

Table S1. Calculated absolute energies at B3LYP/6-31G(d) and at MP4/6-31+G(d,p)//B3LYP/6-31G(d).^a

cpd.	B3LYP/6-31G(d)	ZPVE	MP4/6-31+G(d,p)
H ₂ C=CH ₂	-78.58745734	32.14043	-78.35933431
H ₂ O	-76.4089532	13.27748	-76.24454488
H ₂ C=CH ₂ TS	-154.9194559	45.25288	-154.513700
H ₂ C=CH ₂ Product (EtOH)	-155.0338045	50.38905	-154.628503
H ₂ C=C(CN) ₂	-263.0626863	31.25364	-262.3934121
H ₂ C=C(CN) ₂ TS	-339.4119456	45.27471	-338.5647702
H ₂ C=C(CN) ₂ Product	-339.4977606	49.12846	-338.6562257
H ₂ C=C(CN) ₂ TS rev	-339.381536	42.93836	-338.5405325
H ₂ C=C(CN) ₂ Product rev	-339.4960648	48.22206	-338.6565481
1	-329.9417288	25.24786	-329.3260739
1 complex	-406.359855	40.68838	-405.574074
1 TS	-406.353437	39.52434	-405.563031
1 Product	-406.473868	42.55585	-405.683367
MeOH	-115.714404	32.29088	-115.423510
1 + MeOH complex	-445.664239	59.20306	-444.756691
1 + MeOH TS	-445.659281	57.63993	-444.749046
1 + MeOH Product	-445.778218	60.73105	-444.864866
EtOH	-155.033805	50.38905	-154.628503
1 + EtOH complex	-484.983938	77.20005	-483.962141

1 + EtOH TS	-484.978777	75.60805	-483.954793
1 + EtOH Product	-485.092406	78.4444	-484.065328
t-BuOH	-233.670956	85.44113	-233.042384
1 + t-BuOH complex	-563.619155	111.5989	-562.376634
1 + t-BuOH TS	-563.612880	110.5158	-562.369130
1 + t-BuOH Product	-563.725383	115.4957	-562.477261
2	-990.0080895	82.48117	-988.163697
2 complex	-1066.433450	98.21975	-1064.420086
2 TS	-1066.4291241	96.20858	-1064.413485
2 Product	-1066.5245149	98.49083	-1064.512338
3	-1249.231212	17.76418	-1247.49215
3 complex	-1325.657034	33.12814	-1323.748647
3 TS	-1325.655062	31.80597	-1323.743313
3 Product	-1325.7874628	34.65047	-1323.875032
4	-487.2256818	98.18461	-486.152963
4 TS	-563.6297354	111.5129	-562.384916
4 Product	-563.7540007	114.6442	-562.5121152
5	-989.9806772	83.47452	-988.134573
5 TS	-1066.372817	96.3253	-1064.35399
5 Product	-1066.489125	99.84939	-1064.471089
6	-1316.605959	78.61305	-1314.204829
6 TS	-1392.995272	91.47321	-1390.42363

6 Product	-1393.110234	94.58655	-1390.538024
7	-817.2811172	126.69801	-815.5998422
7 TS	-893.6981933	140.48731	-891.844915
7 + MeOH TS	-933.0035195	158.48223	-931.0317012
8	-445.4286316	51.0864	-444.4993983
8 complex	-521.848574	66.1340	-520.750919
8 TS	-521.8435967	64.90638	-520.7418151
8 + MeOH TS	-561.1488964	82.94954	-559.9287027
9	-777.9503577	109.82591	-776.3822813
9 TS	-854.3588904	123.31159	-852.6182809
9 + MeOH TS	-893.6637404	141.32375	-891.8045178

^a Complex, TS and product are for reaction with water, if not stated otherwise.

Table S2. Absolute energies (Hartrees) of **1**, H₂O, complex **I**, TS **II**, and product **III** calculated at different levels of theory.

Level of theory	1	H ₂ O	complex I	TS II	product III
HF/6-31G(d)//HF/6-31G(d)	-329.0372581	-76.0107465	-405.053049	-405.032086	-405.181069
B3LYP/6-31G(d)//B3LYP/6-31G(d)	-329.9417288	-76.4089532	-406.359855	-406.353437	-406.473868
B3LYP/6-31G(d)//B3LYP/6-31G(d) ΔG^{298}	-329.925393	-76.405461	-406.325071	-406.317060	-406.433391
B3LYP/6-31+G(d)//B3LYP/6-31+G(d)	-329.9462483	-76.422572	-406.373807	-406.365799	-406.484495
B3LYP/6-311G(d)//B3LYP/6-311G(d)	-329.9756846	-76.433933	-406.420427	-406.413353	-406.532053
B3LYP/6-311++G(d,p)//B3LYP/6-311++G(d,p)	-329.9842378	-76.458531	-406.447197	-406.437211	-406.551326
MP4/6-31+G(d,p)//B3LYP/6-31G(d)	-329.3260739	-76.24454488	-405.574074	-405.563031	-405.683367
MP2/6-31G(d)//MP2/6-31G(d)	-329.2506049	-76.1968478	-405.455206	-405.446066	-405.572646
MP2/6-31+G(d)//MP2/6-31+G(d)	-329.2558442	-76.2097766	-405.471980	-405.462512	-405.585300
MP2/6-311G(d)//MP2/6-311G(d)	-329.2901041	-76.2349518	-405.535029	-405.526893	-405.650323
MP2/6-311++G(d,p)//MP2/6-311++G(d,p)	-329.3283368	-76.2749202	-405.609389	-405.599932	-405.716057
MP2/cc-pVTZ//MP2/cc-pVTZ	-329.3826778	-76.3186577	-405.7093441	-405.7056566	
MP2/cc-pVTZ//MP2/cc-pVTZ ΔG^{298}	-329.365432	-76.315336	-405.673264	-405.66833	

6

MP4/6-311++G(d,p)//MP2/6-311++G(d,p)	-329.3743724	-76.2872516	-405.661624	-405.649151	-405.766029
QCISD(T)/6-311++G(d,p)//MP2/6-311++G(d,p)	-329.3764934	-76.2868416	-405.663335	-405.649801	-405.766592
CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p)	-329.3762034	-76.2866116	-405.662815	-405.649214	-405.766132
G2 ΔE^{298}	-329.408917	-76.329222	-405.739156	-405.734962	
G2 ΔG^{298}	-329.435799	-76.349654	-405.777684	-405.766500	
CBS-Q ΔE^{298}	-329.407443	-76.333643	-405.742059	-405.739938	
CBS-Q ΔG^{298}	-329.434266	-76.354052	-405.779348	-405.771476	
PCM/B3LYP/6-31G(d) Toluene	-329.9507523	-76.41148843	-406.3640984	-406.3567593	
PCM/B3LYP/6-31G(d) THF	-329.9610118	-76.41339879	-406.367159	-406.359234	

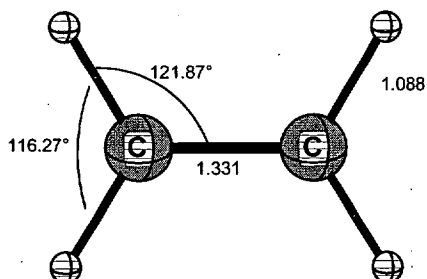
Table S3. Thermochemistry and activation barriers for the addition of water to $\text{H}_2\text{Si}=\text{CH}_2$ (equation 2) at different levels of theory (kcal/mol).^a

Method	Complex I	TS II	Product III
HF/6-31G(d)	-3.17	9.99	-83.50
B3LYP/6-31G(d)//B3LYP/6-31G(d)	-5.76	-1.73	-77.30
B3LYP/6-31+G(d)//B3LYP/6-31+G(d)	-3.13	1.90	-72.59
B3LYP/6-311G(d)//B3LYP/6-311G(d)	-6.78	-2.34	-76.83
B3LYP/6-311++G(d,p)//B3LYP/6-311++G(d,p)	-2.78	3.49	68.12
MP4/6-31G(d)//B3LYP/6-31G(d)	-3.58	5.24	-75.45
MP4/6-31+G(d)//B3LYP/6-31+G(d)	-4.74	3.09	-74.12
MP4/6-311G(d)//B3LYP/6-311G(d)	-4.72	2.03	-75.83
MP4/6-311++G(d,p)//B3LYP/6-311++G(d,p)	-3.22	4.49	-68.92
MP4/6-31+G(d,p)//B3LYP/6-31G(d)	-2.17	4.76	-70.75
QCISD(T)/6-31G(d)//B3LYP/6-31G(d)	-3.52	5.84	-74.58
QCISD(T)/6-31+G(d)//B3LYP/6-31+G(d)	-2.75	5.62	-71.32
QCISD(T)/6-311G(d)//B3LYP/6-311G(d)	-6.20	1.03	-76.75
QCISD(T)/6-311++G(d,p)//B3LYP/6-311++G(d,p)	-2.99	5.37	-68.00
CCSD(T)/6-31G(d)//B3LYP/6-31G(d)	-3.14	6.24	-74.24
CCSD(T)/6-31+G(d)//B3LYP/6-31+G(d)	-2.73	5.68	-71.34
CCSD(T)/6-311G(d)//B3LYP/6-311G(d)	-4.20	3.06	-74.76
CCSD(T)/6-311++G(d,p)//B3LYP/6-311++G(d,p)	-2.97	5.43	-68.02
MP2/6-31G(d)//MP2/6-31G(d)	-4.87	0.87	-78.56
MP2/6-31+G(d)//MP2/6-31+G(d)	-3.99	1.95	-75.10
MP2/6-311G(d)//MP2/6-311G(d)	-6.26	-1.15	-78.61

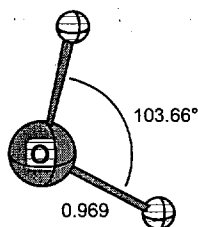
MP2/6-311++G(d,p)//MP2/6-311++G(d,p)	-3.86	2.07	-70.80
MP2/cc-pVTZ//MP2/cc-pVTZ	-5.03	-2.71	
MP4/6-31G(d)//MP2/6-31G(d)	-3.75	4.13	-75.41
MP4/6-31+G(d)//MP2/6-31+G(d)	-3.12	4.89	-73.42
MP4/6-311G(d)//MP2/6-311G(d)	-4.83	2.14	-75.73
MP4/6-311++G(d,p)//MP2/6-311++G(d,p)	-3.36	4.47	-68.87
QCISD(T)/6-31G(d)//MP2/6-31G(d)	-3.37	5.00	-74.14
QCISD(T)/6-31+G(d)//MP2/6-31+G(d)	-2.85	5.76	-71.28
QCISD(T)/6-311G(d)//MP2/6-311G(d)	-4.41	3.09	-74.70
QCISD(T)/6-311++G(d,p)//MP2/6-311++G(d,p)	-3.16	5.33	-67.95
CCSD(T)/6-31G(d)//MP2/6-31G(d)	-3.34	5.07	-74.19
CCSD(T)/6-31+G(d)//MP2/6-31+G(d)	-2.84	5.82	-71.30
CCSD(T)/6-311G(d)//MP2/6-311G(d)	-4.37	3.15	-74.70
CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p)	-3.15	5.39	-67.98
G2 (0K)	-1.18	3.00	
G2 ΔE^{298}	-0.64	1.99	
CBS-Q ΔE^{298}	-0.61	0.72	
PCM/B3LYP/6-31G(d) Toluene	-1.17	3.44	
PCM/B3LYP/6-31G(d) THF	4.55	9.52	

^a All energies are relative to the reactants: $\text{H}_2\text{Si}=\text{CH}_2 + \text{H}_2\text{O}$.

Table S4. Optimized geometries (at B3LYP/6-31G(d)).

H₂C=CH₂

6	-0.665464	0.000000	-0.000107
6	0.665464	0.000000	0.000102
1	-1.239575	0.923582	-0.000187
1	-1.239577	-0.923581	-0.000173
1	1.239577	-0.923580	0.000187
1	1.239579	0.923580	0.000200

H₂O

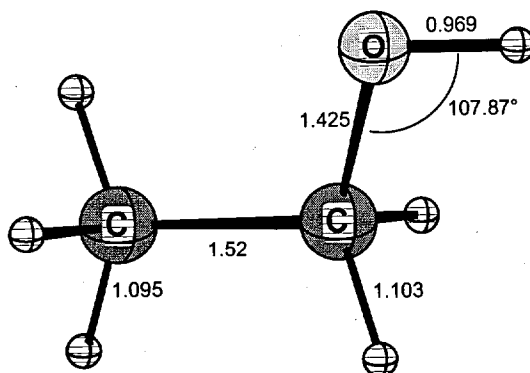
8	0.000000	0.000000	0.119739
1	0.000000	0.761568	-0.478958
1	0.000000	-0.761568	-0.478958

H₂C=CH₂ TS

6	-1.135167	-0.409552	0.015941
6	-0.305374	0.741635	0.006201
1	-1.626117	-0.680486	0.947993
1	-1.681565	-0.654346	-0.891619
1	-0.139600	1.307199	-0.905600
1	-0.099420	1.295695	0.919722
8	1.279669	-0.258291	-0.113947

10

1	0.217047	-0.915826	-0.042497
1	1.735550	-0.278401	0.750726

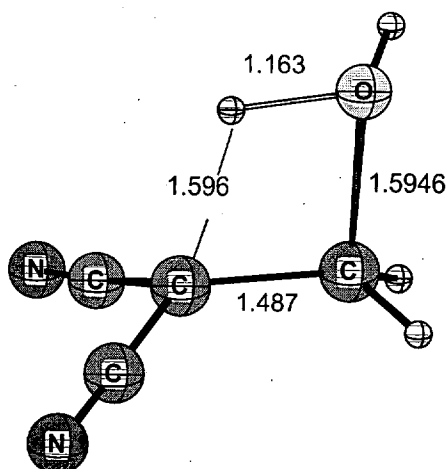
 $\text{H}_2\text{C}=\text{CH}_2$ Product (EtOH)


6	-1.172798	-0.410851	0.000000
6	0.000000	0.555571	0.000000
8	1.198904	-0.214425	0.000000
1	-2.123022	0.134745	0.000000
1	-1.138173	-1.052209	0.886829
1	-1.138173	-1.052209	-0.886829
1	-0.051241	1.207949	-0.887515
1	-0.051241	1.207949	0.887515
1	1.947411	0.400859	0.000000

 $\text{H}_2\text{C}=\text{C}(\text{CN})_2$

6	0.000000	0.000000	1.752402
6	0.000000	0.000000	0.405795
1	0.000000	0.931279	2.307968
1	0.000000	-0.931279	2.307968
6	0.000000	1.225330	-0.348415
7	0.000000	2.215794	-0.956010
6	0.000000	-1.225330	-0.348415
7	0.000000	-2.215794	-0.956010

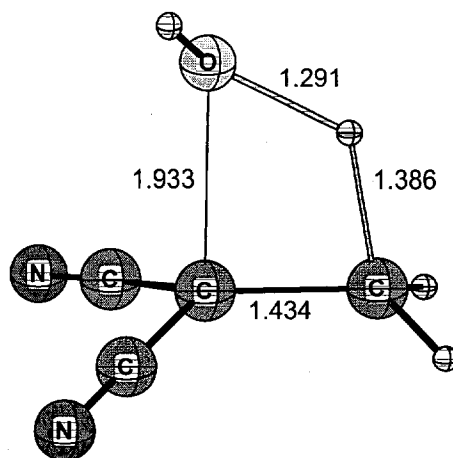
 $\text{H}_2\text{C}=\text{C}(\text{CN})_2$ TS



6	0.111662	0.050489	0.023301
6	-0.888400	-0.764054	0.762872
1	-0.515631	-1.660154	1.251695
1	-1.623160	-0.226524	1.360554
8	-1.670755	-1.333869	-0.504373
1	-0.857566	-0.676975	-1.014524
1	-2.556635	-0.922125	-0.593091
6	-0.102066	1.467744	-0.017215
7	-0.334157	2.608194	-0.076189
6	1.458874	-0.433207	-0.039306
7	2.539673	-0.860923	-0.116320

 $\text{H}_2\text{C}=\text{C}(\text{CN})_2$ Product

6	-0.648455	-1.166319	-0.288056
6	0.209616	-0.068874	0.434460
1	-0.273849	-2.143255	0.026359
1	-0.507526	-1.069828	-1.372439
6	1.634381	-0.198605	0.097719
7	2.748491	-0.355271	-0.183891
6	-0.308550	1.266104	0.094678
7	-0.788463	2.280228	-0.200282
1	0.086455	-0.216149	1.515374
8	-1.993498	-1.089986	0.101901
1	-2.399240	-0.319416	-0.328096

$\text{H}_2\text{C}=\text{C}(\text{CN})_2$ TS rev

6	0.007584	1.237478	-1.178335
6	-0.015949	0.101327	-0.303359
8	0.015091	1.300558	1.211971
1	0.109296	1.863563	0.054039
1	0.770580	1.303870	1.836703
1	-0.924360	1.489791	-1.675880
1	0.918944	1.392109	-1.749901
6	-1.251692	-0.588985	-0.029740
7	-2.251365	-1.157445	0.134504
6	1.188145	-0.664529	-0.082326
7	2.170835	-1.266205	0.065758

 $\text{H}_2\text{C}=\text{C}(\text{CN})_2$ Product rev

6	0.000046	1.414116	-1.007726
6	0.000001	0.310300	0.063509
8	-0.000076	0.963052	1.320520
1	0.891978	2.030187	-0.872394
1	0.000153	0.292833	2.025455
1	-0.892028	2.030081	-0.872603
1	0.000274	0.980548	-2.010269
6	-1.206890	-0.549705	-0.079789
7	-2.164941	-1.199142	-0.158029
6	1.206887	-0.549719	-0.079669
7	2.164936	-1.199145	-0.158014

1

6	-1.157723	0.000000	0.000028
14	0.551984	0.000000	-0.000025
1	-1.739337	0.917287	-0.000023
1	-1.739340	-0.917286	-0.000023
1	1.348620	-1.246244	0.000114
1	1.348616	1.246246	0.000114

1 complex

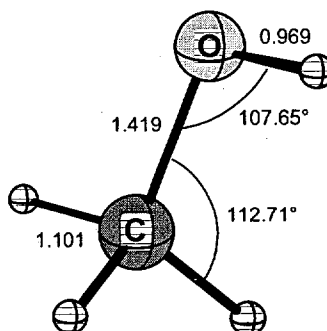
6	1.602791	-0.672853	-0.000016
14	0.410203	0.555384	0.000003
1	1.981271	-1.116754	-0.917035
1	1.981281	-1.116773	0.916991
1	0.005252	1.238554	1.248618
1	0.005239	1.238579	-1.248594
8	-1.934221	-0.278588	0.000008
1	-1.929429	-0.876585	0.766427
1	-1.929437	-0.876576	-0.766418

1 TS

6	-1.249732	-0.724020	0.013224
14	-0.183264	0.680095	0.008706
1	-1.723662	-1.031128	0.945123
1	-1.846266	-0.955917	-0.867663
1	0.074995	1.503738	-1.195589
1	0.209332	1.394611	1.254224
8	1.364283	-0.531880	-0.119076
1	0.529233	-1.212140	-0.074470
1	1.906191	-0.621335	0.689743

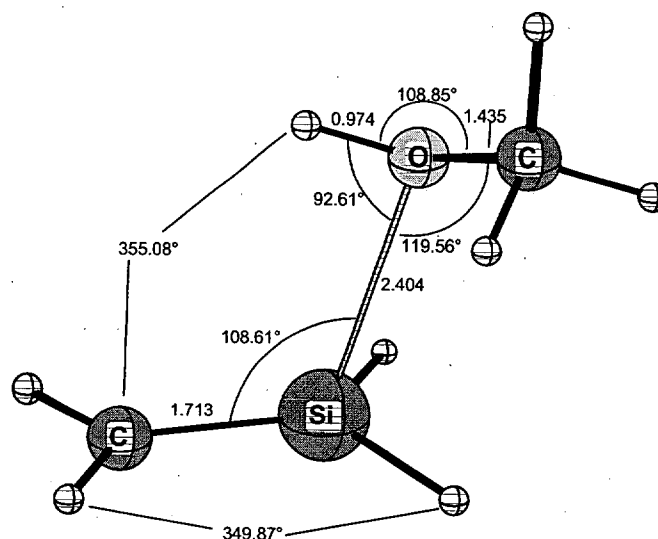
1 Product

6	1.399605	-0.728658	0.000000
14	0.000000	0.514709	0.000000
8	-1.427220	-0.354819	0.000000
1	2.369987	-0.217958	0.000000
1	1.355099	-1.371058	0.886100
1	1.355099	-1.371058	-0.886100
1	0.091788	1.400982	-1.200205
1	0.091788	1.400982	1.200205
1	-2.243629	0.162680	0.000000

MeOH

14

6	0.662312	-0.019521	-0.000001
8	-0.749182	0.122478	-0.000002
1	1.079652	0.991161	-0.000035
1	-1.133838	-0.766462	0.000015
1	1.036883	-0.543659	0.893226
1	1.036886	-0.543743	-0.893178

1 + MeOH complex

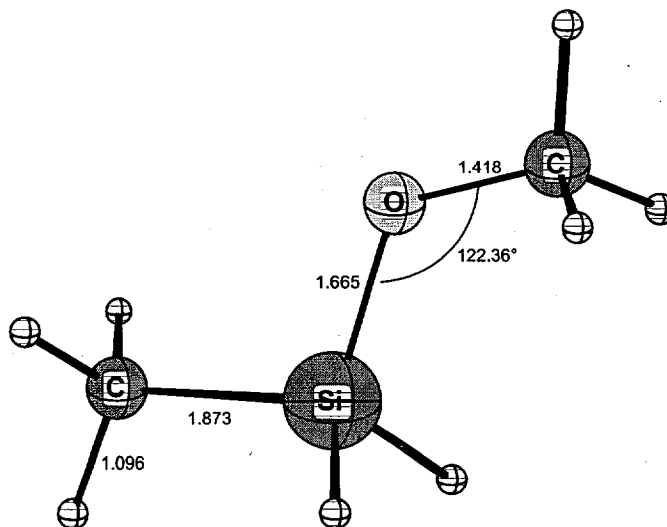
6	-2.015828	0.784740	0.118255
14	-0.983944	-0.580680	0.051989
1	-2.583657	1.125261	-0.743425
1	-2.118615	1.396242	1.010806
1	-0.346766	-1.129626	1.273054
1	-0.972191	-1.500150	-1.106533
8	1.208472	0.145958	-0.616093
1	0.909899	1.061461	-0.759530
6	2.275546	0.151159	0.343446
1	2.569907	-0.889901	0.485420
1	3.134434	0.716150	-0.036004
1	1.956111	0.567029	1.306902

1 + MeOH TS

6	1.567560	0.947816	0.098024
14	0.830204	-0.653686	0.063649
1	1.753769	1.426028	1.059306
1	2.288225	1.230908	-0.667613
1	1.033338	-1.628999	-1.035540

15

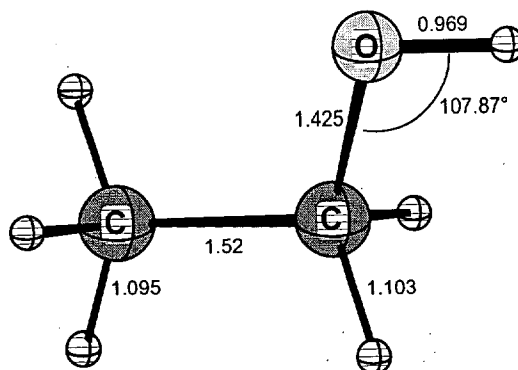
1	0.315137	-1.324989	1.289490
8	-0.838863	0.153978	-0.538077
1	-0.209336	1.015864	-0.411355
6	-2.063327	0.169316	0.227477
1	-2.747787	0.890553	-0.224830
1	-2.499925	-0.829035	0.178485
1	-1.870767	0.436653	1.272577

1 + MeOH Product


6	1.845471	1.024747	0.000000
14	0.000000	0.703446	0.000000
8	-0.225770	-0.946210	0.000000
1	2.047990	2.102546	0.000000
1	2.320982	0.590971	0.886250
1	2.320982	0.590971	-0.886250
1	-0.643372	1.315463	-1.203333
1	-0.643372	1.315463	1.203333
6	-1.515466	-1.535781	0.000000
1	-2.092311	-1.252276	0.891967
1	-2.092311	-1.252276	-0.891967
1	-1.392459	-2.623228	0.000000

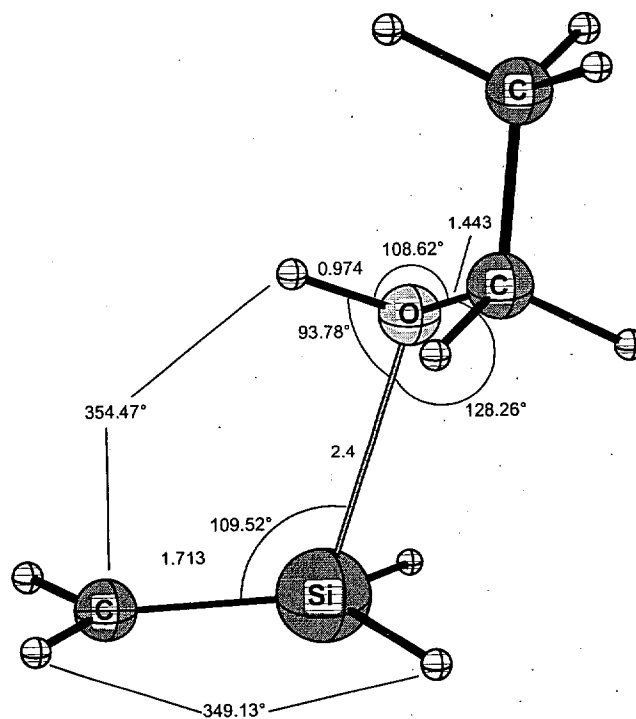
EtOH

16



6	-1.172798	-0.410851	0.000000
6	0.000000	0.555571	0.000000
8	1.198904	-0.214425	0.000000
1	-2.123022	0.134745	0.000000
1	-1.138173	-1.052209	0.886829
1	-1.138173	-1.052209	-0.886829
1	-0.051241	1.207949	-0.887515
1	-0.051241	1.207949	0.887515
1	1.947411	0.400859	0.000000

1 + EtOH complex

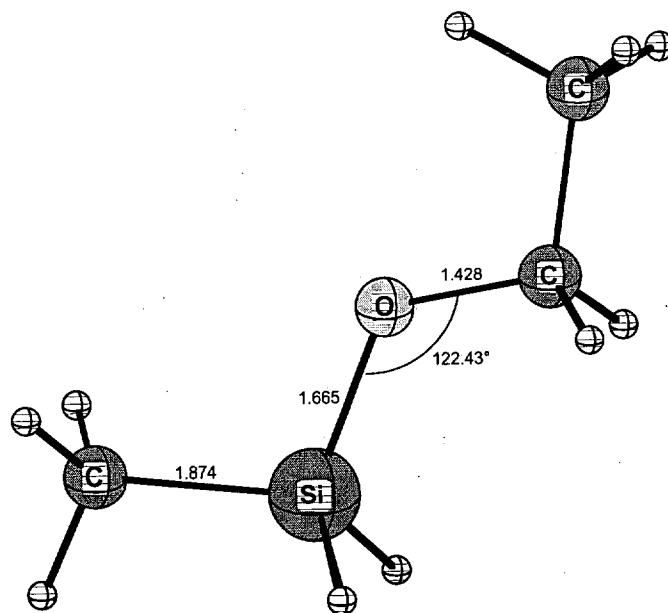


6	-2.527893	0.935104	0.146068
14	-1.651192	-0.529253	0.002172
1	-3.019034	1.403183	-0.702817
1	-2.589830	1.488766	1.079217
1	-1.131893	-1.240134	1.195204
1	-1.708390	-1.358377	-1.221606
8	0.633208	-0.044957	-0.551010
1	0.473956	0.911079	-0.649799
6	1.675163	-0.239663	0.427633
1	1.744556	-1.323348	0.550733
1	1.370396	0.188282	1.392239
6	3.001034	0.342364	-0.040243
1	3.787692	0.136631	0.695015
1	3.297679	-0.094368	-0.998927
1	2.936072	1.430643	-0.162348

1 + EtOH TS

6	1.892705	1.152441	0.142927
14	1.492871	-0.558058	-0.018739
1	2.054748	1.567855	1.137299
1	2.483269	1.646067	-0.627471
1	1.810113	-1.366606	-1.221885
1	1.222459	-1.433502	1.155628
8	-0.341913	-0.071309	-0.444469
1	0.107393	0.889751	-0.267410
6	-1.490977	-0.369674	0.395031
1	-1.632210	-1.451601	0.341290
1	-1.254853	-0.105342	1.433641
6	-2.714263	0.375431	-0.109744
1	-2.565062	1.459213	-0.057461
1	-2.928753	0.105979	-1.148342
1	-3.586789	0.122284	0.503519

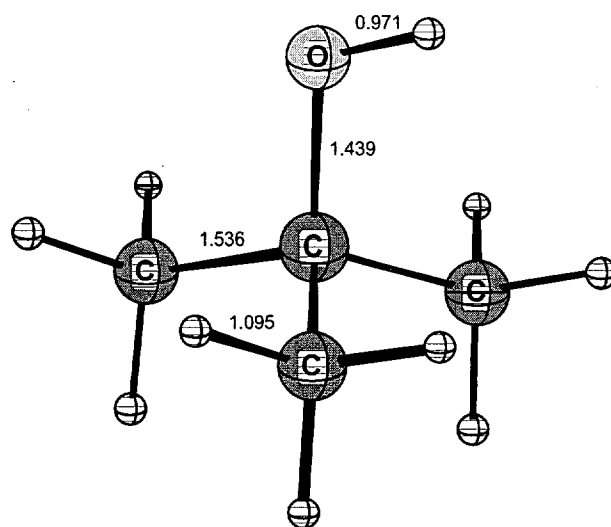
1 + EtOH Product



6	-2.043283	-1.578132	0.000000
14	-0.202158	-1.228947	0.000000
8	0.000000	0.423884	0.000000
1	-2.229504	-2.658842	0.000000
1	-2.525490	-1.151791	0.886265
1	-2.525490	-1.151791	-0.886265
1	0.447804	-1.833935	-1.203250
1	0.447804	-1.833935	1.203250
6	1.289697	1.037791	0.000000
1	1.854033	0.707171	0.884020
1	1.854033	0.707171	-0.884020
6	1.132281	2.567807	0.000000
1	1.584189	3.026273	0.885350
1	1.584189	3.026273	-0.885350
1	0.066480	2.812799	0.000000

t-BuOH

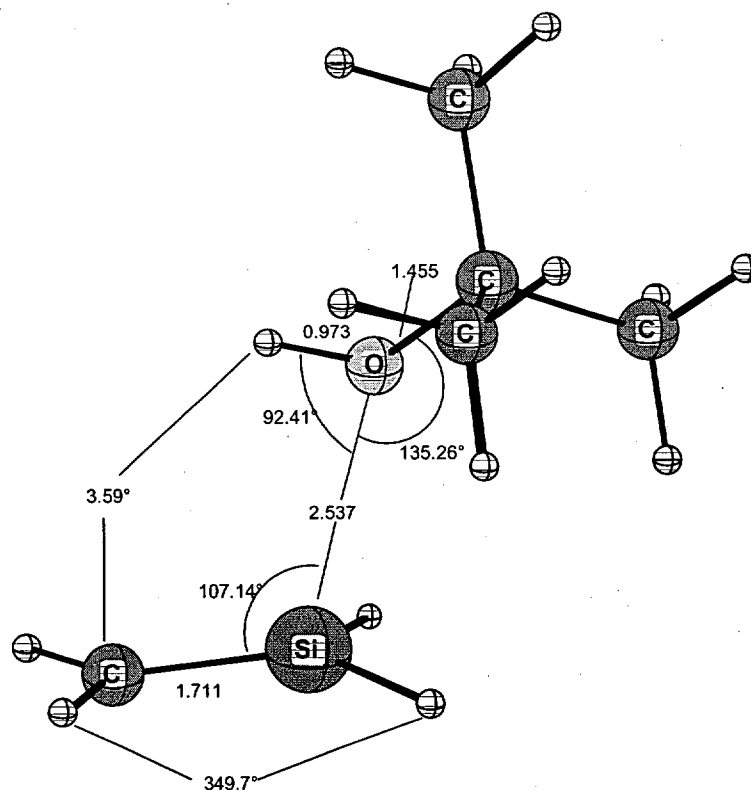
19



8	-0.014135	-0.000364	1.452347
1	-0.944991	0.003336	1.727805
6	0.005421	-0.000051	0.013749
6	-0.684347	1.268969	-0.509737
1	-1.741317	1.288527	-0.212135
1	-0.198844	2.160532	-0.099435
1	-0.648090	1.324807	-1.604010
6	-0.696514	-1.262078	-0.510454
1	-1.754058	-1.270826	-0.214305
1	-0.659417	-1.318466	-1.604663
1	-0.220680	-2.158475	-0.099381
6	1.490501	-0.006939	-0.356799
1	1.979238	-0.896574	0.053780
1	1.622810	-0.005624	-1.444025
1	1.988059	0.876268	0.057041

1 + t-BuOH complex

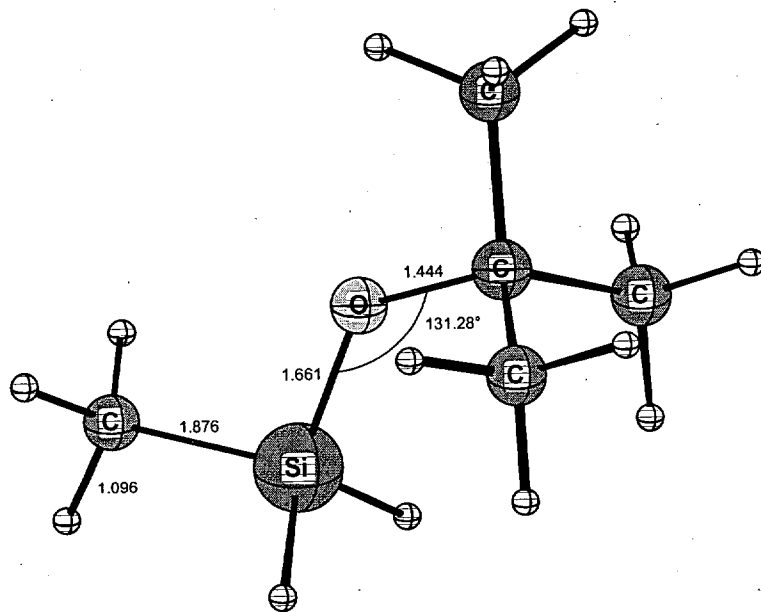
20



6	3.194020	-0.853529	-0.058369
14	2.218363	0.550614	0.014306
1	3.664452	-1.186440	-0.979694
1	3.336822	-1.508961	0.796671
1	1.698395	1.067827	1.300729
1	2.135958	1.512756	-1.105104
8	-0.137453	-0.142336	-0.622237
1	0.113203	-1.080199	-0.692252
6	-1.447251	-0.050511	0.005617
6	-1.407648	-0.718476	1.385868
1	-2.382235	-0.645854	1.881908
1	-1.157623	-1.783499	1.298821
1	-0.658406	-0.242185	2.025791
6	-1.727047	1.448552	0.119643
1	-2.715084	1.622063	0.558879
1	-0.978138	1.934234	0.753496
1	-1.699001	1.917949	-0.868962
6	-2.468337	-0.734242	-0.912558
1	-3.482552	-0.645918	-0.506535
1	-2.450784	-0.279116	-1.907869
1	-2.244891	-1.803327	-1.019469

1 + t-BuOH TS

6	-2.522331	-1.014012	-0.038684
14	-1.866959	0.625567	-0.002757
1	-2.735220	-1.515779	0.905418
1	-3.203119	-1.303319	-0.838200
1	-2.083247	1.611902	-1.091070
1	-1.496061	1.327017	1.257174
8	-0.152622	-0.084926	-0.539806
1	-0.720146	-0.992419	-0.453445
6	1.216301	-0.046517	0.010054
6	2.058321	-0.952734	-0.890802
1	1.695977	-1.985969	-0.853965
1	2.015311	-0.608729	-1.928677
1	3.104393	-0.947600	-0.564177
6	1.199676	-0.551477	1.456837
1	0.821893	-1.578297	1.509338
1	2.214709	-0.541704	1.869958
1	0.568913	0.080772	2.089002
6	1.677629	1.407873	-0.078429
1	1.057280	2.057046	0.547509
1	2.714651	1.493686	0.265616
1	1.625484	1.766061	-1.111299

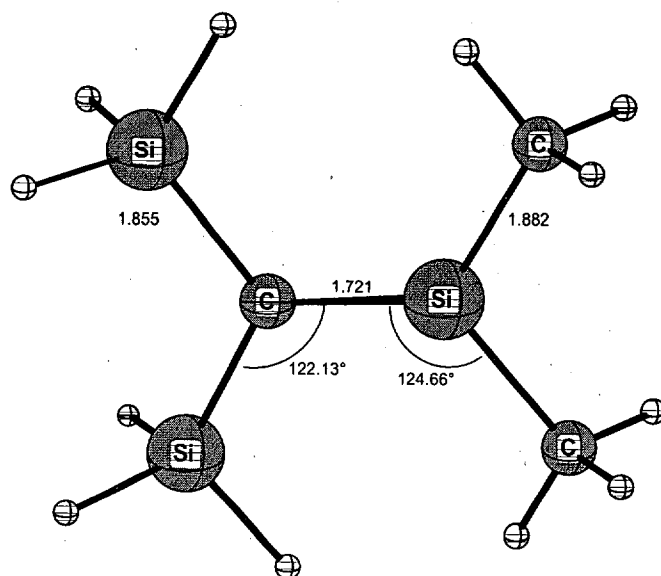
1 + t-BuOH Product

6	-2.529692	1.756994	0.000000
14	-1.623853	0.114686	0.000000
8	0.000000	0.465808	0.000000
1	-3.614629	1.596166	0.000000
1	-2.274963	2.348254	0.886471

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1	-2.274963	2.348254	-0.886471
1	-2.021783	-0.681612	-1.200841
1	-2.021783	-0.681612	1.200841
6	1.160077	-0.393351	0.000000
6	1.150250	-1.267154	-1.262540
1	2.057550	-1.880097	-1.311286
1	0.286792	-1.941581	-1.278446
1	1.111722	-0.638550	-2.158752
6	2.392315	0.549766	0.000000
1	3.020610	0.398615	0.883811
1	3.020610	0.398615	-0.883811
1	2.049523	1.587115	0.000000
6	1.150250	-1.267154	1.262540
1	0.286792	-1.941581	1.278446
1	2.057550	-1.880097	1.311286
1	1.111722	-0.638550	2.158752

2



14	0.000000	0.000000	1.159976
6	0.000000	0.000000	-0.560598
6	0.000000	-1.547984	2.230408
6	0.000000	1.547984	2.230408
14	0.000000	-1.570816	-1.547216
14	0.000000	1.570816	-1.547216
1	0.000000	-2.461953	1.632380
1	0.882270	-1.559772	2.882132
1	-0.882270	-1.559772	2.882132
1	0.000000	2.461953	1.632380
1	0.882270	1.559772	2.882132
1	-0.882270	1.559772	2.882132
1	0.000000	-2.785115	-0.681665
1	-1.194618	-1.665164	-2.437218

1	1.194618	-1.665164	-2.437218
1	0.000000	2.785115	-0.681665
1	-1.194618	1.665164	-2.437218
1	1.194618	1.665164	-2.437218

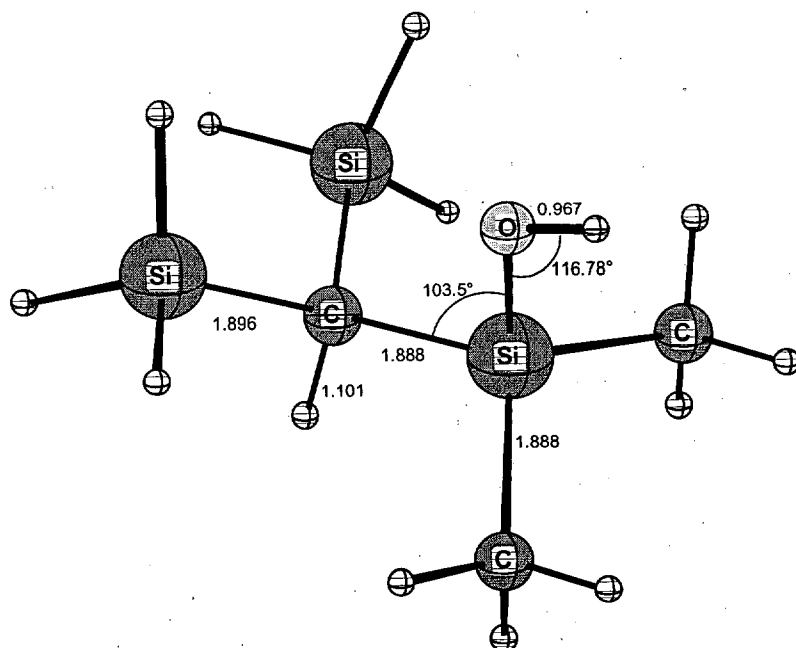
2 complex

14	0.970563	0.070631	-0.263974
6	-0.757611	-0.000277	-0.062082
8	1.582266	-0.086376	1.806423
6	1.988230	-1.416544	-0.821953
6	1.901043	1.667984	-0.599701
14	-1.796927	1.518121	-0.004125
14	-1.654830	-1.606060	-0.068416
1	1.999110	-1.455795	-1.918079
1	3.031880	-1.342433	-0.492733
1	1.571130	-2.365920	-0.471453
1	1.922571	1.867895	-1.677950
1	2.937118	1.597473	-0.251060
1	1.428278	2.525740	-0.113707
1	-2.671480	1.709656	-1.203615
1	-2.732438	1.528219	1.164538
1	-0.972670	2.760647	0.111087
1	-2.384281	-1.922216	-1.336312
1	-2.689432	-1.681059	1.010367
1	-0.732873	-2.764047	0.168700
1	0.660006	-0.060509	2.138597
1	1.921684	-0.971309	2.033865

2 TS

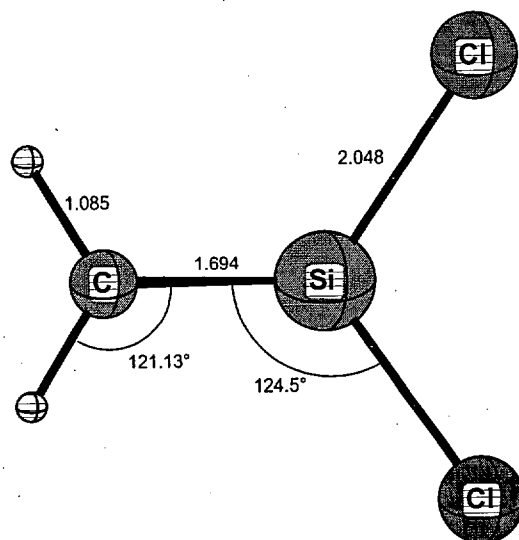
14	1.061351	0.039238	-0.150872
6	-0.716103	-0.000876	0.074781
8	1.212178	0.000249	1.776839
6	2.021062	-1.487198	-0.692511
6	1.969267	1.618293	-0.597819
14	-1.725182	1.538123	-0.091077
14	-1.638146	-1.586246	-0.132429
1	0.121967	-0.046115	1.604898
1	1.531415	-0.829038	2.181473
1	3.075101	-1.434381	-0.394851
1	1.995292	-1.565214	-1.786497
1	1.587689	-2.410505	-0.294434
1	3.025964	1.564209	-0.312789
1	1.921403	1.790126	-1.680045
1	1.521159	2.485506	-0.103710
1	-2.963581	1.458527	0.738963
1	-2.188022	1.857108	-1.479637
1	-0.972702	2.747039	0.367223
1	-2.902060	-1.584888	0.661596
1	-2.035348	-1.935236	-1.533430
1	-0.833368	-2.756051	0.351112

2 Product



14	1.098243	-0.010521	0.032974
6	-0.699194	0.001276	-0.544959
8	0.998383	-0.572026	1.614848
6	2.110822	-1.186870	-1.041344
6	1.904022	1.696408	-0.012427
14	-1.654574	1.567934	-0.095205
14	-1.638198	-1.542994	0.027122
1	1.828170	-0.637801	2.106940
1	-0.677461	-0.044496	-1.644907
1	3.145901	-1.266675	-0.685664
1	2.152306	-0.834527	-2.079875
1	1.681204	-2.194670	-1.045230
1	2.955740	1.644877	0.297870
1	1.886785	2.117311	-1.025394
1	1.398601	2.406671	0.651511
1	-3.104986	1.419778	-0.405559
1	-1.150360	2.739981	-0.865586
1	-1.525535	1.876584	1.353632
1	-2.823244	-1.752134	-0.853651
1	-0.797565	-2.768642	-0.061047
1	-2.127113	-1.396798	1.422084

3



6	-0.000041	2.136142	0.000453
14	0.000000	0.442198	-0.000195
1	0.928559	2.696967	0.000068
1	-0.928688	2.696891	0.000476
17	-1.687399	-0.717709	0.000138
17	1.687421	-0.717672	-0.000169

3 complex

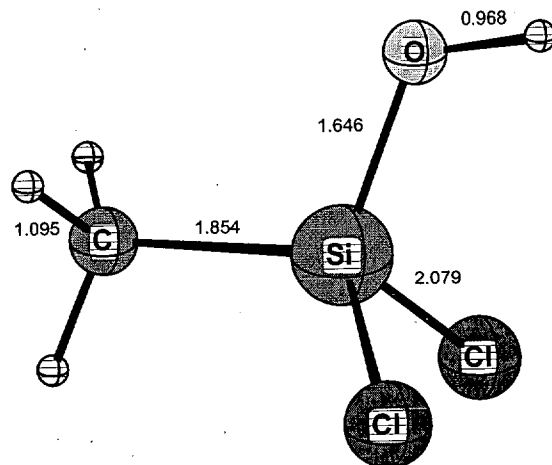
14	0.037975	0.357616	-0.270813
6	0.020223	1.936531	-0.905947
8	-0.112705	0.592122	1.819500
17	-1.661901	-0.850648	-0.283156
17	1.741502	-0.794668	-0.124784
1	0.943343	2.440072	-1.174019
1	-0.906636	2.390776	-1.241974
1	-0.214937	1.566164	1.821996
1	-0.926335	0.210563	2.200035

3 TS

14	0.024917	0.274378	-0.256218
6	-0.028359	1.861379	-0.991639
8	-0.098437	1.052240	1.508069
17	-1.644063	-0.967545	-0.126039
17	1.748497	-0.833007	-0.018432
1	0.868088	2.226324	-1.490612
1	-0.948995	2.133051	-1.508285
1	-0.163427	1.928001	0.916806

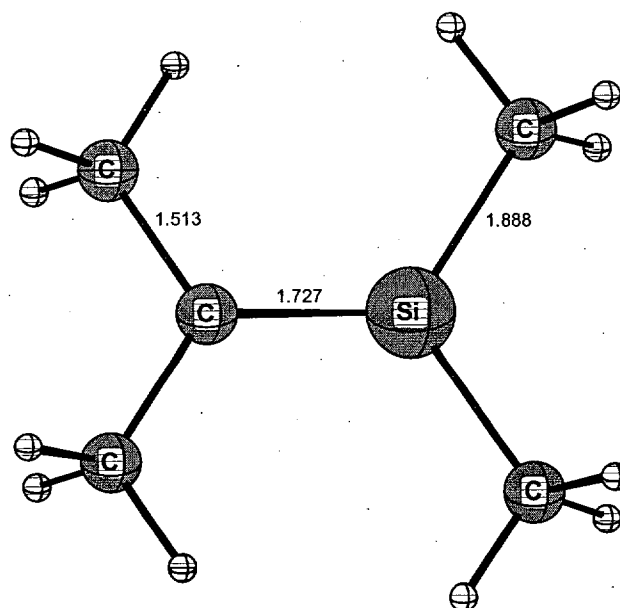
1 -0.922236 0.894527 2.010428

3 Product



6	-1.548640	1.376713	0.000000
14	0.000000	0.357150	0.000000
8	1.294124	1.373533	0.000000
1	-2.438001	0.739622	0.000000
1	-1.576245	2.015444	0.888949
1	-1.576245	2.015444	-0.888949
17	0.069080	-0.882453	-1.667100
17	0.069080	-0.882453	1.667100
1	2.180601	0.984242	0.000000

4



14	0.000000	-0.676674	0.000000
6	0.000000	1.049813	0.000000
6	0.000000	-1.709420	1.580498
6	0.000000	-1.709420	-1.580498
6	0.000000	1.878766	1.265592
6	0.000000	1.878766	-1.265592
1	-0.883774	-2.356418	1.628156
1	0.883774	-2.356417	1.628156
1	0.000000	-1.073269	2.470485
1	-0.883774	-2.356418	-1.628156
1	0.883774	-2.356417	-1.628156
1	0.000000	-1.073269	-2.470485
1	0.880999	2.538649	1.305249
1	-0.880999	2.538649	1.305249
1	0.000000	1.280013	2.182635
1	0.880999	2.538649	-1.305249
1	-0.880999	2.538649	-1.305249
1	0.000000	1.280013	-2.182635

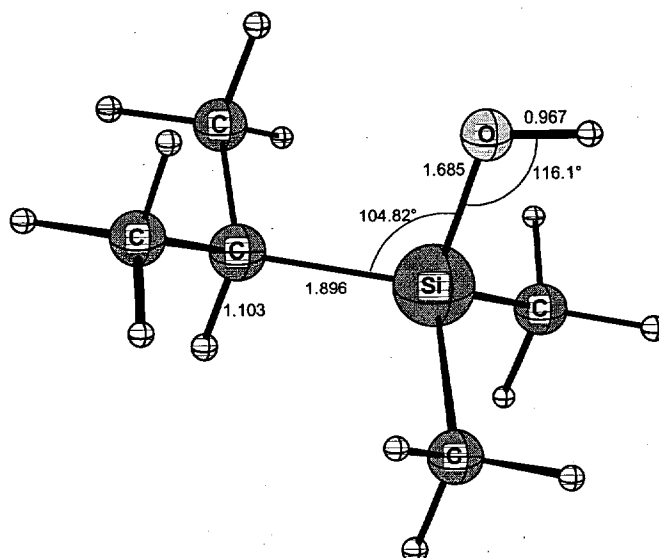
4 TS

14	0.587765	0.027841	-0.221087
6	-1.173571	-0.000018	0.003201
8	0.804701	-0.015787	1.802182
6	1.556521	-1.527963	-0.678052
6	1.534555	1.617079	-0.562770
6	-2.020180	1.258803	-0.137199
6	-1.981134	-1.275384	-0.209760
1	-0.260566	-0.050494	1.596504

28

1	1.080413	-0.871464	2.184886
1	2.564086	-1.535239	-0.245974
1	1.666296	-1.588229	-1.767549
1	1.036994	-2.437530	-0.356656
1	2.540892	1.588490	-0.131071
1	1.631923	1.781446	-1.642506
1	1.011320	2.481658	-0.141540
1	-2.831373	1.277675	0.608036
1	-2.512134	1.330007	-1.122785
1	-1.447048	2.184702	-0.000205
1	-2.796464	-1.359484	0.526706
1	-2.465487	-1.308263	-1.201020
1	-1.382322	-2.191853	-0.121587

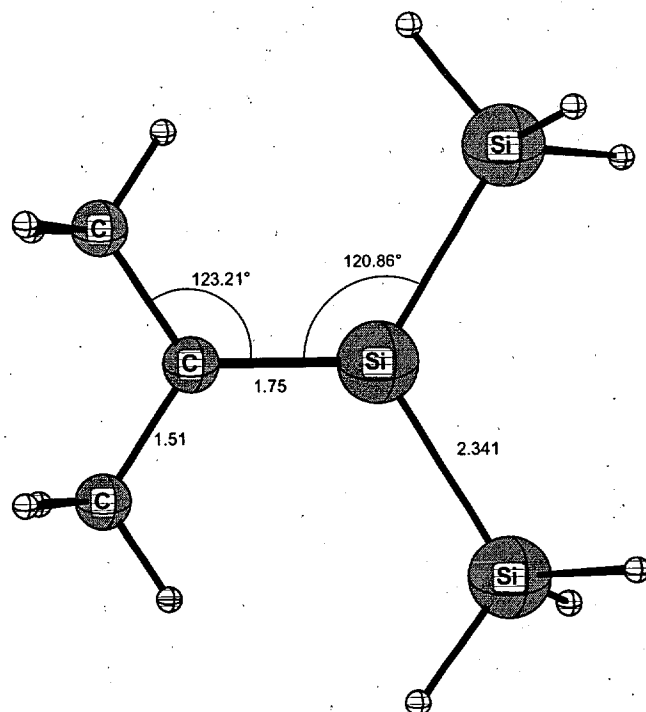
4 Product



14	0.000000	0.640857	0.000000
6	0.442688	-1.202840	0.000000
8	-1.684137	0.679568	0.000000
6	0.684068	1.507278	1.535416
6	0.684068	1.507278	-1.535416
6	-0.058679	-1.921944	-1.267885
6	-0.058679	-1.921944	1.267885
1	-2.089467	1.557332	0.000000
1	1.544427	-1.248806	0.000000
1	0.431943	2.575366	1.543467
1	1.778540	1.434391	1.573680
1	0.288199	1.067092	2.457542
1	0.431943	2.575366	-1.543467
1	1.778540	1.434391	-1.573680
1	0.288199	1.067092	-2.457542
1	0.235226	-2.980387	-1.259863
1	0.346916	-1.475182	-2.183211

1	-1.152159	-1.883298	-1.335667
1	0.235226	-2.980387	1.259863
1	0.346916	-1.475182	2.183211
1	-1.152159	-1.883298	1.335667

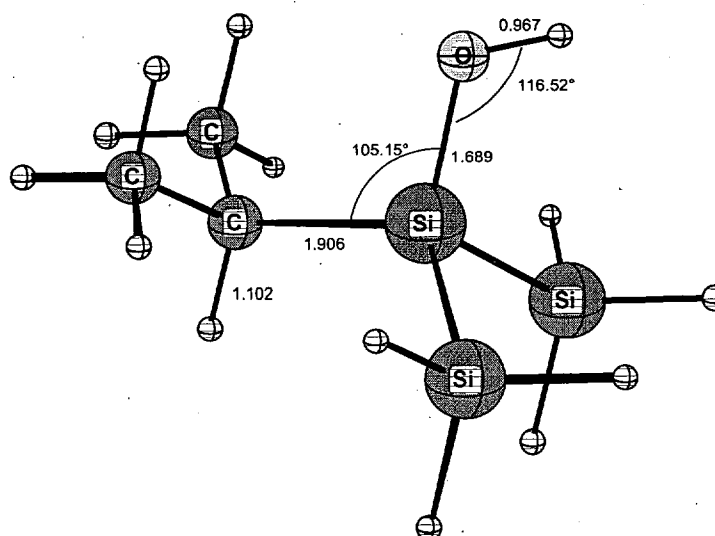
5



14	0.000000	0.000000	0.218742
6	0.000000	0.000000	-1.530746
14	-0.220785	1.996480	1.421139
1	0.777980	2.037960	2.525977
14	0.220785	-1.996480	1.421139
1	-0.777980	-2.037960	2.525977
1	0.000000	3.178943	0.543823
1	-1.570996	2.123860	2.038561
1	0.000000	-3.178943	0.543823
1	1.570996	-2.123860	2.038561
6	0.148194	-1.254438	-2.357939
6	-0.148194	1.254438	-2.357939
1	0.235303	-2.166080	-1.760452
1	-0.235303	2.166080	-1.760452
1	-0.712500	-1.376346	-3.033080
1	1.038315	-1.189113	-3.002107
1	0.712500	1.376346	-3.033080
1	-1.038315	1.189113	-3.002107

5 TS

14	-0.212703	-0.008443	-0.032462
6	1.587420	-0.041853	-0.045545
8	-0.093081	-0.048777	1.984223
14	-1.387975	2.009362	-0.369197
14	-1.488863	-1.960565	-0.324161
6	2.354918	-1.315634	-0.376649
6	2.393260	1.217946	-0.343345
1	0.944129	-0.026104	1.614806
1	-0.299114	0.772280	2.476217
1	-2.764387	1.965977	0.202911
1	-1.507219	2.293933	-1.825712
1	-0.674037	3.151533	0.272116
1	-2.782051	-1.887642	0.411983
1	-1.799831	-2.145092	-1.770200
1	-0.744446	-3.158919	0.150371
1	3.279520	-1.374445	0.217875
1	2.666910	-1.354688	-1.433199
1	1.785607	-2.229942	-0.171586
1	3.327149	1.226967	0.239655
1	2.693809	1.283221	-1.401816
1	1.858601	2.145429	-0.102482

5 Product

14	0.000000	0.325888	0.000000
6	-0.879197	-1.365468	0.000000
8	-1.242953	1.469399	0.000000
14	1.377115	0.582930	1.912971
14	1.377115	0.582930	-1.912971
6	-1.731030	-1.570154	-1.268560
6	-1.731030	-1.570154	1.268560

1	-0.974769	2.398744	0.000000
1	-0.075718	-2.118954	0.000000
1	2.023202	1.928693	1.916153
1	2.466810	-0.436229	1.914827
1	0.620743	0.448710	3.190670
1	2.023202	1.928693	-1.916153
1	2.466810	-0.436229	-1.914827
1	0.620743	0.448710	-3.190670
1	-2.213728	-2.556330	-1.251690
1	-1.133152	-1.511772	-2.185198
1	-2.522664	-0.815480	-1.338397
1	-2.213728	-2.556330	1.251690
1	-1.133152	-1.511772	2.185198
1	-2.522664	-0.815480	1.338397

6

14	-1.074354	2.430438	-0.052001
6	0.591988	-0.627595	-0.119759
14	-0.996771	0.106783	0.137758
6	0.910835	-2.095621	-0.154403
8	1.666081	0.216039	-0.268755
14	-2.880858	-1.262928	0.044413
1	-0.695426	2.905729	-1.411897
1	-2.465891	2.888273	0.222575
1	-0.168083	3.083334	0.932544
1	-2.466278	-2.691910	0.126791
1	-3.802774	-0.979470	1.178990
1	-3.658557	-1.078378	-1.213517
14	3.282559	0.011093	0.135406
1	0.011627	-2.705129	-0.038401
1	1.608851	-2.377664	0.649123
1	1.387175	-2.365892	-1.107641
1	3.914627	-1.088673	-0.640493
1	3.922597	1.299573	-0.208786
1	3.438480	-0.274208	1.587656

6 TS

14	-0.845684	0.085990	-0.047875
6	0.689486	-0.876863	-0.243674
8	-0.556405	-0.052936	1.927068
14	-0.674576	2.397889	-0.459275
14	-2.975873	-0.907711	-0.079875
6	0.746311	-2.313710	-0.716591
8	1.806496	-0.114365	-0.757769
1	0.302897	-0.581054	1.523648
1	-0.249294	0.749706	2.397234
1	-1.899396	3.126757	-0.022036
1	-0.488155	2.630377	-1.915707
1	0.484460	2.975774	0.277445
1	-3.927132	-0.234254	0.847344
1	-3.536330	-0.822362	-1.457492
1	-2.876670	-2.343415	0.300887
1	1.625976	-2.831215	-0.309251

1	0.811248	-2.386076	-1.812179
1	-0.138475	-2.874137	-0.390893
14	3.116587	0.047424	0.251365
1	3.681061	-1.265687	0.672332
1	4.147570	0.808417	-0.499552
1	2.760367	0.798732	1.494669

6 Product

14	0.957552	0.054883	0.316807
6	-0.703853	-0.794680	-0.168938
8	1.275932	-0.090161	1.965186
14	2.691974	-0.948249	-0.949522
14	0.749807	2.361282	-0.089233
6	-0.897359	-2.171581	0.473325
8	-1.757949	0.111150	0.217169
1	-0.709489	-0.908743	-1.266760
1	1.471069	-0.979799	2.292720
1	4.001348	-0.283544	-0.700337
1	2.403262	-0.869861	-2.410771
1	2.847792	-2.392733	-0.600356
1	2.081050	3.030674	-0.049371
1	0.181483	2.568036	-1.452050
1	-0.139383	3.014504	0.906796
1	-1.847663	-2.627717	0.170211
1	-0.900652	-2.090948	1.565908
1	-0.093719	-2.856897	0.175943
14	-3.295242	0.085156	-0.425254
1	-4.106902	-1.067997	0.058223
1	-3.947145	1.345912	-0.000320
1	-3.234923	0.005760	-1.914169

7

14	1.690307	0.618115	0.000000
6	0.000000	0.911966	0.000000
6	2.981736	1.992759	0.000000
1	3.628366	1.927152	0.883296
1	3.628366	1.927152	-0.883296
1	2.501773	2.976211	0.000000
6	2.457331	-1.103771	0.000000
1	1.684065	-1.877768	0.000000
1	3.090132	-1.253617	-0.883005
1	3.090132	-1.253617	0.883005
14	-1.427897	-0.289857	0.000000
6	-1.403533	-1.409078	-1.535650
1	-2.252388	-2.104910	-1.537990
1	-1.453814	-0.815380	-2.456022
1	-0.485862	-2.008727	-1.583313
6	-1.403533	-1.409078	1.535650
1	-0.485862	-2.008727	1.583313
1	-1.453814	-0.815380	2.456022
1	-2.252388	-2.104910	1.537990
6	-3.044989	0.702825	0.000000
1	-3.117473	1.346780	0.884990

1	-3.117473	1.346780	-0.884990
1	-3.919767	0.040881	0.000000
1	-0.279811	1.968735	0.000000

7 TS

14	-1.624024	0.041751	0.205617
6	-0.032887	-0.726038	0.334800
8	-1.901283	-0.964660	-1.488708
6	-3.064913	-0.580085	1.255257
6	-1.913112	1.795920	-0.400395
14	1.672008	-0.055570	0.084596
1	-0.920158	-1.273550	-1.145158
1	-4.035488	-0.445601	0.762875
1	-3.099263	-0.022416	2.199160
1	-2.947607	-1.639320	1.510981
1	-2.920251	1.912648	-0.816032
1	-1.805420	2.507864	0.426801
1	-1.190241	2.070598	-1.173951
6	1.720218	1.328488	-1.221176
1	1.271616	1.012305	-2.171046
1	1.194359	2.230577	-0.885491
1	2.757237	1.620000	-1.430117
6	2.821279	-1.452071	-0.508648
1	2.501710	-1.844614	-1.481711
1	3.857549	-1.105338	-0.611596
1	2.824783	-2.291934	0.197926
6	2.439270	0.649717	1.679630
1	3.468992	0.996515	1.521147
1	1.855822	1.498856	2.057159
1	2.464471	-0.106422	2.474549
1	-0.045089	-1.580824	1.023604
1	-2.513667	-1.724187	-1.449231

7 + MeOH TS

14	-1.290527	-0.619576	-0.185879
6	0.185395	0.202297	-0.722244
8	-1.872561	1.085501	0.603496
6	-2.668226	-0.997949	-1.419437
6	-1.391494	-1.745596	1.316417
14	1.921276	0.123455	-0.094490
1	-0.926393	1.339555	0.149071
1	-3.665084	-0.967581	-0.963135
1	-2.527382	-2.006213	-1.827425
1	-2.653139	-0.299820	-2.263416
1	-2.409163	-1.784656	1.721997
1	-1.098687	-2.767833	1.047930
1	-0.721619	-1.402768	2.110308
6	1.998022	-0.108960	1.793960
1	1.399932	0.643184	2.323033
1	1.640944	-1.098710	2.103984
1	3.032023	-0.015602	2.149545
6	2.813812	1.752231	-0.512846
1	2.341894	2.604830	-0.009333

1	3.868101	1.725575	-0.208897
1	2.787926	1.954054	-1.591453
6	2.948153	-1.282667	-0.869759
1	3.989496	-1.271578	-0.521388
1	2.523903	-2.263613	-0.620829
1	2.964995	-1.204009	-1.964162
6	-2.998515	1.897180	0.220395
1	-3.909720	1.372023	0.513422
1	-2.941823	2.849975	0.752752
1	-3.008360	2.075399	-0.860517
1	0.139285	0.480263	-1.783203

8

14	0.000000	0.421640	0.000000
6	-1.239464	1.598514	0.000000
1	-2.292617	1.333648	0.000000
1	-1.025723	2.663993	0.000000
6	1.837673	0.799512	0.000000
1	2.326529	0.378054	0.884788
1	2.326529	0.378054	-0.884788
1	1.995689	1.882675	0.000000
6	-0.390867	-1.348128	0.000000
6	-0.622848	-2.541802	0.000000
1	-0.837371	-3.587967	0.000000

8 complex

6	-1.172572	-1.201232	-1.277775
14	-0.424034	-0.421269	0.047761
1	-0.601406	-1.639420	-2.091369
1	-2.252723	-1.271793	-1.375596
8	-0.028622	2.042257	-0.688522
1	-0.411046	1.824897	-1.555646
1	0.929535	1.941577	-0.816535
6	1.397288	-0.465234	0.177562
6	2.610086	-0.462290	0.273027
1	3.674261	-0.486898	0.359897
6	-1.292648	0.178132	1.593506
1	-0.989950	1.200546	1.835789
1	-2.376650	0.162856	1.438699
1	-1.059496	-0.468309	2.446369

8 TS

6	1.160437	-1.214831	-1.063378
14	0.285912	0.089468	-0.270048
1	0.600919	-2.009898	-1.554589
1	2.124381	-1.014327	-1.529695
8	0.719551	-0.727672	1.495050
1	1.161618	-1.403322	0.794846
1	-0.038990	-1.168060	1.926164
6	0.955157	1.819559	-0.007804

35

1	0.651018	2.473533	-0.832456
1	0.597318	2.257788	0.929033
1	2.050108	1.796510	0.018428
6	-1.540597	0.020090	-0.139250
6	-2.755448	-0.012048	-0.099285
1	-3.822844	-0.040025	-0.073163

8 + MeOH TS

6	1.160437	-1.214831	-1.063378
14	0.285912	0.089468	-0.270048
1	0.600919	-2.009898	-1.554589
1	2.124381	-1.014327	-1.529695
8	0.719551	-0.727672	1.495050
1	1.161618	-1.403322	0.794846
1	-0.038990	-1.168060	1.926164
6	0.955157	1.819559	-0.007804
1	0.651018	2.473533	-0.832456
1	0.597318	2.257788	0.929033
1	2.050108	1.796510	0.018428
6	-1.540597	0.020090	-0.139250
6	-2.755448	-0.012048	-0.099285
1	-3.822844	-0.040025	-0.073163

9

14	0.105980	-1.360947	0.000000
6	1.611955	-2.195693	0.000000
6	-1.511311	-2.352097	0.000000
1	-2.118763	-2.126876	0.884137
1	-2.118763	-2.126876	-0.884137
1	-1.294171	-3.425549	0.000000
14	0.000000	0.989716	0.000000
1	1.692033	-3.281227	0.000000
6	-0.925775	1.598514	-1.544305
1	-0.416328	1.292019	-2.464892
1	-1.948789	1.206214	-1.583274
1	-0.991532	2.694180	-1.546686
6	-0.925775	1.598514	1.544305
1	-1.948789	1.206214	1.583274
1	-0.416328	1.292019	2.464892
1	-0.991532	2.694180	1.546686
6	1.767751	1.678493	0.000000
1	2.325408	1.352833	0.885191
1	2.325408	1.352833	-0.885191
1	1.750713	2.775760	0.000000
1	2.566641	-1.674862	0.000000

9 TS

6	2.023368	1.202506	-1.120094
14	1.112161	-0.092773	-0.325763
1	2.977805	0.978083	-1.598695

1	1.506828	2.047384	-1.574026
8	1.717840	0.737514	1.457990
1	2.167558	1.329828	0.673379
1	2.420527	0.259110	1.939477
6	1.916787	-1.802731	-0.160868
1	1.604724	-2.438954	-0.997833
1	3.009834	-1.723407	-0.203469
1	1.641377	-2.319000	0.765784
14	-1.220521	0.001554	-0.012079
6	-1.767206	1.818882	-0.014689
1	-2.855311	1.897561	0.104436
1	-1.298649	2.377228	0.803373
1	-1.497199	2.314897	-0.953889
6	-2.074924	-0.918905	-1.439976
1	-1.828750	-0.469783	-2.408954
1	-1.780399	-1.974458	-1.477503
1	-3.165695	-0.884467	-1.323854
6	-1.711068	-0.812414	1.633653
1	-1.424927	-1.870519	1.663344
1	-1.228452	-0.310776	2.479853
1	-2.796691	-0.759793	1.786295

9 + MeOH TS

6	-1.382902	-1.595149	1.406585
14	-0.693813	-0.778378	-0.005934
1	-2.167453	-2.340730	1.269237
1	-0.780585	-1.768828	2.297384
8	-1.755395	0.868465	0.584590
1	-2.008029	0.098932	1.292768
6	-1.453567	-1.090807	-1.715132
1	-0.858927	-1.844101	-2.245788
1	-2.473349	-1.482324	-1.624994
1	-1.482330	-0.192449	-2.342627
14	1.465171	0.162862	-0.004415
6	1.968744	0.559658	1.782520
1	2.978925	0.987255	1.816434
1	1.282078	1.282077	2.237655
1	1.966178	-0.340786	2.407260
6	2.696120	-1.084984	-0.743342
1	2.715658	-2.017005	-0.166954
1	2.444129	-1.339801	-1.779694
1	3.712715	-0.671266	-0.742852
6	1.509582	1.755052	-1.043543
1	1.250620	1.563088	-2.091697
1	0.807022	2.501091	-0.655307
1	2.512456	2.200918	-1.028719
6	-2.872188	1.475184	-0.086099
1	-2.494844	1.999364	-0.966955
1	-3.607044	0.723565	-0.397796
1	-3.347794	2.196783	0.584876

Table S5. Selected geometrical parameters for parent reaction.

1					
B3LYP	6-31G(d)	6-31+G(d)	6-31G(d,p)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.71	1.713	1.710	1.707	1.708
r(C-H)	1.086	1.087	1.086	1.085	1.084
r(Si-H)	1.479	1.478	1.478	1.476	1.476
a(H-C-Si)	122.38	122.33	122.32	122.4	122.24
a((H-Si-C)	122.59	122.56	122.54	122.62	122.61
MP2	6-31G(d)	6-31+G(d)	6-31G(d,p)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.715	1.717	1.714	1.711	1.711
r(C-H)	1.086	1.087	1.081	1.085	1.086
r(Si-H)	1.477	1.476	1.467	1.473	1.468
a(H-C-Si)	122.0	122.0	121.95	122.04	121.92
a(H-Si-C)	122.5	122.54	122.58	122.58	122.82
H₂O					
B3LYP	6-31G(d)	6-31+G(d)	6-31G(d,p)	6-311G(d)	6-311++G(d,p)
r(O-H)	0.969	0.969	0.965	0.962	0.962
a(H-O-H)	103.66	105.46	103.74	105.97	105.05

MP2	6-31G(d)	6-31+G(d)	6-31G(d,p)	6-311G(d)	6-311++G(d,p)
r(O-H)	0.969	0.971	0.961	0.957	0.96
a(H-O-H)	13.97	105.45	103.83	106.67	103.37

1 complex

B3LYP	6-31G(d)	6-31+G(d)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.712	1.716	1.711	1.710
r(Si-O)	2.488	2.589	2.356	2.682
r(O-H)	0.972	0.972	0.967	0.965
a(C-Si-O)	114.58	109.38	109.92	107.6
d(C-Si-O-H)	53.6	352.19	345.93	358.52
a(H-O-H)	104.07	105.77	107.13	105.88

MP2	6-31G(d)	6-31+G(d)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.713	1.717	1.711	1.712
r(Si-O)	2.553	2.604	2.37	2.677
r(O-H)	0.973	0.975	0.961	0.962
a(C-Si-O)	115.75	110.63	116.13	119.84
d(C-Si-O-H)	54.44	351.0	59.08	61.36
a(H-O-H)	104.24	105.62	107.37	103.97

1 TS

B3LYP	6-31G(d)	6-31+G(d)	6-31G(d,p)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.763	1.772	1.762	1.771	1.769
r(Si-O)	1.97	1.953	1.97	1.92	1.940
r ₁ (O-H)	1.078	1.091	1.07	1.088	1.091
r ₂ (O-H)	0.978	0.978	0.973	0.97	0.97
a(C-Si-O)	89.16	88.32	88.97	88.06	87.81
a ₁ (H-O-Si)	77.12	77.95	76.55	79.92	77.47
a(C-H-O)	125.55	124.78	126.52	122.69	125.63
a(Si-C-H)	68.14	68.84	67.92	69.22	68.92
a(H-O-H)	109.72	112.78	110.68	116.03	115.3
a ₂ (H-O-Si)	115.98	120.55	117.07	123.80	123.14
d(C-Si-O-H)	-1.38	-2.6	-1.61	-2.51	-3.05

MP2	6-31G(d)	6-31+G(d)	6-31G(d,p)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.761	1.772	1.769	1.769	1.766
r(Si-O)	1.963	1.945	1.895	1.895	1.931
r ₁ (O-H)	1.089	1.102	1.089	1.089	1.082
r ₂ (O-H)	0.980	0.982	0.966	0.966	0.968
a(C-Si-O)	88.79	88.10	87.9	87.9	87.76
a ₁ (H-O-Si)	76.53	77.67	79.96	79.95	77.14
a(C-H-O)	123.23	125.09	122.98	122.98	126.44
a(Si-C-H)	68.43	69.08	69.08	69.08	68.56

a(H-O-H)	109.38	112.01	116.37	116.37	112.65
a₂(H-O-Si)	115.57	119.8	123.67	123.67	123.01
d(C-Si-O-H)	358.92	358.25	357.77	357.77	357.55

1 Product

B3LYP	6-31G(d)	6-31+G(d)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.872	1.872	1.867	1.867
r(Si-O)	1.671	1.679	1.665	1.673
r(O-H)	0.967	0.967	0.959	0.959
r(Si-H)	1.495	1.493	1.491	1.490
r(C-H)	1.096	1.097	1.094	1.094
a(C-Si-O)	107.03	106.41	106.78	106.56
a(Si-O-H)	116.28	118.49	120.86	119.97

MP2	6-31G(d)	6-31+G(d)	6-311G(d)	6-311++G(d,p)
r(C-Si)	1.866	1.865	1.860	1.860
r(Si-O)	1.676	1.685	1.660	1.671
r(O-H)	0.969	0.970	0.956	0.958
r(Si-H)	1.491	1.498	1.487	1.480
r(C-H)	1.093	1.095	1.093	1.094
a(C-Si-O)	106.42	105.84	106.51	106.41
a(Si-O-H)	116.35	118.36	121.24	118.12