Supplementary Information

Exploration of the mechanism of the dimerization of Hydroxymethylsilanetriol using electronic structure methods.

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Supporting Information : Cartesian coordinates and energies of important stationary points (Optimized geometrical structures at B3LYP/6-31+G(d) level using the SMD solvation model) :

1. **Formation of dimer D1 (Si-O-C-Si)**

- Structure : **RC**

Energy : E= -1264.56587420 a.u.
Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.661786	-0.285438	-0.028299
2	8	0	1.533277	-1.440683	0.341586
3	1	0	0.600381	-1.306189	0.046207
4	8	0	4.079878	-0.802474	0.677168
5	1	0	3.998613	-1.481096	1.368161
6	8	0	2.897629	-0.095401	-1.666126
7	1	0	1.472153	2.154394	-1.138677
8	6	0	2.242330	1.457564	0.565839
9	1	0	1.871618	1.428028	1.595371
10	1	0	3.145177	2.083905	0.573112
11	8	0	1.206007	2.123290	-0.203791
12	14	0	-2.075922	0.092947	0.192589
13	8	0	-1.110970	-1.130753	-0.441003
14	1	0	-1.136325	-1.250223	-1.406696
15	8	0	-2.045402	-0.156749	1.838163
16	1	0	-2.351666	-1.024202	2.153158
17	6	0	-3.812567	0.058708	-0.527923

18	1	0	-3.774383	0.155838	-1.622647
19	1	0	-4.381169	0.919203	-0.147165
20	8	0	-4.457223	-1.178656	-0.152499
21	1	0	-5.360914	-1.169134	-0.510674
22	8	0	-1.462524	1.591182	-0.106960
23	1	0	3.106004	-0.891267	-2.184677
24	1	0	-0.476514	1.713794	-0.097443

- Structure : **TS**

Energy : E= -1264.51289440 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.431173	-0.076422	-0.070432
2	8	0	-1.963579	-0.060677	1.520001
3	1	0	-1.014197	0.120537	1.711452
4	8	0	-3.716166	-1.119605	-0.216917
5	1	0	-3.641031	-1.973870	0.242257
6	8	0	-2.939711	1.408621	-0.610481
7	1	0	0.236268	1.332969	-0.779295
8	6	0	-1.016223	-0.576523	-1.225087
9	1	0	-0.735829	-1.622794	-1.076574
10	1	0	-1.307087	-0.459891	-2.273920
11	8	0	0.198191	0.217134	-1.040381
12	14	0	1.492534	0.057113	0.217377
13	8	0	0.858780	0.185375	1.788078
14	1	0	0.945060	-0.655377	2.271340
15	8	0	1.542313	-1.657359	0.177414
16	1	0	2.387744	-1.970072	-0.191738
17	6	0	3.274901	0.450297	-0.299840
18	1	0	3.735274	1.100059	0.457389
19	1	0	3.260811	1.015066	-1.241435
20	8	0	4.046151	-0.761756	-0.457009
21	1	0	4.930087	-0.524413	-0.784655
22	8	0	1.107460	1.953876	-0.001099
23	1	0	-3.586793	1.885148	-0.062931
24	1	0	0.655312	2.331402	0.773611

- Structure : **PC1**

Energy : E= -1264.56238570 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	14	0	-2.151232	-0.046323	-0.025619
2	8	0	-1.832242	-0.084201	1.602420
3	1	0	-0.879264	-0.182864	1.833980
4	8	0	-3.666791	-0.690601	-0.258279
5	1	0	-3.920025	-1.428582	0.322233
6	8	0	-2.202896	1.507903	-0.637424
7	1	0	-0.657179	2.602778	-0.674993
8	6	0	-0.810166	-0.925584	-1.020652
9	1	0	-0.767761	-1.994005	-0.772398
10	1	0	-1.032807	-0.861488	-2.091785
11	8	0	0.485783	-0.298338	-0.824966
12	14	0	1.623901	-0.736538	0.292867
13	8	0	0.930401	-0.470380	1.791129
14	1	0	1.273615	-0.974374	2.549149
15	8	0	1.992901	-2.358681	0.256879
16	1	0	2.602841	-2.650271	-0.442757
17	6	0	3.119877	0.362159	0.000505
18	1	0	3.788049	0.318442	0.872422
19	1	0	2.800304	1.407977	-0.114262
20	8	0	3.809653	-0.091573	-1.185337
21	1	0	4.571427	0.494281	-1.333506
22	8	0	0.096231	3.231803	-0.684705
23	1	0	-2.846953	2.117015	-0.234937
24	1	0	0.883211	2.662755	-0.647192

2. Formation of dimer D2(Si-O-Si)

- Structure : **RC**

Energy : E= -1264.55822482 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.140162	0.597196	-0.157626
2	6	0	3.914333	0.090644	-0.548619
3	1	0	4.264164	0.632122	-1.434068
4	1	0	4.595483	0.359214	0.272008
5	8	0	4.049407	-1.317416	-0.867508
6	1	0	3.853352	-1.831808	-0.066245
7	8	0	1.642448	-0.400218	1.070734
8	1	0	0.673178	-0.445951	1.250768
9	8	0	2.052111	2.222643	0.206562
10	1	0	2.647176	2.542592	0.905156
11	8	0	1.105171	0.517961	-1.462621
12	14	0	-2.248480	-0.651067	0.265772
13	8	0	-1.107136	-0.567710	1.488741
14	1	0	-1.374341	-0.111353	2.305778
15	8	0	-3.660684	-1.169118	0.978475

16	1	0	-4.466224	-0.749977	0.626437
17	6	0	-2.550543	0.972520	-0.651499
18	1	0	-1.944673	1.777786	-0.214975
19	1	0	-2.258392	0.875430	-1.705258
20	8	0	-3.958583	1.289850	-0.545939
21	1	0	-4.116894	2.124622	-1.018491
22	8	0	-1.622544	-1.730654	-0.827818
23	1	0	0.786264	-0.366517	-1.708755
24	1	0	-1.315417	-2.587546	-0.485097

- Structure : **TS1**

Energy : E= -1264.51519529 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	1.707174	0.512562	0.114276
2	6	0	3.240783	-0.056355	-0.829076
3	1	0	3.160027	0.237885	-1.881180
4	1	0	4.148024	0.428469	-0.438815
5	8	0	3.412696	-1.497245	-0.836296
6	1	0	3.555087	-1.791524	0.079071
7	8	0	1.850832	-0.085550	1.671563
8	1	0	0.960386	-0.302537	2.023106
9	8	0	1.632215	2.187956	0.118022
10	1	0	2.338570	2.646452	0.603117
11	8	0	0.300618	0.014154	-0.572095
12	14	0	-1.636389	-0.421422	0.161586
13	8	0	-0.925250	-0.441342	1.682884
14	1	0	-1.555724	-0.702043	2.377031
15	8	0	-3.127678	-1.134336	0.557229
16	1	0	-3.877952	-0.635177	0.187769
17	6	0	-2.150988	1.160891	-0.732858
18	1	0	-1.624719	2.017090	-0.291712
19	1	0	-1.854043	1.100828	-1.787389
20	8	0	-3.581368	1.333447	-0.621947
21	1	0	-3.834059	2.121626	-1.132129
22	8	0	-1.053837	-1.735625	-0.912622
23	1	0	-0.052232	-1.194397	-0.952825

24	1	0	-1.044598	-2.651504	-0.572987

- Structure : **IM**

Energy : E= -1264.54350032 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.798828	-0.620310	0.005261
2	6	0	-2.692323	0.809397	-0.855077
3	1	0	-2.684441	0.670039	-1.940727
4	1	0	-3.738333	0.930657	-0.551049
5	8	0	-1.981470	2.071360	-0.621267
6	1	0	-2.192175	2.385025	0.275807
7	8	0	-1.972048	-0.456998	1.661657
8	1	0	-1.084195	-0.333189	2.068481
9	8	0	-2.408357	-2.084049	-0.517551
10	1	0	-3.319834	-2.304003	-0.260538
11	8	0	-0.219502	-0.583814	-0.400984
12	14	0	1.269739	0.147313	0.185081
13	8	0	0.777633	-0.056770	1.806264
14	1	0	1.411781	0.338447	2.427248
15	8	0	2.635329	1.164800	0.609824
16	1	0	3.458359	0.778225	0.261214
17	6	0	2.270369	-1.141963	-0.806951
18	1	0	2.013404	-2.145089	-0.438867
19	1	0	1.960616	-1.100222	-1.860149
20	8	0	3.698717	-0.930705	-0.706269
21	1	0	4.151494	-1.583732	-1.265797
22	8	0	0.622874	1.699372	-0.627602
23	1	0	-0.378647	1.887925	-0.652034
24	1	0	1.115530	2.507707	-0.388787

- Structure : **TS2**

Energy : E= -1264.54179114 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.693845	-0.732740	-0.019903
2	6	0	-2.846384	0.630833	-0.641032
3	1	0	-2.864573	0.652627	-1.735313
4	1	0	-3.882893	0.515364	-0.301851
5	8	0	-2.349986	1.945052	-0.232193
6	1	0	-2.547790	2.072393	0.712040

7	8	0	-1.696234	-0.736049	1.651026
8	1	0	-0.843155	-0.402048	2.006905
9	8	0	-2.163926	-2.216549	-0.613293
10	1	0	-3.093508	-2.469254	-0.484191
11	8	0	-0.169200	-0.473254	-0.563272
12	14	0	1.270505	0.283119	0.009495
13	8	0	0.908723	0.298214	1.667492
14	1	0	1.521586	0.819419	2.211512
15	8	0	2.578144	1.392365	-0.158463
16	1	0	3.406261	0.880951	-0.240210
17	6	0	2.301011	-1.258267	-0.494996
18	1	0	1.934112	-2.143624	0.042322
19	1	0	2.171125	-1.454716	-1.568634
20	8	0	3.711887	-1.060961	-0.207440
21	1	0	4.223741	-1.765808	-0.638244
22	8	0	0.315843	1.923718	-0.580939
23	1	0	-0.668360	2.017925	-0.408854
24	1	0	0.760424	2.755773	-0.336950

- Structure : **PC2**

Energy : E= -1264.57168651 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-1.446036	0.132991	0.444150
2	8	0	-1.699209	1.762597	0.163927
3	1	0	-2.367018	1.975755	-0.511583
4	8	0	-1.070070	-0.019266	2.052714
5	1	0	-0.202474	-0.445803	2.211878
6	8	0	-0.154010	-0.375507	-0.459983
7	6	0	-2.999474	-0.832766	0.018344
8	1	0	-3.773457	-0.635882	0.773815
9	1	0	-2.789638	-1.911385	0.040748
10	8	0	-3.460939	-0.431490	-1.291299
11	1	0	-4.271070	-0.930646	-1.492121
12	14	0	1.407290	-0.886773	-0.248941
13	8	0	1.709956	-2.241850	-1.159145
14	1	0	1.153766	-3.025354	-1.006838
15	8	0	1.456806	-1.188417	1.397953
16	1	0	2.288213	-1.514309	1.782258
17	6	0	2.670804	0.389110	-0.811945
18	1	0	3.675078	-0.043211	-0.723473
19	1	0	2.533802	0.629908	-1.876152
20	8	0	2.666779	1.588445	-0.012475
21	1	0	1.892494	2.148254	-0.264717
22	8	0	0.552456	3.300739	-0.620687
23	1	0	-0.243852	2.807811	-0.319061

24	1	0	0.679262	3.998155	0.044944

3. Formation of dimer D3 (Si-C-O-C-Si)

- Structure : **RC**

Energy : E= -1264.56453473 a.u.
Cartesian coordinates :
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-3.039430	-0.266588	-0.088745
2	8	0	-3.755466	0.406380	-1.436279
3	1	0	-4.338568	1.169879	-1.286917
4	8	0	-4.138535	-0.459420	1.147186
5	1	0	-4.981427	-0.899492	0.943264
6	8	0	-2.371953	-1.691841	-0.622782
7	1	0	-2.870831	-2.197371	-1.286697
8	6	0	-1.661248	0.758125	0.671491
9	1	0	-2.061399	1.723971	1.009358
10	1	0	-1.256652	0.249822	1.558629
11	8	0	-0.619118	0.969323	-0.306170
12	6	0	2.571631	1.207364	1.155393
13	1	0	3.560549	1.648776	1.338444
14	1	0	2.180606	0.868351	2.124360
15	14	0	2.739705	-0.266699	-0.009071
16	8	0	3.467936	0.316584	-1.386851
17	1	0	3.532355	-0.294996	-2.140082
18	8	0	1.290379	-1.016505	-0.307533
19	1	0	0.504281	-0.412573	-0.369145
20	8	0	3.765248	-1.411676	0.632230
21	1	0	3.374682	-2.045508	1.256980
22	8	0	1.687551	2.208618	0.587660
23	1	0	0.069038	1.558787	0.086930
24	1	0	1.583169	2.925949	1.236168

- Structure : **TS**

Energy : E= -1264.45617471 a.u.
Cartesian coordinates :
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.798581	-0.204188	0.015315
2	8	0	-3.310024	0.864272	-1.163953
3	1	0	-3.647466	1.721347	-0.852772
4	8	0	-3.908994	-0.279025	1.260221
5	1	0	-4.840069	-0.431297	1.024834

6	8	0	-2.602657	-1.652652	-0.781856
7	1	0	-3.260947	-1.875701	-1.461806
8	6	0	-1.159177	0.239981	0.828673
9	1	0	-1.306868	1.153602	1.430683
10	1	0	-0.895505	-0.561933	1.542968
11	8	0	-0.151431	0.418001	-0.143790
12	6	0	1.856642	0.896879	1.050724
13	1	0	2.425527	1.781342	1.318375
14	1	0	1.132912	0.612921	1.809475
15	14	0	2.661162	-0.423883	-0.025735
16	8	0	3.459216	0.411621	-1.209351
17	1	0	3.903233	-0.106283	-1.902488
18	8	0	1.523293	-1.490224	-0.553036
19	1	0	0.661016	-0.959691	-0.519783
20	8	0	3.811949	-1.200667	0.888055
21	1	0	3.503624	-1.927240	1.457036
22	8	0	1.052784	2.614402	-0.194278
23	1	0	0.351017	1.891950	-0.313207
24	1	0	0.719523	3.186988	0.520086

- Structure : **PC3**

Energy : E= -1264.56565732 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	2.694885	-0.264700	0.066608
2	8	0	2.875112	1.257104	0.721554
3	1	0	3.145599	1.969041	0.117068
4	8	0	3.940777	-0.635216	-0.972222
5	1	0	4.850415	-0.571527	-0.634707
6	8	0	2.586251	-1.283317	1.374533
7	1	0	3.114110	-1.055567	2.158765
8	6	0	1.163509	-0.528550	-0.995061
9	1	0	1.248286	0.016830	-1.946961
10	1	0	1.092464	-1.598106	-1.245535
11	8	0	-0.030540	-0.120646	-0.300691
12	6	0	-1.226953	-0.509384	-1.006393
13	1	0	-1.300312	0.041913	-1.956003
14	1	0	-1.168097	-1.578863	-1.259070
15	14	0	-2.743932	-0.226867	0.073404
16	8	0	-2.969792	1.413811	0.181250
17	1	0	-3.657425	1.731133	0.791352
18	8	0	-2.586433	-0.959280	1.561225
19	1	0	-1.736263	-0.837598	2.018180
20	8	0	-4.113520	-0.865567	-0.618686
21	1	0	-4.216340	-1.832126	-0.592257
22	8	0	0.089387	2.775712	-0.489088
23	1	0	0.016402	1.802921	-0.375442

24	1	0	1.009720	2.972123	-0.246969

Transition states for the determinant steps for the mechanisms of dimerization with one water molecule:

- Structure : **D1'**

Energy: E(RM06)= -1340.84904011 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.414197	-0.252867	-0.141747
2	8	0	-2.036792	-0.704757	1.409652
3	1	0	-1.079756	-0.666975	1.659427
4	8	0	-3.668739	-1.212378	-0.672156
5	1	0	-3.593210	-2.165237	-0.493317
6	8	0	-2.962786	1.316614	-0.224484
7	1	0	0.099959	1.702401	-0.756117
8	6	0	-0.911730	-0.338024	-1.284570
9	1	0	-0.598641	-1.371440	-1.456491
10	1	0	-1.138506	0.102938	-2.261973
11	8	0	0.216287	0.402796	-0.735955
12	14	0	1.449685	-0.218396	0.378793
13	8	0	0.723232	-0.779849	1.847185
14	1	0	0.726424	-1.752307	1.862369
15	8	0	1.415375	-1.864386	-0.231630
16	1	0	2.150127	-2.001331	-0.855492
17	6	0	3.240395	0.137262	-0.212503
18	1	0	3.912142	0.123992	0.658141
19	1	0	3.287319	1.149210	-0.636356
20	8	0	3.697490	-0.823621	-1.197092
21	1	0	4.627478	-0.637473	-1.408457
22	8	0	0.272676	2.805237	-0.522816
23	1	0	-3.665491	1.572048	0.397378
24	1	0	-0.569822	3.186672	-0.206424
25	8	0	1.532412	1.429586	1.182429
26	1	0	1.024123	1.434282	2.010376
27	1	0	0.835789	2.571549	0.309655

- Structure : **D2'**

Energy: E(RM06)= -1340.85504133 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	14	0	-1.445753	-0.237675	0.248050
2	6	0	-2.924660	0.875521	-0.098445
3	1	0	-3.106043	1.537924	0.754367
4	1	0	-2.744567	1.518831	-0.970608
5	8	0	-4.148701	0.120009	-0.280387
6	1	0	-4.076988	-0.381660	-1.109989
7	8	0	-1.616641	-0.884393	1.768351
8	1	0	-0.755345	-1.297793	2.003685
9	8	0	-1.372985	-1.367847	-0.963050
10	1	0	-0.490295	-1.769373	-1.165747
11	8	0	-0.035985	0.727766	0.194396
12	1	0	-0.116060	1.855104	-0.264702
13	14	0	1.634519	0.055081	0.257870
14	8	0	0.088537	2.921990	-0.795736
15	8	0	2.611705	0.452232	1.599344
16	8	0	0.991379	-1.358495	1.156386
17	6	0	2.014955	-0.945534	-1.331335
18	8	0	2.259838	1.540755	-0.542868
19	1	0	-0.033996	3.633758	-0.138056
20	1	0	1.080035	2.748323	-0.858665
21	1	0	2.525023	-0.221841	2.293334
22	1	0	1.047442	-2.172902	0.626794
23	1	0	3.089482	-1.168012	-1.391584
24	1	0	1.756952	-0.340003	-2.207993
25	8	0	1.261433	-2.192280	-1.374515
26	1	0	2.880368	2.005422	0.041591
27	1	0	1.450866	-2.649275	-2.212010

- Structure : **D3'**

Energy: E(RM06)= -1340.75263173 a.u.

Cartesian coordinates :

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-2.620685	-0.600768	0.056337
2	8	0	-2.878051	-0.558640	1.701573
3	1	0	-2.385484	-1.199040	2.243000
4	8	0	-3.285316	-1.924796	-0.691289
5	1	0	-4.237627	-2.079710	-0.568721
6	8	0	-3.387553	0.746649	-0.542652
7	1	0	-3.240606	1.586906	-0.075786
8	6	0	-0.780748	-0.691247	-0.371356
9	1	0	-0.350248	-1.581841	0.095524
10	1	0	-0.625973	-0.772085	-1.453095
11	8	0	-0.077775	0.459485	0.164643
12	1	0	-0.293806	1.246891	-0.403247
13	8	0	-0.595891	2.787969	-1.212999
14	1	0	-1.539146	2.972850	-1.068898

15	1	0	-0.125249	3.033601	-0.329305
16	14	0	2.577680	-0.646632	-0.042449
17	8	0	2.089373	-1.147035	-1.535556
18	1	0	2.789746	-1.350150	-2.178765
19	8	0	1.992151	-1.576768	1.185208
20	1	0	2.100773	-2.541210	1.116320
21	8	0	4.239622	-0.579663	-0.103165
22	1	0	4.723278	-0.494042	0.737137
23	6	0	2.130031	1.126849	0.342916
24	1	0	2.324162	1.503340	1.341252
25	1	0	2.223537	1.875628	-0.438232
26	8	0	0.620635	2.935488	1.031703
27	1	0	1.405448	3.507345	0.979281