

# Supporting Information for “Elucidating the Role of Catalytic Amino Acid Residues in the Silica Oligomerization Reaction Mechanism”

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## Cartesian Coordinates of Optimized Structures 3

### *No Catalyst 3*

RC, Reactant Complexes 3  
TS1, Si-O bond association 15  
IM1, three equatorial OH groups 20  
TS2, water cleavage of IM1 28  
TS-iso, isomerization of IM1 to IM2 33  
IM2, co-linear OH groups on Si 37  
TS3, water cleavage from IM2 45  
TS4, water cleavage from IM2 50  
PC, product complexes 53

### *One H<sub>2</sub>O 59*

RC-w, Reactant Complexes 59  
TS1-w, Si-O bond association 63  
IM1-w, three equatorial OH groups 67  
TS2-cw, water cleavage of IM1, H<sub>2</sub>O acting as catalyst 70  
TS2-sw, water cleavage of IM1, H<sub>2</sub>O acting as spectator 72  
TS-iso-w, isomerization of IM1 to IM2 73  
IM2-w, co-linear OH groups on Si 77  
TS3-cw, water cleavage from IM2, H<sub>2</sub>O acting as catalyst 84  
TS3-sw, water cleavage from IM2, H<sub>2</sub>O acting as spectator 85  
TS4-cw, water cleavage from IM2, H<sub>2</sub>O acting as catalyst 86  
TS4-sw, water cleavage from IM2, H<sub>2</sub>O acting as spectator 88  
PC-w, product complexes 91

### *One C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> 96*

RC-g, Reactant Complexes 96  
TS1-g, Si-O bond association 104  
IM1-g, three equatorial OH groups 107  
TS2-cg, water cleavage of IM1, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as catalyst 115  
TS2-sg, water cleavage of IM1, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as spectator 117  
TS-iso-g, isomerization of IM1 to IM2 120  
IM2-g, co-linear OH groups on Si 124  
TS3-cg, water cleavage from IM2, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as catalyst 137  
TS3-sg, water cleavage from IM2, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as spectator 139  
TS4-sg, water cleavage from IM2, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as spectator 141  
PC-g, product complexes 147

*One CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> 158*

- RC-ma, Reactant Complexes 158
- TS1-ma, Si-O bond association 163
- IM1-ma, three equatorial OH groups 167
- TS2-cma, water cleavage of IM1, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as catalyst 171
- TS2-sma, water cleavage of IM1, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as spectator 174
- TS-iso-ma, isomerization of IM1 to IM2 175
- IM2-ma, co-linear OH groups on Si 181
- TS3-cma, water cleavage from IM2, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as catalyst 191
- TS3-sma, water cleavage from IM2, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as spectator 193
- TS4-cma, water cleavage from IM2, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as catalyst 194
- TS4-sma, water cleavage from IM2, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as spectator 196
- PC-ma, product complexes 199

*Two CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> 207*

- RC-2ma, Reactant Complexes 207
- TS1-2ma, Si-O bond association 208
- IM1-2ma, three equatorial OH groups 209
- TS2-2ma, water cleavage of IM1 213
- TS-iso-2ma, isomerization of IM1 to IM2 215
- IM2-2ma, co-linear OH groups on Si 217
- TS3-2ma, water cleavage from IM2 220
- TS4-2ma, water cleavage from IM2 222
- PC-2ma, product complexes 223

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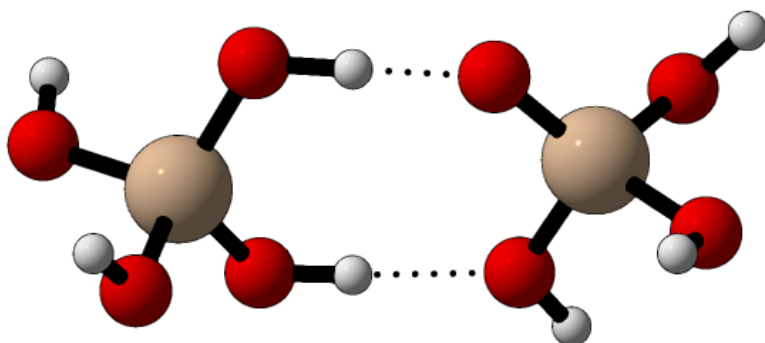
## Cartesian Coordinates of Optimized Structures

The Cartesian coordinates of optimized structures referenced in the manuscript are shown below, optimized at the CAM-B3LYP/6-311++G(2d,2p) level of theory. For each stationary point, the different conformations/configurations for that stationary point are ranked by their relative free energies, with the name of the structure being preceded by its rank (with 00 being the lowest free energy structure for that stationary point). For structures that came from Hu, et al.<sup>1</sup>, the original name of the structure is maintained with the addition of its free energy rank preceding this original name. A folder containing these structures as MOL2 files is included with this Supporting Information. 3D ball-and-stick images of the lowest energy conformation/configuration for each stationary point is also shown here (as well is in the manuscript). The electronic energy (E), enthalpy (H), free energy (G) and free energy using the quasi-RRHO approximation [G(quasi-RRHO)] as calculated by AaronTools<sup>2,3</sup> in Hartrees (a.u.) are also shown for each structure.

### No Catalyst

RC, Reactant Complexes

00\_c3.mol2



E = -1185.693373  
H = -1185.572070  
G = -1185.632124  
G(quasi-RRHO) = -1185.628829

Si	-2.15822	0.05962	0.07752
O	-1.30729	-0.83467	-1.05151
H	-1.82497	-1.37248	-1.65402
O	-3.12455	-1.09028	0.77842
O	-1.15688	0.84081	0.99215
H	0.29703	0.63604	1.15080
H	-3.82684	-0.75945	1.34085
O	-3.24377	1.02588	-0.72745

H	-2.92492	1.91058	-0.91454
Si	2.18231	-0.00434	0.01308
O	2.63222	1.21020	-1.00434
H	3.01298	1.98889	-0.59433
O	1.41336	-1.10398	-0.91264
O	3.59403	-0.65810	0.54658
H	3.52256	-1.29394	1.26083
O	1.31342	0.50275	1.26990
H	0.44262	-1.02440	-0.98710

*01\_c10.mol2*

E = -1185.691518  
H = -1185.569771  
G = -1185.631063  
G(quasi-RRHO) = -1185.627207

Si	-2.38593	-0.01031	0.00431
O	-3.29884	1.17368	-0.68047
H	-2.84820	1.99512	-0.88548
O	-1.43460	-0.79961	-1.05378
O	-1.42455	0.60689	1.16677
H	-0.48067	0.33249	0.98890
H	-0.48790	-0.74455	-0.74262
O	-3.49667	-1.08087	0.56345
H	-4.31621	-0.71482	0.90034
Si	2.31256	-0.01373	0.01471
O	3.27783	-0.02448	1.36350
H	3.38838	-0.87762	1.78672
O	2.45646	1.54072	-0.54269
O	3.10261	-1.03663	-1.03277
H	2.54999	-1.41252	-1.72013
O	0.80194	-0.38905	0.23408
H	3.34830	1.83320	-0.73866

*02\_c6.mol2*

E = -1185.691070  
H = -1185.571125  
G = -1185.631055  
G(quasi-RRHO) = -1185.627912

Si	-2.17963	0.01153	-0.04778
O	-1.47242	-0.53846	1.33748
H	-0.50271	-0.52899	1.33509

O	-3.08321	1.29535	0.49589
O	-1.16063	0.31926	-1.21213
H	0.15896	0.63458	-1.04845
H	-3.65281	1.69962	-0.16053
O	-3.34475	-1.08967	-0.49555
H	-3.03302	-1.77286	-1.09137
Si	2.18761	0.03538	-0.04095
O	2.79472	-1.34104	-0.70082
H	3.46110	-1.23980	-1.38293
O	1.35120	-0.49044	1.28663
O	3.50563	0.92324	0.37961
H	3.35431	1.85783	0.53309
O	1.19773	0.89782	-0.94181
H	1.79642	-1.11566	1.86289

*03\_c2.mol2*

E = -1185.693763  
H = -1185.571400  
G = -1185.629719  
G(quasi-RRHO) = -1185.627167

Si	2.01364	-0.02379	0.00935
O	1.60916	1.52575	-0.34226
H	0.64480	1.65041	-0.40385
O	1.44135	-0.49776	1.46680
O	1.43470	-1.06596	-1.11279
H	0.51245	-1.28845	-0.83264
H	0.51959	-0.82063	1.30881
O	3.64722	-0.08185	0.04322
H	4.11119	0.69347	-0.27632
Si	-1.94245	-0.06522	0.02119
O	-3.04078	-0.43162	-1.16858
H	-2.70657	-1.00088	-1.86404
O	-1.19105	1.37464	-0.38003
O	-2.89269	0.37137	1.30490
H	-3.53070	-0.28289	1.59483
O	-0.85509	-1.17206	0.26612
H	-1.76995	2.11502	-0.57332

*04\_c1.mol2*

E = -1185.694219  
H = -1185.571737  
G = -1185.628690

G(quasi-RRHO) = -1185.626689

Si	1.94136	-0.07339	0.02554
O	1.19472	1.35693	-0.41591
H	1.77669	2.08730	-0.63623
O	0.84953	-1.16518	0.31539
O	3.02780	-0.48582	-1.15995
H	2.68473	-1.07557	-1.83368
H	-0.52389	-1.31996	-0.77541
O	2.90475	0.39917	1.28649
H	3.54561	-0.24674	1.58858
Si	-2.01323	0.00179	0.00331
O	-3.64757	0.04035	0.00035
H	-4.09945	-0.77338	0.22986
O	-1.60950	1.53070	-0.41852
O	-1.43016	-0.40023	1.48000
H	-0.51250	-0.74165	1.33187
O	-1.44221	-1.09789	-1.06838
H	-0.64382	1.64814	-0.46468

*05\_c9.mol2*

E = -1185.692685

H = -1185.570324

G = -1185.627817

G(quasi-RRHO) = -1185.625715

Si	1.91167	-0.08452	0.00140
O	2.58235	-0.33082	-1.49243
H	3.19491	0.34382	-1.79131
O	1.27190	1.46576	-0.06299
O	0.86091	-1.20895	0.31144
H	-0.49330	-0.78297	1.33249
H	1.53444	2.02930	0.66821
O	3.11944	0.09937	1.12426
H	3.32526	-0.68409	1.63681
Si	-1.98249	-0.01665	0.00740
O	-1.44489	-1.12286	-1.07163
H	-0.53007	-1.36401	-0.78763
O	-1.53792	1.51177	-0.38782
O	-3.61675	-0.04812	-0.01607
H	-4.06457	0.79744	0.03953
O	-1.40975	-0.43847	1.48162
H	-0.57741	1.65556	-0.31241

06\_c5.mol2

E = -1185.694389  
H = -1185.572381  
G = -1185.627779  
G(quasi-RRHO) = -1185.626347

Si	-1.87729	-0.09862	-0.05515
O	-1.36283	-0.14040	1.53517
H	-1.71914	0.54148	2.10955
O	-1.40979	1.44535	-0.50511
O	-1.22125	-1.27118	-0.85444
H	0.32304	-1.26731	-0.98599
H	-1.79049	1.76675	-1.32569
O	-3.52911	-0.02469	-0.08960
H	-3.97165	-0.86377	-0.22977
Si	1.89810	-0.01014	-0.02254
O	1.45568	-0.29163	1.53412
H	0.49423	-0.29950	1.68430
O	1.43640	1.49232	-0.48806
O	3.53186	0.05470	-0.08375
H	4.00595	-0.76299	0.07469
O	1.33567	-1.16561	-1.00997
H	0.47371	1.61709	-0.54635

07\_c4.mol2

E = -1185.694473  
H = -1185.572455  
G = -1185.627730  
G(quasi-RRHO) = -1185.626344

Si	1.87398	0.10920	-0.00303
O	1.35511	-0.62131	1.40902
H	1.73714	-1.48108	1.60071
O	1.44039	-1.04554	-1.13567
O	1.19576	1.50866	-0.16123
H	-0.34897	1.59380	-0.29013
H	1.80436	-0.91771	-2.01475
O	3.52718	0.08958	-0.04567
H	3.95181	0.89856	0.24562
Si	-1.89670	0.03461	-0.01215
O	-1.46003	-0.45399	1.49375
H	-0.50179	-0.57266	1.61535
O	-1.40112	-1.07428	-1.11811
O	-3.52956	0.11403	-0.06922

H	-4.01288	-0.69571	0.10224
O	-1.36198	1.52367	-0.35157
H	-0.43765	-1.16496	-1.21692

*08\_c8.mol2*

E = -1185.692970  
H = -1185.571054  
G = -1185.627500  
G(quasi-RRHO) = -1185.625650

Si	1.88003	-0.06505	-0.06728
O	1.34780	1.51938	-0.13590
H	1.73229	2.04132	-0.84364
O	1.42177	-0.37212	1.51320
O	1.24690	-1.03333	-1.12300
H	-0.30036	-1.10882	-1.14746
H	1.68122	-1.23789	1.83736
O	3.53328	-0.00159	-0.10166
H	3.93503	-0.57930	-0.75296
Si	-1.90108	-0.01195	-0.02434
O	-1.49151	1.53591	-0.37822
H	-0.53642	1.70525	-0.31368
O	-1.42642	-0.37920	1.50507
O	-3.53644	-0.00269	-0.06278
H	-3.97518	-0.85434	-0.08815
O	-1.31763	-1.07559	-1.09769
H	-0.46394	-0.41453	1.63903

*09\_c12.mol2*

E = -1185.692087  
H = -1185.569858  
G = -1185.627006  
G(quasi-RRHO) = -1185.624995

Si	-2.01897	-0.03147	0.00771
O	-1.60158	1.23376	-0.97003
H	-1.93691	2.10017	-0.72751
O	-1.36814	-1.35860	-0.67240
O	-1.41979	0.14496	1.51404
H	-0.48667	-0.19966	1.47887
H	-0.45031	-1.43777	-0.29401
O	-3.65158	-0.05847	0.02978
H	-4.07270	-0.64151	0.66454



Si	1.97121	-0.03755	0.03497
O	3.11770	0.59607	1.05255
H	2.84368	1.37802	1.53408
O	1.35211	1.28136	-0.75906
O	2.94341	-0.87595	-1.01854
H	2.56795	-1.70419	-1.32045
O	0.85386	-0.93943	0.69420
H	0.39556	1.28168	-0.89730

*10\_c7.mol2*

E = -1185.693658  
H = -1185.571617  
G = -1185.626864  
G(quasi-RRHO) = -1185.625464

Si	-1.87720	-0.12851	-0.03863
O	-1.36505	0.15757	1.52711
H	-1.67914	0.96552	1.93982
O	-1.42318	1.30746	-0.78168
O	-1.20354	-1.42022	-0.60055
H	0.33159	-1.40938	-0.76759
H	-1.75135	1.42796	-1.67605
O	-3.52698	-0.20814	-0.08923
H	-4.00523	0.59251	0.13409
Si	1.89690	-0.00692	-0.01818
O	1.45646	-0.06680	1.56363
H	0.49591	-0.02919	1.71262
O	1.42261	1.41152	-0.68982
O	3.53021	0.06023	-0.08978
H	4.00936	-0.73076	0.16165
O	1.34236	-1.29505	-0.82955
H	0.46007	1.50711	-0.79024

*11\_c11.mol2*

E = -1185.692431  
H = -1185.570079  
G = -1185.626404  
G(quasi-RRHO) = -1185.624613

Si	-2.00761	-0.03377	-0.00702
O	-1.57358	1.54117	-0.25869
H	-1.85851	2.18050	0.39858
O	-1.37270	-0.87784	-1.24395

O	-1.41094	-0.60765	1.39860
H	-0.48144	-0.89948	1.20080
H	-0.45058	-1.12724	-0.95935
O	-3.64043	-0.05153	0.00677
H	-4.06796	-0.86286	0.28812
Si	1.95174	-0.03865	0.00816
O	2.71793	0.36548	1.42435
H	3.12432	-0.36582	1.89228
O	1.35700	1.40888	-0.52950
O	3.20991	-0.42353	-1.00736
H	2.95726	-0.91116	-1.79307
O	0.85737	-1.17128	0.13364
H	0.40251	1.53037	-0.43422

*12\_c14.mol2*

E = -1185.691615  
H = -1185.569385  
G = -1185.626355  
G(quasi-RRHO) = -1185.624421

Si	2.02168	-0.04161	0.02356
O	1.59436	1.20121	-0.98633
H	1.90057	2.07879	-0.74443
O	1.42646	0.16732	1.52444
O	1.37385	-1.37794	-0.64077
H	0.44970	-1.44135	-0.27384
H	0.49176	-0.17080	1.49149
O	3.64642	-0.12027	0.16716
H	4.17112	0.07302	-0.61166
Si	-1.97305	-0.03418	0.03058
O	-3.01531	-0.90786	-0.92206
H	-2.65363	-1.73599	-1.24077
O	-1.35229	1.20676	-0.87949
O	-3.05924	0.69287	1.05250
H	-2.75387	1.50801	1.45318
O	-0.85118	-0.92023	0.70328
H	-0.39101	1.21447	-0.98184

*13\_c15.mol2*

E = -1185.691863  
H = -1185.569594  
G = -1185.626320  
G(quasi-RRHO) = -1185.624380

Si	-2.02066	-0.03997	0.03322
O	-1.59336	1.41678	-0.63242
H	-1.90216	1.58969	-1.52534
O	-1.44193	-1.29103	-0.83427
O	-1.35697	-0.04791	1.51777
H	-0.43346	-0.40653	1.39857
H	-0.50460	-1.41783	-0.53139
O	-3.64587	-0.19737	0.05618
H	-4.16633	0.58694	0.23830
Si	1.96320	-0.02828	0.01428
O	2.97779	0.55131	1.19211
H	3.53557	-0.10651	1.61045
O	1.35095	1.36558	-0.63373
O	3.01532	-0.67789	-1.09918
H	2.62436	-1.32709	-1.68622
O	0.85204	-1.04519	0.49112
H	0.38729	1.44249	-0.63018

*14\_c16.mol2*

E = -1185.691750

H = -1185.569444

G = -1185.626099

G(quasi-RRHO) = -1185.624316

Si	2.01494	0.02519	0.03918
O	1.57766	-1.15934	-1.03445
H	1.86070	-1.04343	-1.94481
O	1.42980	1.48111	-0.39777
O	1.36578	-0.42103	1.46174
H	0.44087	-0.04643	1.46571
H	0.49777	1.50890	-0.05630
O	3.64064	0.16815	0.09330
H	4.16003	-0.63247	0.00180
Si	-1.96637	0.03619	0.03075
O	-3.19521	-0.61928	0.93169
H	-2.97872	-1.44199	1.37298
O	-1.35636	-1.25224	-0.81777
O	-2.83874	0.99223	-1.01044
H	-2.42121	1.83089	-1.21128
O	-0.85381	0.83812	0.81568
H	-0.39752	-1.25658	-0.94303

*15\_c13.mol2*

E = -1185.689998  
H = -1185.569487  
G = -1185.626096  
G(quasi-RRHO) = -1185.624225

Si	-1.91037	-0.05667	-0.04489
O	-1.58878	0.02205	1.58655
H	-0.64191	0.00133	1.77897
O	-1.50943	1.41181	-0.70640
O	-1.21261	-1.29094	-0.74289
H	0.17546	-1.39079	-0.66129
H	-0.55741	1.52978	-0.82571
O	-3.56071	-0.02514	-0.15129
H	-3.98460	-0.88394	-0.12615
Si	1.90314	-0.07097	-0.01436
O	1.36372	0.18714	1.52565
H	1.61769	1.01261	1.94549
O	1.44208	1.31177	-0.80307
O	3.52701	-0.26007	-0.09715
H	4.07689	0.48890	0.14029
O	1.24245	-1.40713	-0.57767
H	1.78508	1.43314	-1.69184

*16\_c18.mol2*

E = -1185.685939  
H = -1185.563673  
G = -1185.625147  
G(quasi-RRHO) = -1185.621337

Si	2.21050	0.00400	-0.00013
O	1.69030	1.48353	0.48628
H	0.71684	1.42138	0.48555
O	1.70298	-1.15444	1.04788
O	1.73862	-0.32548	-1.53534
H	0.76592	-0.32194	-1.51269
H	0.72956	-1.10797	1.02726
O	3.84308	-0.00303	-0.06331
H	4.31805	0.17203	0.75060
Si	-2.11208	0.00712	-0.00197
O	-2.79168	-1.38752	-0.60955
H	-2.25614	-1.83486	-1.26698
O	-2.68723	1.29994	-0.86814
O	-2.86265	0.17895	1.46999

H	-2.74264	-0.54935	2.08177
O	-0.54197	-0.00333	-0.00146
H	-3.64109	1.35614	-0.94694

*17\_c17.mol2*

E = -1185.687369  
H = -1185.564619  
G = -1185.620780  
G(quasi-RRHO) = -1185.619175

Si	1.92722	0.00697	0.00010
O	1.41959	-0.83063	1.30954
H	0.45213	-0.83547	1.44080
O	1.41603	-0.71131	-1.37694
O	1.46766	1.57211	0.06918
H	0.50397	1.69779	-0.01481
H	0.45281	-0.86334	-1.42403
O	3.55809	0.06330	0.00010
H	4.02963	-0.77090	-0.02039
Si	-2.08315	0.00157	-0.00057
O	-1.33816	-0.89476	-1.20767
H	-1.77941	-1.71838	-1.42636
O	-1.33800	-0.62235	1.36737
O	-1.29938	1.47651	-0.15987
H	-1.74247	2.10193	-0.73731
O	-3.63179	0.03021	-0.00261
H	-1.76598	-0.39570	2.19586

*18\_c19.mol2*

E = -1185.685346  
H = -1185.562417  
G = -1185.617662  
G(quasi-RRHO) = -1185.616271

Si	1.93466	0.00118	-0.03667
O	1.43687	-0.43513	1.48125
H	1.72298	0.13419	2.20048
O	1.35142	-1.14556	-1.02394
O	1.43242	1.50517	-0.39173
H	0.45886	1.59809	-0.43883
H	0.37450	-1.22965	-1.06209
O	3.55846	0.08190	-0.15226
H	4.06167	-0.69658	0.09292

Si	-2.10436	0.00888	0.03599
O	-1.36250	-1.12883	-0.97372
H	-1.84274	-1.95600	-1.05137
O	-1.47558	-0.24216	1.54474
O	-1.31106	1.41043	-0.46417
H	-1.68962	1.81402	-1.24868
O	-3.65390	0.02537	-0.03030
H	-0.51897	-0.37448	1.59816

*19\_c20.mol2*

E = -1185.680500  
H = -1185.557710  
G = -1185.613428  
G(quasi-RRHO) = -1185.611902

Si	-1.95911	0.02936	-0.00226
O	-1.37103	-0.12149	1.52460
H	-1.68854	-0.86083	2.04937
O	-1.32929	1.37620	-0.62913
O	-1.48156	-1.34329	-0.76868
H	-1.83179	-1.50464	-1.64852
H	-0.34508	1.43287	-0.66229
O	-3.58374	0.08048	-0.08045
H	-4.02525	0.89695	0.16228
Si	2.14176	-0.03448	-0.00505
O	1.35213	1.32797	-0.65267
H	1.76105	2.15992	-0.40308
O	1.56387	-0.15433	1.55234
O	1.46454	-1.25997	-0.89730
H	0.50652	-1.37093	-0.85486
O	3.69292	0.02415	-0.07207
H	0.60325	-0.11930	1.64628

*20\_c21.mol2*

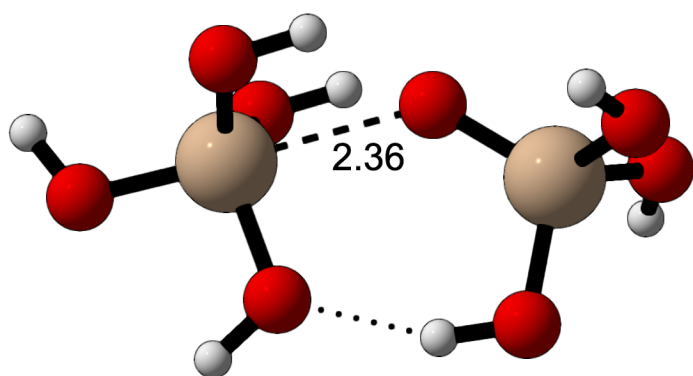
E = -1185.672269  
H = -1185.549658  
G = -1185.607384  
G(quasi-RRHO) = -1185.605312

Si	1.99832	-0.00066	-0.00258
O	1.38908	-0.92162	1.20215
H	1.73952	-0.80280	2.08847
O	1.38475	-0.61152	-1.38880

O	1.38183	1.49896	0.16905
H	1.71967	2.20282	-0.39005
H	1.64762	-1.49175	-1.66844
O	3.61726	0.11907	0.02366
H	4.15473	-0.66263	-0.12033
Si	-2.18742	0.00141	0.00243
O	-1.54940	-0.19845	-1.53268
H	-0.60061	-0.36523	-1.57570
O	-1.53777	-1.22384	0.93990
O	-1.54453	1.43041	0.59135
H	-0.59742	1.55378	0.45882
O	-3.74456	-0.00190	0.00806
H	-0.58950	-1.17332	1.10780

TS1, Si-O bond association

*00\_d3.mol2*



E = -1185.683143  
H = -1185.561176  
G = -1185.618076  
G(quasi-RRHO) = -1185.615415

Si	1.77922	0.04652	0.03873
O	1.11184	-1.14090	-0.91555
H	1.77990	-1.69952	-1.32083
O	1.67985	1.58251	-0.54443
O	1.64119	-0.15710	1.66637
H	0.72713	0.07825	1.88266
H	0.76557	1.86216	-0.39139
O	3.38412	-0.32897	-0.22506
H	4.02216	0.19901	0.25659
Si	-1.86314	0.02271	0.01255

O	-1.64624	-1.31039	-0.94521
H	-0.69397	-1.44260	-1.08541
O	-2.84796	1.10484	-0.77217
O	-2.89592	-0.43623	1.22780
H	-2.67835	-1.26927	1.64854
O	-0.47276	0.62918	0.45640
H	-2.38040	1.75920	-1.29322

*01\_d1.mol2*

E = -1185.684567  
H = -1185.562362  
G = -1185.617581  
G(quasi-RRHO) = -1185.615876

Si	-1.72192	-0.01564	0.01035
O	-1.17155	1.37017	-0.69212
H	-0.21421	1.43934	-0.79987
O	-1.80530	-1.40576	-0.89798
O	-1.61371	-0.19188	1.66044
H	-0.72265	-0.49468	1.86256
H	-0.92610	-1.79789	-0.90884
O	-3.34847	0.42759	-0.07501
H	-3.94065	-0.23014	0.29113
Si	1.81274	-0.05140	0.00732
O	2.57479	0.46647	1.37856
H	3.03389	-0.20396	1.88724
O	1.66007	1.33518	-0.89725
O	2.90666	-1.08306	-0.68335
H	2.53015	-1.74254	-1.26874
O	0.37192	-0.66953	0.15020
H	2.37297	1.97490	-0.85884

*02\_d4.mol2*

E = -1185.683214  
H = -1185.561245  
G = -1185.617214  
G(quasi-RRHO) = -1185.614982

Si	-1.77829	-0.04631	0.03526
O	-1.67730	0.00467	1.67728
H	-0.76340	-0.23459	1.88983
O	-1.10048	1.24392	-0.76651
O	-1.65578	-1.51909	-0.69000



H	-0.74465	-1.81047	-0.53883
H	-1.76347	1.79674	-1.18779
O	-3.38103	0.33542	-0.23545
H	-4.01712	-0.33928	0.00536
Si	1.84705	-0.03247	0.01470
O	2.98178	0.16576	1.21324
H	2.81736	0.89391	1.81478
O	1.65531	1.46291	-0.66981
O	2.62379	-1.04261	-1.04784
H	3.51131	-0.77976	-1.29768
O	0.46472	-0.65560	0.44977
H	0.70917	1.61329	-0.83064

*03\_d2.mol2*

E = -1185.683254  
H = -1185.561281  
G = -1185.617029  
G(quasi-RRHO) = -1185.614916

Si	-1.77648	-0.06242	0.01334
O	-1.11319	1.39036	-0.45301
H	-1.77858	2.07660	-0.54796
O	-1.69414	-1.26358	-1.10862
O	-1.62039	-0.48480	1.59695
H	-0.70664	-0.78868	1.69816
H	-0.77802	-1.57655	-1.08979
O	-3.38321	0.38598	-0.05798
H	-3.99924	-0.20631	0.37506
Si	1.85404	-0.00870	0.00514
O	2.77264	0.12123	1.38078
H	3.15542	-0.69830	1.69798
O	1.64531	1.56289	-0.45620
O	2.90059	-0.74553	-1.05828
H	2.47627	-1.16665	-1.80770
O	0.47388	-0.76503	0.14842
H	0.69301	1.74356	-0.52106

*04\_d5.mol2*

E = -1185.682957  
H = -1185.560993  
G = -1185.616911  
G(quasi-RRHO) = -1185.614595

Si	-1.77652	-0.06112	0.00281
O	-1.10357	1.44721	-0.19813
H	-1.76999	2.13851	-0.22447
O	-1.66952	-1.06454	-1.29763
O	-1.65992	-0.73642	1.49978
H	-0.74734	-1.05208	1.57303
H	-0.75456	-1.38119	-1.30933
O	-3.38049	0.40177	-0.03677
H	-4.01517	-0.27064	0.21382
Si	1.84235	-0.01985	0.00482
O	2.82805	-0.14387	1.33903
H	3.17401	-1.02075	1.51343
O	1.65417	1.61377	-0.14254
O	2.72454	-0.58834	-1.28563
H	3.61624	-0.24405	-1.36145
O	0.46551	-0.78583	0.08234
H	0.70508	1.81379	-0.19547

*05\_d6.mol2*

E = -1185.677808

H = -1185.556165

G = -1185.612804

G(quasi-RRHO) = -1185.610634

Si	-1.79690	0.04370	0.01432
O	-1.16925	-1.14909	-0.92351
H	-0.20661	-1.17113	-1.02688
O	-1.67533	-0.12775	1.65669
O	-1.73715	1.58987	-0.55278
H	-0.80745	1.85135	-0.46082
H	-2.49411	-0.47410	2.01973
O	-3.43211	-0.30046	-0.15227
H	-3.67275	-0.68987	-0.99357
Si	1.87053	0.04995	0.03005
O	1.65431	-1.13982	-1.11993
H	2.30934	-1.83849	-1.16125
O	2.57888	-0.78006	1.27635
O	3.06077	1.09921	-0.45719
H	2.73842	1.89180	-0.88982
O	0.47857	0.72892	0.26765
H	3.03269	-0.24735	1.93143

06\_d7.mol2

E = -1185.676798  
H = -1185.555110  
G = -1185.610020  
G(quasi-RRHO) = -1185.608516

Si	1.70511	0.00351	0.06196
O	1.08914	-1.35490	-0.66091
H	1.72768	-1.77616	-1.24216
O	1.09940	1.37706	-0.63460
O	1.82729	-0.04093	1.68826
H	0.89336	-0.05614	1.98377
H	1.77324	1.87905	-1.10031
O	3.28665	0.04542	-0.45094
H	3.94143	-0.22032	0.19648
Si	-1.80034	-0.01103	0.06651
O	-1.77662	-1.36346	-0.89749
H	-0.85928	-1.66112	-0.97173
O	-1.76569	1.35151	-0.89112
O	-3.35070	-0.06759	0.65398
H	-3.66963	0.75059	1.03766
O	-0.61241	-0.00562	1.09900
H	-0.84997	1.65757	-0.95176

07\_d8.mol2

E = -1185.676798  
H = -1185.555110  
G = -1185.610017  
G(quasi-RRHO) = -1185.608514

Si	1.70510	-0.00353	0.06197
O	1.09937	-1.37711	-0.63451
H	1.77317	-1.87902	-1.10037
O	1.08917	1.35487	-0.66098
O	1.82730	0.04103	1.68826
H	0.89337	0.05633	1.98378
H	1.72776	1.77621	-1.24211
O	3.28663	-0.04549	-0.45096
H	3.94143	0.22056	0.19632
Si	-1.80034	0.01105	0.06652
O	-1.76572	-1.35146	-0.89114
H	-0.85003	-1.65762	-0.95166
O	-1.77659	1.36349	-0.89747
O	-3.35069	0.06762	0.65401

H	-3.66977	-0.75069	1.03729
O	-0.61239	0.00553	1.09899
H	-0.85925	1.66110	-0.97180

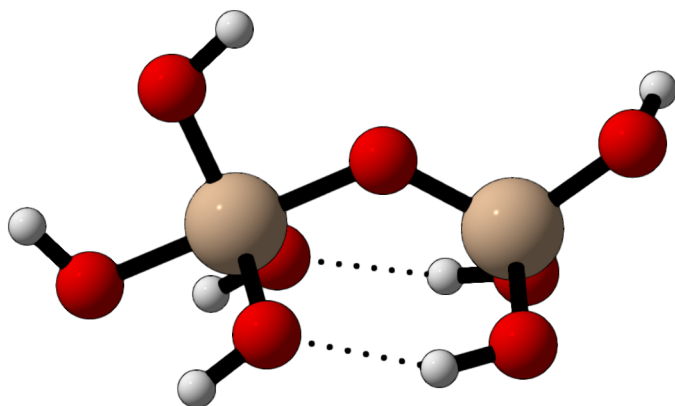
*08\_d9.mol2*

E = -1185.674420  
H = -1185.552962  
G = -1185.608827  
G(quasi-RRHO) = -1185.607013

Si	-1.82418	0.01052	-0.05683
O	-1.08510	-0.42122	1.36715
H	-1.72528	-0.65483	2.04415
O	-1.73417	1.63183	-0.32584
O	-1.62658	-1.01094	-1.31821
H	-0.67301	-0.91633	-1.52853
H	-2.60150	2.04318	-0.30101
O	-3.44369	-0.17652	0.30777
H	-3.86203	-0.94569	-0.08180
Si	1.90042	0.01631	-0.04996
O	1.68641	-0.53780	1.49934
H	0.73426	-0.55869	1.68860
O	2.66703	1.49021	-0.00020
O	3.07437	-0.96289	-0.71202
H	2.90194	-1.90355	-0.64566
O	0.53994	0.12088	-0.82957
H	3.53257	1.49192	0.41200

IM1, three equatorial OH groups

*00\_e1.mol2*



E = -1185.697202  
H = -1185.573186  
G = -1185.625378  
G(quasi-RRHO) = -1185.624548

Si	1.35635	-0.01919	0.12289
O	0.97895	-1.34095	-0.88081
H	1.73853	-1.55583	-1.42655
O	0.98376	1.51924	-0.50294
O	2.01569	-0.22494	1.66073
H	1.31730	-0.30903	2.31259
H	1.74363	1.86362	-0.97726
O	2.97629	0.06730	-0.55788
H	3.64340	-0.01300	0.12403
Si	-1.66897	0.00744	0.03587
O	-1.78422	-1.22324	-1.05207
H	-0.88492	-1.54432	-1.23957
O	-1.78507	1.48348	-0.67634
O	-2.99228	-0.06921	1.00374
H	-3.27885	-0.94897	1.25463
O	-0.27036	-0.10716	0.81944
H	-0.88452	1.83571	-0.78141

*01\_e7.mol2*

E = -1185.692041  
H = -1185.568438  
G = -1185.624078  
G(quasi-RRHO) = -1185.622013

Si	1.47423	0.06911	0.05265
O	0.96821	-1.25860	-0.88339
H	1.73142	-1.73877	-1.21128
O	1.78625	1.58946	-0.61005
O	1.61588	-0.11855	1.72103
H	0.78600	0.10591	2.14613
H	0.99118	2.12518	-0.58644
O	3.12331	-0.42355	-0.22068
H	3.74087	0.29510	-0.08446
Si	-1.73954	0.01568	-0.01193
O	-1.69635	-1.40485	-0.83290
H	-0.76049	-1.62033	-1.01552
O	-2.66002	1.13342	-0.79718
O	-2.64140	-0.18478	1.35187
H	-2.46503	-0.98170	1.85437

O	-0.25629	0.54600	0.25143
H	-2.22620	1.59900	-1.51397

*02\_e9.mol2*

E = -1185.692154  
H = -1185.568538  
G = -1185.623805  
G(quasi-RRHO) = -1185.621845

Si	-1.45966	-0.08860	0.00102
O	-0.97754	1.48907	-0.41905
H	-1.74205	2.06828	-0.44611
O	-1.90492	-1.24516	-1.14377
O	-1.43207	-0.53659	1.62561
H	-0.57954	-0.91214	1.85319
H	-1.13668	-1.75384	-1.40977
O	-3.10175	0.48454	0.10814
H	-3.73695	-0.22332	-0.00031
Si	1.71953	0.00332	-0.02990
O	2.36675	-0.16356	1.47618
H	2.64022	-1.04766	1.72700
O	1.69888	1.61546	-0.31652
O	2.80055	-0.75843	-1.01374
H	2.49655	-0.95124	-1.90252
O	0.25683	-0.61991	-0.19230
H	0.76648	1.89047	-0.41359

*03\_e3.mol2*

E = -1185.692213  
H = -1185.568618  
G = -1185.623778  
G(quasi-RRHO) = -1185.621883

Si	1.46138	-0.08349	0.05068
O	0.98465	1.54671	-0.07004
H	1.73440	2.08300	-0.33700
O	1.87702	-0.69231	1.56386
O	1.47508	-1.12834	-1.27668
H	0.64178	-1.59806	-1.34213
H	1.09294	-1.02961	2.00149
O	3.09838	0.40823	-0.28930
H	3.61086	-0.30122	-0.67696
Si	-1.72056	0.01252	0.00752

O	-2.38001	-0.66594	-1.34118
H	-2.66611	-1.57767	-1.26245
O	-1.68768	1.62215	-0.29137
O	-2.79948	-0.35009	1.20025
H	-2.48824	-0.22810	2.09900
O	-0.26083	-0.52362	0.37628
H	-0.75428	1.91072	-0.27131

*04\_e2.mol2*

E = -1185.692368  
H = -1185.568813  
G = -1185.623609  
G(quasi-RRHO) = -1185.621957

Si	-1.42542	0.01586	-0.09958
O	-0.96893	-0.81195	1.31817
H	-1.74710	-0.96676	1.85765
O	-1.37950	1.69902	-0.05464
O	-1.88460	-0.82274	-1.49218
H	-1.11650	-0.99989	-2.03812
H	-2.24960	2.01985	0.19212
O	-3.11100	0.00983	0.43844
H	-3.66661	-0.46096	-0.18287
Si	1.71945	0.00125	-0.02271
O	1.70213	-0.63947	1.48893
H	0.77218	-0.81006	1.73596
O	2.29122	1.54483	-0.02033
O	2.82874	-0.82531	-0.92066
H	2.79197	-1.78137	-0.85693
O	0.25730	-0.01651	-0.65779
H	3.21629	1.65809	0.20484

*05\_e8.mol2*

E = -1185.692264  
H = -1185.568591  
G = -1185.623180  
G(quasi-RRHO) = -1185.621614

Si	-1.43044	-0.01746	0.11983
O	-0.99362	-1.02637	-1.18538
H	-1.74645	-1.11765	-1.77336
O	-1.97308	-0.73997	1.53797
O	-1.24054	1.65361	-0.04618

H	-0.34351	1.94131	0.14019
H	-1.21913	-0.98412	2.07801
O	-3.07392	0.10476	-0.45572
H	-3.23481	0.96997	-0.83217
Si	1.67882	-0.02008	0.02813
O	2.94976	-0.51924	0.94304
H	3.08948	-1.46668	0.99372
O	1.91942	1.59661	-0.19512
O	1.71297	-0.85001	-1.38776
H	0.79189	-1.06945	-1.62550
O	0.26032	-0.17188	0.74351
H	2.69472	1.87207	-0.68718

*06\_e4.mol2*

E = -1185.693426  
H = -1185.569367  
G = -1185.621141  
G(quasi-RRHO) = -1185.620326

Si	1.37070	-0.01844	0.14427
O	0.98362	-1.37742	-0.81229
H	1.74057	-1.69548	-1.30670
O	0.99025	1.51505	-0.49982
O	1.99997	-0.18725	1.69147
H	1.27865	-0.25443	2.31944
H	1.74843	1.92731	-0.91679
O	3.02007	0.04190	-0.45502
H	3.08570	0.14404	-1.40559
Si	-1.66656	0.00966	0.02406
O	-1.77572	-1.24329	-1.03962
H	-0.87732	-1.58025	-1.19992
O	-1.77940	1.46998	-0.72145
O	-2.99784	-0.04698	0.98320
H	-3.28533	-0.92173	1.25012
O	-0.27453	-0.08746	0.81810
H	-0.87990	1.82733	-0.81376

*07\_e6.mol2*

E = -1185.693542  
H = -1185.569470  
G = -1185.621115  
G(quasi-RRHO) = -1185.620342



Si	-1.33265	-0.01248	0.14476
O	-0.98266	1.52481	-0.49376
H	-1.72574	1.85368	-1.00444
O	-0.97399	-1.38764	-0.80147
O	-1.95852	-0.20564	1.69572
H	-2.91111	-0.10237	1.69573
H	-1.66339	-1.55348	-1.44695
O	-2.94905	0.13779	-0.58512
H	-3.52650	-0.61423	-0.44493
Si	1.67490	0.00651	0.03866
O	3.00006	-0.03611	1.00653
H	3.28568	-0.90664	1.28882
O	1.78773	1.45924	-0.72151
O	1.79309	-1.25846	-1.00972
H	0.89368	-1.59181	-1.17382
O	0.27935	-0.08607	0.82638
H	0.88796	1.81512	-0.81877

*08\_e5.mol2*

E = -1185.693535

H = -1185.569447

G = -1185.621083

G(quasi-RRHO) = -1185.620304

Si	1.33267	-0.01394	0.14468
O	0.97841	-1.44429	-0.70549
H	1.72023	-1.69924	-1.25845
O	0.97696	1.48379	-0.59400
O	1.96004	-0.04897	1.70676
H	2.91242	-0.15301	1.69071
H	1.66519	1.73854	-1.21114
O	2.94777	-0.06230	-0.60096
H	3.52683	0.66078	-0.35518
Si	-1.67469	0.01197	0.03849
O	-1.78288	-1.30197	-0.94901
H	-0.88421	-1.64804	-1.08811
O	-1.79792	1.42619	-0.78953
O	-3.00000	0.00672	1.00713
H	-3.28045	-0.85146	1.32953
O	-0.27916	-0.03325	0.83037
H	-0.89762	1.77261	-0.91388

09\_e10.mol2

E = -1185.693291  
H = -1185.569279  
G = -1185.621002  
G(quasi-RRHO) = -1185.620226

Si	1.33805	-0.01422	0.14808
O	0.96904	-1.40267	-0.77238
H	1.72818	-1.72372	-1.26127
O	0.97176	1.50011	-0.54734
O	1.96663	-0.13677	1.70042
H	2.92519	-0.13597	1.66329
H	1.73098	1.88980	-0.98347
O	3.00485	0.03231	-0.47044
H	3.08785	0.10246	-1.42263
Si	-1.67606	0.00894	0.03861
O	-1.79364	-1.27298	-0.98932
H	-0.89697	-1.61530	-1.14726
O	-1.80045	1.44813	-0.74537
O	-2.99771	-0.02352	1.01188
H	-3.27721	-0.89049	1.31077
O	-0.27832	-0.06436	0.82305
H	-0.90314	1.80518	-0.85712

10\_e11.mol2

E = -1185.686111  
H = -1185.562687  
G = -1185.619065  
G(quasi-RRHO) = -1185.617169

Si	-1.54810	-0.05778	0.01235
O	-1.47782	-0.65786	1.58240
H	-0.60327	-1.00838	1.75588
O	-1.15774	1.54038	-0.32455
O	-3.21770	0.31323	0.25411
H	-3.58562	0.77152	-0.50188
H	-0.22640	1.69652	-0.51208
O	-1.87527	-1.07537	-1.29138
H	-1.05323	-1.43767	-1.62747
Si	1.73292	-0.03311	-0.02303
O	2.81690	-0.96726	-0.83727
H	2.48882	-1.39825	-1.62863
O	2.32854	0.06028	1.50770
O	1.73268	1.52697	-0.56842

H	2.47884	2.08360	-0.33895
O	0.25421	-0.57625	-0.18262
H	2.68312	-0.74777	1.88292

*11\_e14.mol2*

E = -1185.685342  
H = -1185.561969  
G = -1185.619063  
G(quasi-RRHO) = -1185.616778

Si	-1.49680	-0.02501	-0.03338
O	-1.15096	-0.03470	1.60987
H	-0.20972	-0.08263	1.80616
O	-1.38135	1.45380	-0.84070
O	-1.88388	-1.46053	-0.84463
H	-1.08531	-1.86806	-1.18404
H	-2.25093	1.85966	-0.83432
O	-3.20183	0.23550	0.28714
H	-3.72447	-0.48096	-0.07218
Si	1.72738	-0.01754	-0.05638
O	1.74709	-0.03858	1.60004
H	2.52870	0.28304	2.05247
O	2.23813	1.43464	-0.62915
O	2.83623	-1.08612	-0.63861
H	2.78239	-1.98566	-0.31068
O	0.23978	-0.34044	-0.48112
H	3.18556	1.56163	-0.70370

*12\_e13.mol2*

E = -1185.685808  
H = -1185.562397  
G = -1185.618949  
G(quasi-RRHO) = -1185.617030

Si	-1.54246	-0.00869	0.03507
O	-1.14987	1.46462	-0.65784
H	-0.21073	1.67220	-0.63816
O	-1.44380	-1.42912	-0.87106
O	-1.91299	-0.14012	1.67571
H	-1.11051	-0.32027	2.16934
H	-0.57677	-1.82724	-0.77384
O	-3.19663	0.24886	-0.39166
H	-3.75466	-0.45584	-0.06159

Si	1.72586	-0.02927	0.04316
O	1.75787	1.51980	-0.54221
H	2.52975	1.81161	-1.03030
O	2.13632	-1.11325	-1.12272
O	2.88418	-0.21183	1.19724
H	2.90790	0.44599	1.89463
O	0.24707	-0.28180	0.54176
H	3.07023	-1.25242	-1.28897

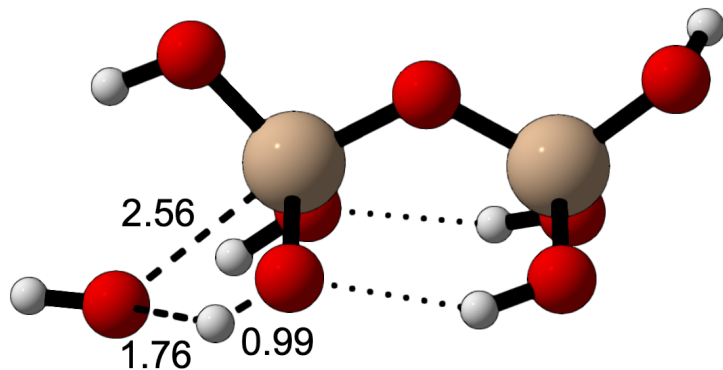
*13\_e12.mol2*

E = -1185.686164  
H = -1185.562691  
G = -1185.618809  
G(quasi-RRHO) = -1185.617017

Si	-1.54872	-0.02944	-0.00471
O	-1.14680	1.47986	-0.60542
H	-0.20539	1.61061	-0.75533
O	-1.88735	-1.31605	-1.04062
O	-1.48736	-0.34175	1.65213
H	-0.62615	-0.68934	1.89045
H	-1.07733	-1.79257	-1.23225
O	-3.20619	0.45226	0.06653
H	-3.75923	-0.25521	0.39923
Si	1.73659	-0.04224	-0.01402
O	2.34431	0.21879	1.49215
H	2.70756	-0.54211	1.94871
O	1.74535	1.44479	-0.73519
O	2.80681	-1.07399	-0.72191
H	2.47058	-1.58697	-1.45910
O	0.25166	-0.58389	-0.10193
H	2.49641	2.01891	-0.57546

TS2, water cleavage of IM1

*00\_h1.mol2*



E = -1185.672731  
 H = -1185.552172  
 G = -1185.605881  
 G(quasi-RRHO) = -1185.604633

Si	1.07563	0.38585	-0.09121
O	1.16696	-0.16963	1.45590
H	2.05726	-0.59828	1.46880
O	1.17126	-0.81617	-1.21154
O	1.99239	1.70439	-0.40756
H	2.92750	1.48330	-0.35091
H	2.06067	-1.20368	-1.02191
O	3.27151	-0.89951	0.22289
H	4.20100	-0.67468	0.16586
Si	-1.77424	-0.04288	-0.00052
O	-1.72692	-0.60902	1.53519
H	-0.82712	-0.64063	1.89141
O	-1.73931	-1.22472	-1.12868
O	-3.19125	0.71978	-0.23432
H	-3.54292	1.22739	0.49952
O	-0.47662	0.92327	-0.22468
H	-0.83986	-1.42222	-1.42611

*01\_h2.mol2*

E = -1185.669444  
 H = -1185.549086  
 G = -1185.604441  
 G(quasi-RRHO) = -1185.602586

Si	-1.19162	0.26096	0.10025
O	-1.09547	-1.07851	-0.85868
H	-2.05879	-1.31945	-0.91236
O	-1.77780	0.05024	1.61548

O	-1.78995	1.59596	-0.66139
H	-1.12470	2.26373	-0.84107
H	-2.69207	-0.25464	1.43466
O	-3.45551	-0.71780	-0.15370
H	-4.05342	-0.15496	-0.64795
Si	1.82779	-0.04845	0.01253
O	1.61519	-1.27299	-1.04679
H	0.67481	-1.49675	-1.16389
O	2.45879	-0.52848	1.44258
O	2.90822	1.01132	-0.61089
H	2.82961	1.21097	-1.54579
O	0.40516	0.64101	0.35505
H	3.36910	-0.83008	1.44422

*02\_h3.mol2*

E = -1185.669461  
H = -1185.548983  
G = -1185.602625  
G(quasi-RRHO) = -1185.601538

Si	1.11044	0.38501	-0.02867
O	1.16836	-0.38545	1.42525
H	2.04714	-0.83789	1.36114
O	1.17280	-0.60233	-1.34508
O	2.04368	1.73063	-0.13032
H	1.55065	2.55032	-0.20855
H	2.04996	-1.04012	-1.21128
O	3.21093	-1.00539	0.08704
H	4.03933	-0.52475	0.05617
Si	-1.75033	-0.05014	-0.00663
O	-1.70718	-0.84496	1.42532
H	-0.80562	-0.91822	1.77246
O	-1.70982	-1.04738	-1.30180
O	-3.17168	0.73374	-0.12466
H	-3.52963	1.11447	0.67947
O	-0.45540	0.93935	-0.07681
H	-0.80684	-1.17768	-1.62673

*03\_h4.mol2*

E = -1185.665004  
H = -1185.544693  
G = -1185.600640  
G(quasi-RRHO) = -1185.598494

Si	-1.20752	-0.27306	-0.00426
O	-1.09488	1.34830	-0.27783
H	-2.07223	1.56341	-0.28918
O	-1.76202	-1.15357	-1.28322
O	-1.76278	-0.80082	1.44951
H	-2.70352	-0.58586	1.47774
H	-1.07483	-1.67996	-1.69694
O	-3.45864	0.67144	-0.05560
H	-3.83999	1.07459	0.72864
Si	1.81934	0.04335	0.03045
O	2.48205	-0.11038	1.51812
H	3.39835	0.15298	1.62117
O	1.60716	1.59722	-0.42618
O	2.87861	-0.67033	-0.99457
H	2.78233	-0.46526	-1.92660
O	0.39536	-0.71818	0.08839
H	0.66550	1.84674	-0.43052

04\_h5.mol2

E = -1185.664783  
H = -1185.544382  
G = -1185.598296  
G(quasi-RRHO) = -1185.597118

Si	-1.12760	0.35756	-0.04124
O	-1.17073	-0.76274	-1.24171
H	-2.09022	-1.12534	-1.07049
O	-1.14034	-0.21102	1.51035
O	-2.04101	1.69769	-0.28725
H	-1.52488	2.49472	-0.42617
H	-1.99834	-0.63622	1.64406
O	-3.31141	-0.81476	0.00972
H	-3.47483	-1.64977	0.45545
Si	1.75178	-0.04708	0.00309
O	1.67477	-1.19585	-1.16202
H	0.76314	-1.34941	-1.45501
O	1.78777	-0.66640	1.51721
O	3.15998	0.75651	-0.14655
H	3.47554	0.92170	-1.03695
O	0.44135	0.90969	-0.13632
H	0.90814	-0.70731	1.91567

05\_h7.mol2

E = -1185.660865  
H = -1185.542638  
G = -1185.598108  
G(quasi-RRHO) = -1185.596326

Si	-1.22395	-0.25515	0.09304
O	-1.13613	1.21165	-0.62407
H	-2.20537	1.32055	-0.64231
O	-1.75360	-1.51237	-0.83632
O	-1.80236	-0.30464	1.64071
H	-1.12572	-0.55786	2.27291
H	-1.05772	-2.15047	-1.00902
O	-3.41395	0.67602	-0.36210
H	-3.74639	0.97089	0.48792
Si	1.79818	0.05274	-0.01722
O	2.80617	0.13207	1.27300
H	2.65395	0.84640	1.89478
O	1.52892	1.56034	-0.58197
O	2.55514	-0.92068	-1.09384
H	3.47911	-0.73991	-1.27561
O	0.38964	-0.66334	0.32676
H	0.57232	1.71165	-0.72756

06\_h8.mol2

E = -1185.660896  
H = -1185.542608  
G = -1185.597945  
G(quasi-RRHO) = -1185.596214

Si	1.22453	-0.25617	0.09327
O	1.13370	1.34022	-0.24980
H	2.20030	1.43783	-0.31700
O	1.78034	-0.67974	1.58857
O	1.77899	-1.24973	-1.10554
H	1.09712	-1.84150	-1.43194
H	1.08998	-1.06553	2.13245
O	3.41244	0.75570	-0.15102
H	3.73693	0.46235	-1.00468
Si	-1.79765	0.04969	-0.02747
O	-2.50890	-0.67255	-1.31300
H	-3.43064	-0.46643	-1.47819
O	-1.53432	1.64599	-0.24323
O	-2.84387	-0.16087	1.21665



H	-2.72426	0.40719	1.98018
O	-0.38960	-0.71361	0.19682
H	-0.57590	1.83346	-0.31748

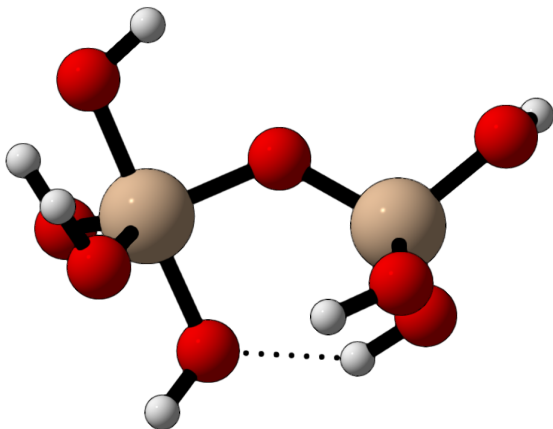
07\_h9.mol2

E = -1185.656649  
H = -1185.537100  
G = -1185.592669  
G(quasi-RRHO) = -1185.591026

Si	1.23977	0.14017	-0.04293
O	1.14531	-0.67923	1.38312
H	0.23448	-0.82041	1.67282
O	1.69741	-0.70812	-1.35357
O	1.89456	1.64992	0.11745
H	1.22819	2.33962	0.07623
H	2.68063	-0.81133	-1.06650
O	3.65810	-0.51960	0.05486
H	4.13475	0.29129	-0.13262
Si	-1.83804	-0.00430	-0.04978
O	-1.71701	-0.71764	1.42520
H	-2.45378	-1.24007	1.74806
O	-2.41366	-1.14402	-1.06601
O	-2.91122	1.22705	-0.09652
H	-2.62453	2.07709	0.24316
O	-0.36109	0.53092	-0.38113
H	-2.76320	-0.85270	-1.91041

TS-iso, isomerization of IM1 to IM2

00\_f1.mol2



E = -1185.687114  
H = -1185.564840  
G = -1185.617065  
G(quasi-RRHO) = -1185.616336

Si	1.34741	0.00244	-0.05384
O	2.37443	0.72661	-1.17708
H	2.94014	0.05019	-1.55631
O	1.78047	-0.03237	1.58330
O	2.12231	-1.56115	-0.34415
H	1.46414	-2.23936	-0.49578
H	2.27271	-0.83710	1.75926
O	0.53659	1.55390	0.23164
H	1.00834	2.09377	0.86664
Si	-1.60892	-0.09990	-0.05457
O	-1.97846	1.34246	-0.74647
H	-1.20437	1.91623	-0.63516
O	-1.72543	-0.09291	1.58503
O	-2.80066	-1.13689	-0.49232
H	-3.13100	-1.05491	-1.38834
O	-0.15549	-0.64524	-0.52142
H	-0.91891	0.20029	2.01917

*01\_f2.mol2*

E = -1185.686076  
H = -1185.563590  
G = -1185.615311  
G(quasi-RRHO) = -1185.614502

Si	1.33966	-0.00694	0.13298
O	0.96515	-1.47028	-0.65382
H	1.71989	-1.74450	-1.18043
O	0.98724	1.50167	-0.56677
O	2.05768	0.06266	1.66077
H	2.29030	-0.78339	2.04405
H	1.72573	1.76775	-1.11950
O	2.91467	-0.03606	-0.69824
H	3.61508	0.20457	-0.09160
Si	-1.67611	0.01141	0.03675
O	-1.79763	-1.32432	-0.92066
H	-0.90222	-1.68191	-1.04887
O	-1.78628	1.40632	-0.82647
O	-3.00393	0.03862	1.00284
H	-3.29460	-0.81094	1.33877

O	-0.28147	-0.02555	0.82913
H	-0.88741	1.76152	-0.93287

*02\_f4.mol2*

E = -1185.685960  
H = -1185.563400  
G = -1185.614948  
G(quasi-RRHO) = -1185.614294

Si	1.38176	-0.02028	0.13873
O	0.91579	-1.36258	-0.79320
H	1.66210	-1.65591	-1.32049
O	1.10352	1.47226	-0.66646
O	1.97895	-0.10675	1.70689
H	1.24206	-0.14349	2.32014
H	1.25002	2.24266	-0.11407
O	3.02648	-0.11769	-0.45875
H	3.14370	0.47927	-1.19788
Si	-1.66105	0.01259	0.02899
O	-1.86646	-1.40956	-0.77765
H	-0.98502	-1.75938	-0.98680
O	-1.68252	1.30429	-0.98860
O	-2.99012	0.21249	0.97229
H	-3.32943	-0.57805	1.39527
O	-0.27379	-0.00494	0.83587
H	-0.76819	1.62227	-1.08726

*03\_f5.mol2*

E = -1185.682968  
H = -1185.560699  
G = -1185.614873  
G(quasi-RRHO) = -1185.613028

Si	-1.45169	-0.07447	0.01015
O	-0.89062	1.55496	-0.20819
H	-1.61748	2.11764	-0.48047
O	-1.84411	-1.62603	-0.60645
O	-1.78327	-0.19531	1.65550
H	-1.29057	0.43355	2.18375
H	-1.08466	-2.20612	-0.53856
O	-2.95416	0.48082	-0.65684
H	-3.49506	-0.25984	-0.93265
Si	1.73909	-0.02844	-0.03739

O	2.56493	-0.46196	1.31899
H	2.08375	-0.38290	2.14422
O	1.74347	1.59512	-0.25488
O	2.68125	-0.73628	-1.18522
H	2.55296	-0.42349	-2.08213
O	0.23523	-0.57657	-0.01621
H	0.80570	1.88393	-0.28637

*04\_f3.mol2*

E = -1185.686749  
H = -1185.563946  
G = -1185.614295  
G(quasi-RRHO) = -1185.613663

Si	1.35562	-0.02295	-0.10171
O	2.94087	0.64659	-0.23377
H	3.57074	-0.02290	-0.50388
O	1.19219	-0.45357	1.53703
O	1.97003	-1.44034	-0.85894
H	1.24707	-2.01057	-1.12440
H	1.60201	-1.29884	1.73048
O	0.77196	1.60536	-0.05565
H	1.49591	2.21576	0.09430
Si	-1.64406	-0.04549	-0.05404
O	-1.95589	1.54229	-0.34906
H	-1.09966	2.00278	-0.33296
O	-1.61668	-0.39445	1.55014
O	-2.91931	-0.89069	-0.64539
H	-3.30396	-0.56172	-1.45958
O	-0.23082	-0.47396	-0.70244
H	-0.69275	-0.49621	1.84134

*05\_f6.mol2*

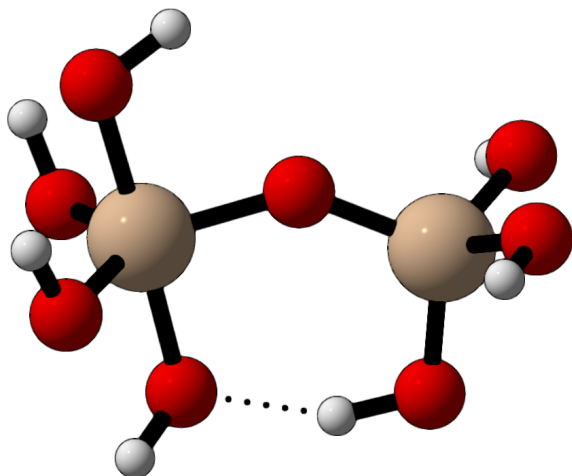
E = -1185.682286  
H = -1185.559493  
G = -1185.611285  
G(quasi-RRHO) = -1185.610156

Si	1.59248	0.00449	-0.15180
O	2.82870	0.02195	-1.22030
H	3.06845	-0.81629	-1.61907
O	1.74977	-1.32185	0.80425
O	1.75838	1.39918	0.69342

H	0.88648	1.62475	1.06619
H	0.87369	-1.52680	1.18068
O	0.13337	-0.02880	-0.85605
Si	-1.32911	-0.00206	-0.00529
O	-2.24276	-1.27748	-0.73320
H	-2.72858	-1.06555	-1.52877
O	-2.25386	1.21702	-0.81029
H	-2.73799	0.95270	-1.59137
O	-1.00343	1.22258	1.19400
H	-1.35795	2.05690	0.88021
O	-1.01114	-1.14072	1.27731
H	-1.36339	-1.99469	1.01818

IM2, co-linear OH groups on Si

[00\\_g3.mol2](#)



E = -1185.688537  
H = -1185.565410  
G = -1185.621543  
G(quasi-RRHO) = -1185.619231

Si	-1.41078	-0.01820	0.02256
O	-0.87000	1.67430	0.09830
H	-1.36143	2.20285	-0.53140
O	-1.99850	-1.68583	-0.12602
O	-2.13740	0.15022	1.53430
H	-2.53154	-0.69115	1.77430
H	-1.26997	-2.30326	-0.06347
O	-2.25192	0.38623	-1.39094
H	-2.67975	-0.40035	-1.73544

Si	1.71250	-0.05981	-0.01314
O	2.62114	-0.71757	1.18468
H	2.45216	-0.39441	2.07119
O	1.72177	1.56779	0.06994
O	2.51368	-0.62708	-1.32922
H	2.10558	-0.46006	-2.18042
O	0.18743	-0.58780	0.01654
H	0.77135	1.85651	0.07281

*01\_g2.mol2*

E = -1185.688933  
H = -1185.565772  
G = -1185.621396  
G(quasi-RRHO) = -1185.619301

Si	-1.41156	-0.05210	0.01298
O	-0.90505	1.68264	-0.06409
H	-1.24968	2.07913	-0.86573
O	-2.10950	-1.65067	0.03786
O	-1.97484	0.22988	1.58350
H	-1.79366	1.13818	1.83287
H	-2.08417	-2.03663	0.91371
O	-2.17771	0.21589	-1.47448
H	-2.67691	-0.56261	-1.72919
Si	1.69563	-0.08081	-0.01999
O	2.58657	-0.72003	1.20197
H	2.44840	-0.33607	2.06936
O	1.69206	1.54729	0.07582
O	2.52955	-0.64197	-1.31912
H	2.08437	-0.58222	-2.16597
O	0.17785	-0.62237	-0.03867
H	0.74323	1.83572	0.02079

*02\_g4.mol2*

E = -1185.688565  
H = -1185.565432  
G = -1185.620556  
G(quasi-RRHO) = -1185.618797

Si	1.40910	-0.02021	-0.01704
O	0.86501	1.66261	-0.19977
H	1.37826	2.23675	0.36984
O	1.98186	-1.67886	0.24512

O	2.20955	0.07145	-1.49792
H	2.62022	-0.77836	-1.67127
H	1.25825	-2.30019	0.16705
O	2.19620	0.45741	1.40439
H	2.61275	-0.30932	1.80329
Si	-1.70846	-0.04597	0.00317
O	-2.62093	-0.78614	-1.14736
H	-2.24403	-0.83377	-2.02796
O	-1.73037	1.57476	-0.13217
O	-2.45604	-0.41643	1.41630
H	-2.69715	-1.33489	1.54922
O	-0.18976	-0.58713	-0.06815
H	-0.78148	1.86496	-0.15957

*03\_g6.mol2*

E = -1185.688589  
H = -1185.565435  
G = -1185.620528  
G(quasi-RRHO) = -1185.618565

Si	1.41244	-0.05190	-0.00560
O	0.89465	1.68099	-0.01597
H	1.23040	2.11926	0.76740
O	2.11748	-1.64675	0.04678
O	1.96466	0.15105	-1.59200
H	1.77573	1.04351	-1.88831
H	2.09389	-2.07372	-0.80989
O	2.18816	0.29717	1.45957
H	2.69468	-0.46402	1.74970
Si	-1.68058	-0.07283	0.01897
O	-1.70343	1.53586	-0.23014
H	-0.76295	1.84397	-0.16058
O	-2.38526	-0.51892	1.43862
O	-2.54586	-0.71426	-1.22440
H	-2.80908	-1.63203	-1.13586
O	-0.17331	-0.62766	0.08816
H	-3.32536	-0.35049	1.52527

*04\_g5.mol2*

E = -1185.688400  
H = -1185.565267  
G = -1185.620403  
G(quasi-RRHO) = -1185.618640

Si	-1.41170	-0.01428	0.02354
O	-2.14952	0.25586	1.51480
H	-2.55308	-0.56530	1.80412
O	-2.24021	0.30457	-1.41900
O	-2.00974	-1.68418	-0.02316
H	-1.28725	-2.30146	0.09046
H	-2.67121	-0.49942	-1.71606
O	-0.85687	1.67486	-0.00666
H	-1.34321	2.16701	-0.66895
Si	1.70051	-0.06603	-0.01113
O	1.73760	1.56235	0.05780
H	0.79411	1.86608	0.00916
O	2.32535	-0.67640	-1.40135
O	2.65359	-0.68205	1.17875
H	2.60823	-0.23965	2.02847
O	0.18195	-0.59430	0.07448
H	3.27189	-0.58866	-1.52637

05\_g8.mol2

E = -1185.688093

H = -1185.564943

G = -1185.619948

G(quasi-RRHO) = -1185.618186

Si	1.41066	-0.01668	-0.02262
O	0.85583	1.67216	-0.07219
H	1.34214	2.19469	0.56639
O	2.00789	-1.68279	0.10396
O	2.14808	0.18214	-1.52514
H	2.55074	-0.65198	-1.77596
H	1.28548	-2.30479	0.01966
O	2.24067	0.37009	1.40238
H	2.67103	-0.41934	1.73707
Si	-1.69815	-0.05363	0.00520
O	-1.74234	1.56703	-0.13119
H	-0.79909	1.87249	-0.10029
O	-2.32314	-0.60220	1.42575
O	-2.61491	-0.62422	-1.23450
H	-2.87871	-1.54481	-1.18595
O	-0.18342	-0.59725	-0.04366
H	-3.25590	-0.44156	1.57975



06\_g7.mol2

E = -1185.688093  
H = -1185.564941  
G = -1185.619944  
G(quasi-RRHO) = -1185.618180

Si	1.41070	-0.01663	-0.02250
O	2.14690	0.18165	-1.52572
H	2.54984	-0.65240	-1.77629
O	2.24202	0.37043	1.40165
O	2.00792	-1.68279	0.10438
H	1.28580	-2.30491	0.01857
H	2.67213	-0.41910	1.73640
O	0.85535	1.67185	-0.07212
H	1.34294	2.19554	0.56449
Si	-1.69814	-0.05358	0.00543
O	-1.74194	1.56714	-0.13072
H	-0.79873	1.87249	-0.09947
O	-2.32415	-0.60236	1.42538
O	-2.61406	-0.62395	-1.23500
H	-2.87969	-1.54396	-1.18574
O	-0.18337	-0.59713	-0.04249
H	-3.25742	-0.44357	1.57813

07\_g1.mol2

E = -1185.687836  
H = -1185.564667  
G = -1185.619722  
G(quasi-RRHO) = -1185.618140

Si	1.35319	0.01789	-0.01171
O	2.12200	-0.44521	1.42133
H	2.69019	0.26997	1.71536
O	2.10170	-0.38200	-1.47039
O	2.16893	1.58540	0.04076
H	1.53570	2.29770	-0.04613
H	2.66490	0.34825	-1.73594
O	0.46872	-1.51963	-0.01118
H	1.01991	-2.26244	0.23723
Si	-1.62059	0.11566	-0.00575
O	-1.87471	-0.65075	1.42890
H	-1.15364	-1.26506	1.60581
O	-1.90292	-0.84927	-1.30300
O	-2.80023	1.24493	-0.14355

H	-2.86022	1.89617	0.55707
O	-0.15536	0.80771	-0.05212
H	-1.17822	-1.48371	-1.37501

*08\_g9.mol2*

E = -1185.688606  
H = -1185.564943  
G = -1185.617302  
G(quasi-RRHO) = -1185.616586

Si	1.32812	0.00902	-0.07429
O	0.67185	1.60473	0.29241
H	1.34789	2.21065	0.59764
O	1.33997	-0.40187	1.57935
O	2.67794	0.76559	-0.75513
H	3.26623	0.10157	-1.12137
H	1.71981	-1.27763	1.68331
O	2.00265	-1.53838	-0.57426
H	1.30674	-2.16610	-0.77046
Si	-1.60564	-0.04676	-0.10022
O	-2.85245	-0.82880	-0.81703
H	-2.94754	-1.76046	-0.61204
O	-1.98726	1.53282	-0.30478
O	-1.55424	-0.49630	1.48078
H	-0.64179	-0.51960	1.81472
O	-0.17356	-0.39912	-0.77569
H	-1.16529	2.03049	-0.15391

*09\_g10.mol2*

E = -1185.688470  
H = -1185.564808  
G = -1185.617170  
G(quasi-RRHO) = -1185.616465

Si	1.32946	0.01261	-0.07763
O	2.67784	0.77880	-0.75136
H	3.26631	0.11997	-1.12652
O	1.34516	-0.41827	1.57089
O	2.00494	-1.52720	-0.59934
H	1.30904	-2.15347	-0.80032
H	1.72745	-1.29428	1.66336
O	0.67384	1.60406	0.30720
H	1.35334	2.21078	0.60298

Si	-1.60523	-0.06176	-0.08689
O	-1.98524	1.52431	-0.26900
H	-1.16016	2.02038	-0.12626
O	-1.55131	-0.53496	1.48344
O	-2.83403	-0.92328	-0.74100
H	-3.24989	-0.55102	-1.52052
O	-0.17466	-0.39153	-0.77616
H	-0.63764	-0.55976	1.81324

*10\_g11.mol2*

E = -1185.685074  
H = -1185.561685  
G = -1185.615454  
G(quasi-RRHO) = -1185.613893

Si	1.39261	-0.01576	-0.00229
O	0.87968	1.67545	-0.25837
H	1.10373	2.19235	0.51687
O	1.98213	-1.66757	0.25867
O	1.90849	-0.01839	-1.61105
H	2.18171	-0.90248	-1.86194
H	2.93407	-1.73966	0.16729
O	2.28737	0.55872	1.32201
H	2.67764	-0.16745	1.81086
Si	-1.68116	-0.06885	0.03154
O	-1.69754	1.42814	-0.60770
H	-0.76437	1.76305	-0.55807
O	-2.42131	-0.16078	1.49904
O	-2.50989	-1.00225	-1.03937
H	-2.76470	-1.87647	-0.73890
O	-0.17409	-0.57339	0.27908
H	-3.36716	-0.00430	1.51602

*11\_g12.mol2*

E = -1185.684442  
H = -1185.560682  
G = -1185.613247  
G(quasi-RRHO) = -1185.612280

Si	1.60274	-0.04896	-0.12308
O	2.84292	-0.69062	-0.97424
H	2.94542	-1.64301	-0.93419
O	1.59491	-0.72247	1.37783

O	1.94575	1.55185	-0.08675
H	1.11294	1.98928	0.16769
H	0.69455	-0.77981	1.73703
O	0.15875	-0.31741	-0.80708
Si	-1.31537	0.01123	-0.04476
O	-1.97269	-1.49897	-0.68333
H	-2.89433	-1.64051	-0.45932
O	-2.53062	0.91222	-0.81288
H	-3.06120	0.36896	-1.39738
O	-0.72409	1.55031	0.61442
H	-1.26625	2.26888	0.28735
O	-1.31174	-0.59923	1.54927
H	-1.57991	-1.52089	1.53074

*12\_g13.mol2*

E = -1185.679583  
H = -1185.556574  
G = -1185.612568  
G(quasi-RRHO) = -1185.611026

Si	1.41607	-0.04707	0.00113
O	2.29341	-0.48363	1.37700
H	2.75058	0.29757	1.69431
O	2.04074	-0.20739	-1.56501
O	2.11482	1.59629	0.12206
H	1.41869	2.25244	0.09420
H	2.45599	0.62213	-1.81066
O	0.79652	-1.67248	-0.03845
H	0.24042	-1.82359	-0.80483
Si	-1.64616	0.10742	0.04580
O	-2.02547	-0.56723	1.48969
H	-2.93022	-0.86503	1.60198
O	-1.93030	-1.02395	-1.11264
O	-2.66324	1.34515	-0.32711
H	-2.44469	2.20532	0.03629
O	-0.14282	0.65799	0.11944
H	-2.13878	-0.69169	-1.98815

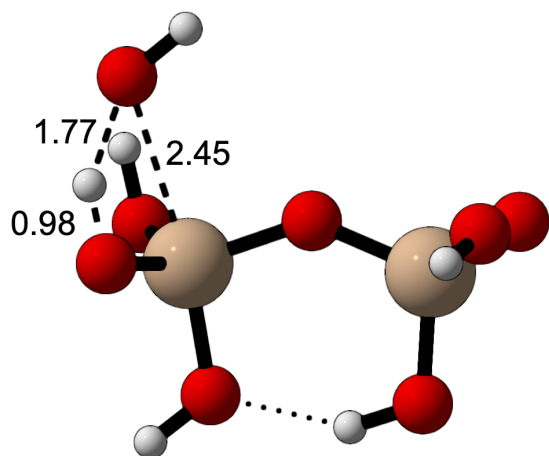
*13\_g14.mol2*

E = -1185.680522  
H = -1185.556752  
G = -1185.610029  
G(quasi-RRHO) = -1185.608871

Si	1.36929	0.05900	-0.07430
O	1.01391	1.74065	0.15960
H	0.08887	1.97033	0.05994
O	1.28936	-0.27006	1.60092
O	2.83688	0.53311	-0.76544
H	3.30533	-0.25229	-1.05587
H	1.57787	-1.17528	1.74379
O	1.83256	-1.61608	-0.44627
H	1.06043	-2.14707	-0.64163
Si	-1.60756	-0.07065	-0.09278
O	-2.76264	-1.04052	-0.72605
H	-3.17632	-0.75191	-1.54150
O	-2.02024	1.51415	-0.29067
O	-1.53257	-0.48444	1.48729
H	-0.61816	-0.43198	1.82091
O	-0.17144	-0.23724	-0.79846
H	-2.78872	1.83454	0.18607

TS3, water cleavage from IM2

[00\\_k1.mol2](#)



E = -1185.668344  
H = -1185.547782  
G = -1185.604143  
G(quasi-RRHO) = -1185.601940

Si	-1.29993	0.32124	0.02647
O	-2.20193	0.21651	1.39138
H	-2.54783	-0.70022	1.32018
O	-2.05231	0.21073	-1.42659

O	-2.40203	-1.86716	-0.03713
H	-1.76830	-2.58596	-0.01706
H	-2.41416	-0.70344	-1.37697
O	-0.76740	1.91428	0.03670
H	-1.35844	2.55378	-0.36417
Si	1.71801	-0.14459	0.00810
O	2.54409	-0.71921	1.29501
H	2.27592	-0.40632	2.16073
O	1.91157	1.46466	-0.18477
O	2.42224	-0.97582	-1.20905
H	2.18977	-0.71945	-2.10317
O	0.13475	-0.47456	0.14119
H	1.05792	1.93310	-0.15735

*01\_k2.mol2*

E = -1185.668359  
H = -1185.547784  
G = -1185.603431  
G(quasi-RRHO) = -1185.601596

Si	1.29880	0.32266	-0.02681
O	2.24361	0.23067	-1.36308
H	2.58260	-0.68888	-1.29171
O	2.00447	0.18818	1.44743
O	2.38669	-1.87484	0.04122
H	1.74505	-2.58478	-0.01353
H	2.36274	-0.72723	1.39727
O	0.77197	1.91740	-0.03134
H	1.35023	2.54775	0.40148
Si	-1.71191	-0.13205	-0.01308
O	-2.56466	-0.77640	-1.25192
H	-2.23605	-0.62244	-2.13984
O	-1.92141	1.47797	0.11763
O	-2.34233	-0.79806	1.33871
H	-2.49772	-1.74439	1.33185
O	-0.13514	-0.46452	-0.20344
H	-1.06890	1.94828	0.11105

*02\_k4.mol2*

E = -1185.664819  
H = -1185.543891  
G = -1185.601138  
G(quasi-RRHO) = -1185.598427

Si	-1.34329	0.33306	0.01230
O	-2.40422	0.32345	1.26725
H	-2.68863	-0.61331	1.27048
O	-1.88338	0.03966	-1.51682
O	-2.21843	-1.89015	0.07876
H	-1.50703	-2.49760	0.28753
H	-2.16041	-0.89603	-1.45074
O	-0.98150	1.95876	-0.03925
H	-0.07735	2.14424	-0.31345
Si	1.68199	-0.14404	0.04727
O	2.61117	-0.42841	1.35713
H	2.41667	0.06890	2.15358
O	1.79273	1.40937	-0.48334
O	2.30453	-1.20370	-1.02635
H	1.90017	-1.24040	-1.89516
O	0.11954	-0.37762	0.34673
H	2.65119	1.73716	-0.75900

03\_k5.mol2

E = -1185.664778

H = -1185.543903

G = -1185.600770

G(quasi-RRHO) = -1185.598324

Si	1.34415	0.32939	-0.01584
O	2.42613	0.27649	-1.25175
H	2.70295	-0.66203	-1.22402
O	1.85711	0.07762	1.52965
O	2.20243	-1.90097	-0.00401
H	1.48855	-2.50822	-0.20473
H	2.12783	-0.86143	1.49656
O	0.99283	1.95846	-0.01555
H	0.07978	2.15923	0.21423
Si	-1.67726	-0.13144	-0.04710
O	-2.58640	-0.58282	-1.32763
H	-2.24847	-0.38228	-2.20280
O	-1.81545	1.45964	0.32904
O	-2.25310	-0.96305	1.23308
H	-2.45843	-1.89135	1.10623
O	-0.11903	-0.37724	-0.35939
H	-2.66498	1.78966	0.62801

04\_k3.mol2

E = -1185.667520  
H = -1185.546566  
G = -1185.599899  
G(quasi-RRHO) = -1185.598839

Si	1.23153	0.35458	-0.05531
O	2.51757	0.51158	-1.05187
H	2.82752	-0.41868	-1.11473
O	1.41666	-0.19728	1.49127
O	2.23684	-1.84803	-0.21493
H	1.63546	-2.47988	-0.61225
H	1.79153	-1.09216	1.30947
O	0.71746	1.93137	0.18684
H	1.25886	2.47203	0.76445
Si	-1.61526	-0.14827	-0.07214
O	-2.11762	1.40951	-0.12495
H	-1.37260	2.01860	-0.02382
O	-1.52624	-0.74364	1.44888
O	-2.72962	-1.06334	-0.82651
H	-3.16126	-0.68469	-1.59462
O	-0.13693	-0.25008	-0.75394
H	-0.63215	-0.70430	1.81747

05\_k6.mol2

E = -1185.665200  
H = -1185.544052  
G = -1185.597390  
G(quasi-RRHO) = -1185.596271

Si	1.27950	0.35173	-0.04543
O	2.61619	0.39239	-0.99043
H	2.84294	-0.55844	-1.05203
O	1.34086	-0.19527	1.51970
O	2.02367	-1.90697	-0.18044
H	1.35888	-2.44360	-0.61491
H	1.61932	-1.12624	1.36692
O	1.02264	1.98744	0.15572
H	0.09487	2.23717	0.19201
Si	-1.59661	-0.12746	-0.08926
O	-1.99636	1.46780	-0.04736
H	-2.78021	1.72341	0.44370
O	-1.54937	-0.79334	1.40053
O	-2.69494	-1.00818	-0.90679



H	-3.09099	-0.61458	-1.68646
O	-0.12846	-0.15131	-0.77332
H	-0.67906	-0.69801	1.81560

*06\_k7.mol2*

E = -1185.662656  
H = -1185.541720  
G = -1185.596239  
G(quasi-RRHO) = -1185.594649

Si	1.62459	-0.12144	-0.09833
O	2.77566	-0.78823	-1.03503
H	2.87617	-1.74120	-0.99612
O	1.61605	-0.89365	1.34795
O	2.05091	1.45243	0.02637
H	1.27610	2.01400	0.16845
H	0.74879	-0.88237	1.77483
O	0.13368	-0.21513	-0.74545
Si	-1.24037	0.34007	-0.01339
O	-2.09342	-1.90672	-0.31731
H	-3.00323	-2.10322	-0.07704
O	-2.49226	0.55642	-1.04608
H	-2.77408	-0.35270	-1.25194
O	-0.84477	1.92260	0.37698
H	-1.21662	2.58398	-0.20927
O	-1.35035	-0.29892	1.50264
H	-1.65023	-1.20978	1.27460

*07\_k8.mol2*

E = -1185.658453  
H = -1185.539130  
G = -1185.595826  
G(quasi-RRHO) = -1185.593511

Si	-1.30224	0.28924	-0.00643
O	-0.79556	1.87362	-0.32286
H	-1.28218	2.30279	-1.02944
O	-2.26861	-1.99268	0.11618
O	-2.10759	0.46277	1.42399
H	-2.10121	1.37250	1.73121
H	-3.00668	-1.93229	0.72575
O	-2.14774	-0.08637	-1.34197
H	-2.44139	-1.02170	-1.00547

Si	1.71684	-0.14421	0.01574
O	2.59476	-0.51780	1.34163
H	2.52051	0.07395	2.09226
O	1.89340	1.42972	-0.37929
O	2.38198	-1.14493	-1.09180
H	1.95382	-1.19452	-1.94824
O	0.13997	-0.46239	0.22319
H	1.02777	1.87334	-0.44897

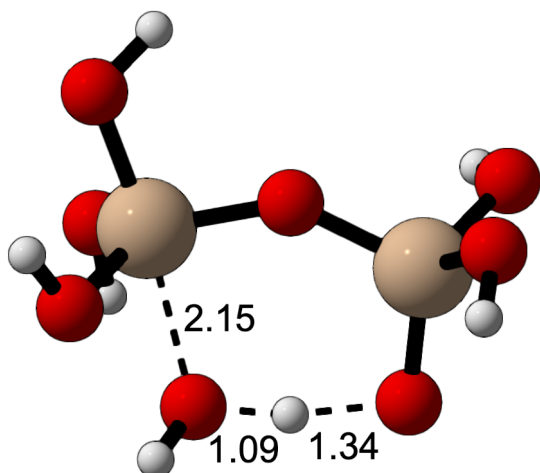
*08\_k9.mol2*

E = -1185.654639  
H = -1185.534595  
G = -1185.590876  
G(quasi-RRHO) = -1185.588766

Si	1.33569	-0.31615	-0.02712
O	0.96574	-1.91844	-0.33318
H	0.05457	-2.06413	-0.60960
O	2.12397	2.01003	0.19738
O	2.33934	-0.50036	1.27292
H	2.34445	-1.41284	1.57340
H	2.92145	1.95417	0.72723
O	1.98394	0.21220	-1.42905
H	2.24623	1.13383	-1.09403
Si	-1.69133	0.14585	0.05698
O	-2.61574	0.20417	1.39938
H	-2.45369	-0.45623	2.07562
O	-1.79694	-1.30546	-0.71105
O	-2.32232	1.36311	-0.82666
H	-1.87751	1.59277	-1.64466
O	-0.12794	0.33914	0.37686
H	-2.65710	-1.59843	-1.01870

TS4, water cleavage from IM2

*00\_m1.mol2*



E = -1185.678569  
 H = -1185.558704  
 G = -1185.613199  
 G(quasi-RRHO) = -1185.611451

Si	1.41920	-0.19272	-0.01738
O	2.09041	0.21482	-1.47767
H	1.89396	1.12707	-1.70242
O	2.10033	-1.73988	0.10988
O	0.74916	1.85061	-0.09002
H	1.07967	2.25477	0.71635
H	1.50699	-2.43773	-0.16843
O	-0.16227	-0.63562	-0.02374
O	2.11138	0.40325	1.37712
Si	-1.69637	-0.03315	0.00173
O	-2.48616	-0.67133	1.30803
O	-1.65715	1.54858	-0.03754
H	-0.34354	1.82693	-0.04967
O	-2.52463	-0.78513	-1.21748
H	-2.15555	-0.67534	-2.09515
H	-2.46080	-0.12491	2.09482
H	2.59101	-0.29113	1.83494

*01\_m2.mol2*

E = -1185.674782  
 H = -1185.553366  
 G = -1185.609160  
 G(quasi-RRHO) = -1185.607322

Si	-1.41592	-0.21633	-0.02309
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O	-1.73132	0.12400	1.56136
H	-2.10230	-0.64370	2.00321
O	-2.08708	-1.75350	-0.16571
O	-0.71216	2.05167	0.14901
H	-0.92220	2.38710	-0.72586
H	-1.44258	-2.44795	-0.30723
O	0.13468	-0.49498	-0.41942
O	-2.33870	0.58363	-1.13888
Si	1.68038	-0.03360	-0.03323
O	2.60567	-0.58819	-1.29373
O	1.76185	1.50111	0.29571
H	0.30215	1.95601	0.19959
O	2.20315	-1.03665	1.18121
H	2.28495	-0.60311	2.03175
H	2.39130	-0.21765	-2.15122
H	-2.90241	-0.02843	-1.61824

*02\_m3.mol2*

E = -1185.674793

H = -1185.553389

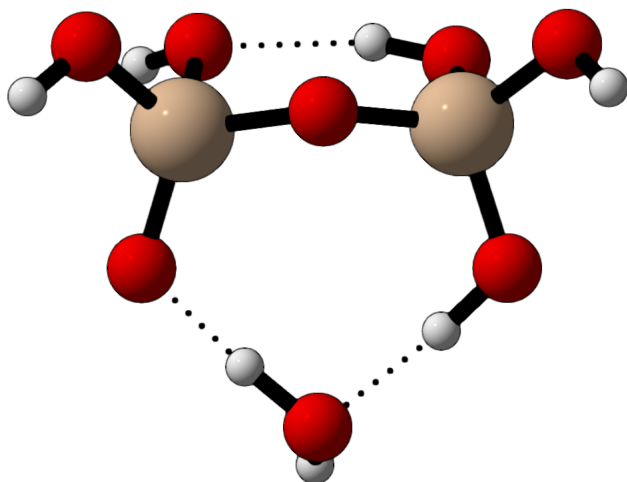
G = -1185.608957

G(quasi-RRHO) = -1185.607094

Si	-1.41941	-0.21818	-0.02802
O	-1.78684	0.10358	1.54852
H	-2.16864	-0.67040	1.96977
O	-2.08984	-1.75115	-0.20878
O	-0.71088	2.05191	0.19476
H	-0.93269	2.40223	-0.67132
H	-1.44625	-2.44057	-0.37641
O	0.14077	-0.49826	-0.38174
O	-2.30335	0.60410	-1.15918
Si	1.68587	-0.01877	-0.01435
O	2.60843	-0.56599	-1.28394
O	1.76883	1.51552	0.30269
H	0.30409	1.96135	0.23205
O	2.21198	-0.94892	1.25242
H	2.20519	-1.89645	1.10615
H	2.45391	-0.12891	-2.12304
H	-2.85906	0.00383	-1.66218

PC, product complexes

*00\_q1.mol2*



E = -1185.700264  
H = -1185.577924  
G = -1185.633606  
G(quasi-RRHO) = -1185.632039

Si	1.49734	-0.30198	-0.06349
O	1.96516	1.25177	-0.14341
H	1.24753	1.92739	-0.06321
O	2.62716	-1.18999	-0.84720
O	-0.09828	2.95533	0.01340
H	-0.14285	3.45041	0.83468
H	3.04901	-0.77225	-1.60005
O	0.01965	-0.50218	-0.71703
O	1.45942	-0.89337	1.46341
Si	-1.50299	-0.28428	-0.10061
O	-1.34789	-1.08110	1.36517
O	-1.96779	1.20883	-0.00488
H	-0.87444	2.29318	0.02885
O	-2.48866	-1.24878	-1.01812
H	-3.10206	-0.76432	-1.57279
H	-2.00013	-0.84837	2.02861
H	0.55194	-1.08233	1.75049

*01\_p2.mol2*

E = -1185.698277  
H = -1185.575784  
G = -1185.633117

G(quasi-RRHO) = -1185.630731

Si	-1.07114	0.70370	0.03861
O	-1.27561	-0.31928	-1.15494
O	-2.07315	0.36479	1.31020
O	-1.26624	2.31207	-0.29466
H	-2.16230	2.58671	-0.49652
H	-2.54346	-0.47083	1.16842
Si	1.74548	-0.22098	0.03071
O	1.21374	-1.10684	-1.22491
H	0.23448	-0.93297	-1.36103
O	2.39916	-1.12629	1.22864
O	3.02922	0.71368	-0.36839
H	2.93527	1.26081	-1.14999
O	0.49597	0.66881	0.58357
H	1.81531	-1.74882	1.66541
H	-3.82967	-1.97892	-0.45997
O	-2.96420	-2.01081	-0.04607
H	-2.36148	-1.44304	-0.60431

*02\_p1.mol2*

E = -1185.698297

H = -1185.575800

G = -1185.633080

G(quasi-RRHO) = -1185.630723

Si	-1.07706	0.70582	0.03805
O	-1.27619	-0.30698	-1.16510
O	-2.08521	0.35723	1.30213
O	-1.27178	2.31675	-0.28190
H	-2.16657	2.59202	-0.48855
H	-2.54278	-0.48528	1.15949
Si	1.74070	-0.21627	0.03274
O	1.21259	-1.09802	-1.22737
H	0.23427	-0.92168	-1.36739
O	2.39578	-1.12487	1.22742
O	3.02221	0.72347	-0.36156
H	2.93000	1.26803	-1.14516
O	0.48803	0.66688	0.58896
H	1.81084	-1.74350	1.66821
H	-2.36727	-1.43318	-0.62739
O	-3.05061	-1.94910	-0.11340
H	-2.66793	-2.81296	0.05621

03\_p3.mol2

E = -1185.698187  
H = -1185.575729  
G = -1185.633007  
G(quasi-RRHO) = -1185.630702

Si	-1.07708	0.70370	0.04025
O	-1.26451	-0.31629	-1.15867
O	-2.04046	0.34533	1.33072
O	-1.43812	2.29138	-0.25012
H	-0.84435	2.75286	-0.84462
H	-2.54134	-0.46909	1.17242
Si	1.74663	-0.22423	0.03081
O	1.21019	-1.12980	-1.20824
H	0.23189	-0.94623	-1.34767
O	2.38492	-1.11182	1.25066
O	3.04319	0.68747	-0.38090
H	2.96248	1.21320	-1.17846
O	0.50558	0.69399	0.55665
H	1.79224	-1.71925	1.69668
H	-3.85714	-1.93236	-0.47950
O	-2.99314	-1.98340	-0.06435
H	-2.37866	-1.42670	-0.61946

04\_p4.mol2

E = -1185.698159  
H = -1185.575694  
G = -1185.632932  
G(quasi-RRHO) = -1185.630657

Si	-1.08357	0.70760	0.03916
O	-1.26532	-0.30174	-1.16963
H	-2.37919	-1.41951	-0.64202
O	-2.05649	0.34064	1.32001
O	-1.44062	2.29825	-0.23860
H	-0.84080	2.76520	-0.82266
H	-2.54144	-0.48322	1.16080
O	-3.07062	-1.92583	-0.13094
H	-2.70113	-2.79574	0.03720
Si	1.74064	-0.22006	0.03340
O	1.20815	-1.11851	-1.21259
H	0.23098	-0.93173	-1.35582
O	2.37896	-1.11377	1.24875
O	3.03581	0.69676	-0.37131

H	2.95842	1.21942	-1.17122
O	0.49647	0.69100	0.56402
H	1.78336	-1.71430	1.70018

*05\_p6.mol2*

E = -1185.698134  
H = -1185.575686  
G = -1185.632590  
G(quasi-RRHO) = -1185.630474

Si	-1.06690	0.70239	0.02881
O	-1.27747	-0.34550	-1.14183
O	-2.08055	0.40630	1.30178
O	-1.23856	2.30506	-0.34251
H	-2.12936	2.58671	-0.55760
H	-2.56270	-0.42500	1.17519
Si	1.74258	-0.22954	0.02232
O	1.20090	-1.17676	-1.17878
H	0.22472	-0.99492	-1.32357
O	2.43681	-1.05958	1.25551
O	2.94912	0.69686	-0.58258
H	3.53264	1.11937	0.05026
O	0.49626	0.65756	0.58534
H	1.84839	-1.52618	1.85209
H	-3.86395	-1.94365	-0.43076
O	-3.00204	-1.98368	-0.01019
H	-2.38497	-1.43840	-0.57532

*06\_p5.mol2*

E = -1185.698200  
H = -1185.575736  
G = -1185.632389  
G(quasi-RRHO) = -1185.630398

Si	-1.07860	0.70535	0.03334
O	-2.07082	0.36553	1.31227
H	-2.52615	-0.48039	1.18341
O	-1.28208	-0.32466	-1.15433
O	-3.04408	-1.95940	-0.07078
H	-2.65519	-2.81858	0.10826
H	-2.36636	-1.44640	-0.59510
O	-1.28923	2.31072	-0.30468
H	-2.18912	2.57732	-0.50013



Si	1.73304	-0.22099	0.02125
O	3.00842	0.74032	-0.35398
H	2.82773	1.50992	-0.89720
O	1.20787	-1.11650	-1.22603
O	2.30714	-1.24253	1.16427
H	2.87122	-0.86632	1.84231
O	0.49362	0.68737	0.56539
H	0.22887	-0.94351	-1.36289

*07\_p7.mol2*

E = -1185.698068  
H = -1185.575604  
G = -1185.632379  
G(quasi-RRHO) = -1185.630338

Si	1.08380	0.70282	0.03347
O	1.27188	-0.31746	-1.16488
H	2.34720	-1.45476	-0.62107
O	1.29427	2.31041	-0.29273
O	2.08909	0.35006	1.29848
H	2.53462	-0.49976	1.16170
H	2.19246	2.57714	-0.49574
O	3.02339	-1.97817	-0.10502
H	2.62582	-2.83352	0.07337
Si	-1.72917	-0.20557	0.03933
O	-2.20964	-1.12969	1.30330
H	-3.07394	-1.54011	1.24149
O	-1.23552	-1.05344	-1.25771
O	-3.03934	0.70612	-0.33911
H	-3.03669	1.12055	-1.20413
O	-0.48200	0.68417	0.58427
H	-0.25146	-0.90697	-1.38767

*08\_p8.mol2*

E = -1185.697998  
H = -1185.575532  
G = -1185.632316  
G(quasi-RRHO) = -1185.630277

Si	-1.07568	0.69957	0.03401
O	-1.27057	-0.33492	-1.15106
O	-2.07486	0.36197	1.30801
O	-1.28441	2.30357	-0.31150

H	-2.18369	2.57018	-0.50969
H	-2.53905	-0.47799	1.17190
Si	1.73599	-0.21202	0.03762
O	1.23607	-1.07273	-1.24853
H	0.25112	-0.92863	-1.37434
O	2.22125	-1.12288	1.30923
O	3.04536	0.69428	-0.35652
H	3.03881	1.09994	-1.22565
O	0.49207	0.68470	0.57895
H	3.08244	-1.53948	1.24571
H	-3.82024	-1.99518	-0.45119
O	-2.95508	-2.02591	-0.03654
H	-2.35226	-1.45924	-0.59591

*09\_p10.mol2*

E = -1185.686673  
H = -1185.564560  
G = -1185.627675  
G(quasi-RRHO) = -1185.623206

Si	1.09599	-0.67784	-0.04488
O	0.48024	-1.94243	-0.92860
H	-0.42496	-1.80229	-1.23027
O	3.90412	1.93987	0.04281
O	1.76411	-1.36314	1.31235
H	1.20390	-1.99290	1.76941
H	4.59032	1.44624	0.49578
O	2.13485	0.22589	-0.78011
H	3.22442	1.25918	-0.24799
Si	-1.78310	0.40171	0.07603
O	-2.81483	0.27151	1.33403
H	-2.82636	-0.56136	1.80913
O	-2.08691	-0.71451	-1.09625
O	-2.08557	1.92435	-0.42822
H	-1.53796	2.27157	-1.13472
O	-0.25311	0.15426	0.49542
H	-2.95291	-0.72111	-1.50878

*10\_p9.mol2*

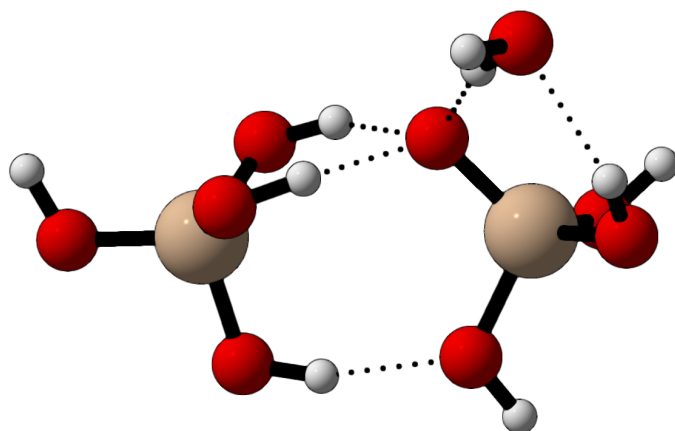
E = -1185.693182  
H = -1185.570164  
G = -1185.625701  
G(quasi-RRHO) = -1185.624109

Si	-1.02686	0.52005	-0.17706
O	-2.27229	0.59948	-1.11631
O	-1.25604	-0.54575	1.09344
O	-0.48131	1.93630	0.52075
H	-1.10915	2.41183	1.06767
H	-2.09860	-1.01786	0.99864
Si	1.78063	-0.25992	-0.07955
O	2.98296	-0.80680	-1.03282
H	2.99070	-1.74557	-1.22846
O	1.48257	-1.36987	1.08803
O	2.34306	1.15897	0.51064
H	1.62247	1.77867	0.68902
O	0.39172	0.01680	-0.88247
H	0.54320	-1.38753	1.33222
H	-4.55912	-0.90248	0.33748
O	-3.76883	-1.27160	-0.06306
H	-3.31691	-0.51913	-0.54956

One H<sub>2</sub>O

RC-w, Reactant Complexes

*00\_sw-c1.mol2*



E = -1262.149718  
H = -1261.999287  
G = -1262.062053  
G(quasi-RRHO) = -1262.059311

Si	-1.68808	-0.56907	0.03636
O	-0.77038	-1.47668	-1.02064
H	-1.16007	-2.30573	-1.30737

O	-0.82603	0.64228	0.58090
O	-3.05701	-0.04914	-0.72833
H	-3.12213	0.91815	-0.72972
H	0.51879	1.32369	-0.43555
O	-2.16569	-1.70436	1.14139
H	-2.91956	-1.46787	1.68455
Si	2.21674	0.09145	0.00516
O	3.83451	0.31272	0.02709
H	4.16437	1.05837	0.53140
O	2.04223	-1.30120	-0.83432
O	1.62080	-0.02020	1.52672
H	0.66149	0.20048	1.48379
O	1.45361	1.33693	-0.73856
H	1.10577	-1.51342	-0.99380
O	-2.48258	2.65574	-0.01120
H	-1.76318	2.03609	0.27412
H	-2.08241	3.26822	-0.63298

*01\_sw-c2.mol2*

E = -1262.149605  
H = -1261.999143  
G = -1262.061614  
G(quasi-RRHO) = -1262.058932

Si	1.69820	-0.56601	0.03650
O	0.74582	-1.55362	-0.91943
H	1.14250	-2.38444	-1.19092
O	0.82188	0.63817	0.57297
O	2.38798	-1.54564	1.17924
H	1.78001	-2.01390	1.75429
H	-0.66887	0.23731	1.47568
O	2.98884	-0.06460	-0.85726
H	3.10073	0.89693	-0.81114
Si	-2.22348	0.09819	0.00021
O	-3.83926	0.33503	0.01106
H	-4.16156	1.11144	0.47195
O	-2.06096	-1.32155	-0.79508
O	-1.44895	1.31494	-0.77842
H	-0.51548	1.30730	-0.47179
O	-1.63027	0.02611	1.52527
H	-1.12566	-1.55581	-0.92923
O	2.42637	2.65556	-0.14492
H	1.76645	2.03023	0.24864
H	2.90422	3.04530	0.59104

*02\_sw-c6.mol2*

E = -1262.144208

H = -1261.994386

G = -1262.061077

G(quasi-RRHO) = -1262.057055

Si	2.14303	0.12936	-0.07604
O	1.46647	-0.26866	1.40019
H	2.05688	-0.24931	2.15638
O	1.02252	0.11284	-1.17954
O	2.93432	1.57860	0.08060
H	2.40843	2.35274	-0.12829
H	-0.46907	0.76296	-0.85439
O	3.36861	-0.97136	-0.22612
H	3.98508	-0.81863	-0.94437
Si	-1.70321	-0.77468	-0.00661
O	-3.29893	-1.11487	0.01913
H	-3.76106	-1.10551	-0.82082
O	-1.25366	-0.95649	1.55346
O	-0.89161	-1.78059	-1.01083
H	-0.05777	-1.31785	-1.26405
O	-1.42035	0.75448	-0.54003
H	-0.31079	-0.75023	1.68539
O	-2.52578	3.19179	0.15504
H	-2.14894	2.32872	-0.10345
H	-3.07299	3.46568	-0.58441

*03\_sw-c3.mol2*

E = -1262.148614

H = -1261.998154

G = -1262.060684

G(quasi-RRHO) = -1262.058057

Si	-2.22408	-0.24481	0.01787
O	-1.89543	1.28917	-0.55262
H	-2.65300	1.79670	-0.85173
O	-0.89898	-0.92975	0.51411
O	-3.40151	-0.13373	1.18138
H	-3.07567	-0.08759	2.08196
H	0.41529	-0.21694	1.18418
O	-2.99981	-0.94759	-1.26330
H	-3.42591	-1.78803	-1.08653

Si	2.22216	-0.31507	-0.02141
O	3.68713	-0.94400	0.35366
H	3.68995	-1.84549	0.68054
O	2.61755	1.00749	-0.89946
O	1.32556	-1.41199	-0.83220
H	0.39216	-1.37904	-0.49132
O	1.34658	0.13850	1.29101
H	1.94527	1.70768	-0.83181
O	0.50888	2.60556	0.05799
H	-0.34726	2.23786	-0.22948
H	0.76625	2.02380	0.78922

*04\_sw-c4.mol2*

E = -1262.148760  
H = -1261.998366  
G = -1262.059504  
G(quasi-RRHO) = -1262.057458

Si	1.89129	-0.34136	-0.08413
O	1.20531	-0.77924	1.38200
H	1.75724	-0.63019	2.15315
O	0.82551	-0.56348	-1.22631
O	2.44585	1.20613	0.05359
H	1.75359	1.89191	0.04553
H	-0.39291	0.48922	-1.18618
O	3.25534	-1.27505	-0.15785
H	3.82815	-1.12528	-0.91181
Si	-1.99217	-0.27259	0.00463
O	-3.61064	-0.07358	0.05282
H	-4.06884	-0.01431	-0.78728
O	-1.55578	-0.21196	1.57811
O	-1.57430	-1.69711	-0.68690
H	-0.64121	-1.60587	-0.98998
O	-1.26143	0.90718	-0.87924
H	-0.60820	-0.40418	1.69870
O	0.26187	2.97683	0.11042
H	-0.41682	2.35593	-0.22422
H	0.26755	3.72036	-0.49802

*05\_sw-c5.mol2*

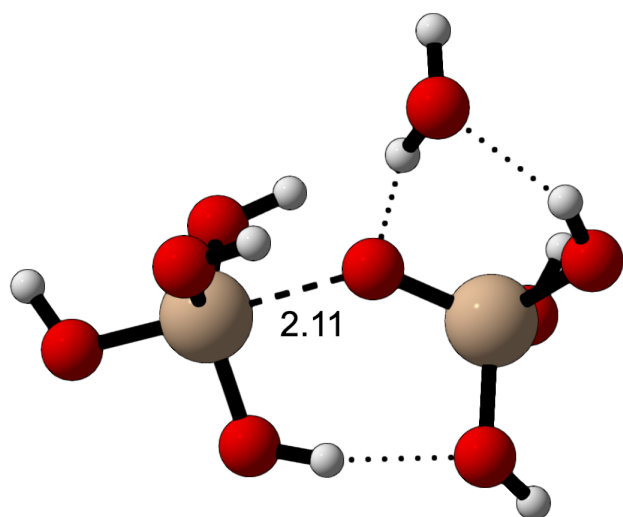
E = -1262.146175  
H = -1261.995816  
G = -1262.058922

G(quasi-RRHO) = -1262.056066

Si	-2.27549	0.26896	0.04191
O	-1.79294	-1.04627	-0.87081
H	-2.47972	-1.48742	-1.37515
O	-1.02415	0.88382	0.76837
O	-3.08641	1.32782	-0.94529
H	-2.54418	2.01900	-1.32951
H	0.42613	1.18868	-0.06685
O	-3.46926	-0.36945	0.99352
H	-3.99484	0.26267	1.48686
Si	1.57990	-0.62562	0.02950
O	3.18347	-0.91292	0.03587
H	3.71709	-0.10304	0.09543
O	0.93863	-1.68835	-1.03553
O	0.91612	-0.81607	1.51469
H	0.09811	-0.26220	1.52918
O	1.32340	0.94034	-0.42163
H	-0.03272	-1.62554	-1.07299
O	3.91128	1.80749	0.04099
H	4.38141	2.17709	-0.71099
H	2.96588	1.81277	-0.19726

TS1-w, Si-O bond association

[00\\_sw-d2.mol2](#)



E	= -1262.137985
H	= -1261.987723
G	= -1262.048927

G(quasi-RRHO) = -1262.046303

Si	1.75405	-0.05176	0.00538
O	1.37265	-1.43935	-0.81021
H	0.44862	-1.54584	-1.06543
O	1.83612	1.36872	-0.86386
O	1.63168	0.04693	1.66719
H	0.73098	0.27450	1.90936
H	0.96772	1.74491	-1.01624
O	3.41883	-0.38693	-0.00784
H	3.90925	0.15551	0.61037
Si	-1.64698	-0.46446	0.00771
O	-2.00997	-1.41797	1.30315
H	-2.48521	-0.99788	2.02213
O	-1.45643	-1.55732	-1.22231
O	-2.94035	0.51563	-0.25481
H	-2.70303	1.45368	-0.31037
O	-0.30531	0.38899	0.09666
H	-1.96494	-2.36871	-1.16618
O	-1.32798	2.86268	-0.14454
H	-0.82731	2.04525	0.08393
H	-1.32895	3.41449	0.64157

*01\_sw-d3.mol2*

E = -1262.136225

H = -1261.986054

G = -1262.047997

G(quasi-RRHO) = -1262.045332

Si	1.26168	-0.48901	0.03400
O	0.49418	-1.54041	-0.97379
H	-0.46161	-1.42754	-1.05877
O	1.64743	1.04906	-0.50953
O	1.07455	-0.68921	1.67170
H	0.23359	-0.29369	1.92210
H	0.86284	1.60078	-0.41372
O	2.79157	-1.16021	-0.14194
H	3.50690	-0.53195	0.00770
Si	-2.19499	0.26779	0.00853
O	-3.11620	-0.29428	1.25880
H	-3.44786	0.36427	1.87144
O	-2.27690	-0.95406	-1.11506
O	-3.01758	1.60355	-0.51636
H	-2.48853	2.24958	-0.98772



O	-0.66770	0.53733	0.28266
H	-3.10878	-1.42025	-1.21236
O	4.32786	1.35694	-0.10666
H	4.54339	1.79925	0.71808
H	3.36865	1.48691	-0.24072

*02\_sw-d\_new-conf-1.mol2*

E = -1262.136225  
H = -1261.986054  
G = -1262.047995  
G(quasi-RRHO) = -1262.045331

Si	1.26167	-0.48900	0.03400
O	0.49418	-1.54046	-0.97374
H	-0.46161	-1.42759	-1.05871
O	1.64747	1.04906	-0.50955
O	1.07449	-0.68911	1.67171
H	0.23354	-0.29354	1.92207
H	0.86291	1.60081	-0.41375
O	2.79156	-1.16022	-0.14187
H	3.50690	-0.53198	0.00775
Si	-2.19498	0.26778	0.00851
O	-3.11609	-0.29415	1.25890
H	-3.44811	0.36451	1.87123
O	-2.27697	-0.95416	-1.11499
O	-3.01761	1.60351	-0.51641
H	-2.48862	2.24947	-0.98794
O	-0.66768	0.53734	0.28249
H	-3.10884	-1.42043	-1.21198
O	4.32790	1.35690	-0.10669
H	3.36869	1.48688	-0.24074
H	4.54343	1.79919	0.71807

*03\_sw-d4.mol2*

E = -1262.136430  
H = -1261.986130  
G = -1262.047825  
G(quasi-RRHO) = -1262.045169

Si	2.04355	-0.20127	0.01392
O	1.20582	-1.27338	-0.91589
H	0.26299	-1.09062	-1.03304
O	2.49529	1.25982	-0.63999

O	1.92300	-0.28660	1.67096
H	1.12472	0.18369	1.93115
H	1.73892	1.85217	-0.58040
O	3.52010	-1.00327	-0.15395
H	4.23730	-0.57932	0.31849
Si	-1.36042	0.66670	-0.00923
O	-2.29910	0.11092	1.25091
H	-2.57461	0.76068	1.90045
O	-1.52395	-0.54557	-1.12475
O	-2.14437	2.03515	-0.50652
H	-1.57535	2.71898	-0.86404
O	0.16882	0.90596	0.27614
H	-2.28560	-1.13466	-0.99366
O	-3.65578	-1.96908	0.00085
H	-3.44569	-1.28614	0.66087
H	-4.56507	-1.81243	-0.26757

*04\_sw-d1.mol2*

E = -1262.138804

H = -1261.988255

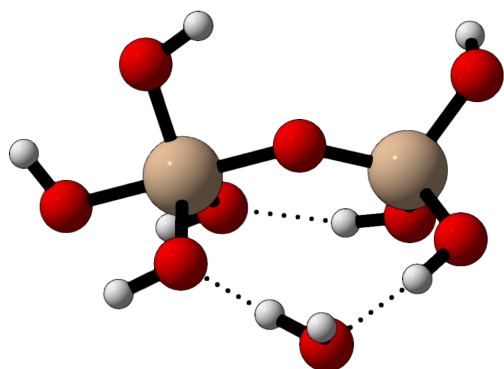
G = -1262.047508

G(quasi-RRHO) = -1262.045874

Si	-1.70367	-0.33431	-0.00976
O	-1.10832	-0.26699	1.52022
H	-0.16903	-0.47263	1.62684
O	-1.46789	0.96859	-1.03772
O	-1.88595	-1.80813	-0.74052
H	-1.01929	-2.07951	-1.06353
H	-0.64633	0.77060	-1.50846
O	-3.29411	-0.02133	0.42522
H	-3.88025	0.10983	-0.32097
Si	1.79448	-0.32545	-0.06486
O	3.09166	-1.18400	-0.62099
H	3.38091	-0.98230	-1.51243
O	1.69791	-0.71872	1.55366
O	2.23682	1.25383	-0.20758
H	1.52206	1.90856	-0.10332
O	0.39815	-0.69887	-0.70171
H	2.32441	-0.28911	2.13895
O	0.05773	2.98535	0.11589
H	-0.63544	2.40428	-0.25377
H	0.04350	3.78922	-0.41037

IM1-w, three equatorial OH groups

*00\_sw-e1.mol2*



E = -1262.152675  
H = -1262.000889  
G = -1262.060060  
G(quasi-RRHO) = -1262.058045

Si	-1.48373	-0.18699	-0.09783
O	-1.10667	-1.10146	1.28391
H	-1.90307	-1.25194	1.79749
O	-1.36557	1.50497	0.04185
O	-1.96615	-0.90340	-1.54635
H	-1.20250	-1.08823	-2.09603
H	-2.22104	1.85508	0.30246
O	-3.17189	-0.11142	0.41144
H	-3.75185	-0.45764	-0.26695
Si	1.66858	-0.43879	-0.01581
O	1.57450	-1.14459	1.46692
H	0.63276	-1.26121	1.69469
O	2.50213	0.96465	0.03617
O	2.63250	-1.37953	-0.96829
H	2.47166	-2.32285	-0.91184
O	0.19418	-0.25051	-0.61822
H	1.95009	1.77321	0.05783
O	0.78920	3.08883	0.10061
H	-0.03475	2.54720	0.04356
H	0.81296	3.62707	-0.69452

*01\_sw-e2.mol2*

E = -1262.151079  
H = -1261.999177  
G = -1262.057690

G(quasi-RRHO) = -1262.056008

Si	-0.89630	-0.61616	-0.11055
O	-0.45916	-0.91009	1.50559
H	-1.24344	-0.94435	2.05718
O	-0.96953	1.00862	-0.57046
O	-1.22751	-1.87373	-1.18092
H	-0.42298	-2.15525	-1.62060
H	-1.83156	1.42663	-0.44240
O	-2.62521	-0.62261	0.34728
H	-3.06914	-1.37799	-0.04128
Si	1.99099	0.26412	-0.02221
O	2.15415	0.03449	1.60011
H	1.32099	-0.33464	1.93998
O	1.67398	1.82938	-0.40489
O	3.45292	-0.02706	-0.70774
H	3.95180	-0.75895	-0.34093
O	0.80648	-0.67451	-0.57148
H	0.71486	1.90692	-0.55218
O	-3.72595	1.75293	-0.03435
H	-3.49432	0.82105	0.19816
H	-3.89324	2.20590	0.79560

*02\_sw-e4.mol2*

E = -1262.148928

H = -1261.997002

G = -1262.057234

G(quasi-RRHO) = -1262.054854

Si	0.90789	-0.24406	0.00350
O	0.43665	-0.57149	1.60443
H	1.08859	-1.14112	2.01861
O	0.34446	-1.31651	-1.18844
O	1.81921	1.14061	-0.37083
H	1.24301	1.89221	-0.52452
H	0.99145	-2.01146	-1.32813
O	2.36972	-1.18497	0.18279
H	3.18285	-0.67202	0.18197
Si	-2.08042	0.23621	-0.03951
O	-2.31833	-0.26672	1.50996
H	-1.45091	-0.48107	1.89506
O	-2.40813	-0.94242	-1.13586
O	-3.19810	1.39511	-0.35642
H	-3.38481	2.00649	0.35808

O	-0.55846	0.72529	-0.20963
H	-1.56426	-1.34043	-1.40962
O	4.48527	0.97617	0.00723
H	4.96844	0.99436	-0.82231
H	3.56276	1.22231	-0.21096

*03\_sw-e3.mol2*

E = -1262.149363  
H = -1261.997610  
G = -1262.056992  
G(quasi-RRHO) = -1262.055170

Si	-1.39254	-0.13598	-0.00438
O	-1.01891	-0.96323	-1.44262
H	-1.78414	-1.47053	-1.72271
O	-1.01768	-0.93782	1.44782
O	-2.03399	1.40930	-0.01729
H	-1.38944	2.12757	-0.01973
H	-1.78201	-1.44166	1.73645
O	-3.00962	-0.82444	0.00104
H	-3.67449	-0.13564	0.00262
Si	1.64913	-0.35277	0.01055
O	1.70965	-1.29428	-1.33446
H	0.80272	-1.39344	-1.67555
O	1.72191	-1.22368	1.39788
O	3.00318	0.57144	0.03762
H	3.32022	0.88194	-0.81231
O	0.28702	0.51773	-0.01038
H	0.81441	-1.32755	1.73417
O	0.24774	3.21090	-0.08715
H	0.49768	3.61166	0.74912
H	0.48849	2.26276	-0.01821

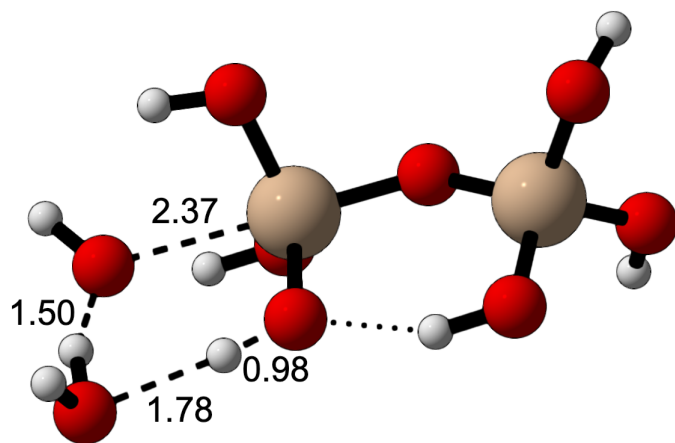
*04\_sw-e\_new-conf-1.mol2*

E = -1262.147381  
H = -1261.995447  
G = -1262.054924  
G(quasi-RRHO) = -1262.052813

Si	0.93365	0.32843	-0.07841
O	0.25508	1.88758	-0.06442
H	0.83362	2.51782	0.36914
O	0.74515	-0.62732	1.30967

O	1.74167	-0.21943	-1.45520
H	1.11413	-0.61488	-2.06435
H	1.45376	-0.47799	1.93912
O	2.47024	0.91262	0.59237
H	2.95024	1.46611	-0.02737
Si	-2.03400	-0.23968	-0.03585
O	-2.47030	1.33859	0.13102
H	-1.66402	1.88146	0.10156
O	-2.01585	-1.03892	1.39882
O	-3.21387	-0.98925	-0.89361
H	-3.59773	-0.48442	-1.61262
O	-0.57794	-0.31499	-0.71459
H	-1.09512	-1.09198	1.70471
O	4.09317	-1.27096	-0.09299
H	3.67100	-0.52284	0.36773
H	3.52031	-1.33923	-0.86676

TS2-cw, water cleavage of IM1, H<sub>2</sub>O acting as catalyst  
*00\_cw-h\_new-conf-1.mol2*



E = -1262.132861  
H = -1261.984592  
G = -1262.045804  
G(quasi-RRHO) = -1262.042879

Si	0.79223	-0.62386	0.01187
O	1.16908	-1.62874	-1.23553
H	2.13705	-1.59874	-1.28669
O	0.94474	0.99598	-0.26102
O	1.07437	-1.13140	1.55512
H	2.01983	-1.08130	1.72517

H	1.83081	1.40759	-0.20540
O	3.16424	-0.54991	-0.02498
H	3.74551	-1.20011	0.37404
Si	-2.14979	0.21658	-0.00869
O	-3.24238	-0.26526	-1.13257
H	-2.90079	-0.50033	-1.99745
O	-1.66686	1.75729	-0.23919
O	-2.96898	0.19811	1.40823
H	-3.51116	-0.57212	1.58809
O	-0.86949	-0.76633	-0.02184
H	-0.69454	1.80760	-0.28709
O	3.52877	1.92060	-0.13015
H	3.74499	2.29697	0.72599
H	3.56611	0.89971	-0.02580

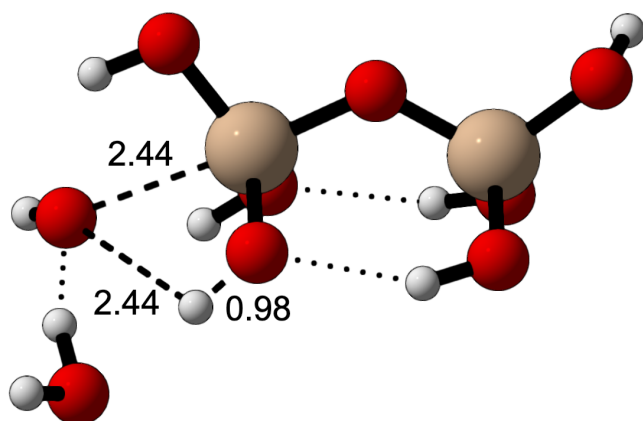
*01\_cw-h\_new-conf-2.mol2*

E = -1262.132690  
H = -1261.984388  
G = -1262.045058  
G(quasi-RRHO) = -1262.042422

Si	0.79639	-0.62224	0.04424
O	1.12452	-1.59541	-1.24168
H	2.08924	-1.56018	-1.33320
O	0.93394	1.00392	-0.19654
O	1.14134	-1.16728	1.56159
H	2.09331	-1.12221	1.69223
H	1.82170	1.41493	-0.17986
O	3.16372	-0.53861	-0.08504
H	3.76362	-1.19782	0.26904
Si	-2.14909	0.19583	-0.01452
O	-2.95090	-0.23297	-1.37619
H	-3.82876	0.13197	-1.50117
O	-1.67463	1.76035	-0.01328
O	-3.22268	-0.03229	1.20312
H	-3.01509	0.38190	2.04292
O	-0.86444	-0.76983	0.08313
H	-0.70664	1.82435	-0.10773
O	3.52187	1.93309	-0.17191
H	3.77349	2.29804	0.67948
H	3.56497	0.91107	-0.08328

TS2-sw, water cleavage of IM1, H<sub>2</sub>O acting as spectator

*00\_sw-h1.mol2*



E = -1262.133706  
H = -1261.985439  
G = -1262.044049  
G(quasi-RRHO) = -1262.042106

Si	-0.71188	-0.58303	-0.24148
O	-0.60042	-0.96820	1.36765
H	-1.46809	-0.89789	1.77820
O	-0.98150	1.01142	-0.53467
O	-1.37096	-1.67124	-1.27094
H	-2.31816	-1.65690	-1.04132
H	-1.85220	1.39763	-0.30256
O	-3.08783	-0.61363	0.31375
H	-3.52099	-1.18205	0.95347
Si	2.08804	0.20862	0.00888
O	2.18391	-0.14451	1.60770
H	1.34363	-0.47785	1.95277
O	1.77701	1.78763	-0.28389
O	3.54911	-0.06226	-0.66021
H	4.04443	-0.81551	-0.33327
O	0.90021	-0.68593	-0.64696
H	0.82961	1.92968	-0.43249
O	-3.46841	1.85182	0.21832
H	-4.05200	2.07965	-0.50882
H	-3.48143	0.82427	0.30444

*01\_sw-h2.mol2*

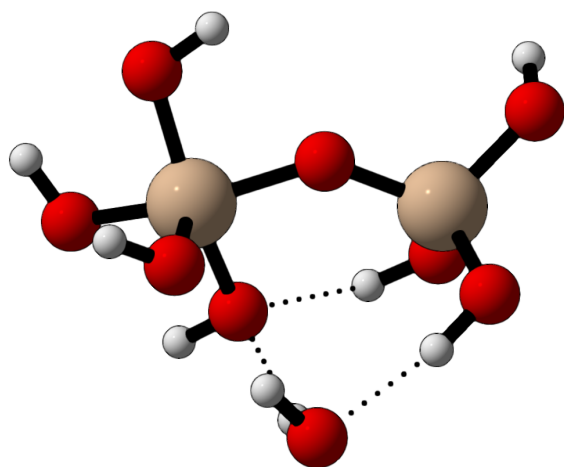
E = -1262.131704



H = -1261.982842  
G = -1262.042158  
G(quasi-RRHO) = -1262.040193

Si	-1.20964	-0.29344	-0.28102
O	-1.17353	-1.03673	1.19322
H	-2.09492	-0.93763	1.51364
O	-1.53094	1.32720	-0.23985
O	-1.95549	-1.11846	-1.48757
H	-2.90481	-1.13820	-1.33689
H	-2.45142	1.34346	0.11029
O	-3.43358	-0.02331	0.68110
H	-4.29106	-0.32276	0.37526
Si	1.79810	-0.37057	0.02619
O	1.57770	-1.05122	1.49966
H	0.63892	-1.16381	1.72129
O	2.43423	1.12077	0.09694
O	2.92326	-1.23249	-0.79060
H	2.87263	-2.18642	-0.70766
O	0.36863	-0.34906	-0.75302
H	1.79624	1.86587	0.09948
O	0.52695	3.06704	0.10772
H	0.57794	3.67911	-0.63111
H	-0.27965	2.52647	-0.03741

TS-iso-w, isomerization of IM1 to IM2  
[00\\_sw-f1.mol2](#)



E = -1262.140769  
H = -1261.989891

G = -1262.046722  
G(quasi-RRHO) = -1262.045450

Si	-1.40636	-0.31883	-0.02177
O	-2.84442	-0.40679	0.92877
H	-3.41891	-1.10377	0.60902
O	-1.70501	0.90501	-1.15365
O	-1.92615	-1.76503	-0.79778
H	-1.21600	-2.13239	-1.32563
H	-2.52153	0.78794	-1.64047
O	-0.74182	0.62544	1.30305
H	-1.44173	0.81593	1.93184
Si	1.71758	-0.33072	0.00136
O	1.82098	-0.28705	1.64372
H	0.96037	0.01418	1.97903
O	2.20283	1.06897	-0.69194
O	2.84011	-1.39873	-0.54001
H	2.82816	-2.26746	-0.13507
O	0.22279	-0.74084	-0.43574
H	1.53716	1.78305	-0.63923
O	0.08168	2.80817	-0.27466
H	-0.12529	2.30896	0.53522
H	-0.56737	2.41409	-0.88313

*01\_sw-f3.mol2*

E = -1262.139059  
H = -1261.988433  
G = -1262.046579  
G(quasi-RRHO) = -1262.044786

Si	0.89836	0.32744	0.00819
O	2.35595	1.22008	-0.17279
H	3.15755	0.68838	-0.17393
O	0.62638	0.30373	1.68587
O	1.80002	-1.11587	-0.32418
H	1.20592	-1.85404	-0.46968
H	1.21562	-0.29037	2.15386
O	0.05958	1.75642	-0.47007
H	0.65398	2.50881	-0.45463
Si	-2.04466	-0.27832	-0.08755
O	-2.58771	1.10112	-0.79906
H	-1.82399	1.69780	-0.87891
O	-2.12851	-0.21774	1.55092
O	-3.08487	-1.47167	-0.51528

H	-3.42887	-1.43302	-1.40933
O	-0.51791	-0.56746	-0.51854
H	-1.23781	-0.06299	1.91233
O	4.46725	-0.94286	-0.39127
H	3.52270	-1.21004	-0.35891
H	4.86158	-1.25810	0.42538

*02\_sw-f2.mol2*

E = -1262.139610  
H = -1261.988896  
G = -1262.046416  
G(quasi-RRHO) = -1262.044689

Si	0.88800	-0.62738	-0.11215
O	2.59848	-0.51951	-0.40550
H	2.96433	-1.37834	-0.62311
O	0.70881	-0.83665	1.56440
O	1.00834	-2.24867	-0.68671
H	0.13615	-2.59671	-0.87680
H	0.80481	-1.75622	1.82048
O	0.83623	1.09554	-0.18068
H	1.68789	1.52340	-0.03798
Si	-1.95139	0.28863	-0.04680
O	-1.77828	1.85619	-0.50988
H	-0.82191	2.03211	-0.52894
O	-1.95971	0.10703	1.58481
O	-3.44661	-0.18104	-0.52825
H	-3.75111	0.16787	-1.36768
O	-0.76731	-0.62034	-0.66373
H	-1.10021	-0.23895	1.88262
O	3.71908	1.86444	-0.01906
H	3.51082	0.91164	-0.14338
H	4.10442	1.94173	0.85695

*03\_sw-f4.mol2*

E = -1262.139621  
H = -1261.988763  
G = -1262.045419  
G(quasi-RRHO) = -1262.044023

Si	0.95323	0.59454	-0.14714
O	2.33631	1.62468	-0.03999
H	3.07680	1.28744	-0.54478

O	1.06143	-0.35116	1.25360
O	1.81151	-0.29104	-1.37417
H	1.19667	-0.86914	-1.83143
H	1.81416	-0.95798	1.22562
O	0.00505	1.94524	0.34383
H	0.57022	2.65406	0.65665
Si	-1.90687	-0.30924	-0.03949
O	-2.62411	1.13807	0.26944
H	-1.91255	1.79273	0.37546
O	-1.60253	-1.16750	1.32593
O	-2.99390	-1.21358	-0.86942
H	-3.53823	-0.74438	-1.50400
O	-0.51785	-0.08022	-0.82676
H	-0.65564	-1.08701	1.54474
O	3.35093	-1.84044	0.29463
H	2.90953	-1.39801	-0.45993
H	3.27531	-2.78433	0.13388

*04\_sw-f5.mol2*

E = -1262.137411

H = -1261.986765

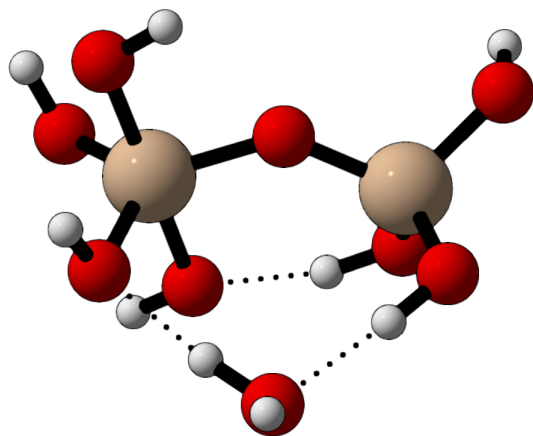
G = -1262.043778

G(quasi-RRHO) = -1262.042474

Si	-1.39019	-0.17864	-0.04795
O	-2.93803	-0.66057	-0.62187
H	-3.55978	0.06503	-0.54815
O	-1.28692	-0.62659	1.58869
O	-1.99565	1.42246	0.03744
H	-1.33048	2.11397	0.10810
H	-1.61359	0.06606	2.16654
O	-0.78552	-1.64973	-0.74272
H	-1.50825	-2.25230	-0.92567
Si	1.60389	-0.33236	0.00713
O	1.90842	-1.48925	-1.11621
H	1.05562	-1.90128	-1.33106
O	1.49927	-0.92324	1.53125
O	2.90919	0.65911	0.01456
H	3.34027	0.80347	-0.82964
O	0.23309	0.47452	-0.32988
H	0.57062	-0.92501	1.82693
O	0.35452	3.20606	-0.17597
H	0.50585	2.25398	-0.33924
H	0.36083	3.62803	-1.03866

IM2-w, co-linear OH groups on Si

*00\_sw-g1.mol2*



E = -1262.147075

H = -1261.995651

G = -1262.054754

G(quasi-RRHO) = -1262.052975

Si	-1.39383	-0.31016	-0.01695
O	-2.42374	-1.46891	0.65381
H	-2.94517	-1.87171	-0.04387
O	-1.93229	1.30832	-0.10573
O	-2.06785	-0.66552	-1.61001
H	-1.37688	-0.69184	-2.27200
H	-2.37987	1.43004	-0.94742
O	-0.74364	-0.00659	1.59601
H	-1.42186	-0.09031	2.26734
Si	1.68527	-0.35989	-0.07878
O	1.78083	-0.80577	1.49537
H	0.89615	-0.62966	1.88086
O	2.18509	1.16682	-0.35628
O	2.76044	-1.25983	-0.93069
H	2.79161	-2.19371	-0.71659
O	0.16788	-0.57845	-0.60789
H	1.51163	1.86474	-0.21735
O	0.19381	2.99069	0.10358
H	-0.61865	2.43636	0.04168
H	0.09863	3.68087	-0.55781

*01\_sw-g9.mol2*

E = -1262.142774  
H = -1261.991760  
G = -1262.054467  
G(quasi-RRHO) = -1262.051269

Si	-0.95878	0.54580	0.07215
O	-0.08834	1.74842	-0.95007
H	-0.47383	1.75519	-1.82759
O	-1.96636	-0.52793	1.05268
O	-1.17570	1.74957	1.23917
H	-0.76334	2.56373	0.94394
H	-1.92979	-0.29488	1.98084
O	-1.89920	0.20021	-1.28031
H	-2.63255	-0.40480	-1.11685
Si	1.99584	-0.40563	0.00928
O	2.86981	-0.54586	1.39169
H	2.69943	0.10893	2.07081
O	2.38838	0.93995	-0.82422
O	2.47864	-1.76392	-0.77612
H	2.20916	-1.84303	-1.69266
O	0.41131	-0.40679	0.30861
H	1.54248	1.42685	-1.00460
O	-4.01472	-1.57639	-0.22805
H	-3.88689	-2.51719	-0.37054
H	-3.31416	-1.29527	0.40953

*02\_sw-g11.mol2*

E = -1262.142347  
H = -1261.991403  
G = -1262.054371  
G(quasi-RRHO) = -1262.051053

Si	0.95677	-0.58526	0.09111
O	0.06370	-1.77855	-0.86839
H	0.55620	-1.99202	-1.66166
O	1.88403	0.64198	1.03698
O	1.30153	-1.75745	1.24869
H	1.80488	-1.35321	1.95846
H	1.27537	1.24695	1.46287
O	1.97457	-0.36051	-1.22881
H	2.67137	0.29246	-1.09296
Si	-2.00853	0.38440	-0.01471
O	-2.95739	0.45077	1.32210

H	-3.04571	-0.36376	1.81979
O	-2.38109	-0.90539	-0.93816
O	-2.40824	1.80655	-0.72924
H	-1.89790	2.05479	-1.50185
O	-0.43696	0.33928	0.35608
H	-1.53897	-1.41355	-1.07227
O	3.94743	1.61647	-0.28914
H	3.79440	2.51496	-0.59092
H	3.20436	1.40021	0.32800

*03\_sw-g3.mol2*

E = -1262.145934  
H = -1261.994597  
G = -1262.053855  
G(quasi-RRHO) = -1262.051990

Si	-1.46306	-0.15608	-0.02174
O	-2.25683	-0.69993	1.36500
H	-2.81209	-1.44751	1.13306
O	-2.16033	1.08390	-0.92361
O	-2.25955	-1.39362	-0.99247
H	-1.61834	-1.90262	-1.48820
H	-2.69382	0.69473	-1.62009
O	-0.65205	1.07953	1.00905
H	-1.27572	1.44607	1.63939
Si	1.59391	-0.53350	-0.03180
O	1.64213	-0.27743	1.58985
H	0.85373	0.24466	1.82376
O	2.33378	0.64999	-0.87703
O	2.50262	-1.84892	-0.38751
H	2.24007	-2.67600	0.01985
O	0.05374	-0.73389	-0.49251
H	1.91138	1.52639	-0.77272
O	0.81626	2.88333	-0.34582
H	1.21225	3.50096	0.27426
H	0.19247	2.32388	0.18060

*04\_sw-g6.mol2*

E = -1262.146876  
H = -1261.995301  
G = -1262.053780  
G(quasi-RRHO) = -1262.052272

Si	-1.39316	-0.29067	-0.00824
O	-0.68863	0.75712	1.27542
H	-1.33366	0.91579	1.96739
O	-2.03751	1.08128	-0.76042
O	-2.28639	-1.05195	1.20421
H	-2.80715	-1.75926	0.81779
H	-2.51422	0.80454	-1.54623
O	-2.09270	-1.36923	-1.21040
H	-1.41876	-1.70486	-1.80145
Si	1.67823	-0.36503	-0.03209
O	2.74602	-1.51219	-0.50806
H	3.07514	-1.44648	-1.40587
O	1.78921	-0.36185	1.60329
O	2.15853	1.03942	-0.71760
H	1.51263	1.77207	-0.64214
O	0.16597	-0.73638	-0.48079
H	0.95459	0.00553	1.94252
O	0.14883	2.85924	-0.20436
H	-0.53243	2.71347	-0.87291
H	-0.15367	2.23537	0.49524

*05\_sw-g2.mol2*

E = -1262.147031  
H = -1261.995387  
G = -1262.053614  
G(quasi-RRHO) = -1262.052116

Si	-1.39447	-0.28790	-0.00609
O	-2.29447	-1.04434	1.20447
H	-2.81752	-1.74960	0.81741
O	-2.02679	1.08754	-0.76194
O	-2.09719	-1.36515	-1.20731
H	-1.42686	-1.69095	-1.80793
H	-2.50333	0.81374	-1.54885
O	-0.69016	0.75738	1.27963
H	-1.33586	0.91518	1.97115
Si	1.67957	-0.36099	-0.04754
O	1.79043	-0.33632	1.59081
H	0.95143	0.02564	1.92720
O	2.16549	1.03242	-0.74406
O	2.76044	-1.45212	-0.61647
H	2.74825	-2.31946	-0.20837
O	0.16358	-0.74105	-0.47645
H	1.53012	1.77125	-0.64681



O	0.16795	2.85762	-0.19300
H	-0.13942	2.23465	0.50503
H	-0.51230	2.71625	-0.86358

*06\_sw-g4.mol2*

E = -1262.141620  
H = -1261.990644  
G = -1262.052229  
G(quasi-RRHO) = -1262.049829

Si	0.89544	0.51383	-0.07583
O	1.25151	1.85593	-1.02966
H	1.87477	1.60115	-1.71318
O	1.83271	0.25099	1.29239
O	1.97980	-0.51360	-1.07739
H	1.45949	-1.14210	-1.57953
H	2.61589	-0.29045	1.13759
O	-0.25124	1.45400	0.88669
H	0.18174	2.01607	1.53001
Si	-1.93680	-0.39133	-0.02800
O	-2.61954	1.03180	-0.48883
H	-2.04765	1.75639	-0.20294
O	-2.09883	-0.68859	1.57853
O	-2.83779	-1.58896	-0.68964
H	-2.93450	-1.58263	-1.64315
O	-0.39671	-0.49478	-0.52689
H	-1.53155	-0.09869	2.08576
O	4.08728	-1.36811	0.27043
H	4.03239	-2.30412	0.47695
H	3.35095	-1.18005	-0.36282

*07\_sw-g10.mol2*

E = -1262.141315  
H = -1261.990150  
G = -1262.052109  
G(quasi-RRHO) = -1262.049371

Si	-1.11294	-0.74292	0.02653
O	-1.04913	0.79452	-0.98709
H	-1.33574	0.57442	-1.87621
O	-1.35503	-2.25304	0.85893
O	-1.99614	0.07246	1.20038
H	-2.14238	1.00942	1.02758

H	-1.42830	-2.12766	1.80524
O	-1.65368	-1.47908	-1.39865
H	-1.88933	-2.39209	-1.22199
Si	1.87810	0.15045	0.02872
O	2.63308	0.59224	1.41702
H	2.23916	1.32066	1.89991
O	1.49781	1.46684	-0.85833
O	3.05180	-0.75860	-0.67082
H	2.78923	-1.28457	-1.42802
O	0.55090	-0.72311	0.29114
H	0.53155	1.41784	-1.05526
O	-2.24565	2.85251	0.22312
H	-3.11449	3.05178	-0.13395
H	-1.83367	2.20689	-0.39632

*08\_sw-g8.mol2*

E = -1262.144319  
H = -1261.992748  
G = -1262.051780  
G(quasi-RRHO) = -1262.049999

Si	-1.42413	-0.27793	-0.03730
O	-0.70408	0.78039	1.27787
H	-1.38851	1.20363	1.80154
O	-2.18783	-1.18209	-1.30869
O	-2.03929	-1.32813	1.13219
H	-1.70870	-1.11964	2.00737
H	-2.03987	-2.12462	-1.22671
O	-2.21463	1.11121	-0.58117
H	-2.77844	0.88983	-1.32595
Si	1.65685	-0.37147	-0.08604
O	2.67314	-1.52394	-0.65472
H	2.57820	-2.40111	-0.28002
O	1.71913	-0.40478	1.55521
O	2.27356	1.00114	-0.71976
H	1.67550	1.76973	-0.62859
O	0.13453	-0.60888	-0.57963
H	0.90306	0.00322	1.89536
O	0.33178	2.86712	-0.13244
H	-0.29098	2.99755	-0.85358
H	-0.09889	2.17669	0.42627

09\_sw-g5.mol2

E = -1262.138529  
H = -1261.987393  
G = -1262.048531  
G(quasi-RRHO) = -1262.046377

Si	-1.34997	-0.32169	0.01072
O	-2.07680	-1.14225	-1.27704
H	-2.67000	-0.54661	-1.73971
O	-2.05933	-0.39707	1.53865
O	-2.22758	1.12778	-0.43497
H	-1.76128	1.95036	-0.26159
H	-2.67589	0.33231	1.63056
O	-0.40466	-1.78717	0.34649
H	-0.87431	-2.58386	0.09750
Si	1.62722	-0.18350	-0.02300
O	1.88815	-1.16680	-1.31360
H	1.19300	-1.82714	-1.39522
O	1.94058	-0.88481	1.42430
O	2.77493	0.98441	-0.10239
H	2.88401	1.42971	-0.94412
O	0.15225	0.51052	-0.08491
H	1.22754	-1.50545	1.62366
O	-0.15693	3.24275	-0.05228
H	0.00990	3.61101	0.81888
H	0.14057	2.31338	-0.01193

10\_sw-g7.mol2

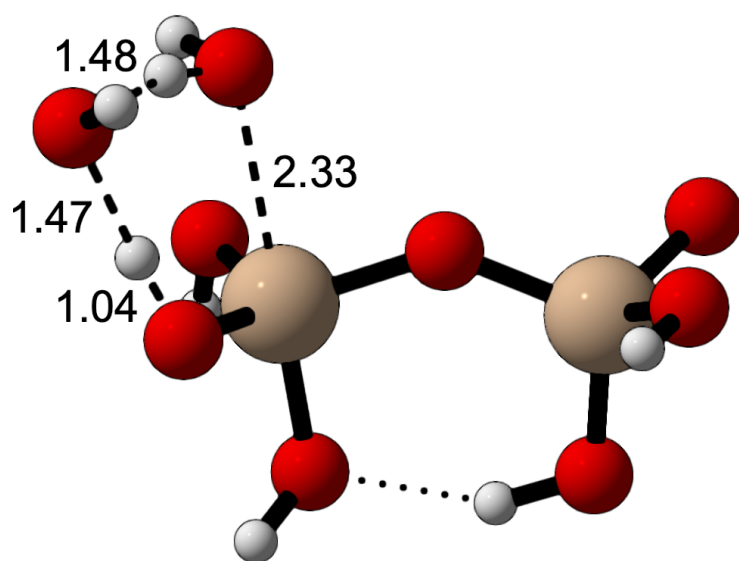
E = -1262.138428  
H = -1261.986956  
G = -1262.047327  
G(quasi-RRHO) = -1262.045348

Si	-1.35990	-0.22826	-0.03477
O	-0.69991	-1.79058	-0.51747
H	-1.38106	-2.46143	-0.57513
O	-1.38504	-0.70658	1.59817
O	-2.70228	-0.55412	-1.01118
H	-3.29111	0.20372	-0.99889
H	-1.73830	0.00889	2.13241
O	-2.02759	1.35326	0.28813
H	-1.38403	2.06378	0.34815
Si	1.58297	-0.29641	-0.02203
O	2.85879	0.71674	-0.17737

H	2.98614	1.36045	0.52163
O	1.93806	-1.50212	-1.06791
O	1.48644	-0.78278	1.54159
H	0.56346	-0.88341	1.83192
O	0.18268	0.45003	-0.41212
H	1.11202	-1.99510	-1.20467
O	0.28386	3.20543	-0.21330
H	0.14620	3.67071	-1.04211
H	0.38384	2.26374	-0.44661

TS3-cw, water cleavage from IM2, H<sub>2</sub>O acting as catalyst

*00\_cw-k1.mol2*

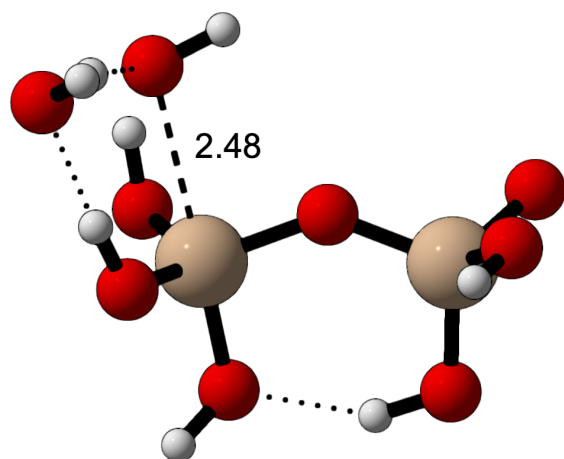


E = -1262.121476  
H = -1261.974558  
G = -1262.034970  
G(quasi-RRHO) = -1262.032248

Si	-0.89998	0.66086	0.00474
O	-1.40094	1.47809	1.35921
H	-1.17425	2.40930	1.30262
O	-1.93722	0.24285	-1.15809
O	0.38466	-0.32904	0.29153
H	-2.65253	-0.49111	-0.99601
O	-2.00034	-0.98367	1.24032
H	-2.42735	-0.46958	1.93013
O	-3.64175	-1.49636	-0.57073
H	-3.48603	-2.34450	-0.99033

H	-2.74176	-1.30209	0.58870
O	-0.10527	1.95241	-0.78599
H	-0.52464	2.18234	-1.61739
Si	1.97506	-0.37964	-0.01577
O	2.85563	-0.64077	1.33638
H	2.95572	0.09968	1.93698
O	2.42345	1.01149	-0.74105
H	1.64083	1.57503	-0.90420
O	2.35871	-1.70356	-0.89561
H	1.86361	-1.84754	-1.70382

TS3-sw, water cleavage from IM2, H<sub>2</sub>O acting as spectator  
*00\_sw-k1.mol2*



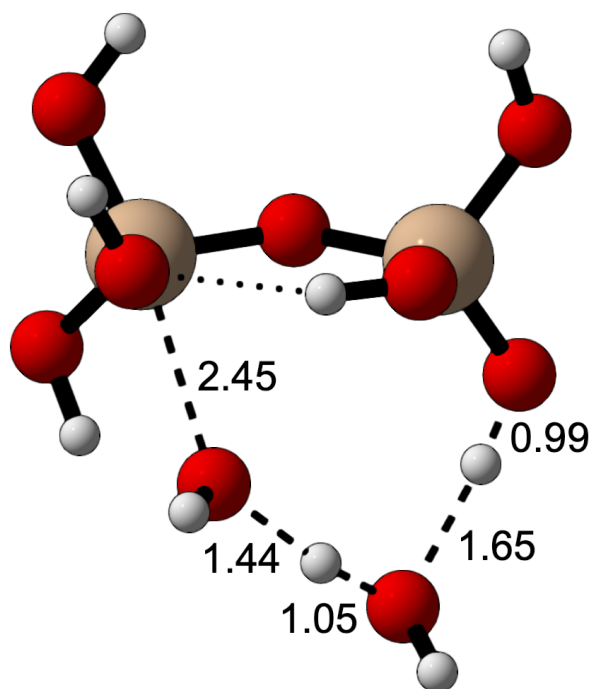
E = -1262.127868  
H = -1261.980330  
G = -1262.041936  
G(quasi-RRHO) = -1262.038877

Si	-0.85189	0.78948	0.03590
O	-1.47226	1.47900	1.38768
H	-1.93397	0.72638	1.81229
O	-1.82951	0.42255	-1.21567
O	-2.16142	-0.94153	1.22981
H	-1.50620	-1.58440	1.50569
H	-2.48418	-0.29735	-1.10373
O	0.00043	2.08192	-0.63576
H	-0.44882	2.51460	-1.36380
Si	1.95734	-0.41008	-0.01977
O	2.83885	-0.74913	1.31311

H	2.93924	-0.04640	1.95753
O	2.47049	0.96090	-0.74050
O	2.24864	-1.73638	-0.92903
H	1.79043	-1.79854	-1.76892
O	0.37855	-0.26498	0.32657
H	1.73375	1.59070	-0.85488
O	-3.61808	-1.57165	-0.67770
H	-3.37428	-2.41737	-1.06022
H	-3.03774	-1.44502	0.18206

TS4-cw, water cleavage from IM2, H<sub>2</sub>O acting as catalyst

*00\_cw-m1.mol2*



E = -1262.130548  
H = -1261.982980  
G = -1262.041149  
G(quasi-RRHO) = -1262.039618

Si	1.59368	-0.02026	-0.15369
O	2.23586	1.29248	-0.88288
H	1.65609	2.01263	-0.55335
O	2.71398	-1.15965	-0.62688
O	0.22581	1.91170	0.46916
H	0.39742	2.08513	1.39639
H	2.38800	-2.05994	-0.66304

O	0.17617	-0.61661	-0.72218
O	1.63640	-0.09849	1.51028
Si	-1.29197	-0.85942	-0.04580
O	-1.12820	-0.83165	1.58555
O	-2.44180	0.12215	-0.61414
H	-1.05046	2.44802	0.06037
O	-1.85752	-2.33484	-0.49539
H	-1.36171	-3.09183	-0.17917
H	-0.26432	-0.49902	1.87153
H	2.27096	-0.74692	1.82677
O	-1.99080	2.70848	-0.32949
H	-2.48838	3.11785	0.38184
H	-2.33075	1.10108	-0.50084

*01\_cw-m2.mol2*

E = -1262.125746

H = -1261.981155

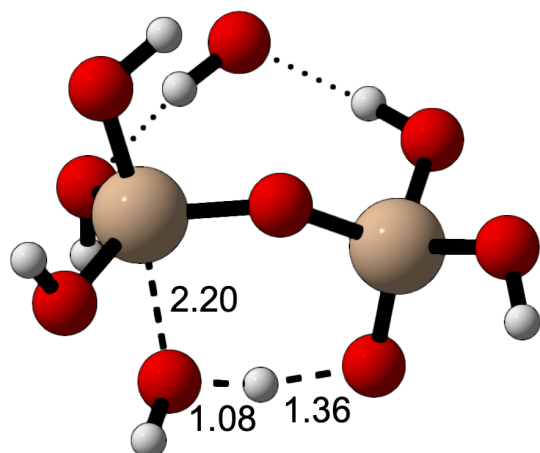
G = -1262.038562

G(quasi-RRHO) = -1262.037149

Si	-1.39972	-0.30471	-0.04050
O	-1.59036	0.27203	1.51669
H	-1.61394	-0.46371	2.13175
O	-1.41557	-1.97490	0.38748
O	-1.55357	1.59309	-0.47919
H	-1.61189	1.68962	-1.43405
H	-0.53949	-2.27767	0.64464
O	0.12089	-0.27299	-0.70995
O	-2.67247	-0.45209	-1.10716
Si	1.62450	-0.31347	-0.08687
O	2.66901	-0.79317	-1.27670
O	2.06471	1.07262	0.55791
H	-0.69785	2.15372	-0.13983
O	1.55341	-1.59203	0.96771
H	2.33678	-1.77261	1.48976
H	3.17354	-0.08231	-1.67537
H	-2.90149	-1.37703	-1.22149
O	0.41400	2.81459	0.36542
H	0.71699	3.48420	-0.25172
H	1.26994	1.96307	0.46192

TS4-sw, water cleavage from IM2, H<sub>2</sub>O acting as spectator

*00\_sw-m1.mol2*



E = -1262.133813  
H = -1261.985568  
G = -1262.044212  
G(quasi-RRHO) = -1262.042475

Si	1.41011	-0.21180	-0.23648
O	1.72567	1.05112	0.81085
H	1.58433	0.77158	1.72060
O	2.07804	0.47666	-1.62418
O	0.77296	-1.12916	1.65732
H	1.10067	-2.03154	1.64524
H	1.42321	0.82077	-2.23218
O	-0.14094	-0.35778	-0.73045
O	2.39367	-1.54633	-0.17960
Si	-1.67083	-0.33818	-0.08971
O	-2.66128	-1.14510	-1.14325
O	-1.63830	-0.96137	1.36606
H	-0.31104	-1.13362	1.61899
O	-2.22423	1.20440	-0.23388
H	-1.57320	1.89457	-0.01343
H	-2.78117	-2.07325	-0.93677
H	2.95878	-1.58297	-0.95524
O	-0.18224	3.03315	0.33561
H	0.55695	2.43016	0.54804
H	-0.29534	3.59929	1.10360

*01\_sw-m2.mol2*

E = -1262.133000



H = -1261.985228  
G = -1262.043744  
G(quasi-RRHO) = -1262.042052

Si	-1.44588	-0.30329	-0.20604
O	-2.37936	-1.51462	0.41483
H	-2.20123	-1.62454	1.35221
O	-2.17056	-0.33748	-1.73081
O	-0.74042	-0.27245	1.87387
H	-0.95972	0.58381	2.24905
H	-1.57040	-0.10038	-2.43872
O	0.10816	-0.57533	-0.62853
O	-1.80202	1.29025	0.20250
Si	1.65463	-0.40202	-0.05826
O	2.24948	0.99626	-0.68988
O	1.64086	-0.51215	1.52390
H	0.36030	-0.37116	1.82752
O	2.59503	-1.52915	-0.81811
H	2.65029	-2.37352	-0.36826
H	1.70741	1.77417	-0.46738
H	-2.39027	1.66883	-0.45752
O	0.44771	2.97300	0.13646
H	-0.37770	2.45187	0.17139
H	0.26771	3.71873	-0.44209

*02\_sw-m3.mol2*

E = -1262.130293  
H = -1261.981485  
G = -1262.043284  
G(quasi-RRHO) = -1262.040452

Si	-0.98377	-0.89999	-0.00952
O	-1.42163	-1.51769	1.46295
H	-1.46483	-0.82507	2.12620
O	-1.18414	-2.33650	-0.89010
O	-0.92436	0.92228	1.10460
H	-1.51467	1.61000	0.75802
H	-0.35416	-2.69625	-1.20314
O	0.60636	-0.66716	-0.32776
O	-2.13364	-0.04147	-0.88017
Si	1.89118	0.32669	-0.02657
O	2.53496	0.77308	-1.48547
O	1.45056	1.52229	0.90536
H	0.07515	1.28159	1.07310

O	3.11310	-0.64266	0.53040
H	2.92170	-1.12047	1.33889
H	2.22199	1.61663	-1.81508
H	-2.47052	-0.58950	-1.59395
O	-2.88867	2.48381	-0.24771
H	-2.75889	1.62527	-0.69493
H	-2.57976	3.15602	-0.86049

*03\_sw-m4.mol2*

E = -1262.127335  
H = -1261.977856  
G = -1262.039642  
G(quasi-RRHO) = -1262.037186

Si	-0.99637	0.27509	0.29414
O	-0.87514	1.29522	1.58513
H	-1.28401	0.91517	2.36631
O	-1.92592	-0.98368	0.95600
O	0.12735	2.17629	-0.67366
H	-0.22571	2.14256	-1.56592
H	-1.41034	-1.74968	1.21525
O	0.35805	-0.51797	-0.11586
O	-1.99101	0.74634	-0.92397
Si	2.00863	-0.34391	-0.14130
O	2.54283	-1.61729	-1.06078
O	2.43411	1.09811	-0.59660
H	1.08808	1.84510	-0.71644
O	2.56886	-0.80097	1.35273
H	2.90213	-0.07324	1.87940
H	2.24513	-1.61674	-1.97176
H	-2.77700	0.18386	-1.02298
O	-4.12380	-1.08691	-0.65763
H	-3.45552	-1.32338	0.01368
H	-4.17705	-1.83334	-1.26016

*04\_sw-m5.mol2*

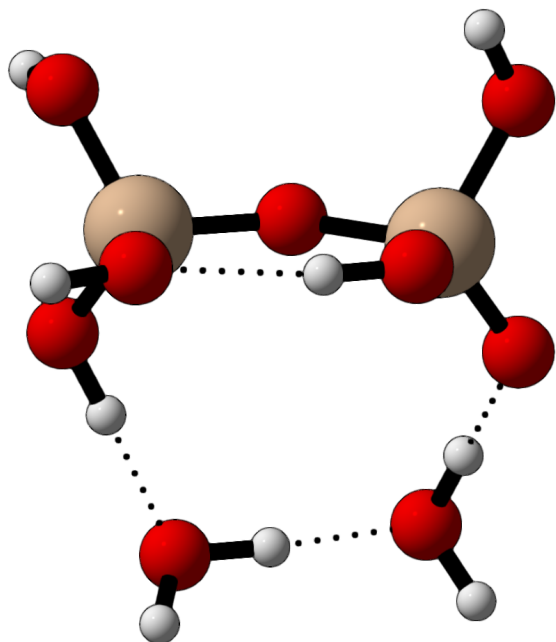
E = -1262.126119  
H = -1261.976360  
G = -1262.038446  
G(quasi-RRHO) = -1262.035974

Si	-0.98366	-0.92420	-0.04446
O	-1.02150	-1.51572	1.49199

H	-1.00844	-2.47619	1.48468
O	-1.16684	-2.33975	-0.93093
O	-0.95731	1.06698	1.30604
H	-1.39306	1.78925	0.83226
H	-0.45281	-2.51367	-1.54550
O	0.42009	-0.34113	-0.60635
O	-2.35402	-0.12569	-0.54770
Si	1.82856	0.32730	-0.04521
O	2.56771	0.98348	-1.38292
O	1.59743	1.34013	1.13108
H	0.03013	1.27693	1.31855
O	2.74134	-1.01849	0.28934
H	3.56543	-0.84592	0.74758
H	2.40418	1.92102	-1.49759
H	-2.81693	-0.64551	-1.21090
O	-2.71507	2.59278	-0.38854
H	-2.69284	1.64630	-0.62350
H	-2.35889	3.06367	-1.14616

PC-w, product complexes

*00\_cw-q1.mol2*



E	= -1262.149873
H	= -1262.000323
G	= -1262.065381
G(quasi-RRHO)	= -1262.061522

Si	1.61702	-0.27879	-0.12561
O	2.12823	1.24436	-0.32125
H	1.51146	1.98396	-0.10650
O	2.65977	-1.24361	-0.93983
O	0.49844	3.29105	0.22587
H	0.54695	3.55844	1.14717
H	3.01207	-0.90322	-1.76417
O	0.09106	-0.48161	-0.60244
O	1.63679	-0.79058	1.44088
Si	-1.39936	-0.92668	-0.00515
O	-1.09837	-1.51692	1.51700
O	-2.46449	0.21711	-0.08730
H	-0.45617	3.07777	0.04616
O	-1.90033	-2.22398	-0.91353
H	-1.37542	-3.01958	-0.80924
H	-0.18946	-1.38580	1.81411
H	2.45545	-0.71588	1.93443
O	-2.01178	2.68493	-0.36297
H	-2.66946	3.15461	0.15467
H	-2.19730	1.68031	-0.23747

*01\_cw-p1.mol2*

E = -1262.151643

H = -1262.001724

G = -1262.064620

G(quasi-RRHO) = -1262.061657

Si	0.65000	-0.43258	0.01300
O	1.29923	-1.25274	-1.27191
H	2.26223	-1.29609	-1.20364
O	0.80191	1.14440	-0.07200
O	1.28728	-1.10838	1.38556
H	2.24966	-1.16949	1.33026
H	2.29076	1.68192	-0.09266
O	3.83573	-0.74650	0.03021
H	4.75638	-1.01749	0.00886
Si	-2.25766	0.11999	-0.00187
O	-3.26504	-0.33809	-1.21229
H	-2.87238	-0.48348	-2.07524
O	-1.75539	1.65776	-0.12076
O	-3.15738	-0.00816	1.35896
H	-3.72317	-0.77825	1.43831
O	-0.94943	-0.85471	0.02655

H	-0.75262	1.67747	-0.11660
O	3.27806	1.89469	-0.13408
H	3.47910	2.41771	0.64554
H	3.81768	0.23786	-0.01256

*02\_sw-p2.mol2*

E = -1262.149006  
H = -1261.998980  
G = -1262.064582  
G(quasi-RRHO) = -1262.060276

Si	0.65695	0.03365	0.25017
O	1.52247	1.32099	0.03237
H	3.01391	1.38268	-0.24670
O	1.35649	-1.39174	-0.17762
O	4.02616	1.36658	-0.39288
H	4.18771	1.76073	-1.25300
H	2.33204	-1.40135	-0.20509
O	0.14510	-0.12754	1.84871
H	0.58038	0.48000	2.44982
Si	-2.36308	0.01018	-0.23296
O	-3.12443	1.31832	-0.85261
H	-2.86606	2.17445	-0.50694
O	-2.55196	-0.08286	1.38727
O	-3.15760	-1.19378	-1.00310
H	-2.88836	-2.09092	-0.79854
O	-0.78158	0.00042	-0.57618
H	-1.69000	-0.10458	1.84246
O	4.12973	-1.30833	-0.27416
H	4.49264	-1.70198	-1.07155
H	4.20852	-0.32907	-0.38583

*03\_cw-h\_new-conf-1.mol2*

E = -1262.151477  
H = -1262.001494  
G = -1262.063886  
G(quasi-RRHO) = -1262.061159

Si	0.65217	-0.43146	0.02589
O	1.29834	-1.25758	-1.25632
H	2.26165	-1.29953	-1.19154
O	0.79614	1.14549	-0.07099
O	1.29947	-1.09432	1.40017

H	2.26168	-1.15305	1.33939
H	2.28344	1.68525	-0.12173
O	3.83968	-0.73666	0.02777
H	4.76098	-1.00487	0.00071
Si	-2.25491	0.10071	-0.01153
O	-3.07471	-0.35275	-1.35420
H	-3.98095	-0.05077	-1.43703
O	-1.76462	1.65068	-0.02079
O	-3.29304	-0.16433	1.22995
H	-3.09352	0.27837	2.05708
O	-0.94471	-0.86255	0.05495
H	-0.76291	1.67767	-0.05733
O	3.26989	1.89871	-0.17897
H	3.47902	2.43699	0.58804
H	3.81742	0.24678	-0.03118

*04\_cw-p2.mol2*

E = -1262.146428  
H = -1261.996146  
G = -1262.063699  
G(quasi-RRHO) = -1262.058928

Si	-0.64906	-0.29874	0.44360
O	-1.47179	-1.39906	-0.49795
H	-0.95254	-2.11439	-0.87070
O	-1.58653	0.85198	0.91494
O	0.66458	0.13909	-0.46448
H	-2.98955	1.36031	0.45196
O	-4.15044	-0.74736	-1.27056
H	-3.25633	-1.06710	-1.07363
O	-3.91978	1.63392	0.16605
H	-3.81636	2.42453	-0.36800
H	-4.18329	0.12170	-0.82731
O	0.08394	-1.15450	1.68488
H	-0.39540	-1.15578	2.51560
Si	2.27403	0.22733	-0.28858
O	3.05643	-0.41667	-1.57009
H	2.96815	-1.36185	-1.70434
O	2.69302	-0.51541	1.10452
H	1.91707	-0.86289	1.57774
O	2.81445	1.76860	-0.34234
H	2.48766	2.37041	0.32871

*05\_sw-q1.mol2*

E = -1262.150053  
H = -1262.000308  
G = -1262.063170  
G(quasi-RRHO) = -1262.060618

Si	1.45249	-0.55824	-0.15226
O	1.59671	1.02984	0.20292
H	1.16519	1.31672	1.05611
O	2.38437	-0.88219	-1.45900
O	0.20696	1.68901	2.33130
H	0.54125	1.35802	3.16815
H	1.96549	-0.80733	-2.31825
O	-0.07135	-0.98381	-0.48069
O	2.07765	-1.37573	1.12038
Si	-1.57438	-0.41353	-0.01528
O	-2.61925	-1.67618	-0.26269
O	-1.57217	0.13470	1.45815
H	-0.55031	1.05392	2.03369
O	-2.02871	0.63330	-1.20666
H	-1.37970	1.33119	-1.40143
H	-2.86715	-2.13865	0.53905
H	1.93954	-2.32457	1.14226
O	0.06150	2.47276	-1.64152
H	0.69245	2.09808	-0.99762
H	-0.08592	3.38375	-1.37397

*06\_sw-p1.mol2*

E = -1262.149739  
H = -1261.999441  
G = -1262.062293  
G(quasi-RRHO) = -1262.059174

Si	-0.59050	-0.58739	0.04986
O	-0.19817	-1.17392	1.57425
H	-0.48332	-2.07566	1.73349
O	-0.83453	1.03289	0.29106
O	-1.71658	-1.39211	-0.67464
H	-3.17252	-0.90609	-0.77792
H	-1.75640	1.32641	0.43685
O	-4.12464	-0.54470	-0.77724
H	-4.37391	-0.42184	-1.69606
Si	2.20419	0.19887	-0.19555
O	2.60403	-0.43520	1.26332

H	1.83652	-0.83583	1.69869
O	1.89080	1.80313	-0.13356
O	3.48790	0.06537	-1.18995
H	4.01080	-0.73544	-1.11981
O	0.87830	-0.57322	-0.73655
H	0.94535	1.96308	0.01074
O	-3.48893	1.68150	0.58166
H	-3.75117	2.48579	0.12667
H	-3.83242	0.92899	0.04019

*07\_cw-h\_new-conf-2.mol2*

E = -1262.142838  
H = -1261.994318  
G = -1262.055557  
G(quasi-RRHO) = -1262.052953

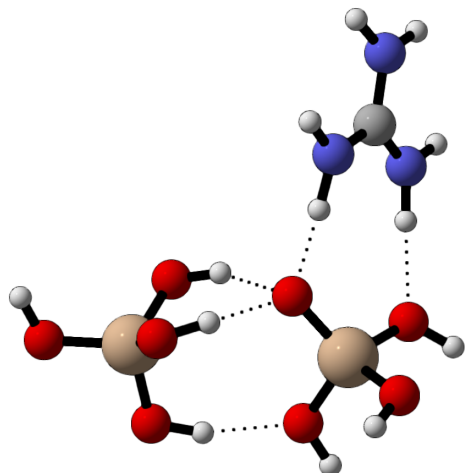
Si	-0.69654	-0.39276	-0.01800
O	-1.43331	-1.11710	1.24283
H	-2.39963	-1.17752	0.99522
O	-0.73514	1.24820	0.12320
O	-1.42541	-0.88997	-1.39009
H	-2.39037	-0.99823	-1.16555
H	-1.65776	1.59752	0.14206
O	-3.67810	-0.82751	-0.05567
H	-4.53290	-1.25835	-0.06403
Si	2.28538	0.05804	0.00511
O	3.01661	-0.40864	1.38651
H	3.93051	-0.14815	1.51617
O	1.97223	1.65628	-0.06900
O	3.30023	-0.35157	-1.20662
H	3.14999	0.05906	-2.06051
O	0.88826	-0.77347	-0.04911
H	1.02724	1.86468	0.02958
O	-3.40156	1.69914	0.18051
H	-3.76608	2.15648	-0.58076
H	-3.63527	0.70780	0.06767

One C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup>

RC-g, Reactant Complexes

*00\_sg-c.mol2*





E = -1391.555489  
 H = -1391.336208  
 G = -1391.410083  
 G(quasi-RRHO) = -1391.405708

Si	-0.32859	1.73146	0.11995
O	1.08330	2.13830	-0.66653
H	1.18491	3.05982	-0.91561
O	-0.23947	0.22727	0.57894
O	-0.60953	2.88056	1.26994
H	0.09195	3.04334	1.90338
H	1.24344	-0.33086	1.45706
O	-1.62012	1.90877	-0.90707
H	-1.97322	2.79296	-1.02564
Si	2.61691	-0.96827	-0.07366
O	3.82453	-2.06417	-0.14141
H	3.65485	-2.92433	0.24651
O	3.28032	0.35938	-0.76009
O	1.30195	-1.48474	-0.90512
H	0.52332	-0.99286	-0.56809
O	2.15538	-0.69678	1.47451
H	2.64488	1.09315	-0.81753
H	-1.61741	-0.68825	0.80901
N	-2.45434	-1.30288	0.89733
H	-2.48060	-1.99141	1.62851
C	-3.41476	-1.28965	-0.00949
N	-4.39599	-2.19459	0.03060
N	-3.41245	-0.36769	-0.96639
H	-5.13805	-2.18300	-0.64520
H	-4.34941	-2.97274	0.66284

H	-4.13793	-0.36277	-1.66045
H	-2.76584	0.41767	-0.94196

*01\_sg-c.mol2*

E = -1391.555451  
H = -1391.336181  
G = -1391.410047  
G(quasi-RRHO) = -1391.405699

Si	0.30012	1.74070	0.12129
O	-1.09226	2.14091	-0.69276
H	-1.23704	3.07406	-0.86496
O	0.24385	0.23988	0.59610
O	1.61243	1.89983	-0.88965
H	1.89604	2.78799	-1.11587
H	-0.50062	-1.00527	-0.54971
O	0.39915	2.91782	1.27285
H	1.18637	2.92418	1.82063
Si	-2.59944	-0.98403	-0.07063
O	-3.79791	-2.09017	-0.13368
H	-3.62098	-2.94706	0.25821
O	-3.26839	0.32877	-0.77973
O	-2.15049	-0.68857	1.47638
H	-1.24089	-0.31526	1.46083
O	-1.27519	-1.50222	-0.88676
H	-2.64340	1.07122	-0.83628
H	1.62439	-0.67528	0.81015
N	2.46101	-1.29053	0.89559
H	2.49015	-1.97729	1.62832
C	3.41984	-1.27676	-0.01290
N	4.40522	-2.17778	0.02958
N	3.41382	-0.35658	-0.97112
H	5.13488	-2.17621	-0.65983
H	4.35090	-2.96473	0.65037
H	4.13770	-0.35161	-1.66686
H	2.76400	0.42660	-0.94722

*02\_sg-c.mol2*

E = -1391.553292  
H = -1391.333942  
G = -1391.409710  
G(quasi-RRHO) = -1391.404643

Si	0.29839	1.83645	-0.01045
O	-1.31498	2.21050	0.15907
H	-1.52449	3.14690	0.18961
O	0.45682	0.26065	-0.04624
O	0.90589	2.60256	-1.34369
H	0.79244	2.14788	-2.18035
H	-0.71518	-0.64487	-1.16385
O	1.01442	2.61395	1.25555
H	1.96532	2.72691	1.20601
Si	-2.48242	-1.05117	0.00611
O	-3.59261	-2.24658	0.00308
H	-3.26715	-3.14652	-0.05428
O	-3.39373	0.30327	0.08612
O	-1.47066	-1.17984	1.28825
H	-0.63936	-0.70761	1.06995
O	-1.56567	-1.09316	-1.35208
H	-2.83799	1.10046	0.12214
H	1.81909	-0.50031	-1.06421
H	3.10899	-1.25223	-2.01401
N	2.69818	-1.01880	-1.12901
C	3.29713	-1.32168	0.01362
N	2.70747	-0.95150	1.14195
N	4.45142	-1.98556	0.03028
H	4.91459	-2.23807	-0.82391
H	4.92357	-2.17697	0.89540
H	1.82644	-0.44294	1.05667
H	3.11202	-1.15605	2.03689

*03\_sg-c.mol2*

E = -1391.547890  
H = -1391.329006  
G = -1391.405367  
G(quasi-RRHO) = -1391.399979

Si	-2.53053	-1.01732	-0.12590
O	-2.22695	-0.33791	1.37057
H	-2.77254	-0.64848	2.09635
O	-1.52312	-0.41421	-1.17489
O	-2.46724	-2.66746	0.01580
H	-1.61594	-3.06125	-0.18320
H	-0.02547	-0.11413	-0.76114
O	-4.13645	-0.70172	-0.35638
H	-4.55945	-1.17019	-1.07807
Si	0.16487	1.85991	0.06777

O	1.32431	3.00328	0.14252
H	1.72405	3.27903	-0.68426
O	-0.40159	1.78426	1.59644
O	-0.99160	2.25446	-1.02045
H	-1.42758	1.41855	-1.29999
O	0.77288	0.40086	-0.40063
H	-1.06673	1.08035	1.70382
H	1.84299	-0.72609	0.76358
N	2.70571	-1.23642	0.92523
H	2.84516	-1.74465	1.77906
C	3.64428	-1.19039	-0.00970
N	4.79884	-1.82959	0.15562
N	3.40905	-0.49663	-1.11542
H	5.51395	-1.79418	-0.54814
H	4.98651	-2.35163	0.99265
H	4.09327	-0.43582	-1.84711
H	2.51826	-0.01937	-1.20338

*04\_sg-c.mol2*

E = -1391.549373

H = -1391.330243

G = -1391.405113

G(quasi-RRHO) = -1391.400361

Si	3.05367	-0.70100	0.07687
O	2.88512	0.46984	-1.10540
H	3.61963	0.56558	-1.71548
O	1.74021	-0.75297	0.94162
O	3.45463	-2.13440	-0.65357
H	2.71250	-2.69687	-0.88225
H	0.24288	-0.73979	0.24465
O	4.44591	-0.24725	0.84445
H	4.80585	-0.87653	1.47190
Si	-0.31048	1.31274	-0.00250
O	-1.78920	2.02593	0.00978
H	-1.90325	2.81284	-0.52764
O	0.50334	1.92338	-1.27794
O	0.46390	1.57192	1.41092
H	1.07980	0.81109	1.53545
O	-0.57581	-0.30022	-0.13505
H	1.39621	1.54014	-1.36402
H	-2.18348	-1.11110	-0.19124
N	-3.09306	-1.57733	-0.23160
H	-3.11541	-2.56367	-0.41916

C	-4.22026	-0.92264	-0.00261
N	-5.38177	-1.57560	0.01377
N	-4.19750	0.38583	0.21594
H	-6.24995	-1.08475	0.12693
H	-5.41857	-2.56867	-0.12770
H	-5.04988	0.87992	0.41024
H	-3.33798	0.92309	0.14756

*05\_sg-c.mol2*

E = -1391.550127  
H = -1391.330337  
G = -1391.404702  
G(quasi-RRHO) = -1391.400040

Si	-0.31182	-0.01340	0.10003
O	0.53198	-0.31348	1.50786
H	0.00854	-0.48456	2.29406
O	0.69428	0.23656	-1.07115
O	-1.39586	-1.25473	-0.13427
H	-1.08966	-1.95923	-0.70958
H	2.08523	-0.85676	-1.27318
O	-1.41114	1.18787	0.44497
H	-1.05254	2.01391	0.77639
Si	3.65203	0.01718	-0.10318
O	5.28397	0.02641	-0.17907
H	5.67762	0.20666	-1.03443
O	3.35924	-0.31724	1.47170
O	3.02997	1.46620	-0.54704
H	2.09386	1.30425	-0.81322
O	3.01939	-1.12064	-1.09770
H	2.40692	-0.35558	1.66592
H	-3.23771	-1.16578	-0.03311
N	-4.25652	-1.13037	-0.03134
H	-4.76473	-1.99542	-0.07470
C	-4.90149	0.02396	-0.12084
N	-6.22831	0.03952	-0.24319
N	-4.22538	1.16251	-0.07692
H	-6.72813	0.90625	-0.32518
H	-6.74521	-0.81268	-0.36346
H	-4.71110	2.03943	-0.13598
H	-3.22031	1.17368	0.09342

06\_sg-c.mol2

E = -1391.548823  
H = -1391.329734  
G = -1391.403428  
G(quasi-RRHO) = -1391.399110

Si	-1.18424	-1.87843	-0.06725
O	-1.84231	-1.25459	1.33667
H	-2.77204	-1.45064	1.47356
O	-1.16647	-0.90051	-1.29701
O	0.38414	-2.21773	0.37762
H	0.48686	-2.76459	1.16023
H	-0.17227	0.35963	-1.03343
O	-2.02446	-3.28490	-0.27416
H	-2.08949	-3.60059	-1.17725
Si	-1.19845	1.94998	-0.01448
O	-1.06204	3.57441	0.02239
H	-0.91155	4.01996	-0.81319
O	-1.38388	1.55664	1.56092
O	-2.46987	1.46540	-0.92463
H	-2.28850	0.54784	-1.22832
O	0.13678	1.24535	-0.66682
H	-1.55612	0.60802	1.68736
H	1.83709	1.09519	-0.08040
N	2.83337	1.08465	0.15642
H	3.28714	1.97022	0.29747
C	3.57217	-0.00410	0.00112
N	4.90190	0.08202	0.02984
N	2.99597	-1.18416	-0.18720
H	5.47464	-0.74258	0.03548
H	5.36067	0.97279	0.08924
H	3.57022	-1.99695	-0.32408
H	2.00418	-1.34534	-0.02240

07\_sg-c.mol2

E = -1391.547936  
H = -1391.328883  
G = -1391.403323  
G(quasi-RRHO) = -1391.398942

Si	0.37760	1.63298	0.00731
O	-0.98954	2.51221	-0.01646
H	-1.81433	1.99046	-0.07537
O	0.52303	0.66468	1.33028

O	0.49004	0.61101	-1.28086
H	-0.12509	-0.14057	-1.05444
H	-0.09243	-0.09542	1.14839
O	1.65167	2.64623	0.03385
H	1.53984	3.51707	-0.35117
Si	-2.67662	-0.87638	0.00199
O	-3.43840	-1.55254	-1.29914
H	-3.48152	-2.51027	-1.31204
O	-3.08841	0.73840	-0.12389
O	-3.46289	-1.53201	1.30450
H	-2.97925	-1.50175	2.13195
O	-1.10825	-0.98681	0.06265
H	-4.02330	0.95061	-0.15745
H	2.16350	-0.27255	1.19013
N	3.03843	-0.79303	1.13941
C	3.58764	-1.13824	-0.01693
H	3.49702	-1.02740	2.00151
N	2.99918	-0.82096	-1.16121
H	2.12113	-0.30175	-1.19420
H	3.42614	-1.08093	-2.03212
N	4.73681	-1.81299	-0.02770
H	5.20887	-2.04541	0.82726
H	5.18091	-2.06560	-0.89194

*08\_sg-c.mol2*

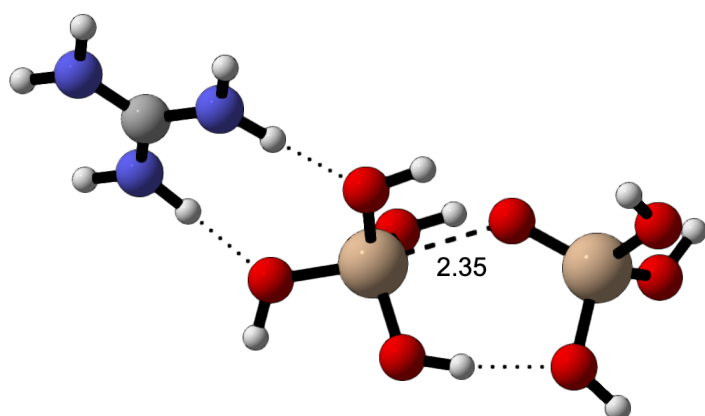
E = -1391.548348  
H = -1391.329286  
G = -1391.401474  
G(quasi-RRHO) = -1391.397523

Si	2.57761	-0.36682	0.05649
O	1.47624	-1.53689	-0.39504
H	1.85383	-2.38400	-0.64404
O	1.80652	0.89095	0.60461
O	3.64202	-1.03651	1.13489
H	3.40654	-0.93164	2.05850
H	0.31709	0.76795	1.04337
O	3.47792	-0.15348	-1.31246
H	4.26665	0.38391	-1.22080
Si	-1.17472	1.91859	-0.06545
O	-2.12069	3.12856	0.49713
H	-1.67740	3.83168	0.97519
O	-2.19012	1.18473	-1.11974
O	0.18518	2.50465	-0.74778

H	0.96901	2.00995	-0.39487
O	-0.69497	0.86114	1.09233
H	-1.95794	0.28221	-1.36223
H	-0.36335	-1.62174	-0.68218
N	-1.32240	-1.87628	-0.93343
H	-1.40854	-2.38707	-1.79726
C	-2.17031	-2.19625	0.05744
N	-3.14647	-3.06834	-0.15749
N	-2.02707	-1.60794	1.23241
H	-3.87673	-3.20736	0.51860
H	-3.18810	-3.60018	-1.00860
H	-2.66135	-1.82814	1.98050
H	-1.48376	-0.74013	1.29269

TS1-g, Si-O bond association

*00\_sg-d.mol2*



E = -1391.543945  
H = -1391.325161  
G = -1391.397953  
G(quasi-RRHO) = -1391.393710

Si	0.16273	-0.89952	0.03545
O	-0.68089	-1.43194	-1.26102
H	-1.59739	-1.12726	-1.35579
O	0.77065	0.64285	0.00290
O	-0.24350	-1.48842	1.51793
H	-1.02580	-1.00065	1.80648
H	0.03581	1.23037	0.23300
O	1.61557	-1.70338	-0.23067
H	1.55790	-2.42380	-0.86042



Si	-3.17234	0.53405	0.04398
O	-4.37760	-0.12332	0.96357
H	-4.70710	0.42077	1.68084
O	-3.23974	-0.34787	-1.36714
O	-3.68882	2.08436	-0.22306
H	-2.99651	2.71213	-0.43758
O	-1.69546	0.43057	0.57647
H	-4.10172	-0.57930	-1.71666
H	2.48952	1.19367	-0.13014
N	3.46302	1.50271	-0.17502
H	3.65116	2.48370	-0.27886
C	4.46176	0.64791	-0.00967
N	5.72051	1.08799	0.02839
N	4.20829	-0.64684	0.10875
H	6.48510	0.45135	0.16301
H	5.92370	2.07084	0.04088
H	4.96326	-1.29511	0.24202
H	3.26150	-1.01739	-0.00753

*01\_sg-d.mol2*

E = -1391.541320  
H = -1391.322386  
G = -1391.394444  
G(quasi-RRHO) = -1391.390639

Si	-0.21237	1.19237	-0.02056
O	1.07545	2.19970	0.01230
H	1.95753	1.79761	0.02622
O	-0.65577	0.42084	-1.42347
O	-0.58828	0.34726	1.36506
H	0.04799	-0.37916	1.42269
H	-0.03135	-0.31067	-1.53129
O	-1.47005	2.29034	-0.03163
H	-1.40338	2.98984	0.61943
Si	2.85161	-0.70988	-0.00837
O	3.46420	-1.34473	1.38740
H	3.48477	-2.30145	1.44475
O	3.50351	0.81973	-0.06338
O	3.50586	-1.66371	-1.19116
H	3.02249	-1.67843	-2.01913
O	1.28969	-0.53719	-0.11563
H	4.41431	0.93616	0.21166
H	-2.37380	-0.23857	-1.20162
N	-3.32538	-0.60347	-1.13881

C	-3.91609	-0.84948	0.02167
H	-3.82867	-0.75212	-1.99521
N	-3.26954	-0.65752	1.16235
H	-2.31332	-0.29963	1.19609
H	-3.73472	-0.83767	2.03422
N	-5.16995	-1.30375	0.04099
H	-5.69057	-1.42006	-0.80921
H	-5.64686	-1.46866	0.90853

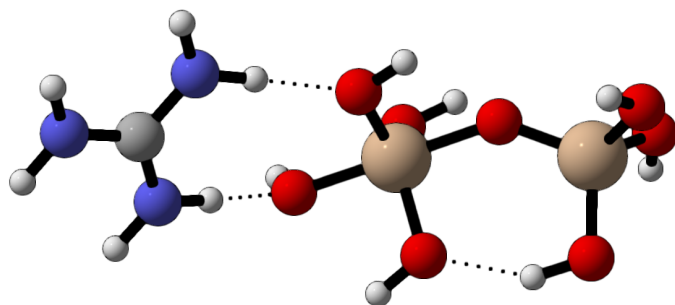
*02\_sg-d.mol2*

E = -1391.539611  
H = -1391.320456  
G = -1391.391949  
G(quasi-RRHO) = -1391.388208

Si	-0.81927	1.81974	0.05930
O	-0.62474	1.18935	1.56387
H	-0.91970	0.27891	1.69406
O	0.19107	1.27096	-1.15900
O	-2.29696	2.39278	-0.41286
H	-2.84101	1.64114	-0.67141
H	-0.22779	0.49069	-1.54284
O	-0.04870	3.27147	0.39312
H	-0.07388	3.90087	-0.32862
Si	-1.54431	-1.57895	-0.05080
O	-2.65607	-2.69827	-0.52590
H	-3.55076	-2.37475	-0.64620
O	-1.36601	-1.56717	1.59893
O	-0.10227	-2.20833	-0.59596
H	-0.14001	-2.68732	-1.42690
O	-1.84612	-0.10080	-0.49451
H	-0.96679	-2.33371	2.01453
H	1.89315	0.80730	-0.77003
N	2.89140	0.67072	-0.58867
H	3.50373	1.45023	-0.75127
C	3.38107	-0.44314	-0.06839
N	4.67538	-0.51207	0.24866
N	2.60204	-1.49775	0.13220
H	5.06097	-1.34119	0.66292
H	5.25469	0.30763	0.22311
H	2.99014	-2.33268	0.53405
H	1.63766	-1.54573	-0.18703

IM1-g, three equatorial OH groups

*00\_sg-e.mol2*



E = -1391.555324

H = -1391.335128

G = -1391.407820

G(quasi-RRHO) = -1391.403292

Si	-0.10698	0.68794	-0.25969
O	-0.48200	0.80944	1.38797
H	0.17147	1.34390	1.84362
O	0.77618	-0.66526	-0.76049
O	-0.55159	1.87396	-1.36623
H	-1.40347	1.67796	-1.75981
H	0.18582	-1.39606	-0.95766
O	1.40563	1.55939	0.02049
H	1.48223	2.30591	-0.57554
Si	-3.03319	-0.50205	0.13090
O	-3.01506	-0.01979	1.69780
H	-2.13543	0.35234	1.90007
O	-3.44108	-2.08819	-0.01060
O	-4.30957	0.19757	-0.63456
H	-4.46596	1.12137	-0.43225
O	-1.61585	-0.19972	-0.55124
H	-2.73953	-2.71959	0.15648
H	2.52631	-0.98296	-0.75777
H	3.87428	-2.01707	-1.17405
N	3.52733	-1.20109	-0.70265
C	4.32520	-0.51428	0.10247
N	5.59483	-0.89515	0.26901
N	3.85938	0.55523	0.72733
H	6.19762	-0.40300	0.90310
H	5.91523	-1.77690	-0.08796
H	4.46978	1.08754	1.32104

H 2.92861 0.93768 0.48803

*01\_sg-e.mol2*

E = -1391.556188

H = -1391.335751

G = -1391.406437

G(quasi-RRHO) = -1391.402882

Si -0.23126 1.04568 -0.21730

O -0.71752 1.25691 1.39488

H 0.00568 1.61041 1.91698

O 0.47241 -0.44902 -0.58491

O -0.41442 2.25922 -1.36736

H -1.27816 2.20524 -1.78045

H -0.17747 -1.14778 -0.71729

O 1.37704 1.68222 0.14582

H 1.52176 2.50974 -0.31558

Si -2.76347 -0.67290 0.08070

O -2.88143 -0.41191 1.69507

H -2.16679 0.19457 1.96075

O -2.03119 -2.10977 -0.26681

O -4.27740 -0.78689 -0.53695

H -4.90968 -0.12519 -0.25014

O -1.85807 0.44645 -0.61638

H -2.32145 -2.89466 0.20106

H 2.85342 0.90344 0.53278

N 3.75565 0.42910 0.70591

H 4.45419 0.88687 1.26351

C 4.05797 -0.68663 0.06152

N 5.27601 -1.22303 0.17689

N 3.13827 -1.27481 -0.68995

H 5.52489 -2.05010 -0.33453

H 6.01201 -0.72372 0.64218

H 3.35051 -2.13758 -1.15770

H 2.16480 -0.94703 -0.67521

*02\_sg-e.mol2*

E = -1391.555685

H = -1391.334986

G = -1391.405126

G(quasi-RRHO) = -1391.401424

Si 0.15995 -0.36367 0.00557

O	0.71329	-1.02144	-1.45624
H	0.10612	-1.65644	-1.83903
O	0.73034	-1.06629	1.43954
O	-0.87978	0.96681	0.03100
H	-0.36402	1.77647	0.04021
H	0.12674	-1.71114	1.81133
O	-1.30166	-1.37221	-0.00145
H	-1.13033	-2.31598	-0.01264
Si	3.09918	0.36364	0.00632
O	3.45234	-0.46133	-1.37290
H	2.63041	-0.83406	-1.73191
O	3.47005	-0.49006	1.35900
O	4.09414	1.66488	0.07092
H	4.26914	2.10525	-0.76249
O	1.53369	0.73325	0.01500
H	2.65325	-0.87590	1.71486
H	-2.63413	1.21071	0.04187
N	-3.64681	1.37255	0.04228
H	-3.98837	2.31604	0.07220
C	-4.49806	0.35874	-0.00151
N	-5.81312	0.58919	0.00051
N	-4.03570	-0.88097	-0.03742
H	-6.46844	-0.16623	-0.08148
H	-6.17288	1.52567	-0.03107
H	-4.67466	-1.65514	-0.07147
H	-3.02219	-1.06558	-0.02448

*03\_sg-e.mol2*

E = -1391.554342

H = -1391.333501

G = -1391.402361

G(quasi-RRHO) = -1391.399250

Si	-1.12918	-1.30081	0.00606
O	-2.02470	-0.84031	1.37306
H	-2.59485	-1.54196	1.69159
O	-1.74036	-0.86179	-1.51545
O	0.37496	-2.05679	0.16140
H	0.25207	-3.00992	0.16125
H	-2.23827	-1.56904	-1.92872
O	-1.85586	-2.90382	-0.05283
H	-2.80951	-2.92881	-0.14290
Si	-0.97609	1.72392	-0.00466
O	-2.01493	1.92024	1.25016

H	-2.25640	1.04311	1.59413
O	-1.69788	1.91137	-1.46344
O	0.14145	2.92174	0.07241
H	0.33002	3.26578	0.94753
O	-0.29339	0.25956	0.07667
H	-1.88044	1.03125	-1.83320
H	1.50032	0.49599	0.03934
N	2.48809	0.76305	0.00757
H	2.71196	1.73908	-0.06646
C	3.44419	-0.15228	0.00880
N	4.72494	0.21192	-0.06477
N	3.11378	-1.43254	0.08409
H	5.45939	-0.47154	-0.03750
H	4.98363	1.18116	-0.09600
H	3.82277	-2.14314	0.07684
H	2.12595	-1.70058	0.11760

*04\_sg-e.mol2*

E = -1391.550417

H = -1391.329920

G = -1391.401756

G(quasi-RRHO) = -1391.397711

Si	-1.45977	-1.23303	0.05151
O	-2.73666	-0.39235	-0.68866
H	-3.33952	-1.01772	-1.09645
O	-0.06245	-1.48409	-0.88138
O	-1.54714	-1.77008	1.64519
H	-1.22608	-1.09586	2.24673
H	-0.13812	-2.33645	-1.31897
O	-2.13269	-2.76190	-0.50197
H	-2.29259	-3.35673	0.23095
Si	-0.72670	1.80724	0.10028
O	-2.09484	2.21224	-0.70313
H	-2.59318	1.39330	-0.88973
O	0.60698	1.98283	-0.86546
O	-0.48606	2.90274	1.30139
H	-1.24425	3.10297	1.85355
O	-0.76889	0.29907	0.61332
H	0.75215	2.85396	-1.24204
H	1.56403	-1.26943	-0.20686
N	2.51509	-1.36859	0.17026
H	2.76111	-2.25464	0.57482
C	3.46307	-0.46977	-0.03854

N	4.72654	-0.74345	0.29154
N	3.16210	0.70854	-0.56812
H	5.45444	-0.06589	0.15409
H	4.99674	-1.67099	0.56493
H	3.88650	1.39046	-0.70600
H	2.19883	1.02351	-0.66903

*05\_sg-e.mol2*

E = -1391.550418  
H = -1391.329918  
G = -1391.401726  
G(quasi-RRHO) = -1391.397694

Si	-1.46135	-1.23195	0.05157
O	-2.73634	-0.38974	-0.69026
H	-3.33908	-1.01442	-1.09926
O	-0.06315	-1.48549	-0.87927
O	-1.55266	-1.76788	1.64545
H	-1.23198	-1.09366	2.24719
H	-0.13918	-2.33820	-1.31613
O	-2.13459	-2.76049	-0.50238
H	-2.30438	-3.35156	0.23136
Si	-0.72486	1.80733	0.10019
O	-2.09361	2.21489	-0.70084
H	-2.59256	1.39665	-0.88872
O	0.60728	1.98034	-0.86809
O	-0.48006	2.90225	1.30091
H	-1.23586	3.10114	1.85683
O	-0.76902	0.29931	0.61354
H	0.75075	2.84968	-1.24942
H	2.19923	1.02192	-0.66898
H	3.88682	1.38949	-0.70357
N	3.16247	0.70731	-0.56668
C	3.46335	-0.47159	-0.03842
N	4.72672	-0.74538	0.29212
N	2.51547	-1.37082	0.16911
H	4.99704	-1.67349	0.56348
H	5.45489	-0.06839	0.15322
H	2.76159	-2.25732	0.57263
H	1.56404	-1.27100	-0.20694

*06\_sg-e.mol2*

E = -1391.549277

H = -1391.328136  
G = -1391.398394  
G(quasi-RRHO) = -1391.394538

Si	1.44479	-1.16066	-0.12243
O	1.75425	-0.62904	1.45834
H	2.15504	-1.33634	1.96801
O	-0.10929	-1.80930	-0.40581
O	2.59299	-1.04693	-1.34975
H	2.51826	-0.20720	-1.80654
H	-0.04363	-2.76843	-0.38396
O	2.03837	-2.76901	0.27080
H	2.79759	-2.99906	-0.26527
Si	0.53648	1.87752	0.05888
O	0.80877	1.87919	1.67698
H	1.17395	1.01037	1.93017
O	-0.99192	2.36655	-0.28995
O	1.44034	3.07452	-0.62113
H	2.32274	3.18434	-0.26277
O	0.80564	0.42373	-0.55226
H	-1.57848	1.65186	-0.56121
H	-1.50999	-0.71592	-1.17269
H	-2.90995	-0.07331	-1.96294
N	-2.42737	-0.27405	-1.10253
C	-3.15617	-0.61838	-0.03019
N	-4.44431	-0.31040	0.03094
N	-2.54939	-1.23168	0.96985
H	-4.98766	-0.52055	0.84936
H	-4.88259	0.22230	-0.69936
H	-3.03831	-1.46136	1.81653
H	-1.58338	-1.51736	0.83597

*07\_sg-e.mol2*

E = -1391.546571  
H = -1391.326209  
G = -1391.397829  
G(quasi-RRHO) = -1391.394280

Si	-0.02936	1.02690	-0.00468
O	-1.10797	2.24273	-0.42571
H	-2.02976	1.98067	-0.34531
O	0.73309	0.85480	1.50139
O	0.31780	-0.16160	-1.16825
H	-0.31413	-0.88721	-1.18067



H	0.20350	0.28975	2.06806
O	1.33079	1.97353	-0.48905
H	1.19333	2.37383	-1.34803
Si	-2.70691	-0.65845	0.11658
O	-2.41405	-1.69183	-1.13282
H	-2.39188	-2.62805	-0.92480
O	-3.62425	0.57414	-0.47367
O	-3.50206	-1.55499	1.23454
H	-3.57343	-1.19291	2.11978
O	-1.38106	0.01311	0.67945
H	-4.43562	0.35958	-0.93766
H	2.42059	0.26124	1.18471
N	3.37550	-0.10452	1.12005
C	3.83609	-0.70739	0.03541
H	3.99210	0.05229	1.89687
N	3.04944	-0.91560	-1.00903
H	2.07665	-0.59417	-1.03627
H	3.42302	-1.36297	-1.82708
N	5.11309	-1.10306	-0.00920
H	5.69472	-1.04450	0.80708
H	5.44763	-1.65831	-0.77553

*08\_sg-e.mol2*

E = -1391.548476

H = -1391.327250

G = -1391.397008

G(quasi-RRHO) = -1391.393506

Si	-0.31109	0.84983	0.01433
O	-0.72719	0.70867	1.65463
H	0.03710	0.61385	2.22523
O	0.06283	-0.56148	-0.84221
O	-0.26162	2.35606	-0.71920
H	0.62438	2.71864	-0.74903
H	0.98085	-0.82556	-0.77180
O	1.46048	0.96383	0.45937
H	1.65000	1.72055	1.02082
Si	-2.97504	-0.53056	-0.12385
O	-3.13760	-0.70229	1.50492
H	-2.38009	-0.27148	1.93479
O	-2.40758	-1.89402	-0.84281
O	-4.47866	-0.34756	-0.75118
H	-5.08827	0.18522	-0.23767
O	-1.98205	0.69524	-0.43136

H	-1.46009	-1.77755	-1.01903
H	4.49047	0.74108	-1.63952
H	3.03037	0.87361	-0.67021
N	3.93248	0.44278	-0.86056
C	4.35397	-0.50593	-0.03494
N	3.58032	-0.84547	0.98746
N	5.52623	-1.10337	-0.22818
H	3.85397	-1.56536	1.63076
H	2.69621	-0.35298	1.09987
H	5.84256	-1.83185	0.38621
H	6.10244	-0.86773	-1.01585

*09\_sg-e.mol2*

E = -1391.549182

H = -1391.328027

G = -1391.396938

G(quasi-RRHO) = -1391.393974

Si	-1.77712	-0.93666	-0.03610
O	-1.86225	-2.68543	-0.02276
H	-2.76590	-2.99332	-0.09724
O	-1.16563	-0.89011	1.54694
O	-3.42170	-0.85855	-0.38028
H	-3.70779	0.05346	-0.45931
H	-1.07885	-1.78282	1.88868
O	-0.55717	-1.00907	-1.24015
H	-0.50641	-1.90842	-1.57585
Si	-0.41933	1.77808	0.09064
O	0.61932	1.49506	-1.17692
H	0.30685	0.70547	-1.64902
O	0.31536	1.47039	1.52131
O	-0.73790	3.38173	0.11956
H	-0.87936	3.80892	-0.72718
O	-1.69898	0.83422	-0.09809
H	-0.01510	0.62144	1.86317
H	1.26652	-1.12397	-0.41821
H	2.14940	-2.35883	0.40288
N	2.14164	-1.44711	-0.01804
C	3.25615	-0.72893	-0.06783
N	3.23208	0.50253	-0.55383
N	4.39661	-1.25328	0.37767
H	5.24586	-0.71812	0.37870
H	4.45125	-2.21964	0.64474
H	4.08048	1.03565	-0.62406

H 2.34575 0.95296 -0.78147

*10\_sg-e.mol2*

E = -1391.548423

H = -1391.327310

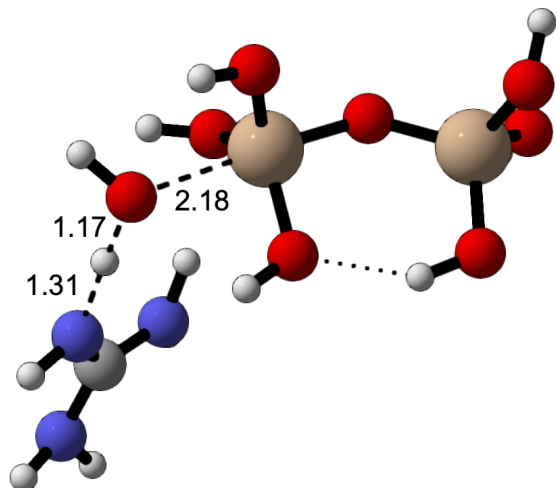
G = -1391.395508

G(quasi-RRHO) = -1391.392578

Si	-0.13191	0.87202	0.19650
O	0.71972	0.56264	1.63230
H	1.38398	1.23306	1.80446
O	0.16311	-0.08159	-1.17241
O	-1.27172	2.12076	0.12151
H	-0.94180	2.91202	-0.30754
H	0.76375	0.34401	-1.78771
O	1.19376	1.94796	-0.38601
H	1.29357	2.78577	0.07082
Si	-2.69345	-0.67327	-0.05597
O	-3.64134	-1.71802	0.77822
H	-3.39666	-2.64369	0.72864
O	-2.28965	-1.39828	-1.47686
O	-3.64764	0.64544	-0.27384
H	-3.10028	1.44213	-0.18814
O	-1.35236	-0.24231	0.71930
H	-1.38428	-1.13504	-1.71065
H	2.73963	1.03405	-0.46100
N	3.60600	0.49465	-0.58935
C	3.81276	-0.67500	-0.00308
H	4.29604	0.85763	-1.22324
N	2.91781	-1.17337	0.83960
H	3.09525	-2.04775	1.30025
H	2.09332	-0.64252	1.11493
N	4.93220	-1.35672	-0.25211
H	5.07862	-2.26690	0.14567
H	5.57419	-1.04998	-0.96003

TS2-cg, water cleavage of IM1, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as catalyst

*00\_cg-h.mol2*

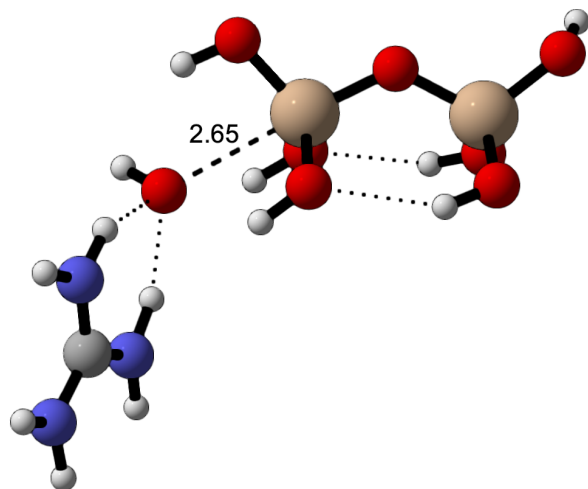


E = -1391.531709  
 H = -1391.316587  
 G = -1391.387248  
 G(quasi-RRHO) = -1391.383260

Si	-0.21170	0.98208	0.24876
O	0.60767	0.56600	1.63204
H	1.36196	1.13064	1.80961
O	0.12441	0.12436	-1.13599
O	-0.84588	2.49581	0.11623
H	-0.24807	3.14881	-0.24990
H	0.84263	0.47488	-1.66629
O	1.67227	1.92495	-0.30971
H	1.97225	2.71857	0.14212
Si	-2.77151	-0.67993	-0.09617
O	-3.35587	-1.82947	0.91501
H	-2.71287	-2.33874	1.41209
O	-2.18695	-1.33007	-1.47510
O	-4.07508	0.21048	-0.52910
H	-4.64843	0.51851	0.17516
O	-1.62075	0.17177	0.64564
H	-1.30004	-0.98667	-1.67060
H	2.57918	1.18916	-0.40849
N	3.57911	0.35610	-0.58867
C	3.75973	-0.81404	-0.04437
H	4.33451	0.65285	-1.18836
N	2.80351	-1.37166	0.72405
H	3.04384	-2.14563	1.31733
H	2.01116	-0.81178	1.00801
N	4.90148	-1.52841	-0.20437

H	4.88521	-2.51514	-0.01192
H	5.53804	-1.24422	-0.92804

TS2-sg, water cleavage of IM1, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as spectator  
*00\_sg-h.mol2*



E	= -1391.535124
H	= -1391.317929
G	= -1391.391791
G(quasi-RRHO)	= -1391.386611

Si	-0.62424	0.93122	-0.13542
O	-0.53809	0.78294	1.49991
H	0.41663	0.84791	1.70056
O	0.08183	-0.33608	-0.91851
O	-0.25508	2.39712	-0.74807
H	0.68497	2.55422	-0.58376
H	1.02724	-0.39324	-0.75138
O	1.91150	1.20444	0.57701
H	2.22216	1.99911	1.01975
Si	-3.08747	-0.60786	-0.05185
O	-3.01521	-0.78252	1.57322
H	-2.23223	-0.37343	1.96701
O	-2.50096	-1.89509	-0.86921
O	-4.64583	-0.50794	-0.50197
H	-5.24274	-0.03476	0.08089
O	-2.21742	0.71201	-0.46341
H	-1.56706	-1.81038	-1.09701
H	4.50234	0.45950	-1.76035
H	3.19771	0.85277	-0.59929

N	4.00156	0.27968	-0.90963
C	4.43768	-0.61261	-0.03060
N	3.75430	-0.74683	1.09717
N	5.52377	-1.34796	-0.27263
H	4.05478	-1.37872	1.81627
H	2.96081	-0.09483	1.21729
H	5.79756	-2.07953	0.35795
H	5.99245	-1.29322	-1.15865

*01\_sg-h.mol2*

E = -1391.533275  
H = -1391.317034  
G = -1391.388596  
G(quasi-RRHO) = -1391.384416

Si	-0.44739	0.81651	-0.39220
O	-0.69051	1.44559	1.11125
H	0.19830	1.71253	1.41029
O	0.41233	-0.59706	-0.38027
O	-0.04720	1.80067	-1.63018
H	0.85104	2.11398	-1.45135
H	-0.15062	-1.37134	-0.25401
O	1.76949	1.72322	0.32974
H	1.92286	2.67103	0.37414
Si	-2.98270	-0.55974	0.11423
O	-3.21737	0.13632	1.57315
H	-2.46873	0.69107	1.83727
O	-2.20832	-2.00387	0.20583
O	-4.42711	-0.81672	-0.58784
H	-5.08377	-0.12009	-0.52508
O	-1.99055	0.35220	-0.78728
H	-2.54117	-2.66756	0.81327
H	4.76987	0.90886	1.15311
N	3.99880	0.48074	0.67048
H	3.05740	1.02692	0.54512
C	4.19846	-0.68485	0.09921
N	3.20296	-1.27895	-0.55875
N	5.38807	-1.30562	0.17795
H	3.33465	-2.19963	-0.93660
H	2.24981	-0.92958	-0.48291
H	5.56176	-2.12864	-0.37118
H	6.19424	-0.78914	0.48136

*02\_sg-h.mol2*

E = -1391.527741  
H = -1391.310273  
G = -1391.382810  
G(quasi-RRHO) = -1391.378546

Si	-1.29758	-1.07026	0.25149
O	-2.39781	-0.79312	-0.94572
H	-2.56967	-1.69480	-1.29649
O	0.13690	-1.69380	-0.26531
O	-1.89109	-1.74524	1.62287
H	-2.14071	-2.66010	1.46313
H	-0.14603	-2.57446	-0.61307
O	-1.75898	-3.24067	-0.82468
H	-2.13134	-4.05521	-0.48381
Si	-0.96966	1.90305	0.04739
O	-2.18810	1.95643	-1.03427
H	-2.49008	1.07043	-1.29584
O	0.50744	2.12352	-0.63770
O	-1.14887	3.11851	1.11893
H	-2.03341	3.28573	1.45074
O	-0.90198	0.45056	0.75487
H	0.66851	2.95785	-1.08477
H	3.23696	-2.06987	0.83895
N	2.83264	-1.26917	0.38641
H	1.84090	-1.31812	0.13712
C	3.62120	-0.28700	-0.01873
N	3.10760	0.80073	-0.57989
N	4.94138	-0.38575	0.13366
H	3.71985	1.53127	-0.89706
H	2.11754	1.01801	-0.54224
H	5.54718	0.38332	-0.08835
H	5.36305	-1.24131	0.44664

*03\_sg-h.mol2*

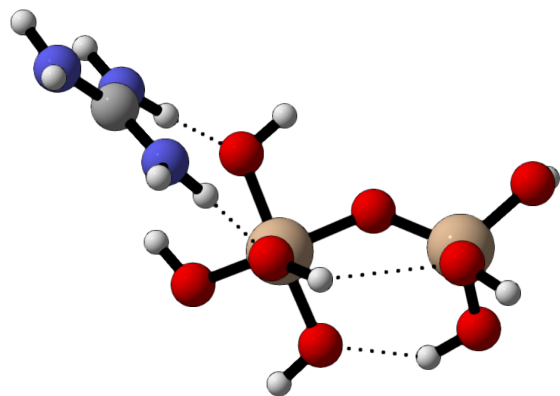
E = -1391.527741  
H = -1391.310272  
G = -1391.382800  
G(quasi-RRHO) = -1391.378542

Si	-1.29749	-1.07020	0.25135
O	-2.39860	-0.79246	-0.94493
H	-2.57105	-1.69390	-1.29589
O	0.13664	-1.69352	-0.26675

O	-1.89000	-1.74539	1.62308
H	-2.13986	-2.66017	1.46324
H	-0.14663	-2.57403	-0.61451
O	-1.75974	-3.24000	-0.82459
H	-2.13155	-4.05472	-0.48356
Si	-0.96920	1.90303	0.04758
O	-2.18888	1.95713	-1.03266
H	-2.49122	1.07127	-1.29433
O	0.50722	2.12276	-0.63923
O	-1.14658	3.11853	1.11937
H	-2.03061	3.28599	1.45242
O	-0.90141	0.45048	0.75490
H	0.66800	2.95674	-1.08704
H	3.23604	-2.06956	0.84023
N	2.83199	-1.26930	0.38668
H	1.84042	-1.31849	0.13671
C	3.62072	-0.28741	-0.01882
N	3.10729	0.79982	-0.58112
N	4.94082	-0.38594	0.13425
H	3.71965	1.53015	-0.89855
H	2.11724	1.01720	-0.54376
H	5.54659	0.38323	-0.08747
H	5.36242	-1.24115	0.44825

TS-iso-g, isomerization of IM1 to IM2

*00\_sg-f.mol2*



E	= -1391.543912
H	= -1391.324855
G	= -1391.393955
G(quasi-RRHO)	= -1391.390685



Si	0.19929	0.99645	0.02853
O	-0.55242	2.52396	-0.04110
H	-1.27550	2.59379	0.58369
O	-0.53695	-0.00005	-1.12649
O	-0.86111	0.63105	1.38070
H	-0.50156	-0.10616	1.87814
H	0.10701	-0.52369	-1.61303
O	1.48677	1.67351	-0.93704
H	1.19727	2.47229	-1.38044
Si	2.68176	-0.70809	0.15788
O	3.78961	0.38328	-0.35461
H	3.28848	1.14024	-0.70839
O	2.11889	-1.65540	-1.06565
O	3.42606	-1.70968	1.21852
H	3.98590	-1.30146	1.88163
O	1.38334	0.00189	0.79412
H	2.76966	-2.05546	-1.64564
H	-2.54561	0.26795	1.13435
N	-3.54513	0.03426	1.03204
H	-4.17095	0.25634	1.78527
C	-3.99575	-0.63669	-0.01632
N	-5.28493	-0.98048	-0.08621
N	-3.17036	-0.95621	-1.00252
H	-5.62557	-1.54474	-0.84319
H	-5.89801	-0.83148	0.69468
H	-3.52402	-1.42831	-1.81544
H	-2.19782	-0.62763	-1.01418

*01\_sg-f.mol2*

E = -1391.544128  
H = -1391.324805  
G = -1391.393554  
G(quasi-RRHO) = -1391.390007

Si	0.24713	1.05621	-0.05339
O	-1.32540	1.68390	-0.37839
H	-1.28393	2.63952	-0.45277
O	0.43940	0.92933	1.62827
O	0.82764	2.65980	-0.32947
H	1.77398	2.65805	-0.47724
H	0.66173	1.77886	2.01604
O	-0.47255	-0.49241	-0.33886
H	0.15811	-1.19647	-0.51729
Si	2.70703	-0.70165	-0.09343

O	2.01538	-2.11280	-0.60386
H	2.31360	-2.93028	-0.19991
O	2.78764	-0.62255	1.53723
O	4.25996	-0.61373	-0.59715
H	4.45519	-0.94922	-1.47394
O	1.76694	0.45967	-0.68265
H	2.02009	-0.13393	1.88483
H	-2.92915	0.99845	-0.41846
N	-3.87385	0.58889	-0.39867
H	-4.66789	1.17882	-0.57063
C	-4.05588	-0.66670	-0.01880
N	-5.29258	-1.15898	0.09856
N	-3.00436	-1.43121	0.23024
H	-5.44444	-2.09339	0.43217
H	-6.09218	-0.55804	0.01508
H	-3.13532	-2.39134	0.49335
H	-2.04936	-1.08526	0.04532

*O2\_sg-f.mol2*

E = -1391.543710  
H = -1391.324220  
G = -1391.393295  
G(quasi-RRHO) = -1391.389756

Si	0.16023	-0.61469	-0.00778
O	-1.31176	-1.45165	-0.31641
H	-1.12482	-2.37655	-0.49049
O	0.46851	-0.59952	1.66105
O	-0.80540	0.82279	-0.09752
H	-0.24423	1.58865	-0.22637
H	0.74218	-1.46629	1.96971
O	0.96275	-2.08319	-0.44602
H	1.90662	-1.97607	-0.58998
Si	2.95659	0.52148	-0.10930
O	3.75471	-0.87331	-0.48483
H	4.61746	-1.01834	-0.09149
O	2.93345	0.80879	1.50117
O	3.73792	1.81242	-0.74085
H	4.13135	1.70252	-1.60827
O	1.46961	0.32583	-0.68164
H	2.13195	0.42374	1.89437
H	-2.49694	1.18477	-0.07852
N	-3.50531	1.40216	-0.06375
H	-3.79948	2.36006	-0.00085

C	-4.40827	0.43464	-0.07213
N	-5.70959	0.72746	0.00404
N	-4.01320	-0.82704	-0.14729
H	-6.40404	0.00758	-0.07876
H	-6.02276	1.68098	0.00556
H	-4.69186	-1.56690	-0.13978
H	-3.01282	-1.06240	-0.20383

*03\_sg-f.mol2*

E = -1391.542680  
H = -1391.322967  
G = -1391.390920  
G(quasi-RRHO) = -1391.387748

Si	1.05993	-1.41090	0.00766
O	1.37998	-2.72294	1.07298
H	2.10015	-3.26305	0.74444
O	-0.23360	-1.93318	-0.95285
O	2.46405	-1.86961	-0.86794
H	2.70498	-1.19290	-1.50188
H	-0.12286	-2.82344	-1.29108
O	0.16934	-0.70726	1.35572
H	0.09310	-1.36419	2.05275
Si	1.15032	1.72559	-0.10302
O	1.28605	1.79201	1.53222
H	0.96297	0.95259	1.89962
O	-0.22123	2.46187	-0.62661
O	2.29582	2.68298	-0.77587
H	3.20880	2.45023	-0.59925
O	1.24332	0.19923	-0.59569
H	-1.03933	2.04994	-0.33033
H	-2.65410	1.09116	1.55930
H	-1.44134	-0.00251	1.00479
N	-2.31160	0.51228	0.81002
C	-3.21128	-0.01586	-0.02915
N	-4.45439	0.45787	-0.04668
N	-2.85144	-0.98628	-0.84745
H	-3.50811	-1.34147	-1.51988
H	-1.88810	-1.34486	-0.86531
H	-5.12106	0.13230	-0.72357
H	-4.71867	1.23377	0.53324

04\_sg-f.mol2

E = -1391.534745

H = -1391.315243

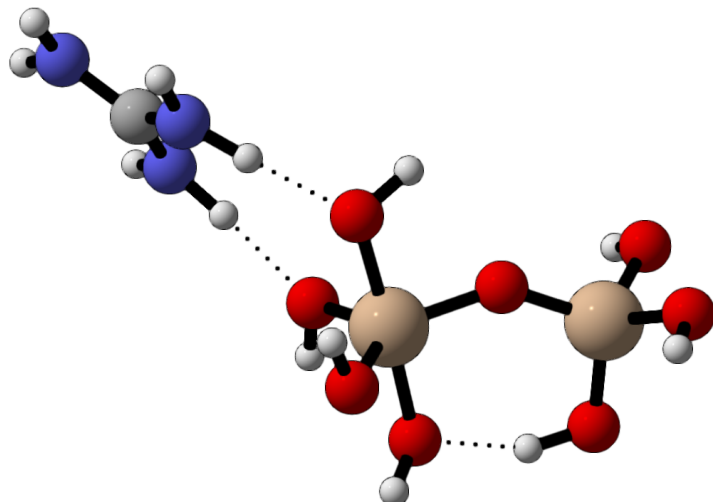
G = -1391.385902

G(quasi-RRHO) = -1391.381776

Si	1.30619	-1.33930	0.00548
O	1.64538	-2.70591	1.00273
H	2.41062	-3.18220	0.67778
O	0.09656	-1.86673	-1.05281
O	2.78606	-1.66064	-0.80742
H	3.02158	-0.92714	-1.37705
H	0.33067	-2.66339	-1.53049
O	0.33478	-0.76137	1.35024
H	0.28823	-1.45124	2.01655
Si	1.00764	1.79917	-0.06967
O	0.85149	1.88443	1.56168
H	0.66360	0.98405	1.88394
O	-0.36000	2.27249	-0.85054
O	2.06526	2.95478	-0.55142
H	2.89278	3.00170	-0.06976
O	1.44297	0.31623	-0.50187
H	-1.05137	1.60499	-0.88773
H	-1.48780	-0.38055	0.71726
H	-1.66937	-0.99763	-0.82857
N	-2.07568	-0.40049	-0.11402
C	-3.38878	-0.21830	-0.03225
N	-4.17411	-0.55007	-1.05055
N	-3.91917	0.31794	1.06054
H	-5.15438	-0.33160	-1.04310
H	-3.78300	-0.92209	-1.89752
H	-4.90443	0.50149	1.12585
H	-3.33543	0.59750	1.82851

IM2-g, co-linear OH groups on Si

00\_sg-g.mol2



E = -1391.552207  
 H = -1391.332218  
 G = -1391.404506  
 G(quasi-RRHO) = -1391.400061

Si	-0.15697	0.81598	0.07012
O	0.89748	0.43208	-1.19961
H	0.59851	0.85539	-2.00817
O	0.01820	2.23969	0.95207
O	-1.36215	-0.31433	0.39559
H	0.55528	2.08629	1.73179
O	0.92273	-0.01788	1.20152
H	0.53314	-0.84676	1.48302
H	4.18618	-0.29485	1.95537
H	2.62790	-0.13690	1.15576
O	-1.18834	1.72203	-1.07130
H	-1.19550	2.65332	-0.84450
Si	-2.89737	-0.66788	0.02810
O	-3.06429	-2.21296	-0.49196
H	-2.74819	-2.40171	-1.37709
O	-3.43843	0.38983	-1.08696
H	-2.71655	1.04828	-1.24402
O	-3.83211	-0.70355	1.37450
H	-3.82990	0.08486	1.91996
N	3.65533	-0.24985	1.10394
C	4.24000	-0.54024	-0.04738
N	3.52875	-0.52592	-1.16552
N	5.53698	-0.85899	-0.08544
H	2.55372	-0.20518	-1.16592
H	3.97274	-0.72907	-2.04296

H	6.09671	-0.82468	0.74703
H	6.01466	-0.95683	-0.96281

*01\_sg-g.mol2*

E = -1391.552193  
H = -1391.332227  
G = -1391.404344  
G(quasi-RRHO) = -1391.400073

Si	-0.16231	0.83265	-0.06836
O	-1.19888	1.71486	1.08702
H	-1.21409	2.64895	0.87245
O	0.92240	0.02236	-1.21196
O	0.00379	2.27085	-0.92828
H	0.54273	2.13290	-1.70961
H	0.53259	-0.79916	-1.51403
O	0.89443	0.43594	1.19550
H	0.59359	0.84576	2.01029
Si	-2.88528	-0.68313	-0.03006
O	-3.85954	-0.72912	-1.34747
H	-4.13887	0.11661	-1.70192
O	-3.43997	0.36809	1.08424
O	-2.98716	-2.24027	0.47180
H	-2.40315	-2.49985	1.18636
O	-1.36040	-0.30025	-0.41081
H	-2.72184	1.02862	1.25022
H	2.62738	-0.10671	-1.15917
N	3.65377	-0.22770	-1.10563
H	4.18723	-0.26081	-1.95597
C	4.23215	-0.54250	0.04246
N	5.52700	-0.86985	0.07975
N	3.51635	-0.54431	1.15781
H	6.00025	-0.98824	0.95698
H	6.09047	-0.82311	-0.74960
H	3.95581	-0.76446	2.03342
H	2.54398	-0.21547	1.15997

*02\_sg-g.mol2*

E = -1391.548614  
H = -1391.328694  
G = -1391.402452  
G(quasi-RRHO) = -1391.397516

Si	0.26885	1.15857	0.17233
O	1.46273	1.74966	-1.04074
H	1.29292	2.62512	-1.39179
O	-0.98856	0.66448	1.28593
O	0.60974	2.46126	1.18971
H	1.38536	2.94520	0.90172
H	-0.78254	0.93021	2.18291
O	-0.92358	1.11067	-1.03691
H	-0.53647	1.24292	-1.90449
Si	2.51635	-0.99522	-0.05719
O	3.43376	-1.38028	1.24642
H	3.60267	-0.67578	1.87426
O	3.32845	-0.08028	-1.13677
O	2.22143	-2.48715	-0.67076
H	1.91839	-2.52018	-1.57958
O	1.16369	-0.24164	0.39620
H	2.81197	0.74332	-1.29250
H	-2.32531	-0.37812	1.11392
N	-3.18588	-0.93220	0.96229
H	-3.48740	-1.58264	1.66545
C	-3.97363	-0.66680	-0.06678
N	-5.15592	-1.27582	-0.18841
N	-3.57743	0.20442	-0.98467
H	-5.76381	-1.07046	-0.96017
H	-5.51561	-1.85094	0.55123
H	-4.16075	0.39067	-1.78051
H	-2.61712	0.56606	-0.98075

*03\_sg-g.mol2*

E = -1391.550904  
H = -1391.330890  
G = -1391.402303  
G(quasi-RRHO) = -1391.398575

Si	-0.18588	0.71586	0.06707
O	-0.11837	2.34656	-0.34300
H	0.46729	2.48082	-1.09070
O	0.89359	0.11096	1.22475
O	0.97206	0.32076	-1.20878
H	0.62920	-0.38190	-1.76285
H	0.53466	0.23097	2.10703
O	-1.37516	1.11513	1.33065
H	-1.35407	2.04416	1.56476
Si	-2.83890	-0.60198	-0.16675

O	-3.75482	0.72075	-0.50810
H	-3.39711	1.53373	-0.14134
O	-2.99582	-1.11314	1.38232
O	-3.49259	-1.83971	-1.01588
H	-3.57388	-1.72274	-1.96366
O	-1.29122	-0.37421	-0.60246
H	-2.52863	-0.49746	1.96209
H	2.68441	0.25037	-1.12724
N	3.71215	0.15134	-1.06910
H	4.27780	0.41704	-1.85533
C	4.26878	-0.47090	-0.04219
N	5.57998	-0.72530	-0.03818
N	3.51776	-0.83127	0.98894
H	6.00731	-1.21411	0.72728
H	6.13398	-0.57136	-0.86087
H	3.93915	-1.28255	1.78086
H	2.54349	-0.51620	1.06114

*04\_sg-g.mol2*

E = -1391.548889

H = -1391.328555

G = -1391.398363

G(quasi-RRHO) = -1391.395026

Si	-0.67365	1.50396	-0.03360
O	-1.64517	2.39477	1.01045
H	-2.19129	2.99789	0.50146
O	0.88641	2.08459	-0.37510
O	-1.31982	2.33784	-1.43401
H	-1.67993	1.72126	-2.07129
H	0.85154	2.60932	-1.17938
O	0.00517	0.64577	1.38440
H	0.23831	1.25861	2.08511
Si	-1.56958	-1.44062	-0.09901
O	-1.76293	-1.38127	1.52344
H	-1.18411	-0.67166	1.86547
O	-0.38950	-2.48577	-0.56540
O	-2.94906	-2.02060	-0.76304
H	-3.77533	-1.66624	-0.42879
O	-1.14467	0.00673	-0.66865
H	-0.58127	-3.42056	-0.46448
H	2.54045	1.40019	-0.04387
N	3.38261	0.81920	0.00506
H	4.26339	1.21323	-0.27473



C	3.22601	-0.50032	0.02633
N	4.21521	-1.30728	-0.35713
N	2.08048	-1.00337	0.45816
H	4.17070	-2.29442	-0.17922
H	5.05222	-0.93810	-0.77010
H	1.80311	-1.93837	0.20893
H	1.34976	-0.37246	0.81009

*05\_sg-g.mol2*

E = -1391.543953

H = -1391.323776

G = -1391.397858

G(quasi-RRHO) = -1391.392978

Si	-0.29670	1.03399	-0.12034
O	0.51667	1.23816	-1.57455
H	1.37110	0.80502	-1.57349
O	-0.13322	2.17098	1.11319
O	1.13497	0.11037	0.52451
H	0.81953	-0.54165	1.15512
H	0.62948	1.97525	1.65979
O	-1.67666	1.93458	-0.74084
H	-1.61209	2.86532	-0.52405
Si	-2.76656	-0.85102	0.09735
O	-2.92486	-2.19577	-0.82743
H	-2.56780	-2.14919	-1.71589
O	-3.73003	0.36789	-0.39461
O	-3.24971	-1.42918	1.55361
H	-3.47716	-0.77475	2.21618
O	-1.22970	-0.34958	0.11270
H	-3.14647	1.14367	-0.58536
H	4.60854	0.95279	1.28930
H	2.92781	0.56349	0.92770
N	3.92648	0.38554	0.82004
C	4.28881	-0.62739	0.04604
N	5.57247	-0.93307	-0.12224
N	3.33897	-1.32888	-0.56039
H	6.29369	-0.39499	0.32275
H	5.85141	-1.67911	-0.73338
H	2.37222	-1.07006	-0.37445
H	3.55739	-2.13759	-1.11309

06\_sg-g.mol2

E = -1391.545881  
H = -1391.326117  
G = -1391.397579  
G(quasi-RRHO) = -1391.393887

Si	1.01422	-1.38369	0.03857
O	1.65837	-2.15859	-1.31436
H	0.99566	-2.62522	-1.82514
O	1.08046	-2.12263	1.54721
O	-0.62116	-2.02950	-0.29456
H	-0.64504	-2.98909	-0.31229
H	0.25620	-2.55996	1.76645
O	2.58551	-0.62604	0.31078
H	3.31237	-1.15130	-0.02556
Si	1.18360	1.56755	-0.03571
O	2.12931	1.73743	-1.36564
H	2.73008	0.99658	-1.48684
O	1.95798	1.80603	1.38667
O	0.11147	2.80757	-0.09469
H	-0.10307	3.14856	-0.96460
O	0.33462	0.17198	-0.05192
H	2.50293	1.03246	1.58077
H	-1.45707	0.59971	0.06400
N	-2.40957	0.95559	0.14631
H	-2.53364	1.94496	0.26349
C	-3.44986	0.14679	0.00717
N	-4.69170	0.63377	0.05883
N	-3.24007	-1.14367	-0.19296
H	-5.48477	0.01895	0.03413
H	-4.85629	1.59794	0.28407
H	-4.01544	-1.77287	-0.29645
H	-2.27537	-1.50522	-0.23823

07\_sg-g.mol2

E = -1391.550916  
H = -1391.330266  
G = -1391.397401  
G(quasi-RRHO) = -1391.394773

Si	0.80258	1.44400	-0.01165
O	-0.36463	1.49954	1.22016
H	0.07641	1.48786	2.07364
O	-0.52363	1.78438	-1.14374

O	2.04443	1.20628	1.24495
H	2.81677	1.74561	1.06840
H	-0.30215	1.45525	-2.01792
O	1.06245	-0.06278	-0.71933
O	1.70299	2.74309	-0.58693
Si	1.40541	-1.55135	-0.18725
O	2.18918	-2.45034	-1.31009
O	2.30703	-1.43118	1.16871
H	2.38557	-0.47474	1.39737
O	0.03038	-2.41229	0.04189
H	-0.74524	-1.90915	0.31607
H	3.13557	-2.31213	-1.37712
H	1.23365	3.21497	-1.27706
H	-1.60833	0.21308	1.17079
H	-2.59944	-1.03143	1.83661
C	-3.25028	-0.26547	0.08987
N	-2.31175	-0.52105	1.01726
N	-4.39003	-0.94976	0.09799
N	-3.01074	0.65042	-0.82682
H	-4.56610	-1.65120	0.79456
H	-5.07183	-0.83140	-0.63000
H	-2.08339	1.11086	-0.89355
H	-3.67968	0.80718	-1.56039

*08\_sg-g.mol2*

E = -1391.545268  
H = -1391.324986  
G = -1391.395477  
G(quasi-RRHO) = -1391.391939

Si	1.48582	-1.22317	-0.02800
O	2.23758	-1.89651	1.32447
H	3.11580	-2.19846	1.08324
O	0.48317	-2.17830	-0.98467
O	2.89889	-1.57971	-1.01265
H	3.17383	-0.81286	-1.51497
H	0.99693	-2.53758	-1.71132
O	0.07817	-0.86163	1.03600
H	0.06641	-1.48658	1.76471
Si	0.83875	1.77503	-0.00262
O	0.40162	1.75988	1.56784
H	0.17937	0.83315	1.78287
O	-0.55451	1.99664	-0.86023
O	1.76264	3.08446	-0.32580

H	2.68810	3.03878	-0.07814
O	1.59997	0.42107	-0.43199
H	-0.48024	2.02121	-1.81720
H	-1.51807	-1.08556	0.26699
N	-2.48849	-1.30364	-0.00236
H	-2.74397	-2.27285	-0.07147
C	-3.43506	-0.38231	-0.04686
N	-4.71835	-0.74072	-0.10745
N	-3.11164	0.90713	-0.03292
H	-5.44295	-0.05503	-0.21883
H	-4.99293	-1.69514	0.03948
H	-3.83896	1.59950	-0.06294
H	-2.16788	1.21271	-0.25719

*09\_sg-g.mol2*

E = -1391.545268

H = -1391.324983

G = -1391.395455

G(quasi-RRHO) = -1391.391922

Si	1.48612	-1.22298	-0.02796
O	2.23914	-1.89392	1.32496
H	3.11758	-2.19518	1.08361
O	0.48443	-2.18036	-0.98340
O	2.89923	-1.57897	-1.01290
H	3.17422	-0.81195	-1.51494
H	0.99859	-2.53944	-1.70988
O	0.07832	-0.86192	1.03603
H	0.06648	-1.48714	1.76452
Si	0.83807	1.77511	-0.00295
O	0.40176	1.75950	1.56775
H	0.17960	0.83274	1.78270
O	-0.55563	1.99763	-0.85980
O	1.76218	3.08440	-0.32593
H	2.68760	3.03886	-0.07809
O	1.59820	0.42096	-0.43354
H	-0.48153	2.02139	-1.81683
H	-1.51790	-1.08566	0.26675
N	-2.48816	-1.30395	-0.00294
H	-2.74336	-2.27323	-0.07215
C	-3.43502	-0.38285	-0.04685
N	-4.71816	-0.74155	-0.10769
N	-3.11190	0.90671	-0.03236
H	-5.44298	-0.05574	-0.21688

H	-4.99258	-1.69595	0.03961
H	-3.83948	1.59882	-0.06230
H	-2.16825	1.21268	-0.25670

*10\_sg-g.mol2*

E = -1391.545268  
H = -1391.324979  
G = -1391.395422  
G(quasi-RRHO) = -1391.391896

Si	1.48613	-1.22289	-0.02793
O	0.07856	-0.86225	1.03645
H	0.06705	-1.48747	1.76494
O	0.48453	-2.18094	-0.98280
O	2.24008	-1.89278	1.32497
H	3.11863	-2.19354	1.08340
H	0.99867	-2.54039	-1.70911
O	2.89915	-1.57858	-1.01313
H	3.17286	-0.81195	-1.51646
Si	0.83757	1.77519	-0.00312
O	1.76229	3.08410	-0.32597
H	2.68801	3.03734	-0.07951
O	0.40153	1.75903	1.56763
O	-0.55627	1.99875	-0.85942
H	-0.48245	2.02348	-1.81644
O	1.59705	0.42090	-0.43434
H	0.17991	0.83207	1.78244
H	-1.51752	-1.08584	0.26694
N	-2.48766	-1.30411	-0.00323
H	-2.74265	-2.27338	-0.07331
C	-3.43465	-0.38316	-0.04677
N	-4.71770	-0.74208	-0.10888
N	-3.11171	0.90645	-0.03093
H	-5.44268	-0.05605	-0.21575
H	-4.99208	-1.69634	0.03955
H	-3.83941	1.59840	-0.06149
H	-2.16822	1.21267	-0.25563

*11\_sg-g.mol2*

E = -1391.545972  
H = -1391.325476  
G = -1391.395285  
G(quasi-RRHO) = -1391.391914

Si	1.01980	-1.33047	-0.13413
O	2.50420	-0.66085	-0.80093
H	3.28606	-1.09869	-0.46231
O	1.85264	-1.61108	1.32002
O	0.92697	-2.41593	-1.41115
H	0.10717	-2.91270	-1.41108
H	1.27278	-1.97179	1.99391
O	-0.50760	-1.93852	0.57044
H	-0.51931	-2.88484	0.73000
Si	1.11737	1.56463	0.10614
O	0.10344	2.83908	0.25139
H	-0.41709	2.88778	1.05503
O	2.10235	2.02310	-1.11495
O	1.88459	1.34945	1.54015
H	2.09215	0.42142	1.72553
O	0.28853	0.20006	-0.25233
H	2.58778	1.23280	-1.39883
H	-1.47968	0.42641	-0.71536
N	-2.47011	0.59621	-0.89394
H	-2.72089	1.33725	-1.52368
C	-3.38342	0.08223	-0.07867
N	-4.65158	0.48864	-0.15315
N	-3.01930	-0.83148	0.80606
H	-5.36981	0.03819	0.38428
H	-4.93198	1.18702	-0.81742
H	-3.70955	-1.25158	1.40247
H	-2.07145	-1.23908	0.76751

*12\_sg-g.mol2*

E = -1391.544809  
H = -1391.324246  
G = -1391.392631  
G(quasi-RRHO) = -1391.389835

Si	-1.76723	-0.92767	-0.07378
O	-2.43038	-1.99190	-1.19865
H	-3.34970	-2.16625	-0.98594
O	-0.85611	-1.42708	1.26775
O	-3.28376	-0.93347	0.79381
H	-3.45139	-0.09322	1.22165
H	-1.43901	-1.54956	2.02107
O	-0.25911	-1.00479	-1.06265
H	-0.35555	-1.67644	-1.74060

Si	-0.45894	1.71141	0.03990
O	0.53296	1.54085	-1.26985
H	0.32974	0.65518	-1.63341
O	0.30094	1.27907	1.42461
O	-0.80551	3.29251	0.22439
H	-0.95268	3.80580	-0.57215
O	-1.75706	0.76980	-0.17556
H	0.11686	0.35835	1.66729
H	1.31235	-1.24516	-0.24738
H	2.30982	-2.29960	0.71140
N	2.22653	-1.45318	0.17696
C	3.28835	-0.68292	0.01246
N	3.18143	0.48993	-0.60111
N	4.47769	-1.07941	0.47137
H	5.28992	-0.49999	0.36042
H	4.61859	-2.02481	0.77883
H	3.99855	1.05623	-0.74335
H	2.27352	0.90333	-0.79966

*13\_sg-g.mol2*

E = -1391.542056  
H = -1391.321675  
G = -1391.392101  
G(quasi-RRHO) = -1391.388576

Si	1.09744	-1.42414	-0.13315
O	0.21017	-0.85873	1.36249
H	-0.00967	-1.60362	1.92748
O	1.81853	-1.99723	-1.60424
O	2.43056	-1.88603	0.78809
H	2.34265	-1.62186	1.70527
H	2.57574	-1.47488	-1.86991
O	-0.20270	-2.46457	-0.39103
H	-0.05697	-2.97050	-1.19375
Si	1.11893	1.64612	-0.00119
O	2.29117	2.63021	-0.57866
H	3.16980	2.52496	-0.20859
O	1.25960	1.57344	1.62370
O	-0.29892	2.33714	-0.48804
H	-0.46342	3.24341	-0.21752
O	1.11055	0.18357	-0.66556
H	0.89085	0.71491	1.91732
H	-1.55674	-0.43617	1.00911
N	-2.58243	-0.38621	1.01962

H	-3.04943	-0.94977	1.70869
C	-3.27999	0.05938	-0.01540
N	-4.57292	-0.24169	-0.12888
N	-2.69567	0.81118	-0.94009
H	-5.14307	0.18599	-0.83579
H	-5.00490	-0.90834	0.48493
H	-3.23335	1.13687	-1.72388
H	-1.80522	1.26972	-0.75888

*14\_sg-g.mol2*

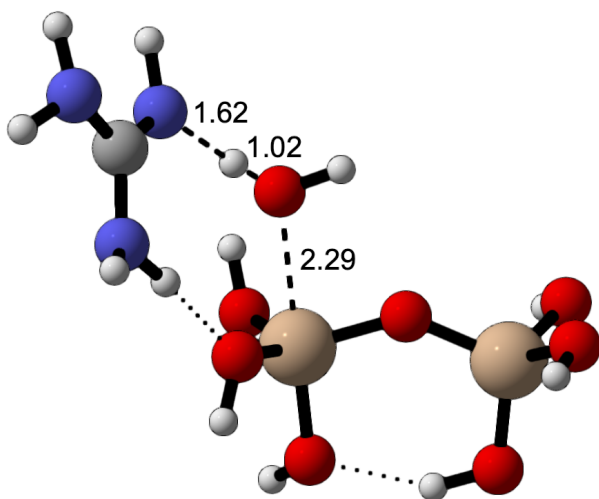
E = -1391.541978  
H = -1391.321182  
G = -1391.389865  
G(quasi-RRHO) = -1391.386910

Si	-0.62679	1.38346	-0.00377
O	0.84505	2.22816	0.03404
H	1.28109	2.17663	-0.81986
O	-1.14047	2.30971	1.36271
O	0.00290	0.43434	-1.42847
H	-0.26408	0.82130	-2.26504
H	-1.71895	1.79791	1.92898
O	-0.84677	-0.08498	0.80637
O	-1.92504	1.85718	-0.98440
Si	-1.60568	-1.37278	0.16955
O	-2.95419	-0.85518	-0.61243
O	-0.62212	-2.25792	-0.79502
H	1.71831	-0.11462	-1.20535
O	-2.04764	-2.45412	1.31272
H	-2.76853	-2.20125	1.89187
H	-2.88993	0.06343	-0.91526
H	-2.46707	2.50034	-0.52077
H	3.00946	-1.12307	-1.78937
H	-0.15157	-1.65208	-1.38314
N	2.65663	-0.51135	-1.07450
C	3.32232	-0.39472	0.06642
N	4.43058	-1.10623	0.26655
N	2.88925	0.43236	1.00911
H	4.98845	-0.97407	1.09060
H	4.72012	-1.80784	-0.39034
H	2.14505	1.09921	0.80967
H	3.38943	0.51204	1.87630



TS3-cg, water cleavage from IM2, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as catalyst

00\_cg-k.mol2



E = -1391.535144  
H = -1391.317180  
G = -1391.389865  
G(quasi-RRHO) = -1391.384873

Si	0.38748	1.06808	0.11085
O	0.22846	2.01070	1.44208
H	-0.33245	1.61068	2.11161
O	-0.87198	0.95644	-0.95366
O	-1.01888	-0.23210	1.37415
H	-0.60469	-1.09861	1.39974
H	-0.70621	1.48947	-1.73670
O	1.44123	2.05279	-0.76720
H	1.50944	2.95523	-0.44914
Si	2.77632	-0.82734	-0.12621
O	3.58319	-1.27633	1.21864
H	3.84319	-0.58294	1.82780
O	3.55683	0.34048	-0.95207
O	2.71990	-2.23397	-0.94930
H	2.29285	-2.22572	-1.80777
O	1.27414	-0.30446	0.22861
H	3.01063	1.14267	-1.04000
N	-3.72287	0.10830	-1.19157
H	-4.06627	-0.12855	-2.10609
C	-4.26677	-0.52698	-0.12056
N	-5.52336	-1.03626	-0.31433

N	-3.59990	-0.62763	0.98218
H	-6.03191	-1.30290	0.51143
H	-6.09243	-0.60245	-1.02222
H	-4.14446	-1.04817	1.72341
H	-2.01297	-0.37009	1.18936
H	-2.73747	0.33382	-1.12709

*01\_cg-k.mol2*

E = -1391.537486  
H = -1391.320866  
G = -1391.386577  
G(quasi-RRHO) = -1391.384137

Si	0.95276	-1.38495	-0.13445
O	1.50358	-2.68566	-1.00832
H	2.37823	-2.97176	-0.73897
O	-0.16974	-1.62858	1.09660
O	1.17494	0.15288	-0.71380
H	0.23067	-1.60057	1.96853
O	-0.54065	-1.44157	-1.30373
H	-0.97839	-2.29829	-1.31484
H	-1.28519	-0.65321	-1.10592
O	2.32323	-1.25575	0.93560
H	2.50143	-2.01353	1.49589
Si	1.27707	1.60410	0.00510
O	2.15613	2.66112	-0.88319
H	1.68448	3.14415	-1.56411
O	2.06961	1.44170	1.42302
H	2.33773	0.51296	1.55029
O	-0.22606	2.21142	0.19548
H	-0.94179	1.61889	-0.10615
N	-2.23914	0.36982	-0.84555
C	-3.16683	0.17320	0.06778
N	-4.41770	0.67320	-0.03391
N	-2.87637	-0.56420	1.14542
H	-5.01057	0.69935	0.77731
H	-4.59973	1.36933	-0.73472
H	-3.58671	-0.80846	1.81046
H	-1.96275	-1.00389	1.20648
H	-2.57990	0.90149	-1.63512

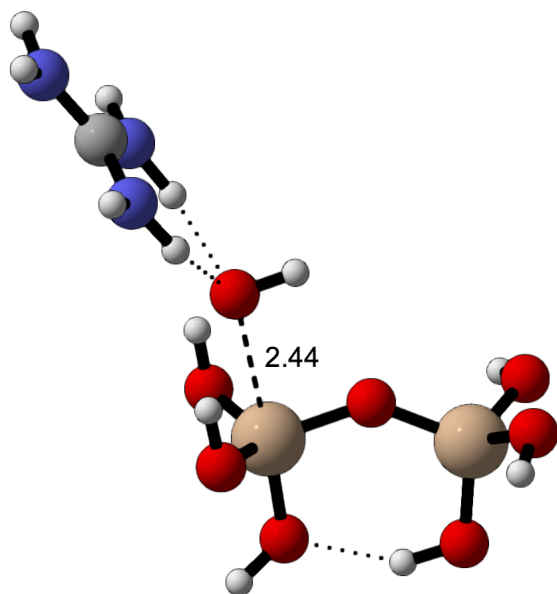
*02\_cg-k.mol2*

E = -1391.534954

H = -1391.316565  
G = -1391.385276  
G(quasi-RRHO) = -1391.381891

Si	0.05572	0.41480	-0.13258
O	-0.73160	1.13864	1.14894
H	-0.51752	2.07402	1.20243
O	-0.82979	0.08653	-1.48188
O	1.43685	-0.39976	0.24008
H	-1.65438	-0.40517	-1.34242
O	-0.84308	-1.28800	0.63975
H	-0.79120	-1.30044	1.60029
H	-3.67539	-1.92383	-0.85116
H	-1.83041	-1.31296	0.36298
O	0.82129	1.81103	-0.76659
H	0.33269	2.21738	-1.48457
Si	3.04726	-0.28579	0.06245
O	3.81869	-0.42941	1.49545
H	3.77370	0.32144	2.08999
O	3.40559	1.12483	-0.67101
H	2.58305	1.62016	-0.85952
O	3.63678	-1.57909	-0.74333
H	3.27198	-1.75612	-1.61222
N	-3.25001	-1.16160	-0.34130
C	-4.12210	-0.27408	0.04590
N	-3.73610	0.75786	0.82914
N	-5.43566	-0.30454	-0.30373
H	-2.74447	0.91865	0.95918
H	-4.33487	1.56076	0.90617
H	-5.79511	-1.16061	-0.68838
H	-6.09268	0.22486	0.24355

TS3-sg, water cleavage from IM2, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as spectator  
*00\_sg-k.mol2*



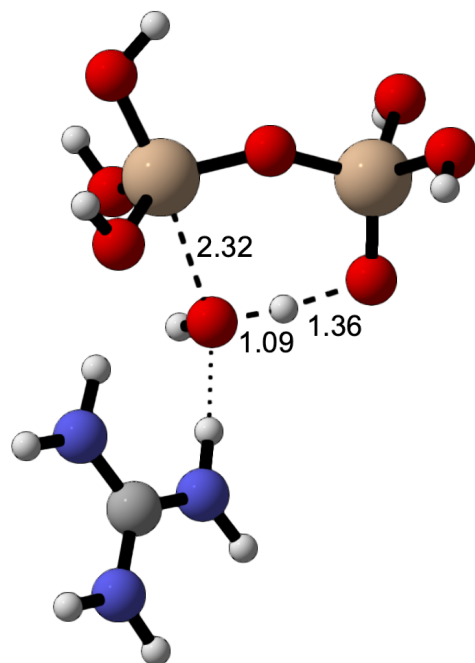
E = -1391.532232  
H = -1391.314613  
G = -1391.389358  
G(quasi-RRHO) = -1391.384066

Si	0.62484	1.18881	0.02657
O	-0.12920	1.64201	1.41121
H	-0.92346	1.09087	1.46419
O	-0.05774	1.57119	-1.41636
O	-1.41866	-0.13996	0.00333
H	-1.01614	-1.01186	0.01357
H	-0.86164	1.03358	-1.47156
O	1.97311	2.18761	0.02201
H	1.85670	3.05107	-0.37771
Si	2.83530	-0.92201	0.00217
O	3.15741	-1.87471	1.28839
H	3.11442	-1.46849	2.15586
O	3.91812	0.28652	-0.16438
O	2.94741	-1.99754	-1.22093
H	2.93861	-1.64802	-2.11367
O	1.34472	-0.28439	0.11570
H	3.48775	1.16001	-0.14577
H	-4.35319	-0.47706	-2.03022
H	-2.87846	-0.32092	-1.02748
N	-3.89977	-0.43149	-1.13644
C	-4.58787	-0.51806	-0.00747
N	-5.91475	-0.65250	-0.01410

N	-3.90916	-0.45511	1.12900
H	-6.41454	-0.76157	-0.87766
H	-6.42106	-0.78414	0.84251
H	-2.88815	-0.33830	1.03129
H	-4.37121	-0.50418	2.01814

TS4-sg, water cleavage from IM2, C(NH<sub>2</sub>)<sub>3</sub><sup>+</sup> acting as spectator

*00\_sg-m.mol2*



E = -1391.533531  
H = -1391.316900  
G = -1391.390566  
G(quasi-RRHO) = -1391.385638

Si	-0.62762	1.46555	0.02600
O	-0.63674	1.88723	1.62571
H	-1.07203	2.73274	1.76051
O	-1.30943	2.85025	-0.64470
O	0.48282	-0.29088	1.05166
H	0.48682	0.02246	1.96112
H	-2.13580	2.69616	-1.10408
O	-1.66429	0.32765	-0.48967
O	0.84955	1.53251	-0.73457
Si	-2.27363	-1.17361	-0.15052
O	-2.65235	-1.84818	-1.61032

O	-1.26212	-1.96711	0.76695
H	-0.24867	-1.09209	0.99239
O	-3.78918	-0.98380	0.48087
H	-3.82872	-0.99936	1.43823
H	-1.91731	-1.97381	-2.21245
H	0.84689	2.23997	-1.38630
N	2.99056	-1.38641	0.47340
H	3.25217	-2.30175	0.79302
C	3.88947	-0.60153	-0.09874
N	5.14770	-1.01501	-0.25114
N	3.52897	0.60240	-0.52096
H	5.82490	-0.44935	-0.72969
H	5.44923	-1.89726	0.12033
H	4.20430	1.21032	-0.94789
H	2.54972	0.89048	-0.51522
H	2.05247	-1.02476	0.68918

*01\_sg-m.mol2*

E = -1391.533612

H = -1391.316847

G = -1391.388999

G(quasi-RRHO) = -1391.384797

Si	0.64905	1.47347	-0.08758
O	0.32478	2.05463	-1.60097
H	0.67728	2.94071	-1.71523
O	1.31602	2.85503	0.60357
O	-0.46883	-0.27582	-1.11520
H	-0.37109	-0.01733	-2.03648
H	2.19488	2.72724	0.96269
O	1.87660	0.42231	0.07826
O	-0.65696	1.28130	0.92398
Si	2.24898	-1.18962	0.13567
O	2.44785	-1.62648	1.71559
O	1.12210	-2.03989	-0.56642
H	0.18616	-1.11967	-0.93559
O	3.77682	-1.31844	-0.48886
H	3.88168	-1.04799	-1.40272
H	3.18516	-1.22276	2.17681
H	-0.59362	1.90095	1.65704
H	-2.37223	0.64109	0.82467
N	-3.35323	0.36988	0.89928
H	-3.91409	0.79917	1.61286
C	-3.86799	-0.57619	0.12673

N	-5.14124	-0.94258	0.27766
N	-3.10967	-1.15501	-0.79010
H	-5.55210	-1.63528	-0.32110
H	-5.73344	-0.49265	0.95169
H	-3.49523	-1.86200	-1.38995
H	-2.13601	-0.85527	-0.92581

*02\_sg-m.mol2*

E = -1391.533630  
H = -1391.316552  
G = -1391.387299  
G(quasi-RRHO) = -1391.383612

Si	-1.09361	-1.44173	-0.15141
O	0.31155	-2.30918	-0.25817
H	0.75080	-2.19099	0.59621
O	-1.89557	-2.16506	-1.42791
O	0.25258	-0.63892	1.64649
H	-0.03389	-1.04730	2.46618
H	-2.42746	-1.56525	-1.95230
O	-1.05197	0.11767	-0.64770
O	-2.08200	-1.76315	1.13163
Si	-1.23291	1.63425	-0.07154
O	-2.80770	2.09121	-0.15804
O	-0.61711	1.71174	1.41477
H	1.82879	-0.22872	1.35202
O	-0.43903	2.69302	-1.03459
H	-0.85097	2.91868	-1.87053
H	-3.44925	1.54285	0.29766
H	-2.86523	-2.24817	0.85912
H	3.32419	0.58297	1.80738
H	-0.22854	0.79023	1.64808
N	2.79257	0.10021	1.10439
C	3.27769	0.03532	-0.12138
N	4.46658	0.57494	-0.40690
N	2.59504	-0.57627	-1.08618
H	4.81494	0.58033	-1.34848
H	4.93227	1.16141	0.26186
H	1.76535	-1.12186	-0.87811
H	2.99881	-0.67214	-2.00062

*03\_sg-m.mol2*

E = -1391.534164

H = -1391.316856  
G = -1391.386386  
G(quasi-RRHO) = -1391.383096

Si	-0.83364	-1.42973	-0.28578
O	0.25958	-1.62008	0.96251
H	-0.16220	-1.53753	1.82189
O	0.21320	-1.87512	-1.53700
O	-2.16579	-1.10011	1.34427
H	-2.97832	-1.57200	1.14449
H	0.61999	-1.13006	-1.98017
O	-1.11624	0.12198	-0.74834
O	-1.96202	-2.61195	-0.57807
Si	-1.45660	1.54676	-0.00230
O	-2.07076	2.58502	-1.13094
O	-2.37516	1.32735	1.26281
H	-2.36088	-0.03737	1.39344
O	0.06655	2.14961	0.30235
H	0.10571	2.96695	0.80333
H	-3.02788	2.60225	-1.18612
H	-1.73871	-3.10515	-1.37116
H	1.95662	-0.95728	0.84248
H	3.57365	-1.46774	1.18300
C	3.47138	0.25179	0.13556
N	2.95940	-0.76054	0.81959
N	4.78450	0.30396	-0.08901
N	2.68982	1.21470	-0.33484
H	5.38617	-0.45354	0.17900
H	5.20834	1.12193	-0.48781
H	1.72490	1.34461	-0.03524
H	3.09673	1.95537	-0.87821

*04\_sg-m.mol2*

E = -1391.534164  
H = -1391.316856  
G = -1391.386382  
G(quasi-RRHO) = -1391.383094

Si	-0.83353	-1.42974	-0.28580
O	0.25972	-1.61988	0.96250
H	-0.16209	-1.53746	1.82188
O	0.21340	-1.87497	-1.53700
O	-2.16576	-1.10030	1.34422
H	-2.97826	-1.57224	1.14440



H	0.62020	-1.12986	-1.98008
O	-1.11639	0.12192	-0.74836
O	-1.96172	-2.61214	-0.57813
Si	-1.45677	1.54667	-0.00228
O	-2.07101	2.58497	-1.13084
O	-2.37531	1.32718	1.26283
H	-2.36092	-0.03756	1.39342
O	0.06638	2.14953	0.30233
H	0.10552	2.96723	0.80273
H	-3.02814	2.60234	-1.18583
H	-1.73831	-3.10530	-1.37121
N	2.68977	1.21475	-0.33486
H	3.09660	1.95539	-0.87833
C	3.47141	0.25191	0.13558
N	4.78451	0.30418	-0.08901
N	2.95952	-0.76041	0.81968
H	5.38626	-0.45321	0.17912
H	5.20828	1.12216	-0.48785
H	3.57383	-1.46758	1.18307
H	1.95676	-0.95723	0.84256
H	1.72479	1.34451	-0.03540

*05\_sg-m.mol2*

E = -1391.535143

H = -1391.316815

G = -1391.385124

G(quasi-RRHO) = -1391.381890

Si	0.62857	1.43717	-0.17860
O	-0.34873	1.49032	1.16188
H	0.17300	1.46086	1.96996
O	-0.63235	1.80791	-1.24945
O	2.14144	1.10597	1.48716
H	2.93106	1.60015	1.25426
H	-0.44803	1.56041	-2.15866
O	1.08203	-0.02001	-0.73522
O	1.68026	2.67644	-0.45996
Si	1.54994	-1.50409	-0.15885
O	2.35770	-2.26899	-1.38235
O	2.37617	-1.33312	1.17309
H	2.34756	0.07419	1.42824
O	0.17340	-2.42116	-0.08305
H	-0.60486	-1.98252	0.27045
H	3.31237	-2.21233	-1.31985

H	1.34613	3.31034	-1.09869
H	-1.68372	0.21784	1.18176
H	-2.60897	-1.05435	1.88929
C	-3.34177	-0.33952	0.14869
N	-2.38810	-0.51397	1.06970
N	-4.44910	-1.07229	0.19468
N	-3.16263	0.55252	-0.81034
H	-4.59312	-1.74622	0.92513
H	-5.14030	-1.01497	-0.53167
H	-2.27102	1.04360	-0.91626
H	-3.84931	0.65443	-1.53693

*06\_sg-m.mol2*

E = -1391.531982

H = -1391.314956

G = -1391.384093

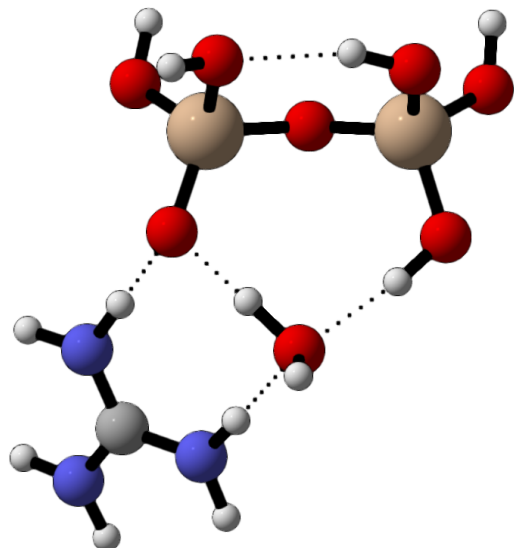
G(quasi-RRHO) = -1391.380792

Si	1.44006	-1.29074	-0.27211
O	2.79026	-2.02354	0.33522
H	2.84228	-1.91380	1.28727
O	1.68449	-1.85005	-1.85054
O	1.15416	-0.78843	1.79076
H	0.38443	-1.25821	2.12101
H	1.43329	-1.21118	-2.51828
O	1.44043	0.32131	-0.57865
O	-0.06597	-1.99383	-0.02060
Si	0.94759	1.73737	0.08873
O	-0.46299	2.05538	-0.73997
O	0.81369	1.60503	1.65806
H	0.96754	0.29418	1.85044
O	1.95860	2.94377	-0.41050
H	2.64902	3.17668	0.21273
H	-0.76969	2.96370	-0.68721
H	-0.29459	-2.53586	-0.78151
H	-1.70757	-1.18164	0.40730
N	-2.67741	-1.03243	0.68284
H	-3.07468	-1.70428	1.31597
C	-3.48389	-0.23981	-0.01182
N	-4.80335	-0.34938	0.12445
N	-2.97753	0.66173	-0.84352
H	-5.42350	0.32046	-0.29374
H	-5.21082	-1.10390	0.64687
H	-3.60262	1.24814	-1.36862

H -2.01025 0.97503 -0.77065

PC-g, product complexes

00\_cg-p3.mol2



E = -1391.562715

H = -1391.343663

G = -1391.415260

G(quasi-RRHO) = -1391.411495

Si	0.54841	1.45556	0.09032
O	-0.73185	0.94167	0.85069
H	-0.70889	-0.52331	1.28486
O	0.14483	2.65439	-0.96460
O	-0.76337	-1.53330	1.42075
H	-0.78128	-1.69591	2.36773
H	0.86715	3.05756	-1.44991
O	1.34078	0.29264	-0.77247
O	1.76647	1.99169	1.09834
Si	2.37080	-0.89734	-0.34681
O	3.39813	-0.29304	0.77824
O	1.56640	-2.21406	0.15708
H	-2.44597	-1.52582	0.62027
O	3.23311	-1.43723	-1.62508
H	3.96950	-0.89159	-1.90700
H	3.09996	0.56123	1.12672
H	1.48544	2.46130	1.88614
H	-3.87602	-2.35454	0.09206

H	0.73104	-2.05108	0.64439
N	-3.35771	-1.49772	0.16334
C	-3.90833	-0.35724	-0.23695
N	-5.14472	-0.37225	-0.74727
N	-3.25068	0.78214	-0.12152
H	-5.53955	0.45668	-1.15293
H	-5.62290	-1.24006	-0.90909
H	-2.27418	0.83753	0.24380
H	-3.68741	1.62911	-0.43992

*01\_sg-p3.mol2*

E = -1391.552095  
H = -1391.333872  
G = -1391.410750  
G(quasi-RRHO) = -1391.405031

Si	0.24121	-1.28295	-0.37174
O	-0.57159	-0.16939	-1.23008
H	-0.05034	0.52685	-1.73240
O	-0.80774	-1.58564	0.86520
O	0.82306	1.69230	-2.36886
H	1.24378	1.43934	-3.19395
H	-0.64938	-2.36692	1.39955
O	1.68746	-0.80123	0.13446
O	0.54206	-2.66232	-1.19984
Si	2.51602	0.56849	0.57007
O	4.03060	0.03431	0.98754
O	2.52616	1.69163	-0.52504
H	1.56247	1.72028	-1.64571
O	1.79490	0.95195	2.01303
H	2.03355	1.80790	2.37290
H	4.69135	0.15407	0.30355
H	-0.20866	-3.10509	-1.60043
H	-2.32459	0.27559	-0.97862
H	-3.78638	0.98488	-1.60273
C	-3.85982	0.50318	0.36009
N	-3.29558	0.55891	-0.83704
N	-5.06686	1.03176	0.55561
N	-3.21998	-0.07790	1.36570
H	-5.54499	1.51464	-0.18316
H	-5.54592	0.91785	1.43042
H	-2.35194	-0.58533	1.21177
H	-3.63355	-0.10315	2.28045

02\_sg-p2.mol2

E = -1391.548748  
H = -1391.330077  
G = -1391.407429  
G(quasi-RRHO) = -1391.401585

Si	-0.44815	0.21763	0.48614
O	0.17933	1.63389	0.66099
H	1.45806	2.06290	-0.05039
O	0.65992	-0.83438	-0.17923
O	2.33046	2.35183	-0.49212
H	2.12480	2.53121	-1.41231
H	0.32126	-1.69994	-0.41968
O	-1.01815	-0.47146	1.90151
H	-0.59950	-0.15804	2.70555
Si	-3.36628	-0.18444	-0.33980
O	-4.26957	1.11210	-0.75372
H	-4.20068	1.88923	-0.19644
O	-3.67013	-0.66443	1.19129
O	-3.88155	-1.28096	-1.43534
H	-3.49923	-2.15891	-1.38862
O	-1.77633	0.10037	-0.49218
H	-2.86310	-0.68768	1.73362
H	5.40633	1.30448	0.00795
N	4.55532	0.78535	-0.11795
H	3.67820	1.31390	-0.25903
C	4.60897	-0.53317	-0.18787
N	3.49832	-1.24692	-0.32043
N	5.78649	-1.15961	-0.11440
H	3.55434	-2.24840	-0.37111
H	2.56706	-0.84247	-0.25730
H	5.84352	-2.15887	-0.19268
H	6.64441	-0.64064	-0.16136

03\_cg-p2.mol2

E = -1391.552260  
H = -1391.333237  
G = -1391.407358  
G(quasi-RRHO) = -1391.402422

Si	-0.18715	-0.30318	-0.08382
O	0.69143	-0.27631	1.27207
H	1.64299	0.00505	1.19208
O	0.62911	0.36982	-1.32311

O	-1.61464	0.43693	0.17589
H	2.63152	-0.44531	-1.24161
O	2.09744	2.49163	-0.57263
H	1.68455	3.18537	-0.05117
O	-0.62365	-1.82668	-0.52858
H	0.04761	-2.51101	-0.55566
Si	-3.20657	0.09030	0.12230
O	-3.93502	0.41242	1.54350
H	-3.70667	-0.14082	2.29263
O	-3.38631	-1.47194	-0.31050
H	-2.55033	-1.93545	-0.46711
O	-3.99511	1.10263	-0.88163
H	-3.74504	1.09342	-1.80726
N	3.53128	-0.78238	-0.93125
C	4.04821	-0.25176	0.20130
N	5.34990	-0.54207	0.45769
N	3.30149	0.49895	0.96321
H	5.69976	-0.35017	1.37991
H	5.77455	-1.32563	-0.00808
H	3.78861	0.77750	1.80530
H	2.56988	1.90157	0.06459
H	4.15168	-1.13406	-1.63873
H	1.04880	1.24092	-1.13885

04\_sg-p3.mol2

E = -1391.552307

H = -1391.333425

G = -1391.407130

G(quasi-RRHO) = -1391.402949

Si	1.18968	1.51461	-0.28800
O	-0.05473	1.48662	0.76316
H	0.08400	0.99085	1.61822
O	0.48139	2.00974	-1.67437
O	0.27928	-0.02870	2.87558
H	0.97862	0.22884	3.48091
H	1.06015	2.28741	-2.38671
O	1.90853	0.06590	-0.39483
O	2.34119	2.61606	0.09182
Si	1.38086	-1.48705	-0.14741
O	2.56624	-2.34737	-0.91668
O	1.09072	-1.87077	1.34073
H	0.63746	-0.80957	2.31434
O	-0.01919	-1.63444	-1.05741

H	0.09454	-1.53547	-2.00577
H	2.61132	-3.27637	-0.68418
H	3.12369	2.28783	0.53861
H	-1.74012	-1.21330	-0.54652
N	-2.74907	-1.20157	-0.39263
H	-3.25007	-2.05327	-0.57449
C	-3.42682	-0.08866	-0.15166
N	-4.75970	-0.11464	-0.15130
N	-2.79262	1.04959	0.08962
H	-5.29324	0.70319	0.08104
H	-5.26078	-0.94870	-0.39754
H	-3.32485	1.88016	0.27963
H	-1.78519	1.09447	0.24447

*05\_sg-p2.mol2*

E = -1391.546214  
H = -1391.328587  
G = -1391.405960  
G(quasi-RRHO) = -1391.399505

Si	0.58921	0.05974	0.13466
O	-0.25853	-1.28554	0.46160
H	-1.10008	-1.26675	-0.08967
O	-0.26752	0.93257	-0.93282
O	-2.28092	-0.72580	-1.09709
H	-2.27430	-1.24269	-1.90617
H	-1.10543	0.42152	-1.15395
O	0.94788	0.91921	1.49955
H	0.22027	1.25382	2.02721
Si	3.63915	-0.02814	-0.06814
O	4.46285	-1.43117	0.03733
H	4.15743	-2.07527	0.67862
O	3.71227	0.83849	1.31210
O	4.42836	0.71663	-1.28493
H	4.21745	1.63773	-1.44760
O	2.07644	-0.29583	-0.43792
H	2.84078	1.05296	1.67884
H	-4.92782	1.69383	-1.13240
H	-3.60434	0.49725	-1.14032
N	-4.50408	0.85327	-0.78561
C	-5.12469	0.07699	0.09109
N	-6.32357	0.40553	0.57690
N	-4.51609	-1.04057	0.46095

H	-6.73078	1.29946	0.36903
H	-6.74104	-0.13375	1.31364
H	-3.61520	-1.23341	-0.00178
H	-4.94612	-1.68510	1.09855

*06\_sg-p2.mol2*

E = -1391.546222  
H = -1391.328497  
G = -1391.405517  
G(quasi-RRHO) = -1391.399218

Si	0.58886	-0.08710	-0.11719
O	-0.26348	1.18392	-0.65872
H	-1.10297	1.25493	-0.10813
O	-0.26393	-0.77482	1.08096
O	-2.27968	0.88443	0.97476
H	-2.27672	1.52394	1.69088
H	-1.10198	-0.23493	1.21745
O	0.94764	-1.15887	-1.32246
H	0.21970	-1.58157	-1.78208
Si	3.63881	0.04379	0.05783
O	4.44827	1.41252	-0.30214
H	4.12460	1.93858	-1.03565
O	3.71117	-1.05569	-1.14519
O	4.44252	-0.46785	1.38085
H	4.24731	-1.35068	1.70025
O	2.07612	0.36195	0.38552
H	2.83964	-1.32938	-1.46996
H	-4.91933	-1.51180	1.35900
H	-3.60134	-0.31944	1.19617
N	-4.50114	-0.72444	0.89885
C	-5.12351	-0.08621	-0.08182
N	-6.31894	-0.48821	-0.51774
N	-4.52130	0.97125	-0.60647
H	-6.72412	-1.34274	-0.18082
H	-6.74100	-0.05844	-1.32079
H	-3.61877	1.22922	-0.18045
H	-4.95086	1.51094	-1.33510

*07\_cg-p2.mol2*

E = -1391.546303  
H = -1391.327963  
G = -1391.405486



G(quasi-RRHO) = -1391.399681

Si	0.24747	0.90116	-0.06724
O	-0.66800	1.06807	1.28411
H	-0.22128	1.10492	2.13279
O	-0.75051	0.57085	-1.27710
O	1.38573	-0.23077	0.20059
H	-1.63656	0.12523	-1.10187
O	-1.59228	-2.68913	0.33997
H	-2.22350	-3.38639	0.53282
H	-3.56400	-0.98800	-1.67350
H	-2.11606	-1.97014	-0.06784
O	1.12765	2.24861	-0.40900
H	0.67350	3.00682	-0.78236
Si	2.99724	-0.41720	0.02121
O	3.68991	-0.93607	1.40083
H	3.76873	-0.30672	2.11994
O	3.63270	0.99921	-0.47835
H	2.98348	1.71176	-0.57146
O	3.33573	-1.64229	-0.99689
H	2.98707	-1.58947	-1.88864
N	-3.13037	-0.57529	-0.85740
C	-4.01472	-0.05176	-0.05628
N	-3.62042	0.51356	1.10713
N	-5.35059	-0.02454	-0.31486
H	-2.63311	0.70038	1.22615
H	-4.25300	1.13040	1.58528
H	-5.69495	-0.63278	-1.03712
H	-5.98575	0.12526	0.45065

*08\_sg-p1.mol2*

E = -1391.547266

H = -1391.329656

G = -1391.405174

G(quasi-RRHO) = -1391.399472

Si	-0.71515	1.04525	-0.02302
O	-0.10420	-0.19953	-0.89224
H	0.68769	-0.58955	-0.36748
O	-0.79851	2.45337	-0.85240
O	0.20158	1.19023	1.31269
H	0.88577	0.46331	1.30226
H	0.03279	2.89718	-1.03132
O	1.80086	-0.82539	0.67917

H	1.60945	-1.61929	1.18427
Si	-3.29088	-0.51202	0.01002
O	-2.48038	-1.61393	-0.87764
H	-1.55277	-1.35724	-1.03676
O	-4.65042	-0.01471	-0.74027
O	-3.89830	-1.13400	1.38990
H	-3.27383	-1.46430	2.03823
O	-2.28321	0.73235	0.32134
H	-4.56925	0.27086	-1.65199
H	4.90282	0.71070	1.66116
H	3.35976	-0.05284	1.20378
N	4.34279	0.18492	1.01574
C	4.85972	-0.32382	-0.09345
N	4.06214	-1.03737	-0.87476
N	6.14191	-0.13252	-0.40921
H	4.40748	-1.48197	-1.70523
H	3.10129	-1.17445	-0.53103
H	6.49477	-0.42866	-1.30134
H	6.71282	0.49180	0.13132

*09\_sg-p1.mol2*

E = -1391.547262

H = -1391.329572

G = -1391.405049

G(quasi-RRHO) = -1391.399462

Si	-0.75833	1.08341	-0.02140
O	-0.12519	-0.11928	-0.93342
H	0.68283	-0.50133	-0.42885
O	-0.89856	2.50852	-0.81298
O	0.17697	1.22178	1.30185
H	0.87704	0.51023	1.26581
H	-0.08383	2.97945	-0.99871
O	1.80715	-0.74518	0.60750
H	1.61787	-1.55954	1.08016
Si	-3.28186	-0.55704	0.02146
O	-2.45023	-1.61633	-0.89793
H	-1.53592	-1.32372	-1.07131
O	-4.66817	-0.09163	-0.69998
O	-3.84697	-1.22245	1.39905
H	-3.20174	-1.53369	2.03640
O	-2.31003	0.71356	0.34044
H	-4.61019	0.20474	-1.61007
H	4.98476	0.50305	1.76520

H	3.39707	-0.07065	1.20482
N	4.39443	0.12402	1.04771
C	4.90166	-0.34105	-0.08640
N	4.07634	-0.94636	-0.92746
N	6.19693	-0.20242	-0.36869
H	4.38987	-1.27863	-1.82064
H	3.10146	-1.04384	-0.60866
H	6.57507	-0.54080	-1.23477
H	6.80484	0.31321	0.24105

*10\_cg-p1.mol2*

E = -1391.552283  
H = -1391.333156  
G = -1391.404898  
G(quasi-RRHO) = -1391.401173

Si	-0.28803	0.97910	0.11378
O	0.61281	0.86504	1.48417
H	1.33582	1.50982	1.49381
O	0.24540	-0.09731	-0.99077
O	-0.27071	2.51785	-0.43010
H	0.62711	2.87655	-0.47539
H	1.24144	-0.19077	-1.04961
O	2.53680	2.34085	0.07930
H	3.32002	2.89257	0.14657
Si	-2.85845	-0.58873	-0.03883
O	-3.52494	-1.30659	1.26510
H	-2.93771	-1.61724	1.95714
O	-2.06049	-1.63288	-0.99604
O	-4.09967	0.01520	-0.90279
H	-4.80431	0.45852	-0.42653
O	-1.82711	0.58518	0.44290
H	-1.15068	-1.35523	-1.19592
H	2.81549	1.47990	-0.31571
N	2.94769	-0.25104	-0.93644
C	3.41629	-1.11604	-0.07665
H	3.48234	-0.25278	-1.79571
N	2.76273	-1.32403	1.08710
H	3.23295	-1.78594	1.84484
H	2.01265	-0.69115	1.32816
N	4.55179	-1.83513	-0.26643
H	4.70479	-2.66028	0.28754
H	4.94087	-1.86026	-1.19243

*11\_cg-p1.mol2*

E = -1391.552284

H = -1391.333151

G = -1391.404874

G(quasi-RRHO) = -1391.401154

Si	-0.28863	0.98049	0.11327
O	0.61379	0.86784	1.48255
H	1.33899	1.51050	1.48742
O	0.24533	-0.09414	-0.99280
O	-0.27480	2.51941	-0.43058
H	0.62182	2.88047	-0.47717
H	1.24127	-0.18903	-1.05020
O	2.53675	2.34070	0.08001
H	3.31928	2.89245	0.15446
Si	-2.85737	-0.58998	-0.03843
O	-3.52122	-1.31072	1.26538
H	-2.93262	-1.61888	1.95739
O	-2.05957	-1.63114	-0.99889
O	-4.10076	0.01391	-0.89940
H	-4.80668	0.45225	-0.42038
O	-1.82664	0.58410	0.44414
H	-1.14982	-1.35295	-1.19827
H	2.81820	1.48065	-0.31467
N	2.94753	-0.25175	-0.93634
C	3.41576	-1.11672	-0.07636
H	3.48151	-0.25464	-1.79601
N	2.76318	-1.32299	1.08803
H	3.23175	-1.78783	1.84494
H	2.01258	-0.69077	1.32892
N	4.55076	-1.83697	-0.26641
H	4.70200	-2.66292	0.28692
H	4.93787	-1.86387	-1.19322

*12\_cg-p2.mol2*

E = -1391.547278

H = -1391.328801

G = -1391.403954

G(quasi-RRHO) = -1391.399046

Si	-0.21109	-0.52107	0.07360
O	0.67983	-0.06714	1.38278
H	0.28863	-0.18660	2.25217
O	0.74057	-0.37215	-1.20553

O	-1.54911	0.39534	-0.02774
H	1.68049	-0.01764	-1.11398
O	1.92549	2.56051	0.60164
H	1.38145	1.95591	1.11878
H	3.67961	0.83300	-1.84984
H	2.41279	1.96280	0.00311
O	-0.80898	-2.04347	0.24400
H	-0.20867	-2.78644	0.15264
Si	-3.16843	0.21175	-0.12521
O	-3.93358	1.05069	1.04176
H	-3.90486	0.69712	1.93256
O	-3.51835	-1.37884	-0.04864
H	-2.74379	-1.95118	0.04993
O	-3.74937	0.91591	-1.47337
H	-3.39006	0.63043	-2.31533
N	3.24912	0.51823	-0.98996
C	4.09911	-0.09774	-0.21929
N	3.71150	-0.51924	1.00673
N	5.38795	-0.36667	-0.56250
H	2.72796	-0.46855	1.22962
H	4.24912	-1.22570	1.47653
H	5.76083	0.10500	-1.36786
H	6.05309	-0.54440	0.17101

*13\_sg-p1.mol2*

E = -1391.548323  
H = -1391.330529  
G = -1391.403011  
G(quasi-RRHO) = -1391.398933

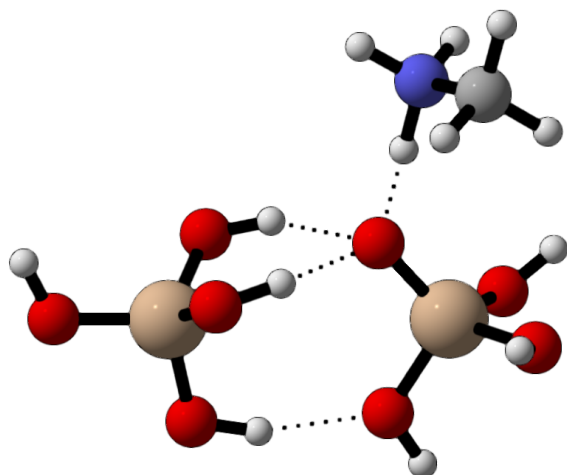
Si	-0.52758	0.73161	0.56917
O	-1.14752	0.20597	2.02981
H	-0.53860	0.16932	2.76943
O	0.36793	-0.51899	-0.08254
O	0.29876	2.05137	0.61581
H	1.51493	2.22431	-0.30386
H	-0.17036	-1.24946	-0.40993
O	2.34524	2.33186	-0.88324
H	2.03429	2.43348	-1.78567
Si	-3.06791	-0.38850	-0.38808
O	-3.72153	-0.61986	1.09164
H	-3.07570	-0.45610	1.79451
O	-2.28079	-1.71475	-0.95081
O	-4.26248	-0.04086	-1.43737

H	-4.93938	0.57667	-1.15325
O	-1.92597	0.76014	-0.32754
H	-2.73870	-2.55754	-0.93166
H	2.19718	-0.84145	0.03438
N	3.08862	-1.30305	0.21210
H	3.05214	-2.22961	0.59819
C	4.26296	-0.76893	-0.09355
N	5.37577	-1.48910	0.08153
N	4.34282	0.45632	-0.58310
H	6.27856	-1.05848	-0.00445
H	5.33620	-2.39538	0.51148
H	5.24457	0.82908	-0.82290
H	3.52446	1.07698	-0.69005

One  $\text{CH}_3\text{NH}_3^+$

RC-ma, Reactant Complexes

*00\_sma-c.mol2*



E = -1282.017323  
H = -1281.809968  
G = -1281.879023  
G(quasi-RRHO) = -1281.875039

Si	-1.33742	-1.20584	0.02105
O	-0.03544	-2.17015	-0.35121
H	-0.22918	-3.09793	-0.50390
O	-0.80216	0.27318	0.22519
O	-2.49595	-1.33999	-1.14783
H	-2.38895	-0.77340	-1.91421
H	0.50944	0.90815	-0.93085

O	-2.00750	-1.93656	1.33627
H	-2.90018	-1.67460	1.56803
Si	2.38169	0.33255	-0.02084
O	3.88834	0.95826	-0.02417
H	3.97355	1.89535	0.15965
O	2.63272	-1.25144	-0.33416
O	1.65537	0.56250	1.43012
H	0.68582	0.50333	1.30647
O	1.44948	1.03902	-1.16941
H	1.79705	-1.74685	-0.37698
N	-2.22753	2.38965	0.60061
H	-1.62872	1.48031	0.46942
H	-1.59744	3.17874	0.71543
C	-3.12591	2.59085	-0.55978
H	-2.51927	2.68568	-1.45347
H	-3.77364	1.72592	-0.64984
H	-3.72114	3.48633	-0.41986
H	-2.75796	2.30375	1.46324

*01\_sma-c.mol2*

E = -1282.016845  
H = -1281.809116  
G = -1281.877943  
G(quasi-RRHO) = -1281.873936

Si	-1.32750	-1.17597	0.00568
O	-0.23902	-1.85547	-1.04838
H	-0.41466	-2.75944	-1.32054
O	-0.77137	0.21222	0.52779
O	-2.77429	-0.86897	-0.73991
H	-3.32563	-1.62084	-0.96468
H	0.45932	1.15487	-0.50333
O	-1.54965	-2.36933	1.12190
H	-2.22222	-2.21951	1.78909
Si	2.36654	0.30294	0.01682
O	3.90181	0.85267	0.05644
H	4.06673	1.65259	0.55860
O	2.49614	-1.11553	-0.78514
O	1.78172	0.11031	1.53528
H	0.80280	0.12588	1.49650
O	1.37987	1.34541	-0.77477
H	1.62957	-1.51313	-0.97352
H	-1.89317	1.26198	0.53416
H	-3.11126	2.17408	1.32433

H	-3.45504	1.32883	-0.04363
C	-2.42921	3.10263	-0.40491
H	-2.05484	2.77154	-1.36726
H	-3.31787	3.70831	-0.54317
H	-1.66553	3.67827	0.10595
N	-2.75303	1.91039	0.41088

*02\_sma-c.mol2*

E = -1282.016803  
H = -1281.809113  
G = -1281.877932  
G(quasi-RRHO) = -1281.873963

Si	1.34995	-1.17047	0.00524
O	0.22784	-1.87484	-1.00378
H	0.42895	-2.76234	-1.31046
O	0.77106	0.21656	0.50597
O	1.75354	-2.28239	1.15438
H	1.03221	-2.70934	1.62041
H	-0.79749	0.15709	1.48811
O	2.77152	-0.88046	-0.78261
H	3.35687	-1.62573	-0.92948
Si	-2.36969	0.29247	0.01345
O	-3.90421	0.84473	0.04831
H	-4.06564	1.65611	0.53290
O	-2.50534	-1.14778	-0.74766
O	-1.38637	1.31099	-0.81232
H	-0.46423	1.12477	-0.54166
O	-1.77587	0.14109	1.53341
H	-1.63866	-1.54730	-0.93220
H	1.88349	1.26945	0.52934
H	3.08085	2.19708	1.33477
H	3.45159	1.37313	-0.03790
N	2.73374	1.93439	0.41673
C	2.39093	3.12722	-0.39054
H	1.61279	3.68248	0.12108
H	3.26787	3.75203	-0.51814
H	2.02873	2.79718	-1.35789

*03\_sma-c.mol2*

E = -1282.014354  
H = -1281.806449  
G = -1281.875427



G(quasi-RRHO) = -1281.871768

Si	-2.27727	-0.48928	0.02444
O	-1.99859	1.07549	-0.49767
H	-2.76181	1.54908	-0.83667
O	-0.94314	-1.09825	0.59243
O	-3.52846	-0.46493	1.10855
H	-3.26810	-0.41778	2.03024
H	0.33753	-0.34747	1.09820
O	-2.92101	-1.20720	-1.31632
H	-3.34060	-2.05858	-1.18086
Si	2.17936	-0.72720	0.01253
O	3.62548	-1.28019	0.53480
H	3.62813	-2.11179	1.01314
O	2.53778	0.45685	-1.07129
O	1.28424	-1.94281	-0.59767
H	0.34174	-1.82183	-0.31517
O	1.28301	0.01803	1.15849
H	3.20824	0.27562	-1.73293
H	-0.46631	1.97582	-0.39642
H	0.85314	1.74655	0.56057
H	1.07982	2.19797	-0.98300
C	0.41928	3.78463	0.21149
H	1.42026	4.12836	0.44617
H	0.01280	4.36252	-0.61066
H	-0.21869	3.88363	1.08232
N	0.47349	2.35784	-0.17887

*04\_sma-c.mol2*

E = -1282.009382

H = -1281.801506

G = -1281.871494

G(quasi-RRHO) = -1281.867033

Si	2.42525	0.50735	-0.08352
O	1.99606	-0.29837	1.31585
H	2.64745	-0.30265	2.02051
O	1.21918	0.45380	-1.09516
O	2.92048	2.03788	0.31468
H	2.23583	2.70866	0.28865
H	-0.24471	0.61400	-0.58991
O	3.81944	-0.25343	-0.53907
H	4.32502	0.17174	-1.23401
Si	-1.09811	-1.27693	0.00564

O	-2.58682	-1.93893	0.05307
H	-3.09843	-1.92936	-0.75788
O	-0.47016	-1.63253	1.46882
O	-0.20892	-1.88436	-1.22701
H	0.47927	-1.22044	-1.44972
O	-1.16352	0.35090	-0.23134
H	0.41187	-1.23748	1.59252
H	-2.28238	1.50078	0.12128
H	-3.12092	2.34071	1.30810
H	-2.78789	3.08373	-0.11319
N	-3.05441	2.19460	0.30361
C	-4.34105	1.70650	-0.25550
H	-4.57950	0.75630	0.20781
H	-5.12085	2.43027	-0.04975
H	-4.22360	1.57714	-1.32500

*05\_sma-c.mol2*

E = -1282.009405  
H = -1281.801192  
G = -1281.871403  
G(quasi-RRHO) = -1281.867025

Si	2.54807	0.48715	-0.05728
O	2.13346	-0.45892	1.25789
H	2.80235	-0.55327	1.93954
O	1.32675	0.55434	-1.04760
O	3.06806	1.96181	0.49315
H	2.39053	2.63801	0.54915
H	-0.19372	0.83305	-0.52243
O	3.92816	-0.23723	-0.60801
H	4.43025	0.25466	-1.26011
Si	-1.05222	-1.06753	-0.00593
O	-2.61935	-1.54713	-0.05920
H	-2.88621	-2.27128	0.51039
O	-0.43713	-1.54411	1.42728
O	-0.20485	-1.66031	-1.26923
H	0.51668	-1.01384	-1.45245
O	-1.09653	0.56854	-0.16443
H	0.49461	-1.27664	1.53611
H	-2.71978	1.17631	-0.47302
H	-4.05370	1.38450	-1.46127
H	-3.94840	0.11462	-0.41101
C	-4.42263	1.93083	0.51578
H	-4.16715	2.97198	0.35779

H	-5.49522	1.79414	0.44483
H	-4.06843	1.60506	1.48690
N	-3.75663	1.11244	-0.52756

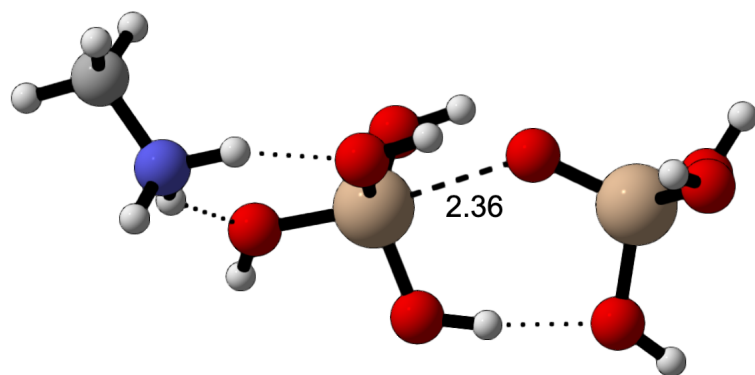
*06\_sma-c.mol2*

E = -1282.014006  
H = -1281.805485  
G = -1281.871396  
G(quasi-RRHO) = -1281.868848

Si	1.80352	-0.82029	-0.11051
O	1.07503	-1.38572	1.27727
H	1.64573	-1.58330	2.02318
O	0.75123	-0.72013	-1.26988
O	2.40249	0.71073	0.21813
H	3.18462	0.75015	0.77397
H	-0.40792	0.36245	-1.08805
O	3.09670	-1.82464	-0.29834
H	3.67038	-1.65682	-1.04836
Si	-2.07410	-0.43468	-0.00745
O	-3.67128	-0.12247	0.07028
H	-4.12170	0.07039	-0.75399
O	-1.64372	-0.61218	1.55796
O	-1.75985	-1.78037	-0.88582
H	-0.82923	-1.73303	-1.19038
O	-1.24924	0.79592	-0.72776
H	-0.72139	-0.90385	1.66079
H	-0.38956	2.10293	0.12341
H	0.18740	2.93194	1.45200
H	1.22289	2.06599	0.47878
N	0.39157	2.68483	0.48738
C	0.60473	3.89176	-0.34702
H	1.44338	4.45419	0.04683
H	0.81580	3.57539	-1.36225
H	-0.29242	4.49960	-0.32869

TS1-ma, Si-O bond association

*00\_sma-d.mol2*



E = -1282.004286  
H = -1281.796259  
G = -1281.864994  
G(quasi-RRHO) = -1281.860848

Si	0.85217	-0.70933	0.07705
O	0.04595	-1.43673	-1.14543
H	-0.89918	-1.23598	-1.23792
O	1.30786	0.87412	-0.11308
O	0.50601	-1.20556	1.60757
H	-0.32726	-0.78400	1.85572
H	0.51736	1.40556	0.06186
O	2.38720	-1.36540	-0.14214
H	2.40805	-2.29122	-0.38898
Si	-2.61009	0.40294	0.02522
O	-3.73377	-0.27168	1.03173
H	-4.10351	0.30617	1.70137
O	-2.61000	-0.62043	-1.28886
O	-3.27885	1.86155	-0.38342
H	-2.65327	2.53005	-0.66823
O	-1.12350	0.49622	0.53194
H	-3.44914	-0.97466	-1.58739
H	3.12037	1.28567	-0.48617
N	4.02188	0.80016	-0.59477
H	4.37754	0.97092	-1.53143
C	5.00292	1.19292	0.44423
H	5.91051	0.61622	0.30921
H	5.21624	2.25126	0.34994
H	4.57385	0.98634	1.41796
H	3.74158	-0.19224	-0.51623

*01\_sma-d.mol2*

E = -1282.004288

H = -1281.796217  
G = -1281.864122  
G(quasi-RRHO) = -1281.860442

Si	-0.85079	-0.79011	-0.02360
O	-0.22490	-0.85125	1.48565
H	0.70145	-0.58311	1.59538
O	-1.31219	0.68494	-0.62607
O	-0.30409	-1.89749	-1.11127
H	0.55842	-1.58637	-1.41615
H	-0.49965	1.12161	-0.92151
O	-2.40708	-1.35971	0.27290
H	-2.47122	-2.06202	0.92183
Si	2.58281	0.41263	-0.04430
O	3.83014	-0.57047	-0.50099
H	4.29733	-0.31758	-1.29899
O	2.39845	0.07361	1.57586
O	3.19675	1.93729	-0.24537
H	2.54154	2.62716	-0.36429
O	1.17958	0.18882	-0.71958
H	3.18716	-0.05460	2.10526
H	-4.62378	0.56735	-1.35617
H	-3.15102	1.09082	-0.77714
H	-3.79536	-0.23597	-0.14828
C	-4.76715	1.51609	0.49496
H	-4.97422	2.49337	0.07493
H	-5.69295	1.02507	0.77092
H	-4.12622	1.61390	1.36357
N	-4.06431	0.69182	-0.51681

*02\_sma-d.mol2*

E = -1282.000484  
H = -1281.792264  
G = -1281.859940  
G(quasi-RRHO) = -1281.855906

Si	2.43999	-0.34699	0.02399
O	1.32331	-1.29538	-0.77146
H	1.74057	-2.02997	-1.22910
O	2.88422	1.06779	-0.69122
O	2.35778	-0.39071	1.66723
H	1.60394	0.15569	1.92470
H	2.16564	1.69604	-0.54117
O	3.78072	-1.29535	-0.28029

H	4.62847	-0.86612	-0.15861
Si	-0.90834	0.95071	-0.00353
O	-1.99131	0.93534	1.27212
H	-1.57695	0.86208	2.13465
O	-1.24200	-0.42421	-0.87924
O	-1.45984	2.14745	-0.99818
H	-1.55428	3.01539	-0.60182
O	0.59428	1.01553	0.45457
H	-0.41478	-0.93509	-0.97385
H	-3.36624	-0.54902	1.04527
H	-3.43850	-2.20042	0.92839
H	-2.68186	-1.26120	-0.23105
C	-4.78763	-1.23937	-0.33786
H	-4.85607	-2.06987	-1.03067
H	-5.60870	-1.27398	0.36857
H	-4.80387	-0.30139	-0.88084
N	-3.50456	-1.33453	0.39972

*03\_sma-d.mol2*

E = -1282.003031

H = -1281.794117

G = -1281.857376

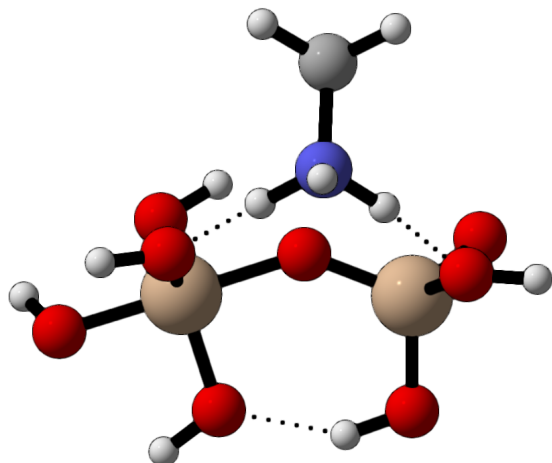
G(quasi-RRHO) = -1281.855474

Si	-1.50886	-0.92756	-0.01171
O	-0.99686	-0.13448	1.35245
H	-0.07451	-0.27965	1.60753
O	-1.53053	-0.03330	-1.42260
O	-1.34319	-2.56672	-0.10587
H	-0.43111	-2.76491	-0.34427
H	-0.66628	-0.13863	-1.83912
O	-3.14064	-0.81447	0.35662
H	-3.72096	-0.99948	-0.38288
Si	1.91257	-0.32938	-0.04950
O	3.37964	-0.96095	-0.43964
H	3.58445	-1.04465	-1.37296
O	1.84624	-0.36736	1.60775
O	1.90002	1.27184	-0.53004
H	2.73247	1.74752	-0.48245
O	0.63004	-1.05266	-0.59768
H	2.41665	0.22561	2.10072
H	-1.20644	1.92154	-0.81500
H	-0.90402	1.84787	0.77657
H	0.32271	2.19016	-0.26353

N	-0.67495	2.38225	-0.06879
C	-0.97003	3.82765	0.05526
H	-0.37788	4.23822	0.86496
H	-0.71467	4.31954	-0.87619
H	-2.02527	3.95730	0.26548

IM1-ma, three equatorial OH groups

[00\\_sma-e.mol2](#)



E = -1282.019407  
H = -1281.809771  
G = -1281.874634  
G(quasi-RRHO) = -1281.871893

Si	1.61070	-0.05363	0.07809
O	1.50810	-1.37692	-0.97763
H	2.38133	-1.59716	-1.30898
O	1.32490	1.48698	-0.58320
O	1.93719	-0.23847	1.71810
H	1.12705	-0.34049	2.22053
H	2.15532	1.89180	-0.84401
O	3.32685	0.09991	-0.25368
H	3.84158	0.07998	0.55337
Si	-1.40135	-1.05012	0.01809
O	-0.99037	-2.33072	-0.91069
H	-0.04613	-2.24901	-1.14864
O	-2.43937	-0.01974	-0.76059
O	-2.27944	-1.59154	1.29589
H	-1.98609	-2.41073	1.69941
O	-0.13197	-0.16414	0.39879

H	-3.35022	-0.29803	-0.87435
N	-1.18342	2.51530	-0.67314
H	-1.77795	1.68489	-0.81402
H	-1.33484	3.15858	-1.44469
H	-0.19095	2.17677	-0.69803
C	-1.47907	3.15354	0.63018
H	-0.82913	4.01114	0.76274
H	-2.51648	3.46783	0.65327
H	-1.29329	2.42570	1.41187

*01\_sma-e.mol2*

E = -1282.017108  
H = -1281.807790  
G = -1281.873130  
G(quasi-RRHO) = -1281.870179

Si	-0.48132	-0.76784	-0.11206
O	0.17659	-1.30247	1.35702
H	-0.51991	-1.58333	1.95407
O	-0.94234	0.85564	-0.17352
O	-0.71352	-1.82499	-1.39765
H	0.07577	-1.87449	-1.94023
H	-0.19884	1.44250	-0.34407
O	-2.12782	-1.17064	0.45027
H	-2.45891	-1.94623	-0.00593
Si	2.35182	0.41522	-0.04928
O	2.64897	-0.10374	1.47731
H	1.87523	-0.60774	1.78741
O	1.87843	1.99432	-0.09110
O	3.75163	0.34939	-0.89931
H	4.27729	-0.44674	-0.80075
O	1.15042	-0.40970	-0.70999
H	2.39657	2.63807	0.39514
N	-3.60834	1.02467	0.53124
H	-3.17287	0.05774	0.56420
H	-3.92423	1.29333	1.45827
H	-2.80091	1.59849	0.27696
C	-4.69762	1.11528	-0.46509
H	-5.06242	2.13492	-0.51685
H	-4.30737	0.81398	-1.43088
H	-5.50108	0.44936	-0.17102



02\_sma-e.mol2

E = -1282.016668

H = -1281.806913

G = -1281.870723

G(quasi-RRHO) = -1281.868166

Si	0.47502	-0.25344	-0.03016
O	-0.11850	-1.61317	0.78928
H	0.50866	-2.33678	0.82735
O	0.06940	-0.08776	-1.66706
O	1.42269	0.89742	0.75911
H	0.85857	1.57635	1.13472
H	0.74605	-0.41662	-2.26066
O	2.00990	-1.08259	-0.42845
H	1.92962	-1.89218	-0.93493
Si	-2.50146	0.27131	0.05516
O	-2.88106	-1.18283	0.72478
H	-2.05917	-1.66541	0.91161
O	-2.70725	0.28319	-1.57359
O	-3.59115	1.36657	0.60276
H	-3.85791	1.27460	1.51909
O	-0.97393	0.63356	0.40827
H	-1.84083	0.17166	-1.99685
N	4.09005	0.19294	0.62482
H	3.45401	-0.49079	0.14253
H	4.55856	-0.26610	1.40050
H	3.41047	0.86309	0.99757
C	5.05626	0.82402	-0.30140
H	5.63404	1.57059	0.23180
H	5.71453	0.06019	-0.69946
H	4.50488	1.29142	-1.10947

03\_sma-e.mol2

E = -1282.011174

H = -1281.802214

G = -1281.870155

G(quasi-RRHO) = -1281.866471

Si	-0.57701	0.44031	0.00098
O	0.01924	1.85836	-0.66539
H	0.95166	1.80382	-0.89547
O	-1.41299	-0.66187	-0.97408
O	-0.34241	0.20716	1.65112
H	0.51726	-0.16552	1.86343

H	-0.79278	-1.27966	-1.36548
O	-2.13801	1.19573	0.33226
H	-2.11730	1.71887	1.13430
Si	2.48082	-0.33727	-0.05445
O	2.78735	-0.35373	1.56314
H	3.06209	-1.19016	1.94408
O	2.93382	1.14320	-0.61392
O	3.38883	-1.55185	-0.67580
H	3.17628	-1.85052	-1.56203
O	0.93524	-0.48069	-0.39957
H	3.81161	1.46389	-0.39900
H	-3.44333	-0.84945	-1.09280
N	-4.11731	-0.29113	-0.56322
H	-4.75030	0.16735	-1.21123
C	-4.84713	-1.10212	0.43506
H	-5.50938	-0.45586	1.00011
H	-5.42192	-1.87170	-0.06789
H	-4.12431	-1.55853	1.10223
H	-3.47752	0.42504	-0.11161

*04\_sma-e.mol2*

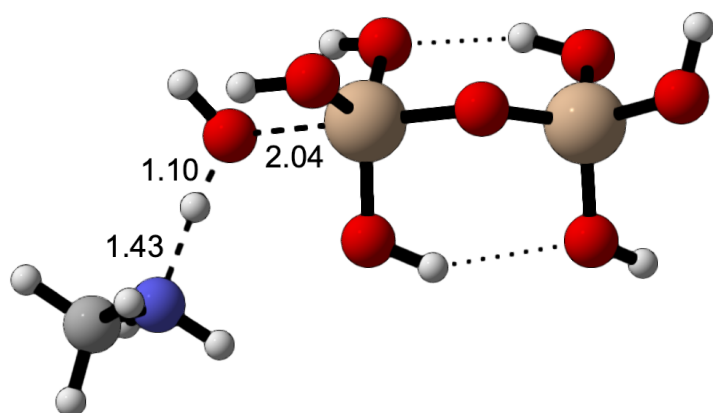
E = -1282.015615  
H = -1281.805817  
G = -1281.870089  
G(quasi-RRHO) = -1281.867199

Si	1.47522	0.22399	0.00928
O	1.37869	-0.44366	1.56722
H	2.24734	-0.64633	1.92001
O	1.61756	-0.81339	-1.31952
O	1.27202	1.89039	-0.19525
H	2.11827	2.32937	-0.29697
H	2.54037	-0.98858	-1.51808
O	3.22834	0.34410	0.05754
H	3.58769	0.87915	0.76693
Si	-1.15584	-1.30528	-0.01254
O	-0.92911	-1.97494	1.46768
H	-0.10900	-1.61449	1.84702
O	-0.72334	-2.30082	-1.23854
O	-2.76101	-1.05542	-0.21948
H	-3.26351	-0.84204	0.56888
O	-0.30229	0.06875	-0.11136
H	0.15802	-2.03866	-1.55425
N	-1.37585	2.50207	-0.59116

H	-1.17115	1.48488	-0.45450
H	-1.75911	2.64895	-1.52044
H	-0.43405	2.90143	-0.55396
C	-2.26351	3.04555	0.46135
H	-2.39299	4.11104	0.30999
H	-3.22269	2.54348	0.40792
H	-1.80532	2.86200	1.42668

TS2-cma, water cleavage of IM1, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as catalyst

*00\_cma-h.mol2*



E = -1282.004980  
H = -1281.800379  
G = -1281.865763  
G(quasi-RRHO) = -1281.862454

Si	0.38844	-0.58355	0.19800
O	-0.19859	-1.60758	-0.98769
H	0.46777	-1.88322	-1.61989
O	0.84694	0.94786	-0.25350
O	0.91157	-1.20491	1.63913
H	1.84551	-1.40745	1.68576
H	0.11925	1.57572	-0.19224
O	2.21636	-1.02870	-0.57906
H	2.61908	-1.88087	-0.39115
Si	-2.45827	0.34762	0.04051
O	-2.82862	-0.61259	-1.23313
H	-2.05933	-1.15028	-1.47968
O	-2.06002	1.87854	-0.40797
O	-3.77549	0.47369	0.99854
H	-4.27300	-0.32965	1.16344
O	-1.15880	-0.21025	0.80509

H	-2.65936	2.36078	-0.98052
H	2.97485	-0.23886	-0.60744
H	3.22981	1.66353	-0.62560
H	4.40244	0.92856	-1.48928
N	3.87250	0.87954	-0.62770
C	4.76744	0.93537	0.53663
H	5.44047	0.08250	0.51208
H	5.35876	1.84900	0.56392
H	4.17255	0.87573	1.44441

*01\_cma-h.mol2*

E = -1282.001842  
H = -1281.798379  
G = -1281.865134  
G(quasi-RRHO) = -1281.861557

Si	0.44875	0.74599	0.10720
O	0.88003	1.00552	1.69208
H	1.82048	1.10235	1.83872
O	0.79171	-0.72304	-0.58974
O	0.07533	2.04582	-0.85999
H	0.83702	2.38178	-1.33473
H	0.02388	-1.30648	-0.64111
O	2.36459	1.10199	-0.40553
H	2.81484	1.86143	-0.02691
Si	-2.44936	-0.38354	0.03734
O	-3.51308	-0.58873	1.26608
H	-3.14356	-0.68455	2.14608
O	-1.84345	-1.80523	-0.53363
O	-3.31624	0.25185	-1.19587
H	-3.93420	0.95426	-0.98478
O	-1.18522	0.45469	0.52766
H	-2.41742	-2.37724	-1.04645
H	4.42900	-0.88082	-1.43102
H	3.06684	0.20324	-0.51353
H	3.07173	-1.61358	-0.88799
N	3.78549	-0.93331	-0.65044
C	4.48809	-1.31858	0.58264
H	4.97849	-2.28515	0.48992
H	5.23390	-0.56489	0.81915
H	3.77122	-1.36308	1.39797

02\_cma-h.mol2

E = -1282.003765  
H = -1281.799748  
G = -1281.863738  
G(quasi-RRHO) = -1281.860913

Si	0.38275	0.50146	0.27570
O	1.06064	0.51832	1.78259
H	1.97623	0.79575	1.80483
O	0.61836	-0.78820	-0.75996
O	-0.21886	1.90565	-0.39908
H	0.37644	2.36287	-0.99494
H	1.28856	-0.65763	-1.43218
O	2.21027	1.12358	-0.43723
H	2.48464	2.01361	-0.19632
Si	-2.44685	-0.34203	-0.02576
O	-3.72929	-0.79457	0.87916
H	-3.77375	-1.71923	1.12916
O	-2.12764	-1.55317	-1.08775
O	-2.93482	1.03738	-0.76348
H	-2.19758	1.66121	-0.83096
O	-1.11636	-0.04058	0.84146
H	-1.17483	-1.61560	-1.24939
H	3.15638	0.45063	-0.49400
N	4.23144	-0.34736	-0.58020
H	5.06269	0.21740	-0.44294
C	4.19430	-1.44952	0.39923
H	3.28275	-2.02164	0.25395
H	5.05196	-2.10932	0.29533
H	4.18801	-1.03307	1.40207
H	4.29170	-0.71562	-1.52346

03\_cma-h.mol2

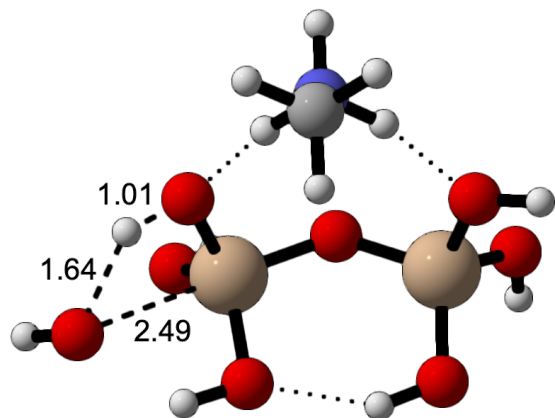
E = -1282.003771  
H = -1281.799751  
G = -1281.863692  
G(quasi-RRHO) = -1281.860916

Si	-0.38053	0.50702	0.26635
O	0.22203	1.89192	-0.44653
H	-0.37410	2.33408	-1.05283
O	-0.62205	-0.80821	-0.73495
O	-1.05468	0.56638	1.77374
H	-1.97016	0.84467	1.78973

H	-1.29394	-0.69351	-1.40834
O	-2.20926	1.11547	-0.45830
H	-2.48015	2.01242	-0.24033
Si	2.44274	-0.36086	-0.02206
O	2.92617	0.99975	-0.80419
H	2.18940	1.62315	-0.88468
O	2.12258	-1.60109	-1.04410
O	3.69536	-0.89444	0.88043
H	4.23247	-0.22534	1.30852
O	1.11835	-0.02488	0.84193
H	1.16978	-1.66513	-1.20306
N	-4.23837	-0.34729	-0.56587
H	-5.06528	0.22378	-0.42849
H	-3.15863	0.44579	-0.49830
C	-4.19929	-1.43793	0.42623
H	-3.29415	-2.01932	0.27788
H	-4.17804	-1.00937	1.42375
H	-5.06342	-2.09177	0.33992
H	-4.30819	-0.72613	-1.50426

TS2-sma, water cleavage of IM1, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as spectator

*00\_sma-h.mol2*



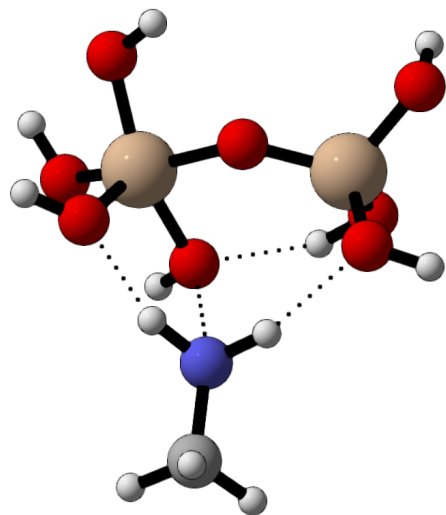
E = -1281.991699  
H = -1281.785600  
G = -1281.851757  
G(quasi-RRHO) = -1281.848780

Si	-1.23372	-0.63574	-0.27123
O	-1.17027	-1.12250	1.30110
H	-2.09563	-0.97783	1.60380
O	-1.67831	0.92830	-0.53021

O	-1.96793	-1.69366	-1.28754
H	-1.36987	-2.16578	-1.87094
H	-2.59166	0.90055	-0.11038
O	-3.45861	-0.19108	0.74973
H	-4.19378	-0.64844	0.33902
Si	1.77484	-0.70693	0.06432
O	1.56876	-1.30369	1.56506
H	0.63489	-1.31976	1.83523
O	2.31409	0.84890	0.05061
O	2.91471	-1.57000	-0.71549
H	2.91172	-2.52128	-0.59055
O	0.36212	-0.64998	-0.72218
H	3.19620	1.02890	0.38381
H	0.42096	3.21741	-1.52255
N	0.32450	2.80242	-0.59965
H	-0.50102	2.16197	-0.61018
C	0.18013	3.84328	0.44671
H	-0.71074	4.42692	0.24465
H	0.08944	3.35284	1.40925
H	1.05429	4.48404	0.43843
H	1.15066	2.21088	-0.42424

TS-iso-ma, isomerization of IM1 to IM2

[00\\_sma-f.mol2](#)



E = -1282.006964  
H = -1281.798309  
G = -1281.861325  
G(quasi-RRHO) = -1281.858999

Si	-1.40936	-0.67074	-0.04170
O	-2.79539	-0.98600	0.92918
H	-3.30201	-1.71967	0.57828
O	-1.87658	0.60193	-1.05508
O	-1.75956	-2.10912	-0.90150
H	-1.03094	-2.34852	-1.47588
H	-2.65303	0.41906	-1.58525
O	-0.79619	0.22865	1.33466
H	-1.48821	0.29329	1.99771
Si	1.73654	-0.62455	0.00083
O	1.77729	-0.67679	1.63714
H	0.91537	-0.37129	1.96841
O	2.25002	0.83641	-0.58549
O	2.82343	-1.70830	-0.56720
H	2.81907	-2.57959	-0.16610
O	0.25253	-0.81825	-0.55849
H	3.15557	1.09109	-0.39444
H	-0.28662	1.97663	0.67782
H	-0.75978	2.11372	-0.85249
H	0.85966	2.16268	-0.47969
N	-0.06969	2.49192	-0.18815
C	-0.14145	3.96089	-0.03914
H	0.58764	4.27939	0.69726
H	0.07302	4.42528	-0.99496
H	-1.13821	4.23496	0.28758

*01\_sma-f.mol2*

E = -1282.006964

H = -1281.798308

G = -1281.861320

G(quasi-RRHO) = -1281.858996

Si	-1.40938	-0.67066	-0.04171
O	-2.79541	-0.98581	0.92918
H	-3.30208	-1.71947	0.57832
O	-1.87651	0.60201	-1.05511
O	-1.75965	-2.10906	-0.90144
H	-1.03105	-2.34852	-1.47582
H	-2.65292	0.41915	-1.58535
O	-0.79614	0.22871	1.33465
H	-1.48814	0.29335	1.99772
Si	1.73647	-0.62461	0.00083
O	1.77718	-0.67693	1.63714



H	0.91526	-0.37139	1.96840
O	2.25005	0.83632	-0.58544
O	2.82331	-1.70841	-0.56720
H	2.81883	-2.57973	-0.16616
O	0.25248	-0.81822	-0.55854
H	3.15565	1.09083	-0.39436
H	-0.28664	1.97648	0.67770
H	-0.75961	2.11382	-0.85266
H	0.85984	2.16259	-0.47961
N	-0.06954	2.49189	-0.18819
C	-0.14122	3.96085	-0.03910
H	0.58798	4.27928	0.69722
H	0.07313	4.42527	-0.99493
H	-1.13793	4.23494	0.28778

*02\_sma-f.mol2*

E = -1282.006179  
H = -1281.797841  
G = -1281.860440  
G(quasi-RRHO) = -1281.858001

Si	1.57634	0.00222	0.06548
O	3.10335	0.75594	0.26322
H	3.63713	0.27689	0.89901
O	1.11679	1.44892	-0.80636
O	1.97018	-1.01059	1.39354
H	1.19993	-1.41739	1.78943
H	1.88057	2.01468	-0.93924
O	1.70903	-1.09877	-1.21932
H	1.78032	-0.65326	-2.06642
Si	-1.31205	-1.06846	0.02464
O	-0.80488	-2.19853	-1.04032
H	0.12488	-2.03329	-1.29125
O	-2.50511	-0.16325	-0.69105
O	-1.96906	-1.74557	1.36244
H	-2.85606	-2.10185	1.28695
O	-0.11521	-0.11943	0.49930
H	-2.72393	-0.40129	-1.59504
H	-1.57014	3.14932	-1.22958
H	-0.35009	2.13366	-0.65024
N	-1.33959	2.47766	-0.50323
C	-1.49418	3.06696	0.84636
H	-1.22794	2.31155	1.57693
H	-0.82934	3.91843	0.93899

H	-2.52133	3.38196	0.99241
H	-1.94252	1.65285	-0.62064

*03\_sma-f.mol2*

E = -1282.004768  
H = -1281.796277  
G = -1281.860232  
G(quasi-RRHO) = -1281.857126

Si	-0.44348	0.92837	-0.07941
O	-2.12192	1.31501	-0.18283
H	-2.22877	2.17389	-0.59516
O	0.10834	1.42504	1.44610
O	-0.16304	2.33766	-1.03361
H	0.72421	2.33169	-1.39472
H	0.26995	2.37096	1.46757
O	-0.98103	-0.66857	0.34635
H	-0.30556	-1.35104	0.28772
Si	2.18153	-0.58344	-0.08990
O	1.59094	-2.11441	0.10962
H	2.06839	-2.70728	0.69354
O	2.59086	0.09723	1.33864
O	3.56861	-0.61706	-0.95455
H	3.61799	-1.24488	-1.67765
O	0.99336	0.23004	-0.79996
H	1.85093	0.63581	1.67150
H	-3.59014	0.16041	0.23268
H	-4.06371	-0.94429	1.39062
H	-2.60628	-1.04781	0.53673
C	-4.31682	-1.64481	-0.55487
H	-4.26508	-2.69229	-0.27999
H	-5.35240	-1.33338	-0.63236
H	-3.81345	-1.48899	-1.50261
N	-3.63239	-0.83751	0.47766

*04\_sma-f.mol2*

E = -1282.006041  
H = -1281.797092  
G = -1281.859452  
G(quasi-RRHO) = -1281.856960

Si	0.42380	1.07066	-0.17459
O	1.38779	2.48720	-0.16131

H	2.18340	2.38936	-0.68587
O	0.91247	0.19282	1.21106
O	1.52407	0.42206	-1.36955
H	1.08963	-0.28530	-1.85179
H	0.88565	0.72769	2.00813
O	-0.87121	2.04432	0.42788
H	-0.56386	2.91815	0.67521
Si	-2.00615	-0.69072	-0.04441
O	-3.09612	0.45956	0.37974
H	-2.60882	1.29400	0.50031
O	-1.42393	-1.52619	1.24326
O	-2.79440	-1.81369	-0.93632
H	-3.47591	-1.48755	-1.52667
O	-0.76241	-0.01070	-0.82128
H	-0.55338	-1.18470	1.49774
H	2.88584	-0.33316	-0.56079
H	2.70098	-0.61515	1.01003
H	4.22894	-0.27659	0.44922
C	3.62296	-2.22344	0.02157
H	4.29169	-2.33567	-0.82406
H	4.07118	-2.65270	0.91020
H	2.67748	-2.71068	-0.18830
N	3.37029	-0.78133	0.24792

*05\_sma-f.mol2*

E = -1282.004196

H = -1281.795818

G = -1281.858777

G(quasi-RRHO) = -1281.856360

Si	0.50531	0.74370	-0.16009
O	1.55069	2.07890	-0.31840
H	2.24783	1.90942	-0.95365
O	1.06239	-0.18097	1.14698
O	1.45391	-0.03143	-1.43659
H	0.91558	-0.69661	-1.87084
H	0.34086	-0.48824	1.70369
O	-0.60802	1.80278	0.66416
H	-0.16183	2.58963	0.98086
Si	-2.25651	-0.45091	-0.05278
O	-3.12652	0.89862	0.26666
H	-2.48585	1.59335	0.50284
O	-1.85878	-1.28279	1.31113
O	-3.19650	-1.44640	-0.95070

H	-3.68961	-1.04691	-1.66976
O	-0.85815	-0.11041	-0.77808
H	-2.56237	-1.45810	1.93899
H	2.77623	-0.92343	-0.72658
H	2.65525	-1.15802	0.85236
N	3.29733	-1.35517	0.07063
C	4.63799	-0.75952	0.26848
H	4.52375	0.30896	0.41235
H	5.10256	-1.20166	1.14250
H	5.24392	-0.95019	-0.61007
H	3.34895	-2.36021	-0.06894

*06\_sma-f.mol2*

E = -1282.004226

H = -1281.795853

G = -1281.858655

G(quasi-RRHO) = -1281.856428

Si	-0.45365	0.98421	0.12952
O	-1.27599	2.46646	0.29196
H	-2.01566	2.39674	0.89713
O	-1.10614	0.18800	-1.21710
O	-1.55788	0.34627	1.35666
H	-1.15029	-0.40830	1.78716
H	-0.42524	-0.22878	-1.75346
O	0.84282	1.86810	-0.63087
H	0.53953	2.72310	-0.93999
Si	2.08498	-0.63489	0.08014
O	3.16896	0.56505	-0.17528
H	2.65521	1.35770	-0.41346
O	1.61111	-1.36450	-1.31743
O	2.82100	-1.78540	0.98309
H	3.33829	-1.48407	1.73242
O	0.73259	-0.09081	0.76746
H	2.30023	-1.63344	-1.92803
H	-2.98691	-0.27238	0.58150
H	-2.86310	-0.49632	-0.99989
H	-4.35699	-0.08218	-0.38312
C	-3.86967	-2.08089	-0.05636
H	-4.51980	-2.18934	0.80431
H	-4.36979	-2.44273	-0.94736
H	-2.95206	-2.63611	0.10316
N	-3.52938	-0.65064	-0.22935

07\_sma-f.mol2

E = -1282.002675

H = -1281.794431

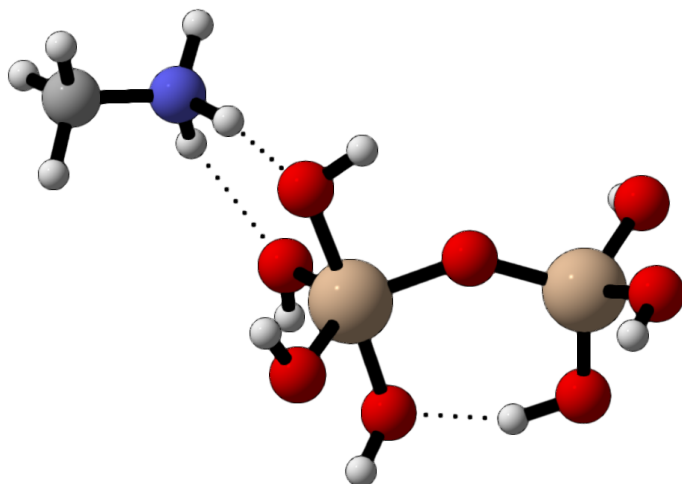
G = -1281.858419

G(quasi-RRHO) = -1281.855505

Si	-0.46813	-0.51725	0.06391
O	-1.96077	-1.25164	-0.39227
H	-1.89031	-1.93497	-1.05730
O	0.02414	-1.25044	1.50691
O	-1.47143	0.76481	0.68238
H	-0.94317	1.54170	0.86986
H	0.00671	-2.20885	1.48637
O	0.39232	-1.46941	-1.12916
H	0.09126	-2.37035	-1.25404
Si	2.35206	0.47439	-0.07487
O	2.89065	-0.35489	-1.38483
H	2.18068	-0.96640	-1.64512
O	2.70175	-0.26835	1.34518
O	3.18222	1.88456	-0.02409
H	3.38654	2.28900	-0.86908
O	0.75028	0.68455	-0.16433
H	1.91243	-0.71896	1.68838
H	-3.11424	0.73745	0.59613
H	-4.63401	0.24791	1.16487
H	-3.82885	-0.53365	-0.06115
N	-4.06908	0.38097	0.33145
C	-4.74037	1.25597	-0.65469
H	-4.91763	2.22562	-0.20343
H	-4.09056	1.36523	-1.51575
H	-5.68135	0.81020	-0.95643

IM2-ma, co-linear OH groups on Si

00\_sma-g.mol2



E = -1282.012984  
 H = -1281.804195  
 G = -1281.871353  
 G(quasi-RRHO) = -1281.867521

Si	0.50935	0.67703	0.08589
O	1.51189	0.34782	-1.23373
H	1.24833	0.89565	-1.97629
O	0.83144	1.95029	1.13761
O	-0.79710	-0.35055	0.34519
H	1.39185	1.65515	1.85784
O	1.53389	-0.41207	1.07610
H	0.99129	-1.07828	1.50102
O	-0.44596	1.80536	-0.91023
H	-0.35561	2.70002	-0.57801
Si	-2.37358	-0.49630	0.00899
O	-2.72786	-1.94838	-0.66243
H	-2.48926	-2.06106	-1.58411
O	-2.82871	0.72587	-0.96733
H	-2.04456	1.31699	-1.08789
O	-3.25942	-0.57600	1.38581
H	-3.12965	0.12952	2.02189
C	4.89762	-0.67526	0.07628
N	3.60093	-1.24213	-0.35424
H	3.24882	-0.79708	-1.20397
H	3.66210	-2.24371	-0.51057
H	5.64776	-0.85505	-0.68562
H	4.77409	0.39136	0.22747
H	5.19601	-1.14430	1.00707
H	2.82042	-1.03158	0.33681

*01\_sma-g.mol2*

E = -1282.013002

H = -1281.804095

G = -1281.870628

G(quasi-RRHO) = -1281.867088

Si	0.46804	-0.96381	0.07185
O	-0.59926	-1.78742	-1.09513
H	-0.68264	-2.71565	-0.87049
O	1.60081	-0.18655	1.22503
O	0.48634	-2.37730	0.98411
H	1.04775	-2.27129	1.75445
H	1.13963	0.47702	1.74069
O	1.60016	-0.68426	-1.15057
H	1.29608	-1.09360	-1.96351
Si	-2.16418	0.69831	0.01627
O	-3.13191	0.77414	1.33688
H	-3.44276	-0.06202	1.68787
O	-2.76414	-0.31730	-1.10734
O	-2.19943	2.26260	-0.47102
H	-1.61178	2.50142	-1.18986
O	-0.65533	0.24732	0.38908
H	-2.08102	-1.01404	-1.27165
H	2.99164	0.34107	0.60788
H	4.64318	0.13951	0.24791
H	3.47169	0.17586	-0.92505
N	3.78682	0.59741	-0.04920
C	3.96193	2.06134	-0.16842
H	3.02046	2.49608	-0.48563
H	4.24305	2.46314	0.79861
H	4.73328	2.27985	-0.89829

*02\_sma-g.mol2*

E = -1282.011706

H = -1281.802889

G = -1281.869653

G(quasi-RRHO) = -1281.866140

Si	0.46596	0.56896	-0.07785
O	0.68641	1.94229	-1.02279
H	1.30639	1.76486	-1.73289
O	1.49292	0.29236	1.23574

O	1.59517	-0.35869	-1.10745
H	1.11841	-1.03105	-1.59704
H	1.14939	0.73580	2.01404
O	-0.67897	1.47389	0.93661
H	-0.56236	2.42170	0.85611
Si	-2.31552	-0.46985	-0.02247
O	-3.05658	0.75553	-0.83075
H	-2.61260	1.60204	-0.73325
O	-2.56575	-0.42174	1.59594
O	-3.09331	-1.84143	-0.46175
H	-3.14710	-2.03162	-1.39956
O	-0.74131	-0.56350	-0.41257
H	-2.03534	0.29333	1.97152
N	3.69573	-1.11055	0.32334
H	3.79860	-2.11104	0.46430
H	3.30660	-0.69791	1.17374
H	2.91843	-0.92590	-0.37653
C	4.97365	-0.48062	-0.07412
H	5.71729	-0.64136	0.69830
H	5.30819	-0.92073	-1.00680
H	4.80717	0.58218	-0.21006

*03\_sma-g.mol2*

E = -1282.011213

H = -1281.802047

G = -1281.869147

G(quasi-RRHO) = -1281.865458

Si	0.44094	1.14211	-0.00882
O	0.91858	-0.37749	-0.89709
H	1.10880	-0.14398	-1.80905
O	0.09371	2.65521	0.80655
O	1.55431	0.69777	1.18468
H	1.53140	1.35575	1.88336
H	-0.79185	2.65841	1.16995
O	0.89297	1.96410	-1.40718
H	0.73076	2.90310	-1.29455
Si	-2.10795	-0.66880	0.00746
O	-2.78451	-1.16632	1.41390
H	-2.21794	-1.65825	2.01053
O	-1.26320	-1.88159	-0.68439
O	-3.44665	-0.26328	-0.84590
H	-3.30583	0.19609	-1.67547
O	-1.14090	0.60984	0.20348



H	-0.36231	-1.54433	-0.88792
N	2.95454	-1.53432	0.42522
H	2.18472	-1.23808	-0.22947
H	2.83935	-0.85667	1.18367
H	2.76284	-2.46620	0.78099
C	4.29204	-1.45182	-0.20265
H	5.05225	-1.69968	0.52935
H	4.33596	-2.14734	-1.03304
H	4.44165	-0.43996	-0.56246

*04\_sma-g.mol2*

E = -1282.009636

H = -1281.800875

G = -1281.868546

G(quasi-RRHO) = -1281.864545

Si	0.51785	0.61851	-0.08478
O	-0.45547	1.74067	0.92876
H	0.00075	2.52968	1.22520
O	1.56678	-0.44681	-1.02901
O	0.78779	1.82308	-1.23418
H	0.24265	2.59578	-1.07758
H	1.55967	-0.21193	-1.95772
O	1.52029	0.27246	1.23580
H	1.16219	0.65099	2.04036
Si	-2.39819	-0.48541	-0.01665
O	-3.24662	-0.61268	-1.41411
H	-3.08123	0.05816	-2.07868
O	-2.88901	0.78006	0.88872
O	-2.79161	-1.90493	0.70313
H	-2.58200	-1.98178	1.63542
O	-0.81523	-0.37004	-0.30866
H	-2.10986	1.35621	1.06178
N	3.70002	-1.19133	0.32162
H	3.78244	-2.19582	0.44628
H	2.91429	-0.97684	-0.36329
H	3.33925	-0.78281	1.18544
C	4.98491	-0.58508	-0.08951
H	4.83932	0.48252	-0.21148
H	5.73754	-0.77026	0.66862
H	5.29474	-1.02184	-1.03226

05\_sma-g.mol2

E = -1282.012939  
H = -1281.803562  
G = -1281.867359  
G(quasi-RRHO) = -1281.865209

Si	-1.53873	-0.18584	-0.00543
O	-2.57983	-0.63802	1.23742
H	-3.28086	-1.19187	0.88701
O	-1.76807	1.29283	-0.79590
O	-2.51666	-1.06212	-1.16252
H	-1.97510	-1.53975	-1.79101
H	-2.31285	1.14918	-1.57323
O	-0.55674	0.66777	1.24990
H	-1.12435	0.96188	1.96571
Si	1.38299	-1.17641	-0.03232
O	1.53552	-1.04573	1.58912
H	0.85017	-0.42503	1.89823
O	2.20267	0.00626	-0.84335
O	2.06656	-2.58243	-0.50474
H	1.87784	-3.36147	0.02216
O	-0.15342	-1.03140	-0.48716
H	3.16109	-0.01697	-0.78973
H	-0.03029	2.56495	-0.97924
N	0.73631	2.47829	-0.31101
H	1.43151	1.83858	-0.71009
H	0.29907	1.94929	0.48006
C	1.31886	3.77792	0.08251
H	0.54328	4.39392	0.52351
H	2.10614	3.60533	0.80782
H	1.72697	4.27069	-0.79280

06\_sma-g.mol2

E = -1282.012939  
H = -1281.803562  
G = -1281.867341  
G(quasi-RRHO) = -1281.865195

Si	-1.53891	-0.18455	-0.00548
O	-2.58024	-0.63489	1.23783
H	-3.28227	-1.18792	0.88814
O	-1.76663	1.29442	-0.79574
O	-2.51821	-1.06004	-1.16177
H	-1.97779	-1.53659	-1.79208

H	-2.31209	1.15168	-1.57276
O	-0.55531	0.66784	1.24991
H	-1.12271	0.96330	1.96538
Si	1.38177	-1.17751	-0.03246
O	1.53497	-1.04729	1.58899
H	0.85025	-0.42604	1.89832
O	2.20226	0.00461	-0.84358
O	2.06399	-2.58431	-0.50490
H	1.87502	-3.36280	0.02274
O	-0.15449	-1.03138	-0.48750
H	3.16061	-0.01774	-0.78776
N	0.73849	2.47748	-0.31217
H	0.30023	1.94832	0.47824
H	-0.02744	2.56618	-0.98080
H	1.43318	1.83727	-0.71136
C	1.32245	3.77601	0.08332
H	2.10838	3.60156	0.80967
H	1.73259	4.26886	-0.79100
H	0.54705	4.39271	0.52368

*08\_sma-g.mol2*

E = -1282.012452

H = -1281.803170

G = -1281.866659

G(quasi-RRHO) = -1281.864229

Si	1.52158	0.35879	0.04214
O	2.60581	0.65821	1.29271
H	2.44358	1.50571	1.71031
O	1.83594	0.55307	-1.59751
O	0.86808	2.04535	0.16247
H	1.48950	2.73678	-0.07495
H	1.48209	1.37603	-1.93666
O	2.17757	-1.27229	-0.10233
H	2.56815	-1.55088	0.72765
Si	-0.96490	-1.39138	0.03192
O	-1.89007	-1.97365	1.25063
H	-1.50158	-2.65704	1.80025
O	-0.06388	-2.57551	-0.62527
O	-2.04465	-0.72267	-1.02256
H	-2.85260	-1.20478	-1.21065
O	-0.02933	-0.15672	0.47318
H	0.88579	-2.30926	-0.54343
N	-1.71760	2.13955	-0.56181

H	-1.93476	1.17839	-0.85608
H	-1.88206	2.75872	-1.35045
H	-0.68708	2.16445	-0.31509
C	-2.54209	2.52898	0.60533
H	-3.59316	2.47563	0.34437
H	-2.32682	1.84511	1.41868
H	-2.28451	3.54032	0.89946

*07\_sma-g.mol2*

E = -1282.012706  
H = -1281.803321  
G = -1281.867048  
G(quasi-RRHO) = -1281.864891

Si	-1.53770	-0.18539	-0.00366
O	-0.55025	0.67209	1.24520
H	-1.11532	0.96662	1.96289
O	-1.76448	1.28907	-0.80247
O	-2.57893	-0.62542	1.24338
H	-3.28225	-1.17934	0.89771
H	-2.31001	1.14168	-1.57858
O	-2.51950	-1.06528	-1.15480
H	-1.98045	-1.55569	-1.77552
Si	1.37817	-1.18331	-0.01758
O	2.02363	-2.64256	-0.36595
H	2.18309	-2.84729	-1.28910
O	1.54912	-1.04282	1.59822
O	2.18960	0.00394	-0.84014
H	3.14729	-0.00183	-0.76785
O	-0.15591	-1.03953	-0.48020
H	0.87180	-0.41466	1.90768
N	0.73506	2.48014	-0.32283
H	0.29766	1.95358	0.46987
H	-0.03193	2.56855	-0.99018
H	1.42653	1.83569	-0.72105
C	1.32349	3.77804	0.06739
H	2.11030	3.60372	0.79282
H	1.73344	4.26711	-0.80916
H	0.55076	4.39842	0.50732

*09\_sma-g.mol2*

E = -1282.011366  
H = -1281.802084

G = -1281.866329  
G(quasi-RRHO) = -1281.864048

Si	-1.21029	-0.92582	-0.00296
O	-1.95779	-1.86318	1.18037
H	-2.30905	-2.66303	0.78331
O	-2.04763	0.32392	-0.75996
O	-1.64469	-2.10047	-1.22818
H	-0.91700	-2.26924	-1.82671
H	-2.42376	0.00161	-1.58204
O	-0.78782	0.23408	1.32389
H	-1.41457	0.14109	2.04463
Si	1.80215	-0.29801	-0.04216
O	1.89307	-0.00140	1.55823
H	0.97968	0.09957	1.88780
O	1.91162	1.17323	-0.78872
O	3.09785	-1.14546	-0.55995
H	3.10373	-2.08985	-0.39199
O	0.42815	-1.05324	-0.41480
H	2.01460	1.16577	-1.74364
N	-0.29237	2.72558	0.33302
H	0.52722	2.43662	-0.21547
H	-0.67138	1.83228	0.73961
H	0.04225	3.30350	1.09946
C	-1.28857	3.45079	-0.48994
H	-0.82405	4.32887	-0.92453
H	-1.64027	2.77721	-1.26100
H	-2.11751	3.74562	0.14374

*10\_sma-g.mol2*

E = -1282.010069  
H = -1281.800622  
G = -1281.864578  
G(quasi-RRHO) = -1281.862362

Si	-1.56764	-0.01074	-0.03014
O	-0.51354	0.72218	1.29498
H	-1.01361	1.31010	1.86666
O	-2.61033	-0.58313	-1.28545
O	-2.51294	-0.76517	1.14118
H	-2.13102	-0.70921	2.01840
H	-2.98622	-1.44080	-1.08563
O	-1.74454	1.56572	-0.61579
H	-2.36002	1.56425	-1.35310

Si	1.24690	-1.28070	-0.07447
O	1.70119	-2.77060	-0.56601
H	1.36708	-3.51856	-0.06692
O	1.35478	-1.21831	1.55469
O	2.28429	-0.23460	-0.82074
H	3.22432	-0.38744	-0.70022
O	-0.21390	-0.84670	-0.58373
H	0.75140	-0.52337	1.87825
H	0.49957	1.82363	0.43784
H	0.27638	2.54896	-1.00109
H	1.63245	1.62444	-0.74639
N	1.00931	2.32491	-0.32943
C	1.74204	3.52231	0.13626
H	2.22884	3.99855	-0.70726
H	1.03967	4.20990	0.59379
H	2.48392	3.21632	0.86555

*11\_sma-g.mol2*

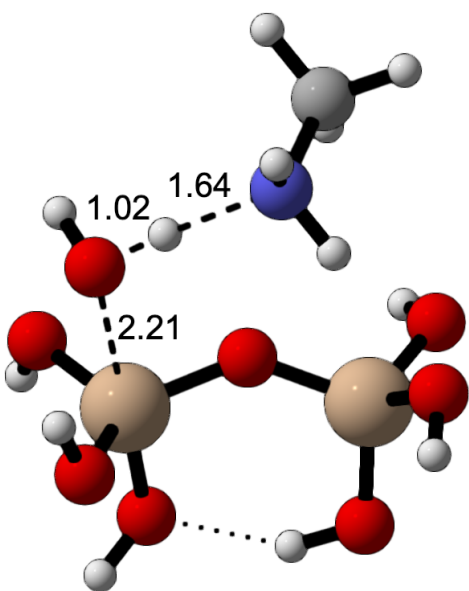
E = -1282.007505  
H = -1281.798313  
G = -1281.863487  
G(quasi-RRHO) = -1281.860559

Si	-0.20297	-1.34475	-0.04251
O	1.32758	-1.60979	-0.85962
H	1.74715	-2.43251	-0.60517
O	0.46393	-1.99572	1.37311
O	-1.00232	-2.25287	-1.20435
H	-1.95528	-2.23572	-1.10503
H	-0.15598	-1.96228	2.10459
O	-1.75373	-0.98315	0.81268
H	-2.30422	-1.73651	1.03364
Si	1.44075	1.05106	-0.03232
O	1.26337	2.67319	0.09124
H	1.04551	3.01712	0.95924
O	2.38637	0.87600	-1.35466
O	2.13127	0.50872	1.35526
H	1.83384	-0.37770	1.60604
O	-0.00728	0.32746	-0.22079
H	2.34342	-0.05728	-1.61448
N	-2.54755	1.50496	0.38986
H	-1.66668	1.82782	-0.00848
H	-2.72856	2.03856	1.23527
H	-2.35090	0.49246	0.64324

C	-3.66431	1.62069	-0.57558
H	-3.80158	2.65930	-0.85402
H	-3.42315	1.03081	-1.45279
H	-4.56711	1.23803	-0.11317

TS3-cma, water cleavage from IM2, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as catalyst

*00\_cma-k.mol2*



E	= -1282.002620
H	= -1281.799392
G	= -1281.866917
G(quasi-RRHO)	= -1281.862949

Si	0.32391	0.90176	-0.04769
O	1.06265	1.05476	-1.52543
H	1.73860	0.39279	-1.67602
O	0.85925	1.72076	1.29746
O	1.70735	-0.45398	0.40729
H	1.34117	-1.33979	0.45856
H	1.51102	1.23620	1.80567
O	-0.86012	2.10376	-0.39577
H	-0.83476	2.82599	0.23370
Si	-2.31064	-0.66410	0.03102
O	-2.66300	-1.99381	-0.85715
H	-2.68599	-1.88318	-1.80966
O	-3.07095	0.62614	-0.61279
O	-2.77962	-1.01840	1.55798

H	-3.67336	-1.34381	1.68009
O	-0.71787	-0.38521	0.11619
H	-2.45387	1.38916	-0.61537
N	4.20686	-0.43146	0.41853
H	2.85729	-0.44222	0.41463
H	4.53437	-0.53580	1.37237
C	4.75801	-1.49949	-0.43452
H	4.40341	-2.46007	-0.07221
H	4.40239	-1.35889	-1.45113
H	5.84524	-1.49825	-0.43406
H	4.53110	0.47574	0.10187

*01\_cma-k.mol2*

E = -1282.006572  
H = -1281.800802  
G = -1281.866658  
G(quasi-RRHO) = -1281.863443

Si	-1.56503	-0.33792	0.05123
O	-2.25516	-1.10286	1.34113
H	-2.87121	-0.53941	1.81482
O	-2.04558	-0.73005	-1.47354
O	-0.02230	0.15801	0.31237
H	-1.81343	-1.62688	-1.72388
O	-0.61957	-2.32524	-0.09766
H	-0.75311	-2.77434	0.74188
H	2.07210	-1.20615	-1.06260
H	0.38610	-2.27580	-0.28221
O	-2.31899	1.18166	0.12213
H	-3.12918	1.24589	-0.38773
Si	0.88271	1.47199	0.01297
O	1.86295	1.77110	1.28209
H	1.45901	1.80696	2.15114
O	-0.09634	2.71943	-0.36241
H	-1.03242	2.46580	-0.26018
O	1.96230	1.18897	-1.18274
H	1.66738	1.35075	-2.08102
N	1.97844	-2.11806	-0.62770
H	2.31037	-2.80025	-1.29782
C	2.78722	-2.17080	0.59631
H	2.41384	-1.42992	1.29950
H	2.68611	-3.15199	1.05441
H	3.84602	-1.97849	0.41998



02\_cma-k.mol2

E = -1281.999401

H = -1281.794070

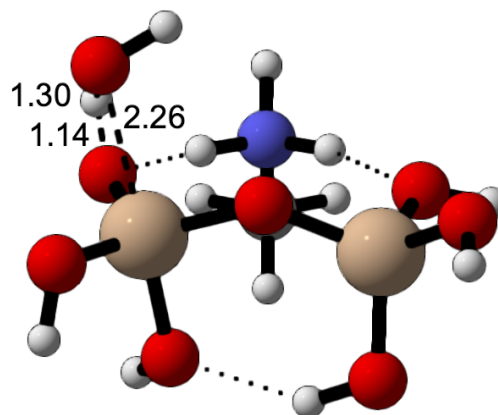
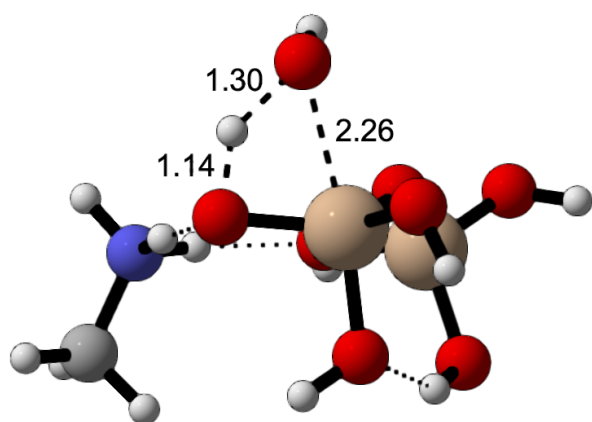
G = -1281.865813

G(quasi-RRHO) = -1281.860472

Si	-0.24470	0.98650	0.00188
O	-0.73333	1.79256	1.34617
H	-0.24926	2.60506	1.51083
O	-1.43677	0.69426	-1.08754
O	0.77709	-0.25309	0.25492
H	-1.24098	1.03595	-1.96357
O	-1.73409	-0.57315	1.23489
H	-2.06531	0.01532	1.91837
H	-3.39756	-0.72219	-1.19793
H	-2.52219	-0.85084	0.69088
O	0.78773	2.05710	-0.77594
H	0.44557	2.91208	-1.04329
Si	2.32585	-0.66953	-0.01939
O	3.06771	-1.10687	1.36524
H	3.14206	-0.44481	2.05474
O	3.08661	0.56772	-0.76074
H	2.49803	1.32276	-0.92471
O	2.42597	-2.04836	-0.88440
H	2.15343	-2.01227	-1.80290
H	-3.84738	-2.21703	-0.73395
C	-5.14507	-0.75271	-0.11750
H	-5.07613	0.28649	0.19757
H	-5.84326	-0.81084	-0.95461
H	-5.55642	-1.32458	0.71142
N	-3.80482	-1.25112	-0.43620

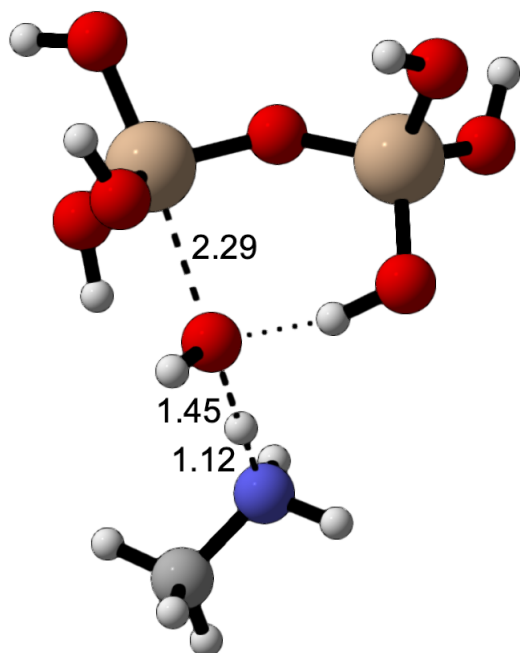
TS3-sma, water cleavage from IM2,  $\text{CH}_3\text{NH}_3^+$  acting as spectator

00\_sma-k.mol2



O	2.15469	0.07441	-0.14739
H	2.24457	-0.44104	-1.15782
O	1.41133	-2.61421	0.50667
O	1.80242	-1.45385	-1.83817
H	1.14036	-1.15316	-2.46439
H	1.30580	-2.84128	1.43381
O	0.57919	-0.55949	1.81096
H	1.24161	-0.02647	2.25415
Si	-1.81797	-0.04956	-0.11475
O	-1.57710	1.48653	-0.66652
H	-2.31738	2.09563	-0.60617
O	-2.10172	-0.10961	1.48887
O	-3.12707	-0.60412	-0.90960
H	-3.56209	-1.38316	-0.55708
O	-0.46707	-0.85339	-0.49392
H	-1.26371	-0.21824	1.97289
H	1.60372	1.60208	-0.40935
N	1.12060	2.53054	-0.56962
H	1.46980	2.93303	-1.43491
H	0.12236	2.31261	-0.69631
C	1.32747	3.45040	0.57329
H	2.38930	3.63440	0.69139
H	0.80773	4.38354	0.38752
H	0.93452	2.98178	1.46870

TS4-cma, water cleavage from IM2, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as catalyst  
*00\_cma-m.mol2*



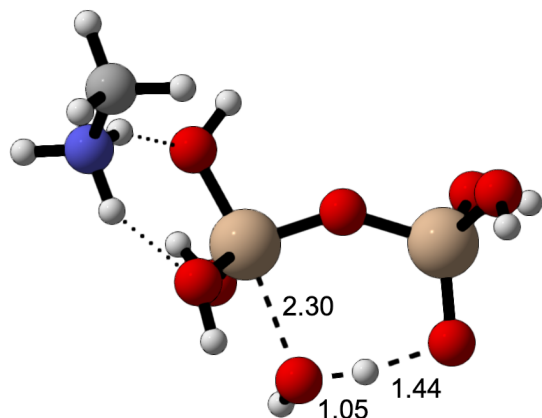
E = -1281.999471  
 H = -1281.793911  
 G = -1281.859799  
 G(quasi-RRHO) = -1281.856616

Si	-0.27925	-1.54201	-0.10202
O	0.99679	-2.02640	-1.02836
H	1.77784	-1.51788	-0.79451
O	-1.38299	-2.70408	-0.61394
O	1.32786	-0.07550	0.62656
H	1.57029	-0.44786	1.47857
H	-0.97715	-3.51008	-0.93600
O	-1.10709	-0.20685	-0.57154
O	-0.27404	-1.82771	1.53252
Si	-1.54119	1.26310	-0.03217
O	-3.01039	1.20548	0.69565
O	-0.37750	1.83846	0.93375
H	2.42553	0.71062	0.09119
O	-1.73179	2.30207	-1.28141
H	-2.53136	2.21712	-1.80389
H	-3.13350	0.55183	1.38670
H	-0.86662	-2.55039	1.75397
H	3.17238	1.37190	-1.32563
H	0.37861	1.17784	0.93674
N	3.26618	1.32465	-0.31497

C	4.57515	0.74951	0.06950
H	4.64439	-0.25560	-0.33218
H	5.38283	1.35839	-0.32168
H	4.63293	0.71221	1.15187
H	3.16896	2.27318	0.03552

TS4-sma, water cleavage from IM2, CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> acting as spectator

*00\_sma-m.mol2*



E = -1281.997612  
H = -1281.790368  
G = -1281.856047  
G(quasi-RRHO) = -1281.852956

Si	0.52567	-0.77042	0.27253
O	0.25617	-2.24953	0.95784
H	0.74545	-2.36539	1.77577
O	1.65518	-0.12197	1.36201
O	-0.77087	-1.79265	-1.32584
H	-0.94927	-2.66359	-0.96147
H	1.27631	0.49264	1.99343
O	-0.65663	0.33117	0.39214
O	1.53069	-0.71292	-1.04167
Si	-2.21950	0.66571	-0.03191
O	-2.26729	2.26387	-0.47438
O	-2.74930	-0.31931	-1.14117
H	-1.66934	-1.24812	-1.31766
O	-2.98034	0.63426	1.43768
H	-3.91994	0.82338	1.42167
H	-2.20160	2.41347	-1.41911
H	1.12732	-1.13901	-1.80363
H	3.23947	0.31387	0.66990

H	3.38313	0.02240	-0.90341
H	4.73099	-0.13490	0.05185
N	3.90360	0.42990	-0.11973
C	4.24979	1.85193	-0.35616
H	4.89436	1.92204	-1.22454
H	3.33324	2.40462	-0.52792
H	4.75847	2.24008	0.51854

*01\_sma-m.mol2*

E = -1282.000666  
H = -1281.793014  
G = -1281.855212  
G(quasi-RRHO) = -1281.853413

Si	-0.25648	-1.42580	-0.19089
O	0.42051	-1.59115	1.30539
H	-0.22887	-1.55750	2.01101
O	1.21505	-1.76820	-0.98095
O	-2.06488	-1.11055	1.04680
H	-2.81302	-1.49928	0.58613
H	1.22343	-1.52616	-1.90984
O	-0.50160	0.09172	-0.75266
O	-1.24320	-2.58866	-0.82160
Si	-0.93307	1.53731	-0.08899
O	-1.40569	2.53750	-1.31333
O	-2.04489	1.38062	1.00839
H	-2.18890	-0.07397	1.08879
O	0.55778	2.08906	0.44923
H	0.54752	2.86385	1.01532
H	-0.72297	2.80278	-1.93228
H	-0.78624	-3.19020	-1.41357
H	2.72611	-0.19133	1.42604
H	1.93833	0.94096	0.51230
C	3.96264	0.70834	0.00647
H	4.68277	-0.10181	-0.00413
H	3.83177	1.09928	-0.99623
H	4.30165	1.49708	0.66831
H	2.28814	-0.56234	-0.11629
N	2.65906	0.19494	0.48769

*02\_sma-m.mol2*

E = -1282.000020  
H = -1281.792927

G = -1281.854990  
G(quasi-RRHO) = -1281.853111

Si	-0.92902	-1.12064	0.20532
O	-1.77451	-0.50039	-1.09581
H	-1.41936	-0.82200	-1.92932
O	-2.04729	-0.55737	1.34109
O	0.29934	-1.89718	-1.36420
H	0.45786	-2.82292	-1.16071
H	-1.64525	-0.26616	2.16042
O	0.37515	-0.25795	0.70742
O	-0.99579	-2.74240	0.54804
Si	1.78529	0.33623	0.10597
O	2.90615	0.37536	1.31364
O	2.29082	-0.48873	-1.13489
H	1.22939	-1.36434	-1.34830
O	1.34619	1.92390	-0.21069
H	2.01206	2.47031	-0.63452
H	2.72943	0.97568	2.04030
H	-1.60419	-2.91860	1.26955
H	-1.66834	1.31644	-1.00326
H	-1.50385	2.82591	-1.68180
N	-1.37464	2.29428	-0.82479
C	-2.13922	2.89035	0.29834
H	-3.18940	2.92645	0.03223
H	-2.00251	2.26485	1.17252
H	-1.76867	3.89100	0.48852
H	-0.35767	2.26113	-0.61703

*03\_sma-m.mol2*

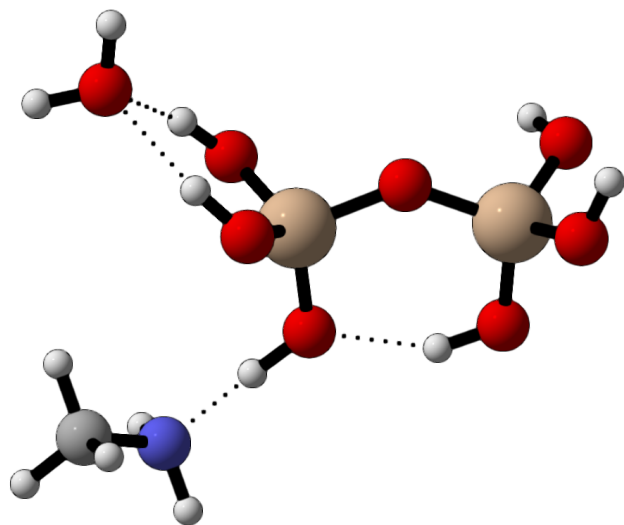
E = -1281.998494  
H = -1281.792206  
G = -1281.854497  
G(quasi-RRHO) = -1281.852578

Si	-1.33773	-0.75604	-0.21157
O	-1.92056	-2.29673	-0.10269
H	-1.69956	-2.69401	0.74241
O	-2.12066	-0.45075	-1.67914
O	-0.56060	-1.23167	1.70158
H	-0.85987	-0.57976	2.34039
H	-1.67158	0.19883	-2.22138
O	0.20446	-0.43373	-0.68260
O	-2.03071	0.49921	0.67977

Si	1.74200	-0.43223	-0.10486
O	2.07107	1.20661	-0.09773
O	1.82647	-1.14882	1.30007
H	0.53838	-1.22005	1.64649
O	2.76055	-1.02927	-1.25350
H	2.98339	-1.95742	-1.16152
H	2.95063	1.46208	0.18960
H	-2.77643	0.86831	0.19712
H	-0.89042	1.93136	0.78907
H	-0.06834	3.13091	1.59693
H	0.71594	2.21620	0.44611
N	-0.18028	2.67973	0.69266
C	-0.57563	3.65724	-0.35120
H	-1.51524	4.11868	-0.07014
H	0.19759	4.41135	-0.44144
H	-0.68857	3.12894	-1.29117

PC-ma, product complexes

*00\_cma-p1.mol2*



E = -1282.021765  
H = -1281.815523  
G = -1281.887725  
G(quasi-RRHO) = -1281.882729

Si	0.45488	0.42677	0.05194
O	1.08441	1.16702	1.36573
H	1.64844	1.92874	1.16796
O	0.59065	-1.18534	0.14281

O	1.16844	1.02594	-1.29031
H	1.72078	1.80663	-1.13937
H	1.49789	-1.64143	0.21727
O	2.60074	3.12484	-0.02250
H	2.32177	4.04444	-0.07526
Si	-2.50473	-0.21270	-0.03960
O	-3.55008	0.30068	1.10625
H	-3.20890	0.43579	1.99259
O	-2.08959	-1.77553	0.13893
O	-3.30647	-0.08563	-1.45413
H	-3.83274	0.70326	-1.59705
O	-1.15681	0.70286	-0.01160
H	-1.12414	-1.89880	0.16817
H	3.56263	3.13878	0.00636
N	2.93478	-2.41759	0.32299
H	2.82208	-3.35716	-0.03787
C	4.00364	-1.72176	-0.40604
H	4.96472	-2.23277	-0.34621
H	3.72334	-1.63207	-1.45269
H	4.11949	-0.71909	-0.00145
H	3.18696	-2.51829	1.29863

*01\_cma-p3.mol2*

E = -1282.021423

H = -1281.815259

G = -1281.887290

G(quasi-RRHO) = -1281.882712

Si	1.68960	0.89945	-0.12484
O	1.07231	2.36372	-0.42448
H	0.13828	2.55100	-0.20992
O	3.13544	0.81868	-0.87508
O	-1.54740	2.95361	0.14880
H	-1.96434	3.42676	-0.57893
H	3.22475	1.27180	-1.71569
O	0.67480	-0.27544	-0.59327
O	1.95400	0.58217	1.46616
Si	0.07306	-1.69579	-0.03127
O	0.52890	-1.84217	1.53568
O	-1.51610	-1.77548	-0.24706
H	-1.63289	3.53015	0.91534
O	0.65661	-2.95296	-0.90267
H	1.56781	-3.20340	-0.74039
H	1.07793	-1.11502	1.85981



H	2.58315	1.12349	1.94713
H	-3.48485	0.09049	1.39247
H	-2.10435	-1.00427	0.04493
H	-2.62545	1.10657	0.45615
N	-3.13693	0.22919	0.45188
C	-4.25674	0.30766	-0.49336
H	-4.80339	-0.63265	-0.48861
H	-4.95593	1.11406	-0.26714
H	-3.86753	0.46256	-1.49722

*02\_cma-p2.mol2*

E = -1282.018667  
H = -1281.811706  
G = -1281.883845  
G(quasi-RRHO) = -1281.878851

Si	-0.26894	0.11009	-0.41819
O	-0.98417	1.60902	-0.27505
H	-0.44112	2.36563	-0.50749
O	-1.28242	-1.01324	-0.02892
O	1.10788	0.18987	0.48518
H	-2.63881	-0.92579	0.46182
O	-3.60942	2.01428	0.48608
H	-2.66360	1.97468	0.24223
H	-3.77448	-1.17976	1.74161
H	-3.66881	2.60597	1.24059
O	0.35314	-0.00709	-1.96280
H	-0.22434	-0.39987	-2.62021
Si	2.68859	-0.13721	0.30883
O	3.62327	1.06083	0.90500
H	3.64251	1.88529	0.41607
O	2.99720	-0.40145	-1.27272
H	2.19786	-0.33698	-1.82152
O	3.15235	-1.39211	1.24518
H	2.69025	-2.22362	1.12497
N	-3.69026	-0.82530	0.79446
C	-4.61002	-1.52884	-0.12097
H	-4.48538	-1.12130	-1.11878
H	-4.36417	-2.58552	-0.13211
H	-5.63840	-1.39666	0.19949
H	-3.87727	0.18685	0.81328

*03\_cma-p1.mol2*

E = -1282.020244

H = -1281.813240

G = -1281.882726

G(quasi-RRHO) = -1281.878960

Si	0.09360	1.26532	-0.32891
O	1.03676	1.92579	0.84387
H	1.69427	1.35248	1.26492
O	0.76495	0.04609	-1.09607
O	-0.38349	2.53573	-1.26986
H	0.31972	3.03199	-1.69207
H	2.12181	-0.43573	-0.91986
O	3.11006	0.31882	1.96790
H	2.85231	-0.27367	2.68183
Si	-2.13316	-0.63430	0.21172
O	-2.50904	-1.21026	1.69963
H	-1.81235	-1.20728	2.35876
O	-1.22464	-1.65498	-0.66733
O	-3.57090	-0.47769	-0.55200
H	-4.29998	-0.11918	-0.04257
O	-1.33803	0.78029	0.35003
H	-0.38952	-1.19606	-0.94836
H	3.78788	-0.45309	-1.39143
H	3.83274	0.85108	2.31667
H	3.39480	-0.53100	0.20857
N	3.13086	-0.85050	-0.72745
C	3.12030	-2.32605	-0.80620
H	2.81723	-2.62526	-1.80383
H	4.10626	-2.72288	-0.58797
H	2.40547	-2.70627	-0.08411

*04\_cma-p3.mol2*

E = -1282.016486

H = -1281.810319

G = -1281.879024

G(quasi-RRHO) = -1281.874731

Si	-0.72384	1.55571	0.09039
O	0.59724	1.77802	-0.73200
H	1.28357	0.70733	-1.17802
O	-0.84061	2.66006	1.30838
O	1.82229	-0.19191	-1.48642
H	1.89814	-0.17628	-2.44436

H	-1.66563	2.66539	1.79730
O	-0.85532	0.05679	0.77467
O	-2.12608	1.61252	-0.81913
Si	-1.22493	-1.39788	0.13815
O	-2.49126	-1.19263	-0.88296
O	0.07268	-2.06735	-0.57039
H	3.24593	-0.34338	-0.74872
O	-1.64619	-2.47679	1.29103
H	-2.53744	-2.40694	1.63785
H	-2.64386	-0.25763	-1.09026
H	-2.13177	2.24817	-1.53754
H	4.44933	-1.40694	-0.22962
H	0.72930	-1.44193	-0.94960
N	4.13075	-0.44326	-0.16461
C	3.86943	-0.05997	1.24564
H	3.09426	-0.70687	1.63993
H	4.77811	-0.16990	1.82607
H	3.53477	0.97068	1.26592
H	4.85421	0.14159	-0.57530

*05\_sma-p1.mol2*

E = -1282.015869  
H = -1281.807756  
G = -1281.877396  
G(quasi-RRHO) = -1281.873172

Si	0.16254	-0.94169	-0.14277
O	-0.79487	-1.81710	-1.19300
H	-0.34462	-2.39452	-1.81186
O	0.81559	0.33363	-1.01273
O	1.26418	-1.74398	0.60853
H	2.72719	-1.47093	0.92650
H	0.16921	1.01406	-1.23912
O	3.71586	-1.25250	1.05029
H	3.85308	-1.08839	1.98621
Si	-2.37286	0.47349	0.26546
O	-3.31022	-0.59623	-0.53833
H	-2.77815	-1.26072	-0.99942
O	-1.83478	1.69360	-0.69317
O	-3.24866	1.13557	1.46605
H	-3.79711	0.55102	1.99324
O	-1.01814	-0.24474	0.79319
H	-2.47206	2.15699	-1.24059
H	3.73630	0.11235	0.05745

H	2.51584	0.79358	-0.84212
H	4.07470	0.81713	-1.42971
N	3.51489	0.91206	-0.58725
C	3.75317	2.21561	0.07327
H	3.14205	2.26604	0.96761
H	4.80092	2.29479	0.34067
H	3.48217	3.01938	-0.60198

*06\_sma-p3.mol2*

E = -1282.016046  
H = -1281.807807  
G = -1281.874823  
G(quasi-RRHO) = -1281.871921

Si	-0.45294	1.47857	-0.45145
O	-1.24998	1.01540	0.89790
H	-0.67876	0.93289	1.71353
O	-1.55182	1.82142	-1.61091
O	0.42425	0.57837	2.87006
H	0.82797	1.35239	3.26987
H	-1.69311	1.15785	-2.28831
O	0.51507	0.30254	-1.00643
O	0.35375	2.84339	-0.05961
Si	1.50382	-0.81755	-0.28768
O	2.70998	-1.13754	-1.37113
O	1.99517	-0.43218	1.14704
H	1.11185	0.17749	2.22718
O	0.51296	-2.17035	-0.37450
H	0.92143	-2.98839	-0.08047
H	3.56927	-0.79248	-1.12272
H	0.93882	3.21956	-0.72020
H	-1.96824	-0.68590	0.79238
H	-2.20747	-2.16234	1.51340
H	-1.15949	-2.01167	0.23164
C	-3.19396	-1.99039	-0.30945
H	-3.25083	-3.06055	-0.47119
H	-4.11804	-1.62960	0.12715
H	-3.00625	-1.48411	-1.24937
N	-2.07294	-1.70077	0.61745

*07\_sma-p3.mol2*

E = -1282.012878

H = -1281.805018  
G = -1281.873586  
G(quasi-RRHO) = -1281.869866

Si	-0.63044	1.32417	-0.29366
O	-1.26656	0.65368	1.04916
H	-0.65348	0.48255	1.82636
O	-1.73481	0.86495	-1.42650
O	0.41302	0.06570	2.93273
H	0.76246	0.81329	3.42349
H	-1.64297	1.22285	-2.31176
O	0.85995	0.81559	-0.62414
O	-0.50149	2.95244	-0.22554
Si	1.80203	-0.50933	-0.28434
O	3.16288	-0.31823	-1.21153
O	2.10453	-0.70774	1.24233
H	1.15456	-0.24776	2.28330
O	0.94393	-1.72238	-1.02660
H	1.28219	-2.60719	-0.87621
H	3.92873	-0.00763	-0.72593
H	-1.30516	3.44985	-0.06169
H	-2.48397	-0.63066	0.65577
H	-3.98714	-1.29677	0.33005
N	-3.02506	-1.23233	0.00816
C	-2.39701	-2.57151	-0.13533
H	-2.41642	-3.06838	0.82777
H	-2.95582	-3.14718	-0.86387
H	-1.37276	-2.43204	-0.46568
H	-3.00649	-0.71529	-0.87401

*08\_sma-p2.mol2*

E = -1282.009030  
H = -1281.801713  
G = -1281.873496  
G(quasi-RRHO) = -1281.868008

Si	-0.08907	0.09978	0.02519
O	-0.77377	0.14386	1.53305
H	-1.61870	-0.32145	1.55066
O	-1.00045	-0.66754	-0.99978
O	-3.02449	-1.38922	0.25966
H	-3.02864	-2.34206	0.38057
H	-2.19561	-1.14504	-0.33394
O	0.27685	1.67509	-0.40078

H	-0.41269	2.15514	-0.86268
Si	2.96631	-0.09294	-0.02500
O	3.87222	-0.26569	1.32372
H	3.57620	0.19700	2.10959
O	3.00057	1.43528	-0.60017
O	3.72578	-1.12055	-1.04285
H	3.46115	-1.09559	-1.96403
O	1.42590	-0.51798	0.24869
H	2.11050	1.82279	-0.65900
H	-5.31957	-0.12319	-1.50018
H	-4.41955	-0.77318	-0.22877
N	-5.32303	-0.27444	-0.49445
C	-5.44653	1.00985	0.23934
H	-5.44334	0.80131	1.30284
H	-4.59840	1.63473	-0.01625
H	-6.37009	1.50244	-0.04167
H	-6.10327	-0.89271	-0.28692

*09\_sma-p1.mol2*

E = -1282.009445

H = -1281.801929

G = -1281.872506

G(quasi-RRHO) = -1281.867388

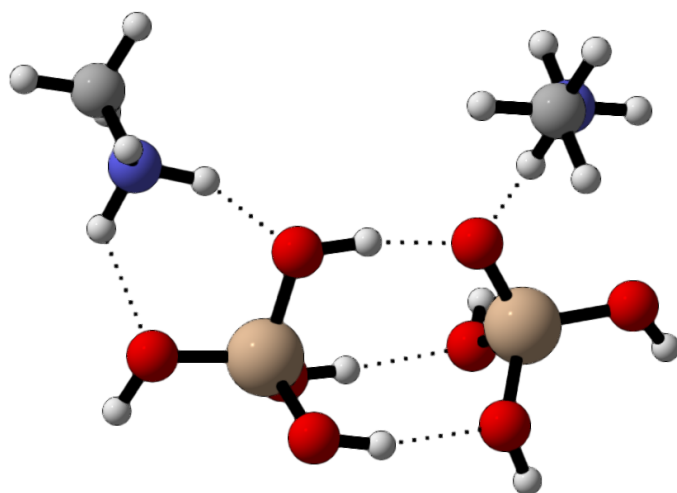
Si	0.01110	0.84674	-0.32227
O	-0.37824	-0.03040	1.05490
H	-1.13569	-0.61001	0.89343
O	0.10167	2.44029	0.10867
O	-0.98529	0.50600	-1.48870
H	-1.93131	-0.49340	-1.03813
H	-0.73658	2.90544	0.12574
O	-2.56467	-1.17446	-0.55270
H	-2.41334	-2.04217	-0.93607
Si	2.75540	-0.39495	0.10496
O	2.12860	-1.09866	1.43864
H	1.18243	-0.89142	1.54749
O	4.08062	0.48623	0.47416
O	3.38740	-1.48342	-0.93695
H	2.77509	-2.08250	-1.36754
O	1.60021	0.49583	-0.60451
H	3.99958	1.10926	1.19840
H	-5.73653	-1.16072	-0.65640
H	-4.11266	-0.74187	-0.47129
N	-5.11775	-0.42508	-0.32414

C	-5.36834	-0.11962	1.10655
H	-5.17751	-1.01434	1.68785
H	-4.69307	0.67070	1.41318
H	-6.39680	0.19717	1.23543
H	-5.28263	0.39087	-0.90828

Two  $\text{CH}_3\text{NH}_3^+$

RC-2ma, Reactant Complexes

*00\_2ma-c.mol2*



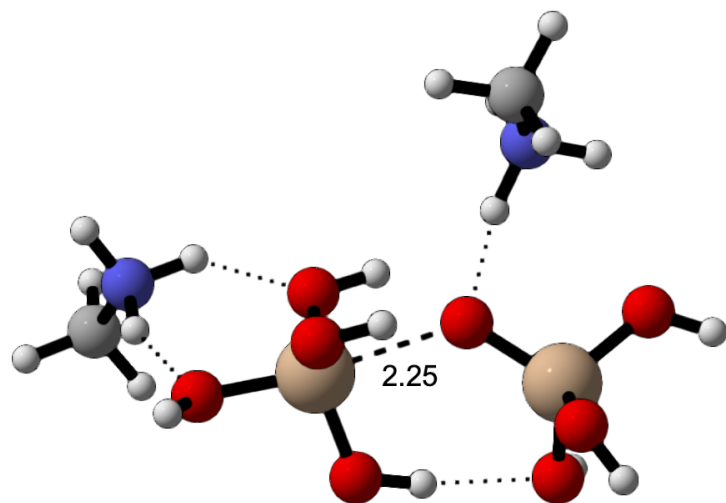
E = -1378.333501  
H = -1378.040494  
G = -1378.120406  
G(quasi-RRHO) = -1378.114850

Si	-1.54511	-1.15693	0.35013
O	-0.82425	-1.60322	1.74437
H	0.14491	-1.67322	1.69941
O	-1.20662	0.39345	-0.03913
O	-1.17744	-2.18528	-0.86211
H	-0.25113	-2.18172	-1.15885
H	-0.22048	0.58785	-0.12674
O	-3.16778	-1.13474	0.56737
H	-3.61389	-1.95062	0.80182
Si	2.15864	-0.72044	-0.29667
O	1.57782	-1.79393	-1.43098
H	1.73456	-1.56717	-2.35112
O	1.92996	-1.56870	1.11366
O	3.74895	-0.43015	-0.58132

H	4.32483	-1.18188	-0.73409
O	1.35830	0.63740	-0.22103
H	2.34586	-2.43267	1.17083
H	-2.62489	1.46195	-0.02106
N	-3.64024	1.66664	0.05409
H	-3.78565	2.34429	0.79831
C	-4.21125	2.13623	-1.23292
H	-5.27607	2.29622	-1.11201
H	-3.72344	3.06173	-1.51495
H	-4.03146	1.37714	-1.98533
H	-4.04828	0.77524	0.34705
H	3.41780	2.91240	-0.34524
N	2.41618	2.98532	-0.18925
H	1.98727	1.97786	-0.23063
C	2.12669	3.62270	1.11583
H	1.05131	3.68307	1.24043
H	2.55017	3.00809	1.90227
H	2.55931	4.61647	1.14914
H	2.03405	3.53223	-0.95570

TS1-2ma, Si-O bond association

[00\\_2ma-d.mol2](#)



E = -1378.320940  
H = -1378.026854  
G = -1378.104440  
G(quasi-RRHO) = -1378.099602

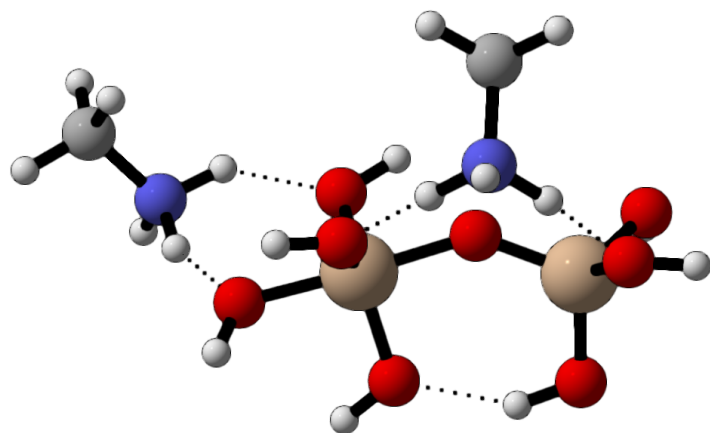
Si	-1.09306	-0.41409	0.64339
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O	-0.46958	0.18010	2.05022
H	0.46827	0.36634	1.95188
O	-1.50208	0.58990	-0.61419
O	-0.77804	-1.97366	0.24322
H	0.02523	-2.16765	-0.25648
H	-0.74033	0.76707	-1.17130
O	-2.68695	-0.59533	1.19550
H	-2.76567	-0.70434	2.14460
Si	2.22075	-0.83013	-0.34486
O	1.78747	-2.26789	-1.04737
H	1.68867	-2.27232	-2.00234
O	2.93836	-1.26526	1.06552
O	3.25668	0.00645	-1.31939
H	4.14442	-0.33881	-1.43418
O	0.97323	0.11859	-0.08017
H	3.48611	-2.05250	1.05982
H	-3.42795	1.13771	-0.95526
N	-4.28036	0.87398	-0.45247
H	-4.70521	1.71423	-0.06948
C	-5.22943	0.12460	-1.30929
H	-6.08776	-0.16338	-0.71346
H	-5.54239	0.75560	-2.13312
H	-4.72831	-0.75889	-1.68771
H	-3.90728	0.29271	0.32729
H	2.76859	2.29143	-1.09014
N	1.92618	2.56925	-0.58733
H	1.43532	1.65344	-0.35621
C	2.24803	3.33980	0.63732
H	1.32257	3.59336	1.14156
H	2.86059	2.72093	1.28323
H	2.78553	4.24213	0.36957
H	1.34664	3.10982	-1.22389

IM1-2ma, three equatorial OH groups

*00\_2ma-e.mol2*



E = -1378.337527  
 H = -1378.041744  
 G = -1378.117489  
 G(quasi-RRHO) = -1378.113266

Si	0.78917	-0.24145	-0.47943
O	0.31363	-1.61858	-1.33646
H	1.03502	-2.04330	-1.80320
O	0.49829	1.28225	-1.16200
O	1.53876	-0.36540	1.02260
H	0.88606	-0.35080	1.72502
H	1.26885	1.65886	-1.59087
O	2.42670	-0.29731	-1.18573
H	2.47433	-0.26497	-2.14242
Si	-2.19799	-0.89798	0.33474
O	-2.18279	-2.26404	-0.56036
H	-1.33411	-2.31898	-1.03787
O	-3.30070	0.20553	-0.21769
O	-2.72615	-1.26143	1.84431
H	-2.42287	-2.09160	2.21690
O	-0.79147	-0.14278	0.28105
H	-4.23048	0.03617	-0.05303
N	-1.83605	2.59769	-0.60162
H	-2.52788	1.83605	-0.53362
H	-2.12601	3.23715	-1.33608
H	-0.93230	2.15058	-0.87715
C	-1.69362	3.29573	0.69748
H	-0.94658	4.07550	0.60117
H	-2.64638	3.72763	0.98204
H	-1.37713	2.57008	1.43804
H	3.53254	-0.49813	1.38873

N	4.29390	-0.47721	0.70475
H	3.76018	-0.43891	-0.19906
C	5.18012	0.69427	0.88578
H	5.93093	0.69277	0.10383
H	4.57938	1.59420	0.81687
H	5.65707	0.64166	1.85781
H	4.80875	-1.35107	0.76150

*01\_2ma-e.mol2*

E = -1378.330900  
H = -1378.034774  
G = -1378.110176  
G(quasi-RRHO) = -1378.106006

Si	0.70330	-0.54616	0.09260
O	1.09233	-0.30178	1.70166
H	1.98528	-0.58138	1.90711
O	-0.05974	-1.98816	-0.37196
O	1.06318	0.60806	-1.08421
H	1.86350	0.42392	-1.57710
H	0.52182	-2.63180	-0.77935
O	2.33707	-1.28758	-0.24353
H	2.46221	-2.14459	0.17242
Si	-1.72922	1.43580	-0.01077
O	-0.89659	2.46405	-0.97042
H	-0.06941	2.03450	-1.25467
O	-2.32288	2.27925	1.26384
O	-3.08096	0.83252	-0.75189
H	-3.84183	1.40887	-0.84665
O	-0.86465	0.14974	0.36305
H	-1.74169	2.93438	1.65486
H	5.04971	-0.09549	-1.35334
N	4.83125	-0.26726	-0.37463
H	5.46857	-0.99063	-0.04974
C	4.97608	0.97230	0.43054
H	4.74806	0.74197	1.46469
H	5.99218	1.33948	0.34621
H	4.27947	1.71235	0.05425
H	3.84266	-0.65273	-0.32109
H	-3.05171	-0.99886	-0.76094
N	-2.79702	-1.98512	-0.59969
H	-1.75327	-2.02756	-0.58753
C	-3.34551	-2.46323	0.69122
H	-3.05054	-3.49536	0.84239

H	-2.93878	-1.84331	1.48204
H	-4.42662	-2.38458	0.67575
H	-3.14175	-2.54073	-1.37749

*02\_2ma-e.mol2*

E = -1378.327499  
H = -1378.031688  
G = -1378.107903  
G(quasi-RRHO) = -1378.103864

Si	-0.60078	-0.72325	0.56326
O	0.18685	0.23961	1.71097
H	1.13002	0.05785	1.80705
O	-1.06907	0.05799	-0.86975
O	-0.90744	-2.32923	0.90747
H	-0.16741	-2.88295	0.64993
H	-0.43302	-0.10969	-1.56849
O	-2.16432	-0.24763	1.20384
H	-2.35087	-0.63282	2.06111
Si	2.39733	-0.56514	-0.40159
O	3.47113	-1.50107	-1.19955
H	3.27288	-1.74029	-2.10723
O	2.99869	-0.33086	1.11107
O	2.23806	0.89357	-1.17560
H	3.00867	1.23756	-1.63392
O	0.95129	-1.20268	-0.23283
H	3.76328	0.23782	1.22202
H	-3.17229	0.41878	-1.42463
N	-3.89664	0.30417	-0.71594
H	-4.37352	1.19339	-0.59778
C	-4.84481	-0.77865	-1.06276
H	-5.56387	-0.88525	-0.25844
H	-5.35588	-0.53429	-1.98705
H	-4.28679	-1.70080	-1.18043
H	-3.33821	0.08177	0.15834
H	1.01181	2.20340	-0.48552
N	0.18024	2.53544	0.02379
H	0.16068	1.99135	0.90077
C	0.17877	4.00115	0.23507
H	-0.71585	4.27776	0.78075
H	1.05962	4.27273	0.80534
H	0.19411	4.49643	-0.72893
H	-0.62559	2.20473	-0.51017

03\_2ma-e.mol2

E = -1378.323194

H = -1378.027686

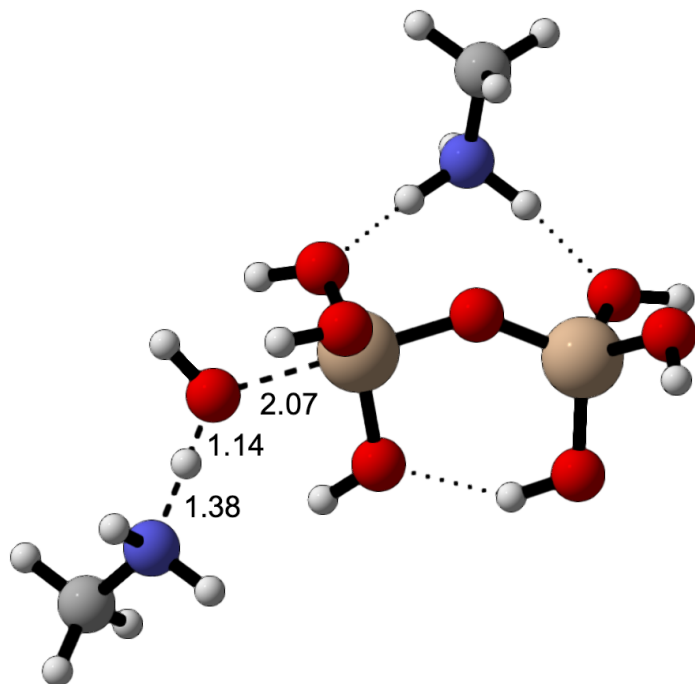
G = -1378.105513

G(quasi-RRHO) = -1378.100879

Si	-0.89177	-0.38309	0.49142
O	-0.39778	0.17477	1.99345
H	0.54404	0.34732	2.03195
O	-1.49595	0.61476	-0.72306
O	-0.74928	-2.00349	0.13438
H	0.03220	-2.27257	-0.35817
H	-0.83798	0.80275	-1.39339
O	-2.51993	-0.57056	1.10749
H	-2.53502	-0.61447	2.06449
Si	2.17806	-0.84118	-0.29465
O	1.94827	-2.29067	-1.04035
H	1.92917	-2.29747	-2.00028
O	2.74782	-1.19827	1.19494
O	3.20232	0.12180	-1.14865
H	4.11940	-0.14943	-1.22833
O	0.83097	0.01557	-0.16164
H	3.35781	-1.93306	1.28459
H	-3.52175	1.18161	-0.94765
N	-4.25361	0.82350	-0.33230
H	-4.69785	1.60829	0.13536
C	-5.23928	-0.00520	-1.06128
H	-5.96280	-0.39395	-0.35368
H	-5.74059	0.59734	-1.81028
H	-4.71481	-0.82615	-1.53716
H	-3.69663	0.25778	0.36983
H	2.62980	2.25423	-1.08756
N	1.77584	2.58850	-0.63836
H	1.24625	1.71809	-0.41557
C	2.07040	3.37908	0.58325
H	1.13354	3.69123	1.02942
H	2.61955	2.75123	1.27555
H	2.66380	4.24462	0.31356
H	1.24998	3.13364	-1.31707

TS2-2ma, water cleavage of IM1

00\_2ma-h.mol2



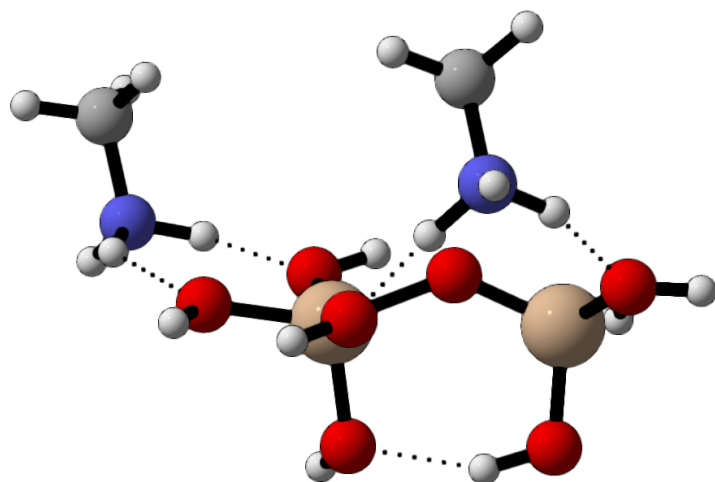
E = -1378.323218  
H = -1378.033062  
G = -1378.109887  
G(quasi-RRHO) = -1378.105027

Si	-0.63119	0.36177	0.28629
O	-0.99919	0.22255	1.88820
H	-1.88761	0.48688	2.12703
O	-0.16061	1.84333	-0.32243
O	-1.09839	-0.81670	-0.79185
H	-1.90643	-0.65384	-1.27967
H	-0.84595	2.37393	-0.73137
O	-2.55514	1.05897	0.00792
H	-2.75360	1.92526	0.37750
Si	1.91151	-1.37433	-0.02983
O	1.08026	-2.48287	-0.89019
H	0.19112	-2.15852	-1.10795
O	2.73069	-2.13316	1.16231
O	3.07527	-0.61190	-0.91774
H	3.86332	-1.10376	-1.15799
O	0.95491	-0.18795	0.47247
H	2.28140	-2.85023	1.61407
H	-5.03008	-0.14336	1.21388
N	-4.58922	-0.38222	0.33247
H	-4.31831	-1.35672	0.40585

C	-5.53805	-0.19624	-0.78032
H	-5.05070	-0.47024	-1.71155
H	-6.43328	-0.80099	-0.65623
H	-5.82121	0.85103	-0.83263
H	-3.46770	0.40015	0.17555
H	2.89008	1.20320	-0.96747
N	2.56459	2.16999	-0.81113
H	1.53345	2.11963	-0.69672
C	3.19914	2.75045	0.39727
H	2.83205	3.76006	0.54105
H	2.93398	2.13505	1.24938
H	4.27501	2.76070	0.26632
H	2.77345	2.71981	-1.64009

TS-iso-2ma, isomerization of IM1 to IM2

*00\_2ma-f.mol2*



E = -1378.322576  
H = -1378.028296  
G = -1378.103460  
G(quasi-RRHO) = -1378.099227

Si	0.71606	-0.24716	-0.70102
O	0.34140	-1.60117	-1.63472
H	0.92425	-2.34526	-1.46844
O	-0.09462	0.98174	-1.62561
O	1.60862	-0.90627	0.63137
H	1.02676	-1.11650	1.36281
H	0.34945	1.28743	-2.41761
O	2.26220	0.29113	-1.24958

H	2.27495	0.78896	-2.06629
Si	-2.07004	-0.85740	0.47337
O	-2.21145	-1.99440	-0.68974
H	-1.39809	-2.05081	-1.22545
O	-3.21428	0.32387	0.32744
O	-2.38380	-1.52795	1.93551
H	-2.06793	-2.42207	2.07946
O	-0.64714	-0.12243	0.37945
H	-4.09849	0.13215	0.64662
N	-1.82066	2.66391	-0.37390
H	-2.54325	1.99672	-0.06983
H	-2.24762	3.35050	-0.98911
H	-1.13261	2.09094	-0.92140
C	-1.16382	3.30789	0.78717
H	-0.39413	3.98263	0.42981
H	-1.90097	3.85761	1.36139
H	-0.72016	2.52968	1.39754
H	3.29694	-0.75295	0.82030
N	4.23637	-0.40293	0.52522
H	4.00135	0.00791	-0.38539
C	4.79068	0.59592	1.46605
H	5.72273	0.98447	1.07160
H	4.07211	1.40024	1.57629
H	4.96265	0.12181	2.42559
H	4.86917	-1.18544	0.38766

01\_2ma-f.mol2

E = -1378.320796

H = -1378.026182

G = -1378.100423

G(quasi-RRHO) = -1378.096542

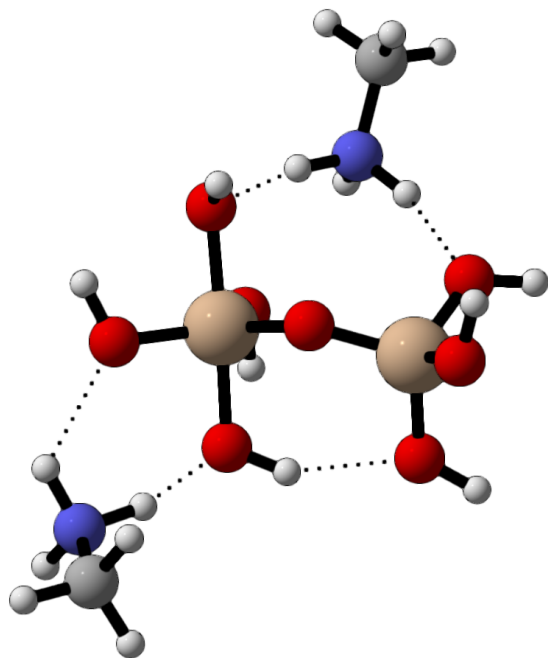
Si	-0.71788	0.33638	0.02660
O	0.19518	1.27904	1.19355
H	0.68651	0.70877	1.78876
O	0.13014	0.80637	-1.35996
O	-1.91832	-0.72552	-0.63448
H	-1.58969	-1.62241	-0.70764
H	-0.42437	0.85203	-2.14191
O	-2.00641	1.44128	0.26284
H	-1.71924	2.16764	0.81906
Si	1.59039	-1.64194	0.09794
O	1.70369	-1.67646	-1.53662
H	1.27801	-0.90672	-1.93705



O	1.90783	-3.14019	0.65882
O	2.74764	-0.66261	0.75468
H	3.63837	-1.01969	0.79588
O	0.16417	-1.06511	0.55978
H	1.48033	-3.87993	0.22293
H	-3.60392	-0.35138	-0.63489
N	-4.39202	0.28907	-0.39704
H	-4.90185	0.53744	-1.23956
C	-5.28280	-0.27419	0.64167
H	-6.03776	0.45769	0.90506
H	-5.75393	-1.17142	0.25671
H	-4.68443	-0.51745	1.51255
H	-3.86630	1.10696	-0.06187
H	2.93548	1.28152	-0.00541
N	2.39517	2.12912	-0.20000
H	1.54230	2.03608	0.39599
C	3.16547	3.36853	0.04482
H	2.53022	4.22244	-0.16057
H	3.48042	3.38466	1.08203
H	4.03255	3.38699	-0.60532
H	2.05286	2.05681	-1.15694

IM2-2ma, co-linear OH groups on Si

[00\\_2ma-g.mol2](#)



E = -1378.329262

H = -1378.034354  
G = -1378.111357  
G(quasi-RRHO) = -1378.106855

Si	-0.41609	-0.97786	-0.00710
O	0.78049	-1.86186	-0.99669
H	0.85584	-1.48000	-1.87413
O	0.37854	-1.60760	1.33299
O	-1.63075	-0.17812	1.01454
H	-1.37519	0.70732	1.29335
H	-0.08322	-1.36712	2.13833
O	-1.68995	-1.76063	-0.78122
H	-1.35895	-2.43252	-1.38034
Si	0.76774	1.86028	-0.09955
O	-0.14493	2.33132	1.17562
H	0.03936	3.16345	1.61528
O	0.72856	3.07497	-1.18603
O	2.32435	1.52337	0.32956
H	2.89326	2.25289	0.58661
O	0.13803	0.49424	-0.63791
H	1.35167	3.04981	-1.91508
H	-3.17430	-0.41737	0.65027
N	-4.08740	-0.74331	0.21484
H	-4.66540	-1.18900	0.92127
C	-4.80725	0.35787	-0.46238
H	-5.69704	-0.02967	-0.94570
H	-5.08156	1.10427	0.27450
H	-4.14727	0.79805	-1.20151
H	-3.76903	-1.45436	-0.44465
H	2.97965	-0.26840	0.42007
N	3.06210	-1.28964	0.33757
H	2.23026	-1.59882	-0.23622
C	4.35267	-1.69556	-0.25902
H	4.38187	-2.77649	-0.33904
H	4.43365	-1.25376	-1.24620
H	5.16890	-1.34999	0.36553
H	2.92424	-1.68089	1.26529

*01\_2ma-g.mol2*

E = -1378.329418  
H = -1378.034471  
G = -1378.110830  
G(quasi-RRHO) = -1378.106621

Si	-0.41801	-0.97575	-0.00377
O	0.77991	-1.85702	-0.99492
H	0.85338	-1.47393	-1.87202
O	0.38488	-1.59769	1.33523
O	-1.63298	-0.17956	1.01862
H	-1.37179	0.70264	1.30310
H	-0.07593	-1.35966	2.14182
O	-1.69024	-1.76520	-0.77380
H	-1.35763	-2.43536	-1.37400
Si	0.77485	1.85585	-0.10187
O	-0.14550	2.31534	1.17778
H	0.09558	3.09609	1.68032
O	0.86570	3.02901	-1.23052
O	2.32967	1.53325	0.32788
H	2.92100	2.27318	0.48446
O	0.12904	0.49715	-0.64023
H	0.06253	3.50718	-1.44676
H	-3.17728	-0.41655	0.65307
N	-4.08867	-0.74474	0.21615
H	-4.66814	-1.18898	0.92228
C	-4.80794	0.35334	-0.46666
H	-5.69619	-0.03679	-0.95074
H	-5.08475	1.10209	0.26690
H	-4.14664	0.79146	-1.20586
H	-3.76734	-1.45747	-0.44019
H	2.99318	-0.26196	0.40671
N	3.06769	-1.28393	0.32942
H	2.23113	-1.59106	-0.23874
C	4.35227	-1.70245	-0.27165
H	4.37337	-2.78404	-0.34496
H	4.43076	-1.26733	-1.26199
H	5.17422	-1.35866	0.34632
H	2.93181	-1.66911	1.25999

*02\_2ma-g.mol2*

E = -1378.329420

H = -1378.034446

G = -1378.110735

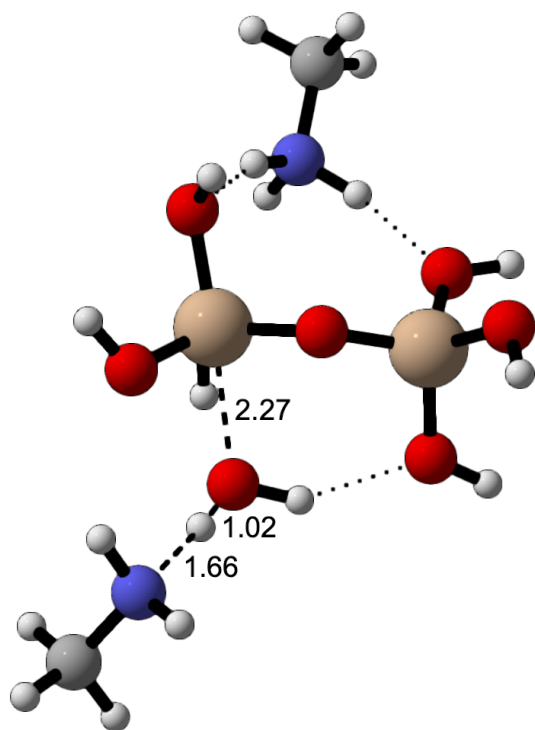
G(quasi-RRHO) = -1378.106536

Si	0.56539	-0.74127	0.18687
O	-0.53380	-1.86323	1.03971
H	-0.78892	-1.51487	1.89705
O	0.07479	-1.50084	-1.22932

O	1.70252	0.30146	-0.69368
H	1.30247	1.11608	-1.01574
H	0.56817	-1.16241	-1.97872
O	1.87224	-1.25895	1.11376
H	1.61663	-1.99089	1.67850
Si	-1.19500	1.77558	0.09658
O	-0.23389	2.44694	-1.05268
H	-0.56901	3.16741	-1.59014
O	-1.68870	2.87935	1.19013
O	-2.57113	1.13282	-0.53585
H	-3.28361	1.72986	-0.77574
O	-0.34787	0.57891	0.73188
H	-1.04296	3.51023	1.51484
H	3.21022	0.37725	-0.15129
N	4.13429	0.17375	0.33253
H	3.85991	-0.50900	1.04005
C	5.14478	-0.36958	-0.60173
H	6.04917	-0.61950	-0.05851
H	4.73769	-1.25876	-1.07014
H	5.36148	0.37624	-1.35812
H	4.46914	1.01011	0.80160
H	-2.82923	-0.75823	-0.66209
N	-2.71706	-1.77392	-0.55278
H	-1.90413	-1.90271	0.11079
C	-3.95764	-2.41717	-0.06904
H	-3.78218	-3.48037	0.05100
H	-4.22642	-1.98072	0.88659
H	-4.75597	-2.25409	-0.78454
H	-2.41457	-2.14602	-1.44899

TS3-2ma, water cleavage from IM2

[00\\_2ma-k.mol2](#)



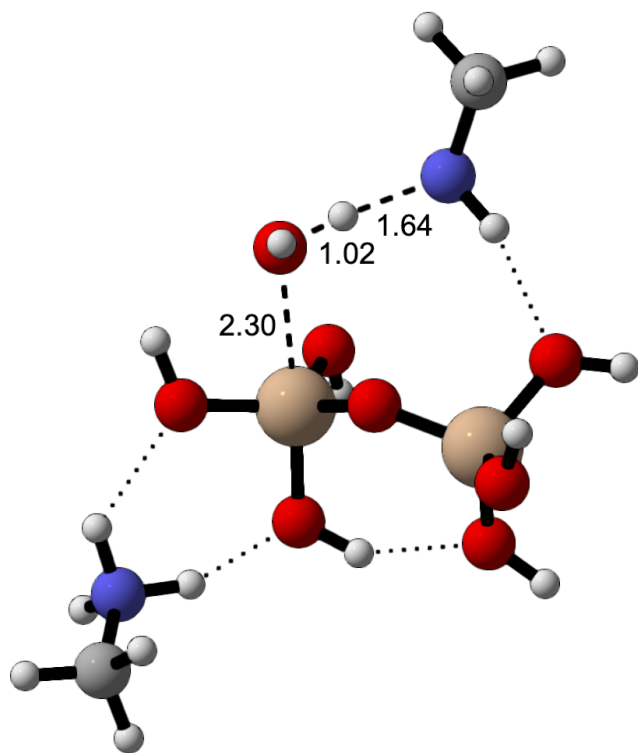
E = -1378.320869  
H = -1378.028749  
G = -1378.107125  
G(quasi-RRHO) = -1378.102103

Si	0.26853	-0.97415	0.38615
O	-0.92476	-1.87785	1.17713
H	-1.12329	-1.59807	2.07364
O	-0.15322	-1.52366	-1.10410
O	1.82631	0.07492	-0.88398
H	1.55702	0.98655	-1.06457
H	0.45393	-1.23040	-1.78843
O	1.64008	-1.46740	1.14140
H	1.48448	-2.17735	1.76911
Si	-0.89502	1.84550	0.12354
O	0.17323	2.37405	-0.99947
H	-0.02378	3.15790	-1.51663
O	-1.25819	2.99280	1.21473
O	-2.32176	1.35656	-0.52436
H	-2.95320	2.03009	-0.79017
O	-0.20051	0.55253	0.78133
H	-0.55057	3.55119	1.54377
H	2.75850	0.09298	-0.48264
N	4.26343	-0.01142	0.20943

H	4.04677	-0.64547	0.96897
C	5.31256	-0.56970	-0.64985
H	6.24453	-0.76898	-0.11922
H	4.95980	-1.50127	-1.08664
H	5.51988	0.12328	-1.46192
H	4.57506	0.85451	0.63062
H	-2.93446	-0.43745	-0.69045
N	-3.03463	-1.46055	-0.63533
H	-2.38653	-1.76620	0.11448
C	-4.43539	-1.87370	-0.38444
H	-4.47755	-2.95494	-0.32251
H	-4.76360	-1.43661	0.55171
H	-5.06165	-1.52333	-1.19666
H	-2.66850	-1.84686	-1.50246

TS4-2ma, water cleavage from IM2

[00\\_2ma-m.mol2](#)

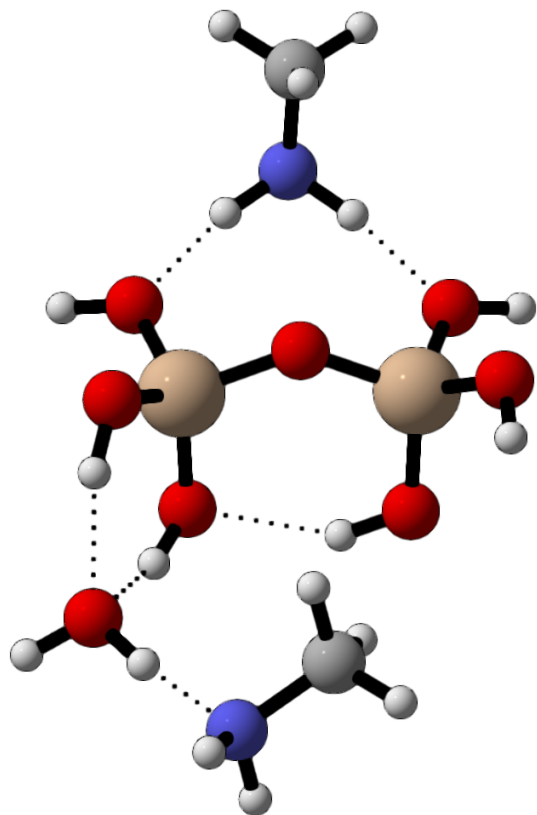


E = -1378.318070  
H = -1378.026135  
G = -1378.105308  
G(quasi-RRHO) = -1378.100061

Si	-0.56246	-0.79128	0.22687
O	0.97203	-2.03524	-0.95177
H	1.06825	-1.63989	-1.82407
O	0.25520	-1.54425	1.43675
O	-1.76705	0.03669	1.06792
H	-1.52557	0.93953	1.31227
H	-0.13123	-1.37483	2.29929
O	-1.58274	-1.68430	-0.70618
H	-1.15126	-2.40931	-1.16424
Si	0.81051	1.88650	-0.10311
O	-0.16607	2.40037	1.10660
H	-0.06260	3.28401	1.46518
O	0.69905	2.97473	-1.30758
O	2.36183	1.64651	0.35213
H	2.91774	2.41183	0.51449
O	0.23982	0.43450	-0.51544
H	1.36024	2.95539	-2.00248
H	-3.42044	-0.36072	0.62014
N	-4.17285	-0.84282	0.08801
H	-4.73858	-1.38809	0.73328
C	-4.99994	0.10505	-0.69766
H	-5.73383	-0.45102	-1.26900
H	-5.49535	0.78570	-0.01523
H	-4.34912	0.65775	-1.36530
H	-3.65257	-1.48767	-0.51159
H	3.13618	-0.42022	0.41771
N	3.24487	-1.42118	0.28629
H	1.86391	-1.85627	-0.48277
C	4.51688	-1.72181	-0.37738
H	4.61202	-2.79714	-0.51006
H	4.52544	-1.26147	-1.36293
H	5.38677	-1.36482	0.17591
H	3.21502	-1.83945	1.20744

PC-2ma, product complexes

*00\_2ma-p1.mol2*



E = -1378.338120  
 H = -1378.045186  
 G = -1378.124952  
 G(quasi-RRHO) = -1378.119754

Si	0.04465	-1.30728	-0.01540
O	-0.87931	-1.98704	-1.15884
H	-1.82124	-2.03516	-0.90627
O	1.39864	-2.19596	0.25145
O	-0.82826	-1.07821	1.34870
H	-1.77031	-1.32675	1.23223
H	1.30258	-3.13005	0.45263
O	-3.21433	-1.80042	0.28902
H	-3.74309	-2.55360	0.56515
Si	0.72984	1.62212	0.14719
O	-0.31425	1.74216	1.38746
H	-0.65215	0.89075	1.70407
O	0.43681	2.78955	-0.94184
O	2.30482	1.78179	0.58190
H	2.62812	2.64353	0.85499
O	0.67226	0.12216	-0.48136
H	-0.47764	3.02960	-1.10667



H	-5.19747	0.65455	0.63036
N	-4.72895	0.34196	-0.21110
H	-5.45819	0.14511	-0.88537
C	-3.84093	1.39708	-0.71810
H	-3.36323	1.05321	-1.63253
H	-4.36222	2.33098	-0.92960
H	-3.06162	1.59315	0.01491
H	-3.84818	-1.02652	0.11095
H	3.38328	0.29574	0.44509
N	3.79553	-0.63564	0.27764
H	3.01848	-1.31490	0.29734
C	4.51412	-0.67776	-1.02133
H	4.91461	-1.67357	-1.17076
H	3.81149	-0.43701	-1.81058
H	5.31728	0.04958	-1.00364
H	4.42018	-0.84890	1.05150

*01\_2ma-p2.mol2*

E = -1378.334442

H = -1378.041737

G = -1378.123134

G(quasi-RRHO) = -1378.117648

Si	0.28204	-0.59465	1.20256
O	-0.86824	-1.32979	2.09512
H	-1.05216	-0.99597	2.97567
O	0.27246	-1.48808	-0.15599
O	1.60853	-0.24406	-2.02238
H	1.06640	0.55777	-2.05603
H	0.79193	-1.10349	-0.92200
O	1.72932	-0.48479	1.94397
H	2.09645	-1.28485	2.32711
Si	-1.10959	1.76434	-0.08661
O	-0.35187	1.84176	-1.53257
H	-0.78658	2.32272	-2.24152
O	-1.50886	3.20650	0.53760
O	-2.52256	0.95057	-0.27899
H	-3.27382	1.26425	0.23230
O	-0.08583	0.96010	0.87704
H	-0.81508	3.79903	0.83457
H	2.44519	0.00494	-1.52786
N	3.79979	0.29010	-0.48860
H	3.40135	0.23176	0.44236
C	4.86835	-0.70246	-0.64720

H	5.67881	-0.58552	0.07398
H	4.45058	-1.70051	-0.53411
H	5.28607	-0.62726	-1.64857
H	4.17254	1.22568	-0.58877
H	-2.72647	-0.97235	-0.48567
N	-2.50443	-1.97493	-0.42941
H	-2.73879	-2.28063	0.51316
C	-3.21100	-2.76955	-1.46379
H	-2.92994	-3.81078	-1.35923
H	-4.27990	-2.65572	-1.32695
H	-2.91981	-2.40218	-2.44096
H	-1.47623	-2.03445	-0.50919

*02\_2ma-p2.mol2*

E = -1378.334940

H = -1378.042160

G = -1378.122703

G(quasi-RRHO) = -1378.117502

Si	-0.38852	-0.31816	1.45908
O	0.39867	-0.15699	2.87325
H	0.53660	-0.94004	3.41003
O	-0.39749	1.19351	0.85344
O	-1.42966	1.17595	-1.53777
H	-0.78093	0.58163	-1.94237
H	-0.83669	1.27349	-0.04689
O	-1.87494	-0.97578	1.61628
H	-2.43738	-0.63105	2.31380
Si	1.50236	-1.29861	-0.71130
O	0.76418	-0.66863	-2.02692
H	1.26646	-0.62771	-2.84483
O	2.15390	-2.76549	-0.94381
O	2.74537	-0.29840	-0.32660
H	3.48290	-0.68294	0.15536
O	0.36564	-1.34503	0.43967
H	1.57670	-3.53047	-0.99413
H	-2.27423	0.64087	-1.43762
N	-3.66599	-0.27940	-1.02729
H	-3.34812	-0.78403	-0.20692
C	-4.83893	0.53897	-0.70209
H	-5.68180	-0.04229	-0.32488
H	-4.56541	1.27436	0.05150
H	-5.16248	1.07649	-1.59053
H	-3.90327	-0.97236	-1.72557

H	2.56855	1.57629	0.10500
N	2.10262	2.43487	0.42710
H	2.59754	2.77596	1.24773
C	2.04790	3.46579	-0.64044
H	1.53714	4.34080	-0.25613
H	3.05828	3.72172	-0.93691
H	1.50364	3.05787	-1.48429
H	1.15306	2.13618	0.71486

*03\_2ma-p3.mol2*

E = -1378.331915  
H = -1378.039524  
G = -1378.122587  
G(quasi-RRHO) = -1378.116228

Si	0.10315	0.32007	-0.57921
O	3.03177	1.12014	1.47736
H	3.01626	1.03295	2.43420
O	1.26110	-0.34932	-1.51784
O	-1.07790	1.07268	-1.43148
H	-1.87087	0.53519	-1.57183
H	1.74297	0.23278	-2.11018
O	0.69446	1.48599	0.37983
H	1.58029	1.35630	0.82510
Si	-1.91002	-1.76644	0.27800
O	-2.80676	-1.11255	-0.92748
H	-3.73538	-1.34218	-1.00280
O	-2.75359	-1.56841	1.65505
O	-1.48497	-3.31878	0.03988
H	-2.14378	-4.00109	0.18432
O	-0.52050	-0.93197	0.24942
H	-2.48331	-2.06328	2.43142
H	-1.29781	3.07643	-0.96947
N	-0.86918	3.70098	-0.27964
H	-0.42254	4.46958	-0.77372
C	-1.85768	4.19032	0.71381
H	-1.34556	4.80976	1.44043
H	-2.61905	4.76602	0.20110
H	-2.30461	3.33345	1.20427
H	-0.13768	3.11521	0.15654
H	3.74025	-1.98693	0.90532
N	3.79907	-1.17751	0.30039
H	3.36760	0.24151	1.10795
C	5.11089	-1.12600	-0.35435

H	5.15303	-0.25525	-1.00484
H	5.88727	-1.01766	0.39949
H	5.33034	-2.01254	-0.95099
H	3.06117	-1.27338	-0.38917

04\_2ma-p3.mol2

E = -1378.331916  
H = -1378.039524  
G = -1378.122577  
G(quasi-RRHO) = -1378.116222

Si	0.10308	0.32016	-0.57934
O	3.03169	1.12100	1.47690
H	3.01608	1.03404	2.43377
O	1.26110	-0.34900	-1.51804
O	-1.07816	1.07247	-1.43161
H	-1.87110	0.53488	-1.57177
H	1.74282	0.23321	-2.11041
O	0.69419	1.48623	0.37965
H	1.58011	1.35679	0.82483
Si	-1.90958	-1.76674	0.27805
O	-2.80654	-1.11302	-0.92735
H	-3.73525	-1.34241	-1.00226
O	-2.75313	-1.56894	1.65515
O	-1.48416	-3.31898	0.03987
H	-2.14287	-4.00143	0.18416
O	-0.52024	-0.93196	0.24943
H	-2.48276	-2.06383	2.43148
H	-1.29867	3.07617	-0.96932
N	-0.86999	3.70079	-0.27960
H	-0.42363	4.46948	-0.77378
C	-1.85834	4.18992	0.71410
H	-1.34617	4.80945	1.44062
H	-2.61995	4.76549	0.20160
H	-2.30498	3.33295	1.20466
H	-0.13827	3.11513	0.15639
H	3.73993	-1.98625	0.90562
N	3.79894	-1.17701	0.30045
H	3.36746	0.24227	1.10772
C	5.11094	-1.12573	-0.35395
H	5.15326	-0.25517	-1.00469
H	5.88712	-1.01717	0.40007
H	5.33055	-2.01246	-0.95027
H	3.06120	-1.27304	-0.38925

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- 2 Y. Guan, V. M. Ingman, B. J. Rooks and S. E. Wheeler, *J. Chem. Theory Comput.*, 2018, **14**, 5249–5261.
- 3 V. M. Ingman, A. J. Schaefer, L. R. Andreola and S. E. Wheeler, *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, 2021, **11**, 1–12.