REFERENCE STATE

0	to 1685	K	crystal
1685	to 3504.616	K	liquid
above	3504.616	K	ideal monatomic gas

Refer to the individual tables for details.

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

	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−3.218	0.	0.	0.
100	7.268	3.833	33.351	−2.952	0.	0.	0.
200	15.636	11.665	20.531	−1.773	0.	0.	0.
298.15	20.000	18.820	18.820	0.	0.	0.	0.
300	20.050	18.943	18.820	0.037	0.	0.	0.
400	22.142	25.032	19.636	2.159	0.	0.	0
500	23.330	30.110	21.237	4.436	0.	0.	0.
600	24.154	34.440	23.086	6.812	0.	0.	0.
700	24.803	38.212	24.983	9.260	0.	0.	0.
800	25.359	41.562	26.850	11.769	0.	0.	0.
900	25.874	44.579	28.655	14.331	0.	0.	0.
1000	26.338	47.329	30.387	16.942	0.	0.	0.
1100	26.778	49.860	32.044	19.598	0.	0.	0.
1200	27.196	52.208	33.627	22.297	0.	0.	0.
1300	27.614	54.401	35.142	25.037	0.	0.	0.
1400	28.033	56.463	36.592	27.820	0.	0.	0.
1500	28.451	58.411	37.982	30.644	0.	0.	0.
1600	28.870	60.261	39.317	33.510	0.	0.	0.
1685.000	29.225	61.765	40.412	35.979	___ CRYSTAL <--> LIQUID ___		
1685.000	27.196	91.562	40.412	86.187	TRANSITION		
1700	27.196	91.803	40.864	86.595	0.	0.	0.
1800	27.196	93.357	43.738	89.315	0.	0.	0.
1900	27.196	94.827	46.388	92.034	0.	0.	0.
2000	27.196	96.222	48.846	94.754	0.	0.	0.
2100	27.196	97.549	51.133	97.473	0.	0.	0.
2200	27.196	98.815	53.272	100.193	0.	0.	0.
2300	27.196	100.023	55.279	102.913	0.	0.	0.
2400	27.196	101.181	57.167	105.632	0.	0.	0.
2500	27.196	102.291	58.950	108.352	0.	0.	0.
2600	27.196	103.358	60.638	111.071	0.	0.	0.
2700	27.196	104.384	62.239	113.791	0.	0.	0.
2800	27.196	105.373	63.762	116.511	0.	0.	0.
2900	27.196	106.327	65.214	119.230	0.	0.	0.
3000	27.196	107.249	66.600	121.950	0.	0.	0.
3100	27.196	108.141	67.925	124.669	0.	0.	0.
3200	27.196	109.005	69.196	127.389	0.	0.	0.
3300	27.196	109.842	70.415	130.109	0.	0.	0.
3400	27.196	110.653	71.586	132.828	0.	0.	0.
3500	27.196	111.442	72.714	135.548	0.	0.	0.
3504.616	27.196	111.478	72.765	135.673	___ LIQUID <--> IDEAL GAS ___		
3504.616	23.023	221.204	72.765	520.221	FUGACITY = 1 bar		
3600	23.046	221.822	76.706	522.419	0.	0.	0.
3700	23.066	222.454	80.637	524.725	0.	0.	0.
3800	23.081	223.070	84.377	527.032	0.	0.	0.
3900	23.093	223.669	87.941	529.341	0.	0.	0.
4000	23.102	224.254	91.341	531.651	0.	0.	0.
4100	23.108	224.825	94.590	533.961	0.	0.	0.
4200	23.111	225.381	97.698	536.272	0.	0.	0.
4300	23.113	225.925	100.673	538.583	0.	0.	0.
4400	23.112	226.457	103.526	540.895	0.	0.	0.
4500	23.111	226.976	106.264	543.206	0.	0.	0.
4600	23.108	227.484	108.893	545.517	0.	0.	0.
4700	23.104	227.981	111.422	547.827	0.	0.	0.
4800	23.100	228.467	113.855	550.138	0.	0.	0.
4900	23.096	228.943	116.199	552.447	0.	0.	0.
5000	23.092	229.410	118.459	554.757	0.	0.	0.
5100	23.089	229.867	120.639	557.066	0.	0.	0.
5200	23.087	230.316	122.744	559.374	0.	0.	0.
5300	23.086	230.755	124.777	561.683	0.	0.	0.
5400	23.086	231.187	126.744	563.992	0.	0.	0.
5500	23.087	231.610	128.647	566.300	0.	0.	0.
5600	23.091	232.026	130.489	568.609	0.	0.	0.
5700	23.098	232.435	132.274	570.918	0.	0.	0.
5800	23.108	232.837	134.005	573.228	0.	0.	0.
5900	23.121	233.232	135.683	575.539	0.	0.	0.
6000	23.135	233.621	137.312	577.851	0.	0.	0.

PREVIOUS. March 1967 (1 atm) CURRENT: March 1967 (1 bar)

Silicon (Si) CRYSTAL $A_r = 28.0855$

$S°(298.15\ K) = 18.820 \pm 0.04\ J·K^{-1}·mol^{-1}$
$T_{fus} = 1685 \pm 3\ K$

$\Delta_f H°(0\ K) = 0\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ·mol^{-1}$
$\Delta_{fus} H° = 50.2 \pm 0.4\ kJ·mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature heat capacities are based on the precise data of Flubacher *et al.* (8–300 K).[1] The entropy is obtained from the heat capacity using $S°(8\ K) = 0.0003\ cal·K^{-1}·mol^{-1}$. The selected values are consistent with recent data of Keesom and Seidel (1.2–4.2 K),[2] and Kalishevich *et al.* (60–300 K).[3] Earlier data have been reviewed by Hultgren *et al.*[10]

High temperature studies are summarized below along with the pertinent low temperatures studies. The selected heat capacities above 300 K are obtained from a Shomate plot of the adopted low temperature heat capacities and the enthalpies reported or derived from the work of Dennison,[5] Kantor *et al.*,[6] Olette,[7] Serebrennikov and Gel'd[8] and Magnus.[9] Discrepancies are apparent in the enthalpy data, particularly in the range of 370–1100 K where only the recent study of Dennison[5] made use of a high purity sample. Enthalpies from Dennison[5] join most smoothly with the low temperature heat capacity but deviate increasingly at higher temperatures, being 1–2% lower than the other measurements above 1000 K. The selected functions agree with Dennison[5] below 600 K, with Magnus[1] from 600 to 1200 K, and with Kantor *et al.*[6] above 1200 K. The resulting heat capacities are slightly different from those selected by Hultgren, *et al.*,[10] the latter are 0.07 $cal·K^{-1}·mol^{-1}$ higher at 800 K and 0.21 $cal·K^{-1}·mol^{-1}$ lower at the melting point.

Source	Method	Quantity Reported	T/K	Sample
1	Calorimetry	$C_p°$	7.7–300	Single crystal, 3mm pieces, Resistance (300 K) = 100 ohm cm, Carrier Concentration $\leq 10^{15}$ cm^{-3}
2	Calorimetry	Specific Heat	1.2–4.2	
3	Calorimetry	$C_p°$	60–300	99.999%
4	Temperature Modulation	$C_p°$	300–900	Resistance (300 K) = 0.027 ohm cm, Carrier Concentration = 10^{19} cm^{-3}
5	Drop Calorimetry	Specific Heat	273–1373	Resistance (300 K) = 107 ohm cm
6	Drop Calorimetry	Enthalpy Equation	1148–1685	"Highly purified"
7	Drop Calorimetry	Specific Enthalpy	1467–1685	99.99%
8	Drop Calorimetry	Specific Enthalpy	302 – 1556	99.3%
9	Drop Calorimetry	Specific Enthalpy	372 – 1175	99.2%

Fusion Data

Refer to the liquid table for details.

Sublimation Data

Refer to the ideal gas table for details.

References

[1]P. Flubacher, A. J. Leadbetter and J. A. Morrison, Phil. Mag. 4, 275 (1959).
[2]P. H. Keesom and G. Seidel, Phys. Rev. 113, 33 (1959).
[3]G. I. Kalishevich, P. V. Gel'd. and R. P. Krentsis, Russ. J. Phys. Chem. 39, 1602 (1965).
[4]D. Gerlich, B. Abeles and R. E. Miller, J. Appl. Phys. 36, 76 (1965).
[5]D. H. Dennison, quoted by H. R. Shanks *et al.*, Phys. Rev. 130, 1743 (1963).
[6]P. B. Kantor, A. M. Kisil and E. M. Fomichev, Ukrain. Fiz. Zhur. 5, 358 (1960).
[7]M. Olette, Phys. Chem. Steelmaking, Proc. Dedham, Mass. 1956, 18–26 (Pub. 1958).
[8]N. N. Serebrennikov and P. v. Gel'd, Dokl. Akad. Nauk SSSR 87, 1021 (1952).
[9]A. Magnus, Ann. Physik 70, 303 (1923).
[10]R. Hultgren, R. L. Orr, and K. K. Kelley, "Supplement to Selected Values of Thermodynamic Properties of Metals and Alloys," University of California, Berkeley, (1965).

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
0	0.	0.	INFINITE	−3.218	0.	0.	0.
100	7.268	3.833	33.351	−2.952	0.	0.	0.
200	15.636	11.665	20.531	−1.773	0.	0.	0.
250	18.221	15.446	19.138	−0.923	0.	0.	0.
298.15	20.000	18.820	18.820	0.	0.	0.	0.
300	20.050	18.943	18.820	0.037	0.	0.	0.
350	21.276	22.132	19.069	1.072	0.	0.	0.
400	22.142	25.032	19.636	2.159	0.	0.	0.
450	22.803	27.680	20.385	3.283	0.	0.	0.
500	23.330	30.110	21.237	4.436	0.	0.	0.
600	24.154	34.440	23.086	6.812	0.	0.	0.
700	24.803	38.212	24.983	9.260	0.	0.	0.
800	25.359	41.562	26.850	11.769	0.	0.	0.
900	25.874	44.579	28.655	14.331	0.	0.	0.
1000	26.338	47.329	30.387	16.942	0.	0.	0.
1100	26.778	49.860	32.044	19.598	0.	0.	0.
1200	27.196	52.208	33.627	22.297	0.	0.	0.
1300	27.614	54.401	35.142	25.037	0.	0.	0.
1400	28.033	56.463	36.592	27.820	0.	0.	0.
1500	28.451	58.411	37.982	30.644	0.	0.	0.
1600	28.870	60.261	39.317	33.510	0.	0.	0.
1685.000	29.225	61.765	40.412	35.979	--- CRYSTAL <--> LIQUID ---		
1700	29.288	62.024	40.602	36.418	−50.177	0.447	−0.014
1800	29.706	63.710	41.839	39.368	−49.947	3.418	−0.099
1900	30.125	65.327	43.033	42.359	−49.675	6.376	−0.175
2000	30.543	66.883	44.187	45.393	−49.361	9.318	−0.243
2100	30.962	68.383	45.303	48.468	−49.006	12.243	−0.305
2200	31.380	69.833	46.386	51.585	−48.608	15.151	−0.360
2300	31.798	71.237	47.436	54.744	−48.169	18.039	−0.410
2400	32.217	72.600	48.456	57.945	−47.688	20.908	−0.455
2500	32.635	73.923	49.448	61.187	−47.165	23.755	−0.496

PREVIOUS: December 1962 CURRENT: December 1966

$S°(298.15\ K) = [44.460]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 1685 \pm 3\ K$

$\Delta_f H°(298.15\ K) = [48.470]\ kJ·mol^{-1}$
$\Delta_{fus} H° = 50.2 \pm 0.4\ kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation, $\Delta_f H°$(Si, l, 298.15 K) is calculated from that of the crystal by adding $\Delta_{fus} H°$ and the difference in enthalpy, $H°(1685\ K) - H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

Enthalpy data for high purity samples in quartz or vitreous silica capsules have been reported for the range 1698–1915 K by Kantor *et al.*[1] and for the range 1686–1825 K by Olette.[2] Due to the limited temperature range and the experimental uncertainty, the data do not appear to justify more than a constant heat capacity. A value of 6.5 $cal·K^{-1}·mol^{-1}$ is selected, intermediate between the values of 6.75 and 6.15 obtained from separate experiments.

The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Modern determinations of the melting point range from 1683 ± 1 to 1690 ± 4 K, the former from the specific volume study of Lucas and Urbain[3] and the later from the enthalpy study of Kantor *et al.*[1] The selected value, $T_{fus} = 1685$ K, is taken from Hultgren *et al.*,[4] who have reviewed the melting data.

The enthalpy of melting is calculated from the selected enthalpy of the crystal and the liquid enthalpy measurements of Kantor *et al.*[1] and Olette,[2] who reported comparable values of $\Delta_{fus} H° = 11.95 \pm 0.18$ and 12.095 ± 0.1 $kcal·mol^{-1}$, respectively.

Vaporization Data

T_{vap} is calculated as the temperature for which $\Delta_r G° = 0$ for Si(l) = Si(g). $\Delta_{vap} H°$ is calculated as the difference between $\Delta_f H°$(g) and $\Delta_f H°$(l) at T_{vap}. The normal boiling for the equilibrium vapor is calculated as the temperature at which Si, Si_2, and Si_3 attain a total pressure of 1 atm; the vapor containing 92.1%, 7.0% and 0.9% (mole) of monomer, dimer, and trimer, repectively. tetramer and high polymers, which are ignored in this calculation, are probably negligible at this temperature (~3490 K).

References

[1] P. B. Kantor, A. M. Kisil, and E. M. Fomichev, Ukrain. Fiz. Zhur. 5, 358 (1960).
[2] M. Olette, Phys. Chem. Steelmaking, Proc. Dedham, Mass. 1956, 18–26 (Pub. 1958).
[3] L. D. Lucas and G. Urbain, Compt. Rend. 255, 2414 (1962).
[4] R. Hultgren, R. L. Orr and K. K. Kelley, "Supplement to Selected Values of Thermodynamic Properties of Metals and Alloys," Univ. of California, Berkeley, (1965).

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
0							
100							
200							
250							
298.15	27.196	44.460	44.460	0.	48.470	40.826	−7.152
300	27.196	44.628	44.461	0.050	48.483	40.778	−7.100
350	27.196	48.821	44.792	1.410	48.808	39.467	−5.890
400	27.196	52.452	45.527	2.770	49.082	38.114	−4.977
450	27.196	55.655	46.478	4.130	49.317	36.728	−4.263
500	27.196	58.521	47.542	5.490	49.523	35.318	−3.690
600	27.196	63.479	49.797	8.209	49.867	32.443	−2.824
700	27.196	67.671	52.059	10.929	50.139	29.517	−2.203
800	27.196	71.303	54.243	13.648	50.349	26.556	−1.734
900	27.196	74.506	56.320	16.368	50.507	23.572	−1.368
1000	27.196	77.372	58.284	19.088	50.616	20.573	−1.075
1100	27.196	79.964	60.139	21.807	50.679	17.565	−0.834
1200	27.196	82.330	61.891	24.527	50.700	14.554	−0.634
1300	27.196	84.507	63.548	27.246	50.679	11.542	−0.464
1400	27.196	86.522	65.118	29.966	50.616	8.534	−0.318
1500	27.196	88.399	66.608	32.686	50.512	5.531	−0.193
1600	27.196	90.154	68.026	35.405	50.365	2.537	−0.083
1685.000	27.196	91.562	69.178	37.717	--- CRYSTAL <--> LIQUID ---		
1700	27.196	91.803	69.376	38.125	0.	0.	0.
1800	27.196	93.357	70.666	40.844	0.	0.	0.
1900	27.196	94.827	71.899	43.564	0.	0.	0.
2000	27.196	96.222	73.081	46.284	0.	0.	0.
2100	27.196	97.549	74.215	49.003	0.	0.	0.
2200	27.196	98.814	75.304	51.723	0.	0.	0.
2300	27.196	100.023	76.353	54.442	0.	0.	0.
2400	27.196	101.181	77.363	57.162	0.	0.	0.
2500	27.196	102.291	78.338	59.882	0.	0.	0.
2600	27.196	103.358	79.280	62.601	0.	0.	0.
2700	27.196	104.384	80.191	65.321	0.	0.	0.
2800	27.196	105.373	81.073	68.040	0.	0.	0.
2900	27.196	106.327	81.928	70.760	0.	0.	0.
3000	27.196	107.249	82.756	73.480	0.	0.	0.
3100	27.196	108.141	83.561	76.199	0.	0.	0.
3200	27.196	109.005	84.343	78.919	0.	0.	0.
3300	27.196	109.842	85.103	81.638	0.	0.	0.
3400	27.196	110.653	85.842	84.358	0.	0.	0.
3500	27.196	111.442	86.562	87.078	0.	0.	0.
3504.616	27.196	111.478	86.595	87.203	----- FUGACITY = 1 bar -----		
3600	27.196	112.208	87.264	89.797	−384.152	10.461	−0.152
3700	27.196	112.953	87.949	92.517	−383.738	21.417	−0.302
3800	27.196	113.678	88.616	95.236	−383.326	32.361	−0.445
3900	27.196	114.385	89.268	97.956	−382.915	43.295	−0.580
4000	27.196	115.073	89.904	100.676	−382.505	54.218	−0.708
4100	27.196	115.745	90.526	103.395	−382.096	65.131	−0.830
4200	27.196	116.400	91.135	106.115	−381.687	76.034	−0.946
4300	27.196	117.040	91.730	108.834	−381.279	86.927	−1.056
4400	27.196	117.665	92.312	111.554	−380.871	97.811	−1.161
4500	27.196	118.277	92.882	114.274	−380.462	108.686	−1.262

PREVIOUS: December 1966 CURRENT: March 1967

CRYSTAL-LIQUID

0 to 1685 K crystal
above 1685 K liquid

Refer to the individual tables for details.

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

	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−3.218	0.	0.	0.
100	7.268	3.833	33.351	−2.952	0.	0.	0.
200	15.636	11.665	20.531	−1.773	0.	0.	0.
250	18.221	15.446	19.138	−0.923	0.	0.	0.
298.15	20.000	18.820	18.820	0.	0.	0.	0.
300	20.050	18.943	18.820	0.037	0.	0.	0.
350	21.276	22.132	19.069	1.072	0.	0.	0.
400	22.142	25.032	19.636	2.159	0.	0.	0.
450	22.803	27.680	20.385	3.283	0.	0.	0.
500	23.330	30.110	21.237	4.436	0	0.	0.
600	24.154	34.440	23.086	6.812	0.	0.	0.
700	24.803	38.212	24.983	9.260	0.	0.	0.
800	25.359	41.562	26.850	11.769	0.	0.	0.
900	25.874	44.579	28.655	14.331	0.	0.	0.
1000	26.338	47.329	30.387	16.942	0.	0.	0.
1100	26.778	49.860	32.044	19.598	0.	0.	0.
1200	27.196	52.208	33.627	22.297	0.	0.	0.
1300	27.614	54.401	35.142	25.037	0.	0.	0.
1400	28.033	56.463	36.592	27.820	0.	0.	0.
1500	28.451	58.411	37.982	30.644	0.	0.	0.
1600	28.870	60.261	39.317	33.510	0.	0.	0.
1685.000	29.225	61.765	40.412	35.979	___ CRYSTAL <--> LIQUID ___		
1685.000	27.196	91.562	40.412	86.187	TRANSITION		
1700	27.196	91.803	40.864	86.595	0.	0.	0.
1800	27.196	93.357	43.738	89.315	0.	0.	0.
1900	27.196	94.827	46.388	92.034	0.	0.	0.
2000	27.196	96.222	48.846	94.754	0.	0.	0.
2100	27.196	97.549	51.133	97.473	0.	0.	0.
2200	27.196	98.815	53.272	100.193	0.	0.	0.
2300	27.196	100.023	55.279	102.913	0.	0.	0.
2400	27.196	101.181	57.167	105.632	0.	0.	0.
2500	27.196	102.291	58.950	108.352	0.	0.	0.
2600	27.196	103.358	60.638	111.071	0.	0.	0.
2700	27.196	104.384	62.239	113.791	0.	0.	0.
2800	27.196	105.373	63.762	116.511	0.	0.	0.
2900	27.196	106.327	65.214	119.230	0.	0.	0.
3000	27.196	107.249	66.600	121.950	0.	0.	0.
3100	27.196	108.141	67.925	124 669	0.	0.	0.
3200	27.196	109.005	69.196	127.389	0.	0.	0.
3300	27.196	109.842	70.415	130 109	0.	0.	0.
3400	27.196	110.653	71.586	132.828	0.	0.	0.
3500	27.196	111.442	72.714	135.548	0.	0.	0.
3504.616	27.196	111.478	72.765	135.673	----- FUGACITY = 1 bar -----		
3600	27.196	112.208	73.800	138.267	−384.152	10.461	−0.152
3700	27.196	112.953	74.848	140.987	−383.738	21.417	−0.302
3800	27.196	113.678	75.861	143.707	−383.326	32.361	−0.445
3900	27.196	114.385	76.840	146.426	−382.915	43.295	−0.580
4000	27.196	115.073	77.787	149.146	−382.505	54.218	−0.708
4100	27.196	115.745	78.704	151.865	−382.096	65.131	−0.830
4200	27.196	116.400	79.594	154.585	−381.687	76.034	−0.946
4300	27.196	117.040	80.458	157.305	−381.279	86.927	−1.056
4400	27.196	117.665	81.296	160.024	−380.871	97.811	−1.161
4500	27.196	118.277	82.111	162.744	−380.462	108.686	−1.262

PREVIOUS: CURRENT: March 1967

IP(Si, g) = 65747.5 ± 0.6 cm^{-1}
$S°(298.15\ K) = 167.980 \pm 0.035\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 446 \pm 8\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 450 \pm 8\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^3P_2$	0.00	5
$^3P_1$	77.115	3
$^3P_0$	223.157	1
$^1D_2$	6298.850	5
$^1S_0$	15394.370	1

Enthalpy of Formation

The enthalpy of formation of silicon gas is chosen to be the value recommended by CODATA.[1] This value was calculated from the sublimation and decomposition measurements of Davis *et al.* (1848–2003 K),[2] Grievison and Alcock (1940–2054 K),[3] Drowart *et al.*,[4] Gulbranson *et al.* (1373–1623 K),[5] Batdorf and Smits (1493–1601 K),[6] and Zenbov *et al.*[7]

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,[8,9] is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels (for $n<11$) and cutting off the summation in the partition function[10] has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than those listed above; the next excited state is approximately 33326 cm^{-1} above the ground state. Although we list only a few levels, all levels given by Moore[8,9] and estimated levels (for $n<11$) are considered in the calculation. The reported uncertainty is $S°(298.15\ K)$ is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states (for $n<10$) and use of different fill and cutoff procedures.[10]

The termal functions at 298.15 K closely agree with the recent CODATA recommendations[1] except for two minor changes. First, the entropy differs by 0.1094 $J \cdot K^{-1} \cdot mol^{-1}$ because this table used a reference pressure of 1 bar, whereas CODATA recommendations are based on 1 atm. Second, the entropy differs by ~0.001 $J \cdot K^{-1} \cdot mol^{-1}$ due to the use of slightly different values for the fundamental constants.

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−7.550	445.668	445.668	INFINITE
100	28.022	140.886	188.980	−4.809	448.142	434.437	−226.927
200	23.796	158.817	170.054	−2.247	449.526	420.095	−109.718
250	22.821	164.013	168.349	−1.084	449.839	412.697	−86.228
298.15	22.251	167.980	167.980	0.	450.000	405.528	−71.047
300	22.234	168.117	167.980	0.041	450.004	405.252	−70.561
350	21.861	171.515	168.249	1.143	450.071	397.787	−59.366
400	21.613	174.417	168.843	2.229	450.071	390.317	−50.970
450	21.440	176.952	169.606	3.305	450.023	382.850	−44.440
500	21.316	179.204	170.456	4.374	449.938	375.391	−39.217
600	21.153	183.075	172.246	6.497	449.684	360.504	−31.385
700	21.057	186.328	174.032	8.607	449.347	345.666	−25.794
800	21.000	189.135	175.748	10.710	448.940	330.881	−21.604
900	20.971	191.607	177.376	12.808	448.476	316.151	−18.349
1000	20.968	193.816	178.911	14.905	447.962	301.476	−15.747
1100	20.989	195.815	180.358	17.002	447.404	286.854	−13.622
1200	21.033	197.643	181.724	19.103	446.806	272.284	−11.852
1300	21.099	199.329	183.014	21.210	446.172	257.766	−10.357
1400	21.183	200.896	184.236	23.323	445.504	243.298	−9.078
1500	21.282	202.360	185.396	25.447	444.803	228.879	−7.970
1600	21.394	203.737	186.500	27.580	444.070	214.508	−7.003
1700	21.513	205.038	187.552	29.726	393.131	200.631	−6.165
1800	21.638	206.271	188.558	31.883	392.569	189.323	−5.494
1900	21.764	207.444	189.522	34.053	392.019	178.047	−4.895
2000	21.889	208.564	190.446	36.236	391.482	166.799	−4.356
2100	22.011	209.635	191.334	38.431	390.958	155.578	−3.870
2200	22.129	210.662	192.190	40.638	390.445	144.382	−3.428
2300	22.241	211.648	193.014	42.857	389.944	133.208	−3.025
2400	22.346	212.597	193.811	45.086	389.454	122.056	−2.656
2500	22.444	213.511	194.581	47.326	388.974	110.924	−2.318
2600	22.535	214.393	195.326	49.575	388.503	99.812	−2.005
2700	22.617	215.245	196.048	51.832	388.041	88.717	−1.716
2800	22.692	216.069	196.748	54.098	387.587	77.639	−1.448
2900	22.759	216.866	197.428	56.370	387.140	66.578	−1.199
3000	22.819	217.639	198.089	58.649	386.700	55.531	−0.967
3100	22.872	218.388	198.732	60.934	386.265	44.500	−0.750
3200	22.918	219.115	199.358	63.223	385.835	33.482	−0.547
3300	22.958	219.821	199.967	65.517	385.409	22.477	−0.356
3400	22.993	220.507	200.561	67.815	384.987	11.486	−0.176
3500	23.022	221.174	201.141	70.116	384.568	0.507	−0.008
3504.616	23.023	221.204	201.167	70.222	---- FUGACITY = 1 bar ----		
3600	23.046	221.822	201.706	72.419	0.	0.	0.
3700	23.066	222.454	202.258	74.725	0.	0.	0.
3800	23.081	223.070	202.798	77.032	0.	0.	0.
3900	23.093	223.669	203.325	79.341	0.	0.	0.
4000	23.102	224.254	203.841	81.651	0.	0.	0.
4100	23.108	224.825	204.346	83.961	0.	0.	0.
4200	23.111	225.381	204.840	86.272	0.	0	0.
4300	23.113	225.925	205.324	88.583	0.	0.	0.
4400	23.112	226.457	205.799	90.895	0.	0.	0.
4500	23.111	226.976	206.264	93.206	0.	0.	0.
4600	23.108	227.484	206.719	95.517	0.	0.	0.
4700	23.104	227.981	207.167	97.827	0.	0.	0.
4800	23.100	228.467	207.605	100.138	0.	0.	0.
4900	23.096	228.943	208.036	102.447	0.	0.	0.
5000	23.092	229.410	208.459	104.757	0.	0.	0.
5100	23.089	229.867	208.874	107.066	0.	0.	0.
5200	23.087	230.316	209.282	109.375	0.	0.	0.
5300	23.086	230.755	209.683	111.683	0.	0.	0.
5400	23.086	231.187	210.077	113.992	0.	0.	0.
5500	23.087	231.610	210.465	116.300	0.	0.	0.
5600	23.091	232.026	210.846	118.609	0.	0.	0.
5700	23.098	232.435	211.221	120.918	0.	0.	0.
5800	23.108	232.837	211.591	123.228	0.	0.	0.
5900	23.121	233.232	211.954	125.539	0.	0.	0.
6000	23.135	233.621	212.312	127.851	0.	0.	0.

PREVIOUS: March 1967 (1 atm) CURRENT: March 1983 (1 bar)

Silicon, Ion (Si^+) IDEAL GAS $M_r = 28.08495$ Silicon, Ion (Si^+) $Si^+_1(g)$

$IP(Si^+, g) = 131838.4 \pm 0.1\ cm^{-1}$
$S°(298.15\ K) = 163.426 \pm 0.02\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 1232.2 \pm 4\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [1242.505]\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2P_{1/2}$	0.0	2
$^2P_{3/2}$	287.32	4
$^4P_{1/2}$	42824.35	4
$^4P_{3/2}$	42932.68	6
$^4P_{5/2}$	43107.97	4

Enthalpy of Formation

$\Delta_f H°(Si^+, g, 0\ K)$ is calculated from $\Delta_f H°(Si, g, 0\ K)$[1] using the spectroscopic value of $IP(Si) = 65747.5 \pm 0.6\ cm^{-1}$ ($786.515 \pm 0.001\ kJ \cdot mol^{-1}$) from Moore.[2,6] The ionization limit is converted from cm^{-1} to $kJ \cdot mol^{-1}$ using the factor, $1\ cm^{-1} = 0.01196266\ kJ \cdot mol^{-1}$, which is derived from the 1973 CODATA fundamental constants.[3] Rosenstock *et al.*[4] and Levin and Lias[5] have summarized additional ionization and appearance potential data.

$\Delta_f H°(Si^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(Si, g, 0\ K)$ by using IP(Si) with JANAF[1] enthalpies, $H°(0\ K) - H°(298.15\ K)$, for Si(g), $Si^+(g)$, and e^-(ref). $\Delta_f H°(Si \rightarrow Si^+ + e^-, 298.15\ K)$ differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[4] $\Delta_f H°(298.15\ K)$ should be changed by $-6.197\ kJ \cdot mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,[2,6] is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[7] has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the first four excited states; the next excited state is $55309.61\ cm^{-1}$ above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state and the first four excited states. The reported uncertainty in $S°(298.15\ K)$ is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states and use of different fill and cutoff procedures.[7]

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

	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−7.343	1232.183		
100	25.060	134.836	186.411	−5.158			
200	26.512	153.262	165.719	−2.491			
250	25.337	159.052	163.832	−1.195			
298.15	24.338	163.426	163.426	0.	1242.505	1193.136	−209.032
300	24.304	163.577	163.427	0.045	1242.551	1192.829	−207.690
350	23.520	167.261	163.719	1.240	1243.750	1184.446	−176.769
400	22.943	170.362	164.361	2.400	1244.864	1175.897	−153.556
450	22.518	173.039	165.180	3.536	1245.915	1167.213	−135.487
500	22.201	175.394	166.086	4.654	1246.918	1158.414	−121.019
600	21.773	179.400	167.982	6.851	1248.818	1140.532	−99.292
700	21.509	182.735	169.858	9.014	1250.611	1122.342	−83.750
800	21.337	185.596	171.651	11.156	1252.323	1103.900	−72.077
900	21.219	188.101	173.342	13.283	1253.967	1085.248	−62.986
1000	21.134	190.332	174.932	15.401	1255.552	1066.416	−55.704
1100	21.072	192.344	176.425	17.511	1257.085	1047.427	−49.738
1200	21.025	194.175	177.829	19.615	1258.570	1028.302	−44.761
1300	20.989	195.857	179.152	21.716	1260.008	1009.054	−40.544
1400	20.960	197.411	180.401	23.814	1261.402	989.697	−36.926
1500	20.937	198.856	181.584	25.908	1262.751	970.243	−33.787
1600	20.918	200.207	182.706	28.001	1264.056	950.699	−31.037
1700	20.903	201.475	183.773	30.092	1215.141	931.522	−28.622
1800	20.890	202.669	184.790	32.182	1216.590	914.797	−26.547
1900	20.879	203.798	185.761	34.270	1218.037	897.991	−24.688
2000	20.870	204.869	186.690	36.358	1219.484	881.109	−23.012
2100	20.862	205.887	187.580	38.444	1220.929	864.155	−21.495
2200	20.855	206.857	188.434	40.530	1222.374	847.132	−20.113
2300	20.849	207.784	189.256	42.615	1223.818	830.043	−18.851
2400	20.844	208.671	190.046	44.700	1225.262	812.892	−17.692
2500	20.839	209.522	190.808	46.784	1226.705	795.680	−16.625
2600	20.835	210.339	191.544	48.868	1228.148	778.410	−15.638
2700	20.831	211.126	192.255	50.951	1229.590	761.085	−14.724
2800	20.828	211.883	192.942	53.034	1231.032	743.707	−13.874
2900	20.825	212.614	193.608	55.117	1232.474	726.277	−13.082
3000	20.823	213.320	194.254	57.199	1233.915	708.797	−12.341
3100	20.820	214.003	194.880	59.281	1235.356	691.270	−11.648
3200	20.818	214.664	195.488	61.363	1236.797	673.696	−10.997
3300	20.816	215.304	196.078	63.445	1238.238	656.076	−10.385
3400	20.814	215.926	196.653	65.526	1239.678	638.414	−9.808
3500	20.813	216.529	197.212	67.608	1241.119	620.708	−9.264
3600	20.811	217.115	197.757	69.689	858.407	613.423	−8.901
3700	20.810	217.685	198.288	71.770	860.261	606.592	−8.564
3800	20.809	218.240	198.806	73.851	862.113	599.711	−8.244
3900	20.808	218.781	199.311	75.932	863.964	592.782	−7.939
4000	20.807	219.308	199.805	78.013	865.814	585.805	−7.650
4100	20.807	219.821	200.286	80.093	867.662	578.782	−7.374
4200	20.806	220.323	200.758	82.174	869.511	571.714	−7.110
4300	20.806	220.812	201.218	84.254	871.359	564.601	−6.859
4400	20.806	221.291	201.669	86.335	873.207	557.446	−6.618
4500	20.806	221.758	202.110	88.416	875.055	550.249	−6.387
4600	20.806	222.216	202.542	90.496	876.903	543.011	−6.166
4700	20.807	222.663	202.966	92.577	878.751	535.732	−5.954
4800	20.808	223.101	203.381	94.658	880.601	528.414	−5.750
4900	20.809	223.530	203.788	96.738	882.450	521.058	−5.555
5000	20.811	223.951	204.187	98.819	884.300	513.664	−5.366
5100	20.813	224.363	204.578	100.901	886.151	506.233	−5.185
5200	20.816	224.767	204.963	102.982	888.002	498.765	−5.010
5300	20.819	225.163	205.340	105.064	889.854	491.262	−4.842
5400	20.822	225.553	205.711	107.146	891.706	483.724	−4.679
5500	20.827	225.935	206.075	109.228	893.559	476.152	−4.522
5600	20.832	226.310	206.433	111.311	895.412	468.546	−4.370
5700	20.838	226.679	206.785	113.395	897.265	460.907	−4.224
5800	20.845	227.041	207.131	115.479	899.117	453.236	−4.082
5900	20.852	227.398	207.472	117.564	900.969	445.532	−3.944
6000	20.861	227.748	207.807	119.649	902.822	437.797	−3.811

PREVIOUS. December 1971 (1 atm) CURRENT: March 1983 (1 bar)

EA(Si, g) = 1.385 ± 0.005 eV
$S°(298.15\ K) = 161.977 \pm 0.001\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 312.04 \pm 3\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = [308.819]\ kJ·mol^{-1}$

Electonic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^4S_3$	0	4
^2D	6952	10
^2P	10937	6

Enthalpy of Formation

$\Delta_f H°(Si^-, g, 0\ K)$ is calculated from $\Delta_f H°(Si, g, 0\ K)$[1] using the adopted electron affinity of EA(Si) = 1.385 ± 0.005 eV (133.631 ± 0.482 $kJ·mol^{-1}$). This value, recommended by Hotop and Lineberger,[2] is based on a laser photodetachment electron spectrometry study.[3] Additional information on $Si^-(g)$ may be obtained in the critical discussions of Hotop and Lineberger,[2,4] Rosenstock *et al.*[5] and Massey.[6]

$\Delta_f H°(Si^-, g, 298.15\ K)$ is obtained from $\Delta_f H°(Si, g, 0\ K)$ by using EA(Si) with JANAF[1] enthalpies, $H°(0\ K)–H°(298.15\ K)$, for $Si^-(g)$, Si(g), and e^-(ref) $\Delta_r H°(Si^- \rightarrow Si + e^-, 298.15\ K)$ differs from a room–temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[5] $\Delta_f H°(298.15\ K)$ should be changed by + 6.197 $kJ·mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

Electronic energy levels are from the laser photodetachment electron spectrometry study of Kasdan *et al.*[3] These workers found that the $Si^-(^2D)$ and $Si^-(^2P)$ states have binding energies of 0.523 ± 0.005 eV and 0.029 ± 0.005 eV, respectively, relative to ground state $Si(^3P_0)$. The electronic energies of 6952 cm^{-1} and 10937 cm^{-1} are the difference in binding energy between ground and excited states. We neglect the spin–orbit splitting of the ^2D and ^2P states; its effect is negligible.

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

	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.197	312.037		
100	20.786	139.270	180.457	−4.119			
200	20.786	153.678	163.878	−2.040			
250	20.786	158.316	162.319	−1.001			
298.15	20.786	161.977	161.977	0.	308.819	272.391	−47.722
300	20.786	162.106	161.977	0.038	308.782	272.165	−47.388
350	20.786	165.310	162.231	1.078	307.747	266.143	−39.720
400	20.786	168.085	162.793	2.117	306.660	260.274	−33.988
450	20.786	170.534	163.520	3.156	305.536	254.543	−29.547
500	20.786	172.724	164.332	4.196	304.382	248.938	−26.006
600	20.786	176.513	166.056	6.274	302.006	238.071	−20.726
700	20.787	179.718	167.785	8.353	299.558	227.608	−16.984
800	20.791	182.494	169.454	10.432	297.050	217.500	−14.201
900	20.803	184.943	171.041	12.511	294.489	207.709	−12.055
1000	20.831	187.136	172.543	14.593	291.881	198.207	−10.353
1100	20.887	189.124	173.961	16.678	289.232	188.967	−8.973
1200	20.981	190.945	175.302	18.771	286.547	179.971	−7.834
1300	21.122	192.629	176.571	20.876	283.833	171.199	−6.879
1400	21.318	194.202	177.775	22.998	281.094	162.638	−6.068
1500	21.572	195.681	178.920	25.142	278.335	154.273	−5.372
1600	21.884	197.082	180.011	27.314	275.562	146.092	−4.769
1700	22.253	198.420	181.055	29.520	222.605	138.532	−4.257
1800	22.674	199.704	182.056	31.766	220.053	133.661	−3.879
1900	23.140	200.942	183.017	34.057	217.545	128.930	−3.545
2000	23.645	202.141	183.944	36.396	215.086	124.329	−3.247
2100	24.179	203.308	184.838	38.787	212.679	119.851	−2.981
2200	24.735	204.445	185.704	41.232	210.326	115.486	−2.742
2300	25.303	205.558	186.543	43.734	208.030	111.227	−2.526
2400	25.876	206.646	187.358	46.293	205.790	107.066	−2.330
2500	26.444	207.714	188.151	48.909	203.608	102.998	−2.152
2600	27.002	208.762	188.923	51.581	201.483	99.015	−1.989
2700	27.542	209.792	189.677	54.309	199.412	95.114	−1.840
2800	28.058	210.803	190.414	57.089	197.394	91.288	−1.703
2900	28.548	211.796	191.134	59.920	195.426	87.533	−1.577
3000	29.005	212.772	191.839	62.797	193.506	83.846	−1.460
3100	29.428	213.730	192.530	65.719	191.629	80.222	−1.352
3200	29.815	214.670	193.207	68.682	189.794	76.657	−1.251
3300	30.164	215.593	193.871	71.681	187.995	73.150	−1.158
3400	30.475	216.498	194.524	74.714	186.229	69.696	−1.071
3500	30.748	217.386	195.164	77.775	184.492	66.294	−0.989
3600	30.982	218.255	195.794	80.862	−201.371	73.402	−1.065
3700	31.180	219.107	196.412	83.970	−202.647	81.052	−1.144
3800	31.343	219.941	197.020	87.097	−203.906	88.736	−1.220
3900	31.472	220.757	197.619	90.238	−205.153	96.454	−1.292
4000	31.568	221.555	198.207	93.390	−206.389	104.203	−1.361
4100	31.635	222.335	198.786	96.550	−207.617	111.983	−1.427
4200	31.674	223.098	199.356	99.716	−208.841	119.793	−1.490
4300	31.687	223.843	199.917	102.884	−210.063	127.632	−1.550
4400	31.676	224.572	200.469	106.053	−211.284	135.500	−1.609
4500	31.643	225.283	201.012	109.219	−212.508	143.395	−1.664
4600	31.591	225.978	201.548	112.381	−213.736	151.317	−1.718
4700	31.521	226.657	202.075	115.536	−214.969	159.267	−1.770
4800	31.435	227.320	202.594	118.684	−216.210	167.242	−1.820
4900	31.336	227.967	203.105	121.823	−217.460	175.244	−1.868
5000	31.224	228.599	203.609	124.951	−218.720	183.271	−1.915
5100	31.101	229.216	204.105	128.067	−219.991	191.323	−1.960
5200	30.969	229.819	204.593	131.171	−221.275	199.401	−2.003
5300	30.829	230.407	205.075	134.261	−222.572	207.503	−2.045
5400	30.683	230.982	205.549	137.337	−223.884	215.630	−2.086
5500	30.531	231.544	206.017	140.397	−225.209	223.781	−2.125
5600	30.374	232.092	206.478	143.443	−226.552	231.957	−2.164
5700	30.214	232.629	206.932	146.472	−227.910	240.156	−2.201
5800	30.051	233.153	207.379	149.485	−229.286	248.380	−2.237
5900	29.886	233.665	207.821	152.482	−230.679	256.627	−2.272
6000	29.720	234.166	208.255	155.463	−232.089	264.899	−2.306

PREVIOUS: CURRENT: March 1983 (1 bar)

Silicon (Si_2) IDEAL GAS $M_r = 56.1710$ Silicon (Si_2) $Si_2(g)$

$S°(298.15\ K) = 229.79\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 587.1 \pm 13\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 589.9 \pm 13\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i	State	ϵ_i, cm^{-1}	g_i	State	ϵ_i, cm^{-1}	g_i
$^3\Sigma_g^-$	0	3	$[^1\Delta_g]$	[10000]	[2]	$^3\Pi_g$	[30000]	6
$^3\Pi_u$	[2000]	6	$[^1\Sigma_g^+]$	[13000]	[1]	$^3\Sigma_u^-$	30769	3
$[^1\Sigma_g^+]$	[6000]	[1]	$[^3\Sigma_u^+]$	[20000]	[3]	$[^1\Pi_g]$	[40000]	[2]
$[^1\Pi_u]$	[8000]	[2]	$^3\Sigma_u^-$	24583	3	$[^1\Sigma_u^+]$	[45000]	[1]
						$^3\Sigma_u^-$	46762	3

$\omega_e = 510.98\ cm^{-1}$ $\omega_e x_e = 2.02\ cm^{-1}$ $\sigma = 2$
$B_e = 0.2390\ cm^{-1}$ $\alpha_e = 0.0013\ cm^{-1}$ $r_e = 2.246$ Å

Enthalpy of Formation

The selected value is based on the spectroscopic and equilibrium data summarized below. Verma and Warsop[1] concluded from analysis of the absorption spectra that $D_0° = 70 \pm 4$ kcal·mol^{-1}. Predissociation of the H state suggested the upper limit $D_0° \leq 74.0$, while linear Birgen–Sponer extrapolations of the H and K states gave 78.4 and 68.9 kcal·mol^{-1} for the ground state. By assuming that the true extrapolation would not reduce the linear extrapolation for the H state by more than half, i.e. from 26 to 13 kcal·mol^{-1}, the authors arrived at the lower limit of $D_0° \geq 65.5$ for the ground state.

Drowart and co-workers have used the Knudsen effusion–mass spectrometric technique to determine the vapor equilibria over the systems SiC–graphite,[2] SiC–silicon[3] and boron–carbon–silicon.[4] Third law analysis of the partial pressures of Si_2 and Si over the three systems yields $D_0°$ values of 73.3, 74.3 and 70.4 kcal·mol^{-1}, which are in good agreement with the spectroscopic values. The selected value, $\Delta_f H°(298.15\ K) = 141 \pm 3$ kcal·mol^{-1}, corresponds to $D_0° = 73.0$ kcal·mol^{-1}.

Source	Method	T/K	Data Points	$\Delta_f H°(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°(298.15\ K)$ kcal·mol^{-1}
1	Prediss. of H state		–	≤75.4		–	≥140.0
	LEX of K state		–	70.3			145.1
	Extrap. of H state		–	≥66.9			≤148.5
2	Mass spec.	2149–2316	7	95.3 ± 7.1	74.68	−9 ± 3	140.7
3	Mass spec.	1703–2160	9	81.0 ± 1.1	75.71	−2.7 ± 0.6	139.7
4	Mass spec.	2166–2344	4	68.0 ± 16	71.76	2 ± 7	143.6

*For the reaction $Si_2(g) = 2\ Si(g)$

Heat Capacity and Entropy

Vibrational and rotational constants are those obtained by Verma and Warsop[1] through combination of their data for the H–X system with those of Douglas.[5] Observation of the same H–X system in matrix isolation by Weltner and McLeod[6] confirms that the lower state is the ground state. Comparison with the isoelectronic molecules C_2, BN, BeO and MgO[7–10] suggest that there are several possible low-lying excited states in Si_2. Tentative estimates for these levels are given above, based on this comparison and on the observed states.[1,5] These estimates are relatively uncertain and probably yield an upper limit for the entropy at temperatures where Si_2 is significant. A probable lower limit may be obtained by increasing the two $^3\Pi$ states by 8000 cm^{-1} and omitting the other estimated levels. This would reduce the entropy by 1.7 cal·K^{-1}·mol^{-1} at 2000 K, corresponding to a change of 3.4 kcal·mol^{-1} in $\Delta_f H°$ values based on equilibrium data.

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K^{-1}·mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−9.263	587.118	587.118	INFINITE
100	29.412	195.317	258.806	−6.349	589.499	570 734	−298.121
200	32.184	216.488	232.879	−3.278	590.212	551.581	−144.058
250	33.463	223.812	230.355	−1.636	590.154	541.924	−113.229
298.15	34.452	229.793	229.793	0.	589.944	532.653	−93.319
300	34.487	230.007	229.794	0.064	589.934	532.298	−92.681
350	35.374	235.390	230.217	1.811	589.611	522.716	−78.011
400	36.227	240.170	231.168	3.601	589.228	513.185	−67.015
450	37.096	244.487	232.412	5.434	588.812	503.705	−58.469
500	37.986	248.441	233.820	7.311	588.382	494.272	−51.636
600	39.743	255.524	236.860	11.198	587.517	475.531	−41.399
700	41.286	261.770	239.981	15.252	586.675	456.933	−34.097
800	42.472	267.365	243.061	19.443	585.848	438.455	−28.628
900	43.274	272.417	246.046	23.734	585.015	420.081	−24.381
1000	43.738	277.003	248.916	28.087	584.146	401.801	−20.988
1100	43.941	281.183	251.663	32.472	583.220	383.611	−18.216
1200	43.963	285.008	254.284	36.869	582.219	365.508	−15.910
1300	43.869	288.524	256.785	41.261	581.130	347.493	−13.962
1400	43.709	291.769	259.169	45.640	579.945	329.564	−12.296
1500	43.520	294.779	261.444	50.002	578.658	311.724	−10.855
1600	43.324	297.581	263.616	54.344	577.268	293.974	−9.597
1700	43.135	300.202	265.692	58.667	475.421	277.207	−8.518
1800	42.962	302.662	267.678	62.972	474.287	265.579	−7.707
1900	42.810	304.981	269.581	67.260	473.136	254.016	−6.983
2000	42.679	307.174	271.406	71.534	471.971	242.513	−6.334
2100	42.569	309.253	273.160	75.797	470.794	231.069	−5.748
2200	42.479	311.231	274.846	80.049	469.607	219.682	−5.216
2300	42.407	313.118	276.469	84.293	468.412	208.348	−4.732
2400	42.352	314.922	278.034	88.531	467.210	197.067	−4.289
2500	42.311	316.650	279.544	92.764	466.004	185.836	−3.883
2600	42.282	318.308	281.003	96.993	464.795	174.653	−3.509
2700	42.264	319.904	282.415	101.221	463.583	163.517	−3.163
2800	42.255	321.441	283.781	105.446	462.369	152.425	−2.844
2900	42.254	322.923	285.106	109.672	461.155	141.377	−2.546
3000	42.259	324.356	286.390	113.897	459.942	130.371	−2.270
3100	42.271	325.742	287.637	118.124	458.729	119.405	−2.012
3200	42.287	327.084	288.849	122.352	457.518	108.479	−1.771
3300	42.307	328.386	290.028	126.581	456.308	97.590	−1.545
3400	42.331	329.649	291.174	130.813	455.101	86.738	−1.333
3500	42.358	330.876	292.291	135.048	453.896	75.921	−1.133
3600	42.388	332.070	293.380	139.285	−315.609	86.060	−1.249
3700	42.420	333.232	294.441	143.525	−315.980	97.223	−1.373
3800	42.455	334.364	295.477	147.769	−316.351	108.396	−1.490
3900	42.492	335.467	296.488	152.016	−316.721	119.578	−1.602
4000	42.531	336.543	297.476	156.267	−317.090	130.770	−1.708
4100	42.571	337.594	298.442	160.523	−317.456	141.971	−1.809
4200	42.614	338.620	299.386	164.782	−317.819	153.181	−1.905
4300	42.658	339.623	300.311	169.045	−318.177	164.399	−1.997
4400	42.704	340.605	301.215	173.313	−318.532	175.626	−2.085
4500	42.751	341.565	302.101	177.586	−318.881	186.861	−2.169
4600	42.800	342.505	302.969	181.864	−319.226	198.103	−2.250
4700	42.850	343.426	303.820	186.146	−319.565	209.353	−2.327
4800	42.902	344.329	304.655	190.434	−319.897	220.610	−2.401
4900	42.955	345.214	305.474	194.726	−320.224	231.874	−2.472
5000	43.010	346.082	306.277	199.025	−320.545	243.145	−2.540
5100	43.066	346.934	307.066	203.328	−320.859	254.422	−2.606
5200	43.123	347.771	307.841	207.638	−321.167	265.705	−2.669
5300	43.181	348.593	308.602	211.953	−321.469	276.994	−2.730
5400	43.241	349.401	309.350	216.274	−321.765	288.288	−2.789
5500	43.302	350.195	310.086	220.601	−322.054	299.588	−2.845
5600	43.364	350.976	310.809	224.935	−322.338	310.893	−2.900
5700	43.427	351.744	311.520	229.274	−322.618	322.204	−2.953
5800	43.492	352.500	312.220	233.620	−322.892	333.519	−3.004
5900	43.557	353.244	312.909	237.973	−323.162	344.838	−3.053
6000	43.623	353.976	313.588	242.332	−323.427	356.163	−3.101

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

$S°(298.15\ K) = 267.90\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 632.7 \pm 42\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 636.0 \pm 42\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^3\Sigma_g^-$	0	3
$^3\Pi_u$	[10000]	[6]
$^1\Pi_u$	[18000]	[2]
$^3\Sigma^1$	21460	3

Vibrational Frequencies and Degeneracies
ν, cm^{-1}
[360](1)
[200](2)
[630](1)

Point Group: [$D_{\infty h}$] σ = [2]
Bond Distance: [2.25] Å
Bond Angle: [180]°
Rotational Constant: B_0 = [0.059282] cm^{-1}

Enthalpy of Formation

The selected value is an average based on the equilibrium data summarized below. Drowart *et al.* have used the Knudsen effusion–mass spectrometric technique to determine the vapor species over the systems SiC–graphite[1] and SiC–silicon.[2] Third law analysis of the partial pressures of Si_3 and Si yields the values 154.0 and 149.9 $kcal·mol^{-1}$. Both drifts suggest that the entropy may be lower than the tabulated values. It is unlikely that the entropy is in error by more than 5 $cal·K^{-1}·mol^{-1}$ so that most of the drift is inherent in the data. The adopted value of $\Delta_f H°(298.15\ K) = 152 \pm 10\ kcal·mol^{-1}$ includes allowance for an error of up to 5 $cal·K^{-1}·mol^{-1}$.

Source	Method	T/K	Data Points	$\Delta_r H°(298.15\ K)$, $kcal·mol^{-1}$* 2nd law	3rd law	$cal·K^{-1}·mol^{-1}$ Drift	$\Delta_f H°(298.15\ K)$ $kcal·mol^{-1}$
1	Mass Spec.	2230–2316	2	209	169.1	−18	154.0
2	Mass Spec.	1703–1890	4	204 ± 3	173.2	−17 ± 2	149.9

*For reaction $Si_3(g) = 3\ Si(g)$

Heat Capacity and Entropy

Weltner and McLeod[3] observed an absorption band near 4660 Å in matrix isolation studies. Their tenative assignment of this band as the $^3\Sigma_u^- \leftarrow {}^3\Sigma_g^-$ transition of Si_3 is adopted here. A $^1\Pi_u$ state is assumed at 18000 cm^{-1}, which is 7000 and 2000 cm^{-1} below the analogous levels[3] for C_3 and C_2Si. Also a $^3\Pi_u$ level is assumed at 10000 cm^{-1}, presumably arising from the same molecular orbital configuration as the $^1\Pi_u$ state. The molecule is assumed to be linear with a bond distance equal to that in Si_2. Vibrational frequencies are estimated from a valence bond calculation using $k_1 = 2.16 \times 10^5$ and $k\sigma/l^2 = 0.11 \times 10^5$ dyn cm^{-1}. The stretching force constant is obtained from Si_2, while the bending force constant is based on C_2Si and the $^1\Pi_u$ excited state[3] of C_3.

References

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[3] W. Weltner, Jr. and D. McLeod, Jr., J. Chem. Phys. 41, 235 (1964); 40, 1305 (1964); 45, 3096 (1966).

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
0	0.	0.	INFINITE	−12.919	632.703	632.703	INFINITE
100	39.149	216.004	312.988	−9.698	635.125	614.674	−321.073
200	49.903	246.896	272.794	−5.180	636.108	593.728	−155.066
250	52.965	258.381	268.794	−2.603	636.134	583.123	−121.837
298.15	55.055	267.898	267.898	0.	635.968	572.927	−100.374
300	55.122	268.239	267.899	0.102	635.959	572.536	−99.687
350	56.664	276.859	268.577	2.899	635.651	561.989	−83.872
400	57.787	284.502	270.099	5.761	635.254	551.492	−72.017
450	58.621	291.359	272.087	8.673	634.792	541.048	−62.803
500	59.255	297.570	274.329	11.620	634.279	530.660	−55.438
600	60.129	308.457	279.135	17.593	633.123	510.042	−44.403
700	60.686	317.770	284.005	23.636	631.823	489.629	−36.537
800	61.060	325.900	288.745	29.724	630.384	469.412	−30.649
900	61.323	333.108	293.281	35.844	628.818	449.383	−26.082
1000	61.516	339.579	297.593	41.986	627.128	429.536	−22.437
1100	61.663	345.450	301.681	48.146	625.319	409.863	−19.463
1200	61.781	350.820	305.555	54.318	623.395	390.360	−16.992
1300	61.884	355.769	309.230	60.501	621.357	371.022	−14.908
1400	61.981	360.359	312.720	66.695	619.203	351.846	−13.128
1500	62.081	364.639	316.040	72.898	616.934	332.827	−11.590
1600	62.190	368.649	319.204	79.111	614.549	313.964	−10.250
1700	62.312	372.423	322.225	85.336	461.519	296.594	−9.113
1800	62.451	375.988	325.114	91.574	459.598	286.948	−8.327
1900	62.610	379.369	327.881	97.827	457.692	277.408	−7.626
2000	62.789	382.585	330.536	104.097	455.803	267.969	−6.999
2100	62.989	385.653	333.089	110.385	453.933	258.623	−6.433
2200	63.208	388.588	335.545	116.695	452.084	249.366	−5.921
2300	63.445	391.403	337.913	123.028	450.258	240.192	−5.455
2400	63.699	394.109	340.198	129.385	448.456	231.098	−5.030
2500	63.966	396.714	342.407	135.768	446.681	222.078	−4.640
2600	64.244	399.228	344.545	142.178	444.932	213.128	−4.282
2700	64.531	401.658	346.615	148.617	443.212	204.246	−3.951
2800	64.824	404.011	348.623	155.085	441.521	195.426	−3.646
2900	65.121	406.291	350.573	161.582	439.860	186.666	−3.362
3000	65.420	408.503	352.467	168.109	438.228	177.963	−3.099
3100	65.718	410.653	354.309	174.666	436.626	169.314	−2.853
3200	66.013	412.744	356.103	181.252	435 054	160.717	−2.623
3300	66.304	414.780	357.850	187.868	433.511	152.168	−2.409
3400	66.589	416.764	359.554	194.513	431.997	143.665	−2.207
3500	66.867	418.698	361.216	201.186	430.511	135.206	−2.018
3600	67.136	420.586	362.839	207.886	−723.403	158.172	−2.295
3700	67.396	422.429	364.425	214.613	−723.593	182.663	−2.579
3800	67.646	424.229	365.975	221.365	−723.763	207.158	−2.848
3900	67.886	425.990	367.492	228.142	−723.913	231.658	−3.103
4000	68.114	427.711	368.976	234.942	−724.042	256.162	−3.345
4100	68.330	429.396	370.429	241.764	−724.151	280.668	−3.576
4200	68.535	431.045	371.853	248.607	−724.241	305.177	−3.795
4300	68.727	432.660	373.248	255.471	−724.312	329.688	−4.005
4400	68.908	434.242	374.616	262.353	−724.363	354.200	−4.205
4500	69.077	435.792	375.959	269.252	−724.398	378.713	−4.396
4600	69.233	437.312	377.276	276.167	−724.415	403.227	−4.579
4700	69.379	438.803	378.569	283.098	−724.416	427.741	−4.754
4800	69.512	440.265	379.839	290.043	−724 402	452.255	−4.922
4900	69.635	441.699	381.087	297.000	−724.374	476.769	−5.082
5000	69.747	443.107	382.314	303.969	−724.333	501.281	−5.237
5100	69.848	444.490	383.519	310.949	−724.280	525.793	−5.385
5200	69.939	445.847	384.705	317.939	−724.217	550.304	−5.528
5300	70.020	447.180	385.871	324.937	−724.145	574.813	−5.665
5400	70.091	448.489	387.018	331.942	−724.065	599.321	−5.797
5500	70.154	449.776	388.148	338.955	−723 976	623.827	−5.925
5600	70.208	451.041	389.260	345.973	−723.885	648.332	−6.047
5700	70.254	452.284	390.354	352.996	−723.790	672.835	−6.166
5800	70.291	453.506	391.433	360.023	−723.693	697.336	−6.280
5900	70.322	454.708	392.495	367.054	−723.596	721.836	−6.391
6000	70.345	455.890	393.542	374.087	−723.498	746.334	−6.497

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

REFERENCE STATE

0	to 820	K	crystal, alpha
820	to 1050	K	crystal, beta
1050	to 1685.492	K	liquid
above	1685.492	K	ideal monatomic gas

Refer to the individual tables for details.

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

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−6.568	0.	0.	0.
100	23.481	28.050	78.738	−5.069	0.	0.	0.
200	25.757	45.209	58.112	−2.581	0.	0.	0.
298.15	26.791	55.694	55.694	0.	0.	0.	0.
300	26.809	55.859	55.694	0.050	0.	0.	0.
400	27.777	63.704	56.757	2.779	0.	0.	0.
500	28.785	70.010	58.797	5.607	0.	0.	0.
600	29.814	75.349	61.122	8.536	0.	0.	0.
700	30.864	80.023	63.495	11.570	0.	0.	0.
800	31.935	84.214	65.827	14.710	0.	0.	0.
820.000	32.151	85.005	66.285	15.351	ALPHA <--> BETA TRANSITION		
820.000	29.790	86.026	66.285	16.188			
900	30.125	88.814	68.165	18.584	0.	0.	0.
1000	30.543	92.010	70.393	21.618	0.	0.	0.
1050.000	30.752	93.505	71.458	23.150	BETA <--> LIQUID TRANSITION		
1050.000	39.463	100.582	71.458	30.581			
1100	39.463	102.418	72.824	32.554	0.	0.	0.
1200	39.463	105.852	75.435	36.500	0.	0.	0.
1300	39.463	109.010	77.898	40.446	0.	0.	0.
1400	39.463	111.935	80.226	44.393	0.	0.	0.
1500	39.463	114.658	82.432	48.339	0.	0.	0.
1600	39.463	117.204	84.526	52.285	0.	0.	0.
1685.492	39.463	119.259	86.236	55.659	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
1685.492	20.834	200.650	86.236	192.844			
1700	20.839	200.829	87.214	193.146	0.	0.	0.
1800	20.882	202.021	93.559	195.232	0.	0.	0.
1900	20.949	203.152	99.297	197.323	0.	0.	0.
2000	21.049	204.229	104.517	199.423	0.	0.	0.
2100	21.191	205.259	109.290	201.534	0.	0.	0.
2200	21.383	206.249	113.675	203.662	0.	0.	0.
2300	21.636	207.205	117.721	205.813	0.	0.	0.
2400	21.959	208.132	121.469	207.992	0.	0.	0.
2500	22.361	209.036	124.953	210.207	0.	0.	0.
2600	22.849	209.923	128.204	212.467	0.	0.	0.
2700	23.430	210.796	131.247	214.780	0.	0.	0.
2800	24.109	211.660	134.104	217.157	0.	0.	0.
2900	24.889	212.519	136.793	219.606	0.	0.	0.
3000	25.770	213.377	139.331	222.138	0.	0.	0.
3100	26.753	214.238	141.734	224.763	0.	0.	0.
3200	27.834	215.104	144.013	227.492	0.	0.	0.
3300	29.008	215.978	146.181	230.333	0.	0.	0.
3400	30.270	216.863	148.246	233.296	0.	0.	0.
3500	31.611	217.759	150.220	236.389	0.	0.	0.
3600	33.022	218.670	152.108	239.620	0.	0.	0.
3700	34.493	219.594	153.920	242.995	0.	0.	0.
3800	36.011	220.534	155.660	246.520	0.	0.	0.
3900	37.565	221.490	157.336	250.199	0.	0.	0.
4000	39.142	222.461	158.952	254.034	0.	0.	0.
4100	40.730	223.447	160.513	258.027	0.	0.	0.
4200	42.304	224.446	162.023	262.176	0.	0.	0.
4300	43.874	225.460	163.487	266.485	0.	0.	0.
4400	45.418	226.486	164.907	270.950	0.	0.	0.
4500	46.927	227.524	166.287	275.568	0.	0.	0.
4600	48.214	228.556	167.628	280.269	0.	0.	0.
4700	49.584	229.608	168.936	285.159	0.	0.	0.
4800	50.884	230.665	170.211	290.182	0.	0.	0.
4900	52.114	231.727	171.455	295.332	0.	0.	0.
5000	53.254	232.791	172.671	300.596	0.	0.	0.
5200	55.250	234.914	175.024	311.429	0.	0.	0.
5400	56.945	237.032	177.282	322.655	0.	0.	0.
5600	58.296	239.129	179.453	334.184	0.	0.	0.
5800	59.317	241.193	181.547	345.951	0.	0.	0.
6000	59.709	243.172	183.564	357.650	0.	0.	0.

PREVIOUS: December 1970 (1 atm) CURRENT: September 1983 (1 bar)