Supporting Information

Computational Study of the Effect of Mineral Dust on Secondary Organic Aerosol Formation by Accretion Reactions of Closed-Shell Organic Compounds

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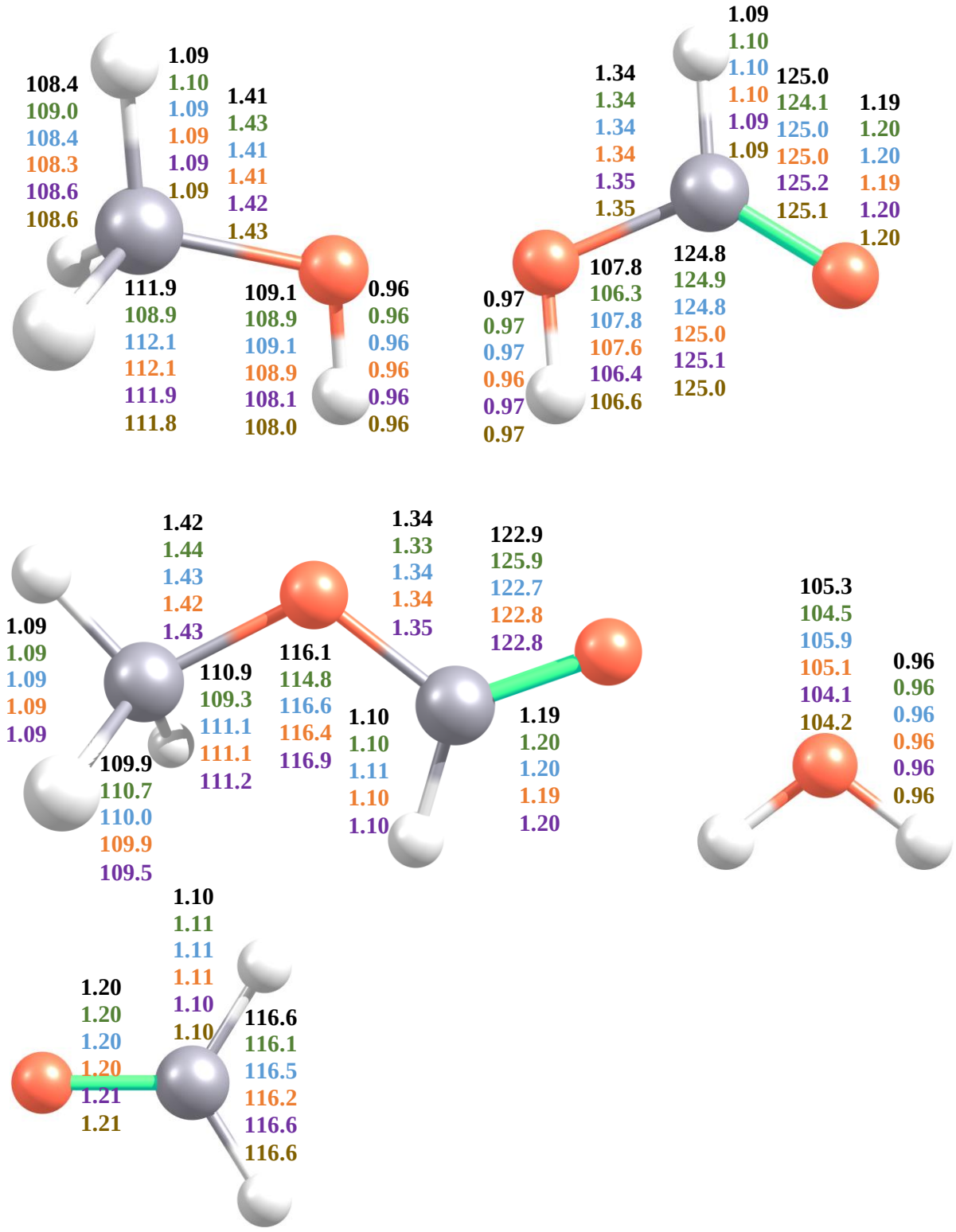


Figure S1. Geometries of the reactants and products at the M06-2X/aug-cc-pVTZ (black), ωB97X-D/6-31++G** (blue), ωB97X-D/aug-cc-pVTZ (orange), MP2/aug-cc-pVTZ (purple) and CCSD(T)/aug-cc-pVTZ (dark yellow) levels of theory as compared with the experimentally determined structures (green: CH_3OH[1], syn-$HCOOH$[2], CH_3CHO[3], H_2O[4] and CH_2O[5]).

Table S1. Reaction Enthalpy at Different Levels of Theory as Compared with Experimental Data, at 0 K

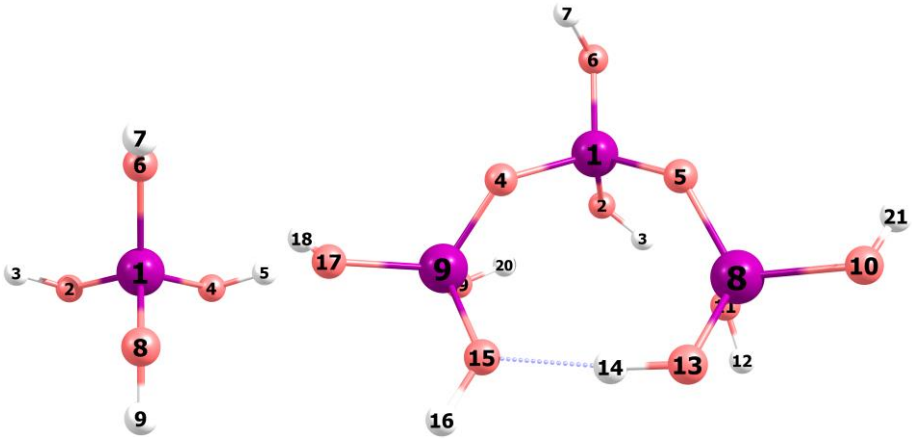
Products	CH_3OH+syn-HCOOH to $CH_3OCHO+H_2O$	syn-HCOOH to anti-HCOOH	CH_2O+H_2O to $CH_2(OH)_2$	MAE* (%)
ATcT**	-19.0	16.4	-34.9	-
ωB97X-D/6-31++G**	-17.1	20.0	-47.5	22.68
CCSD(T)/aug-cc-pVTZ//wB97X-D/6-311++G**	-20.8	16.7	-34.1	4.50
MPWB1K/aug-cc-pVTZ	-16.8	17.1	-49.4	19.15
wB97X-D/aug-cc-pVTZ	-17.2	16.4	-39.5	7.53
CBS-QB3	-26.2	15.7	-9.3	38.47
M06-2X/aug-cc-pVTZ	-18.5	17.5	-50.1	17.64
MP2/aug-cc-pVTZ	-22.5	16.8	-34.5	7.33
CCSD(T)/aug-cc-pVTZ	NA***	16.6	NA	-
CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ	-21.0	16.8	-35.1	4.54
DLPNO-CCSD(T)/aug-cc-pVTZ// ωB97X-D/6-31++G**	-21.0	16.8	-34.1	5.05
M06-2X/6-311++G**	-17.9	19.6	-49.2	22.06

***** Mean Absolute Error

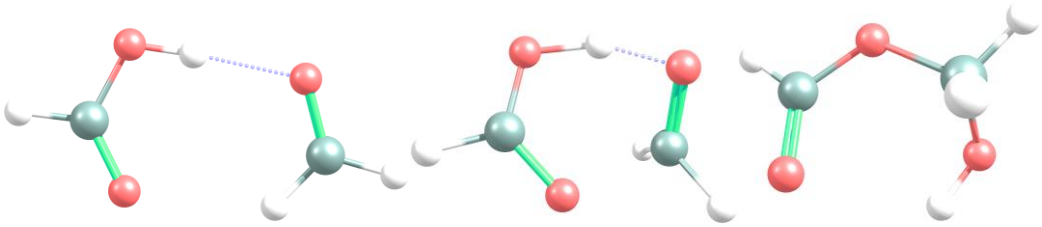
** Active Thermochemical Tables (version 1.122d); https://atct.anl.gov/

*** Not available

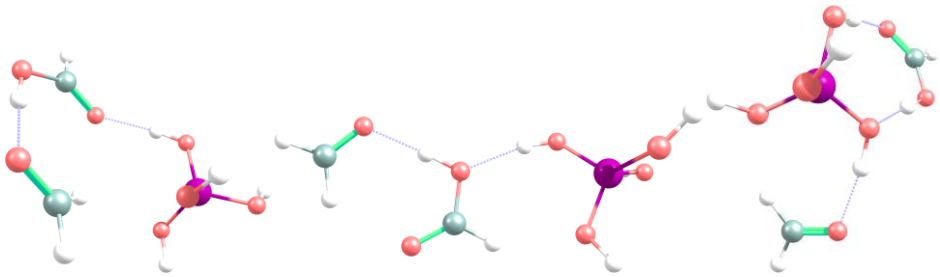
Table S2. Comparison of the Geometry of the Mono- and Tri-Silicic acid Models Optimized at the ωB97X-D/6-31++G** Level of Theory with the Experimentally Resolved SiO_2 Units' of Quartz, K-Feldspar and Kaolinite, as the Materials Representing Dust Particles



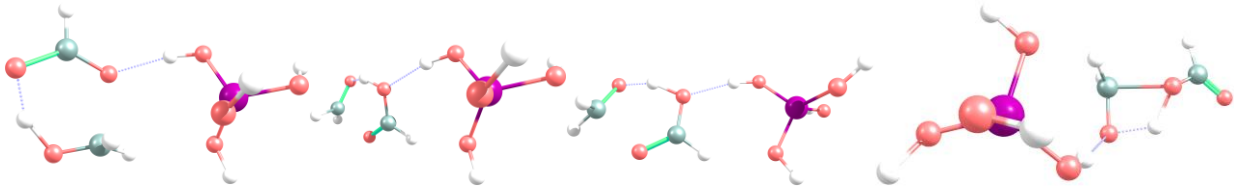
Structure	O6-H7 (Å)	Si1-O6 (Å)	H7-O6-Si1 (°)	H5-O4-Si1 (°)	O2-Si1-O4 (Mcat.) O4-Si1-O5 (Tcat.) (°)	O6-Si1-O2 (Mcat.) O6-Si1-O4 (Tcat.) (°)
ωB97X-D/6-31++G** (Mcat.)	0.96	1.64	116.1	117.4	102.8	112.5
ωB97X-D/6-31++G** (Tcat.)	0.96	1.63	117.8	-	109.1	109.5
Quartz[6]	-	1.60	-	-	89.4	112.5
Quartz[7]	-	1.58	-	-	109.7	109.9
Quartz[8]	-	1.59	-	-	107.4	110.1
K-Feldspar[9]	-	1.65	-	-	109.0	111.6
Orthoclase Feldspar[10]	-	1.62	-	-	109.5	112.0
Monoclinic K-feldspar[11]	-	1.64	-	-	104.4	111.8
Kaolinite[12]	-	1.60	-	-	106.6	111.6
Kaolinite[13]	-	1.61	-	-	106.4	111.6



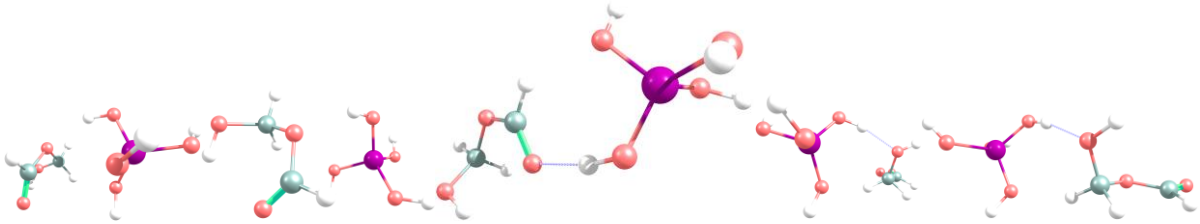
RC-FFA **TS-FFA** **HCO_2CH_2OH**



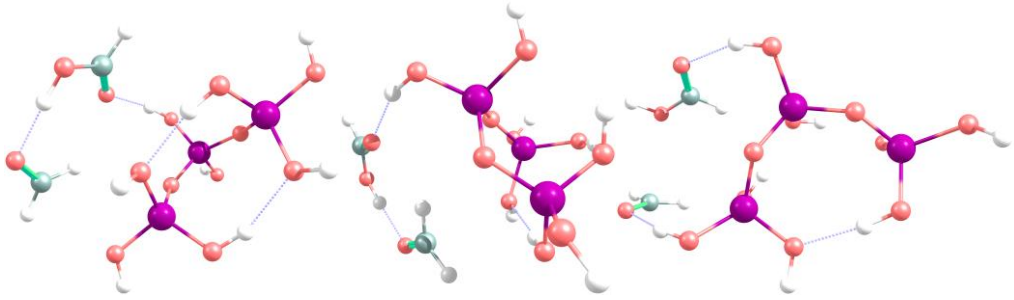
RC1(M)-FFA **RC2(M)-FFA** **RC3(M)-FFA**



TSM1-FFA **TSM2-FFA** **TSM2-FFA** **TSM3-FFA**



PC1(M)-FFA **PC1(M)-FFA** **PC2(M)-FFA** **PC3(M)-FFA** **PC3(M)-FFA**



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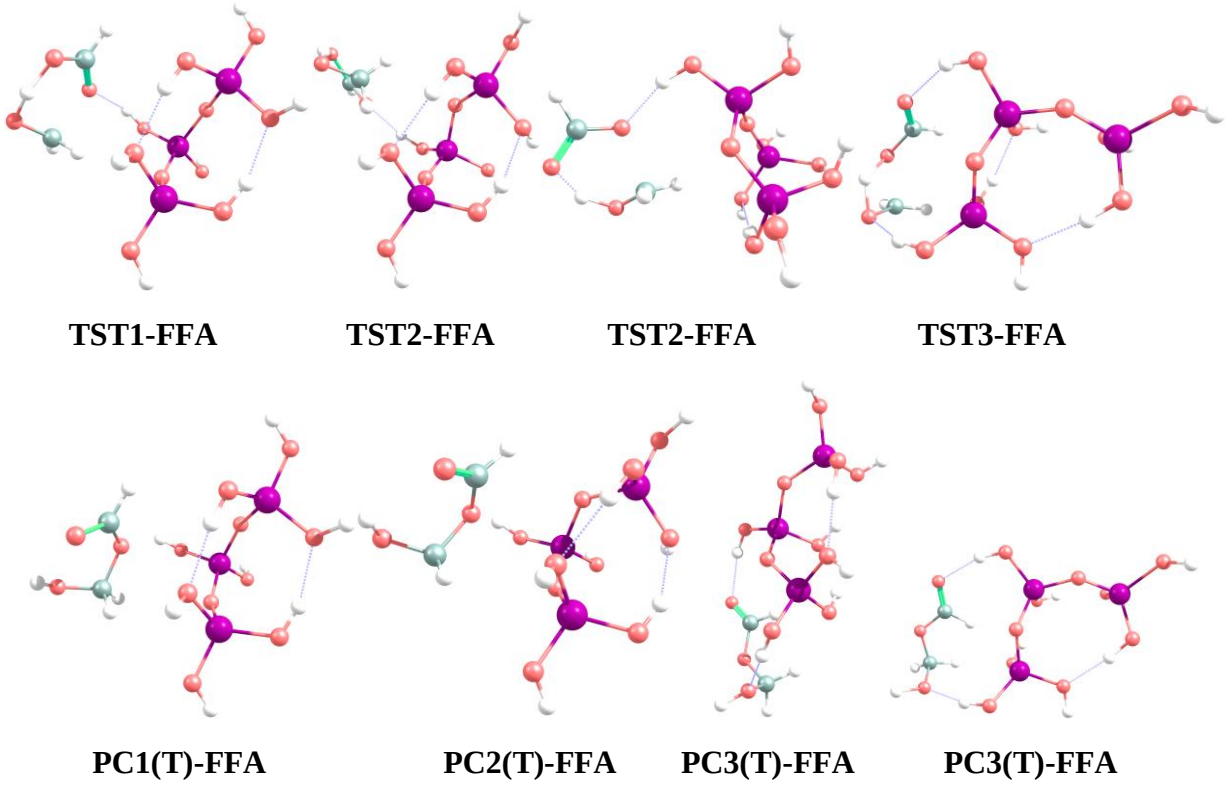
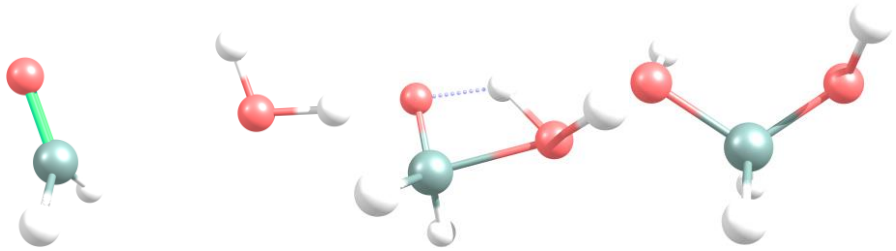
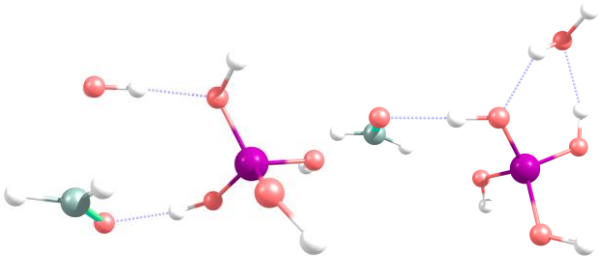


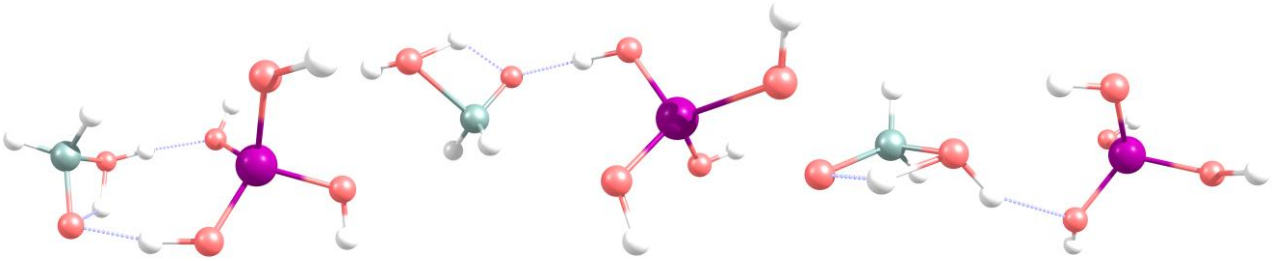
Figure S2. Geometries of the species involved in R7. The blue dotted lines represent H-bonding.



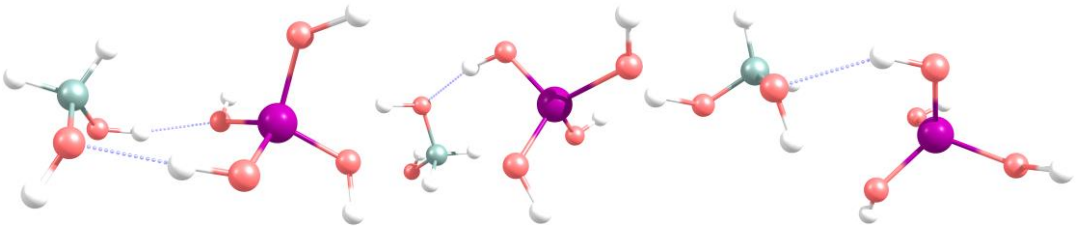
RC-FW **TS-FW** **$CH_2(OH)_2$**



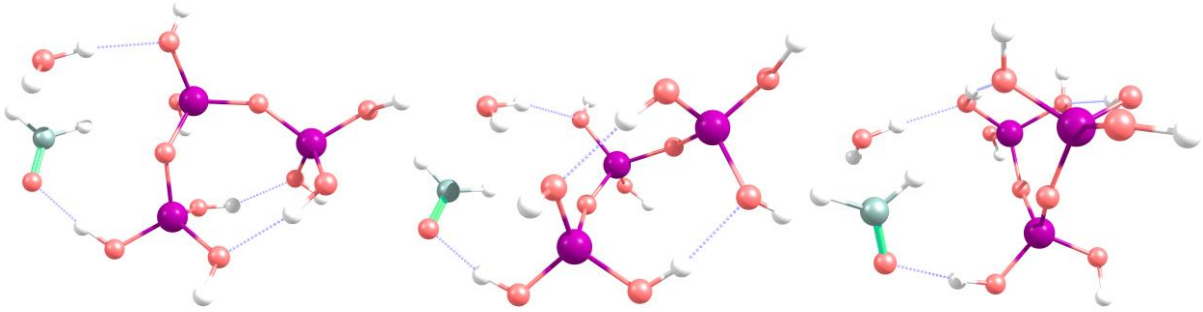
RC1(M)-FW **RC2(M)-FW**



TSM1-FW **TSM2-FW** **TSM3-FW**



PC1(M)-FW **PC2(M)-FW** **PC3(M)-FW**



RC1(T)-FW **RC2(T)-FW** **RC3(T)-FW**

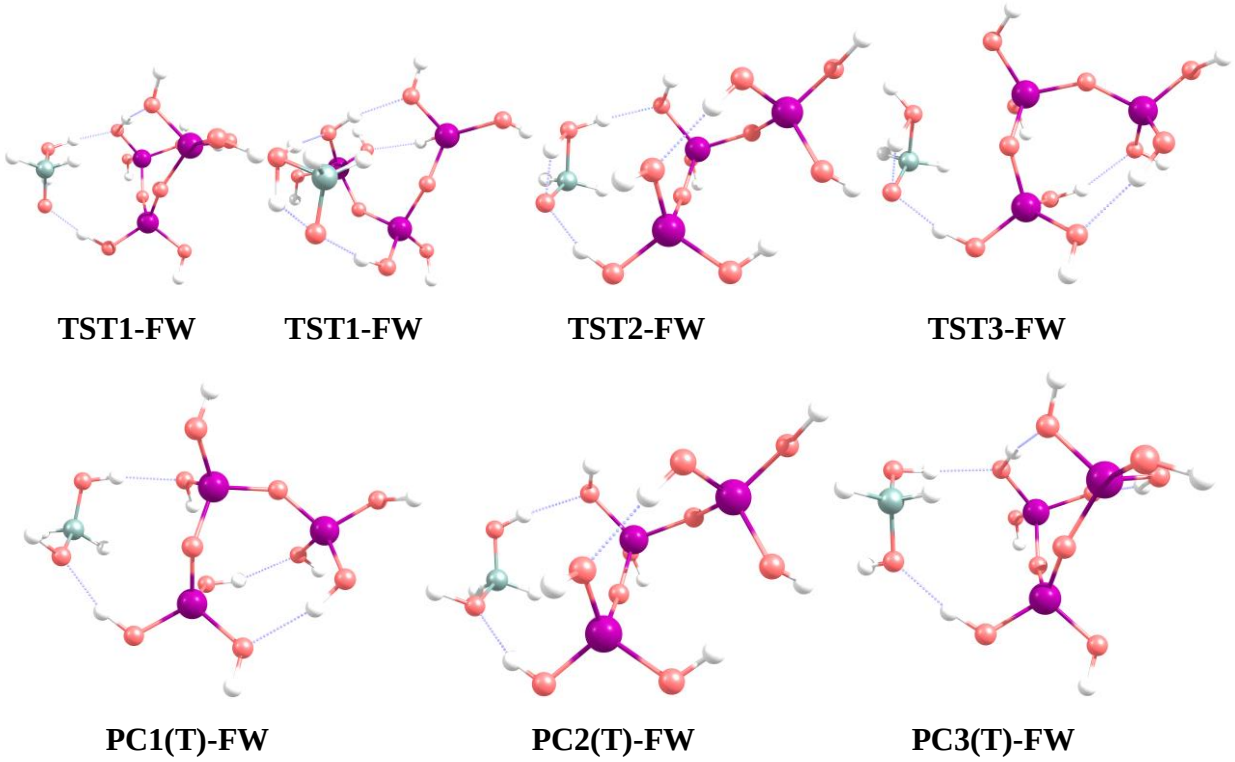
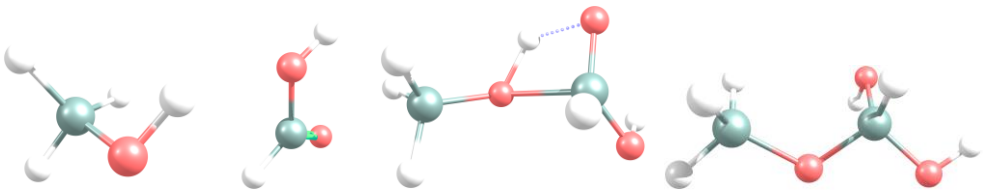
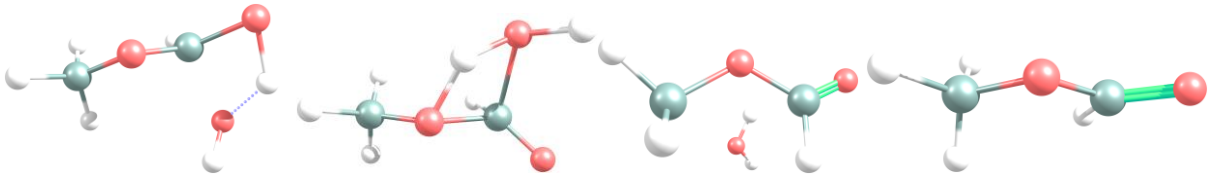


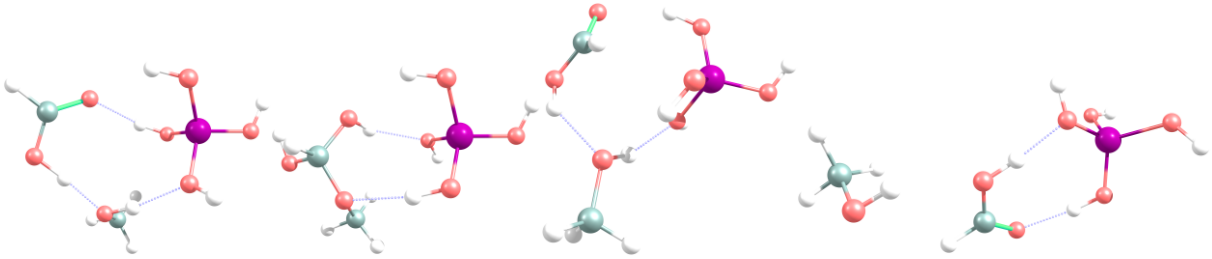
Figure S3. Geometries of the species involved in R8. The blue dotted lines represent H-bonding.



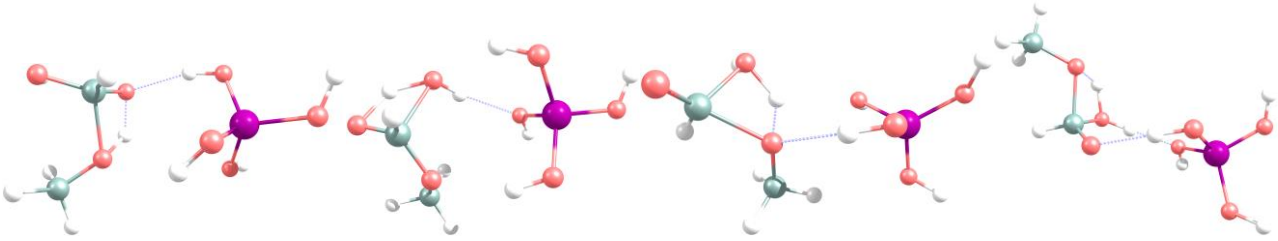
RC-FAM **TS1-FAM** **INT**



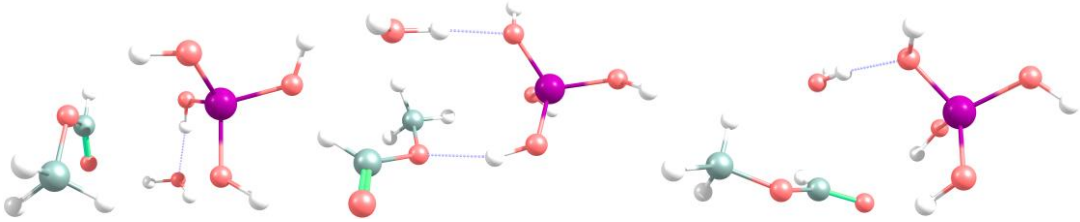
TS2-FAM **TS3-FAM** **PC-FAM** **CH_3OCHO**



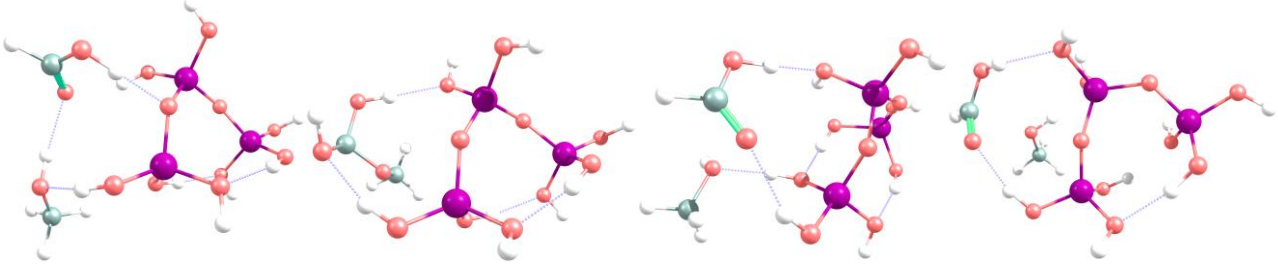
RC1(M)-FAM **INTM** **RC2(M)-FAM** **RC3(M)-FAM**



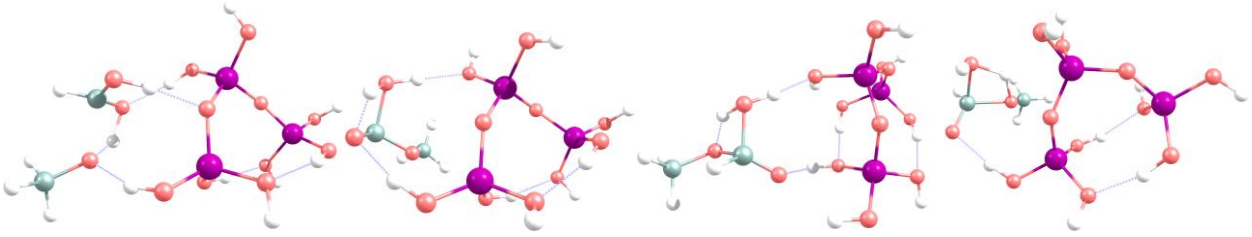
TSM1-FAM **TSM2-FAM** **TSM3-FAM** **TSM4-FAM**



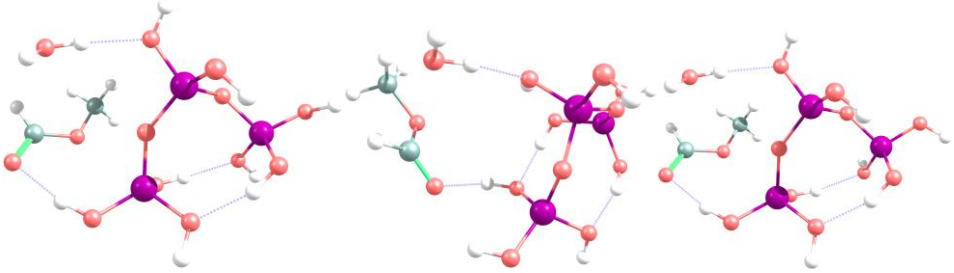
PC1(M)-FAM **PC2(M)-FAM** **PC3(M)-FAM**



RC1(T)-FAM **INTT** **RC2(T)-FAM** **RC3(T)-FAM**



TST1-FAM **TST2-FAM** **TST3-FAM** **TST4-FAM**



PC1(T)-FAM **PC2(T)-FAM** **PC3(T)-FAM**

Figure S4. Geometries of the species involved in R9. The blue dotted lines represent H-bonding.

Table S3. The Gibbs Free Energy Values of the Pre- and Post-Reaction Complexes Relative to the Reactants in kJ mol^{-1}, at 1 atm

	298 K	198 K		298 K	198 K
			R7		
RC1(M)-FFA	-3.7	-33.4	PC1(M)-FFA	-1.1	-34.2
RC2(M)-FFA	2.2	-25.9	PC2(M)-FFA	-11.9	-44.0
RC3(M)-FFA	-19.2	-49.0	PC3(M)-FFA	16.2	-14.2
RC-FFA	-10.9	-24.8	PC1(T)-FFA	-12.5	-43.9
RC1(T)-FFA	-9.7	-40.1	PC2(T)-FFA	-6.3	-39.9
RC2(T)-FFA	-7.1	-37.8	PC3(T)-FFA	-4.7	-38.8
RC3(T)-FFA	8.0	-22.2			
			R8		
RC1(M)-FW	26.9	-1.4	PC1(M)-FW	1.3	-30.1
RC2(M)-FW	17.7	-10.2	PC2(M)-FW	-0.1	-27.9
RC-FW	17.2	8.7	PC3(M)-FW	11.4	-18.8
RC1(T)-FW	22.8	-4.9	PC1(T)-FW	3.4	-27.4
RC2(T)-FW	152.6	123.3	PC2(T)-FW	9.0	-22.3
RC3(T)-FW	22.0	-5.6	PC3(T)-FW	-2.7	-33.2
			R9		
RC1(M)-FAM	25.0	-54.8	PC1(M)-FAM	-10.4	-42.9
RC2(M)-FAM	9.2	-21.8	PC2(M)-FAM	6.8	-23.3
RC3(M)-FAM	-3.8	-31.7	PC3(M)-FAM	-1.8	-32.0
RC-FAM	4.5	-6.5	PC-FAM	-0.2	-11.4
RC1(T)-FAM	-15.3	-46.0	PC1(T)-FAM	-3.3	-33.0
RC2(T)-FAM	-11.7	-43.1	PC2(T)-FAM	-5.6	-35.9
RC3(T)-FAM	3.0	-27.8	PC3(T)-FAM	2.2	-28.7

Table S4. The Imaginary Frequency (υ*; cm^{-1}), $\Delta_r^{\#}G$ (kJ mol^{-1}), $\Delta_r^{\#}H$ (kJ mol^{-1}), $\Delta_r^{\#}S$ (J mol^{-1}) and κ_r Values of the Studied Reaction Paths, at 1 atm

Reaction path	υ*	κ_r (298 K)	κ_r (198 K)	$\Delta_r^{\#}G$ (298 K)	$\Delta_r^{\#}G$ (198 K)	$\Delta_r^{\#}H$ (298 K)	$\Delta_r^{\#}H$ (198 K)	$\Delta_r^{\#}S$ (298 K)	$\Delta_r^{\#}S$ (198 K)
r0 (TS-FFA; R7)	1075.765	2.26	3.74	67.1	49.3	13.8	14.8	-178.8	-115.8
r1 (TSM1-FFA)	1128.974	2.25	3.82	77.8	45.4	-18.7	-18.8	-323.7	-215.3
r2 (TSM2-FFA)	1065.428	1.88	3.16	78.0	45.7	-18.1	-18.0	-322.4	-213.8
r3 (TSM3-FFA)	1717.919	3.33	6.67	204.0	173.1	112.2	111.8	-308.0	-205.8
r1 (TST1-FFA)	1151.572	2.13	3.67	69.9	38.2	-23.9	-24.5	-314.7	-210.4
r2 (TST2-FFA)	1034.359	1.90	3.13	75.6	42.5	-22.9	-23.2	-330.3	-220.4
r3 (TST3-FFA)	1710.352	3.90	7.50	191.8	156.8	87.7	87.6	-349.0	-232.0
r0 (TS-FW; R8)	1696.876	3.82	7.35	191.6	176.4	145.3	147.3	-155.3	-97.7
r1 (TSM1-FW)	1517.524	3.29	6.13	168.2	134.9	67.6	70.0	-337.4	-217.6
r2 (TSM2-FW)	1513.426	3.26	6.07	191.0	160.8	100.1	101.7	-304.7	-198.3
r3 (TSM3-FW)	1679.596	3.78	7.24	197.9	168.2	108.5	110.0	-299.8	-195.4
r1 (TST1-FW)	1502.738	3.26	6.05	157.0	124.3	58.5	60.4	-330.2	-214.2
r2 (TST2-FW)	1491.015	3.21	5.95	168.6	135.1	67.7	69.8	-338.3	-218.9
r3 (TST3-FW)	1525.924	3.30	6.16	197.2	164.4	98.7	100.1	-330.4	-215.5
r0 (TS2-FAM; R9)	1783.048	4.12	8.02	188.8	171.9	138.6	138.7	-168.5	-111.3
r0 (TS3-FAM; R9)	1335.441	2.75	4.93	204.3	187.8	155.4	155.4	-163.9	-108.8
r1 (TSM2-FAM)	1798.032	4.20	8.18	190.7	156.3	88.4	88.2	-343.2	-228.4
r2 (TSM3-FAM)	1283.003	2.61	4.63	231.7	199.8	137.3	136.4	-316.6	-212.8
r3 (TSM4-FAM)	1364.731	2.84	5.13	194.7	161.0	94.3	94.3	-336.6	-223.7
r1 (TST2-FAM)	1649.173	3.71	7.07	172.2	136.4	65.8	65.6	-356.7	-237.5
r2 (TST3-FAM)	1376.308	2.88	5.21	192.5	156.6	85.5	85.8	-358.9	-237.6
r3 (TST4-FAM)	1414.709	2.97	5.43	204.3	170.8	105.1	104.2	-332.7	-223.4

Section S.A. The Cartesian coordinates of the geometries optimized at the ωB97X-D/6-31++G** level.

Mcat

Si	-0.02408	0.00002	-0.01490
O	-1.04470	1.28060	-0.08022
H	-0.65897	2.14416	-0.23593
O	-1.04460	-1.28046	-0.08364
H	-0.65868	-2.14364	-0.24096
O	1.06831	0.00179	-1.24634
H	1.99320	0.00142	-0.99052
O	0.91917	-0.00186	1.34519
H	0.47619	-0.00287	2.19606

Tcat

Si	-0.008980	1.458860	-0.180210
O	0.080940	1.474160	1.466840
H	-0.665430	1.023960	1.892420
O	1.269520	0.588880	-0.744310
O	-1.401410	0.724070	-0.635790
O	0.074890	2.982830	-0.750800
H	0.377300	3.106200	-1.652570
Si	-2.200910	-0.600810	-0.081570
Si	2.179850	-0.584860	-0.055160
O	-3.742610	-0.633640	-0.620210
O	-2.111760	-0.364050	1.572410
H	-2.394120	-1.090250	2.133140
O	-1.537610	-2.012460	-0.529700
H	-0.568680	-2.079140	-0.469160
O	1.257590	-1.961380	-0.179840
H	1.708240	-2.796430	-0.030490
O	3.574020	-0.892540	-0.852100
H	4.346900	-0.390070	-0.585560
O	2.535040	-0.178270	1.492810
H	1.892500	0.417330	1.904280
H	-4.265100	0.162840	-0.509400

CH_2O

C	0.52978	0.00000	0.00000
O	-0.67543	0.00000	0.00000
H	1.11234	0.94104	0.00001
H	1.11239	-0.94101	0.00001

syn-HCO_2H

C	0.13126	0.40136	0.00000
O	1.13344	-0.26445	0.00000
O	-1.11357	-0.09153	0.00000
H	0.10347	1.49814	0.00000
H	-1.04998	-1.05849	0.00000

H_2O

O	0.00000	0.00000	0.11568
H	0.00000	0.76648	-0.46273
H	0.00000	-0.76648	-0.46273

CH_3OH

C	0.66286	-0.02061	0.00000
H	1.02454	-0.54695	-0.89318
H	1.08116	0.98744	-0.00137
H	1.02473	-0.54462	0.89448
O	-0.74484	0.12207	0.00000
H	-1.14887	-0.74879	0.00002

Reaction R7

RC-FFA

C	2.00453	0.51052	-0.00046
O	1.66464	-0.65530	0.00076
H	3.07461	0.77641	-0.00229
O	-1.06818	1.15990	0.00027
H	-0.07642	-0.98082	-0.00044
O	-1.05845	-1.09462	-0.00039
H	1.25443	1.31719	0.00057
C	-1.64150	0.09201	0.00003
H	-2.73483	-0.00785	-0.00036

TS-FFA

C	1.29462	0.41113	0.21512
O	1.27435	-0.76622	-0.26223
H	1.87827	1.17557	-0.30501
O	-0.37432	1.13329	-0.10832
H	0.10619	-1.13304	0.05296
O	-1.03758	-0.99731	0.15745
H	1.17595	0.56915	1.29513
C	-1.25512	0.23776	-0.06647
H	-2.29700	0.53690	-0.23013

HCO_2CH_2OH

C	-1.02132	-0.39258	0.39233
O	-1.47250	0.66835	-0.35961
H	-1.77162	-1.17919	0.35901
O	0.16446	-1.00827	-0.16750
H	-0.87920	1.41486	-0.20959
O	1.30004	0.89909	0.23267
H	-0.78352	-0.10956	1.42343
C	1.25297	-0.24229	-0.16537
H	2.10848	-0.79023	-0.57921

RC1(M)-FFA

Si	-1.81355	-0.12562	0.03398
O	-1.68310	0.36590	-1.53453
H	-2.17127	1.15403	-1.78161
O	-1.10106	-1.57876	0.19710
H	-0.17136	-1.65969	-0.07212
O	-1.12100	1.10145	0.90670
H	-1.24033	1.07561	1.85881
O	-3.36646	-0.26528	0.56125
H	-3.77507	-1.12780	0.46005
C	1.22418	1.90981	-0.36228
O	2.27173	1.85173	0.25433
H	0.85913	1.06085	-0.95821
H	0.61759	2.82665	-0.34617
C	2.73318	-1.44452	-0.03006
H	3.19229	-2.43788	0.04662
O	3.56670	-0.49430	0.31536
O	1.58627	-1.27042	-0.40048
H	3.10985	0.39260	0.27301

RC2(M)-FFA

Si	-2.31675	-0.12660	0.01112
O	-1.67770	1.39998	-0.00565

H	-2.11875	2.04184	0.55597
O	-1.19502	-1.12179	-0.63218
H	-0.26227	-0.94435	-0.43834
O	-2.74491	-0.39337	1.57802
H	-3.39750	-1.07872	1.73580
O	-3.68965	-0.31464	-0.87841
H	-3.56845	-0.54269	-1.80260
C	4.84939	-0.53824	0.12071
O	3.91707	-1.31608	0.08245
H	4.67888	0.54938	0.08629
H	5.88254	-0.91552	0.19048
C	1.58809	1.13400	-0.12810
H	0.61188	1.62862	-0.20468
O	1.44166	-0.19294	-0.09232
O	2.65557	1.70056	-0.07790
H	2.32709	-0.63438	-0.02637

RC3(M)-FFA

Si	-0.44723	-1.12651	-0.05584
O	-1.28365	-2.12482	-1.06126
H	-0.75750	-2.64582	-1.67198
O	-1.45639	-0.86082	1.22943
H	-1.88872	-1.64164	1.58345
O	0.98672	-1.81664	0.26541
H	1.72938	-1.23021	0.50794
O	-0.14939	0.38441	-0.66742
H	-0.90386	1.00856	-0.70447
C	-2.89330	1.95933	0.57713
O	-2.28446	2.10734	-0.46235
H	-3.73953	2.62146	0.82634
H	-2.61955	1.16280	1.28804
C	3.09699	1.10153	0.12999
H	4.01457	1.70061	0.18121
O	2.98146	0.03917	0.71266
O	2.18837	1.68077	-0.61956
H	1.34300	1.15494	-0.64677

TSM1-FFA

Si	-1.88633	-0.03130	0.02638
O	-1.54995	1.34840	-0.81729
H	-1.92317	2.16066	-0.46707
O	-1.19990	-1.28291	-0.75962
H	-0.23865	-1.23256	-0.89117
O	-1.29185	0.25219	1.54248
H	-1.60799	-0.31990	2.24528
O	-3.49172	-0.34772	0.18797
H	-3.90271	-0.86879	-0.50522
C	1.59744	1.22880	-0.09520
O	2.84115	1.46061	-0.11051
H	1.09024	0.93525	0.82899
H	0.96927	1.64841	-0.88259
C	2.48677	-1.27579	-0.08619
H	2.55843	-2.36250	-0.22687
O	3.39153	-0.72016	0.60368
O	1.51099	-0.67872	-0.62177
H	3.27584	0.50602	0.41809

TSM2-FFA

Si	-2.23295	-0.04342	0.01304
O	-1.42784	1.35026	-0.38254

H	-1.82228	2.16269	-0.05609
O	-1.21749	-1.28149	-0.29242
H	-0.27206	-1.15793	-0.11269
O	-2.70674	0.17211	1.57452
H	-3.43219	-0.37381	1.88480
O	-3.60599	-0.31747	-0.85214
H	-3.50162	-0.80363	-1.67294
C	4.14528	-0.01286	0.32916
O	3.74744	-1.14541	-0.07452
H	3.96851	0.30021	1.36538
H	5.00264	0.45008	-0.16609
C	1.70621	0.68970	-0.25263
H	0.82912	1.27520	-0.55175
O	1.47965	-0.52799	0.10159
O	2.83939	1.21883	-0.25769
H	2.51297	-1.05686	0.13318

TSM3-FFA

Si	-2.25540	-0.12780	0.03579
O	-3.22801	1.10046	-0.47079
H	-3.99645	0.85585	-0.99056
O	-1.39488	0.51966	1.29912
H	-1.90122	1.08045	1.89185
O	-3.25576	-1.36659	0.45636
H	-2.87918	-2.24787	0.40618
O	-1.17687	-0.71882	-1.02878
H	-0.34120	-0.23666	-1.17795
C	1.50681	1.05519	0.11591
O	1.23786	0.62247	-1.08377
H	2.13638	1.94625	0.22668
H	0.80898	0.83700	0.93005
C	4.03566	-0.16128	0.50451
H	4.24184	0.40342	1.42549
O	4.86939	-0.66375	-0.19243
O	2.70742	-0.24602	0.25597
H	2.17846	-0.19202	-0.82064

PC1(M)-FFA

Si	-1.78656	0.08525	0.06231
O	-0.73696	0.10108	1.33365
H	-0.74867	-0.66469	1.91297
O	-1.20612	1.13693	-1.05260
H	-0.27245	1.02183	-1.26996
O	-1.84235	-1.48829	-0.42645
H	-2.61113	-1.76014	-0.93253
O	-3.32453	0.54405	0.40696
H	-3.52377	1.48188	0.37113
C	2.19976	1.04923	0.16352
O	3.55807	0.85068	0.22915
H	1.68023	0.87215	1.10933
H	2.01769	2.05504	-0.20947
C	1.57034	-1.11792	-0.51882
H	0.99652	-1.69088	-1.25667
O	2.13325	-1.59565	0.43651
O	1.56081	0.18611	-0.82315
H	3.71545	0.02424	0.70224

PC2(M)-FFA

Si	-2.26314	-0.03481	0.00344
O	-1.40945	1.18344	-0.72909

H	-1.79973	2.05822	-0.66165
O	-1.27442	-1.32547	0.09162
H	-0.32556	-1.17420	0.24995
O	-2.78464	0.61417	1.42412
H	-3.53420	0.18621	1.84307
O	-3.61647	-0.50904	-0.80670
H	-3.49846	-1.20887	-1.45263
C	3.90465	0.30182	0.36688
O	4.18943	-0.91249	-0.21097
H	3.61559	0.21631	1.41961
H	4.76671	0.95258	0.24138
C	1.63917	0.44017	-0.24007
H	0.86261	1.02855	-0.74163
O	1.41914	-0.61720	0.32736
O	2.83139	1.00556	-0.31401
H	3.49415	-1.53523	0.03425

PC3(M)-FFA

Si	2.23363	0.14267	-0.00086
O	3.22976	-1.15862	0.16017
H	4.04842	-1.13561	-0.33970
O	1.28418	0.12715	1.35597
H	1.73160	-0.11257	2.17089
O	3.21797	1.45478	-0.14175
H	2.84180	2.22247	-0.57794
O	1.23069	0.15551	-1.28641
H	0.40067	-0.34317	-1.22787
C	-1.74273	-0.68612	0.45909
O	-1.15076	-1.20568	-0.69409
H	-2.27277	-1.46863	1.01859
H	-0.93410	-0.25972	1.05048
C	-3.95726	0.09921	0.14405
H	-4.19445	-0.93737	0.45182
O	-4.78512	0.90887	-0.15467
O	-2.63886	0.37022	0.14749
H	-1.79490	-1.65913	-1.24672

RC1(T)-FFA

Si	0.98135	0.58049	1.69647
O	1.71931	1.74417	2.57690
H	1.49272	1.76659	3.50870
O	-0.18487	1.22788	0.72839
O	2.10999	-0.06932	0.70222
O	0.31860	-0.49770	2.71891
H	-0.39668	-1.05066	2.35436
Si	2.36851	-0.77624	-0.73704
Si	-0.69432	1.54156	-0.77781
O	3.72874	-1.68154	-0.77651
O	2.58218	0.49529	-1.78833
H	2.98259	0.28245	-2.63512
O	1.10194	-1.72444	-1.17321
H	0.26283	-1.25426	-1.32075
O	-1.08456	0.04446	-1.39847
H	-1.58332	0.03842	-2.22007
O	-2.08741	2.41370	-0.77046
H	-2.00640	3.36693	-0.84795
O	0.40545	2.32827	-1.68803
H	1.27227	1.89538	-1.77766
H	3.66796	-2.59562	-0.49270
C	-3.87105	0.37983	0.32201

O	-4.18382	-0.50186	-0.45520
H	-2.98658	0.27695	0.96943
H	-4.47355	1.29668	0.39797
C	-1.65487	-2.55709	0.41507
H	-0.88718	-3.33627	0.35088
O	-2.50589	-2.62173	-0.57975
O	-1.69661	-1.73198	1.31189
H	-3.15109	-1.86612	-0.51912

RC2(T)-FFA

Si	-0.45122	0.46707	1.60223
O	0.61731	1.25407	2.52658
H	1.50916	1.36479	2.14814
O	-1.01335	1.34668	0.32938
O	0.20362	-0.90718	0.98227
O	-1.78330	0.10206	2.51107
H	-1.66985	0.06531	3.46288
Si	0.01782	-2.08419	-0.12675
Si	-2.22364	0.99362	-0.72343
O	1.08118	-3.31176	0.06274
O	0.38487	-1.35916	-1.58861
H	0.74926	-1.94765	-2.25616
O	-1.49739	-2.69230	-0.12574
H	-2.21775	-2.03912	-0.14184
O	-3.05901	-0.29704	-0.07447
H	-3.25590	-0.21198	0.86877
O	-3.13212	2.33677	-0.90714
H	-3.69049	2.39355	-1.68496
O	-1.66261	0.51496	-2.18143
H	-1.02631	-0.21900	-2.17127
H	0.78127	-4.08131	0.55098
C	1.61724	1.16076	-2.00382
O	2.76855	0.90361	-2.30414
H	1.31332	1.29713	-0.95621
H	0.84868	1.28101	-2.78179
C	3.94916	0.82995	0.82435
H	4.60816	0.63119	1.67797
O	4.50531	0.49819	-0.31189
O	2.83398	1.30850	0.94376
H	3.87422	0.67148	-1.06741

RC3(T)-FFA

Si	-0.70927	1.11705	-0.46984
O	-0.38142	1.18174	1.17141
H	-1.17680	1.19863	1.72532
O	0.24780	-0.10369	-1.01310
O	-2.28968	0.76545	-0.66405
O	-0.37649	2.49625	-1.24952
H	0.56174	2.74165	-1.26109
Si	-3.38778	-0.09517	0.19670
Si	0.77910	-1.49499	-0.33158
O	-4.93516	0.31838	-0.13226
O	-3.06165	0.37360	1.75815
H	-3.67427	0.09828	2.44316
O	-3.22077	-1.69622	-0.06392
H	-2.32017	-2.04175	-0.19954
O	-0.53917	-2.50977	-0.34191
H	-0.34838	-3.45030	-0.30226
O	1.97407	-2.24526	-1.12728
H	2.89127	-1.97321	-0.93848

O	1.28554	-1.14220	1.20380
H	0.77039	-0.41809	1.59333
H	-5.37766	-0.18418	-0.81966
C	4.48977	-1.14731	0.94912
O	4.49256	-1.40882	-0.23656
H	5.41947	-0.83948	1.45715
H	3.56496	-1.20727	1.54503
C	2.70093	2.09841	0.34698
O	2.42846	2.63301	-0.70244
O	3.93746	1.73547	0.69265
H	1.97391	1.84931	1.12889
H	4.53021	1.95970	-0.04206

TST1-FFA

Si	-0.74365	-0.34779	1.77332
O	-1.72734	-1.19697	2.76296
H	-1.87872	-0.83634	3.63871
O	-0.08404	-1.40508	0.70859
O	-1.58402	0.76231	0.90239
O	0.39141	0.39207	2.68010
H	0.99581	0.97513	2.19431
Si	-1.96914	1.34163	-0.56486
Si	-0.02329	-1.99081	-0.80703
O	-2.86792	2.70584	-0.49756
O	-2.90101	0.15237	-1.25960
H	-3.43311	0.41825	-2.01404
O	-0.62316	1.66728	-1.44383
H	-0.03381	0.91372	-1.62299
O	0.78859	-0.79083	-1.63853
H	1.13332	-1.02776	-2.50402
O	0.89977	-3.33499	-0.92191
H	0.46929	-4.18284	-0.79307
O	-1.49839	-2.30050	-1.42524
H	-2.15332	-1.58299	-1.37442
H	-2.40904	3.54524	-0.56553
C	3.30760	-0.14666	0.60780
O	4.27597	0.27656	-0.09153
H	2.45547	-0.63872	0.13417
H	3.48427	-0.36901	1.66211
C	2.20358	2.08452	-0.25099
H	1.55723	2.96651	-0.31712
O	2.90980	1.80108	-1.26381
O	2.18822	1.42079	0.82538
H	3.70756	0.94978	-0.89821

TST2-FFA

Si	-0.30448	0.21799	1.62883
O	0.96823	-0.10067	2.57789
H	1.79387	-0.31251	2.10365
O	0.07977	1.33157	0.47159
O	-0.85092	-1.10863	0.84132
O	-1.54019	0.81268	2.54528
H	-1.32389	1.06151	3.44658
Si	-1.76739	-1.77758	-0.32504
Si	-0.87530	1.96092	-0.70664
O	-1.97930	-3.38715	-0.14555
O	-0.85197	-1.56545	-1.70645
H	-1.04121	-2.16690	-2.43196
O	-3.22745	-1.05846	-0.44325
H	-3.21315	-0.08658	-0.43914

O	-2.45484	1.68373	-0.24196
H	-2.65268	1.90030	0.67815
O	-0.50558	3.54566	-0.83849
H	-0.72094	3.98515	-1.66354
O	-0.65180	1.23348	-2.14915
H	-0.75212	0.26736	-2.18421
H	-2.75559	-3.68078	0.33582
C	2.27506	-0.38134	-1.14083
O	3.20803	-0.92806	-1.79569
H	2.26301	0.69654	-0.96898
H	1.32855	-0.91612	-1.04476
C	4.21765	-0.31088	0.70486
H	4.75692	-0.28978	1.66177
O	4.89458	-0.12633	-0.34676
O	2.97015	-0.51467	0.74197
H	4.15176	-0.46523	-1.32369

TST3-FFA

Si	-0.72389	1.14762	-0.42501
O	-0.43669	1.16666	1.22377
H	-1.24682	1.15403	1.75607
O	0.21263	-0.08568	-0.98351
O	-2.30510	0.82268	-0.66360
O	-0.35559	2.53843	-1.16761
H	0.58521	2.76394	-1.13703
Si	-3.40760	-0.08850	0.13713
Si	0.79069	-1.44134	-0.27654
O	-4.95280	0.30497	-0.22348
O	-3.13094	0.33186	1.72175
H	-3.75343	0.01920	2.38136
O	-3.20574	-1.67872	-0.16715
H	-2.29769	-2.02039	-0.24339
O	-0.49441	-2.49272	-0.24016
H	-0.28760	-3.42542	-0.14241
O	2.00466	-2.17849	-1.06014
H	2.90604	-1.83088	-0.94076
O	1.31008	-1.02579	1.24237
H	0.76040	-0.31310	1.61271
H	-5.36582	-0.18169	-0.94000
C	4.35294	-0.63525	0.94159
O	4.43952	-0.95021	-0.31596
H	5.26869	-0.42531	1.50091
H	3.45047	-0.90635	1.50014
C	2.90718	1.80585	0.42032
O	2.43583	2.33165	-0.55751
O	4.03384	1.08570	0.37409
H	2.47389	1.87396	1.42687
H	4.27482	0.25687	-0.50700

PC1(T)-FFA

Si	0.62585	0.28710	1.78230
O	1.48695	1.21457	2.81416
H	1.68125	0.84629	3.67816
O	-0.10685	1.28832	0.71508
O	1.58569	-0.73497	0.93102
O	-0.45535	-0.57680	2.65249
H	-1.01400	-1.16853	2.13317
Si	2.27268	-1.11237	-0.49312
Si	-0.19240	1.85759	-0.80643
O	3.39627	-2.29346	-0.36717

O	3.04263	0.27957	-0.97846
H	3.72183	0.17331	-1.64971
O	1.13759	-1.60272	-1.56952
H	0.44287	-0.94767	-1.75882
O	-0.68474	0.54254	-1.70757
H	-1.10352	0.72859	-2.55260
O	-1.36006	2.98833	-0.98606
H	-1.12875	3.90238	-0.80803
O	1.23396	2.46352	-1.31179
H	2.00717	1.88752	-1.18794
H	3.11586	-3.19202	-0.55185
C	-3.16561	-0.20409	0.54361
O	-4.44516	-0.70573	0.57254
H	-2.98499	0.47259	-0.29587
H	-2.95543	0.27939	1.49503
C	-2.12805	-1.91305	-0.71155
H	-1.29259	-2.62317	-0.72953
O	-2.90794	-1.74395	-1.61833
O	-2.16515	-1.25947	0.45344
H	-4.67635	-0.98613	-0.32142

PC2(T)-FFA

Si	-0.57135	0.24936	1.65691
O	0.44755	1.06963	2.63080
H	1.13777	1.55179	2.16087
O	-1.13090	1.23651	0.46241
O	0.11560	-1.06390	0.96951
O	-1.83451	-0.29406	2.56395
H	-2.01876	0.18562	3.37468
Si	0.23914	-2.01318	-0.34962
Si	-2.20591	0.92204	-0.73947
O	1.44965	-3.10485	-0.21147
O	0.68485	-0.97566	-1.57516
H	1.16547	-1.36074	-2.31313
O	-1.15990	-2.78767	-0.66907
H	-1.94773	-2.21872	-0.66285
O	-2.91817	-0.54441	-0.37387
H	-3.29335	-0.61139	0.51250
O	-3.27919	2.15212	-0.78304
H	-3.72997	2.32100	-1.61278
O	-1.47682	0.76584	-2.18709
H	-0.69657	0.18695	-2.20027
H	1.23749	-3.96267	0.16239
C	3.21419	0.30132	0.43273
O	4.43394	0.92934	0.33102
H	3.07567	-0.49378	-0.30531
H	3.10120	-0.07945	1.44569
C	1.93236	1.69866	-0.96889
H	1.01329	2.29296	-1.02627
O	2.69007	1.49854	-1.88751
O	2.10516	1.22454	0.27111
H	4.59128	1.12541	-0.60075

PC3(T)-FFA

Si	0.68239	-1.11453	-0.25675
O	0.54755	-0.99511	1.40199
H	1.39343	-1.02981	1.87265
O	-0.26544	0.11883	-0.80934
O	2.24241	-0.88198	-0.67204
O	0.17916	-2.52675	-0.86309

H	-0.76768	-2.72961	-0.79008
Si	3.47255	-0.02173	-0.01259
Si	-0.71656	1.53493	-0.12052
O	4.94685	-0.50740	-0.52611
O	3.34792	-0.39170	1.60207
H	4.06081	-0.11307	2.18034
O	3.32124	1.57072	-0.33914
H	2.42452	1.94748	-0.32769
O	0.64450	2.48532	-0.12737
H	0.51771	3.42050	0.05168
O	-1.88707	2.32230	-0.92496
H	-2.79296	1.99782	-0.80085
O	-1.26460	1.20596	1.40530
H	-0.70298	0.54904	1.84797
H	5.30218	-0.06378	-1.29923
C	-4.49871	0.16744	0.65047
O	-4.38708	1.09608	-0.38509
H	-5.50450	0.14481	1.07295
H	-3.75477	0.45435	1.39809
C	-2.98777	-1.55380	0.11579
O	-2.66413	-2.57919	-0.42342
O	-4.26767	-1.15467	0.17349
H	-2.28664	-0.86758	0.61327
H	-5.05656	0.92753	-1.05706

Reaction R8

RC-FW

C	0.96176	0.56175	0.00195
O	1.32507	-0.59059	0.00478
H	0.80144	1.12352	0.93964
H	0.77374	1.11101	-0.93767
O	-1.73076	0.00443	-0.02972
H	-1.43489	-0.91062	-0.00450
H	-2.66537	-0.00512	0.19037

TS-FW

C	0.34550	0.62851	0.00071
O	1.02804	-0.48236	0.02692
H	0.25841	1.23096	0.92005
H	0.33031	1.23236	-0.91661
O	-1.12694	-0.16706	-0.11034
H	-0.23404	-0.90374	-0.05211
H	-1.63650	-0.13529	0.71181

$CH_2(OH)_2$

C	0.00003	0.52966	0.00001
O	1.16298	-0.24672	0.09447
H	0.00066	1.15834	0.89652
H	-0.00077	1.15815	-0.89666
O	-1.16299	-0.24673	-0.09447
H	1.24308	-0.77348	-0.70751
H	-1.24309	-0.77342	0.70765

RC1(M)-FW

Si	1.20726	-0.00706	-0.01195
O	1.12732	-0.45486	1.57260
H	1.73054	-1.14369	1.86006
O	0.43793	1.46988	-0.04513
H	0.74632	2.10556	0.60694
O	2.79503	0.09348	-0.42403
H	3.01107	-0.06730	-1.34517
O	0.46878	-0.98857	-1.07030
H	-0.46252	-1.25042	-0.91873
C	-2.48092	-0.81776	0.54580
O	-2.16008	-1.44798	-0.44276
H	-3.53884	-0.65080	0.79710
H	-1.73313	-0.42497	1.25304
O	-2.37202	1.68860	-0.11042
H	-2.73969	1.85628	-0.98158
H	-1.40559	1.69642	-0.21890

RC2(M)-FW

Si	-0.64465	-0.66587	-0.00996
O	0.41123	-1.09170	1.19361
H	0.27911	-1.96677	1.56578
O	0.03884	0.63355	-0.75893
H	1.01109	0.65746	-0.84327
O	-0.80390	-2.02397	-0.92928
H	-1.61294	-2.09251	-1.44068
O	-2.13797	-0.20919	0.46788
H	-2.26294	0.75147	0.57076
O	-1.72985	2.54353	0.22872
H	-0.97516	2.20529	-0.28315
H	-2.22695	3.12214	-0.35376
C	3.21212	0.30501	0.42883
H	2.51663	-0.12848	1.16605
H	4.28611	0.34744	0.67890
O	2.81382	0.72229	-0.63877

TSM1-FW

Si	1.19434	-0.04536	-0.00063
O	1.45429	0.25491	1.59732
H	2.12872	-0.26571	2.03866
O	0.31709	1.31312	-0.47769
H	0.70500	2.15333	-0.21567
O	2.66552	-0.11942	-0.72829
H	2.71431	-0.64846	-1.52789
O	0.33267	-1.34619	-0.39362
H	-0.65983	-1.40151	-0.25027
C	-2.40230	-0.02696	0.65710
O	-2.24451	-1.13878	-0.08772
H	-3.39232	0.12809	1.09782
H	-1.59387	0.23265	1.35620
O	-2.33511	0.96275	-0.51982
H	-2.33528	-0.08654	-0.97340
H	-1.39330	1.27371	-0.58069

TSM2-FW

Si	1.42614	-0.03346	-0.03330
O	2.17542	1.04407	0.96687

H	2.92094	0.70927	1.46924
O	0.59042	0.91743	-1.10599
H	1.04924	1.71277	-1.38617
O	2.63331	-0.92639	-0.72050
H	2.38277	-1.81088	-0.99579
O	0.37540	-1.07608	0.62960
H	-0.53480	-0.76472	0.85243
C	-2.45403	0.65743	0.01453
O	-2.10876	-0.16073	1.00052
H	-3.04958	1.54446	0.27392
H	-1.73075	0.82610	-0.79004
O	-3.51390	-0.38817	-0.62676
H	-4.43563	-0.12006	-0.49965
H	-3.05911	-0.85414	0.30512

TSM3-FW

Si	1.50961	-0.00865	-0.01416
O	1.79143	-1.54381	-0.51824
H	2.60108	-1.71048	-1.00548
O	0.42251	-0.17470	1.24161
H	0.59667	-0.88281	1.86729
O	2.96019	0.62393	0.41559
H	3.03687	1.58066	0.41851
O	0.80163	1.00959	-1.07454
H	-0.16481	1.03076	-1.10642
O	-1.87136	0.55422	-0.04021
H	-1.24996	0.28478	0.67250
H	-2.90098	0.88974	0.35687
C	-3.04686	-0.59670	-0.31443
H	-2.66838	-1.49038	0.20849
H	-3.01276	-0.69389	-1.40882
O	-3.99081	0.11739	0.23603

PC1(M)-FW

Si	-1.26881	0.01844	-0.00312
O	-1.59537	-0.21305	1.59292
H	-2.33802	0.26962	1.96174
O	-0.33324	-1.29840	-0.41189
H	-0.62197	-2.14030	-0.04927
O	-2.71626	0.07770	-0.77987
H	-2.73206	0.54249	-1.61934
O	-0.42871	1.34624	-0.41029
H	0.53257	1.38501	-0.23090
C	2.61048	-0.11091	0.48897
O	2.26665	1.20572	0.06230
H	3.65555	-0.13256	0.81011
H	1.94839	-0.30427	1.34022
O	2.47283	-1.04577	-0.52058
H	2.80556	1.41837	-0.70798
H	1.52336	-1.21052	-0.65551

PC2(M)-FW

Si	1.39416	0.03124	-0.00930
O	1.12739	1.30404	1.00847
H	1.68074	1.34860	1.79120
O	0.72737	0.49148	-1.44776

H	0.92453	1.38515	-1.73725
O	3.02308	-0.20568	-0.04244
H	3.32184	-1.08595	-0.28028
O	0.70150	-1.37944	0.42335
H	-0.26870	-1.42756	0.35092
C	-2.31042	0.27884	-0.08332
O	-2.05523	-1.10074	0.12715
H	-1.71592	0.79511	0.67716
H	-1.98802	0.58598	-1.08048
O	-3.66950	0.57430	0.00358
H	-3.96503	0.41835	0.90646
H	-2.48210	-1.60170	-0.57642

PC3(M)-FW

Si	-1.38367	0.03757	0.00248
O	-1.31870	1.46641	-0.80980
H	-2.03633	1.65953	-1.41660
O	-0.39561	0.25803	1.32108
H	-0.45732	1.10712	1.76562
O	-2.96639	-0.22821	0.35448
H	-3.22290	-1.13771	0.52202
O	-0.80532	-1.27652	-0.77326
H	0.15418	-1.41540	-0.69542
O	1.85112	-0.97022	0.11595
H	1.37533	-0.58533	0.87096
H	4.18931	-0.06756	0.47227
C	2.54381	0.07103	-0.53112
H	1.87433	0.90188	-0.77752
H	2.94807	-0.37217	-1.44742
O	3.54540	0.62020	0.27382

RC1(T)-FW

Si	0.11264	1.27396	0.21243
O	0.58554	1.38326	1.77940
H	0.35612	0.61759	2.31889
O	0.76931	-0.02677	-0.53393
O	-1.51666	1.22474	0.09480
O	0.71611	2.58283	-0.58323
H	0.43628	3.45284	-0.28975
Si	-2.81570	0.25017	-0.08712
Si	0.58953	-1.61515	-0.10182
O	-4.21346	1.09632	-0.06195
O	-2.75152	-0.73520	1.25361
H	-3.53584	-1.25979	1.43396
O	-2.76232	-0.60593	-1.47578
H	-2.03432	-1.24422	-1.56854
O	-0.50635	-2.30455	-1.14637
H	-0.15093	-2.94694	-1.76561
O	1.99044	-2.40702	-0.19779
H	2.82239	-1.90390	-0.05570
O	-0.07388	-1.61194	1.40405
H	-1.04112	-1.54269	1.47321
H	-4.63759	1.25829	-0.90732
C	4.05997	0.26966	0.67047
O	4.17869	-0.84093	0.18826
H	4.92093	0.94800	0.74722
H	3.10282	0.62637	1.08187
O	3.46123	1.98921	-1.19566

H	3.42194	1.39612	-1.95093
H	2.55181	2.30241	-1.07228

RC2(T)-FW

Si	-0.37160	-1.45202	-0.79213
O	0.19175	-2.47222	0.37301
H	-0.21447	-3.33925	0.44098
O	-1.89163	-0.92782	-0.47348
O	0.65854	-0.19836	-0.78190
O	-0.37916	-2.28142	-2.20060
H	-0.90825	-1.94169	-2.92491
Si	1.03263	1.37712	-0.51270
Si	-2.57626	0.22825	0.47001
O	2.52307	1.76094	-0.99041
O	0.85984	1.46511	1.16805
H	1.15895	2.29224	1.55873
O	-0.01272	2.39092	-1.23739
H	-0.94993	2.29032	-1.00303
O	-2.63780	1.63096	-0.43138
H	-3.27551	1.65163	-1.14989
O	-4.07089	-0.31161	0.84847
H	-4.48684	0.05114	1.63323
O	-1.72180	0.55536	1.81220
H	-0.82678	0.92986	1.73442
H	3.26247	1.24123	-0.60801
C	3.95243	-0.98294	0.45154
O	4.30330	0.17420	0.31792
H	3.15656	-1.41916	-0.17173
H	4.44800	-1.64720	1.17298
O	2.01610	-1.09773	2.15877
H	1.66984	-0.20112	2.05555
H	1.35574	-1.66389	1.73374

RC3(T)-FW

Si	-0.26523	-0.29208	1.73820
O	0.51184	-1.58207	2.32607
H	0.92548	-2.21430	1.69992
O	0.74982	0.88726	1.19859
O	-1.18957	-0.71697	0.44298
O	-1.17115	0.36904	2.93093
H	-1.33820	-0.19532	3.68870
Si	-2.05914	-0.24631	-0.84571
Si	1.13294	1.77881	-0.10024
O	-3.33192	-1.21664	-1.17706
O	-0.97569	-0.42756	-2.10515
H	-1.34982	-0.43170	-2.99015
O	-2.59899	1.28893	-0.70717
H	-1.93443	1.95613	-0.46926
O	-0.18127	2.77670	-0.33864
H	-0.07180	3.46814	-0.99717
O	2.52233	2.60587	0.13737
H	2.72290	2.87390	1.03659
O	1.39324	0.89372	-1.45992
H	0.60827	0.44395	-1.82833
H	-4.17982	-0.97594	-0.79777
O	3.12376	-1.30421	-1.76279
H	2.71011	-0.43108	-1.66117
H	3.96611	-1.25954	-1.30429

C	1.39113	-2.96089	-0.72437
H	1.82863	-3.56657	-1.53025
H	0.71365	-2.14524	-1.02284
O	1.61412	-3.21444	0.44363

TST1-FW

Si	-0.02260	-0.67135	1.61851
O	0.99580	-1.89840	1.80878
H	1.66290	-2.08676	1.08028
O	0.76575	0.74587	1.25849
O	-1.05287	-0.89599	0.35221
O	-0.89527	-0.44991	2.98693
H	-0.64847	-1.01181	3.72468
Si	-2.18417	-0.37375	-0.68188
Si	0.87051	1.82276	0.05723
O	-3.34762	-1.46623	-1.02843
O	-1.30841	-0.14931	-2.09126
H	-1.82058	-0.03221	-2.89558
O	-2.89802	1.00954	-0.18171
H	-2.29131	1.71422	0.09252
O	-0.54952	2.68486	0.07349
H	-0.57597	3.48568	-0.45681
O	2.19542	2.76469	0.21163
H	2.54678	2.89087	1.09566
O	1.03357	1.11261	-1.43236
H	0.20899	0.73169	-1.80410
H	-4.12669	-1.47836	-0.46837
O	2.82266	-0.82910	-1.77620
H	2.24845	-0.01905	-1.70578
H	3.20932	-1.13560	-0.75461
C	2.01756	-2.07153	-1.38136
H	2.24509	-2.81888	-2.14883
H	0.95329	-1.79261	-1.37660
O	2.61233	-2.24179	-0.18262

TST2-FW

Si	0.18443	1.28462	-0.74270
O	-0.31323	1.97535	0.68980
H	0.25738	1.75870	1.43890
O	1.80822	1.06798	-0.68836
O	-0.56098	-0.14600	-0.94027
O	-0.28297	2.32503	-1.90369
H	-0.41164	1.97984	-2.78944
Si	-0.84316	-1.64781	-0.31051
Si	2.65777	0.09289	0.32746
O	-2.35511	-2.14000	-0.54230
O	-0.49982	-1.39873	1.32565
H	-0.83752	-2.08356	1.90999
O	0.20544	-2.73029	-0.93493
H	1.13545	-2.51218	-0.77614
O	2.77881	-1.42336	-0.34324
H	3.35478	-1.50452	-1.10864
O	4.11226	0.80167	0.53361
H	4.67254	0.48841	1.24640
O	1.85211	-0.05891	1.74257
H	1.07620	-0.65575	1.75601
H	-3.02258	-1.49490	-0.17201
C	-3.65839	1.00061	0.07478

O	-3.77975	-0.24477	0.57373
H	-3.00795	1.12609	-0.80320
H	-4.57994	1.58674	-0.00622
O	-2.91658	1.57663	1.28753
H	-3.09688	0.48133	1.52564
H	-1.96326	1.77359	1.08984

TST3-FW

Si	0.07996	1.34689	-0.07663
O	0.61535	1.56147	1.45945
H	0.52421	0.76755	2.00187
O	0.68765	-0.04975	-0.69551
O	-1.56398	1.25128	-0.13494
O	0.53275	2.64003	-0.97417
H	-0.18876	3.11872	-1.38720
Si	-2.78410	0.17490	-0.01619
Si	0.68592	-1.57169	-0.05257
O	-4.24074	0.92049	0.01675
O	-2.51920	-0.57796	1.44809
H	-3.25168	-1.09664	1.79068
O	-2.80644	-0.89925	-1.24733
H	-2.05477	-1.51439	-1.30555
O	-0.46050	-2.45775	-0.87501
H	-0.12258	-3.17428	-1.41766
O	2.12922	-2.27336	-0.18590
H	2.92063	-1.67477	-0.27495
O	0.18116	-1.42154	1.51212
H	-0.77772	-1.33680	1.64960
H	-4.78317	0.82985	-0.76952
C	3.86895	0.46110	0.60785
O	4.02977	-0.45598	-0.34770
H	4.77218	0.96005	0.98516
H	3.13646	0.25875	1.39838
O	3.14410	1.49179	-0.32808
H	3.44004	0.62157	-0.98838
H	3.59349	2.33662	-0.47639

PC1(T)-FW

Si	-0.02104	-1.27455	-0.55157
O	-0.88672	-1.70621	0.79707
H	-0.73748	-1.10576	1.53956
O	-0.48416	0.20462	-1.06913
O	1.57248	-1.24544	-0.16947
O	-0.34084	-2.34462	-1.73558
H	-0.03018	-3.24541	-1.62822
Si	2.79647	-0.24559	0.24245
Si	-0.58004	1.59823	-0.19059
O	4.20699	-1.05294	0.41377
O	2.33109	0.34721	1.72915
H	3.01057	0.80016	2.23530
O	3.02549	0.95418	-0.84087
H	2.31189	1.60492	-0.94999
O	0.67045	2.58110	-0.66902
H	0.43806	3.34436	-1.20335
O	-1.98686	2.35797	-0.43304
H	-2.77024	1.77281	-0.46547
O	-0.33193	1.18514	1.38662
H	0.58844	1.09215	1.68751

H	4.83642	-0.98570	-0.30736
C	-4.03954	-0.36708	0.88302
O	-3.88470	0.40604	-0.30460
H	-5.08312	-0.33319	1.20943
H	-3.39663	0.12833	1.62006
O	-3.72121	-1.69691	0.68809
H	-4.27241	-0.08374	-1.03793
H	-2.75401	-1.80077	0.65429

PC2(T)-FW

Si	0.03058	-1.27705	0.62368
O	-0.55182	-1.92834	-0.77673
H	-0.05661	-1.71043	-1.57317
O	1.67076	-1.24104	0.60043
O	-0.52222	0.24652	0.81821
O	-0.55825	-2.23025	1.80601
H	-0.56493	-1.88140	2.69924
Si	-0.61129	1.77658	0.23394
Si	2.68658	-0.29695	-0.27857
O	-2.08330	2.42285	0.42653
O	-0.21231	1.58292	-1.39025
H	-0.38261	2.35006	-1.94360
O	0.48011	2.75125	0.95476
H	1.39332	2.44246	0.85432
O	2.90161	1.14970	0.52067
H	3.38814	1.10061	1.34838
O	4.08184	-1.13207	-0.42214
H	4.70949	-0.84565	-1.08850
O	2.04425	0.04812	-1.73895
H	1.30730	0.68900	-1.76546
H	-2.80615	1.82919	0.14782
C	-3.79570	-0.90291	-0.01857
O	-3.72933	0.42895	-0.52360
H	-3.15793	-0.89503	0.87118
H	-4.82818	-1.13667	0.25810
O	-3.40558	-1.83885	-0.95707
H	-4.20033	0.45522	-1.36300
H	-2.43556	-1.89427	-0.98363

PC3(T)-FW

Si	-0.21051	-0.22123	1.77315
O	0.82939	-1.32589	2.34406
H	1.53517	-1.63400	1.74193
O	0.57087	1.09080	1.14779
O	-1.12875	-0.81893	0.55203
O	-1.17643	0.26083	3.00316
H	-0.96569	-0.10233	3.86575
Si	-2.10561	-0.61938	-0.72832
Si	0.82397	1.83008	-0.27607
O	-3.24074	-1.78352	-0.89064
O	-1.05856	-0.77957	-2.01903
H	-1.45807	-0.92001	-2.88119
O	-2.84951	0.83568	-0.71235
H	-2.26804	1.60188	-0.57901
O	-0.60574	2.62060	-0.61000
H	-0.58393	3.23830	-1.34591
O	2.09858	2.84857	-0.19375
H	2.30613	3.22342	0.66452

O	1.16338	0.79749	-1.50882
H	0.41235	0.26576	-1.83892
H	-4.08854	-1.63406	-0.46682
O	2.98902	-1.31846	-1.72639
H	2.55922	-0.44857	-1.65832
H	3.62866	-2.02177	0.53480
C	2.31860	-2.20668	-0.90656
H	2.59057	-3.21456	-1.23392
H	1.23064	-2.07855	-0.93437
O	2.66849	-2.03859	0.46496

Reaction R9

RC-FAM

C	-1.35252	-0.26112	-0.14093
O	-0.89291	0.96936	0.16511
O	1.76420	0.07524	-0.71845
H	1.23407	0.86056	-0.54869
O	-2.48056	-0.62420	0.06008
C	2.37853	-0.32264	0.49241
H	3.07905	0.43478	0.86632
H	1.63992	-0.53788	1.27698
H	2.93746	-1.23612	0.28181
H	-1.62504	1.47378	0.55017
H	-0.54743	-0.85579	-0.58940

TS1-FAM

C	-1.99996	-0.21223	0.15957
H	-2.81838	0.08222	-0.50093
H	-2.11627	-1.26646	0.42447
H	-2.03510	0.40150	1.06983
O	-0.77596	-0.03913	-0.53538
C	0.67234	-0.00518	0.38923
H	0.29796	-0.25968	1.38753
O	1.51154	-0.95584	-0.03916
O	0.87662	1.23454	0.03128
H	-0.23625	1.02709	-0.51941
H	1.97622	-0.59686	-0.80819

INT

C	-1.89557	-0.03295	0.08810
H	-1.95644	1.04667	-0.08802
H	-2.66613	-0.54252	-0.49017
H	-2.05549	-0.23350	1.15621
O	-0.65600	-0.56103	-0.34746
C	0.43740	-0.02725	0.30571
H	0.28662	-0.01467	1.39650
O	1.49504	-0.84416	-0.07110
O	0.66975	1.30924	-0.03637
H	0.77104	1.33953	-0.99674
H	2.29912	-0.46677	0.29891

TS2-FAM

C	-1.94386	0.18659	0.09312
H	-1.81097	1.27359	0.10823
H	-2.75877	-0.07809	-0.57840
H	-2.16947	-0.17101	1.10309

O	-0.77711	-0.44843	-0.42430
C	0.31731	-0.34782	0.33679
H	0.11273	-0.18918	1.40386
O	1.37939	-0.97141	-0.05314
O	1.12726	1.21062	0.02474
H	0.78679	1.62820	-0.77772
H	1.76277	0.17760	-0.21699

TS3-FAM

C	-0.64674	-0.36620	0.36040
O	-0.88504	1.30887	0.11746
O	0.72345	-0.03278	-0.54390
H	0.12502	1.00198	-0.47064
O	-1.44872	-1.09361	-0.14159
C	1.95502	-0.13363	0.15632
H	2.74613	0.24729	-0.49228
H	1.94242	0.44984	1.08608
H	2.15244	-1.18437	0.38522
H	-1.65952	1.38524	-0.45555
H	-0.27372	-0.36087	1.39110

CH_3OCHO

C	-0.44315	0.84232	0.33203
O	2.01738	-0.71460	0.00288
O	-0.86274	-0.12918	-0.48395
H	1.82855	-0.12177	-0.73185
O	-0.05188	1.90217	-0.07850
C	-1.12493	-1.40135	0.11592
H	-1.67915	-1.97493	-0.62516
H	-0.17939	-1.89604	0.35085
H	-1.73524	-1.29149	1.01835
H	2.84991	-0.41135	0.37330
H	-0.49829	0.58265	1.40341

RC1(M)-FAM

C	-2.33530	-1.70701	0.04426
O	-1.16627	-1.71856	0.40671
O	-3.00311	-0.66645	-0.36207
H	-2.94618	-2.61892	0.03331
H	-2.43124	0.17451	-0.39933
C	-1.63245	2.41173	0.55823
H	-1.38483	3.42186	0.21790
H	-2.63845	2.41864	0.98162
H	-0.91283	2.09298	1.31868
O	-1.64250	1.50751	-0.54373
H	-0.72633	1.37733	-0.85690
Si	1.63899	-0.08070	0.00639
O	3.19881	0.38663	0.17592
H	3.79996	-0.23988	0.58386
O	1.61556	-1.64331	-0.50008
H	0.77466	-2.09720	-0.36196
O	0.75452	0.14205	1.36625
H	-0.04377	-0.40688	1.37500
O	0.98220	0.95696	-1.12357
H	1.45601	1.06041	-1.95210

INTM

C	-2.12729	-0.57516	-0.45285
O	-1.13784	-1.32190	0.19205
O	-3.30551	-0.55978	0.29005

H	-2.26168	-1.04571	-1.43089
H	-3.45708	-1.45161	0.61798
C	-1.94245	1.68689	0.35214
H	-1.47467	2.60677	0.00159
H	-3.00499	1.84902	0.53734
H	-1.44898	1.36364	1.27450
O	-1.75169	0.74074	-0.70407
H	-0.77750	-0.83394	0.95448
Si	1.74621	0.00628	-0.02917
O	3.30676	0.46529	0.15921
H	3.94574	-0.23731	0.29311
O	1.70299	-1.56388	-0.49973
H	0.82074	-1.95423	-0.50730
O	0.91946	0.06303	1.43350
H	1.11967	0.81306	1.99819
O	1.06678	1.06817	-1.06771
H	0.10271	0.99867	-1.15280

RC2(M)-FAM

C	-2.82273	2.21194	-0.04273
H	-2.23315	3.13234	-0.10716
H	-3.49092	2.15906	-0.90305
H	-3.42176	2.22652	0.87385
O	-1.98313	1.06358	-0.09067
H	-1.32468	1.09137	0.62868
Si	1.49235	0.37813	-0.02509
O	0.40071	0.70919	1.20021
H	0.71612	0.61453	2.10220
O	2.78123	1.37297	0.15937
H	3.64162	0.99843	-0.04178
O	2.07961	-1.14394	0.02010
H	1.46443	-1.88754	-0.07634
O	0.61279	0.66380	-1.37910
H	-0.27466	1.02818	-1.25866
C	-1.09111	-1.92690	-0.30623
H	-0.90997	-1.27326	-1.17377
O	-2.19316	-1.64132	0.37497
H	-2.49637	-0.75333	0.09911
O	-0.33312	-2.81683	0.00286

RC3(M)-FAM

Si	-2.32003	0.18981	0.00805
O	-0.93369	1.05978	-0.35684
H	-0.95898	1.98877	-0.10952
O	-2.77808	0.80264	1.46041
H	-3.69497	0.68821	1.71875
O	-3.56156	0.46040	-1.03205
O	-1.91122	-1.37570	-0.08052
C	1.68135	-1.15377	0.06732
O	0.75853	-1.84394	0.44955
O	1.57089	0.07174	-0.42073
H	2.72963	-1.47499	0.08479
H	0.62916	0.38532	-0.42002
H	-3.61726	-0.12296	-1.79234
C	4.82626	0.89230	0.54483
H	5.77739	0.46698	0.87037
H	4.08185	0.72725	1.33639
H	-1.00841	-1.63943	0.18076
H	4.95862	1.97330	0.40755
O	4.47143	0.24403	-0.66055

H	3.60711	0.56751	-0.93659

TSM1-FAM

C	-1.84021	-0.81617	-0.28755
O	-1.27528	-1.03203	0.88560
O	-3.11474	-1.19973	-0.45569
H	-1.26518	-0.91211	-1.20936
H	-3.47383	-1.39676	0.42103
C	-2.94249	1.61668	0.05209
H	-3.56770	1.27918	0.88531
H	-2.66750	2.66161	0.20442
H	-3.49292	1.51025	-0.88512
O	-1.74155	0.85715	-0.03569
H	-1.33683	0.23385	0.89849
Si	1.88346	0.05242	-0.05846
O	3.43493	-0.07145	-0.58198
H	3.75255	-0.96395	-0.73347
O	1.50499	-1.41566	0.57232
H	0.56410	-1.51766	0.79756
O	1.74686	1.28847	1.03028
H	2.33178	1.26382	1.79000
O	0.85849	0.47289	-1.27727
H	0.17395	1.10777	-1.03822

TSM2-FAM

C	-2.08678	-0.40083	-0.63998
O	-1.21251	-1.45306	0.49073
O	-3.20263	-0.74777	-0.07508
H	-1.74866	-0.84908	-1.57653
H	-2.43773	-1.41438	0.60906
C	-2.13468	1.66375	0.51903
H	-1.73464	2.66129	0.34595
H	-3.22431	1.67328	0.52000
H	-1.76130	1.27168	1.46871
O	-1.64497	0.86502	-0.56919
H	-0.69622	-0.95310	1.15229
Si	1.73242	0.01938	-0.05120
O	3.34693	0.22447	0.11047
H	3.86906	-0.56796	0.24937
O	1.40211	-1.45972	-0.67015
H	0.56306	-1.86175	-0.40308
O	0.93808	0.04206	1.42958
H	1.15071	0.77430	2.01296
O	1.22628	1.28950	-0.95011
H	0.26851	1.33282	-1.06611

TSM3-FAM

C	-1.27659	1.87588	0.10717
H	-0.20887	2.10922	0.12571
H	-1.77913	2.52889	-0.61227
H	-1.68588	2.05770	1.11132
O	-1.44600	0.52317	-0.28343
H	-1.39263	-0.32027	0.62364
Si	1.88348	-0.14341	-0.05834
O	0.97557	-0.38582	1.30524
H	1.39847	-0.14013	2.13124
O	2.43679	1.40553	0.08350
H	3.19059	1.64295	-0.46097
O	3.21527	-1.10159	-0.18118
H	3.08880	-1.95172	-0.60853

O	0.92958	-0.44388	-1.34436
H	-0.00213	-0.17777	-1.26336
C	-3.06241	-0.11956	-0.06439
H	-3.50770	0.67926	0.54248
O	-2.21374	-1.05818	1.03918
H	-2.46904	-0.88768	1.95403
O	-3.51838	-0.69806	-0.99186

TSM4-FAM

Si	-2.01006	0.15234	-0.01810
O	-1.12553	-0.61252	1.18484
H	-1.59349	-1.30896	1.65403
O	-2.99704	-1.04344	-0.56381
H	-3.79128	-0.77570	-1.03040
O	-2.98592	1.34749	0.55340
O	-0.94388	0.82284	-1.03225
C	2.07368	-0.77411	-0.38552
O	1.25090	-0.70470	-1.28569
O	1.55342	-0.85210	1.08262
H	2.94299	-1.44437	-0.40475
H	0.56349	-0.77379	1.09861
H	-2.61501	2.23265	0.53389
C	4.13944	0.77281	0.05921
H	4.46467	0.76419	-0.98512
H	4.62759	-0.04753	0.60165
H	-0.12112	0.32295	-1.23928
H	4.42579	1.72271	0.51479
O	2.72646	0.66911	0.10934
H	2.13115	0.16938	1.08032

PC1(M)-FAM

C	2.13935	-0.11233	-0.86252
O	0.44413	2.72581	0.29331
O	2.58888	0.82383	-0.24495
H	1.93772	-0.11879	-1.93823
H	1.36607	2.45209	0.19295
C	2.01274	-1.40983	1.09766
H	1.74807	-2.43748	1.33888
H	3.05384	-1.20590	1.35200
H	1.35205	-0.71168	1.61568
O	1.82143	-1.29229	-0.32569
H	0.12129	2.24034	1.06482
Si	-1.47333	-0.18262	-0.08471
O	-3.11069	-0.06025	-0.04754
H	-3.60767	-0.61454	-0.65247
O	-0.67310	0.71316	-1.19060
H	-0.36460	1.58765	-0.87205
O	-0.96143	0.38055	1.39808
H	-1.56422	0.22392	2.12929
O	-1.12340	-1.76509	-0.35994
H	-0.21509	-1.93164	-0.63715

PC2(M)-FAM

C	1.55988	1.33699	-1.23371
H	0.54623	1.72827	-1.31556
H	2.28068	2.11618	-1.49570
H	1.67545	0.46314	-1.87915
O	1.72870	0.95463	0.14037
H	0.67013	-1.72827	-0.90361
Si	-1.74627	-0.00707	0.14271

O	-1.11400	-1.16945	-0.86282
H	-1.54573	-1.27340	-1.71484
O	-1.97037	1.29766	-0.84149
H	-2.60082	1.95725	-0.54326
O	-3.21178	-0.40158	0.76919
H	-3.21405	-0.84771	1.61901
O	-0.71249	0.19029	1.38013
H	0.20567	0.43406	1.18213
C	2.81548	0.21327	0.43150
H	3.49148	0.06471	-0.42355
O	1.62399	-1.85759	-1.03428
H	1.88663	-2.54286	-0.41485
O	3.00593	-0.21070	1.53701

PC3(M)-FAM

Si	-1.77409	-0.02169	-0.10357
O	-0.98526	1.31282	-0.71713
H	-1.16261	1.52803	-1.63580
O	-1.45607	-0.02144	1.50390
H	-0.66236	-0.51166	1.75322
O	-3.36317	0.21824	-0.42510
O	-1.30107	-1.41175	-0.83733
C	2.00763	-0.77902	0.62178
O	1.00432	-1.40931	0.88633
O	1.38125	1.94767	0.61986
H	2.63210	-0.29815	1.38626
H	0.56075	1.81123	0.11100
H	-3.93803	-0.54688	-0.35945
C	3.57176	0.20112	-0.82874
H	4.43114	-0.16162	-0.25752
H	3.31394	1.22302	-0.54357
H	-0.44160	-1.73989	-0.53522
H	3.79143	0.14081	-1.89279
O	2.43503	-0.65291	-0.62077
H	1.11597	2.45975	1.38748

RC1(T)-FAM

Si	0.60345	1.60998	-0.22324
O	-0.24626	1.94482	-1.57705
H	-1.12011	1.53253	-1.63785
O	-0.36345	0.71227	0.79131
O	1.95378	0.76095	-0.51308
O	1.02733	3.00155	0.52478
H	0.58596	3.79826	0.22421
Si	3.04673	-0.42766	-0.32345
Si	-0.57300	-0.93125	0.94549
O	4.50904	-0.08175	-0.96369
O	2.38112	-1.67219	-1.20220
H	2.92558	-2.45088	-1.33968
O	3.24729	-0.80536	1.25313
H	2.42849	-0.97113	1.74966
O	0.56896	-1.36342	2.07368
H	0.39018	-2.17139	2.56166
O	-2.05689	-1.25568	1.50106
H	-2.74793	-1.43271	0.82030
O	-0.33780	-1.67430	-0.49209
H	0.56243	-1.76658	-0.85061
H	5.14795	0.34493	-0.38870
C	-3.41443	-2.64572	-1.43375
H	-3.65598	-3.55589	-0.88260

H	-4.01404	-2.61937	-2.34974
H	-2.34761	-2.64623	-1.67940
O	-3.74076	-1.55025	-0.58323
H	-3.55931	-0.71813	-1.04303
C	-3.40632	1.83938	-0.04765
H	-4.38840	2.32643	-0.04542
O	-2.74879	2.07224	1.06139
O	-3.00225	1.17091	-0.98646
H	-1.89392	1.57478	1.06605

INTT

Si	0.42169	-1.42349	-0.57552
O	-0.70192	-2.36314	0.18474
H	-0.51882	-3.30374	0.24666
O	-0.29443	-0.01341	-0.91203
O	1.72325	-1.18487	0.39368
O	0.85405	-2.23989	-1.93191
H	1.57042	-1.87558	-2.45692
Si	2.94555	-0.09920	0.47973
Si	-0.40123	1.57715	-0.47892
O	4.37126	-0.80270	0.86458
O	2.48972	0.90934	1.71395
H	3.16147	1.50200	2.06017
O	3.12518	0.68410	-0.94706
H	2.44645	1.34791	-1.17850
O	0.88422	2.32781	-1.25246
H	0.65355	2.82226	-2.04279
O	-1.75561	2.24005	-1.06871
H	-2.56027	1.69727	-0.98766
O	-0.16245	1.76692	1.12360
H	0.72436	1.57952	1.47007
H	5.00317	-0.92851	0.15389
C	-2.58376	-0.01342	2.37178
H	-2.32864	-1.06688	2.52940
H	-1.77948	0.62144	2.74064
H	-3.51826	0.22163	2.89726
O	-2.69806	0.28352	0.98974
H	-2.49742	-1.86265	0.07554
C	-3.71555	-0.37753	0.32363
H	-4.66658	-0.29483	0.86727
O	-3.82448	0.30072	-0.90665
O	-3.46198	-1.72230	0.13597
H	-3.80826	-0.36585	-1.60113

RC2(T)-FAM

Si	1.00433	1.46989	0.61807
O	0.22891	1.86762	-0.79856
H	0.53734	1.30660	-1.52997
O	0.13423	0.36011	1.45509
O	2.45748	0.82585	0.23617
O	1.11297	2.83357	1.50095
H	1.02660	2.74716	2.45217
Si	2.76913	-0.46753	-0.75872
Si	-0.59169	-1.07914	1.18890
O	4.13201	-0.21989	-1.61816
O	1.52463	-0.51293	-1.84675
H	0.76211	-1.04157	-1.55204
O	2.89571	-1.82798	0.13761
H	2.21934	-1.99308	0.81381
O	0.50516	-2.19697	1.72850

H	0.21821	-3.11327	1.74405
O	-1.99286	-1.23883	2.00845
H	-2.60499	-0.50775	1.84534
O	-0.74977	-1.35801	-0.43221
H	-1.58081	-1.10335	-0.88471
H	4.95868	-0.17099	-1.13505
C	-3.19695	1.70446	-0.35578
O	-2.86907	0.96667	0.55519
O	-2.38391	2.36764	-1.13938
H	-4.24571	1.89978	-0.61286
H	-1.42973	2.18191	-0.92691
C	-4.09588	-1.68461	-1.16364
H	-5.06471	-1.51166	-1.64262
H	-3.86269	-2.75436	-1.17050
H	-4.13819	-1.33687	-0.13131
O	-3.06880	-0.92448	-1.80013
H	-2.99688	-1.18562	-2.72255

RC3(T)-FAM

Si	-0.25072	1.37378	-0.00986
O	0.37746	1.53529	1.50743
H	0.59080	2.42452	1.80139
O	0.18915	-0.06409	-0.57808
O	-1.88199	1.48628	-0.02500
O	0.39995	2.60183	-0.90755
H	-0.08261	2.87106	-1.69347
Si	-2.98703	0.26771	0.13966
Si	0.33659	-1.70144	-0.54016
O	-4.40821	1.01548	0.43951
O	-2.47057	-0.68334	1.41109
H	-2.39432	-0.24454	2.26330
O	-3.12089	-0.69660	-1.15709
H	-2.40504	-1.31979	-1.38260
O	-0.83932	-2.27849	-1.57527
H	-0.54350	-2.51006	-2.45908
O	1.79936	-2.16656	-1.05103
H	2.44682	-1.44973	-1.17570
O	-0.03479	-2.24132	0.95617
H	-0.90836	-1.95954	1.26750
H	-5.20785	0.53230	0.22110
C	2.86658	-1.33613	2.39337
H	1.99813	-1.99875	2.31617
H	3.74970	-1.87755	2.04772
H	3.02200	-1.05108	3.44242
O	2.72779	-0.19716	1.56057
H	1.90982	0.27053	1.77322
C	3.64437	0.99855	-0.74489
H	4.55028	0.78609	-0.17064
O	3.14799	0.23676	-1.54815
O	3.17698	2.20702	-0.46725
H	2.32127	2.35056	-0.91986

TST1-FAM

Si	0.63910	1.56697	0.26641
O	-0.15981	2.36442	-0.90695
H	-0.98291	1.95246	-1.22160
O	-0.36885	0.38285	0.86825
O	1.99451	0.83367	-0.23692
O	1.04709	2.61307	1.45678
H	0.59671	3.45992	1.44480

Si	3.15777	-0.27645	-0.46059
Si	-0.41784	-1.26432	0.62983
O	4.57820	0.34055	-0.98191
O	2.52896	-1.21387	-1.67937
H	3.10250	-1.88211	-2.06142
O	3.43201	-1.11810	0.91342
H	2.62923	-1.42093	1.36919
O	0.76440	-1.88029	1.62192
H	0.62272	-2.77979	1.92838
O	-1.85848	-1.83571	1.10872
H	-2.62285	-1.59649	0.54691
O	-0.16236	-1.62176	-0.94061
H	0.72367	-1.52533	-1.33032
H	5.20787	0.61024	-0.30983
C	-4.99260	-1.15370	-0.91260
H	-5.59374	-1.30040	-0.01012
H	-5.50311	-0.44189	-1.57560
H	-4.89619	-2.10994	-1.43427
O	-3.70516	-0.68663	-0.55703
H	-3.01359	-0.00550	-1.36527
C	-3.45249	1.10868	-0.17733
H	-4.49243	1.43225	-0.25533
O	-2.97073	1.26782	1.02463
O	-2.66924	1.11725	-1.23314
H	-2.01800	1.00461	1.05264

TST2-FAM

Si	0.42000	-1.39927	-0.54957
O	-0.70144	-2.40052	0.14945
H	-0.49981	-3.33984	0.15533
O	-0.34935	-0.01757	-0.87107
O	1.67159	-1.14326	0.47958
O	0.92342	-2.17529	-1.90393
H	1.60068	-1.74290	-2.43021
Si	2.91408	-0.07256	0.45552
Si	-0.45900	1.58292	-0.45445
O	4.34956	-0.77414	0.80387
O	2.53414	1.00281	1.65544
H	3.23167	1.59390	1.94914
O	3.01863	0.62683	-1.02322
H	2.35317	1.31039	-1.23896
O	0.81421	2.32077	-1.26321
H	0.56157	2.82744	-2.03914
O	-1.83177	2.22315	-1.00654
H	-2.63787	1.65924	-0.95186
O	-0.16939	1.77637	1.14176
H	0.74215	1.65767	1.44985
H	4.93626	-0.96689	0.06981
C	-2.41853	-0.32830	2.40826
H	-2.14145	-1.38633	2.34606
H	-1.59924	0.24166	2.84353
H	-3.32336	-0.21091	3.01520
O	-2.60927	0.21382	1.10836
H	-2.41231	-1.89987	-0.14958
C	-3.67814	-0.22117	0.40480
H	-4.55329	-0.44751	1.02824
O	-3.85174	0.39576	-0.75085
O	-3.35202	-1.64086	-0.28730
H	-3.50192	-0.81736	-1.10550

TST3-FAM

Si	-0.81609	-0.71359	1.40174
O	0.25455	-1.63992	0.52093
H	-0.08076	-1.77760	-0.38310
O	-0.39314	0.86775	1.31121
O	-2.30214	-0.92049	0.75816
O	-0.70124	-1.20756	2.94859
H	-0.82357	-0.54565	3.63182
Si	-2.78226	-0.77395	-0.82617
Si	-0.11925	1.95818	0.11729
O	-3.85718	-1.93517	-1.21635
O	-1.42672	-1.05843	-1.73068
H	-0.90696	-0.25699	-1.91856
O	-3.42770	0.70780	-1.06032
H	-2.96377	1.46896	-0.67637
O	-1.57099	2.71502	-0.11600
H	-1.55563	3.52008	-0.63992
O	1.02012	3.04802	0.53137
H	1.91163	2.67256	0.49560
O	0.23767	1.16654	-1.29465
H	1.16238	0.85512	-1.25964
H	-4.73508	-1.87349	-0.83596
C	3.44636	-0.08807	0.18372
O	2.65206	0.80421	-0.12788
O	2.88969	-1.42009	0.65931
H	4.32615	0.10284	0.81324
H	1.89000	-1.44752	0.61344
C	5.46481	-0.94460	-1.22975
H	5.97526	-1.26005	-0.31165
H	5.70786	-1.63843	-2.03580
H	5.79225	0.06056	-1.50804
O	4.05258	-0.94439	-1.06853
H	3.45919	-1.73943	-0.33034

TST4-FAM

Si	0.47786	-1.41949	-0.53653
O	-0.22124	-2.01900	0.83451
H	-0.17539	-2.97249	0.94015
O	-0.25425	-0.01143	-0.86327
O	2.09123	-1.20435	-0.35738
O	0.20798	-2.52922	-1.71497
H	0.80511	-2.53329	-2.46607
Si	3.04612	-0.03737	0.29957
Si	-0.45657	1.57009	-0.41737
O	4.48872	-0.74930	0.59092
O	2.29151	0.47097	1.70109
H	2.12584	-0.21142	2.35808
O	3.24361	1.26900	-0.63955
H	2.45911	1.79846	-0.87996
O	0.77878	2.42545	-1.15205
H	0.55163	2.84364	-1.98629
O	-1.84755	2.16236	-0.97918
H	-2.64508	1.59095	-0.99233
O	-0.23430	1.72659	1.19507
H	0.64776	1.48321	1.51850
H	5.25712	-0.17528	0.61614
C	-2.81986	0.13017	2.36775
H	-1.83286	0.20919	2.82111
H	-3.34379	1.08207	2.47642
H	-3.39342	-0.67973	2.83180

O	-2.61153	-0.11898	0.98145
H	-2.39492	-1.21274	0.51617
C	-3.85972	-0.34503	0.04573
H	-4.68469	-0.65705	0.70013
O	-3.97177	0.44596	-0.88053
O	-3.13977	-1.76209	-0.28802
H	-2.81401	-1.70934	-1.19895

PC1(T)-FAM

Si	-0.54441	1.41026	-0.51620
O	0.38921	2.64954	0.04151
H	0.00154	3.52789	0.04024
O	0.46206	0.15175	-0.68379
O	-1.72239	1.05050	0.57499
O	-1.21493	1.90270	-1.93017
H	-1.90052	1.33175	-2.29125
Si	-2.93764	-0.04802	0.52449
Si	0.52223	-1.49107	-0.52485
O	-4.37793	0.56752	0.99188
O	-2.47367	-1.20331	1.61406
H	-3.13725	-1.83926	1.89205
O	-3.08076	-0.62410	-1.00719
H	-2.38523	-1.24881	-1.29540
O	-0.76269	-2.05346	-1.45071
H	-0.53106	-2.70053	-2.12143
O	1.85337	-2.12923	-1.17763
H	2.73342	-1.75532	-0.97366
O	0.25457	-1.91135	1.03081
H	-0.64066	-1.76986	1.37538
H	-4.98090	0.86178	0.30629
C	2.43851	0.47427	2.22356
H	1.78908	1.26025	1.83467
H	1.89927	-0.14295	2.94024
H	3.32223	0.91975	2.68957
O	2.80928	-0.39098	1.14971
H	2.27249	2.50710	-0.23397
C	3.95011	-0.18437	0.51261
H	4.62475	0.55089	0.96920
O	4.21758	-0.80921	-0.49196
O	3.22795	2.35744	-0.29965
H	3.38525	2.09923	-1.21188

PC2(T)-FAM

Si	-0.63307	-0.80956	1.35879
O	0.44275	-1.70309	0.47871
H	0.19237	-1.76363	-0.45620
O	-0.24934	0.78758	1.31516
O	-2.13679	-1.00428	0.74684
O	-0.48030	-1.33698	2.89629
H	-0.72485	-0.72323	3.59169
Si	-2.63404	-0.80169	-0.82533
Si	-0.14380	2.02129	0.25023
O	-3.61912	-2.01562	-1.28979
O	-1.27157	-0.92177	-1.75201
H	-0.80824	-0.07937	-1.89910
O	-3.39717	0.63787	-0.95820
H	-2.99371	1.39187	-0.50031
O	-1.66305	2.66820	0.16929
H	-1.74079	3.51479	-0.27840
O	0.91429	3.16253	0.73952

H	1.84283	2.92654	0.62235
O	0.21067	1.43928	-1.26014
H	1.16719	1.30396	-1.37659
H	-4.48960	-2.05552	-0.88992
C	3.58682	0.37909	-0.54759
O	2.87316	1.35981	-0.46953
O	3.09241	-1.71225	1.34184
H	4.42347	0.18876	0.13567
H	2.16602	-1.78704	1.04746
C	4.29139	-1.65127	-1.51537
H	4.29322	-2.14224	-0.54026
H	3.89413	-2.31830	-2.27773
H	5.29327	-1.32159	-1.80214
O	3.39454	-0.52436	-1.48861
H	3.08434	-1.93775	2.27471

PC3(T)-FAM

Si	-0.57546	1.40325	-0.56874
O	0.37478	2.65241	-0.06130
H	-0.00164	3.53431	-0.11388
O	0.41807	0.12968	-0.69512
O	-1.74286	1.09579	0.55059
O	-1.24874	1.85021	-1.99349
H	-1.95462	1.28858	-2.32866
Si	-2.91646	-0.05049	0.54141
Si	0.54155	-1.50584	-0.55119
O	-4.30702	0.68727	0.98268
O	-2.48348	-1.25131	1.60867
H	-2.56119	-1.03909	2.54266
O	-3.05014	-0.72617	-0.93882
H	-2.35046	-1.34915	-1.22074
O	-0.71913	-2.07105	-1.50539
H	-0.60313	-2.95080	-1.87281
O	1.90582	-2.10306	-1.16971
H	2.77636	-1.74321	-0.90909
O	0.26275	-1.96287	0.99728
H	-0.65760	-1.88489	1.29210
H	-5.13038	0.22753	0.80645
C	2.35338	0.56357	2.21780
H	1.68132	1.30808	1.78808
H	1.83053	-0.03804	2.95995
H	3.21568	1.06246	2.66963
O	2.76407	-0.33389	1.18694
H	2.25799	2.49391	-0.30017
C	3.93330	-0.14898	0.59411
H	4.58697	0.60215	1.05537
O	4.24516	-0.80798	-0.37435
O	3.21617	2.34845	-0.32691
H	3.41172	2.08386	-1.22983

REFERENCES

(1) Venkateswarlu, P.; Gordy, W. Methyl Alcohol II. Molecular Structure. *J. Chem. Phys.* **1955**, *23*, 1200-1202.
(2) Herzberg, G. Electronic Spectra and Electronic Structure of Polyatomic Molecules, Van Nostrand, New York, 1966.
(3) Hellwege, K. H.; Hellwege, A. M. Landolt-Bornstein: Group II: Atomic and Molecular Physics Volume 7: Structure Data of Free Polyatomic Molecules. Springer-Verlag. Berlin, 1976.
(4) Hoy, A. R.; Bunker, P. R. A Precise Solution of the Rotation Beninding Schrodinger Equation for a Triatomic Molecule with Application to the Water Molecule. *J. Mol. Spect.* **1979**, *74*, 1-8.
(5) Gurvich, L. V.; Veyts, I. V.; Alcock, C. B. Thermodynamic Properties of Individual Substances, Hemisphere Pub. Co., New York, 1989.
(6) Glinnemann, J.; King Jr, H. E.; Schulz, H.; Hahn, T.; La Placa, S. J.; Dacol, F.; Crystal Structures of the Low-Temperature Quartz-Type Phases of SiO_2 and GeO_2 at Elevated Pressure. *Zeitschrift für Kristallographie-Crystalline Materials* **1992**, *198*, 177-212.
(7) Arnold, H. Die Struktur des Hochquarzes. *Zeitschrift für Kristallographie-Crystalline Materials* **1962**, *117*, 467-469.
(8) Kihara, K. An X-ray Study of the Temperature Dependence of the Quartz Structure. *Eur. J. Miner.* **1990**, 63-78.
(9) Viswanathan, K.; Brandt, K. The Crystal Structure of a Ternary (Ba, K, Na)-Feldspar and its Significance. *Am. Mineral.* **1980**, *65*, 472-476.
(10) Ribbe, P. H. A Refinement of the Crystal Structure of Sanidinized Orthoclase. *Acta Crystallogr.* **1963**, *16*, 426-427.
(11) Phillips, M. W.; Ribbe, P. H. The Structures of Monoclinic Potassium-Rich Feldspars. *Am. Mineral.* **1973**, *58*, 263-270.
(12) Gruner, J. W. The Crystal Structure of Kaolinite. *Zeitschrift für Kristallographie-Crystalline Materials* **1932**, *83*, 75-88.
(13) Bish, D. L. Rietveld Refinement of the Kaolinite Structure at 1.5 K. *Clays Clay Miner.* **1993**, *41*, 738-744.