Table S1. Calculated molecular parameters (B3LYP/6-311+G(2d,p)) and heats of formation (CBS-Q) of stationary points on the OH + SiO potential energy surface.[a]

Species	Geometry [b]	Dipole moment [c]	Rotational constants [d]	Vibrational frequencies [e]	ΔH_f^o(0 K) [f]
HOSiO-*cis* (^{2}A')	*r*(H-O)=0.968	2.696	55.69	278 (a')	-324.0
planar C_s	*r*(O-Si)=1.639		7.575	390 (a'')	
	r(Si-O)=1.534		6.668	763 (a')	
	∠(H-O-Si)=117.43^o			864 (a')	
	∠(O-Si-O)=126.79^o			1161 (a')	
				3792 (a')	
TS1 (^{2}A)	*r*(H-O)= 0.964	4.018	63.89	-386 (a)	-311.7
C_1	*r*(O-Si)= 1.640		7.252	299 (a)	
	r(Si-O)= 1.537		6.611	615 (a)	
	∠(H-O-Si)= 124.08^o			829 (a)	
	∠(O-Si-O)= 128.34^o			1178 (a)	
	∠(H-OSiO)= 93.17^o			3853 (a)	
HOSiO-*trans* (^{2}A')	*r*(H-O)= 0.965	4.745	62.09	294 (a')	-323.6
planar C_s	*r*(O-Si)= 1.645		7.412	359 (a'')	
	r(Si-O)= 1.530		6.621	783 (a')	
	∠(H-O-Si)= 118.19^o			824 (a')	
	∠(O-Si-O)= 124.62^o			1178 (a')	
				3842 (a')	

TS2 (^{2}A')	r(H-O)= 1.470	2.234	134.0	-1255 (a')	-134.4
planar C_s	r(O-Si)= 1.590		6.843	299 (a')	
	r(Si-O)= 1.514		6.517	333 (a'')	
	∠(H-O-Si)= 62.76^o			882 (a')	
	∠(H-Si-O)= 153.41^o			1287 (a')	
				1825 (a')	
$HSiO_2$ ($^2B_2$)	r(H-Si)= 1.468	3.352	36.23	307 (a_1)	-174.0
planar C_{2v}	r(Si-O)= 1.565		8.982	546 (b_2)	
	∠(O-Si-O)= 115.81^o		7.198	573 (b_1)	
				912 (b_2)	
				1020 (a_1)	
				2298 (a_1)	
TS3 (^{2}A')	r(H-O)= 1.882	0.315	299.9	-596 (a')	-49.1
planar C_s	r(O-Si)= 1.523		6.175	83 (a')	
	r(Si-O)= 1.513		6.051	293 (a'')	
	∠(H-O-Si)= 137.41^o			298 (a')	
	∠(O-Si-O)= 175.53^o			955 (a')	
				1402 (a')	
HSiOO (^{2}A')	r(H-Si)= 1.518	2.273	90.86	249 (a')	193.0
planar C_s	r(Si-O)= 1.692		5.952	253 (a'')	
	r(O-O)= 1.319		5.586	643 (a')	
	∠(H-Si-O)= 89.63^o			824 (a')	
	∠(Si-O-O)= 133.5^o			1156 (a')	
				2053 (a')	

TS4 (^{2}A')	r(H-Si)= 1.524	2.403	37.85	-357	(a')	200.2
planar C_s	r(Si-O)= 1.675		8.536	602	(a'')	
	r(O-O)= 1.427		6.965	692	(a')	
	∠(H-Si-O)= 91.85^o			798	(a')	
	∠(Si-O-O)= 93.60^o			922	(a')	
				1992	(a')	

[a] The molecular parameters at the B3LYP/6-311+G(2d,p) level of theory and heats of formation at the CBS-Q level of theory for SiO, SiO_2, SiH, SiH_2($^1A_1$) and SiC were benchmarked against experimental data in the ESI of Part I of this series.[1] The accuracy of the *ab initio* results is stated following the convention of the CCCBDB-NIST database.[2] This is also broadly consistent with the accuracy of the experimental data reported for the silicon benchmarking species.[1] [b] Geometrical parameters: r in Å and ∠ in degrees. [c] In Debye (= 3.336 x 10^{-30} Cm). [d] In GHz. [e] In cm^{-1}. The symmetry of the vibration is shown in parenthesis. [f] In kJ mol^{-1}. Evaluated uncertainty = ± 7 kJ mol^{-1}.[3] 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}; and H(^{2}S), 216.164±0.004 kJ mol^{-1} [4]

References:

1 J. C. Gómez Martín, M. A. Blitz and J. M. C. Plane, *Phys. Chem. Chem. Phys.*, 2009, **11**, 671-678.

2 NIST, Computational Chemistry Comparison and Benchmark DataBase Release 14, NIST Standard Reference Database 101, 2006, http://srdata.nist.gov/cccbdb

3 L. A. Curtiss, K. Raghavachari, P. C. Redfern and B. B. Stefanov, *J. Chem. Phys.*, 1998, **108**, 692-697.

4 L. A. Curtiss, K. Raghavachari, P. C. Redfern and J. A. Pople, *J. Chem. Phys.*, 1997, **106**, 1063-1079.

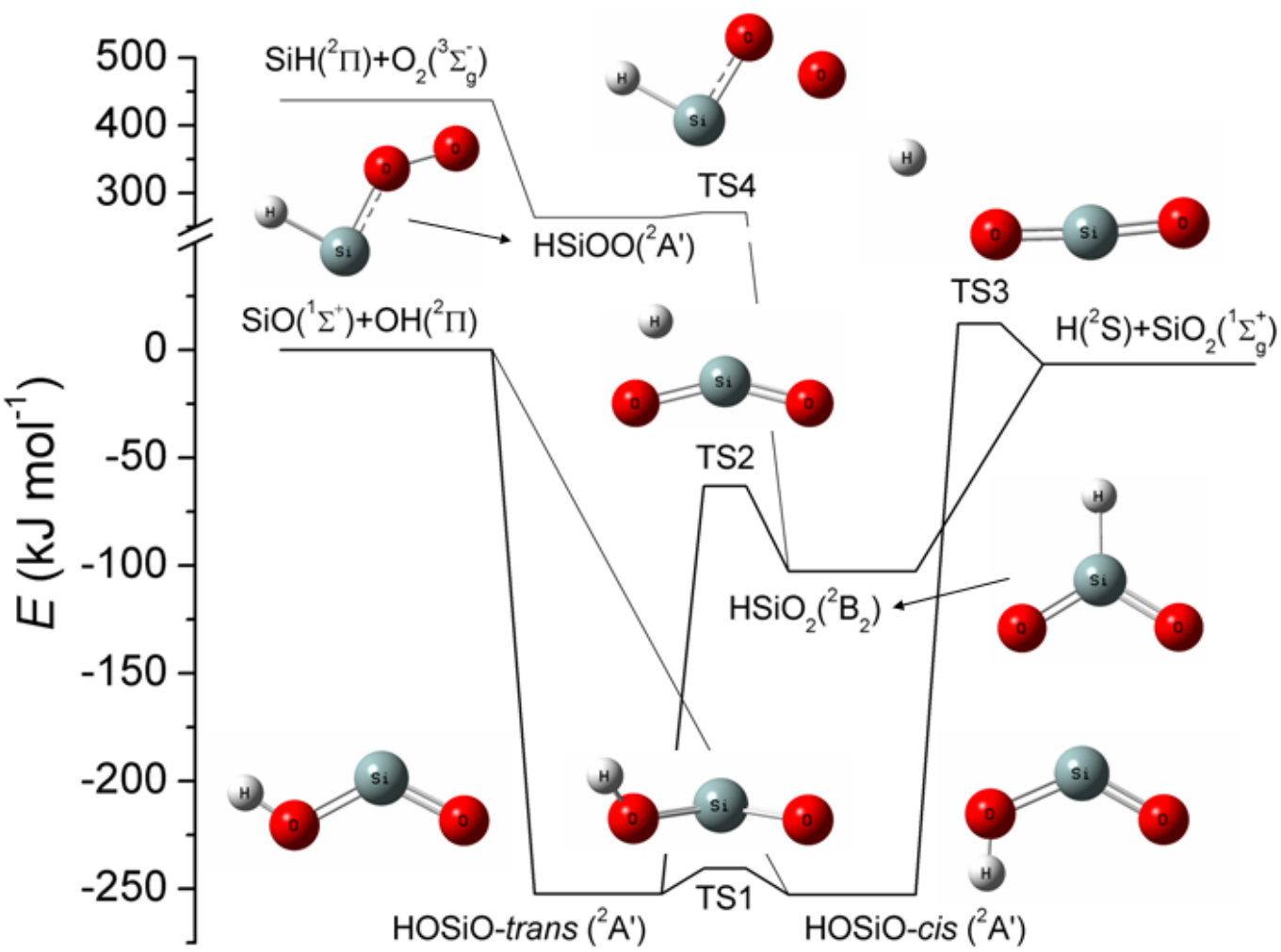

Figure S1. Stationary points on the SiO + OH potential surface, using the data in Table S1.

Table 2. Calculated molecular parameters (B3LYP/6-311+G(2d,p)) and heats of formation (CBS-Q)

for stationary points on the SiO + H_2O potential energy surface

Species	Geometry	Dipole moment	Rotational constants	Vibrational frequencies	ΔH_f^o(0 K) [a]
TS5 (^{1}A)	r(H-O)= 0.967	2.996	19.23	-1358 (a)	-330.8
C_1	r(O-Si)=1.966		10.11	418 (a)	
	r(Si-O)=1.583		6.712	474 (a)	
	r(O-H)= 1.343			692 (a)	
	∠(H-O-Si)= 123.87^o			696 (a)	
	∠(O-Si-O)= 79.43^o			1064 (a)	
	∠(Si-O-H)= 80.16^o			1315 (a)	
	∠(H-OSiO)=-113.1^o			1912 (a)	
				3800 (a)	
$Si(OH)_2$ (^{1}A')	r(H-O)= 0.967	1.826	26.08	321 (a')	-498.3
planar C_s	r(O-Si)=1.652		8.834	443 (a'')	
	r(Si-O)=1.675		6.599	515 (a'')	
	r(O-H)= 0.963			778 (a')	
	∠(H-O-Si)=117.4^o			797 (a')	
	∠(O-Si-O)=126.8^o			832 (a')	
	∠(Si-O-H)=116.9^o			893 (a')	
				3794 (a')	
				3859 (a')	

[a] Units as indicated in the footnote to Table S1.

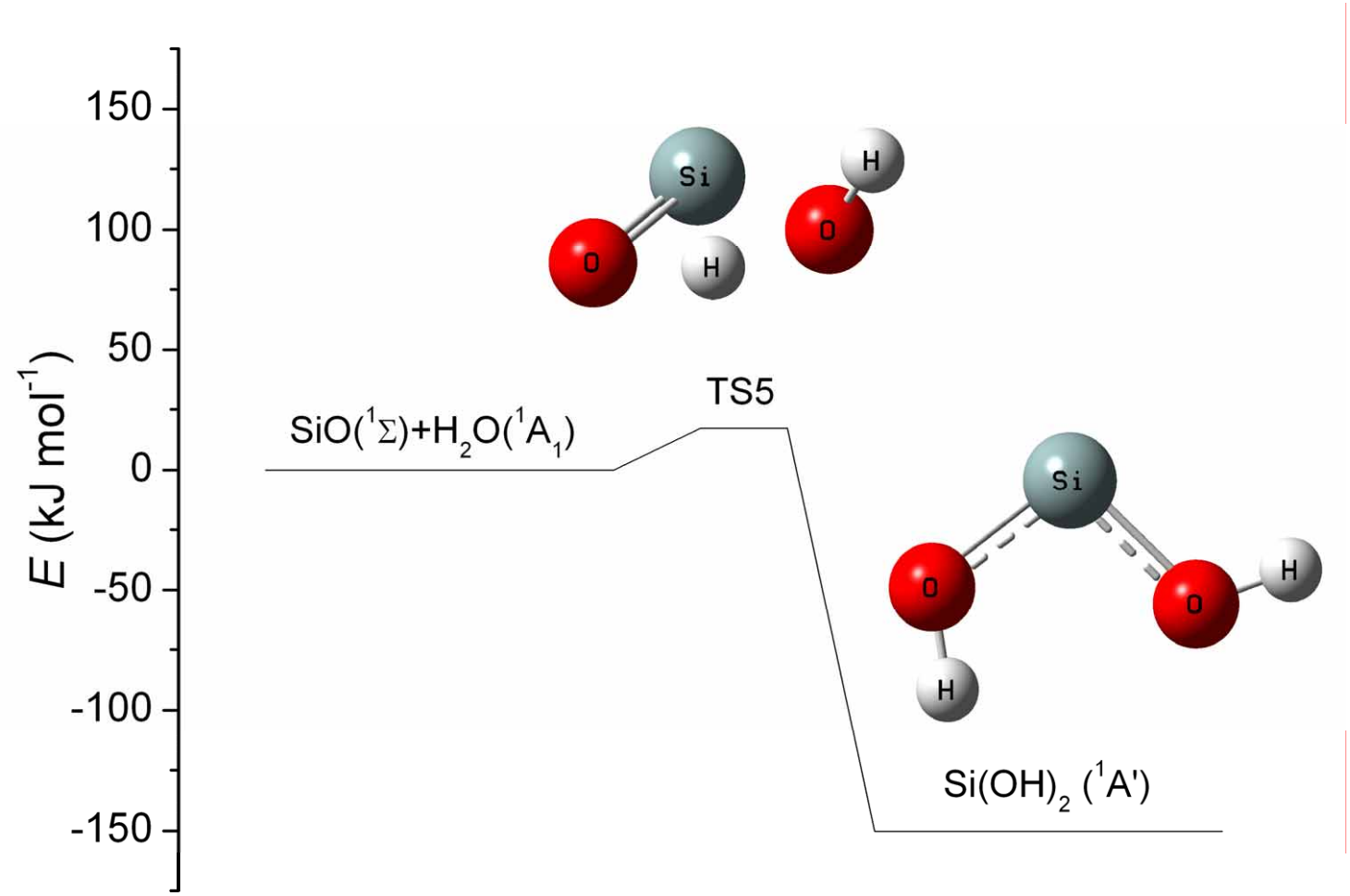

Figure S2. Stationary points on the SiO + H_2O potential surface, using the data in Table S2.

Table S3. Calculated molecular parameters (B3LYP/6-311+G(2d,p)) and heats of formation (CBS-Q) of stationary points on the SiO_2 + O potential energy surface

Species	Geometry	Dipole moment	Rotational constants	Vibrational frequencies	ΔH_f^o(0 K) [a]
TS6 (^{3}A")	r(O-O)= 1.702	1.760	21.960	-773 (a')	57.6
planar C_s	r(O-Si)= 1.591		3.545	111 (a')	
	r(Si-O)= 1.518		3.052	225 (a")	
	∠(O-O-Si)= 118.89^o			324 (a')	
	∠(O-Si-O)= 151.76^o			787 (a')	
				1265 (a')	
TS7 (^{3}A)	r(O-O)= 1.348	2.305	28.769	-160 (a)	-18.8
C_1	r(O-Si)= 1.756		3.788	78 (a)	
	r(Si-O)= 1.529		3.669	252 (a)	
	∠(O-O-Si)= 100.6^o			624 (a)	
	∠(O-Si-O)= 120.8^o			1092 (a)	
	∠(OOSi-O)= 126.1^o			1154 (a)	
TS8 (^{1}A)	r(O-O)= 1.391	2.853	24.568	-317 (a)	-7.1
C_1	r(O-Si)= 1.664		4.074	99 (a)	
	r(Si-O)= 1.519		3.610	165 (a)	
	∠(O-O-Si)= 104.5^o			634 (a)	
	∠(O-Si-O)= 143.1^o			913 (a)	
	∠(OOSi-O)= -70.96^o			1229 (a)	

$OSiO_2$ ($^3B_1$)	r(O-Si)= 1.511	1.556	13.180	258	(a_1)	-201.8
C_{2v}	r(O-Si)= 1.632		6.269	282	(b_2)	
	∠(O-Si-O)= 137.9°		4.249	288	(b_1)	
				843	(a_1)	
				918	(b_2)	
				1301	(a_1)	

[a] Units as indicated in the footnote to Table S1.

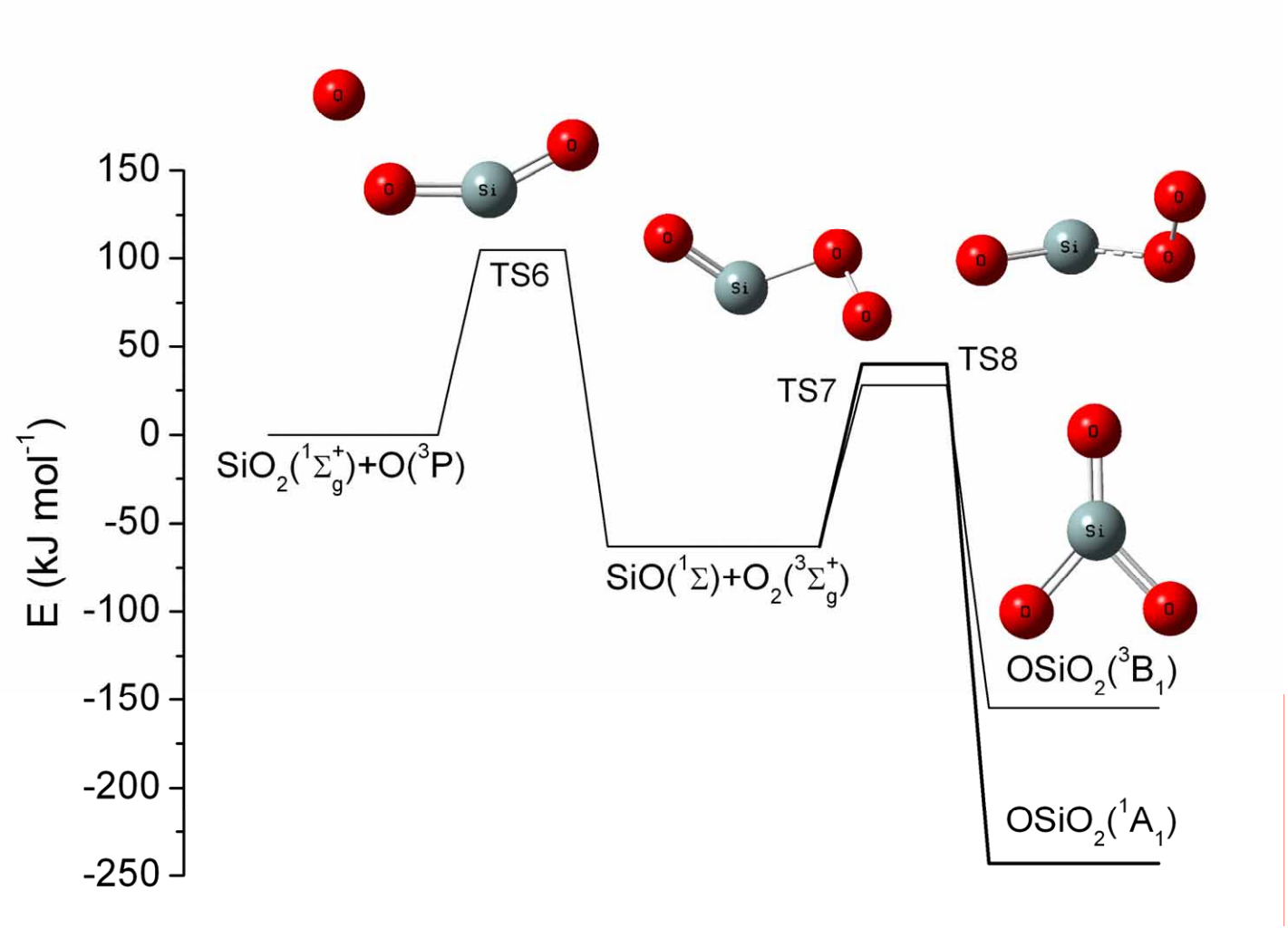

Figure S4. Stationary points on the SiO_2 + O potential surface, using the data in Table S3.

Supplementary Material (ESI) for *PCCP*