Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information
for
Aluminium Catalysed Oligomerisation in Cement-Forming Silicate Systems

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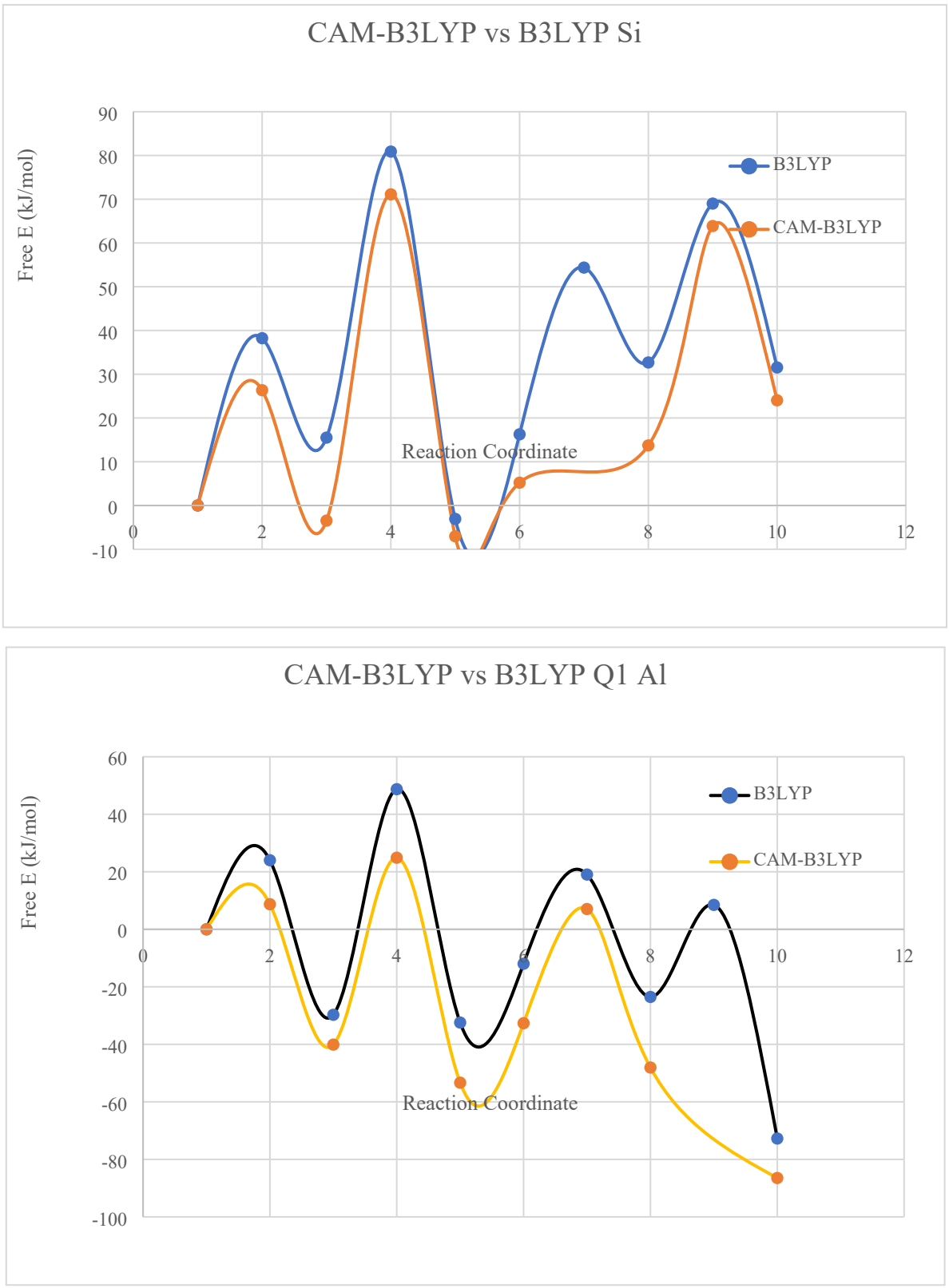


Figure S1 Free energies (kj•mol^{-1}) of the B3LYP-D3 and CAM-B3LYP optimised geometries for each stationary (critical) point along the reaction profiles for Si-only (Upper) and Q1 Al (Lower) systems.

Table S1 Energy barriers for each TS in CAM-B3LYP and B3LYP-D3 (see main text).

	Si		Al-Q1	
Barriers	**B3LYPD3**	**CAM-B3LYP**	**B3LYPD3**	**CAM-B3LYP**
TS1	38.2	26.3	24	8.7
TS2	65.4	74.5	78.4	64.9
TS3	38.1	-	31	39.6
TS4	36.2	49.3	32	-

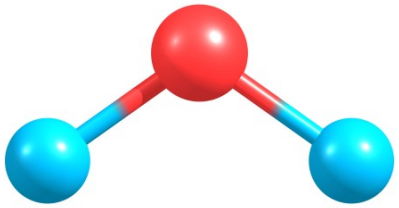
Table S2 Free energies of stationary points and transition states for CAM-B3LYP and B3LYP Si + Q1.

	Si		Al-Q1	
Step	**B3LYPD3**	**CAM-B3LYP**	**B3LYPD3**	**CAM-B3LYP**
RCT1	0.00	0.00	0.00	0.00
TS1	38.24	26.35	24.01	8.71
INT	15.51	-3.46	-29.73	-40.10
TS2	80.88	71.11	48.71	24.89
PRD1	-3.06	-7.04	-32.44	-53.34
RCT2	16.27	5.22	-11.98	-32.65
TS3	54.37		19.04	7.04
INT2	32.69	13.73	-23.52	-48.07
TS4	69.00	63.87	8.48	
PRD2	31.55	24.04	-72.75	-86.48

Exemplary Data Card of geometry optimised stationary points

Example: H_2O molecule

FILE NAME + Graphical Representation



Cartesian Coordinates of all geometry optimised stationary points

Atom type	X	Y	Z
O	1.34146346	1.62020904	0.00000000
H	2.30146346	1.62020904	0.00000000
H	1.02100888	2.52514487	0.00000000

First nine analytical frequencies of normal modes of vibration

Frequencies --	1664.9645	3800.9563	3914.2425
Frequencies --	##########	##########	##########
Frequencies --	##########	##########	##########

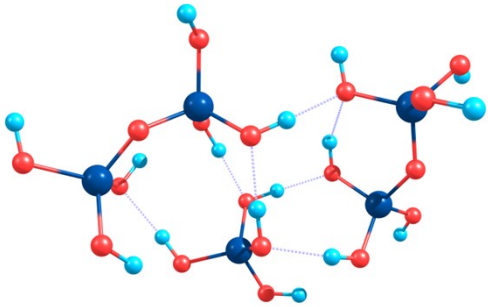
Note: *In this case, H_2O only has 3 (3N-6 = 3(3) -6 = 3 normal modes of vibration. Else for systems with 4 atoms 3N-6 = 6 modes would be listed. Systems with 5 atoms or more, would have 3N-6 = 9 or more modes, listing the first 9 modes.*

Thermodynamic properties reported

Zero-point correction=	0.021370 (Hartree/Particle)
Thermal correction to Energy=	0.024205
Thermal correction to Enthalpy=	0.025149
Thermal correction to Gibbs Free Energy =	0.003713
Sum of electronic and zero-point Energies =	-76.398367
Sum of electronic and thermal Energies =	-76.395532
Sum of electronic and thermal Enthalpies =	-76.394588
Sum of electronic and thermal Free Energies =	-76.416024

Neutral Si

PENT-Si-RCT-Bondi2.log



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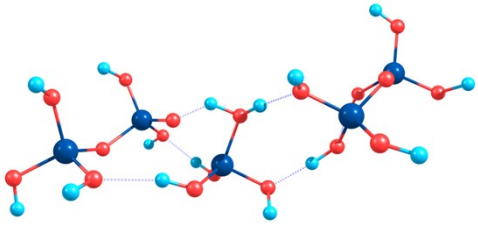
O	2.070028	0.844995	1.350396
O	2.302371	2.232653	-0.967287
O	4.379147	2.176312	0.700142
O	3.739412	-0.040456	-0.550676
O	4.872293	-2.406274	0.122378
O	2.206869	-1.855588	0.540028
O	3.131928	-2.331306	-1.898769
O	-3.896017	0.553984	-1.712491
O	-2.906428	-1.615847	-0.342671
O	-5.528811	-1.206281	-0.717676
O	-4.043817	0.442344	0.946913
O	-0.309498	-1.274151	-0.438633
O	-1.635047	-0.884244	1.924959
O	-1.353954	-3.337144	1.05745
H	2.144381	-2.689915	1.02892
H	4.18454	3.064111	1.030794
H	3.803928	-2.284851	-2.593205
H	-5.672845	-2.027019	-0.226728
H	-3.527599	0.029881	1.662275
H	-1.226253	0.009781	1.860416
H	-1.511723	-4.015915	0.386611
H	2.002735	-0.125245	1.439815
H	1.471488	1.826855	-1.303572
Si	3.533419	-1.664051	-0.460607
Si	-4.088788	-0.468983	-0.447484
H	5.343269	-1.938891	0.826913
H	-3.371776	1.34601	-1.496813
Si	3.105274	1.315895	0.133093
Si	-1.532473	-1.786163	0.553085
H	0.597696	-1.473318	-0.113508
O	-0.279042	1.364898	-1.216507
H	-0.309191	0.395486	-1.038156
O	-0.543083	1.604075	1.466504
O	-0.206817	3.805266	-0.186684
O	-2.504579	2.518196	-0.088998
H	-3.045717	1.981709	0.527153
H	0.415622	1.384919	1.560336
Si	-0.874165	2.317737	0.004561
H	0.736077	3.782862	-0.415327
O	-0.391411	-3.029703	-1.877166
H	-1.081508	-2.731646	-2.489627
H	0.44782	-2.964603	-2.360728
H	-1.986905	0.121185	3.733266
H	1.490218	2.195165	-0.666244
H	-0.80065	-0.154491	1.745554
H	-1.439827	0.099448	-1.568613

Frequencies -- 26.9289 35.2399 37.8426
Frequencies -- 44.2435 50.3114 57.1260
Frequencies -- 60.0850 83.3463 94.3697

Zero-point correction= 0.250112 (Hartree/Particle)
Thermal correction to Energy= 0.282877
Thermal correction to Enthalpy= 0.283822
Thermal correction to Gibbs Free Energy= 0.187032
Sum of electronic and zero-point Energies= -2812.065269
Sum of electronic and thermal Energies= -2812.032503
Sum of electronic and thermal Enthalpies= -2812.031559
Sum of electronic and thermal Free Energies= -2812.128349

PENT-Si-TS-Bondi5.log



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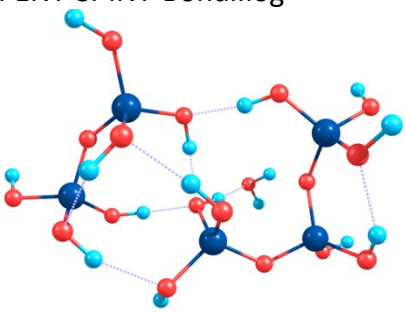
O	-4.737521	-1.715632	-0.669112
O	-7.003794	-0.336134	-0.395412
O	-6.112088	-1.754607	1.665014
O	-4.773336	0.464988	0.928558
O	-2.086159	0.837282	1.256622
O	-3.180326	0.599999	-1.148948
O	-3.582794	2.844209	0.459774
O	2.051164	-0.628761	0.261359
O	4.673937	-0.578414	-0.323118
O	3.054732	-2.452144	-1.359789
O	3.739473	-2.567421	1.238543
O	4.064312	1.908893	0.29613
O	5.070559	0.139366	2.166163
O	6.689448	1.128497	0.296394
H	-2.273728	0.754244	-1.527526
H	-5.411024	-1.9773	2.292944
H	-4.426267	3.214195	0.163576
H	3.831641	-2.764665	-1.843969
H	4.173438	-2.104646	1.972339
H	4.932276	0.797079	2.8609
H	6.854562	1.479876	-0.589915
H	-4.093842	-1.15782	-1.14559
H	-7.566653	0.270251	0.105654
Si	-3.434128	1.214626	0.347543
Si	3.349053	-1.540347	0.001804
H	-1.863605	1.422521	1.995211
H	0.689454	-0.769172	0.545991
Si	-5.643865	-0.838331	0.383049
Si	5.138157	0.686158	0.611424
H	4.255137	2.780774	0.669133
O	1.492008	1.755434	-0.83125
H	2.352306	1.644785	-0.379005
O	-0.210017	-0.461573	0.053172
O	-0.69051	1.077362	-1.929538
H	-0.586794	2.021446	-2.11039
O	1.167618	-0.641028	-2.385422
H	1.838032	-1.31378	-2.14942
H	-0.901248	0.047698	0.586922
Si	0.675259	0.384465	-1.206676

Frequencies -- -405.9059 13.8913 15.3554
Frequencies -- 23.2401 29.3736 30.9908
Frequencies -- 42.7704 55.8849 62.4931

Zero-point correction= 0.244484 (Hartree/Particle)
Thermal correction to Energy= 0.278070
Thermal correction to Enthalpy= 0.279015
Thermal correction to Gibbs Free Energy= 0.176921
Sum of electronic and zero-point Energies= -2812.013231
Sum of electronic and thermal Energies= -2811.979645
Sum of electronic and thermal Enthalpies= -2811.978700
Sum of electronic and thermal Free Energies= -2812.080794

PENT-Si-INT-Bondi.log



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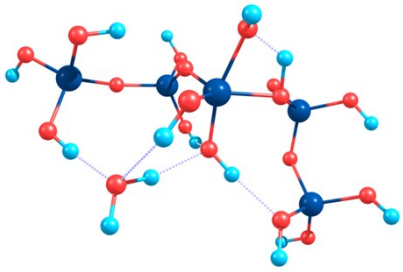
O	5.512671	-0.95045	0.252311
O	3.427536	-1.011362	-1.374508
O	3.138585	-1.73588	1.25076
O	3.523485	0.84799	0.531358
O	0.976094	1.662263	0.937343
O	2.711681	3.429341	0.15605
O	1.981702	1.431543	-1.569735
O	-1.620952	-2.107534	-0.428448
O	-2.74635	0.104677	0.575211
O	-3.752928	-2.381877	1.014726
O	-4.012374	-1.213689	-1.413244
O	-1.591157	2.547083	0.41578
O	-3.183792	1.470967	-1.602155
O	-4.227772	2.401816	0.643591
H	3.31411	3.78221	-0.513224
H	2.172418	-1.583418	1.319499
H	2.564106	0.714191	-1.892282
H	-4.63546	-2.127163	1.317691
H	-3.913013	-0.332249	-1.823134
H	-3.57068	2.230185	-2.059685
H	-4.101676	2.823799	1.504398
H	5.960674	-0.559394	1.014952
H	2.686595	-1.639388	-1.48742
Si	2.325108	1.848144	0.005367
Si	-3.064302	-1.382895	-0.086899
H	0.78532	0.711935	1.10737
H	-1.900125	-0.278848	2.411035
Si	3.889259	-0.73539	0.192256
Si	-2.898554	1.660287	0.01956
H	-0.70035	2.143099	0.488798
O	-1.247805	-0.847034	2.857573
O	-0.295733	-0.134738	-1.565497
H	0.448795	0.500259	-1.639846
O	0.948978	-2.467738	-1.278752
H	1.175877	-3.246479	-0.748327
O	0.460034	-1.034857	0.919621
H	-0.192645	-1.064784	1.692871
H	-1.735689	-1.658405	3.064892
Si	-0.135331	-1.425842	-0.582675

Frequencies --	24.9448	38.4501	40.9426
Frequencies --	50.5097	57.3970	65.1214
Frequencies --	72.4298	89.4894	92.4663

Zero-point correction=	0.249923 (Hartree/Particle)
Thermal correction to Energy=	0.282899
Thermal correction to Enthalpy=	0.283843
Thermal correction to Gibbs Free Energy=	0.187332
Sum of electronic and zero-point Energies=	-2812.072998
Sum of electronic and thermal Energies=	-2812.040022
Sum of electronic and thermal Enthalpies=	-2812.039077
Sum of electronic and thermal Free Energies=	-2812.135588

PENT-Si-TS2-Bondi4.log



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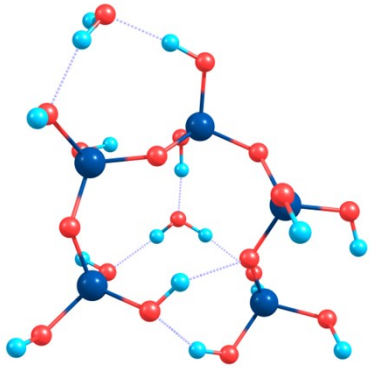
O	3.980728	0.054855	1.380214
O	4.025861	2.011151	-0.549688
O	5.831908	0.066866	-0.491651
O	3.286565	-0.529014	-1.152627
O	0.711573	-0.513993	-2.077012
O	1.843521	-2.774224	-1.387955
O	1.608176	2.935313	0.205348
H	2.609873	-3.24793	-1.037389
H	6.209838	0.480201	-1.279644
H	1.351071	3.826489	-0.070646
H	3.172437	-0.461432	1.521487
H	3.141188	2.389906	-0.315659
Si	1.777594	-1.172553	-1.022726
H	0.166655	0.153619	-1.602578
Si	4.251449	0.429794	-0.203873
O	-1.558697	-0.713125	1.293918
O	-2.962798	-0.227005	-0.93311
O	-3.897202	-1.993941	0.890653
O	-1.682206	-2.594147	-0.543973
O	-4.510101	1.702094	-2.056596
O	-5.026062	0.717086	0.371772
O	-2.743603	2.207167	-0.00876
H	-4.586322	-1.319146	1.021277
H	-2.072681	-3.061302	-1.29606
H	-5.351792	1.393015	0.981983
H	-2.915685	3.156125	-0.082099
Si	-2.568214	-1.406408	0.137222
Si	-3.829588	1.151075	-0.674028
H	-3.902356	1.944767	-2.769862
O	1.294805	-0.926237	0.543393
O	0.672144	1.250287	2.303985
H	0.898426	2.058813	1.806731
O	-0.245726	0.981133	-0.069386
H	-1.081993	1.485933	-0.000181
Si	0.157467	0.016157	1.314523
O	0.051823	-1.099185	2.752863
H	0.109918	-0.621759	3.593315
H	-1.173785	-1.197088	2.223867
H	0.937606	2.326241	-0.181296

Frequencies --	-877.0619	20.5845	23.8283
Frequencies --	31.5076	40.1434	51.6285
Frequencies --	53.6438	61.2818	82.4871

Zero-point correction=	0.246136 (Hartree/Particle)
Thermal correction to Energy=	0.279027
Thermal correction to Enthalpy=	0.279971
Thermal correction to Gibbs Free Energy=	0.182185
Sum of electronic and zero-point Energies=	-2812.015823
Sum of electronic and thermal Energies=	-2811.982931
Sum of electronic and thermal Enthalpies=	-2811.981987
Sum of electronic and thermal Free Energies=	-2812.079773

PENT-Si-PRD-Bondi.log



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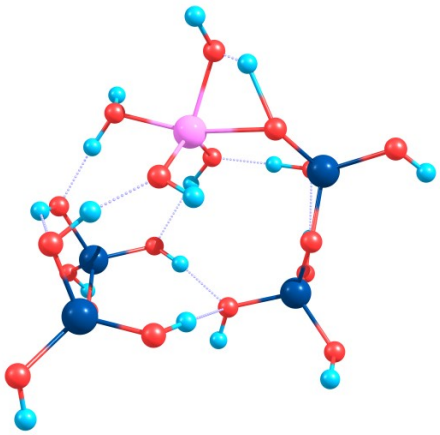
O	-0.162922	2.743949	1.226975
O	-0.528763	4.415668	-0.819845
O	0.86155	2.147087	-1.159945
O	-1.824748	2.056907	-0.80509
O	-1.501287	-0.562363	-0.45235
O	-3.009617	0.814903	1.314556
O	-3.935103	0.467508	-1.127868
O	0.319135	-2.42769	0.10365
O	1.928481	-0.332092	-0.441528
O	0.827946	-1.810671	-2.399387
O	2.782523	-2.865824	-0.772902
O	3.11711	-0.052459	1.874177
O	4.619134	-0.605298	-0.240563
O	3.453726	1.840419	-0.115811
H	-2.57933	0.156926	1.891409
H	0.904897	1.172691	-1.130607
H	-3.851492	0.565085	-2.087375
H	1.401857	-1.459474	-3.094388
H	3.637584	-2.407217	-0.699994
H	5.008229	-0.32411	-1.081534
H	2.624906	2.238275	-0.452279
H	-0.876418	3.093968	1.781378
H	-0.853806	4.59995	-1.71246
Si	-2.549194	0.688997	-0.254116
Si	1.486067	-1.866185	-0.896271
H	1.400078	0.176369	2.512728
Si	-0.430002	2.83515	-0.403169
Si	3.304124	0.257431	0.262674
H	3.806722	0.277192	2.468274
O	0.476224	0.409223	2.730359
O	-1.259127	-1.414473	2.074242
O	-2.243163	-3.089926	0.213816
H	-3.175933	-2.782447	0.053126
O	-4.709228	-2.115858	-0.197781
H	-4.591803	-1.270887	-0.675345
H	-0.551641	-0.750605	2.352094
H	0.282891	1.189158	2.174206
H	-5.04247	-1.845125	0.670478
Si	-1.185225	-1.885524	0.504643

Frequencies -- 26.8733 27.9839 40.7045
Frequencies -- 44.4592 46.4420 57.2100
Frequencies -- 61.9579 80.5306 86.6182

Zero-point correction= 0.250245 (Hartree/Particle)
Thermal correction to Energy= 0.283530
Thermal correction to Enthalpy= 0.284474
Thermal correction to Gibbs Free Energy= 0.186739
Sum of electronic and zero-point Energies= -2812.078640
Sum of electronic and thermal Energies= -2812.045355
Sum of electronic and thermal Enthalpies= -2812.044411
Sum of electronic and thermal Free Energies= -2812.142145

Neutral 4

PENT-4-TS-fix3-Bondi3.log



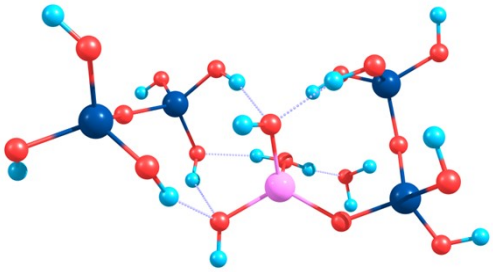
40

O	2.930734	1.672643	0.751902
O	3.682395	0.101591	2.72007
O	1.117902	-0.022852	1.906762
O	3.033769	-0.969722	0.285243
O	1.533515	-1.759707	-1.798444
O	2.838906	0.654289	-1.847808
O	4.218266	-1.55295	-2.088787
O	-2.374075	1.441541	-1.097672
O	-2.366471	-1.157391	-0.635682
O	-4.691603	0.142779	-1.177101
O	-3.42591	0.465996	1.218451
O	-0.139048	-2.04909	0.452331
O	-2.47599	-2.104743	1.898326
O	-2.127787	-3.821398	-0.054377
H	1.899462	1.005287	-1.780756
H	0.620901	-0.692494	1.387103
H	4.461223	-2.444626	-1.804462
H	-5.279678	-0.572757	-0.899688
H	-2.589922	0.935443	1.520021
H	-2.934954	-1.244608	1.984458
H	-1.678408	-4.128285	-0.854093
H	3.193913	1.583442	-0.189739
H	3.465334	-0.569608	3.382036
Si	2.881259	-0.923694	-1.372412
Si	-3.24329	0.240025	-0.411309
H	0.861413	-1.828927	-1.090662
H	0.675485	3.875533	1.00894
Si	2.681792	0.165673	1.423842
Si	-1.805293	-2.283255	0.415843
H	0.350952	-2.78649	0.851148
Al	-0.659803	2.170829	-0.241702
O	-1.098662	1.638281	1.386618
H	-0.371399	1.208831	1.866368
O	0.857852	3.26922	0.274004
O	-1.734753	3.600745	-0.720285
H	-1.455664	4.190013	-1.434865
O	0.354778	1.266249	-1.375061
H	-0.149974	0.579752	-1.831111
H	-2.426232	2.628521	-1.075899
H	1.661875	2.733854	0.531933

Frequencies -- -1057.8772 38.5750 40.6676
Frequencies -- 45.3048 46.4108 57.7779
Frequencies -- 60.1246 81.4158 98.4860

Zero-point correction= 0.256988 (Hartree/Particle)
Thermal correction to Energy= 0.289186
Thermal correction to Enthalpy= 0.290130
Thermal correction to Gibbs Free Energy= 0.196226
Sum of electronic and zero-point Energies= -2765.617589
Sum of electronic and thermal Energies= -2765.585392
Sum of electronic and thermal Enthalpies= -2765.584447
Sum of electronic and thermal Free Energies= -2765.678351

PENT-4-INT-Bondi.log



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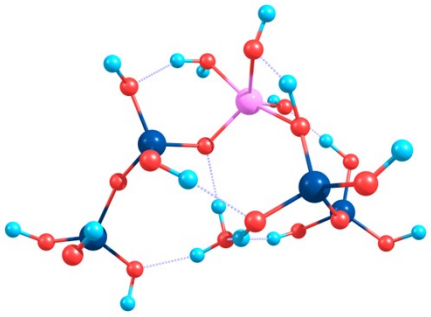
O	-3.958603	-0.878137	2.311422
O	-2.648896	-2.01205	0.404835
O	-5.395501	-1.770292	0.239583
O	-3.860805	0.350767	-0.149818
O	-2.031598	1.141568	-1.909184
O	-3.496219	3.00339	-0.601297
O	-1.676454	1.738766	0.736246
O	1.880431	-1.651727	-1.056461
O	3.420878	0.261956	0.022493
O	4.485943	-1.839494	-1.312858
O	3.431758	-2.199503	1.135039
O	1.924573	2.379709	0.751555
O	1.990923	0.106326	2.290847
O	4.142119	1.725385	2.106646
H	-4.179511	3.073357	-1.281464
H	-5.705687	-1.536814	-0.646251
H	-1.061657	0.977444	0.8653
H	5.384958	-1.741635	-0.970696
H	2.961858	-1.757017	1.863181
H	1.113206	-0.14691	1.90757
H	3.949642	2.251824	2.894794
H	-4.741187	-0.447123	2.680079
H	-2.233484	-1.951322	-0.488553
Si	-2.767109	1.54078	-0.466162
Si	3.287647	-1.379099	-0.288775
H	-2.011726	0.177045	-2.088589
H	3.368112	1.253203	-1.719191
Si	-3.968368	-1.07127	0.679535
Si	2.837514	1.131386	1.313073
H	1.195414	2.139706	0.158556
Al	0.343509	-0.86108	-0.907167
O	2.833544	1.505041	-2.496983
O	0.612804	0.861071	-1.531215
H	-0.209287	1.296039	-1.859032
O	-0.151105	-0.522633	0.765112
H	-0.804261	-1.148452	1.121105
O	-1.072839	-1.494457	-1.73273
H	-0.994527	-2.056471	-2.513614
H	1.474482	1.148087	-2.036198
H	3.124836	0.912453	-3.207067

Frequencies -- 27.3024 28.0682 31.9175
Frequencies -- 46.7162 56.2288 62.2464
Frequencies -- 70.1664 75.2842 87.2025

Zero-point correction= 0.259247 (Hartree/Particle)
Thermal correction to Energy= 0.293315
Thermal correction to Enthalpy= 0.294259
Thermal correction to Gibbs Free Energy= 0.194593
Sum of electronic and zero-point Energies= -2765.639096
Sum of electronic and thermal Energies= -2765.605028
Sum of electronic and thermal Enthalpies= -2765.604083
Sum of electronic and thermal Free Energies= -2765.703749

PENT-4-TS2-Bondi10.log



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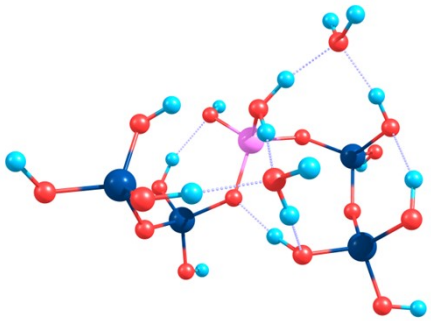
O	3.929931	0.024353	-1.269952
O	2.259036	-2.087958	-1.766211
O	4.639154	-2.478517	-0.709155
O	2.718098	-1.321871	0.765749
O	1.7913	1.164233	0.894085
O	0.311446	-0.938583	1.87236
O	2.40106	-0.120767	3.195643
O	-0.564155	0.868613	-0.646629
O	-3.105452	0.053054	-0.688472
O	-2.505139	2.612392	-0.143561
O	-1.966478	0.647645	1.669077
O	-2.891112	-2.546524	-0.879415
O	-3.967787	-1.414218	1.403682
O	-5.323761	-1.509949	-0.921157
H	0.049279	-1.474509	1.0814
H	5.436477	-2.13349	-0.285338
H	3.147168	0.487509	3.28805
H	-2.77153	3.084693	0.657732
H	-1.144453	0.158604	1.908725
H	-3.336971	-0.813092	1.843728
H	-6.032321	-1.000171	-0.504129
H	3.248997	0.724764	-1.461257
H	1.354023	-2.164959	-1.386582
Si	1.819901	-0.287887	1.666563
Si	-2.014743	1.036742	0.06139
H	-0.309057	-0.933772	-0.881335
Si	3.36955	-1.423884	-0.758609
Si	-3.841841	-1.350301	-0.23392
H	-3.151498	-3.454484	-0.668601
Al	0.774443	2.038266	-0.563809
O	-0.192572	-1.871654	-0.613323
O	2.085116	1.892353	-1.719666
H	1.949464	2.177004	-2.631263
O	0.736934	3.163647	0.913041
H	1.147761	4.037805	0.863448
H	-1.054477	-2.294709	-0.810594
H	1.43754	2.214116	1.312249
O	-0.252856	3.427356	-1.556149
H	-1.164214	3.429686	-1.178745
H	-0.356192	3.303295	-2.513469

Frequencies -- -1040.2364 29.7363 35.0527
Frequencies -- 42.7669 44.2258 65.1007
Frequencies -- 76.1679 84.9571 93.5537

Zero-point correction= 0.256835 (Hartree/Particle)
Thermal correction to Energy= 0.289738
Thermal correction to Enthalpy= 0.290682
Thermal correction to Gibbs Free Energy= 0.195069
Sum of electronic and zero-point Energies= -2765.628498
Sum of electronic and thermal Energies= -2765.595595
Sum of electronic and thermal Enthalpies= -2765.594650
Sum of electronic and thermal Free Energies= -2765.690263

PENT-4-PRD-Bondi2.log



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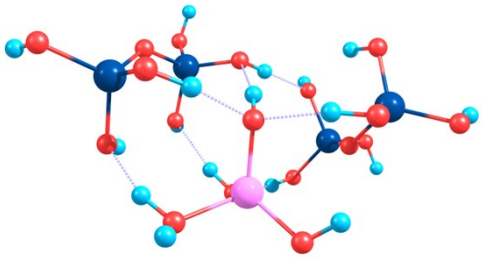
O	-2.996919	-1.689063	-1.735789
O	-2.839975	-3.49974	0.263656
O	-0.712143	-2.084934	-0.325949
O	-2.808932	-0.83155	0.810831
O	-1.742645	1.634167	0.962854
O	-3.527407	0.986317	-0.984004
O	-4.368211	1.246001	1.516842
O	0.604533	-0.14723	0.992825
O	3.107313	-0.981347	0.437874
O	1.994448	-1.882249	2.574664
O	2.640038	0.751301	2.499935
O	3.072006	-0.951974	-2.278088
O	3.092477	1.383137	-0.863495
O	5.240707	-0.243446	-0.864275
H	-3.044798	1.694465	-1.465173
H	-0.239028	-1.461886	0.282382
H	-4.262506	1.117638	2.469574
H	1.436008	-1.802735	3.359542
H	2.191953	1.588033	2.238282
H	2.311656	1.607751	-1.390633
H	5.686428	0.257306	-1.561004
H	-3.264824	-0.750376	-1.803928
H	-3.790031	-3.67212	0.207222
Si	-3.07861	0.792654	0.597344
Si	2.067842	-0.5293	1.63837
H	-0.066287	-1.396217	-1.782644
Si	-2.365168	-2.013739	-0.250777
Si	3.597131	-0.192896	-0.924167
H	2.099	-0.937525	-2.420596
Al	-0.040804	1.457571	0.637734
O	0.33949	-0.740751	-2.404961
O	0.129573	1.535214	-1.215062
H	-0.556684	2.107906	-1.673098
O	0.973187	2.678564	1.367552
H	0.551515	3.285212	1.988777
O	-1.90782	2.851035	-2.204351
H	-1.95949	2.920238	-3.170389
H	0.168126	0.647313	-1.716234
H	-0.144099	-0.812008	-3.241618
H	-2.000956	3.75691	-1.870251

Frequencies -- 23.7519 27.1700 35.9852
Frequencies -- 41.1256 56.6500 64.5113
Frequencies -- 67.7479 73.3558 92.1374

Zero-point correction= 0.260828 (Hartree/Particle)
Thermal correction to Energy= 0.294486
Thermal correction to Enthalpy= 0.295430
Thermal correction to Gibbs Free Energy= 0.197175
Sum of electronic and zero-point Energies= -2765.653963
Sum of electronic and thermal Energies= -2765.620305
Sum of electronic and thermal Enthalpies= -2765.619361
Sum of electronic and thermal Free Energies= -2765.717615

PENT-4-RCT-Bondi.log



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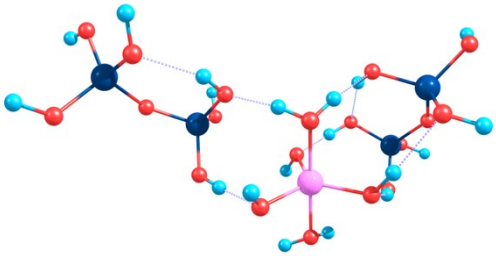
O	-2.701562	0.317435	-2.422307
O	-4.489694	-1.495936	-1.478283
O	-2.006046	-2.195648	-1.541722
O	-2.688316	-0.274252	0.18883
O	-2.085033	1.191611	2.335529
O	-1.99455	2.188788	-0.258921
O	-4.306467	1.816213	0.951513
O	2.892593	-1.654873	-1.375236
O	3.06872	1.040359	-0.908107
O	5.233129	-0.571413	-1.088869
O	3.523695	-0.7003	1.060926
O	0.490091	1.410467	-1.006281
O	1.872263	1.740396	1.338146
O	2.133572	3.57572	-0.557579
H	-2.12709	3.144665	-0.179091
H	-1.059584	-1.990707	-1.341384
H	-4.852516	1.459188	1.665515
H	5.866424	0.000878	-0.634664
H	3.320904	0.103142	1.571701
H	1.741725	2.519375	1.897432
H	1.993217	3.900366	-1.458396
H	-2.390177	1.148654	-2.026867
H	-5.195772	-0.836532	-1.509812
Si	-2.777119	1.2223	0.866907
Si	3.676036	-0.461177	-0.594968
H	-1.270557	0.603193	2.371889
H	1.919507	-1.668734	-1.181412
Si	-2.969257	-0.887449	-1.326109
Si	1.86465	1.980582	-0.305776
H	-0.372063	1.793161	-0.716947
Al	0.102416	-1.708054	1.179642
O	0.062566	-0.297186	2.221467
H	0.719139	0.396362	2.024696
O	0.356667	-1.331779	-0.540162
O	1.739317	-2.515719	1.684907
H	1.954287	-3.395739	1.33691
O	-1.078672	-2.944015	1.449311
H	-1.697103	-3.030025	0.711052
H	2.531209	-1.917029	1.528755
H	0.288518	-0.384055	-0.780785

Frequencies -- 18.4649 35.5017 41.3036
Frequencies -- 48.0029 56.6064 62.4830
Frequencies -- 63.9582 71.7643 79.2418

Zero-point correction= 0.258888 (Hartree/Particle)
Thermal correction to Energy= 0.292929
Thermal correction to Enthalpy= 0.293873
Thermal correction to Gibbs Free Energy= 0.194088
Sum of electronic and zero-point Energies= -2765.633674
Sum of electronic and thermal Energies= -2765.599633
Sum of electronic and thermal Enthalpies= -2765.598689
Sum of electronic and thermal Free Energies= -2765.698474

Neutral 5

PENT-5-RCT-Bondi.log



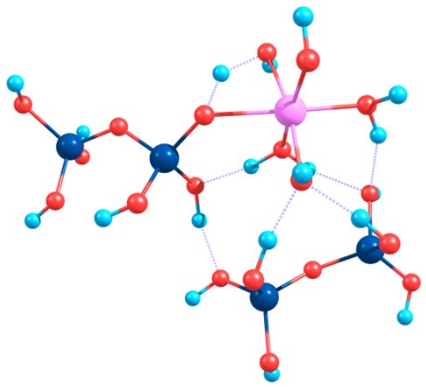
43

O	-2.176923	2.014839	0.422835
O	-4.534601	3.37	-0.095521
O	-3.35611	1.810386	-1.88492
O	-4.520117	0.711418	0.35439
O	-3.826131	-1.858446	-0.073344
O	-2.580945	-0.335815	1.851475
O	-5.065421	-1.163369	2.224415
O	2.6311	-1.939101	-0.204988
O	4.513977	-0.312146	0.812477
O	2.355191	-0.995106	2.248613
O	2.155659	0.739293	0.142547
O	6.508348	-0.133287	-0.850908
O	4.564849	1.814933	-0.766591
O	6.325499	1.697979	1.195011
H	-1.752805	-0.74075	1.429529
H	-4.115072	1.859358	-2.48329
H	-5.972704	-1.289489	1.914066
H	2.581019	-0.345747	2.928737
H	2.805345	1.333616	-0.28939
H	4.756781	2.75614	-0.651064
H	6.989305	1.243153	1.732158
H	-2.134493	1.38446	1.175673
H	-4.927061	3.513956	0.777077
Si	-3.986622	-0.698017	1.07441
Si	2.891387	-0.63764	0.735399
H	-3.344819	-1.50794	-0.881785
H	1.988695	-1.804003	-0.962434
Si	-3.684303	1.979007	-0.275513
Si	5.519576	0.769855	0.102831
H	7.178211	0.362401	-1.342453
Al	-0.642871	-1.126977	-1.204063
O	-2.246526	-0.865396	-1.918996
H	-2.513089	0.046821	-2.118943
O	0.85047	-1.499545	-2.10197
O	-0.212092	0.793878	-1.097939
H	-0.868637	1.339738	-0.603296
O	-0.52193	-1.248324	0.585492
H	-0.363916	-2.141965	0.914758
O	-1.10505	-3.122971	-1.31641
H	-0.402702	-3.753311	-1.092867
H	-1.870259	-3.359661	-0.766368
H	0.649874	0.869312	-0.607015
H	1.239129	-0.734013	-2.545409

Frequencies --	11.8595	20.7377	24.8581
Frequencies --	33.6098	34.7896	42.8809
Frequencies --	57.1240	62.7128	77.9601

Zero-point correction= 0.284787 (Hartree/Particle)
Thermal correction to Energy= 0.320839
Thermal correction to Enthalpy= 0.321784
Thermal correction to Gibbs Free Energy= 0.216409
Sum of electronic and zero-point Energies= -2842.050434
Sum of electronic and thermal Energies= -2842.014381
Sum of electronic and thermal Enthalpies= -2842.013437
Sum of electronic and thermal Free Energies= -2842.118812

PENT-5-INT-Bondi2.log



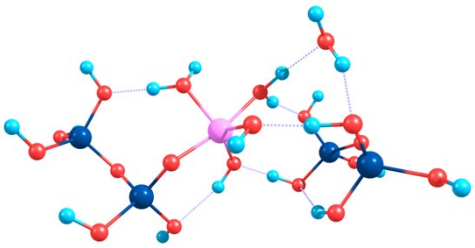
43

O	1.199742	-1.519142	1.668251
O	2.275564	-3.788745	0.975963
O	0.323599	-2.760623	-0.621315
O	2.643634	-1.604988	-0.642039
O	3.473998	0.742151	-1.608248
O	3.923341	0.197978	0.939819
O	5.28496	-1.120725	-1.006577
O	2.436339	3.038041	-0.45042
O	-3.524172	0.539169	-0.193328
O	-1.977059	-0.695071	1.656391
O	-1.197227	-0.523663	-0.965414
O	-5.009135	-1.073148	-1.873869
O	-4.42606	-1.756971	0.624375
O	-6.182188	0.323788	0.052595
H	3.045047	0.607054	1.206731
H	5.427561	-2.05138	-0.785608
H	-2.697634	-1.349172	1.641788
H	-0.775964	-1.399075	-0.799461
H	-4.96298	-2.556482	0.542814
H	1.214243	-0.52097	1.547834
H	2.503158	-4.462122	0.320275
Si	3.850172	-0.489191	-0.531496
Si	-1.969334	0.239722	0.301262
H	3.718656	0.616837	-2.536858
H	3.020812	2.386874	-0.897124
Si	1.619081	-2.403919	0.375168
Si	-4.805642	-0.479117	-0.356112
H	-5.418181	-0.469213	-2.508811
Al	0.713921	2.38035	0.34296
O	-0.384985	3.530508	-0.801589
O	1.483949	1.052375	1.387817
H	1.434362	1.361561	2.304123
O	-1.230011	1.657575	0.601462
O	0.767391	3.586912	1.661463
H	0.365019	4.420926	1.391014
H	-0.301438	3.248292	-1.725665
H	2.963481	3.485261	0.228534
H	-1.293119	2.693533	-0.305065
O	0.783423	1.191975	-1.253971
H	1.647036	0.843246	-1.552245
H	0.109357	0.461871	-1.271608
H	-6.090447	0.943098	0.79025
H	-0.230628	-3.488828	-0.30384

Frequencies --	-1564.5968	20.7597	25.9591
Frequencies --	37.5108	43.0935	60.1080
Frequencies --	62.9151	69.4520	84.4349

Zero-point correction= 0.279840 (Hartree/Particle)
Thermal correction to Energy= 0.315333
Thermal correction to Enthalpy= 0.316277
Thermal correction to Gibbs Free Energy= 0.214819
Sum of electronic and zero-point Energies= -2842.026033
Sum of electronic and thermal Energies= -2841.990540
Sum of electronic and thermal Enthalpies= -2841.989596
Sum of electronic and thermal Free Energies= -2842.091054

PENT-5-TS-Bondi4.log



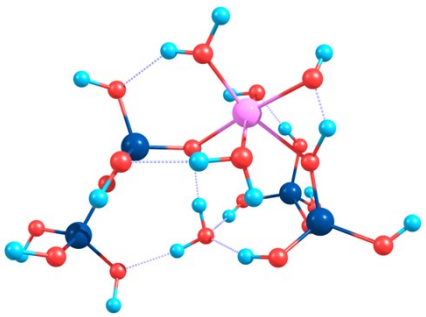
43

O	-2.910502	-2.159078	-0.110533
O	-3.064504	-0.506742	-2.238079
O	-5.315799	-1.62551	-1.317255
O	-4.168918	0.207227	0.149688
O	-2.82299	2.104303	1.555433
O	-4.797374	0.69179	2.710781
O	-2.407498	-0.445734	2.084231
O	1.77358	-0.777607	-0.686554
O	3.862888	-0.273156	0.958821
O	3.704859	-2.656882	-0.271762
O	1.94181	-2.003287	1.65488
O	6.180634	1.139879	1.088654
O	5.646043	-0.479868	-0.958898
O	4.145025	1.80968	-0.613497
H	-5.579468	0.175498	2.47213
H	-5.316622	-2.20132	-2.093863
H	-1.459637	-0.231923	1.747389
H	4.479449	-2.331587	-0.758877
H	2.448697	-2.133405	2.468069
H	6.060525	-0.1135	-1.751683
H	4.63688	2.418548	-1.183134
H	-2.630541	-1.852515	0.77443
H	-2.046258	-0.474154	-2.137578
Si	-3.56187	0.615587	1.628814
Si	2.802136	-1.421218	0.357955
H	-3.380641	2.835735	1.251688
H	-3.053862	1.284364	-2.42498
Si	-3.83649	-1.037252	-0.890884
Si	4.982338	0.572021	0.122763
H	5.915563	1.786225	1.758216
Al	0.344783	0.35198	-0.532497
O	-0.976421	1.824997	-0.468135
H	-1.618045	1.990048	-1.224475
O	-2.759863	2.219706	-2.34631
O	1.508728	1.821997	-0.91569
H	1.177692	2.709162	-0.715875
O	-0.076771	0.024501	1.183404
H	0.478473	-0.678577	1.562072
O	-0.539771	-0.301541	-1.951399
H	-0.075603	-1.073238	-2.301502
H	2.497261	1.791038	-0.809491
H	-2.325055	2.410689	-3.190175
H	-1.481807	1.987871	0.356785

Frequencies --	11.9011	24.4991	36.7782
Frequencies --	44.1229	50.4136	52.2444
Frequencies --	61.4198	76.8058	86.6521

Zero-point correction=	0.283881 (Hartree/Particle)
Thermal correction to Energy=	0.320409
Thermal correction to Enthalpy=	0.321353
Thermal correction to Gibbs Free Energy=	0.215806
Sum of electronic and zero-point Energies=	-2842.065171
Sum of electronic and thermal Energies=	-2842.028643
Sum of electronic and thermal Enthalpies=	-2842.027699
Sum of electronic and thermal Free Energies=	-2842.133246

PENT-5-TS2-Bondi8.log



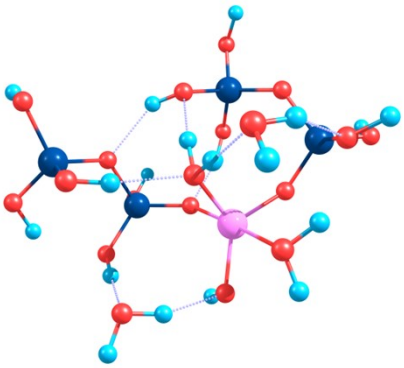
43

O	4.238234	-2.710155	-1.424271
O	3.333306	-0.250291	-1.854222
O	1.5595	-2.300715	-1.647263
O	2.949791	-1.589269	0.536159
O	2.321081	0.955151	0.661433
O	1.103875	-0.7248	2.345189
O	3.626869	-0.1949	2.780089
O	-0.620465	0.744605	-0.627422
O	-3.039219	-0.435683	-0.806748
O	-2.593575	2.097972	-1.697403
O	-2.646947	1.570421	0.955877
O	-2.892225	-2.707933	0.512945
O	-4.334604	-0.714917	1.544992
O	-5.194557	-1.908688	-0.786969
H	0.493619	-1.235295	1.753469
H	0.857121	-2.303708	-0.954738
H	4.465591	0.205185	2.511783
H	-3.492528	2.455869	-1.665693
H	-3.202211	0.967856	1.484323
H	-5.227373	-0.341432	1.57343
H	-5.714081	-2.660867	-0.470271
H	4.485385	-2.781469	-2.355815
H	2.644731	0.474606	-1.823382
Si	2.524319	-0.384458	1.574266
Si	-2.216572	0.967719	-0.537959
H	-0.422042	-0.937756	-0.109086
Si	2.986913	-1.670814	-1.124383
Si	-3.912329	-1.462642	0.128639
H	-3.078438	-3.172712	1.34152
Al	0.713043	1.994849	-0.292009
O	-0.243127	-1.818352	0.300214
O	0.012376	1.954381	1.640056
H	-0.971994	1.924852	1.634676
O	1.533984	1.755709	-1.889179
H	0.908684	1.388266	-2.527955
O	1.983905	3.237589	0.383675
H	2.531323	3.584909	-0.334771
H	0.284392	1.106265	2.050901
H	-1.114992	-2.259269	0.369775
H	2.496515	2.050719	0.75521
O	-0.50235	3.492441	-0.660883
H	-1.247014	3.337613	-1.283308
H	-0.085701	4.345518	-0.851985

Frequencies --	-590.4352	23.1192	26.9842
Frequencies --	34.4653	44.7270	53.4526
Frequencies --	66.5102	69.2180	100.8637

Zero-point correction=	0.282816 (Hartree/Particle)
Thermal correction to Energy=	0.317670
Thermal correction to Enthalpy=	0.318614
Thermal correction to Gibbs Free Energy=	0.218868
Sum of electronic and zero-point Energies=	-2842.045603
Sum of electronic and thermal Energies=	-2842.010750
Sum of electronic and thermal Enthalpies=	-2842.009805
Sum of electronic and thermal Free Energies=	-2842.109552

PENT-5-PRD-Bondi.log



43

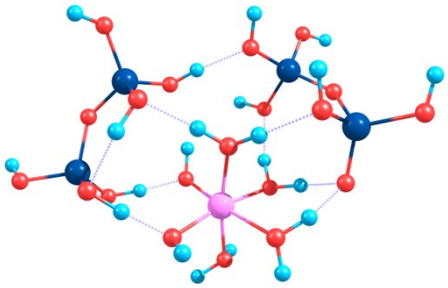
O	4.708733	-0.267423	0.482541
O	3.461981	-1.832342	2.262849
O	2.634809	0.662858	1.984237
O	2.17266	-1.100107	-0.001054
O	0.359861	0.188889	-1.468273
O	3.040828	0.852893	-1.626343
O	2.206665	-1.371818	-2.695308
O	-2.234404	0.82101	-1.014462
O	-2.892568	-1.344266	0.422945
O	-4.857947	0.045554	-0.802536
O	-3.586818	1.159073	1.22758
O	-1.973974	-3.866889	0.162981
O	-1.173672	-2.109694	-1.588466
O	-0.369785	-1.774092	0.987609
H	2.856892	1.727734	-1.179492
H	1.717768	0.881911	1.738317
H	1.628967	-2.146712	-2.722367
H	-4.98403	-0.702437	-1.402362
H	-4.478381	1.190266	1.602514
H	-0.714412	-1.25285	-1.74875
H	0.533238	-1.977828	0.67394
H	4.584964	0.238247	-0.340842
H	3.896676	-2.626791	1.923455
Si	1.895761	-0.318403	-1.463161
Si	-3.375718	0.155274	-0.098117
H	-1.496238	2.430404	3.283933
Si	3.253321	-0.623026	1.1681
Si	-1.607567	-2.278794	-0.0189
H	-2.423048	-4.104999	0.985541
Al	-0.634063	1.501536	-0.664354
O	-0.096289	0.869532	1.064358
H	-0.593745	1.195874	1.898751
O	-1.507353	1.476895	3.111236
O	-1.511479	2.977704	0.485883
H	-1.596741	3.794596	-0.029146
O	0.038952	2.899024	-1.5378
H	0.467872	2.608971	-2.3547
O	2.444606	3.105122	-0.343344
H	1.559045	3.244099	-0.764632
H	-2.409851	2.726535	0.777901
H	-2.377605	1.310633	2.694512
H	2.993503	3.844779	-0.640344
H	-0.161673	-0.12849	1.092408

Frequencies --	25.7238	38.6431	44.6304
Frequencies --	48.7337	60.3229	66.8359
Frequencies --	70.3552	80.8982	91.8817

Zero-point correction=	0.287006 (Hartree/Particle)
Thermal correction to Energy=	0.322972
Thermal correction to Enthalpy=	0.323917
Thermal correction to Gibbs Free Energy=	0.222185
Sum of electronic and zero-point Energies=	-2842.073643
Sum of electronic and thermal Energies=	-2842.037676
Sum of electronic and thermal Enthalpies=	-2842.036732
Sum of electronic and thermal Free Energies=	-2842.138464

Neutral 6

PENT-6-RCT-Bondi.log



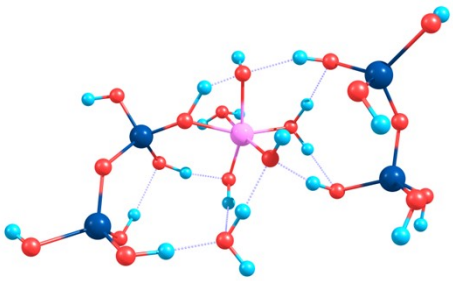
46

O	1.69046	-1.090572	1.767654
O	2.419283	-3.592886	0.966837
O	1.054477	-2.039158	-0.694013
O	3.572997	-1.381753	-0.119764
O	3.725144	0.966373	-1.457988
O	3.481188	0.908761	1.26456
O	5.759671	0.159097	0.131966
O	-3.306416	1.949388	0.220931
O	-3.694052	-0.719713	-0.264078
O	-5.317442	0.596687	1.381749
O	-2.685206	0.138597	2.056702
O	-1.811128	-0.973163	-2.07749
O	-1.543797	-2.401181	0.135386
O	-3.493644	-3.089968	-1.509179
H	2.733409	1.592466	1.057144
H	0.140221	-2.228952	-0.385788
H	6.228651	-0.452278	-0.452056
H	-5.719454	-0.263359	1.565039
H	-2.735556	-0.77807	2.364977
H	-1.78961	-3.195454	0.630064
H	-4.30341	-2.884497	-1.99726
H	2.331345	-0.351502	1.909041
H	2.951114	-3.706256	1.767187
Si	4.123521	0.198855	-0.073901
Si	-3.762052	0.546118	0.823672
H	2.709588	0.972911	-1.549455
H	-2.27054	1.770226	-0.928441
Si	2.195538	-2.035355	0.487318
Si	-2.668098	-1.798457	-0.921044
H	-1.07631	-1.452776	-2.486385
Al	0.184531	1.923089	-0.289456
O	1.161596	0.887642	-1.422757
H	0.935061	-0.054388	-1.39149
O	-1.396497	1.657917	-1.440395
O	-0.339568	0.412199	0.812934
H	0.363767	-0.154467	1.214841
O	1.577586	2.502472	0.748778
H	1.271446	2.871096	1.587134
O	0.424297	3.56883	-1.416992
H	1.331436	3.908577	-1.369264
O	-1.084599	2.984629	0.82575
H	-1.089075	3.925007	0.594032
H	-2.054949	2.644479	0.715645
H	-1.149018	0.354616	1.38132
H	-1.428965	0.752263	-1.818861
H	0.222423	3.420352	-2.353863

Frequencies --	34.2119	38.3488	53.9537
Frequencies --	54.9167	60.6202	61.6042
Frequencies --	71.3585	78.8796	86.2087

Zero-point correction=	0.310435 (Hartree/Particle)
Thermal correction to Energy=	0.347623
Thermal correction to Enthalpy=	0.348567
Thermal correction to Gibbs Free Energy=	0.244820
Sum of electronic and zero-point Energies=	-2918.490858
Sum of electronic and thermal Energies=	-2918.453671
Sum of electronic and thermal Enthalpies=	-2918.452726
Sum of electronic and thermal Free Energies=	-2918.556473

PENT-6-TS-Bondi.log



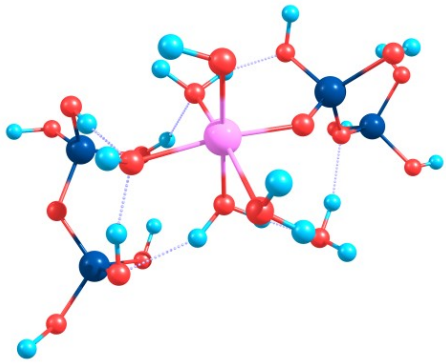
46

O	3.796497	2.495384	-0.770092
O	5.00359	2.098502	1.705164
O	2.416815	1.444521	1.319669
O	4.473213	0.129536	0.087514
O	3.047996	-2.055825	-0.456995
O	2.955851	0.003109	-2.161273
O	5.213366	-1.419333	-1.990248
O	-0.963774	0.106421	1.896533
O	-4.088746	-0.184623	-0.947365
O	-3.293769	-0.956688	1.506478
O	-3.793187	-2.804014	-0.458275
O	-5.893689	1.760953	-1.410867
O	-4.691965	1.519658	1.025356
O	-3.417151	2.447518	-1.216595
H	3.153514	0.955159	-2.189932
H	1.691765	1.205849	0.654757
H	5.855509	-1.94638	-1.49425
H	-2.450131	-0.458577	1.788307
H	-4.751438	-2.871252	-0.568657
H	-4.370629	0.727692	1.49564
H	-2.544424	2.47214	-0.744245
H	3.17627	3.237033	-0.737563
H	4.744554	2.858001	2.244431
Si	3.937306	-0.838553	-1.135059
Si	-3.218582	-1.304417	-0.111639
H	2.146923	-2.199204	-0.839065
H	-1.064087	1.015958	1.562306
Si	3.894662	1.582922	0.612505
Si	-4.502113	1.390882	-0.61078
H	-6.644015	1.187394	-1.206001
Al	-0.096678	-0.923561	0.68945
O	1.58023	-1.219033	1.698642
H	1.96339	-0.348492	1.944114
O	-1.136048	2.383689	0.165495
O	0.622938	0.466312	-0.281986
H	1.060311	0.263453	-1.122796
O	-1.630537	-1.240762	-0.530538
H	-0.806399	-1.979152	-0.88796
O	0.397839	-2.300679	-0.628531
H	0.357417	-3.197775	-0.262894
O	-0.742085	-2.528504	1.804784
H	-0.16738	-2.671359	2.574074
H	-1.640384	-2.409883	2.159619
H	-0.445816	1.771668	-0.207257
H	-0.684545	3.220361	0.343753
H	2.259506	-1.627158	1.105425

Frequencies -- -993.9082 23.7138 26.0656
Frequencies -- 31.1098 42.0689 45.6836
Frequencies -- 60.5548 68.0173 72.3926

Zero-point correction= 0.307353 (Hartree/Particle)
Thermal correction to Energy= 0.344620
Thermal correction to Enthalpy= 0.345564
Thermal correction to Gibbs Free Energy= 0.239837
Sum of electronic and zero-point Energies= -2918.467561
Sum of electronic and thermal Energies= -2918.430294
Sum of electronic and thermal Enthalpies= -2918.429350
Sum of electronic and thermal Free Energies= -2918.535078

PENT-6-INT-Bondi.log



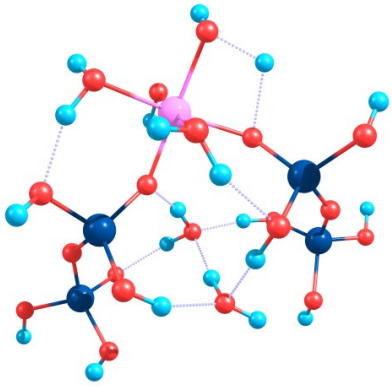
46

O	4.105696	1.134131	-3.055459
O	1.990483	1.333275	-1.483861
O	3.083671	-1.123267	-1.960669
O	4.344891	0.684503	-0.398286
O	3.175676	-0.154904	1.876057
O	5.169522	1.661058	2.003824
O	2.874507	2.433227	1.032959
O	-1.578954	-1.474616	0.541395
O	-3.175081	0.633156	0.201603
O	-4.121336	-1.872445	-0.236515
O	-2.338684	-0.687657	-1.934007
O	-4.043071	2.818561	-0.959319
O	-5.642642	0.588003	-0.913435
O	-5.162787	1.855597	1.387071
H	5.676616	0.964471	2.44214
H	2.791975	-1.552898	-1.096061
H	2.307652	2.369722	0.242461
H	-4.933835	-1.414556	-0.510321
H	-2.657366	-1.382356	-2.528592
H	-5.580696	0.625607	-1.878763
H	-6.073102	2.182254	1.393329
H	5.037005	0.903752	-3.177673
H	1.209757	0.75651	-1.368102
Si	3.881006	1.131971	1.12995
Si	-2.783566	-0.908382	-0.322087
H	2.893286	-0.919682	1.271068
H	-2.204767	0.937902	1.762965
Si	3.387061	0.472074	-1.733779
Si	-4.536601	1.511752	-0.092163
H	-4.722716	3.474432	-1.168209
Al	0.216543	-1.843404	0.386802
O	0.502584	-0.041322	1.162288
H	-0.249456	0.367849	1.680663
O	-1.531602	1.026626	2.466961
O	0.27899	-0.921124	-1.428296
H	0.862898	-1.341835	-2.081752
O	-0.026564	-3.531684	-0.192336
H	0.789476	-3.94059	-0.503104
O	2.115416	-1.9204	0.326249
H	2.441008	-2.801361	0.553934
O	0.221497	-2.48681	2.327233
H	-0.45412	-2.020404	2.845102
H	-0.073567	-3.411373	2.279113
H	-0.626632	-0.828945	-1.826051
H	-1.792572	0.369075	3.128375
H	1.335811	0.091605	1.656524

Frequencies -- 16.0050 21.1071 34.9654
Frequencies -- 37.6156 43.4178 54.2035
Frequencies -- 64.9199 65.4818 84.7507

Zero-point correction= 0.311166 (Hartree/Particle)
Thermal correction to Energy= 0.349661
Thermal correction to Enthalpy= 0.350605
Thermal correction to Gibbs Free Energy= 0.242315
Sum of electronic and zero-point Energies= -2918.475148
Sum of electronic and thermal Energies= -2918.436653
Sum of electronic and thermal Enthalpies= -2918.435709
Sum of electronic and thermal Free Energies= -2918.543999

PENT-6-TS2-Bondi.log

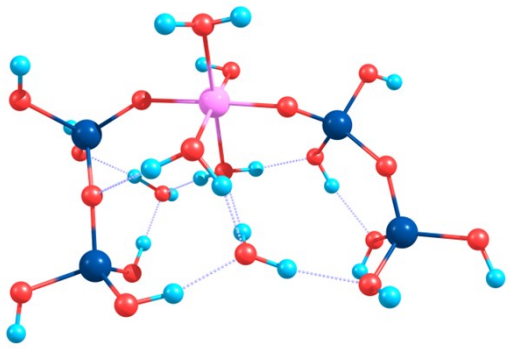


46

O	2.374702	-3.229053	0.836748
O	4.558417	-3.002671	-0.669345
O	2.235588	-2.280533	-1.755103
O	3.284394	-0.843303	0.306129
O	1.888499	1.273247	-0.629777
O	1.599232	0.4966	1.949015
O	3.849402	1.589335	1.261141
O	-0.898318	1.037744	-0.326681
O	-3.264196	-0.16341	-0.201253
O	-2.944275	2.277863	0.839266
O	-1.892969	0.188305	2.104195
O	-2.805906	-2.375103	-1.549112
O	-3.155776	-2.591645	1.065798
O	-5.277229	-1.781218	-0.486984
H	0.988719	-0.280491	1.848226
H	1.32098	-1.911697	-1.663061
H	4.489814	1.897908	0.606216
H	-3.268308	2.458043	1.732354
H	-1.278045	-0.572493	2.1104
H	-3.403717	-2.202832	1.916455
H	-5.692365	-2.652035	-0.419231
H	2.139287	-4.130701	0.576248
H	5.004351	-2.669767	-1.460268
Si	2.642777	0.628705	0.662015
Si	-2.189239	0.806867	0.606619
H	-0.401573	-0.422538	-1.045939
Si	3.088082	-2.325996	-0.361668
Si	-3.646703	-1.748756	-0.260729
H	-2.827509	-3.338202	-1.643827
Al	0.237631	2.431045	-0.768975
O	0.069686	-1.679828	1.498693
H	-0.063015	-1.691313	0.517384
O	-0.207706	-1.385346	-1.185297
O	0.504699	2.81122	1.207623
H	-0.170935	3.305829	1.692418
O	0.017217	2.352372	-2.55064
H	-0.423646	1.528194	-2.790176
O	1.435939	3.961876	-0.995976
H	1.482868	4.138462	-1.951422
H	0.712815	1.983088	1.711748
H	-1.04036	-1.786178	-1.508628
H	2.553692	2.909712	-0.90602
H	0.72182	-2.38662	1.654967
O	-1.233539	3.809035	-0.540099
H	-1.993597	3.431942	-0.029606
H	-1.57222	4.012701	-1.425626

Frequencies -- -1422.3532 27.2155 35.6015
Frequencies -- 41.3729 47.9053 56.0851
Frequencies -- 65.5624 68.9984 73.8402

Zero-point correction= 0.304445 (Hartree/Particle)
Thermal correction to Energy= 0.342733
Thermal correction to Enthalpy= 0.343678
Thermal correction to Gibbs Free Energy= 0.237389
Sum of electronic and zero-point Energies= -2918.415121
Sum of electronic and thermal Energies= -2918.376833
Sum of electronic and thermal Enthalpies= -2918.375889
Sum of electronic and thermal Free Energies= -2918.482177



46

O	-2.504389	2.460352	1.362269
O	-4.472846	2.764726	-0.510332
O	-1.901215	2.923597	-1.211437
O	-3.019036	0.585788	-0.557836
O	-2.100196	-1.863416	-0.148668
O	-4.140908	-0.806318	1.365562
O	-4.608073	-1.533784	-1.134675
O	1.51321	-1.534805	-0.732241
O	3.844569	-0.166021	-0.525209
O	3.69417	-2.739555	0.198697
O	2.462142	-0.790458	1.678594
O	3.282387	2.502267	-0.853696
O	4.01504	1.542782	1.486664
O	5.825519	1.515372	-0.607609
H	-4.597859	-1.600783	1.676596
H	-0.960246	2.70447	-1.023069
H	-4.279699	-2.068757	-1.869881
H	4.516931	-2.688943	0.704068
H	2.956857	0.01412	1.930695
H	3.653057	2.393305	1.772322
H	6.226735	2.381888	-0.451793
H	-2.391391	1.68282	1.954742
H	-4.61838	3.687975	-0.263402
Si	-3.417527	-0.965043	-0.136402
Si	2.836295	-1.325948	0.130123
H	0.456804	1.38132	0.202547
Si	-2.958333	2.190878	-0.189378
Si	4.259067	1.363493	-0.142748
H	3.430643	2.652626	-1.799097
Al	-0.260294	-1.785663	-0.266353
O	-0.559005	-0.304286	-1.677547
H	0.061852	0.442306	-1.49383
O	0.564198	1.879572	-0.63076
O	-2.082737	0.186217	2.773054
H	-2.897756	-0.303239	2.512907
O	0.063831	-3.082349	0.94112
H	-0.779342	-3.394717	1.291112
O	-0.093514	-0.250293	1.054447
H	0.769549	-0.400653	1.516868
O	-0.391411	-3.029703	-1.877166
H	-1.081508	-2.731646	-2.489627
H	0.44782	-2.964603	-2.360728
H	-1.986905	0.121185	3.733266
H	1.490218	2.195165	-0.666244
H	-0.80065	-0.154491	1.745554
H	-1.439827	0.099448	-1.568613

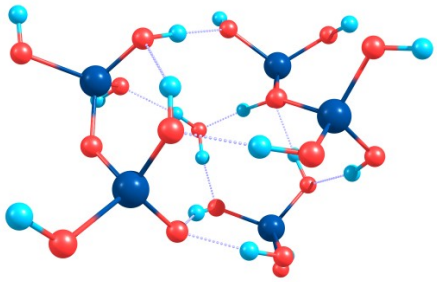
Frequencies -- 25.1072 27.3950 34.5487
Frequencies -- 39.8249 44.6113 55.3400
Frequencies -- 59.3975 71.2665 80.2297

Zero-point correction= 0.311957 (Hartree/Particle)
Thermal correction to Energy= 0.350817
Thermal correction to Enthalpy= 0.351762
Thermal correction to Gibbs Free Energy= 0.243564
Sum of electronic and zero-point Energies= -2918.487062
Sum of electronic and thermal Energies= -2918.448201
Sum of electronic and thermal Enthalpies= -2918.447257
Sum of electronic and thermal Free Energies= -2918.555454

Anionic Si

PENT-6-PRD-Bondi2.log

bondi-Si-RCT.log

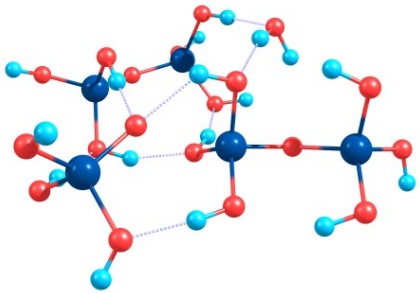


O	-2.275838	-3.325833	-0.189937
O	0.374822	-2.89017	-0.821514
O	-1.65356	-1.55404	-2.049648
O	-0.922421	-1.1049	0.538883
O	-3.330377	-0.155903	1.392994
O	-2.15786	-2.261053	2.537418
O	-1.064864	0.238945	2.84126
O	0.77037	2.390583	0.466132
O	2.986271	0.903113	-0.017735
O	1.523648	0.318442	2.136821
O	2.891989	2.622713	2.055551
O	4.908767	-0.823697	-0.350598
O	2.433624	-1.692042	0.395937
O	2.798869	-0.861607	-2.094789
H	-2.956695	-2.32812	3.078635
H	-0.902787	-1.101202	-2.568545
H	-0.094628	0.29599	2.64081
H	1.685817	-0.548691	1.711033
H	3.565817	2.176242	2.586064
H	1.692813	-2.15986	-0.060973
H	3.340569	-0.411095	-2.759234
H	-2.373711	-3.377805	0.778098
H	0.554008	-3.384931	-1.633144
Si	-1.87832	-0.770253	1.848757
Si	1.971591	1.59316	1.127413
H	-3.299713	0.295463	0.521868
H	0.184332	2.073513	-0.913573
Si	-1.141396	-2.225754	-0.646743
Si	3.283014	-0.62088	-0.521349
H	5.235327	-1.707372	-0.570694
O	-2.930164	0.801224	-1.216951
H	-2.490197	0.003791	-1.586386
O	-0.483845	1.928834	-1.68443
O	-2.815686	3.395792	-1.821917
H	-3.301698	3.128641	-2.613636
O	-1.852671	2.598864	0.509969
H	-0.889606	2.534838	0.765253
O	0.249202	-0.230595	-3.161097
H	0.039096	0.607139	-2.682129
H	1.093549	-0.529718	-2.767835
Si	-1.998067	2.169712	-1.06925

Frequencies --	22.4097	32.4709	41.0579
Frequencies --	51.0458	53.0401	57.7673
Frequencies --	60.3426	68.8644	77.2226

Zero-point correction= 0.262225 (Hartree/Particle)
Thermal correction to Energy= 0.296280
Thermal correction to Enthalpy= 0.297224
Thermal correction to Gibbs Free Energy= 0.197576
Sum of electronic and zero-point Energies= -2888.047128
Sum of electronic and thermal Energies= -2888.013074
Sum of electronic and thermal Enthalpies= -2888.012130
Sum of electronic and thermal Free Energies= -2888.111778

bondi-Si-TS1freqb.log



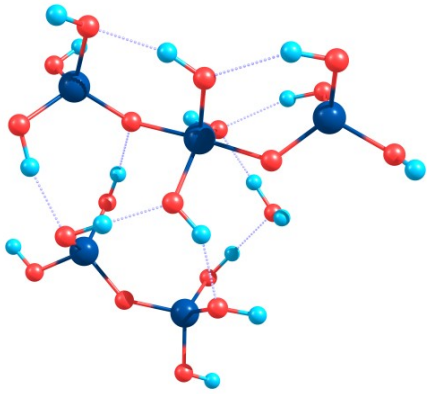
41
Si5H17O19

O	-0.023436	-0.082378	-1.160194
O	-2.059282	1.766633	-0.841303
O	-1.301684	0.205153	1.409667
O	0.340807	1.96214	0.693605
O	1.147847	4.513901	1.381212
O	2.103219	3.455109	-0.791295
O	-0.557744	4.022081	-0.6787
O	4.696213	0.17258	0.1113
O	2.95648	-1.700687	-0.329178
O	2.52991	0.750691	-1.36957
O	2.247949	0.358139	1.297385
O	0.682688	-2.681352	-1.191649
O	2.869627	-4.264709	-0.651914
O	1.421898	-3.230294	1.366001
H	2.354316	2.557681	-1.095385
H	-0.684126	0.878931	1.758691
H	-0.323955	4.487142	-1.493632
H	1.562698	0.578692	-1.470804
H	1.491014	1.012126	1.090597
H	2.553081	-5.12722	-0.351542
H	0.473334	-2.964805	1.525624
H	0.073857	-1.06051	-1.245057
H	-1.564587	2.619063	-0.802925
Si	0.767145	3.420538	0.183741
Si	3.072697	-0.082672	-0.036104
H	0.421177	4.683609	1.995581
H	4.927648	0.987213	0.577097
Si	-1.31553	0.417819	-0.255738
Si	1.960429	-2.983745	-0.152327
H	-0.040949	-3.323713	-1.172008
O	-4.90145	-2.004146	-0.628223
H	-5.179286	-1.973716	-1.55365
O	-2.466743	-0.767015	-0.599113
O	-4.7211	0.674866	-0.757671
H	-4.031167	1.341492	-0.936008
O	-4.124239	-0.758945	1.52428
H	-3.309957	-0.424793	1.934835
O	-1.119352	-2.53159	1.713436
H	-1.552493	-2.696189	0.862464
H	-1.121106	-1.551459	1.771878
Si	-4.043481	-0.693724	-0.123884

Frequencies --	-124.6731	17.4249	26.4137
Frequencies --	33.0364	41.4922	44.5765
Frequencies --	57.4560	60.0535	64.9373

Zero-point correction= 0.263062 (Hartree/Particle)
Thermal correction to Energy= 0.296946
Thermal correction to Enthalpy= 0.297890
Thermal correction to Gibbs Free Energy= 0.197613
Sum of electronic and zero-point Energies= -2888.031767
Sum of electronic and thermal Energies= -2887.997883
Sum of electronic and thermal Enthalpies= -2887.996938
Sum of electronic and thermal Free Energies= -2888.097215

Bondi-Si-INT.log



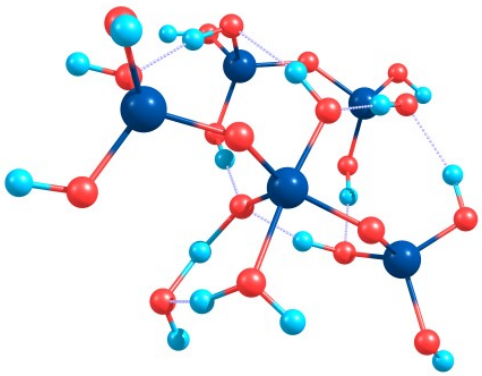
41
Si5H17O19

O	0.081232	-0.07152	-1.031285
O	-2.347872	1.507374	-0.794946
O	-1.383228	0.065448	1.576178
O	-0.126885	1.842304	0.46296
O	0.607668	4.227109	1.488056
O	1.439133	3.605337	-0.928771
O	-1.203036	4.04829	-0.540618
O	4.643756	0.723027	0.120343
O	3.116771	-1.324498	-0.358555
O	2.420613	1.065619	-1.378946
O	2.213087	0.648105	1.297769
O	1.046923	-2.679139	-1.265319
O	3.389082	-3.891682	-0.480434
O	1.695789	-2.909683	1.36723
H	1.897016	2.764594	-1.153505
H	-0.935894	0.705847	2.145774
H	-1.067289	4.561077	-1.349314
H	1.494912	0.713336	-1.481941
H	1.332618	1.047665	1.10536
H	3.172412	-4.760774	-0.117002
H	0.704383	-2.817686	1.446612
H	0.042441	-1.011971	-1.279052
H	-2.122942	2.456501	-0.754551
Si	0.190463	3.397208	0.117616
Si	3.065459	0.290009	-0.060207
H	-0.036847	4.162591	2.205984
H	4.779781	1.583518	0.53935
Si	-1.208957	0.485019	-0.084374
Si	2.280267	-2.715548	-0.143144
H	0.459793	-3.448413	-1.255589
O	-4.292936	-2.657837	-0.537531
H	-4.390256	-2.823328	-1.484944
O	-2.164918	-0.949949	-0.491096
O	-4.637868	-0.052489	-1.06409
H	-4.064372	0.730779	-1.19045
O	-4.024658	-0.974408	1.457049
H	-3.22647	-0.587946	1.864548
O	-0.940743	-2.653908	1.49847
H	-1.213846	-2.579673	0.567683
H	-1.068262	-1.725002	1.790327
Si	-3.756691	-1.136053	-0.170676

Frequencies -- 25.0957 32.2350 37.7888
Frequencies -- 43.6271 45.7100 56.4328
Frequencies -- 65.9176 70.3868 81.0679

Zero-point correction= 0.264851 (Hartree/Particle)
Thermal correction to Energy= 0.299264
Thermal correction to Enthalpy= 0.300208
Thermal correction to Gibbs Free Energy= 0.199622
Sum of electronic and zero-point Energies= -2888.040642
Sum of electronic and thermal Energies= -2888.006229
Sum of electronic and thermal Enthalpies= -2888.005285
Sum of electronic and thermal Free Energies= -2888.105871

bondi-Si-TS2-d3d.log



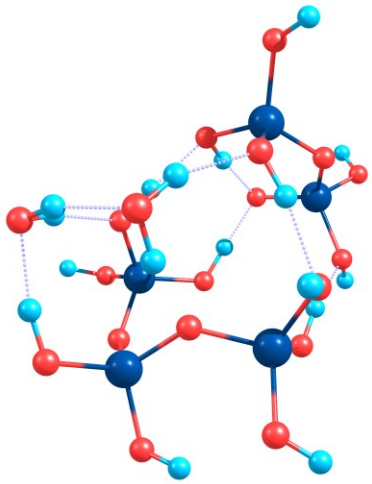
41
Si5H17O19

O	-0.020778	-0.034436	-1.333162
O	2.352243	-2.280104	0.363889
O	0.698373	-0.443393	1.158408
O	0.186775	-2.399677	-0.809212
O	-1.515178	-1.979921	1.234203
O	-2.510367	-2.84105	-1.11465
O	-0.956094	-4.497549	0.276894
O	-4.702368	1.41574	-0.77729
O	-2.302546	2.229763	-0.216987
O	-2.582109	-0.116602	-1.494712
O	-3.34377	0.07078	1.105181
O	0.243138	2.749016	-0.687007
O	-1.28153	4.241396	1.049454
O	-0.450892	1.792719	1.761872
H	-2.730948	-1.911073	-1.348475
H	1.487499	-0.827223	2.002489
H	-1.701016	-4.933673	0.712536
H	-1.566807	-0.091323	-1.50166
H	-2.753629	-0.713241	1.185774
H	-0.5779	4.669516	1.555336
H	0.00786	0.931142	1.508598
H	0.224557	0.907001	-1.354212
H	1.951751	-3.160941	0.360331
Si	-1.207872	-2.913746	-0.115236
Si	-3.214274	0.863279	-0.326486
H	-0.737278	-1.393393	1.436772
H	-5.420753	0.781672	-0.651902
Si	1.068238	-1.007975	-0.36251
Si	-0.909677	2.724741	0.507196
H	1.166008	2.6222	-0.369954
O	2.775857	2.053461	0.092311
H	3.337163	2.719666	0.513017
O	2.419788	-0.292499	-1.100909
O	4.38541	1.371277	-1.890186
H	4.908554	0.725899	-2.3859
O	4.548146	-0.005975	0.471296
H	5.246476	0.544203	0.852006
O	2.385475	-1.380183	2.586296
H	1.970644	-2.006363	3.197771
H	2.503815	-1.969407	1.493591
Si	3.552687	0.753934	-0.603796

Frequencies -- -1300.8456 30.9186 33.5073
Frequencies -- 42.8499 52.7951 76.1003
Frequencies -- 78.5861 82.2401 85.8875

Zero-point correction= 0.257526 (Hartree/Particle)
Thermal correction to Energy= 0.290324
Thermal correction to Enthalpy= 0.291268
Thermal correction to Gibbs Free Energy= 0.195320
Sum of electronic and zero-point Energies= -2888.018766
Sum of electronic and thermal Energies= -2887.985968
Sum of electronic and thermal Enthalpies= -2887.985023
Sum of electronic and thermal Free Energies= -2888.080971

bondi-Si-PRD1.log

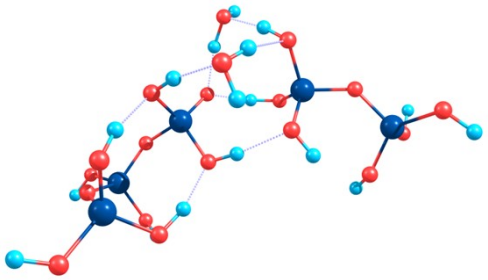


41
Si5H17O19

O	1.211944	-0.940758	2.226143
O	1.913744	1.537688	1.234828
O	3.482576	0.269937	2.933614
O	3.132725	-0.681893	0.379482
O	2.601233	1.403638	-1.235532
O	4.782331	-0.196825	-1.719852
O	2.38364	-1.248003	-2.040729
O	-1.448021	-0.735378	3.098084
O	-1.779663	-0.901129	0.179792
O	-3.934154	-0.813879	-1.446717
O	-3.987527	0.457291	0.910812
O	-0.073684	-2.867727	0.717694
O	-2.348176	-3.220777	-0.831371
O	-0.192226	-1.979296	-1.800224
H	5.272191	0.634512	-1.658577
H	3.726595	-0.52956	3.419834
H	2.435456	-1.138293	-3.001312
H	-3.769084	-1.771309	-1.402722
H	-2.162145	-3.952267	-1.436809
H	0.747734	-1.679103	-1.756632
H	0.903344	-1.621526	1.589006
Si	3.218088	-0.072428	-1.177907
Si	-3.047152	0.040187	-0.353946
H	1.103961	1.393081	-1.642552
Si	2.428994	0.035062	1.688671
Si	-1.066253	-2.243221	-0.461352
H	-0.535102	-3.214715	1.496622
O	0.115773	1.327019	-1.877225
O	-2.441307	1.366452	-1.114602
O	-0.618901	2.202507	0.632846
H	-1.820732	2.08653	2.01806
O	-1.151579	3.651438	-1.601211
H	-1.682718	4.250622	-1.058906
H	0.287984	1.931179	0.920469
H	-1.765763	-0.956474	2.206527
H	-0.4844	-0.650388	2.955092
O	-2.486222	1.769864	2.664539
H	-2.078777	0.935063	2.998424
H	-3.519497	1.006742	1.605819
H	2.208329	1.667358	0.261332
Si	-0.974207	2.126626	-0.980941

Frequencies -- 34.8368 41.1537 48.0232
Frequencies -- 49.7354 55.6699 67.4363
Frequencies -- 72.4757 80.7284 88.1637

Zero-point correction= 0.263864 (Hartree/Particle)
Thermal correction to Energy= 0.297663
Thermal correction to Enthalpy= 0.298607
Thermal correction to Gibbs Free Energy= 0.201044
Sum of electronic and zero-point Energies= -2888.050126
Sum of electronic and thermal Energies= -2888.016326
Sum of electronic and thermal Enthalpies= -2888.015382
Sum of electronic and thermal Free Energies= -2888.112945



41
Si5H17O19

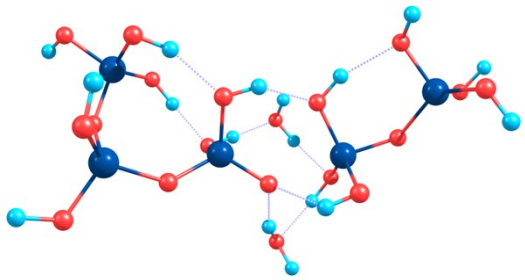
O	2.647846	1.574071	1.563462
O	1.922683	-0.724795	0.475801
O	2.308369	1.44929	-1.145754
O	4.390134	0.241171	0.000699
O	5.979943	-0.880384	-1.899967
O	5.933226	-1.725212	0.733147
O	3.906458	-2.239853	-0.95852
O	0.476151	0.350949	2.858723
O	-4.402848	-0.370247	0.001522
O	-3.488572	-0.747141	-2.503475
O	-5.005056	1.401704	-1.959693
O	-4.766405	-2.753507	1.270179
O	-2.554825	-2.321967	-0.041724
O	-3.078717	-0.896315	2.26184
H	6.424178	-2.542091	0.56717
H	1.347032	1.780383	-1.045033
H	3.630551	-2.214672	-1.88616
H	-3.134947	-1.565389	-2.119377
H	-1.751758	-1.76085	-0.17251
H	-2.629565	-0.037388	2.080027
H	2.190541	2.464949	1.430276
H	2.303399	-1.500191	0.021897
Si	5.082571	-1.144504	-0.546918
Si	-3.86026	0.387142	-1.363337
H	6.551503	-0.099776	-1.875931
Si	2.806338	0.673942	0.196979
Si	-3.687091	-1.57309	0.895571
H	-5.568679	-2.452098	1.717565
O	-1.605541	1.304878	1.445681
H	-0.84011	1.058317	2.033288
O	-2.590663	1.353956	-1.002884
O	-0.061815	2.266837	-0.612977
O	-0.689376	-0.386901	-0.453872
H	0.223785	-0.585843	-0.151554
H	0.559911	-0.496064	2.394209
H	1.277188	0.830112	2.556491
H	-5.807096	0.969573	-2.283258
O	1.219682	3.712809	1.144393
H	1.713792	4.367822	0.631247
H	0.644377	3.237591	0.466959
Si	-1.160094	1.20443	-0.166435

Frequencies -- 17.5744 19.8219 31.5465
Frequencies -- 35.7919 43.6967 52.4490
Frequencies -- 61.5397 69.5081 79.7683

Zero-point correction= 0.263611 (Hartree/Particle)
Thermal correction to Energy= 0.297979
Thermal correction to Enthalpy= 0.298923
Thermal correction to Gibbs Free Energy= 0.197177
Sum of electronic and zero-point Energies= -2888.039147
Sum of electronic and thermal Energies= -2888.004780
Sum of electronic and thermal Enthalpies= -2888.003836
Sum of electronic and thermal Free Energies= -2888.105582

d3-Si-RCT2-fromIRC.log

bondi-Si-TS3h-d3e.log



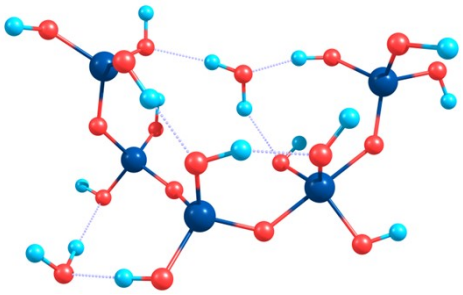
41
Si5H17O19

O	2.594242	1.512946	1.551275
O	1.818504	-0.717126	0.021209
O	2.636	1.703083	-1.32107
O	4.210093	0.270545	0.063555
O	5.472501	-0.860454	-2.108375
O	6.345713	-1.132507	0.487289
O	4.067279	-2.337746	-0.450544
O	0.922717	-0.398959	2.830738
O	-4.353477	-0.064473	0.104342
O	-3.679304	0.1205	-2.495167
O	-4.624798	2.290931	-1.219279
O	-5.282525	-2.576478	0.607496
O	-3.080024	-2.27129	-0.754491
O	-3.131686	-1.598493	1.91842
H	6.963516	-1.840725	0.259635
H	1.729539	2.03143	-1.449962
H	4.007901	-2.844528	-1.27274
H	-3.511876	-0.829978	-2.380597
H	-2.152922	-1.934249	-0.767251
H	-2.508389	-0.834487	1.973725
H	1.994469	2.295121	1.644
H	2.458386	-1.448699	-0.098662
Si	5.046316	-0.989511	-0.517962
Si	-3.724032	0.928546	-1.05732
H	5.963409	-0.059835	-2.340014
Si	2.586035	0.782351	0.05924
Si	-3.94698	-1.627239	0.495461
H	-5.969376	-2.252414	1.205815
O	-1.360315	0.504923	1.699595
H	-0.574827	0.213932	2.23576
O	-2.246414	1.460347	-0.58986
O	0.429341	1.570344	-0.081718
O	-0.813546	-0.764529	-0.646724
H	0.121136	-1.052172	-0.561817
H	1.108522	-1.021973	2.108417
H	1.53663	0.333206	2.611831
H	-5.52159	2.155279	-1.553896
O	0.825692	3.567645	1.551025
H	1.252589	4.293761	1.074484
H	0.517537	2.941832	0.835846
Si	-0.919524	0.735913	0.101559

Frequencies -- -116.1612 10.8567 16.0988
Frequencies -- 28.6405 31.9399 40.0768
Frequencies -- 48.1367 59.3327 73.3710

Zero-point correction= 0.264286 (Hartree/Particle)
Thermal correction to Energy= 0.298360
Thermal correction to Enthalpy= 0.299304
Thermal correction to Gibbs Free Energy= 0.197493
Sum of electronic and zero-point Energies= -2888.024275
Sum of electronic and thermal Energies= -2887.990200
Sum of electronic and thermal Enthalpies= -2887.989256
Sum of electronic and thermal Free Energies= -2888.091068

bondi-Si-INT2.log



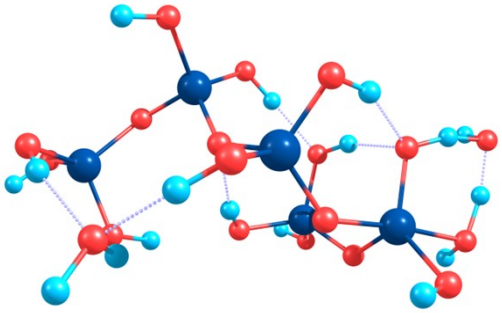
41
Si5H17O19

O	1.5421	0.72956	1.413454
O	2.028477	0.690797	-1.508409
O	3.047	2.917556	0.122214
O	3.782391	0.552868	0.312783
O	3.310979	-2.037948	1.072806
O	4.043643	-1.508188	-1.421126
O	5.796126	-1.192027	0.621091
O	-4.290387	2.847352	-0.40544
O	-3.268996	-0.758821	0.04459
O	-3.858518	1.17192	1.835197
O	-2.143618	-0.805557	2.491659
O	-1.906452	-1.769389	-2.036345
O	-1.853285	-2.895724	0.502488
O	-3.982225	-3.154846	-1.05513
H	4.694709	-1.124896	-2.026071
H	3.984723	2.740686	0.272358
H	6.155625	-0.404546	1.051358
H	-4.639733	0.735713	2.204298
H	-1.73226	-3.851688	0.41098
H	-4.415836	-2.989126	-1.90344
H	2.215489	0.208505	1.872446
H	2.684203	-0.000571	-1.694796
Si	4.214014	-1.002689	0.166844
Si	-2.67233	0.163749	1.273389
H	2.354192	-2.07788	0.824855
Si	2.226912	1.448674	0.016937
Si	-2.745308	-2.13984	-0.689435
H	-1.435461	-0.896783	-1.980989
O	-0.616617	0.567135	-1.754197
H	0.356219	0.406988	-1.863562
O	-1.499931	1.147618	0.734034
O	0.711035	2.329551	-0.248102
O	-1.7024	2.9969	-1.185575
H	-2.648577	2.972698	-0.892289
H	-4.69132	2.205086	-1.009094
H	-4.27827	2.381168	0.45452
H	-1.923395	-1.703319	2.187632
O	0.742079	-1.711153	0.292341
H	0.679351	-0.854231	0.758319
H	-0.051169	-2.21729	0.54194
Si	-0.763267	1.782153	-0.6131

Frequencies -- 19.3647 28.0869 35.1820
Frequencies -- 50.5970 58.1803 66.3557
Frequencies -- 70.2175 75.8113 82.9376

Zero-point correction= 0.266174 (Hartree/Particle)
Thermal correction to Energy= 0.300247
Thermal correction to Enthalpy= 0.301191
Thermal correction to Gibbs Free Energy= 0.202184
Sum of electronic and zero-point Energies= -2888.035337
Sum of electronic and thermal Energies= -2888.001264
Sum of electronic and thermal Enthalpies= -2888.000320
Sum of electronic and thermal Free Energies= -2888.099328

bondi-Si-TS4f.log



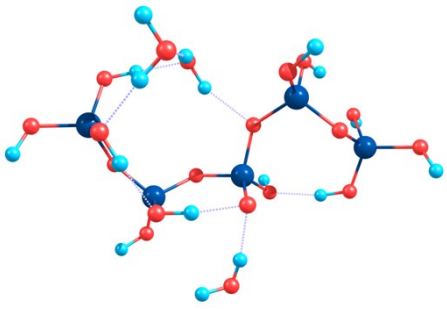
41
Si5H17O19

O	4.756077	0.381092	-0.576194
O	2.948378	-0.653737	0.930234
O	3.676709	-1.402715	-1.850366
O	2.462287	1.170875	-1.181685
O	1.625507	3.595798	-0.588756
O	-0.230995	1.71628	-0.960193
O	1.353568	1.543856	1.222812
O	0.929756	-2.348504	1.342254
O	-2.932859	0.824088	1.026247
O	-0.782292	0.607311	2.641138
O	-2.395503	-1.446205	2.429483
O	-2.937327	1.01238	-1.687075
O	-4.494789	-0.782455	-0.532732
O	-5.04077	1.8256	-0.079815
H	-0.50879	0.805724	-0.72504
H	-0.013374	1.03687	2.1963
H	-3.939485	-1.355828	-1.106143
H	-5.692111	1.900121	-0.790574
Si	1.295863	1.998678	-0.38314
Si	-1.752843	-0.183452	1.59508
H	0.942445	4.206879	-0.280807
Si	2.961213	-0.394539	-0.716265
Si	-3.855055	0.7163	-0.336487
O	-0.513758	-3.080753	-0.790142
H	-1.262379	-2.762512	-1.343339
O	-0.928462	-0.668512	0.248223
O	1.352279	-1.094443	-1.006083
O	-2.539766	-1.815129	-2.181667
H	-2.305828	-0.872969	-2.283183
H	-3.135758	-1.890312	1.992762
H	-2.791252	-2.115206	-3.067505
O	5.060263	0.094097	1.794954
H	3.955225	-0.339424	1.494755
H	3.001076	-2.009682	-2.183198
H	-2.196195	1.630928	-1.57128
H	5.055242	0.344639	0.520752
H	4.889539	0.941357	2.231594
H	1.771736	-1.828544	1.434721
Si	0.253008	-1.822675	-0.061681
H	4.693389	1.31214	-0.833038
H	1.959506	0.764047	1.343052

Frequencies -- -1154.9764 29.1423 33.3000
Frequencies -- 41.6423 51.9118 55.7552
Frequencies -- 63.0710 64.8653 90.1258

Zero-point correction= 0.260274 (Hartree/Particle)
Thermal correction to Energy= 0.292814
Thermal correction to Enthalpy= 0.293758
Thermal correction to Gibbs Free Energy= 0.198657
Sum of electronic and zero-point Energies= -2888.023878
Sum of electronic and thermal Energies= -2887.991339
Sum of electronic and thermal Enthalpies= -2887.990394
Sum of electronic and thermal Free Energies= -2888.085496

bondi-Si-PRD2.log



41
Si5H17O19

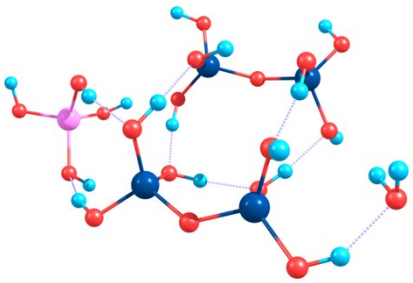
O	2.277139	1.482811	1.317388
O	1.833583	-3.007233	1.731516
O	2.701456	3.170253	-0.843278
O	3.593674	0.645324	-0.835033
O	5.828804	-0.790567	-0.331779
O	3.64549	-0.924761	1.319388
O	3.743995	-2.059503	-1.166761
O	0.097425	4.063454	1.288649
O	-3.305209	-0.604292	0.6918
O	-1.404909	-2.424324	1.313988
O	-2.666014	-2.550362	-1.065598
O	-4.252061	1.767147	-0.203602
O	-4.75718	-0.646983	-1.463209
O	-5.953104	-0.014954	0.832548
H	3.149254	-0.122551	1.599304
H	3.542248	3.5441	-0.544931
H	2.765723	-2.259313	-1.158517
H	-1.981045	-3.08071	1.72874
H	-5.241816	-0.198881	-2.169133
H	-6.002169	0.495791	1.652458
Si	4.184456	-0.790856	-0.249377
Si	-2.085533	-1.549252	0.104128
H	6.266781	-0.097357	0.180006
Si	2.383256	1.64072	-0.328756
Si	-4.569045	0.172001	-0.034556
H	-3.315079	1.952224	-0.44879
O	-1.631175	1.948023	-0.950352
H	-1.652851	1.833446	-1.911879
O	-0.887932	-0.593639	-0.497279
O	0.948935	1.207292	-1.006161
O	-0.351561	1.359113	1.370499
H	1.029892	4.091606	1.541279
H	-0.139838	3.11384	1.418895
H	-3.417745	-2.151278	-1.54082
H	1.298746	1.419129	1.565054
H	2.513704	-2.300847	1.689054
O	1.158509	-2.584871	-0.882146
H	0.638712	-1.761604	-0.891253
H	1.269957	-2.786703	0.080138
Si	-0.486712	0.998891	-0.16638
H	2.346684	-3.827369	1.694939

Frequencies -- 20.9911 25.7436 34.2773
Frequencies -- 35.3646 44.3204 47.0790
Frequencies -- 49.2684 59.2881 76.0000

Zero-point correction= 0.262802 (Hartree/Particle)
Thermal correction to Energy= 0.298781
Thermal correction to Enthalpy= 0.299726
Thermal correction to Gibbs Free Energy= 0.194630
Sum of electronic and zero-point Energies= -2888.031591
Sum of electronic and thermal Energies= -2887.995612
Sum of electronic and thermal Enthalpies= -2887.994668
Sum of electronic and thermal Free Energies= -2888.099763

Anionic Q0

bondi-4-RCT-d3c.log



42

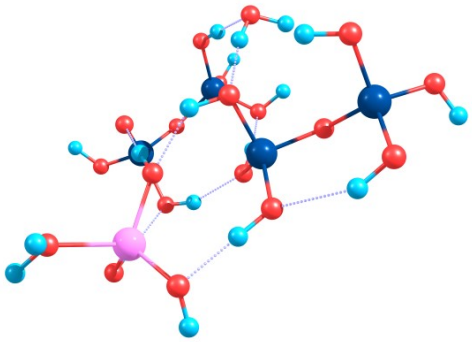
AlSi4H18O19

O	-3.996766	-3.175596	-0.158806
O	-3.631431	-0.713595	-1.187848
O	-2.987186	-1.165915	1.340185
O	-1.499687	-2.285741	-0.614896
O	-0.068417	-1.309347	1.437584
O	0.297495	-3.859094	0.44955
O	1.155269	-1.72894	-0.913049
O	1.213226	1.092481	1.541298
O	-0.275231	2.899762	0.155388
O	1.005014	0.946205	-1.156776
O	2.394054	2.96623	0.041142
O	-2.82577	3.568964	-0.235908
O	-1.7173	1.257205	-1.267323
O	-2.23812	1.419835	1.334144
H	1.162685	-4.031638	0.846234
H	-2.831332	-0.190858	1.359819
H	1.192324	-0.745315	-1.010701
H	0.101466	0.953939	-1.537622
H	3.203509	2.412205	-0.227678
H	-2.420057	0.58217	-1.372297
H	-2.476314	1.926068	2.124272
H	-3.545701	-4.0307	-0.186026
H	-3.884872	-1.026559	-2.069497
Si	-0.005344	-2.284816	0.090155
Si	1.11142	1.979473	0.15688
H	-0.95522	-1.273178	1.838739
H	3.25885	-1.856232	-1.294947
Si	-3.017926	-1.863442	-0.142311
Si	-1.802872	2.314317	-0.004587
H	-3.73435	3.199059	-0.316418
Al	4.516552	-0.346628	-0.129765
O	6.237833	-0.382307	0.290616
H	6.413775	-1.030797	0.983625
O	4.147176	-1.495102	-1.427142
O	3.532804	-0.687045	1.296127
H	2.863686	-0.016312	1.493699
O	4.216608	1.324642	-0.76345
H	3.944413	1.277747	-1.689864
H	0.691718	0.256709	1.545336
O	-4.972596	1.773207	-0.196829
H	-4.889686	1.538288	0.739301
H	-4.699761	0.957328	-0.653036

Frequencies -- 23.1443 24.2845 31.1403
Frequencies -- 40.8922 52.2903 54.6028
Frequencies -- 61.2287 70.2804 80.2821

Zero-point correction= 0.270915 (Hartree/Particle)
Thermal correction to Energy= 0.307391
Thermal correction to Enthalpy= 0.308335
Thermal correction to Gibbs Free Energy= 0.202994
Sum of electronic and zero-point Energies= -2841.594240
Sum of electronic and thermal Energies= -2841.557764
Sum of electronic and thermal Enthalpies= -2841.556820
Sum of electronic and thermal Free Energies= -2841.662161

bondi-4-TS1-d3b.log



42

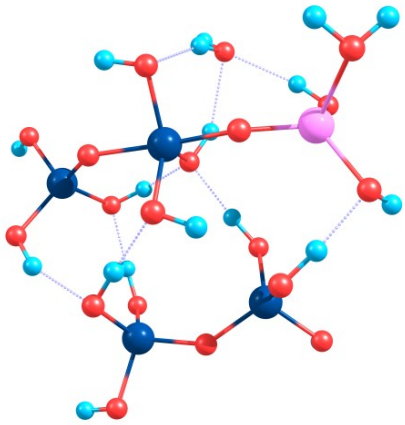
AlSi4H18O19

O	-0.056851	-0.025542	-1.203437
O	-1.955928	1.94803	-0.721985
O	-1.327531	0.169645	1.404249
O	0.450999	1.841311	0.716906
O	1.587568	4.425823	1.518816
O	2.467775	3.342831	-0.918235
O	-0.420494	4.139319	-0.566319
O	4.708147	-0.089769	-0.009969
O	2.815683	-1.910396	-0.415872
O	2.628914	0.553355	-1.420089
O	2.288219	0.164547	1.286603
O	0.388531	-2.681012	-1.104723
O	2.461472	-4.448733	-0.739236
O	1.261916	-3.32161	1.383275
H	2.700114	2.432454	-1.186588
H	-0.696854	0.762003	1.848869
H	-0.347692	4.597675	-1.412728
H	1.657119	0.481238	-1.532581
H	1.200474	1.170524	0.939672
H	2.039542	-5.274183	-0.46586
H	0.341084	-3.012003	1.607
H	-0.00238	-1.00935	-1.260582
H	-1.427134	2.787122	-0.659038
Si	3.047092	-0.288176	-0.026704
H	0.948408	4.945386	2.033295
H	5.051061	-0.057094	0.8925
Si	-1.291997	0.517195	-0.244647
Si	1.721119	-3.084774	-0.166249
H	-0.413493	-3.196375	-0.939223
O	-5.046302	-1.600048	-0.845823
H	-5.313843	-1.412129	-1.75545
O	-2.529423	-0.553609	-0.673702
O	-4.66492	1.053206	-0.564824
H	-3.91864	1.664543	-0.720764
O	-4.177259	-0.765223	1.454183
H	-3.364788	-0.491017	1.908825
O	-1.208907	-2.516384	1.936767
H	-1.79599	-2.828355	1.233317
H	-1.199246	-1.540818	1.81291
Si	-4.089029	-0.445493	-0.164932
Al	1.027354	3.340976	0.041501
H	2.39319	4.959242	1.419692

Frequencies -- -131.5985 19.2614 22.6686
Frequencies -- 33.9443 36.8286 39.9822
Frequencies -- 52.1488 57.2609 63.5802

Zero-point correction= 0.272234 (Hartree/Particle)
Thermal correction to Energy= 0.307718
Thermal correction to Enthalpy= 0.308663
Thermal correction to Gibbs Free Energy= 0.204552
Sum of electronic and zero-point Energies= -2841.567242
Sum of electronic and thermal Energies= -2841.531758
Sum of electronic and thermal Enthalpies= -2841.530813
Sum of electronic and thermal Free Energies= -2841.634924

bondi-4-INT-d3l.log



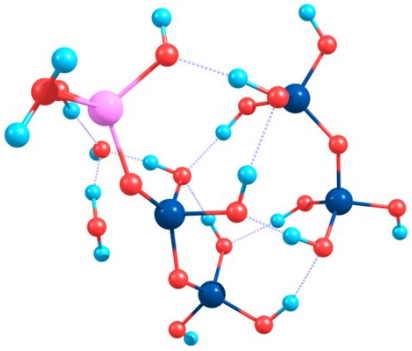
42
AlSi4H18O19

O	-0.119094	-0.20462	-1.700142
O	1.404456	-2.86846	-1.043399
O	0.435725	-1.039178	1.018189
O	-0.933476	-2.261632	-0.754461
O	-2.114124	-1.516907	1.546618
O	-3.639141	-1.922636	-0.63335
O	-2.464156	-4.024127	0.505227
O	-4.009854	2.71662	-0.499357
O	-1.439856	2.691895	-0.155155
O	-2.599623	0.556977	-1.31467
O	-3.017001	1.032993	1.33084
O	0.994956	2.464425	-1.118562
O	0.543202	4.202549	0.85042
O	0.480427	1.62935	1.465179
H	-3.494536	-1.024682	-1.000603
H	1.217956	-1.392468	1.485916
H	-3.189012	-4.206402	1.118296
H	-1.658482	0.25902	-1.505436
H	-2.725018	0.093916	1.431646
H	0.266409	4.362006	1.763064
H	0.424192	0.659381	1.279396
H	0.467074	0.568073	-1.78923
H	0.734533	-3.56641	-1.061284
Si	-2.264223	-2.41808	0.139096
Si	-2.754485	1.706063	-0.13996
H	-1.145419	-1.330404	1.640363
H	-4.883695	2.361032	-0.290181
Si	0.631999	-1.374315	-0.684861
Si	0.15027	2.704029	0.271214
H	1.966206	2.320219	-0.931865
O	3.489731	1.956789	-0.369627
H	3.655686	2.519468	0.397663
O	2.140599	-0.587248	-0.815405
O	4.855086	-0.43266	-1.156653
H	4.633439	-1.245708	-1.639206
O	3.867607	-0.141384	1.607434
H	3.590187	-1.047058	1.826448
O	2.683942	-2.739695	1.457292
H	2.385482	-3.471741	2.014145
H	2.388351	-2.96583	0.547308
Al	3.419133	0.22219	-0.034211
H	5.752802	-0.533036	-0.8019

Frequencies --	27.1298	32.4197	49.5250
Frequencies --	58.2087	60.6165	65.2226
Frequencies --	80.1016	82.0370	86.2939

Zero-point correction=	0.274969 (Hartree/Particle)
Thermal correction to Energy=	0.309957
Thermal correction to Enthalpy=	0.310901
Thermal correction to Gibbs Free Energy=	0.210486
Sum of electronic and zero-point Energies=	-2841.587474
Sum of electronic and thermal Energies=	-2841.552486
Sum of electronic and thermal Enthalpies=	-2841.551542
Sum of electronic and thermal Free Energies=	-2841.651957

bondi-4-TS2-d3fs3.log



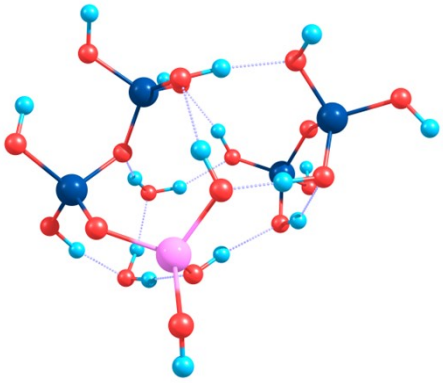
42
AlSi4H18O19

O	0.121652	0.082567	-1.3064
O	-2.175085	2.541761	0.474806
O	-0.62185	0.540519	1.148359
O	-0.030372	2.475987	-0.804762
O	1.664861	2.008289	1.236781
O	2.697197	2.716885	-1.138109
O	1.256033	4.522587	0.19172
O	4.660761	-1.676197	-0.545292
O	2.193223	-2.35968	-0.142884
O	2.685118	-0.02667	-1.393854
O	3.244185	-0.258822	1.251025
O	-0.319016	-2.661373	-0.909025
O	0.907807	-4.367709	0.867437
O	0.181954	-1.922176	1.665101
H	2.895222	1.767082	-1.301365
H	-1.38799	0.768154	1.837412
H	2.035578	4.931994	0.591316
H	1.673918	0.027641	-1.440688
H	2.768172	0.601476	1.261152
H	0.114218	-4.787523	1.225871
H	-0.111654	-0.994023	1.452614
H	-0.181703	-0.84272	-1.366847
H	-1.652999	3.324762	0.699624
Si	1.406469	2.914394	-0.142605
Si	3.178832	-1.043875	-0.189935
H	0.859668	1.490305	1.482754
H	5.40234	-1.076427	-0.389066
Si	-0.953303	1.114239	-0.405176
Si	0.697536	-2.800385	0.385915
H	-1.295632	-2.566714	-0.698763
O	-2.8659	-2.232186	-0.45926
H	-3.218126	-2.827822	0.214463
O	-2.347745	0.563102	-1.079775
O	-4.77665	-0.682132	-1.828175
H	-4.893232	0.091738	-2.403731
O	-4.423774	-0.152563	0.970054
H	-3.89826	0.337712	1.648676
O	-2.635624	1.192758	2.443921
H	-2.560119	1.626975	3.303297
H	-2.484235	2.083793	1.418423
Al	-3.482862	-0.577731	-0.411047
H	-4.735647	-1.466687	-2.399653

Frequencies --	-241.7482	25.5368	43.2708
Frequencies --	47.0537	60.3243	70.6650
Frequencies --	74.5687	77.3407	91.1015

Zero-point correction=	0.271361 (Hartree/Particle)
Thermal correction to Energy=	0.304545
Thermal correction to Enthalpy=	0.305489
Thermal correction to Gibbs Free Energy=	0.209381
Sum of electronic and zero-point Energies=	-2841.574800
Sum of electronic and thermal Energies=	-2841.541616
Sum of electronic and thermal Enthalpies=	-2841.540672
Sum of electronic and thermal Free Energies=	-2841.636780

bondi-4-PRD1-d3.log



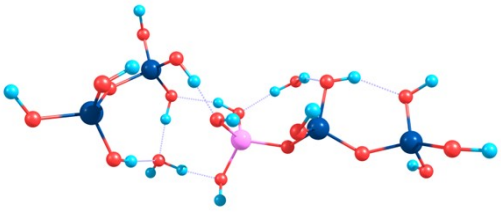
42
AlSi4H18O19

O	1.326696	-0.72919	2.329251
O	1.887656	1.706993	1.186964
O	3.556552	0.620061	2.905346
O	3.205239	-0.509859	0.437046
O	2.485645	1.225922	-1.48132
O	4.818588	-0.119228	-1.709305
O	2.555813	-1.51612	-1.876201
O	-1.35314	-0.442321	3.158713
O	-1.811288	-0.957159	0.318745
O	-4.06325	-1.227231	-1.127726
O	-4.054389	0.322078	1.041896
O	0.170013	-2.701504	0.816712
O	-2.078345	-3.359942	-0.639108
O	-0.132789	-1.753643	-1.651769
H	5.171961	0.77274	-1.830837
H	3.837207	-0.130748	3.446547
H	2.720036	-1.613627	-2.825796
H	-3.735071	-2.137836	-1.046702
H	-1.813104	-4.053822	-1.258885
H	0.85276	-1.796349	-1.656365
H	1.005711	-1.438853	1.727177
Si	3.262656	-0.178525	-1.179688
Si	-3.168282	-0.136176	-0.258876
H	1.468158	1.167996	-1.725084
Si	2.486599	0.25866	1.710506
Si	-0.948	-2.201465	-0.305273
H	-0.175493	-3.27206	1.519732
Al	-1.214012	2.06354	-1.189391
O	0.045569	1.081598	-2.001649
H	-0.157764	0.129663	-2.009256
O	-2.703763	1.091019	-1.195961
O	-0.795915	2.468573	0.484299
H	-1.905979	2.229409	1.745942
O	-1.431958	3.525038	-2.145338
H	-1.57201	4.311718	-1.604839
H	0.056244	2.141528	0.81668
H	-1.658342	-0.757448	2.290257
H	-0.390394	-0.356314	3.019833
O	-2.532788	1.965982	2.472665
H	-2.070266	1.201965	2.886168
H	-3.584267	1.003021	1.605556
H	2.11798	1.849545	0.242504

Frequencies -- 23.6933 37.3367 46.2985
Frequencies -- 50.0667 54.2550 58.9031
Frequencies -- 66.2008 75.1112 80.1130

Zero-point correction= 0.272566 (Hartree/Particle)
Thermal correction to Energy= 0.307927
Thermal correction to Enthalpy= 0.308872
Thermal correction to Gibbs Free Energy= 0.207456
Sum of electronic and zero-point Energies= -2841.624746
Sum of electronic and thermal Energies= -2841.589385
Sum of electronic and thermal Enthalpies= -2841.588440
Sum of electronic and thermal Free Energies= -2841.689855

bondi-4-RCT2k-d3b.log



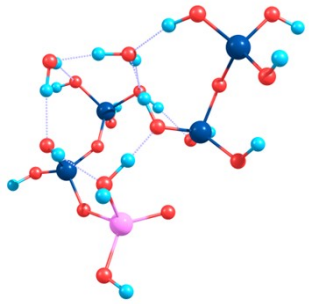
42
AlSi4H18O19

O	3.060832	2.040599	0.532509
O	2.374944	0.508547	-1.655845
O	4.257548	2.428574	-1.772996
O	4.711106	0.143312	-0.382546
O	6.044258	-2.209639	-0.186548
O	3.796813	-1.884976	1.145664
O	3.767254	-2.076641	-1.584797
O	-1.970585	3.210434	-0.296594
O	-4.250611	-0.786981	0.359356
O	-1.95329	-1.793222	-0.704453
O	-2.854088	0.640443	-1.43731
O	-6.786247	-0.159366	1.113531
O	-5.635218	0.776884	-1.193773
O	-6.331662	-1.87642	-0.853263
H	3.580198	-1.111815	1.725921
H	4.277039	2.22444	-2.717757
H	3.138222	-1.416548	-1.927322
H	-2.214357	-2.084633	-1.588976
H	-6.359859	0.923876	-1.816913
H	-7.288499	-1.932515	-0.981341
H	3.149147	1.490009	1.35432
H	1.647714	0.095233	-1.072938
Si	4.55657	-1.501847	-0.251747
Si	-2.720824	-0.419177	-0.164578
H	6.541467	-2.186532	-1.015445
Si	3.573119	1.265652	-0.827657
Si	-5.781442	-0.50144	-0.142994
H	-6.682827	0.720563	1.501967
O	0.494332	-0.06272	2.800359
O	-1.860295	0.151829	1.067598
O	0.233252	2.125596	0.985501
O	0.676316	-0.570834	-0.081069
H	0.074142	-1.208936	-0.495191
H	-2.229585	2.423814	-0.804194
H	-1.144434	2.914262	0.144929
H	-3.782449	0.882702	-1.624535
H	1.146843	2.317199	0.714892
O	3.076887	0.287047	2.563691
H	3.523045	0.488071	3.398223
H	2.100282	0.142922	2.772198
Al	-0.109589	0.412615	1.189744
H	0.352273	-0.990479	3.031039

Frequencies -- 10.4357 19.2773 20.8373
Frequencies -- 29.1131 35.7458 39.5164
Frequencies -- 47.2307 48.9352 64.7404

Zero-point correction= 0.270410 (Hartree/Particle)
Thermal correction to Energy= 0.307211
Thermal correction to Enthalpy= 0.308155
Thermal correction to Gibbs Free Energy= 0.199655
Sum of electronic and zero-point Energies= -2841.607599
Sum of electronic and thermal Energies= -2841.570798
Sum of electronic and thermal Enthalpies= -2841.569854
Sum of electronic and thermal Free Energies= -2841.678354

bondi-fs3-TS3.log



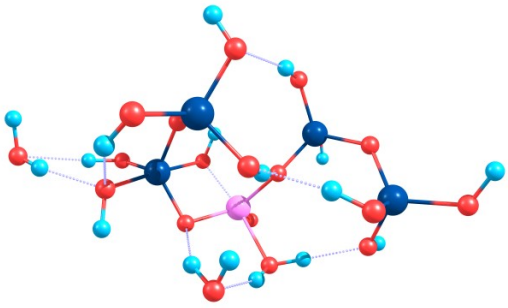
42
AlSi4H18O19

O	-3.766911	-1.109936	1.747945
O	-5.482113	-1.215161	-0.233084
O	-4.595401	1.244684	0.588758
O	-2.979505	-0.297821	-0.723878
O	-2.474307	2.262258	-1.209582
O	-0.929496	0.743472	0.534141
O	-0.882837	0.137556	-2.157839
O	1.125332	-2.244531	2.719029
O	2.275536	-0.806198	-0.711031
O	2.527823	0.01197	1.87253
O	4.649548	-0.515327	0.314927
O	0.052951	-2.279563	-1.084654
O	2.4261	-2.79203	-2.382693
O	1.987062	-3.35967	0.260013
H	0.060491	1.704127	1.184819
H	-5.149683	1.466795	1.348645
H	-1.466985	-0.171236	-2.867946
H	1.633141	-1.42614	2.525423
H	2.120415	-3.643291	-2.726065
H	2.905203	-3.65492	0.340443
H	-2.829326	-1.416302	1.743483
H	-5.934868	-0.805634	-0.983323
H	-3.34318	2.287911	-0.769741
Si	-4.207137	-0.355099	0.364514
Si	1.699753	-2.302132	-0.986358
H	-0.287133	-1.473175	-1.534173
O	0.46795	2.694278	-1.335145
O	3.080041	1.681139	-0.172314
O	2.407778	4.362743	0.310808
O	0.875678	2.224815	1.501369
H	1.954532	0.775891	2.079089
H	-0.35514	-1.901674	2.039803
H	1.435555	-2.842188	2.011251
H	5.266591	-0.111898	0.940479
H	1.769547	5.084084	0.249978
O	-1.130044	-1.701599	1.437735
H	-0.902782	-2.149333	0.598363
H	-0.962229	-0.171263	0.953486
Si	3.136273	0.153862	0.322043
H	0.593446	2.923012	2.110723
Al	1.691672	2.826215	-0.200782
Si	-1.741805	0.82164	-0.903831

Frequencies -- -112.6713 19.6431 33.1817
Frequencies -- 38.1705 44.4941 57.4538
Frequencies -- 61.4399 68.1938 72.8740

Zero-point correction= 0.273125 (Hartree/Particle)
Thermal correction to Energy= 0.308206
Thermal correction to Enthalpy= 0.309150
Thermal correction to Gibbs Free Energy= 0.208049
Sum of electronic and zero-point Energies= -2841.536158
Sum of electronic and thermal Energies= -2841.501077
Sum of electronic and thermal Enthalpies= -2841.500133
Sum of electronic and thermal Free Energies= -2841.601234

bondi-4-INT2-d3k.log



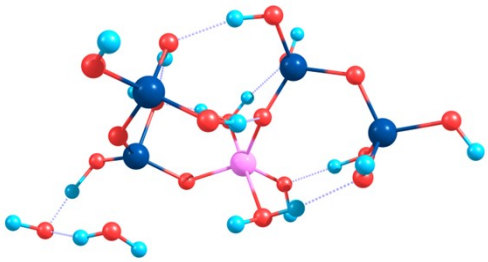
42
AlSi4H18O19

O	3.910146	-1.338589	0.792785
O	1.463123	-1.707594	1.26519
O	3.441144	0.416532	-1.058191
O	1.961125	0.735951	0.939857
O	2.341073	2.927437	-0.607766
O	-0.002532	1.563005	-0.729357
O	0.52839	2.943621	1.440406
O	-0.318256	-3.612345	0.164375
O	-3.214697	0.546483	0.892958
O	-1.225002	0.920046	2.680567
O	-2.349592	-1.404228	2.598149
O	-2.694173	1.622654	-1.56372
O	-3.438506	-0.932636	-1.399593
O	-5.203131	0.96015	-0.862116
H	-0.358814	0.701158	-0.369477
H	-0.750457	1.681493	2.2972
H	-3.995666	-1.62419	-1.013322
H	-5.491195	1.729421	-0.351398
Si	1.255455	2.040534	0.249317
Si	-1.89129	-0.152548	1.626365
H	2.971491	2.269323	-0.979498
Si	2.559369	-0.632396	0.115122
Si	-3.611807	0.571583	-0.707084
O	-0.884003	-1.939852	-1.862488
H	-0.50053	-1.254887	-2.476807
O	-0.894896	-0.607307	0.432567
O	1.616692	-1.344417	-1.067834
O	0.521769	-0.024739	-3.118132
H	0.222593	0.760399	-2.62771
H	-2.592239	-2.209682	2.121456
H	1.152329	-0.430353	-2.471543
O	6.019088	0.215104	-0.259269
H	5.173081	0.488551	-0.68699
H	3.383774	0.044691	-1.94827
H	-1.780211	1.794299	-1.266324
H	4.740819	-0.940861	0.459299
H	6.127108	0.849955	0.463293
H	-1.807481	-1.643194	-1.691322
H	1.166684	-1.209885	2.03855
H	1.114777	3.214415	2.161986
Al	0.165882	-1.951875	-0.156731
H	0.081205	-3.94093	0.979199

Frequencies -- 31.8614 35.5369 40.4879
Frequencies -- 57.4879 62.5289 79.6887
Frequencies -- 83.9326 87.9272 97.4035

Zero-point correction= 0.276856 (Hartree/Particle)
Thermal correction to Energy= 0.311240
Thermal correction to Enthalpy= 0.312184
Thermal correction to Gibbs Free Energy= 0.214433
Sum of electronic and zero-point Energies= -2841.612339
Sum of electronic and thermal Energies= -2841.577954
Sum of electronic and thermal Enthalpies= -2841.577010
Sum of electronic and thermal Free Energies= -2841.674762

Bondi-4-TS4d-d3h



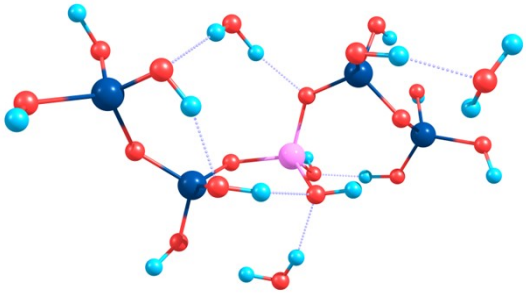
42

O	4.209306	-0.97334	1.003662
O	2.098413	0.184865	1.853292
O	3.550227	-1.30461	-1.566157
O	2.785415	0.939126	-0.520612
O	2.436995	3.403034	-1.356653
O	0.394446	1.71262	-1.620439
O	1.123471	2.502781	0.873905
O	0.044492	-1.333334	2.246139
O	-3.483498	0.911353	0.232785
O	-1.622554	2.622465	1.040223
O	-2.1059	0.35149	2.514491
O	-2.93736	-0.43458	-2.0768
O	-3.789275	-1.81391	0.027727
O	-5.483191	-0.054499	-1.093733
H	-0.222925	1.119696	-1.136406
H	-0.641302	2.729952	1.043767
H	-2.883247	-2.197077	0.198893
H	-5.920197	-0.728129	-1.632277
Si	1.668906	2.123259	-0.65735
Si	-2.015049	1.031039	0.994515
H	1.853004	4.044261	-1.783046
Si	2.802752	-0.513865	0.338233
Si	-3.913337	-0.372116	-0.718513
O	-1.335754	-2.82549	0.445698
H	-1.330498	-3.411317	-0.323029
O	-0.929015	0.148646	0.184534
O	1.555375	-1.536162	0.028128
O	-0.432301	-1.605724	-1.751024
H	-1.290365	-1.184755	-1.999498
H	-2.594186	0.829934	3.19761
H	0.266419	-1.122823	-2.218153
O	5.798072	-1.822025	-0.628435
H	4.537482	-1.589322	-1.338033
H	3.042149	-2.123953	-1.644858
H	-2.808702	0.419357	-2.516484
H	5.00916	-1.372586	0.306725
H	6.332215	-1.050316	-0.86546
H	0.858906	-0.738767	2.302623
H	2.794298	0.267872	2.519937
H	1.417289	1.772349	1.477795
Al	-0.18049	-1.475237	0.283194
H	-0.69786	-0.824374	2.638138

Frequencies -- -472.9287 17.5542 33.4068
Frequencies -- 39.4911 55.1366 66.6910
Frequencies -- 80.7584 89.9484 94.6874

Zero-point correction= 0.271535 (Hartree/Particle)
Thermal correction to Energy= 0.304743
Thermal correction to Enthalpy= 0.305687
Thermal correction to Gibbs Free Energy= 0.209690
Sum of electronic and zero-point Energies= -2841.590633
Sum of electronic and thermal Energies= -2841.557424
Sum of electronic and thermal Enthalpies= -2841.556480
Sum of electronic and thermal Free Energies= -2841.652477

bondi-4-PRD2e-d3.log



42

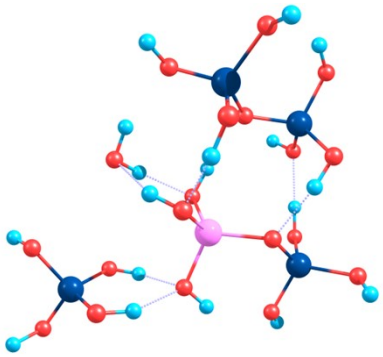
O	2.109244	0.726727	1.514576
O	2.989368	2.986858	0.207555
O	3.938005	0.535566	-0.368012
O	5.823901	-1.060482	0.778045
O	3.191505	-1.753816	0.837406
O	-3.130718	-2.005316	2.932346
O	0.308926	4.08981	0.983406
O	-2.915995	-0.415735	0.491346
O	-1.054333	-2.217607	1.1458
O	-2.593302	-2.636105	-1.021986
O	-3.849079	1.890788	-0.602104
O	-4.583588	-0.625212	-1.494636
O	-5.487754	0.328571	0.826184
H	2.640336	-1.095643	1.312238
H	3.635643	3.187258	0.899273
H	-3.426895	-1.258971	2.384357
H	-1.677553	-2.299995	1.905895
H	-5.142112	-0.241508	-2.183627
H	-5.432206	0.94561	1.568452
Si	4.390896	-1.014366	-0.03638
Si	-1.794908	-1.496671	-0.12933
H	5.745319	-1.022976	1.741415
Si	2.584228	1.384113	0.05825
Si	-4.2051	0.348744	-0.206866
H	-2.943346	2.031816	-1.004057
Al	-0.304178	1.038148	-0.695758
O	-1.391037	2.10758	-1.597294
H	-1.461773	1.937574	-2.545835
O	-0.719481	-0.661386	-1.019748
O	1.408987	1.292393	-1.046664
O	-0.461496	1.38676	1.049673
H	-1.277091	1.095681	1.47755
H	1.231175	3.927965	0.725527
H	-0.023092	3.193488	1.190959
H	-3.334742	-2.240834	-1.514147
H	1.140542	0.87597	1.649532
O	1.382385	-2.5036	-1.327266
H	0.729033	-1.779128	-1.299718
H	1.892376	-2.375933	-0.509134
O	4.625507	-1.736466	-1.490697
H	5.042712	-2.607948	-1.462283
H	-3.764	-2.708436	2.725577

Frequencies -- 19.9538 26.0958 29.5715
Frequencies -- 32.5176 42.5798 45.4181
Frequencies -- 53.1002 56.8552 63.5006

Zero-point correction= 0.271828 (Hartree/Particle)
Thermal correction to Energy= 0.309299
Thermal correction to Enthalpy= 0.310243
Thermal correction to Gibbs Free Energy= 0.202101
Sum of electronic and zero-point Energies= -2841.615189
Sum of electronic and thermal Energies= -2841.577718
Sum of electronic and thermal Enthalpies= -2841.576774
Sum of electronic and thermal Free Energies= -2841.684916

Anionic Q1

switch-4-RCT-d3e.log



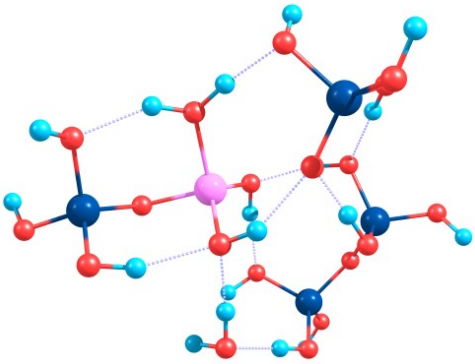
42

O	4.846777	-0.753831	0.773662
O	3.04891	0.975983	1.812562
O	3.280867	0.736442	-0.833749
O	2.192424	-1.267005	0.624297
O	1.447869	-2.152647	-1.862417
O	3.654861	-3.069088	-0.68179
O	1.237001	-3.656542	0.449231
O	-0.747491	-0.845671	-1.394978
O	0.669357	1.632459	-0.798574
O	-0.421793	-0.047624	1.377686
O	-2.184434	1.438313	-0.297795
O	-0.635558	3.874673	-0.281173
O	1.424068	3.215892	1.300986
O	1.957165	3.971068	-1.186749
H	3.939095	-3.049442	-1.606381
H	2.360069	1.018625	-1.039392
H	1.109513	-4.508764	0.007938
H	0.462862	-0.41657	1.514897
H	-2.052731	2.399633	-0.261445
H	2.013235	2.471185	1.539995
H	1.782058	3.911314	-2.13618
H	4.903233	-1.626922	0.3473
H	2.854642	0.579109	2.674054
Si	2.100755	-2.547268	-0.426554
H	0.591923	-1.619078	-1.778051
H	-5.242643	-2.560324	0.852408
Si	3.358778	-0.086684	0.580043
Si	0.866194	3.156873	-0.244286
H	-0.725971	4.681768	0.243779
O	-4.200987	-0.021518	-1.327556
H	-3.472046	0.63187	-1.19427
O	-4.784763	-2.137482	0.113427
O	-3.913712	0.169254	1.349887
O	-6.359078	0.057137	0.387452
H	-7.024028	-0.331361	-0.197355
H	-1.177568	-1.576268	-0.903242
O	-1.510995	-2.559232	0.740937
H	-1.233069	-1.726723	1.182489
H	-0.690929	-3.083816	0.734918
Si	-4.810973	-0.481416	0.131832
Al	-0.645113	0.53672	-0.280453
H	-3.221645	0.762678	0.967184

Frequencies -- 15.8038 26.9513 31.7847
Frequencies -- 34.0591 43.9119 45.4994
Frequencies -- 58.9411 62.6662 67.2532

Zero-point correction= 0.271682 (Hartree/Particle)
Thermal correction to Energy= 0.307954
Thermal correction to Enthalpy= 0.308898
Thermal correction to Gibbs Free Energy= 0.203213
Sum of electronic and zero-point Energies= -2841.607952
Sum of electronic and thermal Energies= -2841.571680
Sum of electronic and thermal Enthalpies= -2841.570736
Sum of electronic and thermal Free Energies= -2841.676421

switch-4-TS1-try4.log



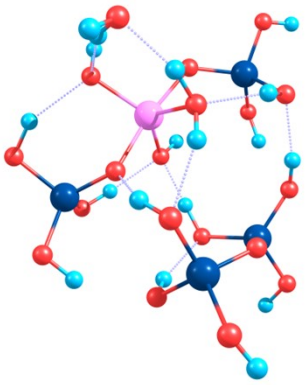
42

O	0.018622	-0.219517	-1.540725
O	-2.252511	1.497725	-1.010552
O	-1.299168	-0.265663	1.298735
O	0.064016	1.923792	0.878948
O	0.271841	4.516051	1.585773
O	1.553081	3.676988	-0.625073
O	-1.140058	3.785666	-0.607621
O	4.485952	1.146999	-0.058414
O	3.275134	-1.199796	-0.478394
O	2.273649	1.120177	-1.435138
O	2.15264	0.532922	1.236062
O	1.193467	-2.708176	-1.065027
O	3.716867	-3.727427	-0.640891
O	2.222115	-2.887396	1.436027
H	1.860604	2.842963	-1.044795
H	-0.822991	0.523085	1.628072
H	-0.913144	4.184562	-1.460233
H	1.374765	0.698191	-1.581964
H	1.317179	1.12516	1.12627
H	3.538179	-4.644378	-0.392831
H	1.258047	-2.762202	1.679216
H	0.39732	-1.120505	-1.530506
H	-1.903818	2.430855	-0.829982
Si	3.011425	0.400896	-0.140589
H	-3.226683	1.417159	-0.879855
H	4.871858	1.15473	0.827571
Si	2.580102	-2.642134	-0.134489
H	0.529533	-3.3476	-0.771318
O	-5.103794	-2.360912	-0.532957
H	-5.454288	-2.289359	-1.431091
O	-2.629323	-1.213182	-0.893613
O	-4.672935	0.350061	-0.50166
H	-5.364054	0.682439	0.087813
O	-3.872304	-1.327713	1.523724
H	-2.995438	-0.96463	1.775603
O	-0.327745	-2.636831	2.03993
H	-0.824867	-3.230369	1.459596
H	-0.658834	-1.728186	1.803924
Si	-4.047009	-1.165036	-0.109623
H	0.293872	5.441246	1.30566
Si	0.232051	3.412037	0.341561
Al	-1.352738	-0.040307	-0.464637

Frequencies -- -102.1227 24.4562 28.6825
Frequencies -- 38.7986 42.3900 47.6357
Frequencies -- 53.1924 60.5744 69.5344

Zero-point correction= 0.271663 (Hartree/Particle)
Thermal correction to Energy= 0.306299
Thermal correction to Enthalpy= 0.307243
Thermal correction to Gibbs Free Energy= 0.205732
Sum of electronic and zero-point Energies= -2841.601344
Sum of electronic and thermal Energies= -2841.566709
Sum of electronic and thermal Enthalpies= -2841.565764
Sum of electronic and thermal Free Energies= -2841.667275

switch-4-INTc-d3.log



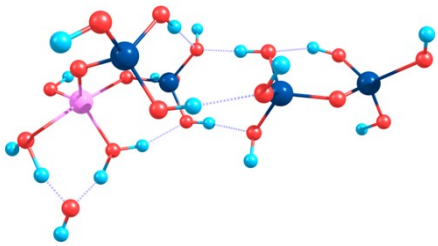
42

O	-3.10604	-0.890542	-0.223075
O	-1.814197	0.065337	1.963679
O	-3.400953	-1.985114	2.256807
O	-1.095371	-2.317145	0.870921
O	-0.964848	-4.239413	-1.055578
O	-0.797382	-1.654646	-1.705592
O	1.211601	-2.966029	-0.324553
O	1.049191	3.21717	-0.081114
O	2.73315	1.076069	-0.056559
O	0.694422	0.462191	-1.671868
O	0.893553	0.667339	1.774469
O	2.749169	-1.320678	1.175877
O	3.283341	-1.25008	-1.429323
O	5.058931	-0.137941	0.233302
H	-0.222042	-0.820047	-1.706028
H	-3.690714	-2.878203	2.02561
H	1.641589	-2.455242	0.401993
H	1.528587	0.211141	-2.093254
H	1.078135	1.497579	2.319057
H	2.573677	-1.915013	-1.379914
H	5.598343	-0.931081	0.113105
H	-2.516111	-1.026063	-0.993154
H	-1.599348	0.758519	1.254259
Si	-0.401551	-2.770417	-0.566434
H	-1.637188	-4.19963	-1.749096
H	1.911523	3.545066	-0.3686
Si	-2.349522	-1.29005	1.202945
Si	3.440577	-0.366308	-0.028891
H	2.169605	-0.759489	1.72814
O	-1.622818	3.897071	-0.855202
H	-0.682139	4.002944	-0.596233
O	-0.91448	1.478971	0.073061
O	-3.477238	2.021262	-0.60096
H	-3.650628	1.067623	-0.493673
O	-1.594661	1.714329	-2.518282
H	-0.738365	1.230952	-2.514701
H	0.010797	0.336628	2.059057
O	1.268376	3.101615	2.654621
H	0.451288	3.401911	3.079322
H	1.181978	3.388779	1.710343
Si	-1.884426	2.263998	-0.978114
Al	0.929996	1.408028	-0.111875

Frequencies -- 37.4052 42.1313 44.2776
Frequencies -- 48.6772 54.2097 62.7211
Frequencies -- 75.5097 81.0579 89.4547

Zero-point correction= 0.275904 (Hartree/Particle)
Thermal correction to Energy= 0.309551
Thermal correction to Enthalpy= 0.310495
Thermal correction to Gibbs Free Energy= 0.213503
Sum of electronic and zero-point Energies= -2841.625345
Sum of electronic and thermal Energies= -2841.591698
Sum of electronic and thermal Enthalpies= -2841.590754
Sum of electronic and thermal Free Energies= -2841.687746

switch-4-TS2b-d3b.log



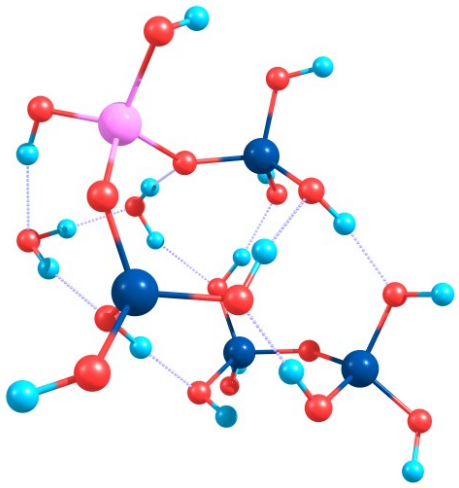
42

O	-4.992159	1.272412	-0.793415
O	-6.109558	0.658299	1.589686
O	-6.551447	-0.964244	-0.349123
O	-4.039351	-0.827655	0.58349
O	-1.706153	-2.088587	0.185896
O	-2.347953	0.330535	-1.048293
O	-1.654727	0.17729	1.510875
O	5.251598	1.281991	-0.48029
O	3.276497	-1.102794	-0.914358
O	3.050862	0.542519	1.742853
O	5.112868	-0.86763	0.992652
O	1.874825	-3.283734	-1.685219
O	1.056428	-1.680747	0.393362
O	0.841943	-1.012845	-2.237987
H	-1.504827	0.827119	-1.189918
H	-6.232445	-1.62072	-0.98279
H	-1.419025	-0.359051	2.282168
H	3.239465	-0.334955	2.399586
H	0.11814	-1.947244	0.360839
H	0.575967	-0.099496	-2.024434
H	-4.076955	1.19429	-1.126352
Si	-2.44116	-0.613023	0.286651
H	-2.05436	-2.719839	-0.459357
Si	-5.40126	0.054861	0.235208
Si	1.803529	-1.726727	-1.091624
H	2.543474	-3.82354	-1.243597
O	-0.011651	1.59728	-1.46099
H	-0.080458	2.125986	-2.270249
O	2.604387	1.543068	-0.679529
O	1.131003	3.813956	-0.521261
H	2.003195	4.200529	-0.675691
O	0.60974	1.732507	1.122043
H	2.117074	0.833192	1.720821
H	-0.221808	1.218985	1.190442
H	5.861481	-0.330482	1.28598
H	4.918876	2.07751	-0.913638
H	-5.725531	1.481859	1.918939
O	3.766354	-1.450891	2.903493
H	4.571622	-1.254858	1.964932
H	4.231725	-1.192164	3.711775
Al	3.84424	0.314202	0.038659
Si	1.171122	2.16149	-0.379027

Frequencies -- -899.5750 14.3685 20.8563
Frequencies -- 27.5302 35.1969 36.4513
Frequencies -- 38.5656 47.1999 50.7078

Zero-point correction= 0.265666 (Hartree/Particle)
Thermal correction to Energy= 0.301490
Thermal correction to Enthalpy= 0.302435
Thermal correction to Gibbs Free Energy= 0.196360
Sum of electronic and zero-point Energies= -2841.588562
Sum of electronic and thermal Energies= -2841.552737
Sum of electronic and thermal Enthalpies= -2841.551793
Sum of electronic and thermal Free Energies= -2841.657868

switch-4-PRD1-d3.log



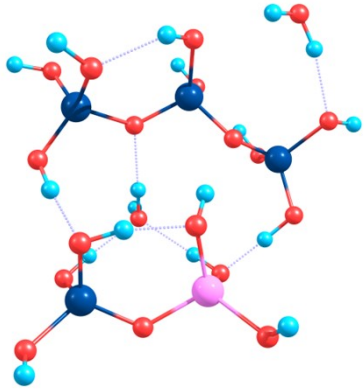
42

O	-1.106338	-0.228548	2.288254
O	-1.921733	-2.092863	0.460357
O	-3.374073	-1.622321	2.59932
O	-3.165839	0.289099	0.660097
O	-2.685399	-0.568664	-1.836833
O	-4.929111	0.827433	-1.337045
O	-2.606093	2.109881	-1.128633
O	1.620566	-0.374421	3.11513
O	1.90346	0.834578	0.61972
O	4.001756	1.575087	-1.203589
O	4.41603	-0.627058	0.674865
O	-0.176082	2.240639	1.622291
O	1.986052	3.470469	0.45629
O	0.134809	2.07685	-0.990302
H	-5.397871	0.022611	-1.598436
H	-3.545927	-1.11275	3.403323
H	-2.802303	2.563893	-1.961469
H	3.824992	2.402539	-0.736763
H	1.594799	4.293824	0.132793
H	-0.836731	2.223759	-0.938491
H	-0.855658	0.683313	2.003207
Si	-3.349241	0.637429	-0.939181
H	-1.699789	-0.517391	-1.983387
Si	-2.386609	-0.892226	1.508149
Si	0.992511	2.147952	0.426262
H	0.143102	2.56434	2.47778
O	-0.049577	-0.403462	-2.05266
H	0.135345	0.504037	-1.711045
O	2.58044	-0.900757	-1.579388
O	0.750867	-2.292293	-0.231633
H	2.029267	-2.599499	1.09128
O	0.955202	-2.619871	-2.922511
H	1.31696	-3.495579	-2.731834
H	-0.186209	-2.26469	0.057964
H	1.816404	0.132514	2.298418
H	0.66907	-0.556134	3.011695
O	2.675798	-2.590509	1.824871
H	2.314946	-1.887481	2.411103
H	3.974273	-1.37874	1.117194
H	-2.277054	-1.949281	-0.438108
Al	3.278591	0.202166	-0.366731
Si	1.105825	-1.541982	-1.669982

Frequencies -- 30.9153 37.8275 43.5672
Frequencies -- 53.7344 55.7228 60.6355
Frequencies -- 64.4383 73.2046 77.5754

Zero-point correction= 0.273680 (Hartree/Particle)
Thermal correction to Energy= 0.309363
Thermal correction to Enthalpy= 0.310307
Thermal correction to Gibbs Free Energy= 0.208419
Sum of electronic and zero-point Energies= -2841.623514
Sum of electronic and thermal Energies= -2841.587831
Sum of electronic and thermal Enthalpies= -2841.586887
Sum of electronic and thermal Free Energies= -2841.688775

switch-4-RCT2-d3.log



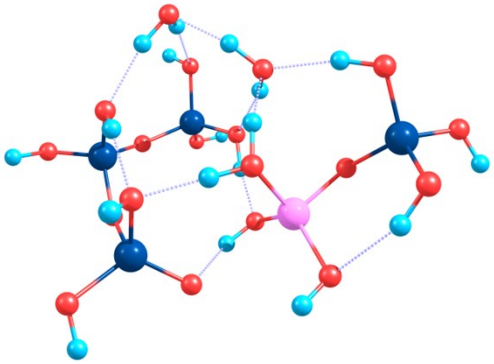
42

O	3.586807	0.501884	1.563991
O	2.836134	0.793616	-1.038989
O	5.370021	0.191582	-0.271051
O	3.353495	-1.656248	-0.098408
O	1.859435	-3.766576	-1.461742
O	0.871843	-2.707979	1.017254
O	0.911223	-0.973972	-1.346973
O	-5.126858	0.243482	-1.399624
O	-0.607275	1.676071	0.44548
O	-3.111292	1.081308	1.370203
O	-2.71593	1.853934	-1.207502
O	1.793293	2.89718	0.168145
O	-0.235326	3.07486	-1.690387
O	-0.402262	4.291184	0.781786
H	0.82005	-1.915039	1.585109
H	5.651094	-0.058685	-1.161113
H	0.053364	-0.743308	-0.960653
H	-3.41104	1.944871	1.685751
H	0.019263	3.86042	-2.193767
H	0.124952	5.101989	0.769472
H	2.672073	0.35893	1.892614
H	2.028885	0.241398	-1.277165
H	1.590508	-3.625776	-2.377615
Si	3.768147	-0.094785	0.03689
Si	0.195312	3.029617	-0.085654
H	2.23567	2.134867	-0.302676
O	-1.501526	-3.195799	0.221174
O	-1.852991	-0.545509	-0.227879
O	-3.828607	-2.208136	-0.653558
O	-2.973398	-1.728023	1.922902
H	-3.271468	-0.819357	2.102409
H	-4.381428	0.77592	-1.718444
H	-4.734154	-0.638138	-1.268605
H	-2.040226	2.329377	-1.730302
H	-4.445143	-2.898061	-0.371197
O	0.923512	-0.079203	2.076041
H	0.563124	0.165386	2.94064
H	0.440472	0.479005	1.436292
H	-0.566557	-3.039323	0.606155
Si	-2.529935	-1.952657	0.349644
Si	-2.090915	1.047132	0.080575
Al	1.742435	-2.308772	-0.489552

Frequencies -- 22.1570 29.6914 40.7750
Frequencies -- 49.1975 51.5229 57.8354
Frequencies -- 62.2637 67.0943 72.4498

Zero-point correction= 0.270784 (Hartree/Particle)
Thermal correction to Energy= 0.307576
Thermal correction to Enthalpy= 0.308521
Thermal correction to Gibbs Free Energy= 0.203305
Sum of electronic and zero-point Energies= -2841.613505
Sum of electronic and thermal Energies= -2841.576713
Sum of electronic and thermal Enthalpies= -2841.575769
Sum of electronic and thermal Free Energies= -2841.680984

switch-4-TS3e-d3b.log



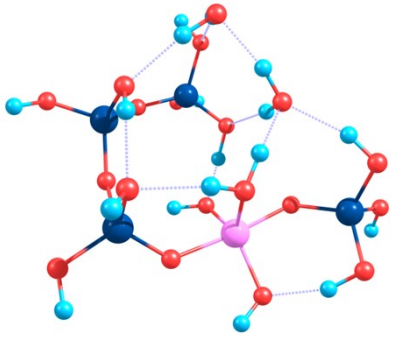
42

O	-3.9135	-1.279419	1.588962
O	-5.555526	-1.232159	-0.43211
O	-4.741221	1.128345	0.601287
O	-2.979061	-0.365344	-0.773973
O	-2.76409	2.436903	-0.993076
O	-1.175394	0.903675	0.922291
O	-0.540393	0.514275	-1.952533
O	1.089155	-2.430294	2.656088
O	2.841437	-1.243743	-0.679518
O	2.424965	-0.140095	1.763841
O	4.819455	-0.063725	0.455884
O	0.168033	-1.748093	-0.982382
O	2.143509	-2.890554	-2.525163
O	1.66207	-3.568706	0.091361
H	-0.375625	1.430845	1.199295
H	-4.21033	1.7943	0.114307
H	0.085698	1.279257	-1.85426
H	1.628403	-1.634515	2.462921
H	1.510734	-3.48464	-2.951736
H	2.47551	-4.091808	0.133822
H	-2.960282	-1.503139	1.64047
H	-6.035208	-0.724992	-1.10065
H	-2.275974	3.241941	-0.777498
Si	-4.26455	-0.418986	0.22371
Si	1.683606	-2.348488	-1.03712
H	-0.011499	-0.837625	-1.411684
O	0.483199	2.806993	-1.136597
O	2.710513	1.424397	-0.391624
O	2.554706	4.017656	0.233252
O	1.055391	2.199253	1.476213
H	1.86701	0.64539	1.954774
H	-0.393732	-1.902465	2.044235
H	1.309536	-3.017352	1.907021
H	5.209434	0.60444	1.036065
H	2.332908	4.755201	-0.350238
O	-1.138405	-1.591624	1.45546
H	-0.834056	-1.8443	0.555663
H	-1.088709	-0.057172	1.256923
Si	1.635773	2.666211	-0.074246
Si	3.183001	0.02115	0.299695
Al	-1.823222	0.963261	-0.827903
H	0.9797	2.923886	2.113474

Frequencies --	-43.4060	27.9476	32.6088
Frequencies --	41.4575	45.0137	57.8075
Frequencies --	58.9542	68.5086	73.7133

Zero-point correction=	0.273711 (Hartree/Particle)
Thermal correction to Energy=	0.307867
Thermal correction to Enthalpy=	0.308811
Thermal correction to Gibbs Free Energy=	0.209858
Sum of electronic and zero-point Energies=	-2841.605317
Sum of electronic and thermal Energies=	-2841.571161
Sum of electronic and thermal Enthalpies=	-2841.570217
Sum of electronic and thermal Free Energies=	-2841.669170

switch-4-INT2d-d3.log



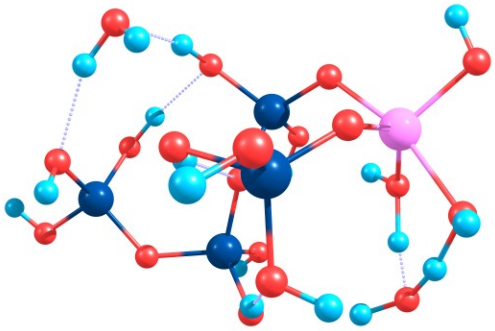
42

O	-3.774447	-1.269693	1.644595
O	-4.959032	-1.689403	-0.640518
O	-4.741613	0.857421	0.277303
O	-2.545791	-0.409992	-0.627597
O	-2.8879	2.163301	-1.171246
O	-1.171937	0.866422	1.176754
O	-0.387171	0.222019	-1.880107
O	1.358099	-2.242435	2.774439
O	2.739037	-1.083745	-0.746445
O	2.516972	0.079867	1.678003
O	4.630847	0.494982	-0.020995
O	0.175782	-1.996033	-0.848702
O	2.238654	-3.000335	-2.381067
O	1.981217	-3.482693	0.302081
H	-0.447145	1.382996	1.586073
H	-4.195336	1.518528	-0.224498
H	0.433648	0.709057	-2.029865
H	1.815887	-1.420391	2.503489
H	1.68463	-3.717254	-2.719171
H	2.856096	-3.89601	0.320927
H	-2.845492	-1.543698	1.783212
H	-5.212201	-1.401211	-1.527673
H	-2.650913	3.095808	-1.095441
Si	-3.95213	-0.599608	0.13397
Si	1.752414	-2.387133	-0.927634
H	-0.066849	-1.086516	-1.30361
O	-0.312478	2.592308	-0.646807
O	2.188554	1.548707	-0.541987
O	1.878958	4.170059	-0.2556
O	1.082724	2.399625	1.663244
H	2.024079	0.862171	2.004553
H	-0.211464	-1.897141	2.190728
H	1.605889	-2.858574	2.057514
H	4.978696	1.287513	0.410219
H	1.273697	4.884292	-0.49714
O	-1.010933	-1.669326	1.643692
H	-0.742796	-1.902556	0.726662
H	-1.091888	-0.105705	1.449335
Si	1.138805	2.717234	-0.002587
Si	3.005052	0.278164	0.108208
Al	-1.493664	1.107412	-0.726627
H	0.994782	3.162689	2.251138

Frequencies --	37.4929	39.1676	42.9589
Frequencies --	50.7211	56.6334	68.8351
Frequencies --	72.5122	77.4218	89.1701

Zero-point correction=	0.274894 (Hartree/Particle)
Thermal correction to Energy=	0.309312
Thermal correction to Enthalpy=	0.310256
Thermal correction to Gibbs Free Energy=	0.212035
Sum of electronic and zero-point Energies=	-2841.622522
Sum of electronic and thermal Energies=	-2841.588104
Sum of electronic and thermal Enthalpies=	-2841.587160
Sum of electronic and thermal Free Energies=	-2841.685381

switch-4-TS4-d3d.log



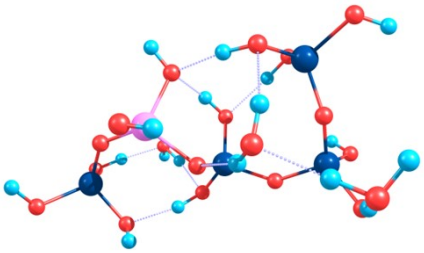
42

O	3.905495	-0.491483	0.903347
O	2.298734	-2.161978	-0.032551
O	4.203698	-0.637139	-1.856557
O	2.489509	1.301115	-0.372015
O	2.164796	3.757444	0.543329
O	-0.036979	2.371062	-0.020464
O	1.350727	1.640322	2.083033
O	-0.209589	-2.64637	-1.472652
O	-2.650349	-0.334772	1.454934
O	-0.207409	-0.511492	2.609964
O	-1.18787	-2.607438	1.226685
O	-3.195637	1.733413	-0.204623
O	-3.59142	-0.734077	-1.104445
O	-5.138222	0.116762	0.911075
H	-0.460844	1.493335	-0.040513
H	0.281541	0.338896	2.470418
H	-2.820441	-0.623757	-1.707148
H	-5.867049	0.363409	0.325151
Si	1.536712	2.225882	0.507238
Si	-1.130297	-0.960633	1.334737
H	1.658613	4.384451	1.077567
Si	-3.641022	0.194928	0.239079
O	-1.254863	-0.440888	-2.592342
H	-1.28917	0.556614	-2.655271
O	-0.460466	-0.39002	-0.051168
O	1.416905	-0.550599	-1.96738
O	-1.524075	2.21264	-2.456647
H	-2.254442	2.147216	-1.809376
H	-1.986273	-3.034691	1.566226
H	-0.782644	2.500439	-1.892711
O	2.540038	-1.858421	2.319093
H	2.291011	-2.180462	1.143983
H	3.876875	-0.633914	-2.764732
H	-2.833506	2.285815	0.503097
H	3.276766	-1.06732	1.775261
H	1.744882	-1.384577	2.614744
H	1.565979	-2.635217	-0.45661
H	4.117534	0.414297	1.159999
H	2.180764	1.338422	2.479908
H	-0.733132	-2.938483	-0.704448
Al	2.839457	-0.464835	-0.731108
Si	-0.064221	-0.990625	-1.577202

Frequencies -- -1208.1165 42.3936 44.1189
Frequencies -- 63.3319 67.5041 70.7550
Frequencies -- 80.7354 88.4800 91.9720

Zero-point correction= 0.270039 (Hartree/Particle)
Thermal correction to Energy= 0.303513
Thermal correction to Enthalpy= 0.304457
Thermal correction to Gibbs Free Energy= 0.209395
Sum of electronic and zero-point Energies= -2841.612545
Sum of electronic and thermal Energies= -2841.579071
Sum of electronic and thermal Enthalpies= -2841.578127
Sum of electronic and thermal Free Energies= -2841.673190

switch-4-PRD2-d3g.log



42

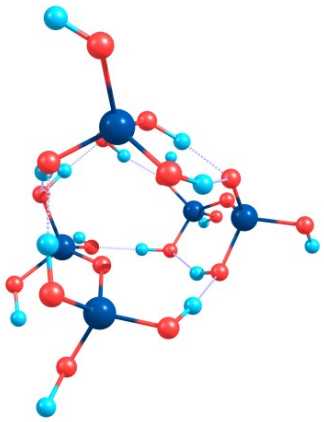
O	-3.542051	-2.663974	-0.330887
O	-3.329471	-1.111009	-2.441106
O	-3.005794	-0.001839	-0.047524
O	-4.381288	1.225151	1.912811
O	-2.484124	-0.577522	2.539657
O	-0.0245	-1.175245	1.399529
O	2.955325	-2.628369	1.706396
O	3.228288	1.146039	0.397699
O	0.712925	1.376376	1.842549
O	1.364534	3.174098	-0.45335
O	4.875223	-1.004131	0.691796
O	3.544029	-0.714428	-1.575282
O	5.544304	0.963668	-0.975834
H	-1.646616	-1.012524	2.275041
H	-3.419962	-0.142618	-2.67049
H	-2.740838	1.845534	-2.355436
H	1.110338	1.777499	2.6258
H	3.151669	-0.151809	-2.258619
H	5.664201	1.843312	-0.59374
Si	-2.919629	0.604743	1.481434
H	-5.143572	0.708528	1.61817
Si	-2.74468	-1.356722	-0.941465
Si	4.269681	0.135469	-0.317708
H	4.198565	-1.592032	1.11649
O	0.623586	0.372571	-0.711763
O	-1.348022	2.302709	-1.364833
O	-1.128257	-1.693847	-0.970074
O	1.447595	-2.204514	-0.623664
H	2.207809	-1.762969	-1.072976
H	3.347282	-3.513521	1.708544
H	2.355184	-2.627797	0.930491
H	0.495096	3.283375	-0.868714
H	-3.100931	-3.099976	0.410847
O	-3.522485	1.508746	-2.858537
H	-4.277	1.746488	-2.300407
H	-1.686196	2.289475	-0.446895
O	-1.890855	1.890421	1.466487
H	-0.938562	1.713818	1.704007
H	0.340624	-0.353446	1.814621
Si	0.238529	-1.135116	-0.246362
Al	1.533519	1.58353	0.250281
H	-0.779131	1.506325	-1.385536

Frequencies -- 19.8129 31.2603 39.2229
Frequencies -- 46.4418 57.9558 60.7917
Frequencies -- 71.1998 73.0328 79.8920

Zero-point correction= 0.275094 (Hartree/Particle)
Thermal correction to Energy= 0.310578
Thermal correction to Enthalpy= 0.311522
Thermal correction to Gibbs Free Energy= 0.209468
Sum of electronic and zero-point Energies= -2841.638504
Sum of electronic and thermal Energies= -2841.603020
Sum of electronic and thermal Enthalpies= -2841.602076
Sum of electronic and thermal Free Energies= -2841.704130

CAM-B3LYP
Anionic Si

Bondi-Si-RCT1-CAMhighb.log



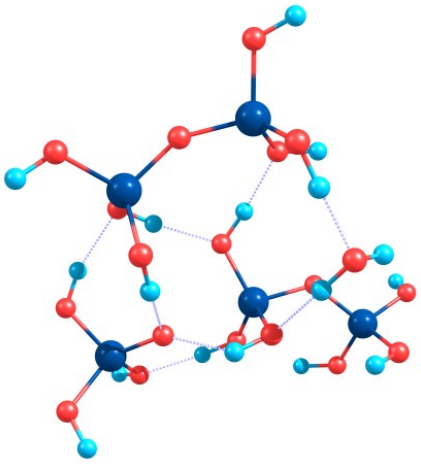
41

O	-2.410463	-3.282252	-0.348473
O	0.256108	-2.898194	-0.862408
O	-1.666503	-1.443294	-2.082026
O	-1.052461	-1.15355	0.529447
O	-3.356091	0.001774	1.340508
O	-2.441787	-2.241924	2.427264
O	-1.130222	0.109439	2.866185
O	0.938246	2.399228	0.472781
O	3.064841	0.771342	0.109126
O	1.421477	0.251428	2.105946
O	2.949757	2.449065	2.191344
O	4.868354	-1.048575	-0.291876
O	2.32766	-1.758432	0.356036
O	2.819905	-0.832699	-2.067432
H	-3.195729	-2.284929	3.023609
H	-0.899692	-1.026342	-2.585296
H	-0.172496	0.208748	2.649658
H	1.582695	-0.621145	1.704236
H	3.618693	1.989192	2.707028
H	1.597463	-2.222347	-0.110367
H	3.397626	-0.417715	-2.718202
H	-2.595143	-3.371985	0.59823
H	0.420059	-3.50546	-1.592163
Si	-2.000185	-0.771798	1.817847
Si	2.032015	1.513515	1.184964
H	-3.28598	0.451786	0.476404
H	0.333553	2.145441	-0.947486
Si	-1.23417	-2.204768	-0.707231
Si	3.276962	-0.723953	-0.483778
H	5.176387	-1.923647	-0.548931
O	-2.798104	0.953966	-1.203256
H	-2.42604	0.142471	-1.602063
O	-0.350252	2.02256	-1.690906
O	-2.633427	3.541389	-1.771693
H	-3.116856	3.348686	-2.580476
O	-1.654009	2.685336	0.517981
H	-0.690085	2.610742	0.759124
O	0.312252	-0.175432	-3.144015
H	0.128867	0.672153	-2.68332
H	1.155478	-0.488283	-2.769162
Si	-1.842554	2.292947	-1.05588

Frequencies --	34.6537	40.8047	50.0038
Frequencies --	53.8102	60.2415	66.4083
Frequencies --	68.2812	74.7637	85.3556

Zero-point correction=	0.265191 (Hartree/Particle)
Thermal correction to Energy=	0.298632
Thermal correction to Enthalpy=	0.299576
Thermal correction to Gibbs Free Energy=	0.202579
Sum of electronic and zero-point Energies=	-2888.177292
Sum of electronic and thermal Energies=	-2888.143851
Sum of electronic and thermal Enthalpies=	-2888.142907
Sum of electronic and thermal Free Energies=	-2888.239904

Bondi-Si-TS1freqb-CAMhighb.log



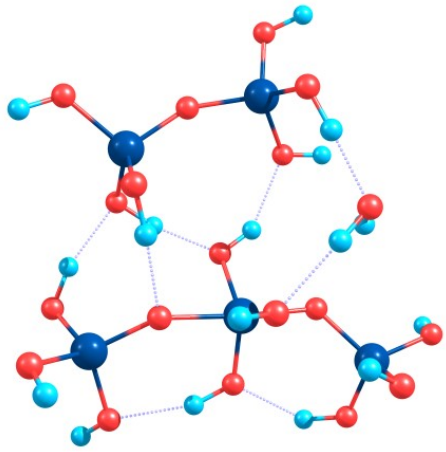
41

O	0.004583	-0.038354	-1.160094
O	-1.856895	1.976849	-0.8237
O	-1.226052	0.363124	1.383862
O	0.563283	1.968285	0.683615
O	1.607764	4.425993	1.34681
O	2.429021	3.283172	-0.814764
O	-0.162103	4.064453	-0.67067
O	4.651231	-0.414167	0.100931
O	2.60347	-1.931045	-0.323354
O	2.608059	0.550081	-1.334642
O	2.30446	0.189792	1.311921
O	0.268399	-2.703797	-1.165429
O	2.346769	-4.449225	-0.797351
O	1.038616	-3.466054	1.30645
H	2.627978	2.375294	-1.107679
H	-0.570495	0.995812	1.730727
H	0.036362	4.730742	-1.335286
H	1.637011	0.490688	-1.472654
H	1.614218	0.905641	1.123548
H	1.921915	-5.307859	-0.710538
H	0.218697	-3.008315	1.62521
H	-0.019349	-1.01215	-1.289693
H	-1.306766	2.788007	-0.799864
Si	1.112281	3.371505	0.170681
Si	3.019055	-0.379001	-0.029763
H	0.963859	4.614292	2.035869
H	5.077967	0.377849	0.440954
Si	-1.2386	0.563906	-0.269052
Si	1.545573	-3.152636	-0.201176
H	-0.532393	-3.238459	-1.132521
O	-4.986532	-1.518614	-0.876926
H	-5.172354	-1.402685	-1.813436
O	-2.481309	-0.494827	-0.629312
O	-4.577141	1.117006	-0.510764
H	-3.850499	1.729523	-0.711792
O	-4.172539	-0.764855	1.437784
H	-3.455982	-0.418607	1.982228
O	-1.16912	-2.262637	2.120302
H	-1.940396	-2.573594	1.63314
H	-1.13621	-1.300416	1.939301

Frequencies --	-124.9361	26.0658	33.4627
Frequencies --	37.8110	43.1313	48.9599
Frequencies --	58.4262	61.7659	69.2394

Zero-point correction=	0.265221 (Hartree/Particle)
Thermal correction to Energy=	0.298989
Thermal correction to Enthalpy=	0.299933
Thermal correction to Gibbs Free Energy=	0.200627
Sum of electronic and zero-point Energies=	-2888.165275
Sum of electronic and thermal Energies=	-2888.131507
Sum of electronic and thermal Enthalpies=	-2888.130563
Sum of electronic and thermal Free Energies=	-2888.229869

Bondi-Si-INT-CAMhighb.log



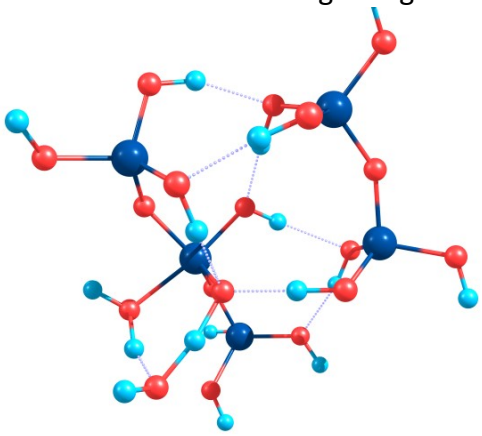
41

O	0.089008	-0.053676	-1.019996
O	-2.362002	1.484173	-0.782567
O	-1.356361	0.089682	1.576795
O	-0.152552	1.872975	0.428515
O	0.643795	4.250265	1.394183
O	1.349248	3.607266	-1.037613
O	-1.264296	4.020991	-0.535253
O	4.604893	0.703627	0.208318
O	3.011186	-1.287024	-0.23391
O	2.41601	1.091841	-1.305433
O	2.175363	0.734999	1.352745
O	1.020473	-2.636283	-1.268335
O	3.424655	-3.792456	-0.653795
O	1.719443	-3.131692	1.290764
H	1.879967	2.803803	-1.205817
H	-0.941688	0.736211	2.156339
H	-1.241194	4.799724	-1.099695
H	1.498544	0.742979	-1.441949
H	1.296411	1.122668	1.159563
H	3.225578	-4.728534	-0.556814
H	0.762674	-2.93673	1.46109
H	0.067095	-0.989729	-1.273877
H	-2.179922	2.437332	-0.764698
Si	0.15685	3.415009	0.063796
Si	3.026981	0.32074	0.019
H	0.076212	4.193146	2.169086
H	4.806162	1.592772	0.515884
Si	-1.195826	0.495838	-0.080044
Si	2.269865	-2.729476	-0.183706
H	0.465761	-3.416871	-1.371636
O	-4.206021	-2.703955	-0.524469
H	-4.210618	-2.939605	-1.456957
O	-2.131712	-0.946562	-0.460328
O	-4.605307	-0.11578	-1.033622
H	-4.069136	0.688002	-1.158481
O	-3.979832	-1.032069	1.463997
H	-3.206211	-0.633766	1.893864
O	-0.865011	-2.612077	1.547073
H	-1.177073	-2.608719	0.630971

Frequencies --	19.3005	25.4514	36.9296
Frequencies --	40.0520	55.8106	57.4804
Frequencies --	70.3159	74.0295	80.9330

Zero-point correction= 0.266976 (Hartree/Particle)
Thermal correction to Energy= 0.301069
Thermal correction to Enthalpy= 0.302013
Thermal correction to Gibbs Free Energy= 0.202162
Sum of electronic and zero-point Energies= -2888.176407
Sum of electronic and thermal Energies= -2888.142315
Sum of electronic and thermal Enthalpies= -2888.141370
Sum of electronic and thermal Free Energies= -2888.241222

Bondi-Si-TS2-D3d-CAMhighb.log



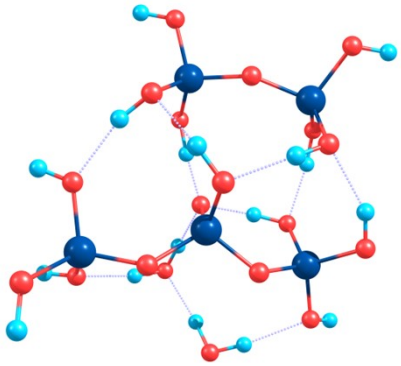
41

O	0.048729	0.039094	-1.245262
O	-2.31314	2.331814	0.35797
O	-0.686865	0.51972	1.211082
O	-0.135708	2.406383	-0.752161
O	1.629578	1.935678	1.178169
O	2.550574	2.744512	-1.193461
O	1.140886	4.464357	0.233116
O	4.623125	-1.633021	-0.78818
O	2.201835	-2.223658	-0.101669
O	2.60477	0.020187	-1.494104
O	3.441933	-0.110711	1.058467
O	-0.297886	-2.722821	-0.701527
O	1.113455	-4.243701	1.077708
O	0.277401	-1.815526	1.778579
H	2.77289	1.818183	-1.41432
H	-1.421638	0.968863	2.042143
H	1.931553	4.930965	0.521135
H	1.599329	0.044329	-1.497157
H	2.866137	0.674081	1.16809
H	0.411562	-4.696971	1.554133
H	-0.102874	-0.915485	1.558762
H	-0.231926	-0.884365	-1.325521
H	-1.947472	3.218902	0.27019
Si	1.302215	2.8796	-0.148364
Si	3.207338	-0.958067	-0.319335
H	0.848824	1.397198	1.449536
H	5.382085	-1.048468	-0.873555
Si	-1.037107	1.035028	-0.322836
Si	0.78742	-2.728271	0.538056
H	-1.24819	-2.635995	-0.478141
O	-2.907041	-2.160771	-0.231915
H	-3.476633	-2.833848	0.155791
O	-2.377273	0.299171	-1.025613
O	-4.550849	-0.995465	-1.912589
H	-5.048704	-0.254662	-2.272504
O	-4.393165	-0.057655	0.640721
H	-5.088498	-0.587237	1.043192
O	-2.287684	1.583649	2.630167

Frequencies --	-1250.2500	27.6218	37.6242
Frequencies --	42.6682	50.5735	59.7337
Frequencies --	67.1712	77.1885	81.4622

Zero-point correction= 0.259587 (Hartree/Particle)
Thermal correction to Energy= 0.292317
Thermal correction to Enthalpy= 0.293261
Thermal correction to Gibbs Free Energy= 0.197203
Sum of electronic and zero-point Energies= -2888.150434
Sum of electronic and thermal Energies= -2888.117704
Sum of electronic and thermal Enthalpies= -2888.116760
Sum of electronic and thermal Free Energies= -2888.212818

Bondi-Si-PRD1-CAMhighb.log



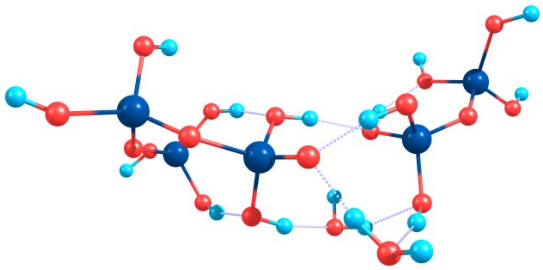
41

O	0.152716	-0.360219	-1.718888
O	-3.23126	3.088006	0.796617
O	-0.483775	0.028904	0.931577
O	-0.707537	1.937474	-0.897172
O	0.87856	2.245836	1.219557
O	1.551198	3.433445	-1.088627
O	-0.628787	4.295097	0.189396
O	4.903734	-0.270085	-0.595422
O	2.678697	-1.484559	-0.085743
O	2.55082	0.826502	-1.406461
O	3.265284	0.866511	1.165087
O	0.524865	-2.842859	-0.672634
O	2.492582	-3.866084	0.915972
O	0.840864	-1.965669	1.852597
H	2.115251	2.673459	-1.325722
H	-1.782268	0.553435	1.972892
H	-0.26046	5.010626	0.71719
H	1.72886	0.393686	-1.728166
H	2.486416	1.450654	1.258493
H	2.02111	-4.634617	1.251453
H	0.267203	-1.178954	1.600277
H	0.31067	-1.317229	-1.59264
H	-2.4167	3.579976	0.625586
Si	0.302208	2.986998	-0.138513
Si	3.335668	-0.00177	-0.214575
H	0.386632	1.3883	1.366359
H	5.490914	0.491713	-0.613945
Si	-0.859572	0.323489	-0.59181
Si	1.608753	-2.541002	0.544353
H	-0.414198	-2.961872	-0.435121
O	-2.244277	-2.706051	-0.264289
H	-2.604646	-3.519443	0.106738
O	-2.392151	-0.162865	-0.9539
O	-4.294095	-1.913503	-1.721661
H	-4.993062	-1.306634	-1.987066
O	-4.091938	-1.016954	0.839048
H	-4.69292	-1.65173	1.243837

Frequencies --	31.3849	41.2130	49.3708
Frequencies --	50.7612	55.4922	61.7436
Frequencies --	79.9100	85.6138	93.5894

Zero-point correction= 0.266359 (Hartree/Particle)
Thermal correction to Energy= 0.300428
Thermal correction to Enthalpy= 0.301373
Thermal correction to Gibbs Free Energy= 0.203032
Sum of electronic and zero-point Energies= -2888.179259
Sum of electronic and thermal Energies= -2888.145190
Sum of electronic and thermal Enthalpies= -2888.144245
Sum of electronic and thermal Free Energies= -2888.242586

Bondi-Si-RCT2-CAMhighb.log



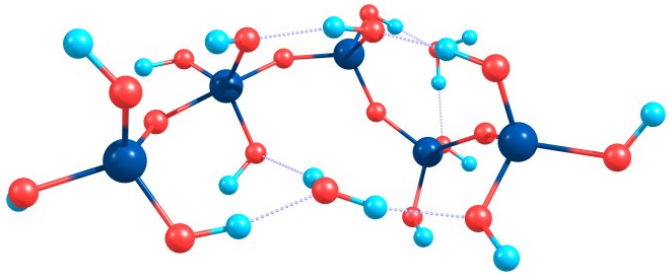
41

O	2.698423	1.574834	1.518066
O	1.911048	-0.691216	0.40339
O	2.270176	1.505903	-1.149476
O	4.353067	0.222701	-0.112637
O	5.535441	-1.174891	-2.137525
O	6.427674	-1.215867	0.437078
O	4.032698	-2.34082	-0.324976
O	0.591633	0.269297	2.838263
O	-4.438645	-0.407586	-0.021976
O	-3.593951	-0.572247	-2.550398
O	-5.040409	1.537501	-1.798592
O	-4.784113	-2.819932	1.164084
O	-2.581973	-2.308865	-0.114157
O	-3.140234	-0.987947	2.221431
H	7.07032	-1.917268	0.290502
H	1.32062	1.831704	-1.02416
H	4.117869	-3.166597	-0.811424
H	-3.191106	-1.408774	-2.287586
H	-1.781636	-1.755053	-0.25171
H	-2.647966	-0.148686	2.095742
H	2.267384	2.47107	1.42271
H	2.377031	-1.514572	0.173964
Si	5.133181	-1.138172	-0.554818
Si	-3.920327	0.458528	-1.315301
H	6.212114	-0.567009	-2.45263
Si	2.805633	0.690781	0.145052
Si	-3.726914	-1.62298	0.836963
H	-5.584733	-2.593662	1.646968
O	-1.585223	1.170276	1.510836
H	-0.813543	0.951209	2.086117
O	-2.616242	1.328912	-0.889594
O	-0.094333	2.253353	-0.505526
O	-0.695899	-0.394994	-0.470453
H	0.223042	-0.611774	-0.214704
H	0.730969	-0.533081	2.317616

Frequencies --	18.3091	22.4987	27.8662
Frequencies --	34.6621	35.7885	46.5917
Frequencies --	53.3260	68.5050	70.3060

Zero-point correction= 0.264880 (Hartree/Particle)
Thermal correction to Energy= 0.299594
Thermal correction to Enthalpy= 0.300538
Thermal correction to Gibbs Free Energy= 0.197552
Sum of electronic and zero-point Energies= -2888.170590
Sum of electronic and thermal Energies= -2888.135875
Sum of electronic and thermal Enthalpies= -2888.134931
Sum of electronic and thermal Free Energies= -2888.237917

Bondi-Si-INT2-CAMhighb.log



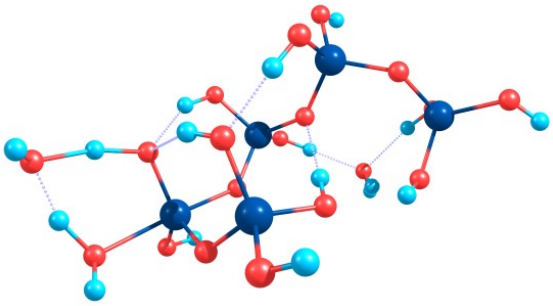
41

O	1.506442	0.765568	1.440349
O	1.992714	0.610077	-1.46595
O	2.99076	2.897286	0.065203
O	3.719518	0.55654	0.354703
O	3.425377	-2.068438	0.993617
O	4.199783	-1.384414	-1.434178
O	5.850905	-1.038319	0.634366
O	-4.208952	3.048755	-0.23794
O	-3.264164	-0.825234	0.052751
O	-3.909852	1.131042	1.786945
O	-2.138668	-0.768425	2.468586
O	-1.964477	-1.789128	-2.058949
O	-1.790655	-2.90924	0.449495
O	-3.958255	-3.227925	-1.019268
H	4.83441	-0.962955	-2.023145
H	3.928855	2.755063	0.21883
H	6.118805	-0.403196	1.30537
H	-4.679322	0.72881	2.203636
H	-1.672471	-3.864893	0.412123
H	-4.495941	-3.065571	-1.800728
H	2.178983	0.306987	1.953133
H	2.680268	-0.031276	-1.686279
Si	4.276966	-0.942838	0.166738
Si	-2.710574	0.151537	1.243172
H	2.453284	-2.085265	0.848808
Si	2.183471	1.42841	0.020854
Si	-2.748364	-2.186732	-0.696004
H	-1.476955	-0.931346	-2.022128
O	-0.638636	0.516973	-1.769382
H	0.326707	0.352118	-1.885184
O	-1.58732	1.151058	0.657037
O	0.668116	2.267536	-0.279777
O	-1.718109	2.948365	-1.276087
H	-2.627614	3.031387	-0.908104
H	-4.796494	2.574441	-0.837169
H	-4.202501	2.50994	0.573705

Frequencies --	21.5015	29.6744	34.6417
Frequencies --	43.7905	53.6359	61.0921
Frequencies --	71.2300	74.9332	77.1537

Zero-point correction= 0.267911 (Hartree/Particle)
Thermal correction to Energy= 0.301943
Thermal correction to Enthalpy= 0.302888
Thermal correction to Gibbs Free Energy= 0.203757
Sum of electronic and zero-point Energies= -2888.170521
Sum of electronic and thermal Energies= -2888.136488
Sum of electronic and thermal Enthalpies= -2888.135544
Sum of electronic and thermal Free Energies= -2888.234675

Bondi-Si-TS4f-CAMhighb.log



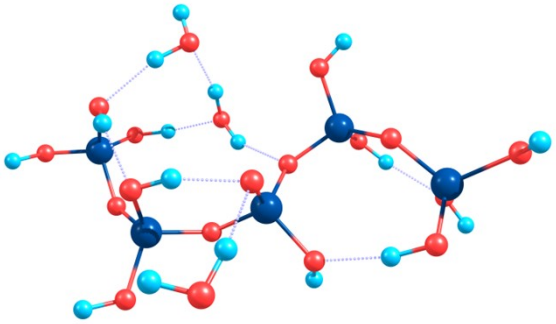
41
Si5H17O19

O	4.762944	0.325555	-0.654416
O	3.011242	-0.67194	0.89428
O	3.576258	-1.382488	-1.92486
O	2.472646	1.174923	-1.145587
O	1.592446	3.587535	-0.604167
O	-0.217001	1.680508	-0.946206
O	1.348071	1.560677	1.219543
O	0.984853	-2.348234	1.37095
O	-3.076427	0.625971	1.021144
O	-0.90398	0.897618	2.576283
O	-2.2354	-1.337652	2.664245
O	-2.861253	0.942746	-1.650921
O	-4.57209	-0.804746	-0.740334
O	-5.039754	1.773736	-0.181527
H	-0.493326	0.77671	-0.709257
H	-0.081662	1.228162	2.15495
H	-3.994337	-1.403433	-1.250393
H	-5.650823	1.926728	-0.909048
Si	1.296836	1.999389	-0.382994
Si	-1.775153	-0.127441	1.668023
H	0.909015	4.214885	-0.348761
Si	2.945592	-0.399148	-0.736745
Si	-3.88855	0.637163	-0.397422
O	-0.525518	-3.035819	-0.710243
H	-1.25336	-2.735269	-1.292183
O	-0.89925	-0.659202	0.387133
O	1.32379	-1.049412	-0.934957
O	-2.476707	-1.826329	-2.223733
H	-2.276904	-0.877063	-2.303607
H	-2.865417	-1.982666	2.328166
H	-2.628791	-2.143514	-3.121866
O	5.138854	0.045207	1.71591
H	4.014854	-0.369553	1.427672
H	2.888553	-1.963486	-2.26473
H	-2.150004	1.588784	-1.530862

Frequencies --	-1033.1083	27.2715	32.0430
Frequencies --	44.5207	48.9944	55.6892
Frequencies --	60.9553	71.0551	89.0957

Zero-point correction= 0.262607 (Hartree/Particle)
Thermal correction to Energy= 0.295010
Thermal correction to Enthalpy= 0.295954
Thermal correction to Gibbs Free Energy= 0.201186
Sum of electronic and zero-point Energies= -2888.154156
Sum of electronic and thermal Energies= -2888.121754
Sum of electronic and thermal Enthalpies= -2888.120809
Sum of electronic and thermal Free Energies= -2888.215577

Bondi-Si-PRD2-CAMhighb.log



41

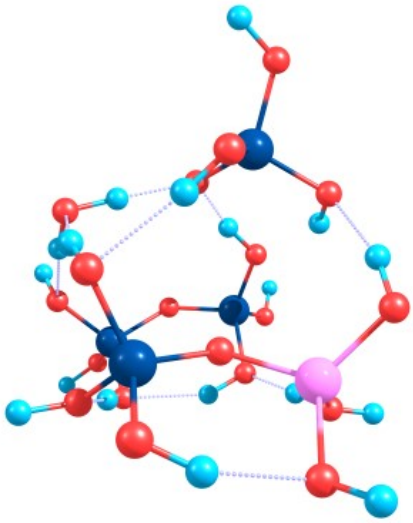
O	2.343185	1.551181	1.217974
O	1.645802	-2.628301	1.937111
O	2.737346	3.043649	-1.064743
O	3.582839	0.525574	-0.867885
O	5.857301	-0.817723	-0.334953
O	3.729914	-0.860673	1.373821
O	3.776304	-2.173223	-0.996449
O	0.365393	3.982183	1.354255
O	-3.328192	-0.613825	0.619737
O	-1.619329	-2.657021	1.067849
O	-2.775312	-2.34149	-1.333578
O	-4.187762	1.833149	-0.064854
O	-4.902701	-0.462017	-1.404311
O	-5.914271	0.10402	0.981117
H	3.308298	-0.024443	1.65115
H	3.581611	3.449074	-0.842305
H	2.80032	-2.350376	-1.011085
H	-2.227412	-3.345922	1.354124
H	-5.498863	-0.036326	-2.027885
H	-5.92983	0.575712	1.819567
Si	4.228803	-0.8367	-0.205287
Si	-2.165893	-1.575807	-0.022056
H	6.333145	-0.121275	0.127456
Si	2.408491	1.576113	-0.431299
Si	-4.589536	0.260307	0.042764
H	-3.270473	1.992961	-0.373133
O	-1.614668	1.859535	-0.941342
H	-1.613991	1.824092	-1.904471
O	-0.877478	-0.653251	-0.421569
O	0.95348	1.11927	-1.013317
O	-0.292765	1.348228	1.350705
H	1.291235	3.903134	1.604642
H	0.022651	3.065391	1.449238
H	-3.547373	-1.893915	-1.715543

Frequencies -- 14.9297 27.2657 32.2508
Frequencies -- 37.2042 45.0666 50.7023
Frequencies -- 51.9581 56.6458 60.2091

Zero-point correction= 0.264478 (Hartree/Particle)
Thermal correction to Energy= 0.300359
Thermal correction to Enthalpy= 0.301304
Thermal correction to Gibbs Free Energy= 0.196295
Sum of electronic and zero-point Energies= -2888.162563
Sum of electronic and thermal Energies= -2888.126681
Sum of electronic and thermal Enthalpies= -2888.125737
Sum of electronic and thermal Free Energies= -2888.230746

Anionic Q1 CAM-B3LYP

Switch-4-RCT1-CAMhighd2.log



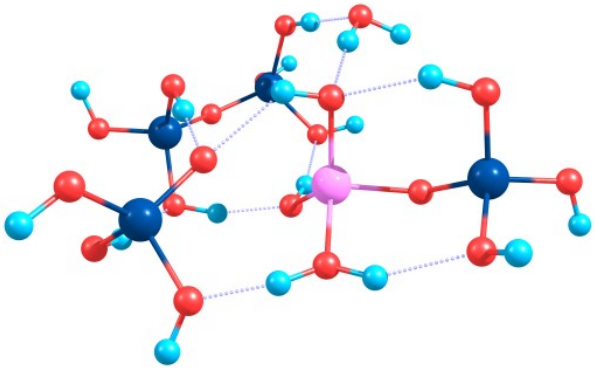
42

O	-2.244935	-3.244398	-0.761602
O	0.39286	-2.672148	-1.147502
O	-1.543867	-1.260515	-2.361055
O	-1.096242	-1.079063	0.307981
O	-3.332784	0.2083	1.856917
O	-2.810881	-2.64837	1.861982
O	-0.841968	-0.787408	3.016547
O	0.736636	2.182082	0.905603
O	2.962112	0.864265	0.210323
O	1.459528	-0.168535	2.119722
O	2.751052	2.029874	2.648556
O	4.973992	-0.691839	-0.31465
O	2.514708	-1.742225	0.096777
O	2.980603	-0.441599	-2.159614
H	-3.708395	-2.753723	2.186129
H	-0.790116	-0.716252	-2.741978
H	0.086017	-0.509502	2.7212
H	1.752648	-0.949255	1.607733
H	1.735909	-2.108546	-0.391948
H	3.505961	0.141234	-2.719623
H	-2.565605	-3.26784	0.166252
H	0.569795	-3.233401	-1.910035
H	-3.067186	1.054435	1.4601
Si	-1.144354	-2.046312	-0.979002
Si	3.370428	-0.515554	-0.562757
H	5.393044	-1.485966	-0.662233
O	-2.877065	1.115586	-1.594023
H	-2.460553	0.262221	-1.806287
O	-0.335306	2.075487	-1.314382
O	-2.541301	3.720152	-1.524386
H	-2.646238	3.797904	-2.477075
O	-2.101692	2.391941	0.661045
H	-1.251558	2.397002	1.128203
O	0.396306	0.299105	-3.080478
H	0.166901	1.014049	-2.419112
H	1.251828	-0.055765	-2.789345
Si	-1.886571	2.289809	-0.995397
H	2.927987	2.968752	2.533718
H	0.381898	2.108415	-0.086296
Al	-2.141049	-1.031925	1.709731
Si	1.94902	1.272718	1.440345
H	-1.022086	-0.463514	3.907376

Frequencies -- 34.3052 41.7932 51.0259
Frequencies -- 52.9620 56.3121 57.5068
Frequencies -- 67.3850 70.8678 76.8622

Zero-point correction= 0.273514 (Hartree/Particle)
Thermal correction to Energy= 0.307974
Thermal correction to Enthalpy= 0.308918
Thermal correction to Gibbs Free Energy= 0.209785
Sum of electronic and zero-point Energies= -2841.729071
Sum of electronic and thermal Energies= -2841.694612
Sum of electronic and thermal Enthalpies= -2841.693668
Sum of electronic and thermal Free Energies= -2841.792801

Switch-4-TS1-CAMhighB.log



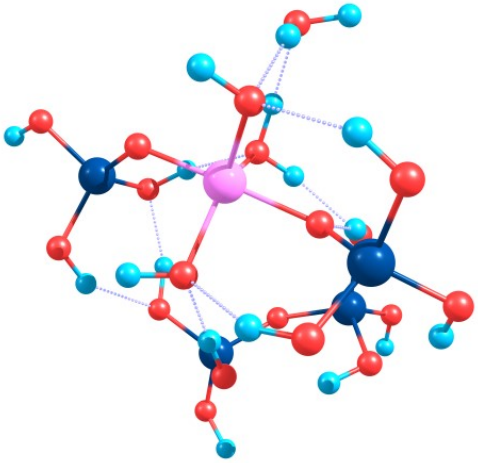
42

O	0.054317	-0.253287	-1.48027
O	-2.241529	1.453492	-1.034597
O	-1.31308	-0.189657	1.31437
O	0.064202	1.981727	0.880993
O	0.232349	4.586964	1.493553
O	1.530154	3.699937	-0.658565
O	-1.150111	3.741249	-0.667277
O	4.48627	1.120183	-0.020106
O	3.206276	-1.187197	-0.369155
O	2.277819	1.128366	-1.369621
O	2.154074	0.600958	1.290476
O	1.265392	-2.724474	-1.168416
O	3.772685	-3.68686	-0.626229
O	2.141787	-3.008775	1.36872
H	1.863877	2.876544	-1.064886
H	-0.851878	0.613964	1.619032
H	-1.011356	4.288356	-1.447639
H	1.394353	0.699889	-1.541863
H	1.318596	1.175048	1.181124
H	3.649846	-4.622173	-0.438596
H	1.20213	-2.820713	1.631508
H	0.421268	-1.153303	-1.524681
H	-1.913195	2.395141	-0.900613
Si	3.004829	0.415344	-0.07791
H	-3.216754	1.374819	-0.962
H	4.979225	1.030832	0.800686
Si	2.57748	-2.668817	-0.156068
H	0.697549	-3.501226	-1.128287
O	-5.054584	-2.410652	-0.487071
H	-5.297861	-2.498963	-1.413611
O	-2.608304	-1.231756	-0.844615
O	-4.661198	0.295064	-0.544483
H	-5.434267	0.626004	-0.07619
O	-3.873999	-1.291993	1.53468
H	-3.019622	-0.902123	1.802684
O	-0.364247	-2.571325	2.036745
H	-0.951168	-3.151929	1.540264
H	-0.68389	-1.655549	1.840152
Si	-4.035272	-1.188788	-0.096714
H	0.312547	5.505971	1.221514
Si	0.209625	3.444812	0.298026
Al	-1.338373	-0.05631	-0.451872

Frequencies --	-99.3800	22.5648	29.9862
Frequencies --	32.5386	42.6769	47.8927
Frequencies --	51.6409	56.9010	66.6368

Zero-point correction=	0.273861 (Hartree/Particle)
Thermal correction to Energy=	0.308419
Thermal correction to Enthalpy=	0.309363
Thermal correction to Gibbs Free Energy=	0.207901
Sum of electronic and zero-point Energies=	-2841.723523
Sum of electronic and thermal Energies=	-2841.688964
Sum of electronic and thermal Enthalpies=	-2841.688020
Sum of electronic and thermal Free Energies=	-2841.789482

Switch-4-INTc-CAMhighB.log



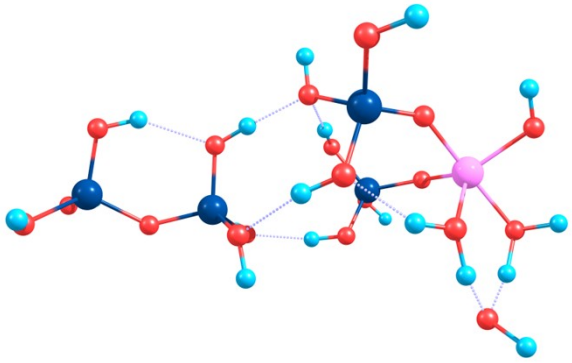
42

O	-3.170127	-0.746874	-0.184699
O	-1.758274	0.078849	1.941306
O	-3.480611	-1.839346	2.282935
O	-1.280009	-2.343135	0.822071
O	-1.021348	-4.234292	-1.099709
O	-0.882589	-1.629468	-1.689882
O	1.078888	-2.947502	-0.297657
O	1.166648	3.167588	-0.137601
O	2.748841	0.942856	-0.109002
O	0.69199	0.438282	-1.697036
O	0.942572	0.700258	1.766182
O	2.697228	-1.382587	1.203293
O	3.274752	-1.438725	-1.364661
O	5.039984	-0.294973	0.25599
H	-0.286369	-0.820973	-1.721277
H	-3.852609	-2.707662	2.099953
H	1.516864	-2.480282	0.444277
H	1.50347	0.181236	-2.146806
H	1.170041	1.514373	2.301561
H	2.521203	-2.048114	-1.339475
H	5.590268	-1.081685	0.1959
H	-2.64375	-0.929648	-0.982117
H	-1.525432	0.769435	1.244331
Si	-0.519294	-2.76947	-0.575945
H	-1.840951	-4.275127	-1.601498
H	2.015992	3.48355	-0.459168
Si	-2.417999	-1.225417	1.210005
Si	3.431786	-0.498479	-0.015237
H	2.172836	-0.799543	1.777158
O	-1.47098	3.940146	-0.828289
H	-0.525173	4.024454	-0.59698
O	-0.849632	1.501065	0.062155
O	-3.388127	2.146901	-0.573253
H	-3.618864	1.213766	-0.438506
O	-1.54225	1.786912	-2.496362
H	-0.714515	1.265129	-2.520462
H	0.067452	0.388911	2.075729
O	1.446921	3.135426	2.587316
H	0.701183	3.529891	3.053906
H	1.341818	3.402504	1.645438
Si	-1.800532	2.329889	-0.957695

Frequencies --	34.5540	42.7975	45.7332
Frequencies --	48.7962	53.8515	55.2022
Frequencies --	69.1654	77.1472	91.4873

Zero-point correction=	0.277635 (Hartree/Particle)
Thermal correction to Energy=	0.311263
Thermal correction to Enthalpy=	0.312207
Thermal correction to Gibbs Free Energy=	0.215232
Sum of electronic and zero-point Energies=	-2841.745673
Sum of electronic and thermal Energies=	-2841.712045
Sum of electronic and thermal Enthalpies=	-2841.711100
Sum of electronic and thermal Free Energies=	-2841.808075

Switch-4-TS2-CAMhighB.log



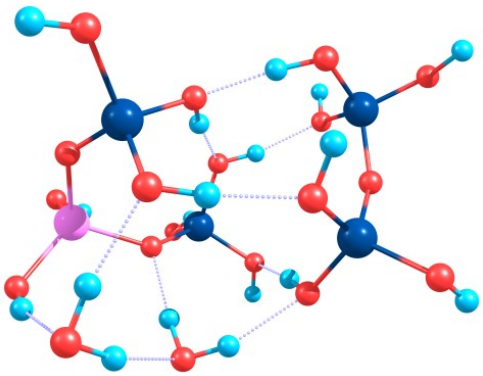
42

O	-5.071054	1.153499	-0.97823
O	-6.210875	0.720565	1.439125
O	-6.520135	-1.071934	-0.334942
O	-4.042567	-0.691897	0.627343
O	-1.754839	-1.995539	0.167836
O	-2.347698	0.462281	-0.962746
O	-1.638708	0.217188	1.559415
O	5.263594	1.201906	-0.522911
O	3.176367	-1.09396	-0.88482
O	3.059664	0.499409	1.7387
O	5.094266	-0.893011	0.961937
O	1.918101	-3.284553	-1.803488
O	1.010545	-1.903378	0.368999
O	0.754275	-1.05365	-2.184589
H	-1.49167	0.903075	-1.16002
H	-6.227567	-1.709026	-0.993271
H	-1.482547	-0.277112	2.37214
H	3.320983	-0.278287	2.450901
H	0.053832	-2.073154	0.339297
H	0.510919	-0.135803	-1.985651
H	-4.134321	1.162232	-1.237452
Si	-2.451224	-0.51874	0.334239
H	-2.165626	-2.647353	-0.410426
Si	-5.44233	0.045602	0.168012
Si	1.756226	-1.792479	-1.102897
H	2.603929	-3.843081	-1.427144
O	0.041113	1.592462	-1.459296
H	-0.017788	2.08993	-2.284335
O	2.640475	1.571781	-0.629183
O	1.101972	3.792989	-0.52586
H	1.907046	4.280255	-0.327057
O	0.653123	1.668084	1.114738
H	2.136559	0.808931	1.769002
H	-0.220053	1.251075	1.235946
H	5.923434	-0.424198	1.098375
H	4.987604	2.016947	-0.94808
H	-5.802903	1.487382	1.851633
O	3.953948	-1.336424	3.027626
H	4.673056	-1.195607	1.985215
H	4.460903	-1.017938	3.780903

Frequencies --	-786.7007	13.7601	19.5438
Frequencies --	27.5185	33.4122	40.0155
Frequencies --	42.7715	46.8714	54.1336

Zero-point correction=	0.268006 (Hartree/Particle)
Thermal correction to Energy=	0.303579
Thermal correction to Enthalpy=	0.304523
Thermal correction to Gibbs Free Energy=	0.198800
Sum of electronic and zero-point Energies=	-2841.714113
Sum of electronic and thermal Energies=	-2841.678541
Sum of electronic and thermal Enthalpies=	-2841.677597
Sum of electronic and thermal Free Energies=	-2841.783319

Switch-4-PRD1-CAMhighB.log



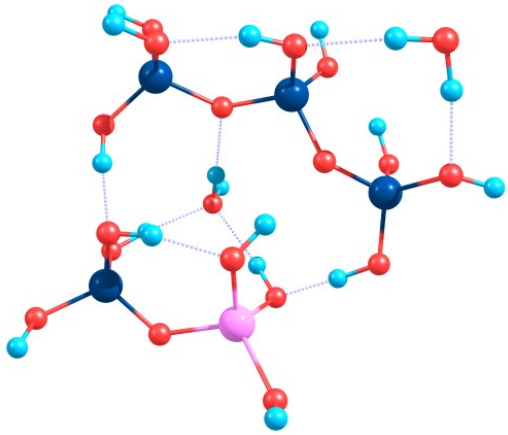
42

O	-1.19944	-0.031681	2.415532
O	-1.655941	-2.021722	0.701874
O	-3.423197	-1.526212	2.574641
O	-3.089542	0.24702	0.564971
O	-2.742555	-0.686516	-1.920989
O	-4.971874	0.640873	-1.336061
O	-2.701009	1.992786	-1.301234
O	1.541385	-0.354786	2.994563
O	1.902722	0.961486	0.588383
O	4.034733	1.638937	-1.184963
O	4.403824	-0.509143	0.738589
O	-0.187812	2.333001	1.587396
O	1.822797	3.554827	0.208347
O	0.00207	1.929442	-1.000691
H	-5.476029	-0.169665	-1.458682
H	-3.918037	-0.970552	3.185156
H	-2.923962	2.429091	-2.131544
H	3.77394	2.499192	-0.844401
H	1.394054	4.360025	-0.098693
H	-0.95317	2.143943	-1.018972
H	-0.921682	0.858034	2.101254
Si	-3.377022	0.511874	-1.021772
H	-1.759425	-0.752645	-1.964361
Si	-2.355661	-0.806523	1.571424
Si	0.909625	2.194949	0.346667
H	0.09679	2.812469	2.373794
O	-0.069862	-0.594969	-1.933014
H	0.05492	0.33948	-1.656192
O	2.588297	-0.844009	-1.503884
O	0.895497	-2.404584	-0.173879
H	2.169213	-2.621274	1.127355
O	1.134553	-2.679459	-2.853111
H	1.6995	-3.454928	-2.790713
H	0.001669	-2.292217	0.206164
H	1.734002	0.172821	2.194363
H	0.5783	-0.467888	2.954868
O	2.769549	-2.542186	1.890869
H	2.339798	-1.841991	2.424524
H	4.008596	-1.275172	1.184931
H	-2.177636	-2.385908	-0.023479
Al	3.287518	0.2921	-0.339795
Si	1.187905	-1.614941	-1.596801

Frequencies --	30.0090	44.4743	47.5511
Frequencies --	54.0265	56.7613	58.4027
Frequencies --	62.0592	66.3373	71.8763

Zero-point correction=	0.274904 (Hartree/Particle)
Thermal correction to Energy=	0.310785
Thermal correction to Enthalpy=	0.311730
Thermal correction to Gibbs Free Energy=	0.209236
Sum of electronic and zero-point Energies=	-2841.747450
Sum of electronic and thermal Energies=	-2841.711569
Sum of electronic and thermal Enthalpies=	-2841.710625
Sum of electronic and thermal Free Energies=	-2841.813118

Switch-4-RCT2-CAMhighB.log



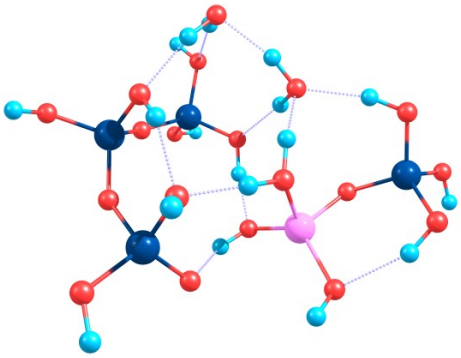
42

O	3.633887	0.457277	1.454843
O	2.755339	0.725458	-1.082053
O	5.311964	0.096884	-0.449324
O	3.282785	-1.701481	-0.164927
O	1.729349	-3.936827	-1.235283
O	0.846605	-2.623403	1.11382
O	0.852219	-1.100177	-1.380355
O	-4.860594	0.153267	-1.823044
O	-0.611312	1.737155	0.457507
O	-3.174924	1.199706	1.192915
O	-2.527927	1.723759	-1.388986
O	1.820233	2.873968	0.125126
O	-0.296241	3.311262	-1.544206
O	-0.253562	4.27191	1.021485
H	0.860262	-1.816669	1.654134
H	5.593048	-0.195176	-1.321197
H	-0.055838	-0.906229	-1.12078
H	-3.542764	2.064898	1.400199
H	0.154349	3.936548	-2.120206
H	0.250156	5.091878	1.037942
H	2.734966	0.377273	1.82975
H	1.960327	0.182926	-1.336945
H	1.70722	-3.936937	-2.194399
Si	3.735473	-0.160838	-0.061755
Si	0.224864	3.08734	0.006
H	2.21494	2.107787	-0.366189
O	-1.571773	-3.155906	0.536096
O	-1.811413	-0.548111	-0.123142
O	-3.75797	-2.189094	-0.648339
O	-3.178108	-1.554915	1.944236
H	-3.480448	-0.640811	2.047524
H	-4.080483	0.699884	-1.990023
H	-4.499453	-0.702483	-1.543394
H	-1.880765	2.3201	-1.806978
H	-4.372521	-2.910439	-0.478711
O	0.984408	0.031863	2.098244
H	0.66036	0.266626	2.975567
H	0.455876	0.564618	1.478713
H	-0.618435	-2.983902	0.84169
Si	-2.571634	-1.898028	0.458686
Si	-2.041124	1.059322	0.021933

Frequencies --	16.6159	21.5417	25.9530
Frequencies --	44.1111	50.2663	52.4183
Frequencies --	61.3186	66.2271	69.6764

Zero-point correction= 0.272776 (Hartree/Particle)
Thermal correction to Energy= 0.309422
Thermal correction to Enthalpy= 0.310366
Thermal correction to Gibbs Free Energy= 0.204328
Sum of electronic and zero-point Energies= -2841.736790
Sum of electronic and thermal Energies= -2841.700144
Sum of electronic and thermal Enthalpies= -2841.699200
Sum of electronic and thermal Free Energies= -2841.805238

Switch-4-TS3-CAMhighb.log



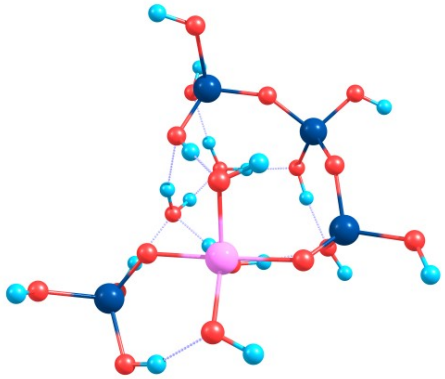
42

O	-3.908537	-1.194502	1.628224
O	-5.544024	-1.244581	-0.384916
O	-4.794925	1.147887	0.580492
O	-3.005571	-0.317062	-0.738621
O	-2.768542	2.45886	-0.931683
O	-1.135602	0.910655	0.880894
O	-0.597352	0.517233	-1.990939
O	1.074652	-2.444005	2.612413
O	2.7329	-1.192669	-0.658464
O	2.420315	-0.138471	1.798102
O	4.806207	-0.23102	0.512599
O	0.118395	-1.774653	-1.039561
O	2.151956	-2.865308	-2.52007
O	1.630139	-3.546024	0.06495
H	-0.3505	1.446646	1.171092
H	-4.24511	1.825406	0.142821
H	0.067473	1.245214	-1.917907
H	1.609599	-1.643328	2.45356
H	1.576039	-3.478938	-2.987401
H	2.386141	-4.143472	0.068172
H	-2.970078	-1.460007	1.669299
H	-5.984301	-0.851868	-1.144415
H	-2.327274	3.290046	-0.740422
Si	-4.285487	-0.389369	0.247417
Si	1.643876	-2.334564	-1.056925
H	-0.086371	-0.886244	-1.476905
O	0.612533	2.706269	-1.200174
O	2.848793	1.449799	-0.281678
O	2.603743	4.019656	0.166612
O	1.062087	2.23235	1.431717
H	1.868004	0.643408	1.989169
H	-0.443053	-1.932553	2.008134
H	1.299535	-3.014845	1.857317
H	5.278167	0.361109	1.106365
H	2.2247	4.823485	-0.20059
O	-1.174894	-1.61082	1.424729
H	-0.886722	-1.860967	0.523871
H	-1.075933	-0.02668	1.240836
Si	1.717965	2.650186	-0.092733
Si	3.19691	-0.005631	0.347716

Frequencies --	-44.5494	24.7724	40.7080
Frequencies --	44.5853	47.3825	61.4808
Frequencies --	63.7183	68.2469	83.6329

Zero-point correction= 0.276064 (Hartree/Particle)
Thermal correction to Energy= 0.310017
Thermal correction to Enthalpy= 0.310961
Thermal correction to Gibbs Free Energy= 0.212993
Sum of electronic and zero-point Energies= -2841.727046
Sum of electronic and thermal Energies= -2841.693093
Sum of electronic and thermal Enthalpies= -2841.692149
Sum of electronic and thermal Free Energies= -2841.790118

Switch-4-INT2-CAMhighb.log



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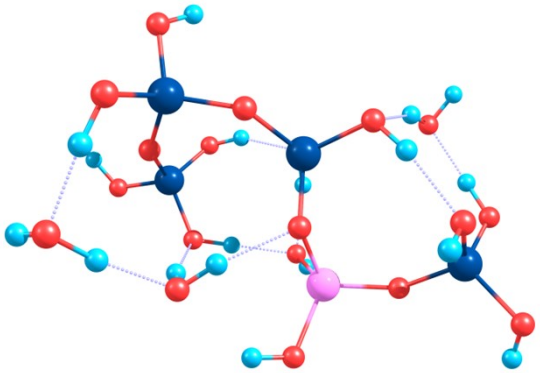
O	-3.766991	-1.237584	1.639657
O	-4.935248	-1.688859	-0.636629
O	-4.764278	0.849036	0.262841
O	-2.56124	-0.368407	-0.621189
O	-2.880359	2.209857	-1.073786
O	-1.122486	0.840807	1.154985
O	-0.409959	0.220632	-1.885337
O	1.372499	-2.214829	2.744062
O	2.681665	-1.086652	-0.697017
O	2.552338	0.111839	1.691155
O	4.624551	0.455943	-0.049018
O	0.160003	-2.01665	-0.86562
O	2.246484	-3.002524	-2.35347
O	1.948899	-3.485466	0.303722
H	-0.412521	1.348397	1.589885
H	-4.217505	1.537368	-0.188452
H	0.402735	0.694144	-2.084658
H	1.833685	-1.393952	2.491083
H	1.728742	-3.720006	-2.732442
H	2.770925	-3.987757	0.302376
H	-2.855114	-1.544456	1.789401
H	-5.146431	-1.475492	-1.550123
H	-2.636001	3.135394	-0.997422
Si	-3.956642	-0.588646	0.131389
Si	1.734534	-2.397215	-0.919641
H	-0.100981	-1.127856	-1.318101
O	-0.29095	2.563894	-0.652104
O	2.203016	1.547899	-0.514027
O	1.873287	4.161781	-0.297698
O	1.094749	2.428844	1.644074
H	2.070506	0.891108	2.026637
H	-0.243543	-1.9302	2.179555
H	1.620485	-2.833769	2.035203
H	5.031157	1.223228	0.365668
H	1.294248	4.886676	-0.552427
O	-1.035315	-1.72167	1.629079
H	-0.762222	-1.947434	0.715888
H	-1.088219	-0.116873	1.441515
Si	1.15177	2.718001	-0.01648
Si	3.009197	0.274906	0.11458

Frequencies --	34.9003	40.7319	45.1474
Frequencies --	49.4853	61.2069	63.5846
Frequencies --	70.3486	75.7855	89.2960

Zero-point correction= 0.277407 (Hartree/Particle)
Thermal correction to Energy= 0.311674
Thermal correction to Enthalpy= 0.312618
Thermal correction to Gibbs Free Energy= 0.214595
Sum of electronic and zero-point Energies= -2841.748299
Sum of electronic and thermal Energies= -2841.714032
Sum of electronic and thermal Enthalpies= -2841.713088
Sum of electronic and thermal Free Energies= -2841.811111

Switch-4-PRD2-CAMhighb.log



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O	3.515673	-2.746434	0.50136
O	3.357523	-1.003702	2.429334
O	3.133622	-0.121379	-0.062536
O	4.311547	1.236153	-2.041309
O	2.41156	-0.563763	-2.604724
O	0.011935	-1.142914	-1.371261
O	-2.892401	-2.731263	-1.620447
O	-3.236649	1.168365	-0.33221
O	-0.752485	1.416398	-1.8262
O	-1.373377	3.205007	0.473691
O	-4.787673	-1.008087	-0.773788
O	-3.577794	-0.748776	1.546313
O	-5.593968	0.870867	0.916215
H	1.59726	-1.018747	-2.321456
H	3.436911	-0.0397	2.650384
H	2.716475	1.921867	2.351568
H	-1.135477	1.812298	-2.613791
H	-3.295606	-0.232744	2.309773
H	-5.816737	1.716098	0.514905
Si	2.912968	0.565057	-1.530992
H	5.114003	0.713055	-1.952567
Si	2.787179	-1.35216	0.955583
Si	-4.273604	0.111495	0.294126
H	-4.117797	-1.632328	-1.137788
O	-0.631388	0.409051	0.703293
O	1.336871	2.289038	1.360149
O	1.165601	-1.593452	0.961855
O	-1.401102	-2.169453	0.676787
H	-2.181806	-1.763424	1.111692
H	-3.24706	-3.625675	-1.670293
H	-2.304587	-2.725812	-0.841687
H	-0.508658	3.356381	0.871057
H	3.058791	-3.286143	-0.150691
O	3.500177	1.601867	2.854656
H	4.262475	1.928169	2.363728
H	1.649724	2.25009	0.436694
O	1.857508	1.808453	-1.377826
H	0.918265	1.690551	-1.6726
H	-0.371831	-0.348839	-1.805608
Si	-0.223429	-1.091752	0.270984

Frequencies --	23.3708	29.4132	38.5859
Frequencies --	40.6683	50.8224	58.4387
Frequencies --	68.6466	71.7474	78.9716

Zero-point correction= 0.276158 (Hartree/Particle)
Thermal correction to Energy= 0.311740
Thermal correction to Enthalpy= 0.312684
Thermal correction to Gibbs Free Energy= 0.210215
Sum of electronic and zero-point Energies= -2841.759798
Sum of electronic and thermal Energies= -2841.724216
Sum of electronic and thermal Enthalpies= -2841.723272
Sum of electronic and thermal Free Energies= -2841.825741