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Calculated molecular parameters (B3LYP\6-311+G(2d,p)) and heats of formation (CBS-Q) of silicon-bearing species.

For comparison, experimental values (where available) are shown in brackets.[12,13,37,41,48]

Species	Geometry [a]	Dipole moment [b]	Rotational constants [c]	Vibrational freqs. [d]	ΔH_f^o(0 K) [e]
SiO ($^1\Sigma^+$)	r(Si-O)=1.515 [1.510]	3.2320 [3.0982]	21.629 [21.787]	1247.4 [1241.6] (σ)	-109.87 [-104.3±0.8 [13]]
SiO_2 ($^1\Sigma^+$)	r(Si-O)=1.512	0	6.912	297.6(×2) [272.5](π_u)	-295.09 [-305±33 [12]]
				991.4 (σ_g)	[-320.72 [41]]
				1437.8 [1416.5] (σ_u)	
SiH ($^2\Pi_J$)	r(Si-H)=1.529 [1.520]	0.1118	222.2 [224.8]	2021.2 [2041.8] (σ)	366.20 [375±8 [12]]
					[366.9 [41]]
SiH_2 ($^1A_1$)	r(Si-H)=1.523 [1.514]	0.1464	238.144	1023.1 [1001.8] (a_1)	264.30 [275±3 [13]]
	∠(H-Si-H)=91.53 [92.0]		210.611	2043.0 [1981.6] (a_1)	
			111.766	2043.5 [1993.4] (b_2)	
SiC ($^*{}^3\Pi_J$) [f]	r(Si-C)=1.717	1.7634	20.417 [18.167]	976.5 [983] (σ)	731.4 [715±33 [12]]
SiOCO (^{3}A)	r(Si-O)=1.706	2.3104	46.878	21.9 [g] (a)	63.30
C_1	r(O-C)=1.325		3.265	173.5 (a)	
	r(C-O)=1.179		3.110	539.0 (a)	
	∠(Si-O-C)=137.70			740.5 (a)	
	∠(O-C-O)=130.62			1045.9 (a)	
	∠(SiOC-O)=-83.69			1855.2 (a)	

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OSiCO (^{3}A")	*r*(O-Si)=1.551	2.7713	38.510	118.0	(a')	54.79
planar C_s	*r*(Si-C)=1.827		3.246	290.8	(a")	
	r(C-O)=1.155		2.993	398.3	(a')	
	∠(O-Si -C)=118.44			567.0	(a')	
	∠(Si-C-O)=170.96			1070.7	(a')	
				2021.8	(a')	
SiOH (^{2}A')	r(Si-O)=1.662	1.4871	793.38952	766.1	(a')	-7.80
C_s	r(O-H)=0.965		16.57278	848.8	(a')	
	∠(Si-O-H)=119.76		16.23369	3809.9	(a')	
HSiO (^{2}A')	r(H-Si)=1.528	3.4073	305.85407	613.1	(a')	19.32
C_s	r(Si-O)=1.532		19.71012	1163.7	(a')	
	∠(H-Si-O)=118.60		18.51684	1910.5	(a')	
HSiOH-*cis* (^{1}A')	*r*(H-Si)=1.543	1.5970	171.885	634.1	(a")	-101.01
planar C_s	*r*(Si-O)=1.665		16.172	742.9	(a')	
	r(O-H)=0.963		14.781	835.9	(a')	
	∠(H-Si-O)=97.73			963.8	(a')	
	∠(Si-O-H)=119.50			1931.1	(a')	
				3841.7	(a')	
HSiOH-*trans* (^{1}A')	*r*(H-Si)= 1.526	1.2157	174.997	673.0	(a")	-101.09
planar C_s	*r*(Si-O)= 1.670		16.159	806.7	(a')	
	r(O-H)= 0.964		14.793	830.7	(a')	
	∠(Hi-Si-O)=94.38			962.5	(a')	
	∠(Si-O-H)=114.85			2013.2	(a')	
				3846.0	(a')	

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HSiOH (^{3}A)	r(H-Si)= 1.497	1.3790	214.505	368.4 (a)	67.65
C_1	r(Si-O)= 1.667		15.339	656.2 (a)	
	r(O-H)= 0.963		14.857	795.2 (a)	
	∠(H-Si-O)=115.43			876.4 (a)	
	∠(Si-O-H)=117.47			2073.6 (a)	
	∠(HSiO-H)=-99.82			3842.0 (a)	
$SiOH_2$ (^{1}A')	r(Si-O)= 2.050	4.7986	395.264	205.6 (b_1)	240.40
planar C_{2v}	r(O-H)= 0.965		10.236	303.3 (a_1)	
	∠(H-O-H)=111.47		9.978	428.2 (b_2)	
				1585.6 (a_1)	
				3762.6 (a_1)	
				3842.6 (b_2)	
$SiOH_2$ (^{3}A)	r(Si-O)= 2.246	3.8737	311.891	239.7 (a')	166.82
C_s	r(O-H)= 0.966		8.768	425.5 (a')	
	∠(Si-O-H)=108.74		8.648	469.6 (a")	
	∠(HOH-Si)=117.09			1623.7 (a')	
				3772.4 (a')	
				3872.3 (a")	
H_2SiO (^{1}A')	r(Si-O)=1.523	3.8195	166.12548	682.4 (b_2)	-104.35
planar C_{2v}	r(Si-H)=1.481		18.533	697. 8 (b_1)	
	∠(H-Si-H)=112.12		16.673	1009.4 (a_1)	
				1219.1 (a_1)	
				2219.7 (a_1)	
				2237.4 (b_2)	

[a] Geometrical parameters: *r* in Å and ∠ in degrees. [b] In Debye (= 3.336 x 10^{-30} Cm). [c] In GHz. [d] In cm^{-1}. The symmetry of the vibration is shown in parenthesis. [e] In kJ mol^{-1}. Evaluated uncertainty = ± 7 kJ mol^{-1}.[40] The heats of formation at 0 K of the corresponding atomic species are: Si(^{3}P), 446±8 kJ mol^{-1}; O(^{3}P), 246.98±0.08 kJ mol^{-1}; H(^{2}S), 216.164±0.004 kJ mol^{-1}; and C(^{3}P), 711.7±0.4 kJ mol^{-1}.[13] [f] The nature of the ground state is uncertain.[49] [g] Hindered rotor.

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