Supporting Information Available (Total 12 pages)

for

Insights into the Mechanism of Selective Olefin Epoxidation Catalyzed by $[\square(\text{SiO}_4)\text{W}_{10}\text{O}_{32}\text{H}_4]^{4-}$. A Computational Study

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a. Complete Ref. 34: Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Table S1: Structure **I_S**

W	0.441995	-0.224072	-0.237927
O	0.052391	0.191655	-2.029330
O	1.388277	-1.656510	-0.394153
O	-0.750106	1.760475	0.166401
O	0.156494	-0.365288	1.658607
O	1.803101	1.112823	-0.074156
H	2.763646	1.066332	0.068167
H	-0.416778	0.262936	2.139936
H	-0.782817	0.362726	-2.525207
H	-0.143989	2.517915	0.058170
H	-1.611319	1.853548	-0.331588
O	-1.472338	-0.911328	-0.330871
H	-1.827235	-1.484892	0.380719
C	-2.285397	-3.726287	1.373988
C	-2.124561	-2.867877	2.405082
H	-3.256097	-4.152546	1.126535
H	-1.444233	-4.039116	0.758109
H	-2.962844	-2.570200	3.033644
H	-1.149227	-2.452381	2.651056
H	-2.307159	-0.353576	-1.324400
O	-2.690709	0.259664	-2.123659
O	-2.865668	1.573192	-1.407209
H	-3.822038	1.758373	-1.526811

Table S2: Structure **TS1_S**

W	0.379348	-0.614791	-0.094641
O	0.732539	0.665590	-1.364694
O	-0.986762	-1.413635	-0.808748
O	1.811779	0.757265	1.014495
O	0.084236	-1.105245	1.743304
O	1.750701	-1.838195	-0.404474
H	1.972357	-2.718354	-0.740834
H	-0.460812	-0.649779	2.408948
H	0.581886	1.756465	-1.260550
H	2.013332	0.553754	1.943812
H	1.887603	1.730686	0.762922
O	-0.968241	1.050192	0.589114
H	-1.939821	0.921229	0.503915
C	-3.882470	0.287459	-0.633250
C	-4.301800	0.254472	0.651927
H	-4.118658	1.126973	-1.285703
H	-3.299668	-0.524026	-1.064656
H	-4.893329	1.058818	1.086105
H	-4.088586	-0.597188	1.296117
H	-0.624151	1.980644	0.216290
O	0.198493	2.909328	-0.625689
O	1.400783	3.180767	0.257256
H	1.815488	3.955174	-0.179480

Table S3: Structure **II_S**

W	0.555413	-0.446824	-0.075019
O	0.945515	0.553614	-1.635074
O	-0.280178	-1.758228	-0.833212
O	1.768471	1.283985	0.836375
O	-0.108627	-0.647102	1.679410
O	2.243424	-1.261746	0.248842
H	2.578091	-2.164694	0.113344
H	-0.709059	0.018364	2.096086
H	1.034653	1.518159	-1.770642
H	2.633830	1.116420	1.248140
H	1.591761	2.208743	0.482080
O	-0.889008	1.106741	-0.057757
O	-1.760522	1.251577	1.152819
C	-4.404142	0.157581	-0.523402
C	-3.850671	-0.966568	-0.013087
H	-5.309361	0.594956	-0.104260
H	-3.981299	0.652273	-1.396223
H	-4.288057	-1.476066	0.844612
H	-2.957999	-1.417066	-0.443856
H	-0.203667	2.550438	-0.296213
O	0.609939	3.141738	-0.433440
H	-2.613023	0.859364	0.817930
H	0.420343	4.093386	-0.484349

Table S4: Structure **TS2_S**

W	0.990038	0.096044	-0.065443
O	1.515032	0.636231	1.678543
O	1.880046	1.228858	-1.027208
O	-0.352527	-1.361063	1.348860
O	0.210454	-1.127473	-1.437405
O	2.142747	-1.467306	0.053356
H	2.184846	-2.097551	-0.693055
H	-0.511889	-0.757651	-1.982327
H	1.308426	0.214006	2.531853
H	-0.065956	-2.262325	1.105226
H	-1.252447	-1.135481	1.008796
O	-0.708720	0.947174	-0.108285
O	-2.354271	-0.111374	-0.029543
C	-4.232360	-1.000850	0.510787
C	-3.752923	-0.992933	-0.807348
H	-3.970207	-1.799577	1.197843
H	-4.857427	-0.198431	0.892494
H	-3.246422	-1.861437	-1.215767
H	-4.139740	-0.284796	-1.535426
H	-2.730827	0.867622	0.067774
O	-2.732668	2.350917	0.194457
H	-1.732943	2.284950	0.104186
H	-3.137262	3.118379	-0.241615

Table S5: Structure III_S

W	1.023891	0.022429	-0.080062
O	1.816154	0.553470	1.556499
O	2.336415	0.268721	-1.177453
O	-0.746852	-0.509637	1.469465
O	-0.193811	-0.965004	-1.340652
O	1.260197	-1.840708	0.533477
H	1.196225	-2.549326	-0.136327
H	-0.264626	-0.577792	-2.237246
H	1.557984	0.434436	2.485982
H	-0.492193	-1.453079	1.570039
H	-1.697851	-0.370222	1.224723
O	0.011720	1.555264	-0.372896
O	-3.250316	-0.053173	0.454600
C	-4.236362	-1.161204	0.164996
C	-3.289176	-0.745074	-0.906640
H	-4.046670	-2.069292	0.730779
H	-5.269563	-0.826779	0.134920
H	-2.374099	-1.298161	-1.107374
H	-3.644953	-0.091003	-1.698033
H	-2.948814	1.692938	0.295701
O	-2.371395	2.440234	0.003565
H	-0.894444	1.988432	-0.265657
H	-2.632604	3.304418	0.364116

Table S6: Structure I_r

Si	0.017269	0.003002	0.387252
O	1.701685	2.608918	1.657956
O	2.610696	0.722354	-2.480717
O	1.847909	3.427141	-3.122952
O	2.956759	2.638056	-0.648494
O	0.443282	3.196339	-0.613796
O	-0.037989	1.375041	-2.584677
O	-3.028648	1.790878	2.469502
O	-2.387983	1.695335	-1.371068
O	-4.489924	2.634906	0.263973
O	-0.849058	-1.219442	-3.261163
O	1.557736	-1.312747	3.863741
O	1.483540	-1.775238	-1.949262
O	-2.119721	-2.858779	-1.576417
O	0.038477	-3.958841	-3.039222
O	0.029590	-3.317941	-0.233523
O	-3.300862	0.027399	0.478254
O	-4.673631	-2.341801	-0.342320
O	-3.190790	-0.602752	-2.090310
O	1.416828	-3.376824	2.095050
O	2.910198	-1.813287	0.300629
O	-1.008826	-4.885079	1.868279
O	4.061011	0.386613	-0.248090
O	2.898488	0.118729	2.110543
O	4.566483	2.405110	1.735556

O	3.950816	-2.480754	2.817280
O	4.288033	-1.576876	-2.264832
O	-2.314359	1.024892	-4.226882
O	0.401937	-1.175209	1.420922
O	1.432047	0.567057	-0.251991
O	-0.916631	-0.686022	-0.790763
O	-0.703775	-2.620475	3.448907
O	-0.803768	1.291004	0.930763
O	-2.152465	-2.453545	1.022080
O	-0.726464	3.071984	3.002151
O	0.390506	5.102395	1.465141
O	-1.889915	3.528490	0.693069
W	2.482876	-1.825596	2.138441
W	3.016451	-0.786829	-1.375399
W	-1.673246	0.413951	-2.727739
W	0.005625	3.413178	1.280746
W	1.522613	2.255953	-1.875450
W	-2.876237	1.950096	0.412693
W	-0.242014	-2.607845	-1.976288
W	-3.091249	-1.619216	-0.444467
W	-0.517386	-3.225281	1.653334
W	3.208546	1.607090	0.989258
H	-1.562067	2.513921	3.064479
H	1.461138	-0.345606	3.979059
H	0.033645	-2.020479	3.807222
C	-4.549585	-0.356731	4.584755
C	-3.874162	-1.335478	3.943250
H	-3.056650	0.873196	2.815481
H	-3.016951	-1.849156	4.375136
H	-4.123998	-1.629533	2.926379
H	-4.269535	-0.032045	5.588005
H	-5.361340	0.190568	4.108498
O	-6.181906	2.530366	2.418209
H	-5.740231	2.641148	1.521120
O	-5.160556	3.134419	3.353361
H	-4.315888	2.607682	3.114310

Table S7: Structure TS_{I_r}

Si	0.006608	0.011943	0.383138
O	1.584528	2.733908	1.570322
O	2.638377	0.736223	-2.470239
O	1.808191	3.395775	-3.202536
O	2.894905	2.720167	-0.695780
O	0.372523	3.182698	-0.688986
O	-0.036405	1.325176	-2.614458
O	-3.295294	1.714307	2.340969
O	-2.403711	1.566726	-1.397942
O	-4.608071	2.465159	0.106565
O	-0.740678	-1.299328	-3.250314
O	1.505834	-1.148599	3.907693
O	1.593822	-1.761107	-1.885916
O	-1.976405	-2.975704	-1.580409
O	0.254435	-3.998724	-2.981822
O	0.159109	-3.323257	-0.181841

O	-3.323378	-0.123859	0.405506
O	-4.577908	-2.564343	-0.420278
O	-3.128740	-0.765991	-2.134343
O	1.497596	-3.274887	2.187337
O	2.970717	-1.704872	0.399698
O	-0.839309	-4.902724	1.925701
O	4.044991	0.528435	-0.193392
O	2.845842	0.280268	2.145125
O	4.432638	2.625847	1.749322
O	3.963539	-2.256983	2.967294
O	4.403518	-1.489870	-2.131575
O	-2.289231	0.880427	-4.256590
O	0.415128	-1.132813	1.445699
O	1.413304	0.614207	-0.244517
O	-0.872252	-0.738054	-0.799204
O	-0.692616	-2.598891	3.473216
O	-0.877954	1.275671	0.898964
O	-2.080594	-2.541654	1.012359
O	-0.615667	3.062042	3.007540
O	0.023197	5.157213	1.299389
O	-2.044804	3.455759	0.629819
W	2.494539	-1.672734	2.228204
W	3.086557	-0.718718	-1.293017
W	-1.642483	0.306593	-2.744538
W	-0.185089	3.432865	1.136679
W	1.510400	2.241558	-1.931890
W	-3.001367	1.803318	0.366376
W	-0.098420	-2.646728	-1.941678
W	-3.025100	-1.777511	-0.484475
W	-0.422363	-3.225398	1.692999
W	3.114452	1.761840	1.002269
H	-1.059211	3.668138	3.629123
H	1.307574	-0.190829	3.960647
H	-0.005534	-1.954020	3.840887
C	-4.261086	-0.003161	5.020812
C	-3.777663	-0.947575	4.184348
H	-2.792126	1.092420	2.902702
H	-3.038947	-1.688154	4.484803
H	-4.078987	-0.977296	3.139177
H	-3.941525	0.048684	6.063798
H	-4.953836	0.764564	4.673026
O	-6.374732	2.508421	2.310468
H	-5.878230	2.646934	1.450561
O	-5.346918	2.915689	3.341678
H	-4.502748	2.410766	3.015534

Table S8: Structure II_f

Si	-0.028316	-0.007438	-0.399833
O	-2.323095	1.892085	-1.942183
O	-2.752873	0.372891	2.418085
O	-2.715777	3.246345	2.695291
O	-3.559914	1.892153	0.370359
O	-1.267692	3.061653	0.207072
O	-0.367483	1.687217	2.396762

O	2.473556	2.341270	-2.727905
O	1.819422	2.454022	1.110082
O	3.675163	3.694494	-0.560691
O	1.100828	-0.504242	3.350108
O	-1.146481	-2.094285	-3.649949
O	-1.001718	-1.792910	2.170668
O	2.760284	-1.951002	1.842290
O	0.946844	-3.381780	3.486934
O	0.811524	-3.116760	0.627042
O	3.172090	0.873757	-0.613699
O	5.088059	-0.954309	0.477465
O	3.202516	0.556406	2.040038
O	-0.488015	-3.818887	-1.644985
O	-2.351535	-2.478729	-0.025532
O	2.252113	-4.602237	-1.278200
O	-4.043422	-0.603649	0.280306
O	-2.831885	-0.853522	-2.056370
O	-5.039729	0.950987	-1.922571
O	-3.158051	-3.704152	-2.414716
O	-3.762928	-2.292330	2.524387
O	1.912920	2.137758	4.013229
O	-0.085640	-1.363857	-1.273498
O	-1.549917	0.233404	0.204618
O	1.042693	-0.280207	0.831462
O	1.389360	-2.731139	-3.131333
O	0.422645	1.379049	-1.103427
O	2.696146	-1.865820	-0.783874
O	-0.076102	2.766005	-3.398258
O	-1.672027	4.626105	-2.104073
O	0.920154	3.835532	-1.188507
W	-1.918302	-2.609815	-1.858665
W	-2.733418	-1.315347	1.515607
W	1.459317	1.213087	2.609558
W	-0.880054	3.123330	-1.711660
W	-2.089027	2.045901	1.600240
W	2.278345	2.642491	-0.697159
W	0.878479	-2.148315	2.259428
W	3.374671	-0.644386	0.548169
W	1.330767	-3.121157	-1.268732
W	-3.527915	0.628605	-1.117737
H	0.850647	2.390504	-3.458033
H	-1.279614	-1.153110	-3.883382
H	0.543014	-2.374441	-3.555278
C	5.758045	-1.687662	-4.303911
C	4.824011	-2.017453	-3.388154
H	5.043059	-2.019449	-2.321539
H	3.801128	-2.277210	-3.658915
H	6.768782	-1.397001	-4.015065
H	5.525749	-1.654004	-5.368976
O	5.558510	3.562943	-2.722361
H	5.019833	2.817559	-3.081599
O	3.586806	1.464394	-3.203601
H	3.642986	0.789733	-2.465739
H	5.097839	3.837927	-1.894773

Table S9: Structure TS2_r

Si	0.003380	0.001873	0.390337
O	1.989232	2.357817	1.734259
O	2.712797	0.470526	-2.429011
O	2.306790	3.271139	-3.003630
O	3.275666	2.281074	-0.548002
O	0.844515	3.147477	-0.520186
O	0.176719	1.452555	-2.552844
O	-2.829168	2.292430	2.568563
O	-2.129701	2.055317	-1.374481
O	-4.117778	3.164103	0.291516
O	-0.935463	-1.003414	-3.313502
O	1.318646	-1.581060	3.841116
O	1.289052	-1.885002	-1.983182
O	-2.430757	-2.513097	-1.695909
O	-0.395710	-3.835930	-3.154541
O	-0.378722	-3.274501	-0.336187
O	-3.266210	0.452950	0.420065
O	-4.914731	-1.722229	-0.493274
O	-3.192871	-0.117017	-2.140138
O	0.951988	-3.567448	2.004403
O	2.652289	-2.147274	0.285940
O	-1.633351	-4.765558	1.694190
O	4.076426	-0.093933	-0.187899
O	2.856156	-0.279147	2.146463
O	4.796389	1.795753	1.861191
O	3.559185	-3.010276	2.793888
O	4.102111	-2.018402	-2.248990
O	-2.093031	1.421788	-4.244427
O	0.226645	-1.240369	1.393860
O	1.485005	0.411228	-0.215075
O	-0.977302	-0.532983	-0.829885
O	-1.087590	-2.620384	3.361861
O	-0.681581	1.362073	0.962455
O	-2.454278	-2.181020	0.915323
O	-0.313254	3.036027	3.108098
O	0.968788	5.002869	1.618384
O	-1.443815	3.723047	0.786664
W	2.197252	-2.154380	2.117992
W	2.922714	-1.099395	-1.356764
W	-1.554463	0.702261	-2.753239
W	0.391977	3.378475	1.368575
W	1.824115	2.115743	-1.792761
W	-2.619594	2.254805	0.403821
W	-0.519467	-2.490788	-2.055208
W	-3.251743	-1.209847	-0.534019
W	-0.937621	-3.173210	1.553288
W	3.359389	1.195346	1.078226
H	-1.141346	2.484503	3.194807
H	1.309579	-0.612090	3.979293
H	-0.320037	-2.098199	3.763108
C	-5.644583	-0.193909	4.094612
C	-4.351857	-0.484935	4.439307

H	-3.746796	-1.156691	3.839026
H	-3.918950	-0.156366	5.382066
H	-6.060270	-0.532102	3.149642
H	-6.261926	0.464208	4.705852
O	-5.416081	3.477505	2.818834
H	-5.242965	3.533628	1.848815
O	-3.945817	1.216855	3.327222
H	-5.143872	2.554914	3.111382
H	-3.280982	3.130351	2.839418

Table S10: Structure III_r

Si	-0.037381	0.000528	-0.392170
O	-2.146845	2.210981	-1.787585
O	-2.690142	0.456795	2.473831
O	-2.380834	3.284353	2.941307
O	-3.371508	2.168813	0.537824
O	-0.993134	3.144358	0.421676
O	-0.180339	1.553297	2.476311
O	2.572606	2.154184	-2.621968
O	2.078975	2.157175	1.176787
O	4.017052	3.281670	-0.540099
O	1.067300	-0.806625	3.289731
O	-1.354521	-1.754915	-3.758502
O	-1.160090	-1.838967	2.070005
O	2.570329	-2.341042	1.694670
O	0.640381	-3.656490	3.287623
O	0.515579	-3.223047	0.433331
O	3.249382	0.552035	-0.571192
O	4.996472	-1.484742	0.356204
O	3.268464	0.085685	2.043707
O	-0.858064	-3.661309	-1.875328
O	-2.576650	-2.261140	-0.152291
O	1.773574	-4.746179	-1.579346
O	-4.081381	-0.258135	0.290012
O	-2.911912	-0.465629	-2.067688
O	-4.939044	1.529050	-1.795610
O	-3.506851	-3.240916	-2.611581
O	-3.955259	-2.102406	2.421685
O	2.155521	1.722431	4.062316
O	-0.227511	-1.283199	-1.351744
O	-1.523776	0.352641	0.239974
O	1.016672	-0.450455	0.801361
O	1.126564	-2.644916	-3.289833
O	0.534477	1.379673	-1.013607
O	2.512791	-2.099189	-0.927956
O	0.176450	2.961949	-3.194566
O	-1.248620	4.888784	-1.788807
O	1.255598	3.779960	-0.933653
W	-2.169676	-2.304240	-1.993055
W	-2.843065	-1.162282	1.465183
W	1.607859	0.912282	2.620812
W	-0.594054	3.298917	-1.494634
W	-1.875382	2.110972	1.756393
W	2.499969	2.396321	-0.656126

W	0.684739	-2.354105	2.130902
W	3.313063	-1.029551	0.470891
W	1.013871	-3.179453	-1.453247
W	-3.457832	1.019206	-1.029883
H	1.095270	2.522385	-3.228711
H	-1.379780	-0.788802	-3.914352
H	0.302809	-2.207298	-3.680118
C	5.240894	-0.317325	-2.955855
C	4.018951	-0.854069	-3.607023
H	4.105186	-1.508750	-4.470707
H	3.104656	-0.943733	-3.031288
H	6.223914	-0.584704	-3.340366
H	5.185831	-0.020497	-1.914617
O	5.981201	3.161736	-2.517181
H	5.508640	2.539845	-3.108008
H	5.394983	3.326373	-1.731525
H	3.249230	1.611413	-3.100561
O	4.458488	0.578455	-3.900775

Table S11: Structure I_{1CC}

Si	0.022068	0.038862	0.235036
O	1.534593	2.981989	0.471883
O	2.530444	-0.146427	-2.842109
O	1.618272	2.124908	-4.336132
O	2.771617	2.283733	-1.750594
O	0.256790	2.712550	-1.866406
O	-0.159109	0.315000	-3.069405
O	-3.088476	2.384041	1.634049
O	-2.487369	0.934323	-1.938912
O	-4.628621	2.250476	-0.669814
O	-0.850866	-2.367991	-2.796098
O	1.768645	-0.214305	4.105887
O	1.541291	-2.371151	-1.479108
O	-1.999800	-3.404876	-0.620236
O	0.168631	-4.845121	-1.732828
O	0.204460	-3.313720	0.694550
O	-3.278955	-0.031986	0.418672
O	-4.525030	-2.593526	0.502198
O	-3.183454	-1.488198	-1.788831
O	1.629708	-2.599272	2.812543
O	3.007922	-1.616960	0.610994
O	-0.705817	-4.252520	3.185001
O	3.997110	0.339621	-0.645886
O	2.863733	0.814796	1.701990
O	4.390949	2.925081	0.550121
O	4.069067	-1.304713	3.199682
O	4.327250	-2.163531	-1.932010
O	-2.468958	-0.656509	-4.395594
O	0.517068	-0.668106	1.618961
O	1.385759	0.397635	-0.626985
O	-0.883657	-1.054065	-0.605192
O	-0.471767	-1.616553	4.039865
O	-0.858572	1.400567	0.334023
O	-1.975081	-2.181547	1.716083

O	-0.878656	3.878702	1.591661
O	0.169069	5.213639	-0.616759
O	-2.068594	3.376190	-0.668298
W	2.582967	-1.019681	2.325360
W	3.021686	-1.197098	-1.323483
W	-1.760341	-0.700501	-2.813529
W	-0.171598	3.561510	-0.196747
W	1.363547	1.425684	-2.769262
W	-2.981217	1.746973	-0.342270
W	-0.154726	-3.237277	-1.165659
W	-2.985467	-1.897639	0.099648
W	-0.297499	-2.716814	2.483367
W	3.086569	1.860712	0.109009
H	-1.764041	3.416589	1.762356
H	2.347181	-0.503622	4.841835
H	0.286673	-0.970789	4.213292
C	-4.682958	1.035630	4.450130
C	-4.253597	-0.073039	3.807683
H	-3.105057	1.654902	2.288880
H	-3.542806	-0.771303	4.247867
H	-4.586033	-0.304510	2.798047
H	-4.350404	1.273368	5.462830
H	-5.370771	1.735186	3.977850
O	-6.292704	2.870560	1.449045
H	-5.908887	2.710523	0.535277
O	-5.306800	3.852602	2.033420
H	-4.432697	3.341668	1.948965
N	0.380215	2.933056	4.538946
C	1.624607	3.018670	3.653743
C	-0.305676	4.286554	4.567389
C	0.787753	2.499932	5.927608
H	1.465878	3.245981	6.354717
H	-0.106626	2.401812	6.550972
C	-0.570417	1.881658	3.959926
H	1.288813	1.534043	5.834968
H	0.393141	5.027621	4.970955
H	-0.579623	4.532184	3.534639
H	-1.197845	4.221816	5.198963
H	-1.488125	1.873581	4.555812
H	-0.773111	2.141734	2.925521
H	-0.063142	0.923217	3.992439
H	2.326957	3.719891	4.119105
H	2.055636	2.019854	3.565434
H	1.325203	3.367487	2.665778

Table S12: Structure TS_{2,1CC}

Si	0.096302	-0.015214	0.292542
O	1.244454	2.545261	2.103649
O	3.248337	1.117584	-1.820735
O	2.463705	3.836280	-2.380681
O	3.003627	2.857959	0.197573
O	0.505461	3.260981	-0.324120
O	0.677184	1.642390	-2.515191
O	-3.813271	1.667354	1.635554

O	-1.879226	1.736192	-1.870818
O	-4.356264	2.469807	-0.951702
O	0.224538	-0.918593	-3.577892
O	0.904150	-1.676170	3.906310
O	2.216532	-1.470763	-1.786335
O	-1.274601	-2.767249	-2.366041
O	1.246271	-3.599333	-3.383288
O	0.527933	-3.260756	-0.622128
O	-3.154945	-0.133892	-0.426370
O	-4.057689	-2.511645	-1.725420
O	-2.356928	-0.513336	-2.918205
O	1.336917	-3.487532	1.957824
O	3.071634	-1.669739	0.721238
O	-0.861185	-5.082394	1.007724
O	4.127679	0.640322	0.668213
O	2.476280	0.060203	2.651096
O	3.985861	2.472117	2.887096
O	3.570700	-2.519014	3.333211
O	4.998781	-1.091686	-1.385512
O	-1.120425	1.333810	-4.673102
O	0.327404	-1.275246	1.278080
O	1.571040	0.684867	0.050644
O	-0.468240	-0.615820	-1.140847
O	-1.081105	-3.008692	2.841557
O	-0.950924	1.141054	0.777719
O	-1.935817	-2.605744	0.185536
O	-1.316749	2.707631	2.982326
O	-0.264580	4.962401	1.809228
O	-2.117257	3.330756	0.439382
W	2.250082	-1.884208	2.396416
W	3.504251	-0.461785	-0.770455
W	-0.791397	0.623683	-3.124460
W	-0.395418	3.288581	1.372754
W	1.960674	2.522678	-1.364141
W	-2.889716	1.763301	-0.325756
W	0.636512	-2.376250	-2.314975
W	-2.551625	-1.698494	-1.413736
W	-0.409612	-3.401423	1.065027
W	2.909144	1.687737	1.771860
H	-1.589968	1.768582	2.995690
H	0.778694	-0.752291	4.198845
H	-0.422919	-2.477259	3.418245
C	-7.546146	0.220158	1.113352
C	-7.482212	1.192069	2.071328
H	-7.480306	0.952396	3.132634
H	-7.613686	2.241522	1.827517
H	-7.464802	-0.836507	1.358950
H	-7.571382	0.472070	0.057672
O	-5.584469	3.856343	1.297558
H	-5.118304	4.062101	0.460334
O	-5.456738	1.127235	1.649250
H	-5.755332	2.876232	1.291552
H	-3.961388	2.593599	1.958382
N	-4.071300	-1.541500	3.558285
C	-4.375173	-1.945871	2.112165
C	-2.898738	-0.563674	3.555141

C	-5.281070	-0.835699	4.131407
C	-3.711069	-2.772676	4.366616
H	-6.125728	-1.533397	4.144412
H	-5.051671	-0.506947	5.151059
H	-5.492013	0.018307	3.474204
H	-2.045194	-1.064478	3.099004
H	-3.195711	0.305977	2.962824
H	-2.680890	-0.291328	4.594682
H	-3.480408	-2.392084	1.678012
H	-5.199010	-2.668029	2.131299
H	-4.655437	-1.045049	1.559565
H	-2.800263	-3.200994	3.929519
H	-3.529755	-2.471135	5.404467
H	-4.546043	-3.479811	4.321025

Table S13: Structure I_{2CC}

Si	-0.268517	-0.012097	0.248599
O	1.530772	-2.781605	0.561454
O	-1.465521	-2.039784	-2.960432
O	1.053491	-2.341995	-4.293179
O	0.468632	-3.456907	-1.756573
O	2.084016	-1.504127	-1.726123
O	0.295173	0.069790	-3.010384
O	3.199164	1.505848	1.922889
O	1.916381	1.772344	-1.755163
O	4.057781	2.916047	-0.295140
O	-1.703391	2.002209	-2.855565
O	-1.629241	-1.488587	4.010769
O	-2.986004	-0.096623	-1.670128
O	-2.184086	3.476408	-0.683987
O	-4.431155	2.328015	-1.969383
O	-3.277969	1.487704	0.518737
O	1.304727	2.892650	0.586236
O	-0.308634	5.245044	0.599622
O	0.148967	3.568178	-1.691218
O	-3.516278	-0.136838	2.599306
O	-3.195455	-1.776508	0.387021
O	-3.809050	2.707280	2.993650
O	-1.907335	-3.593384	-0.824110
O	-1.102960	-2.889259	1.603429
O	0.062455	-5.232547	0.483411
O	-3.650987	-2.906839	2.915107
O	-4.168467	-2.604525	-2.223213
O	0.694575	2.573063	-4.284021
O	-1.205772	-0.106438	1.574847
O	-0.578891	-1.352776	-0.662955
O	-0.689830	1.335280	-0.596542
O	-1.709565	1.179402	3.980443
O	1.352411	0.050062	0.459810
O	-1.289596	2.804332	1.704495
O	3.491835	-1.147056	1.829104
O	4.264682	-2.589948	-0.340575
O	3.710063	0.180674	-0.382132
W	-2.599209	-1.741162	2.161303

W	-2.730666	-1.961861	-1.508585
W	0.185924	1.964835	-2.745592
W	2.870581	-1.563000	-0.015848
W	0.442896	-1.810835	-2.762548
W	2.727428	1.783413	-0.094915
W	-2.921036	1.798730	-1.311936
W	-0.454850	3.576082	0.156157
W	-2.636269	1.599433	2.362889
W	-0.210476	-3.570941	0.057848
H	3.386089	-0.163239	2.053368
H	-2.214160	-1.852285	4.707852
H	-1.530183	0.205117	4.162672
C	2.719286	3.588112	4.551181
C	1.472238	3.672084	4.033305
H	2.562097	1.923069	2.540161
H	0.592563	3.291013	4.550850
H	1.300951	4.118089	3.053411
H	2.903058	3.151417	5.535882
H	3.589549	3.947768	4.002500
O	5.574369	3.711292	1.886156
H	5.179982	3.594451	0.969118
O	5.650558	2.290057	2.390134
H	4.685654	1.962934	2.262685
N	1.721619	-1.957123	4.705489
C	1.245159	-3.049697	3.748064
C	3.225220	-2.050900	4.854868
C	1.015166	-2.124450	6.032724
H	1.264076	-3.101968	6.456580
H	1.328075	-1.326786	6.713008
C	1.355253	-0.587444	4.134312
H	-0.057607	-2.050869	5.834298
H	3.482193	-3.040651	5.247521
H	3.648623	-1.895915	3.855919
H	3.563767	-1.268904	5.542348
H	1.761180	0.180715	4.798717
H	1.774198	-0.507903	3.136282
H	0.273695	-0.535384	4.071030
H	1.459724	-4.022225	4.204465
H	0.177089	-2.917063	3.581455
H	1.773076	-2.939150	2.801530
N	7.224215	-0.781280	-0.208105
C	8.604300	-0.182355	-0.373008
C	7.312029	-2.174153	0.401520
C	6.394872	0.133827	0.718743
C	6.553041	-0.895737	-1.577760
H	5.564519	-0.450368	1.134061
H	7.017924	0.537560	1.517520
H	6.004539	0.956262	0.124175
H	9.183253	-0.789507	-1.075264
H	8.500647	0.835532	-0.755691
H	9.100935	-0.154837	0.599624
H	7.180542	-1.524588	-2.218646
H	5.576835	-1.363368	-1.438990
H	6.447856	0.105572	-1.999907
H	7.980153	-2.786025	-0.211812
H	7.698403	-2.086411	1.421410

H 6.300953 -2.596509 0.400458

Table S14: Structure TS2_{2CC}

Si	-0.296861	0.018380	0.286579
O	0.671077	-2.871189	1.659807
O	-2.260953	-2.626273	-1.926857
O	-0.010868	-4.110894	-2.956636
O	-0.704267	-4.012572	-0.239641
O	1.382962	-2.649479	-0.863024
O	-0.020012	-1.292919	-2.743830
O	3.947995	1.191470	1.221032
O	2.076058	0.198715	-2.168923
O	4.554044	1.099602	-1.439334
O	-1.423089	1.039834	-3.393930
O	-1.527044	0.476671	4.151174
O	-3.096881	-0.015443	-1.500977
O	-1.305115	3.279871	-1.953567
O	-3.884337	2.394270	-2.767640
O	-2.788923	2.301298	-0.120649
O	2.029596	2.285331	-0.479159
O	1.052945	4.809040	-1.395184
O	0.888192	2.321034	-2.848451
O	-3.262407	1.671138	2.438145
O	-3.556411	-0.692566	1.045526
O	-2.742360	4.422991	1.724597
O	-2.923361	-3.120916	0.617640
O	-1.768774	-1.842581	2.620753
O	-1.385024	-4.671206	2.492626
O	-4.015579	-0.638723	3.838237
O	-4.947728	-2.114780	-1.074461
O	0.912762	0.333156	-4.860153
O	-1.132147	0.703374	1.495291
O	-1.011206	-1.431459	-0.039096
O	-0.416296	1.001848	-1.031301
O	-1.048719	2.826831	3.237529
O	1.301401	-0.251965	0.543653
O	-0.409658	3.313184	0.543594
O	2.839475	-1.535138	2.491120
O	3.383431	-3.623793	0.848439
O	3.540597	-1.081775	-0.123639
W	-2.794781	-0.172408	2.691601
W	-3.331974	-1.699921	-0.617875
W	0.381407	0.497390	-3.220235
W	2.258449	-2.277771	0.770439
W	-0.352607	-2.909196	-1.756236
W	3.027899	0.686617	-0.678296
W	-2.522824	1.748742	-1.917757
W	0.436496	3.200921	-1.180343
W	-2.007370	2.859617	1.564294
W	-1.208231	-3.260694	1.499410
H	2.269903	-0.895418	2.957235
H	-1.717443	0.194060	5.064741
H	-1.111191	1.940908	3.750977
C	5.774206	4.663713	0.422984

C	6.166677	4.203714	1.648160
H	5.706625	4.569931	2.560251
H	7.066584	3.606525	1.771853
H	4.898942	5.296335	0.305400
H	6.258826	4.331366	-0.490701
O	6.618791	0.834170	0.338598
H	6.127863	0.805546	-0.524732
O	4.831513	2.678835	1.227467
H	6.256994	1.664146	0.764317
H	4.713158	0.576740	1.322412
N	2.281414	3.253468	3.722816
C	2.157264	4.044900	2.417320
C	1.904486	1.797588	3.457677
C	3.721512	3.298821	4.192995
C	1.353786	3.850544	4.766147
H	3.970520	4.330548	4.464370
H	3.826775	2.648038	5.067486
H	4.347377	2.955529	3.361494
H	0.902503	1.764031	3.034835
H	2.628925	1.393753	2.746509
H	1.925652	1.263293	4.414690
H	1.136359	3.952195	2.047664
H	2.397381	5.092040	2.633591
H	2.867277	3.628502	1.697105
H	0.329175	3.763892	4.387078
H	1.467823	3.289412	5.699892
H	1.629737	4.898560	4.921423
N	6.770997	-2.842747	0.656980
C	8.280354	-2.739180	0.643846
C	6.228589	-1.977475	1.798739
C	6.334169	-4.286456	0.863488
C	6.230357	-2.333366	-0.683014
H	5.147149	-2.101549	1.863526
H	6.704164	-2.313581	2.726535
H	6.478183	-0.936714	1.565277
H	6.771071	-4.901873	0.070512
H	6.689769	-4.622414	1.842992
H	5.238347	-4.316923	0.826568
H	6.455770	-3.082136	-1.448079
H	5.154716	-2.155415	-0.599642
H	6.724757	-1.386654	-0.906811
H	8.669949	-3.292274	-0.215712
H	8.551602	-1.683427	0.565235
H	8.679742	-3.162036	1.570617

Table S15: Structure I_{CC}

Si	0.026757	0.013906	0.327642
O	1.738246	2.570082	1.654405
O	2.698900	0.646271	-2.469986
O	2.017394	3.357776	-3.137803
O	3.030729	2.552080	-0.620509
O	0.544695	3.185919	-0.654485
O	0.060063	1.366725	-2.614095
O	-3.059259	1.753262	2.405715

O	-2.293801	1.766334	-1.422828
O	-4.410167	2.726891	0.171433
O	-0.822205	-1.200616	-3.307527
O	1.500570	-1.472809	3.934470
O	1.483112	-1.815811	-1.967325
O	-2.150712	-2.804420	-1.625349
O	-0.007633	-3.961481	-3.054693
O	-0.038086	-3.279137	-0.245817
O	-3.291153	0.107447	0.393575
O	-4.715263	-2.218122	-0.441439
O	-3.152143	-0.515761	-2.161929
O	1.272519	-3.384404	2.075350
O	2.820194	-1.880139	0.325042
O	-1.164212	-4.891387	1.759933
O	4.074370	0.269283	-0.192422
O	2.857972	0.042700	2.152309
O	4.595667	2.274906	1.793204
O	3.856713	-2.548441	2.836733
O	4.299871	-1.707766	-2.195177
O	-2.207714	1.092857	-4.281644
O	0.304097	-1.090952	1.492104
O	1.467833	0.515252	-0.265619
O	-0.896692	-0.669120	-0.841558
O	-0.843493	-2.670207	3.436001
O	-0.767493	1.313885	0.882109
O	-2.230594	-2.397038	0.981273
O	-0.570681	3.149119	3.019152
O	0.521757	5.123116	1.336816
O	-1.804266	3.563422	0.725623
W	2.402095	-1.881635	2.157209
W	3.029673	-0.876918	-1.356643
W	-1.605457	0.458691	-2.785293
W	0.110554	3.441686	1.201634
W	1.641192	2.199934	-1.903326
W	-2.817052	2.013863	0.344013
W	-0.265699	-2.592756	-2.021494
W	-3.116908	-1.544797	-0.526117
W	-0.639436	-3.244833	1.596836
W	3.241912	1.514715	1.016810
H	-1.537161	3.010256	3.136533
H	1.997579	-0.945135	4.586611
H	-0.038906	-2.281095	3.892675
C	-4.927997	-0.402158	4.262739
C	-4.325346	-1.400119	3.577176
H	-3.585631	0.946023	2.605334
H	-3.505728	-1.993972	3.984469
H	-4.613931	-1.646048	2.557830
H	-4.631110	-0.142659	5.279836
H	-5.721795	0.203651	3.823170
O	-6.072033	2.824386	2.364645
H	-5.684100	2.932238	1.443842
O	-5.018874	3.485300	3.219167
H	-4.232464	2.874451	3.053466
N	-0.812526	0.370516	3.536172
H	-0.379717	-0.265060	2.814085
H	-0.138439	1.115595	3.758349

H	-1.634056	0.864552	3.116569
H	-1.071825	-0.191128	4.348171

Table S16: Structure TS_{2CC}

Si	-0.035763	-0.005811	-0.358657
O	-1.704364	2.536069	-1.761680
O	-2.728023	0.724893	2.397081
O	-2.039260	3.466562	2.985735
O	-3.040197	2.591627	0.501390
O	-0.529391	3.165727	0.538375
O	-0.112240	1.422541	2.602968
O	3.238505	2.119388	-2.387070
O	2.241471	1.809801	1.469125
O	4.412523	2.769549	-0.007022
O	0.748739	-1.151750	3.347813
O	-1.496334	-1.513920	-3.893774
O	-1.530230	-1.766353	1.966062
O	2.095795	-2.762660	1.688875
O	-0.071477	-3.898377	3.135384
O	0.009000	-3.313905	0.322842
O	3.267906	0.155289	-0.355194
O	4.655979	-2.196216	0.516197
O	3.087776	-0.461923	2.198517
O	-1.294761	-3.445012	-2.062142
O	-2.873122	-1.883860	-0.321164
O	1.144137	-4.885386	-1.713299
O	-4.079246	0.304169	0.121295
O	-2.855639	0.002078	-2.196736
O	-4.558958	2.270237	-1.924371
O	-3.875594	-2.627052	-2.805039
O	-4.351281	-1.610755	2.182869
O	2.116375	1.139881	4.323126
O	-0.365303	-1.198104	-1.393087
O	-1.463921	0.561185	0.211810

O	0.861615	-0.634909	0.869798
O	0.844635	-2.600585	-3.357174
O	0.832824	1.228097	-1.000023
O	2.174419	-2.366532	-0.921334
O	0.726851	3.071462	-3.057395
O	-0.478865	5.072723	-1.530380
O	1.806649	3.547923	-0.694152
W	-2.429038	-1.922550	-2.147627
W	-3.073131	-0.817087	1.322011
W	1.526102	0.500001	2.823378
W	-0.058169	3.401944	-1.327516
W	-1.657422	2.261904	1.797179
W	2.847457	2.025268	-0.254671
W	0.198437	-2.555912	2.071890
W	3.057843	-1.519744	0.579943
W	0.576537	-3.253041	-1.525112
W	-3.218618	1.520439	-1.115690
H	1.608949	2.619489	-3.102111
H	-1.566607	-0.592383	-4.208329
H	-0.008230	-2.242547	-3.782939
C	5.905027	-0.766481	-3.286555
C	5.269446	-0.296951	-4.404350
H	4.404436	-0.817082	-4.810520
H	5.681819	0.502292	-5.012766
H	5.496438	-1.583964	-2.699753
H	6.796057	-0.280456	-2.896547
O	5.963682	2.983586	-2.356996
H	5.757919	3.079050	-1.397429
O	4.299540	0.917499	-3.037124
H	5.617083	2.095525	-2.646698
H	3.816788	2.899944	-2.579379
N	1.841887	-0.096262	-3.378128
H	1.638633	-1.136024	-3.356314
H	1.357506	0.342256	-2.564897
H	2.875767	0.142825	-3.286436
H	1.462573	0.312454	-4.235321

Figure S1

Figure S2