	93.2184	332.68	136.92	7.48
4200.00	98.3739	332.33	127.14	6.62
4400.00	103.5303	331.99	117.38	5.83
4600.00	108.6877	331.67	107.63	5.11
4800.00	113.8458	331.37	97.89	4.46
5000.00	119.0046	331.09	88.17	3.85
5200.00	124.1640	330.82	78.46	3.30
5400.00	129.3239	330.57	68.77	2.78
5600.00	134.4843	330.33	59.07	2.31
5800.00	139.6452	330.11	49.38	1.86
6000.00	144.8064	329.91	39.71	1.45

TABLE II (Cont'd)

TABLE III. Thermodynamic Properties of Germanium Difluoride (M = 110.5868)

T (DEG.K.)	$-(G^\circ-H^\circ_0)/T$ (GIBBS/MOL)	$(H^\circ-H^\circ_0)/T$ (GIBBS/MOL)	S° (GIBBS/MOL)	C°_p (GIBBS/MOL)
0.00	0.000	0.0000	0.000	0.0000
100.00	45.748	8.1259	53.874	8.6482
200.00	51.567	8.7658	60.333	10.1697
273.15	54.375	9.2796	63.655	11.1580
298.15	55.195	9.4489	64.644	11.4355
300.00	55.254	9.4612	64.715	11.4548
400.00	58.062	10.0703	68.132	12.2719
500.00	60.364	10.5641	70.928	12.7665
600.00	62.326	10.9588	73.285	13.0756
700.00	64.040	11.2766	75.317	13.2779
800.00	65.564	11.5360	77.100	13.4161
900.00	66.935	11.7506	78.686	13.5143
1000.00	68.183	11.9308	80.114	13.5862
1100.00	69.327	12.0838	81.411	13.6404
1200.00	70.385	12.2154	82.600	13.6822
1300.00	71.367	12.3295	83.696	13.7150
1400.00	72.284	12.4294	84.714	13.7413
1500.00	73.145	12.5176	85.663	13.7626
1600.00	73.955	12.5960	86.551	13.7802
1700.00	74.721	12.6661	87.387	13.7948
1800.00	75.447	12.7292	88.176	13.8071
1900.00	76.137	12.7862	88.923	13.8175
2000.00	76.794	12.8380	89.632	13.8265
2200.00	78.022	12.9285	90.950	13.8409
2400.00	79.150	13.0050	92.155	13.8518
2600.00	80.194	13.0705	93.264	13.8604
2800.00	81.165	13.1272	94.292	13.8672
3000.00	82.072	13.1767	95.249	13.8727
3200.00	82.924	13.2204	96.144	13.8773
3400.00	83.726	13.2591	96.986	13.8810
3600.00	84.485	13.2938	97.779	13.8841
3800.00	85.205	13.3249	98.530	13.8868
4000.00	85.889	13.3531	99.242	13.8891
4200.00	86.541	13.3786	99.920	13.8910
4400.00	87.164	13.4020	100.566	13.8927
4600.00	87.760	13.4233	101.184	13.8942
4800.00	88.332	13.4430	101.775	13.8955
5000.00	88.881	13.4611	102.342	13.8967
5200.00	89.410	13.4779	102.887	13.8977
5400.00	89.919	13.4934	103.412	13.8986
5600.00	90.410	13.5079	103.917	13.8994
5800.00	90.884	13.5214	104.405	13.9001
6000.00	91.342	13.5341	104.876	13.9008

TABLE III. Thermodynamic Properties of
Ortho-Hydrogen Dihydride (M = 110.588)

T	$-(G^{\circ}-H^{\circ}_{0})/T$	$(H^{\circ}-H^{\circ}_{0})/T$	S°	C°_{p}
(DEG.K.)	(CIBBS/MOL)	(CIBBS/MOL)	(CIBBS/MOL)	(CIBBS/MOL)
0.00	0.000	0.000	0.000	0.0000
100.00	45.764	6.1295	53.874	8.0482
200.00	51.562	6.7038	60.393	10.1697
273.15	54.325	9.2740	63.599	11.1580
298.15	55.195	9.4685	64.664	11.4353
300.00	55.254	9.4812	64.735	11.4548
400.00	58.002	10.0703	68.132	12.2119
500.00	60.304	10.5641	70.868	12.7685
600.00	62.326	10.9885	73.315	13.0758
700.00	64.140	11.2766	75.317	13.2175
800.00	65.804	11.5340	77.100	13.4161
900.00	66.935	11.7606	78.695	13.5143
1000.00	68.283	11.9608	80.244	13.5982
1100.00	69.327	12.0938	81.421	13.6466
1200.00	70.435	12.2154	82.650	13.6822
1300.00	71.347	12.3235	83.670	13.7150
1400.00	72.284	12.4274	84.712	13.7413
1500.00	73.145	12.5176	85.663	13.7626
1600.00	73.955	12.5940	86.551	13.7802
1700.00	74.723	12.6661	87.387	13.7948
1800.00	75.447	12.7242	88.171	13.8071
1900.00	76.137	12.7842	88.923	13.8175
2000.00	76.794	12.8380	89.632	13.8265
2200.00	78.022	12.9285	90.950	13.8409
2400.00	79.175	13.0050	92.155	13.8518
2600.00	80.262	13.0705	93.264	13.8604
2800.00	81.285	13.1272	94.292	13.8672
3000.00	82.272	13.1767	95.247	13.8727
3200.00	83.224	13.2204	96.144	13.8773
3400.00	83.724	13.2591	96.984	13.8810
3600.00	84.485	13.2938	97.779	13.8841
3800.00	85.209	13.3249	98.530	13.8868
4000.00	85.889	13.3531	99.242	13.8891
4200.00	86.541	13.3786	99.920	13.8910
4400.00	87.164	13.4020	100.566	13.8924
4600.00	87.760	13.4235	101.184	13.8942
4800.00	88.332	13.4430	101.779	13.8955
5000.00	88.881	13.4611	102.348	13.8967
5200.00	89.410	13.4779	102.889	13.8977
5400.00	89.919	13.4934	103.412	13.8986
5600.00	90.410	13.5079	103.917	13.8994
5800.00	90.884	13.5214	104.405	13.9001
6000.00	91.342	13.5341	104.878	13.9008

TABLE III (Contd.)

T (DEG.K.)	$(H^\circ - H^\circ_{298})$ (KCAL/MOL)	$-\Delta H_f$ (KCAL/MOL)	$-\Delta G_f$ (KCAL/MOL)	LOG K_f
0.00	-2.8172	156.89	156.89	INF
100.00	-2.0046	157.12	155.86	340.62
200.00	-1.0640	157.27	154.53	168.86
273.15	-0.2825	157.32	153.54	122.85
298.15	0.0000	157.33	153.17	112.27
300.00	0.0212	157.33	153.14	111.56
400.00	1.2109	157.34	151.74	82.91
500.00	2.4649	157.33	150.34	65.71
600.00	3.7581	157.31	148.94	54.25
700.00	5.0765	157.29	147.55	46.07
800.00	6.4116	157.26	146.16	39.93
900.00	7.7584	157.24	144.78	35.16
1000.00	9.1136	157.21	143.39	31.34
1100.00	10.4750	157.19	142.01	28.22
1200.00	11.8412	157.16	140.63	25.61
1300.00	13.2112	157.14	139.26	23.41
1400.00	14.5840	157.12	137.88	21.52
1500.00	15.9593	157.10	136.51	19.89
1600.00	17.3364	157.09	135.14	18.46
1700.00	18.7152	157.07	133.76	17.20
1800.00	20.0953	157.06	132.39	16.07
1900.00	21.4766	157.05	131.02	15.07
2000.00	22.8588	157.04	129.65	14.17
2200.00	25.6256	157.03	126.92	12.61
2400.00	28.3949	157.03	124.18	11.31
2600.00	31.1661	157.04	121.44	10.21
2800.00	33.9389	157.05	118.70	9.27
3000.00	36.7130	157.07	115.96	8.45
3200.00	39.4880	157.10	113.22	7.73
3400.00	42.2638	157.14	110.48	7.10
3600.00	45.0403	157.18	107.73	6.54
3800.00	47.8174	157.24	104.98	6.04
4000.00	50.5950	157.30	102.23	5.59
4200.00	53.3730	157.37	99.47	5.18
4400.00	56.1514	157.45	96.71	4.80
4600.00	58.9301	157.54	93.95	4.46
4800.00	61.7091	157.64	91.18	4.15
5000.00	64.4883	157.74	88.41	3.86
5200.00	67.2677	157.86	85.64	3.60
5400.00	70.0474	157.98	82.86	3.35
5600.00	72.8272	158.11	80.07	3.12
5800.00	75.6071	158.24	77.28	2.91
6000.00	78.3872	158.39	74.49	2.71

T (DEG.K)	$H^\circ-H^\circ_{298}$ (KCAL/MOL)	$-\Delta H^\circ_f$ (KCAL/MOL)	$-\Delta G^\circ_f$ (KCAL/MOL)	LOG K
0.00	-2.8172	156.84	156.84	INF
100.00	-2.0044	158.12	153.96	340.02
200.00	-1.0640	157.27	154.53	166.06
273.15	-0.2825	157.12	151.54	122.45
298.15	0.0000	157.33	151.27	111.27
300.00	0.0172	157.32	151.14	110.24
400.00	1.2109	157.34	147.79	82.61
500.00	2.4649	157.39	150.34	65.71
600.00	3.7381	157.31	148.09	54.25
700.00	5.0705	157.20	145.85	46.07
800.00	6.4116	157.26	143.63	39.83
900.00	7.7596	157.24	141.38	35.15
1000.00	9.1136	157.21	139.16	31.46
1100.00	10.4720	157.15	136.97	28.22
1200.00	11.8342	157.16	134.83	25.61
1300.00	13.1992	157.16	132.64	23.46
1400.00	14.5660	157.12	130.88	21.52
1500.00	15.9343	157.10	129.27	19.87
1600.00	17.3046	157.09	127.39	18.46
1700.00	18.7752	157.07	125.76	17.220
1800.00	20.0493	157.08	124.31	16.07
1900.00	21.4180	157.08	123.02	15.07
2000.00	22.8838	157.06	121.77	14.17
2100.00	24.3494	157.05	120.52	13.31
2200.00	25.6254	157.03	119.40	12.63
2300.00	26.9746	157.03	118.34	11.91
2400.00	28.3241	157.04	117.44	11.24
2500.00	29.7737	157.05	116.47	10.77
2600.00	31.1232	157.05	115.57	10.27
2700.00	32.4730	157.02	114.70	9.85
2800.00	33.8230	157.00	113.85	9.43
2900.00	35.1730	157.00	113.02	9.03
3000.00	36.5230	157.00	112.20	8.68
3100.00	37.8730	157.00	111.38	8.34
3200.00	39.2230	157.00	110.57	8.03
3300.00	40.5730	157.00	109.76	7.73
3400.00	41.9230	157.00	108.95	7.46
3500.00	43.2730	157.00	108.14	7.20
3600.00	44.6230	157.00	107.33	6.96
3700.00	45.9730	157.00	106.52	6.73
3800.00	47.3230	157.00	105.71	6.52
3900.00	48.6730	157.00	104.90	6.32
4000.00	50.0230	157.00	104.09	6.13
4100.00	51.3730	157.00	103.28	5.95
4200.00	52.7230	157.00	102.47	5.78
4300.00	54.0730	157.00	101.66	5.62
4400.00	55.4230	157.00	100.85	5.46
4500.00	56.7730	157.00	100.04	5.31
4600.00	58.1230	157.00	99.23	5.17
4700.00	59.4730	157.00	98.42	5.03
4800.00	60.8230	157.00	97.61	4.90
4900.00	62.1730	157.00	96.80	4.78
5000.00	63.5230	157.00	95.99	4.66
5100.00	64.8730	157.00	95.18	4.55
5200.00	66.2230	157.00	94.37	4.44
5300.00	67.5730	157.00	93.56	4.34
5400.00	68.9230	157.00	92.75	4.24
5500.00	70.2730	157.00	91.94	4.15
5600.00	71.6230	157.00	91.13	4.06
5700.00	72.9730	157.00	90.32	3.97
5800.00	74.3230	157.00	89.51	3.89
5900.00	75.6730	157.00	88.70	3.81
6000.00	76.3272	157.00	87.89	3.73

has been used to estimate a value of 1.70 ± 0.03 Å for ℓ(Ge - F). The moment of intertia of GeF is calculated to be 7.2256 x 10^{-39} g cm^2. The values of σ and g_i were taken to be 1 and 2, respectively.

The enthalpy of formation of GeF(g) is based on a value of 7.7 ± 0.3 kcal mol^{-1}, determined by Margrave et al.,[22] for the enthalpy of the reaction

$$Ge(g) + CaF(g) \rightarrow Ca(g) + GeF(g). \quad (4)$$

The enthalpy of formation of CaF(g) has been calculated from the relationship

$$\Delta Hf^\circ(CaF,g) = \Delta Hf^\circ(Ca,g) + \Delta Hf^\circ(F,g) - D^\circ_{298}(CaF). \quad (5)$$

In Eq. 5, $\Delta Hf^\circ(Ca,g)$ was taken to be 42.6 ± 0.4 kcal mol^{-1},[8b] $\Delta Hf^\circ(F,g)$ was taken to be 18.9 ± 0.1 kcal mol^{-1},[24] and $D^\circ_{298}(CaF)$ was taken to be 127.5 ± 2.5 kcal mol^{-1}.[25] Thus, $\Delta Hf^\circ(CaF,g)$ is calculated to be -66.0 ± 2.6 kcal mol^{-1}; insertion of this value into Eq. 4 yields

$$\Delta Hf^\circ(GeF,g) = -11.4 \pm 3 \text{ kcal mol}^{-1}.*$$

On the basis of the reaction

$$\tfrac{1}{2}Ge_2(g) + \tfrac{1}{2}F_2(g) \rightarrow GeF(g), \quad (6)$$

$\Delta Hf(GeF,g)$ is calculated to be -68.2 ± 3.1 kcal mol^{-1}.

The thermodynamic properties of GeF(g) are given in Table IV.

The value of 114 kcal mol^{-1} for D(GeF), obtained by linear extrapolation of the spectroscopic data of Barrow et al.,[26] is surprisingly close to the value of 120 ± 3 kcal mol^{-1}, which can be derived from $\Delta Hf^\circ(GeF)$.

has been used to estimate a value of 1.70 ± 0.04 Å for $R(Ge - F)$. The moment of inertia of GeF_2 is calculated to be 7.2250×10^{-39} g cm^2. The values of φ_1 and φ_2 were taken to be 1 and 2, respectively.

The enthalpy of formation of $GeF_2(g)$ is based on a value of 7.7 ± 0.3 kcal mol^{-1}, determined by Margrave *et al.*[24] for the enthalpy of the reaction

$$Ge(g) + CaF_2(g) \rightarrow Ca(g) + GeF_2(g) \qquad (4)$$

The enthalpy of formation of $CaF_2(g)$ has been calculated from the relationship

$$\Delta H_f^\circ(CaF_2,g) = \Delta H_f^\circ(Ca,g) + \Delta H_f^\circ(F_2,g) + D_{298}^\circ(CaF). \qquad (5)$$

In Eq. 5, $\Delta H_f^\circ(Ca,g)$ was taken to be 42.6 ± 0.4 kcal mol^{-1},[25] $\Delta H_f^\circ(F_2,g)$ was taken to be 18.9 ± 0.1 kcal mol^{-1},[24] and $D_{298}^\circ(CaF)$ was taken to be 127.5 ± 2.5 kcal mol^{-1}.[26] Thus, $\Delta H_f^\circ(CaF_2,g)$ is calculated to be −63.0 ± 2.6 kcal mol^{-1}; insertion of this value into Eq. 4 yields

$$\Delta H_f^\circ(GeF_2,g) = -11.4 \pm 3 \text{ kcal mol}^{-1}.*$$

On the basis of the reaction

$$\tfrac{1}{2}Ge_2(g) + \tfrac{1}{2}F_2(g) \rightarrow GeF_2(g), \qquad (6)$$

$\Delta H_f^\circ(GeF_2,g)$ is calculated to be −58.2 ± 3.1 kcal mol^{-1}.

The thermodynamic properties of $GeF_2(g)$ are given in Table IV.

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* The value of 114 kcal mol^{-1} for $D(GeF)$, obtained by Jervis using the law of the geometric mean, is lower than that given by Margrave *et al.*[26] is surprisingly close to the value of −10.4 ± 3 kcal mol^{-1}, which is obtained from $\Delta H_f^\circ(GeF)$.

TABLE IV. Thermodynamic Properties of Germanium Monofluoride (M = 91.5884)

T	$-(G^\circ - H^\circ_0)/T$	$(H^\circ - H^\circ_0)/T$	S°	C°_p
(DEG.K.)	(GIBBS/MOL)	(GIBBS/MOL)	(GIBBS/MOL)	(GIBBS/MOL)
0.00	0.000	0.0000	0.000	0.0000
100.00	40.754	6.9528	47.707	6.9686
200.00	45.590	7.0359	52.626	7.3509
273.15	47.803	7.1745	54.978	7.7465
298.15	48.434	7.2274	55.661	7.8636
300.00	48.478	7.2314	55.710	7.8718
400.00	50.588	7.4390	58.027	8.2236
500.00	52.268	7.6192	59.887	8.4395
600.00	53.670	7.7681	61.438	8.5751
700.00	54.877	7.8901	62.767	8.6639
800.00	55.938	7.9909	63.928	8.7247
900.00	56.884	8.0749	64.959	8.7679
1000.00	57.738	8.1459	65.884	8.7996
1100.00	58.518	8.2065	66.724	8.8234
1200.00	59.234	8.2587	67.493	8.8418
1300.00	59.897	8.3041	68.201	8.8563
1400.00	60.514	8.3440	68.858	8.8679
1500.00	61.091	8.3792	69.470	8.8773
1600.00	61.632	8.4106	70.043	8.8850
1700.00	62.143	8.4387	70.582	8.8914
1800.00	62.626	8.4640	71.090	8.8968
1900.00	63.084	8.4869	71.571	8.9014
2000.00	63.520	8.5077	72.028	8.9054
2200.00	64.333	8.5442	72.877	8.9117
2400.00	65.078	8.5750	73.653	8.9166
2600.00	65.765	8.6015	74.367	8.9203
2800.00	66.404	8.6243	75.028	8.9233
3000.00	66.999	8.6444	75.644	8.9258
3200.00	67.558	8.6620	76.220	8.9277
3400.00	68.083	8.6777	76.761	8.9294
3600.00	68.580	8.6917	77.271	8.9308
3800.00	69.050	8.7043	77.754	8.9320
4000.00	69.497	8.7157	78.212	8.9330
4200.00	69.922	8.7261	78.648	8.9338
4400.00	70.328	8.7356	79.064	8.9346
4600.00	70.717	8.7442	79.461	8.9352
4800.00	71.089	8.7522	79.841	8.9358
5000.00	71.447	8.7595	80.206	8.9363
5200.00	71.790	8.7664	80.557	8.9367
5400.00	72.121	8.7727	80.894	8.9371
5600.00	72.440	8.7786	81.219	8.9375
5800.00	72.749	8.7840	81.533	8.9378
6000.00	73.047	8.7892	81.836	8.9381

TABLE IV. Thermodynamic Properties of Carrollite, Metaborate (M = 81.5984)

T (deg.K)	$-(G^{\circ}_{T}-H^{\circ}_{0})/T$ (DIMBS/MOL)	$H^{\circ}_{T}-H^{\circ}_{0}$ (DIMBS/MOL)	S°_{T} (DIMBS/MOL)	C°_{p} (DIMBS/MOL)
0.00	0.000	0.000	0.000	0.0000
100.00	4.755	475.507	4.755	9.4884
200.00	4.5.590	1,117.180	5.590	7.3709
273.15	4.7.803	1,511.365	7.803	7.7485
298.15	4.8.434	1,623.974	8.434	7.8834
300.00	4.8.478	1,631.410	8.478	7.9118
400.00	5.8.588	2,030.027	8.588	8.2361
500.00	5.9.262	2,426.887	9.262	8.4395
600.00	6.9.670	2,824.464	9.670	8.5781
700.00	6.9.927	3,223.767	9.927	8.6639
800.00	7.10.118	3,625.918	10.118	8.7247
900.00	7.10.283	4,029.983	10.283	8.7719
1000.00	7.10.434	4,434.539	10.434	8.7996
1100.00	7.10.574	4,839.724	10.574	8.8234
1200.00	7.10.704	5,245.487	10.704	8.8418
1300.00	7.10.827	5,651.801	10.827	8.8543
1400.00	7.10.944	6,058.658	10.944	8.8679
1500.00	7.11.056	6,465.970	11.056	8.8773
1600.00	7.11.163	6,873.663	11.163	8.8850
1700.00	7.11.267	7,281.667	11.267	8.8914
1800.00	7.11.367	7,689.910	11.367	8.8968
1900.00	7.11.464	8,098.329	11.464	8.9014
2000.00	7.11.557	8,506.871	11.557	8.9054
2200.00	7.11.737	9,324.372	11.737	8.9117
2400.00	7.11.913	10,142.653	11.913	8.9166
2600.00	7.12.085	10,961.707	12.085	8.9203
2800.00	7.12.253	11,781.529	12.253	8.9233
3000.00	7.12.418	12,601.999	12.418	8.9258
3200.00	7.12.580	13,422.920	12.580	8.9277
3400.00	7.12.739	14,244.277	12.739	8.9294
3600.00	7.12.895	15,065.980	12.895	8.9308
3800.00	7.13.049	15,887.993	13.049	8.9320
4000.00	7.13.200	16,710.297	13.200	8.9330
4200.00	7.13.349	17,532.861	13.349	8.9338
4400.00	7.13.495	18,355.668	13.495	8.9346
4600.00	7.13.639	19,178.682	13.639	8.9352
4800.00	7.13.781	20,001.881	13.781	8.9358
5000.00	7.13.921	20,825.263	13.921	8.9363
5200.00	7.14.059	21,648.777	14.059	8.9367
5400.00	7.14.195	22,472.419	14.195	8.9371
5600.00	7.14.329	23,296.173	14.329	8.9375
5800.00	7.14.461	24,119.033	14.461	8.9378
6000.00	7.14.592	24,942.000	14.592	8.9381

TABLE IV (Contd.)

T (DEG.K.)	$(H^\circ - H^\circ_{298})$ (KCAL/MOL)	$-\Delta Hf$ (KCAL/MOL)	$-\Delta Gf$ (KCAL/MOL)	LOG Kf
0.00	-2.1549	68.15	68.15	INF
100.00	-1.4596	68.15	68.31	149.28
200.00	-0.7477	68.18	68.45	74.80
273.15	-0.1952	68.20	68.56	54.86
298.15	0.0000	68.20	68.58	50.27
300.00	0.0146	68.20	68.58	49.96
400.00	0.8207	68.21	68.71	37.54
500.00	1.6548	68.22	68.83	30.09
600.00	2.5060	68.22	68.95	25.12
700.00	3.3682	68.23	69.07	21.57
800.00	4.2378	68.24	69.19	18.90
900.00	5.1126	68.24	69.31	16.83
1000.00	5.9910	68.25	69.43	15.17
1100.00	6.8722	68.26	69.55	13.82
1200.00	7.7555	68.27	69.67	12.69
1300.00	8.6405	68.29	69.78	11.73
1400.00	9.5267	68.30	69.90	10.91
1500.00	10.4140	68.31	70.01	10.20
1600.00	11.3021	68.33	70.12	9.58
1700.00	12.1909	68.35	70.23	9.03
1800.00	13.0804	68.36	70.34	8.54
1900.00	13.9703	68.38	70.45	8.10
2000.00	14.8606	68.40	70.56	7.71
2200.00	16.6424	68.44	70.78	7.03
2400.00	18.4252	68.49	70.99	6.46
2600.00	20.2089	68.54	71.19	5.98
2800.00	21.9933	68.60	71.39	5.57
3000.00	23.7782	68.66	71.59	5.22
3200.00	25.5636	68.72	71.78	4.90
3400.00	27.3493	68.79	71.97	4.63
3600.00	29.1353	68.86	72.16	4.38
3800.00	30.9216	68.94	72.34	4.16
4000.00	32.7081	69.02	72.52	3.96
4200.00	34.4948	69.11	72.69	3.78
4400.00	36.2816	69.20	72.86	3.62
4600.00	38.0686	69.29	73.02	3.47
4800.00	39.8557	69.39	73.18	3.33
5000.00	41.6429	69.49	73.34	3.21
5200.00	43.4302	69.59	73.49	3.09
5400.00	45.2176	69.70	73.64	2.98
5600.00	47.0051	69.82	73.78	2.88
5800.00	48.7926	69.94	73.92	2.79
6000.00	50.5802	70.06	74.06	2.70

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