

Supporting Information

Theoretical Characterizations of the Mechanism for the Dimerization of Monosilicic Acid in Basic Solution

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Figure S1. The geometries of the prereactive hydrogen bond complexes (RC) formed between $\text{Si}(\text{OH})_4$ and $\text{Si}(\text{OH})_3\text{O}^-$.

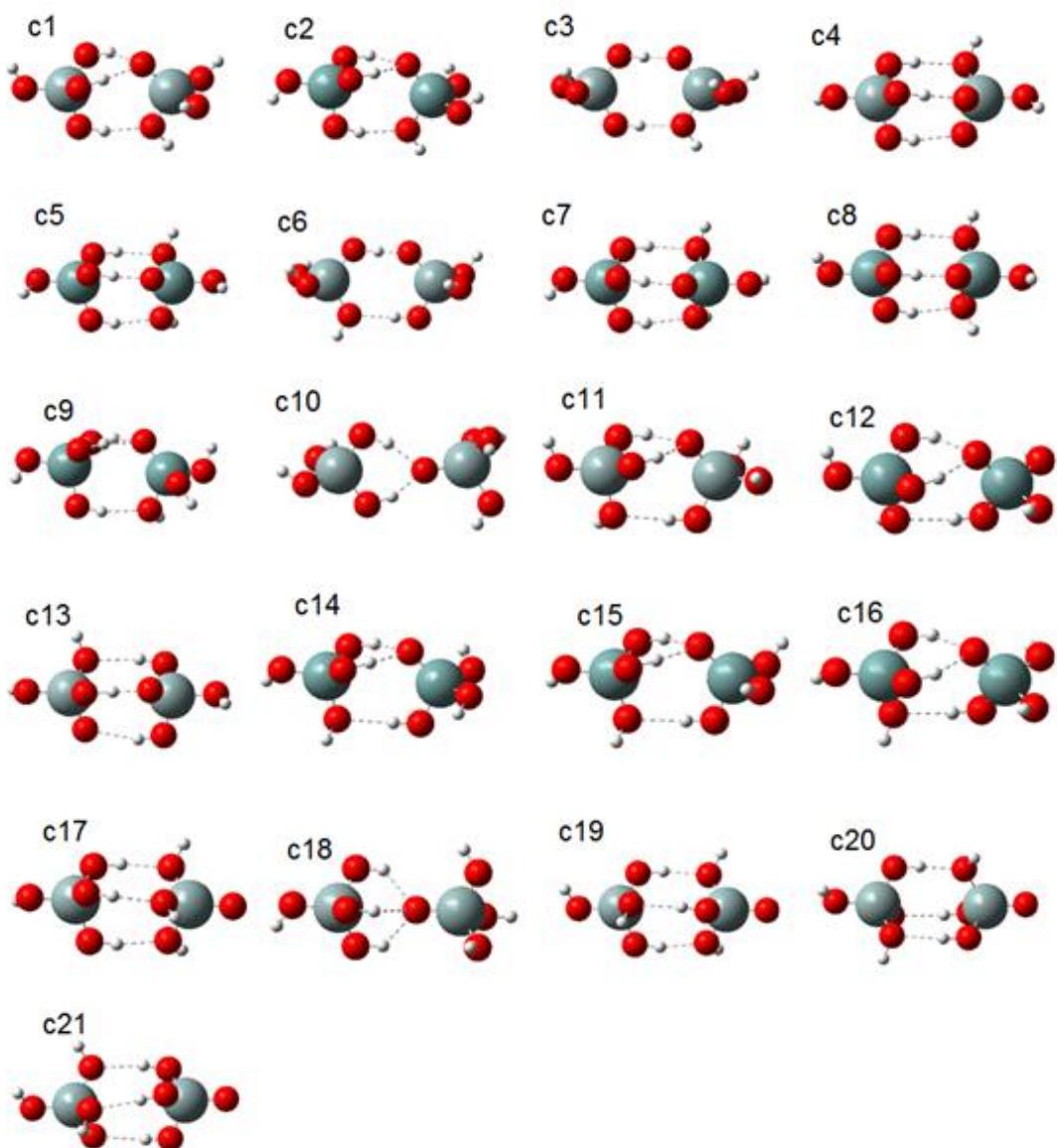


Figure S2. The geometries of the transition state (TS1) for the Si-O bond association path.

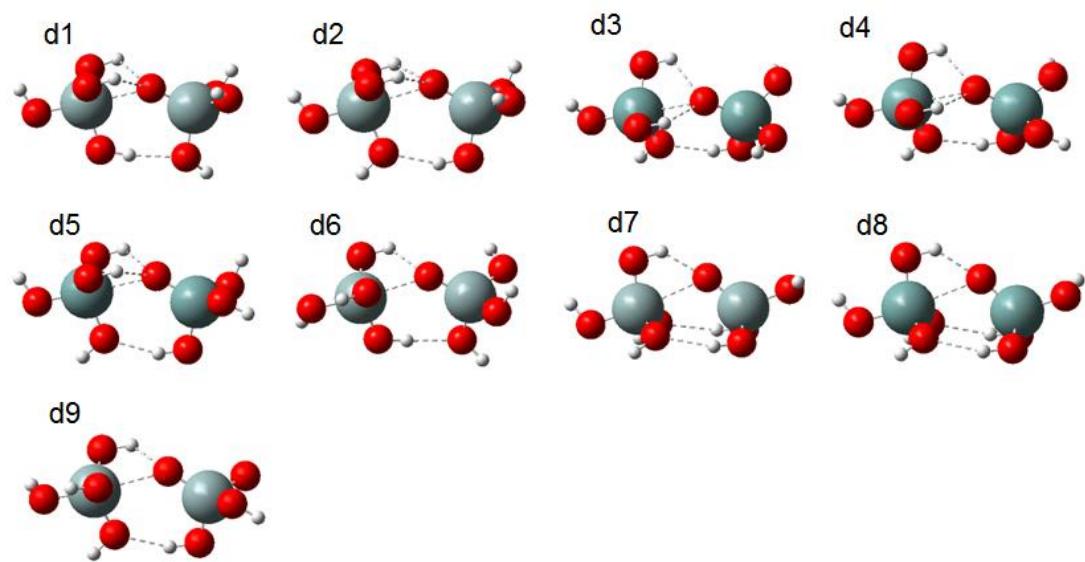


Figure S3. The geometries of the intermediates (IM1) with three OH groups equatorially bound to the five-coordinated silicon atom.

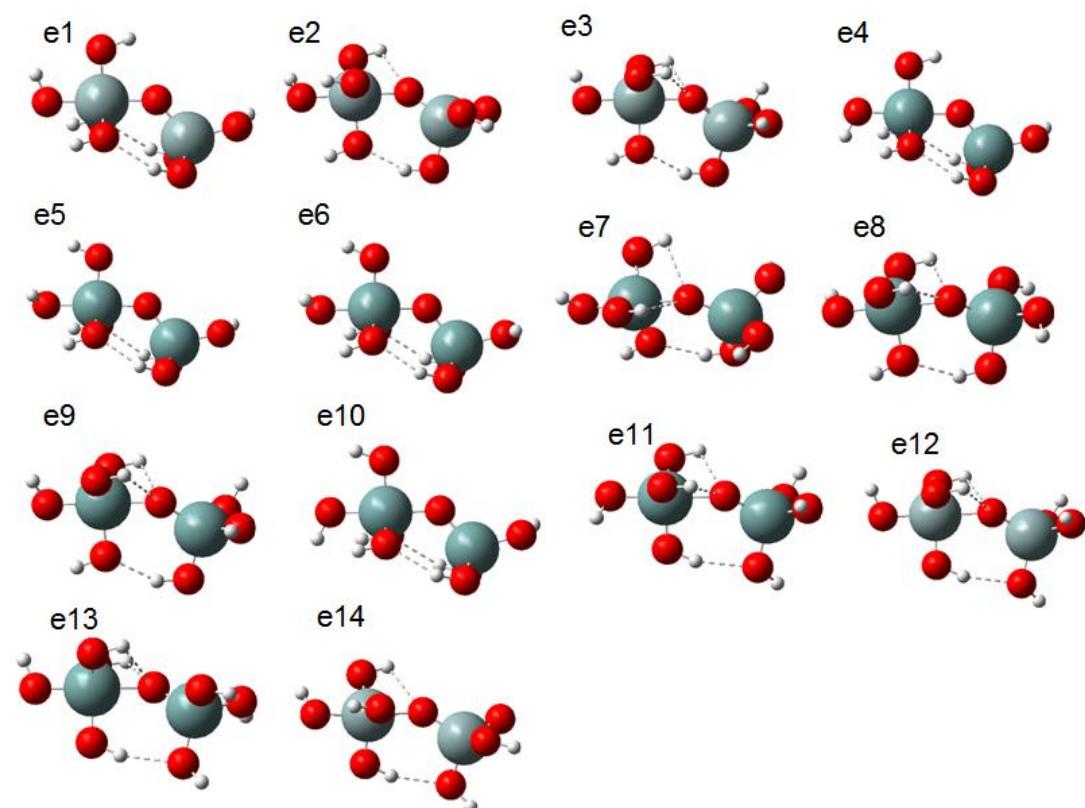


Figure S4. The geometries of the transition state (TS-iso) for the isomerization of IM1.

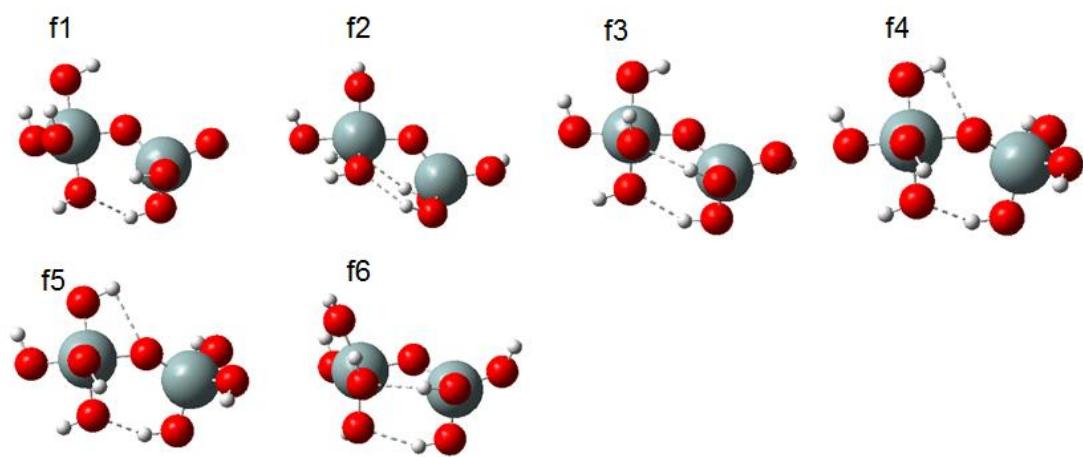


Figure S5. The geometries of the intermediate (IM2) with two nearly collinear SiOH bonds and the bridge oxygen atom in the apical position.

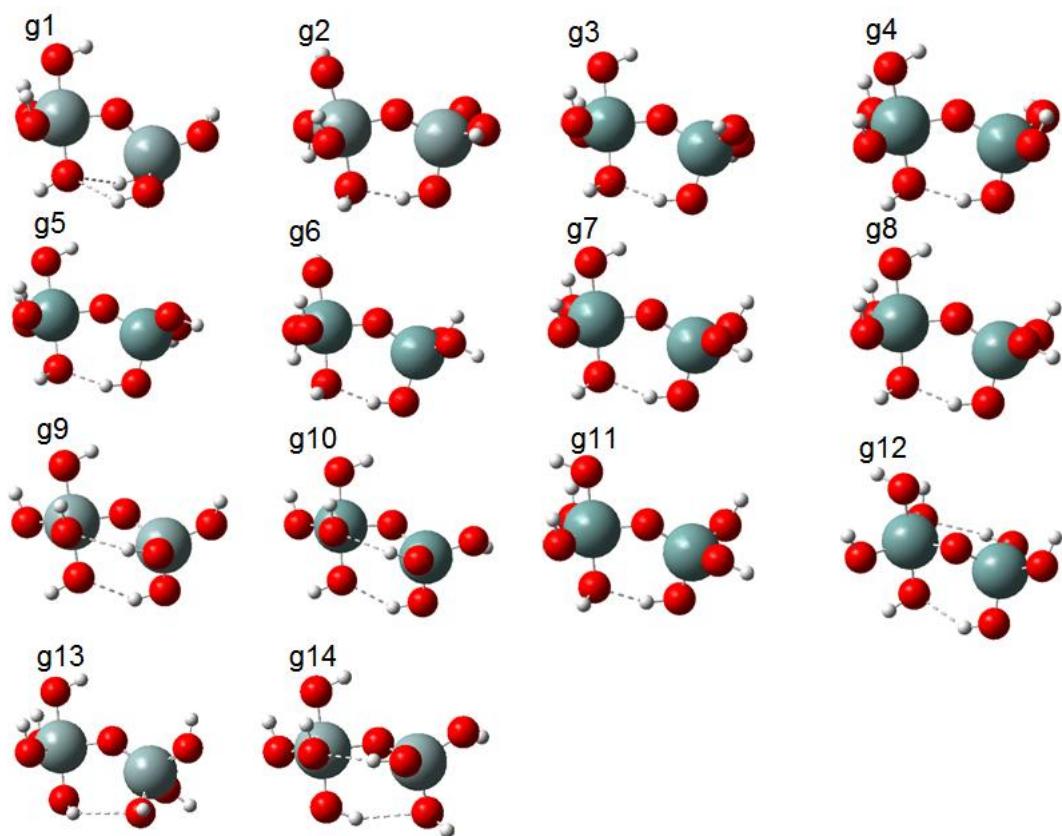


Figure S6. The geometries of the 4-center transition state (TS2) connected to IM1 for water cleavage.

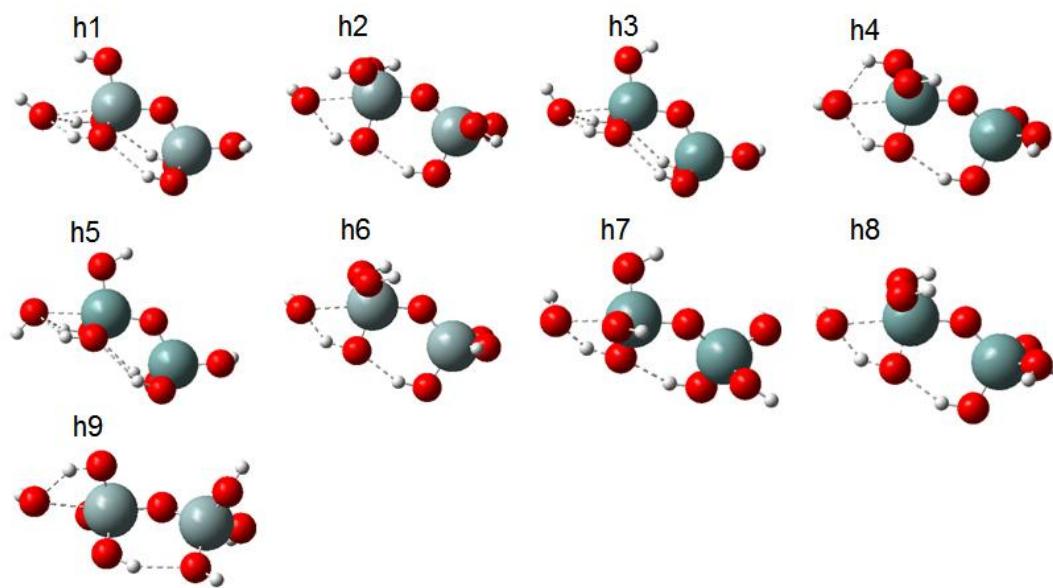


Figure S7. The geometries of the 4-center transition state (TS3) connected to IM2 for water cleavage.

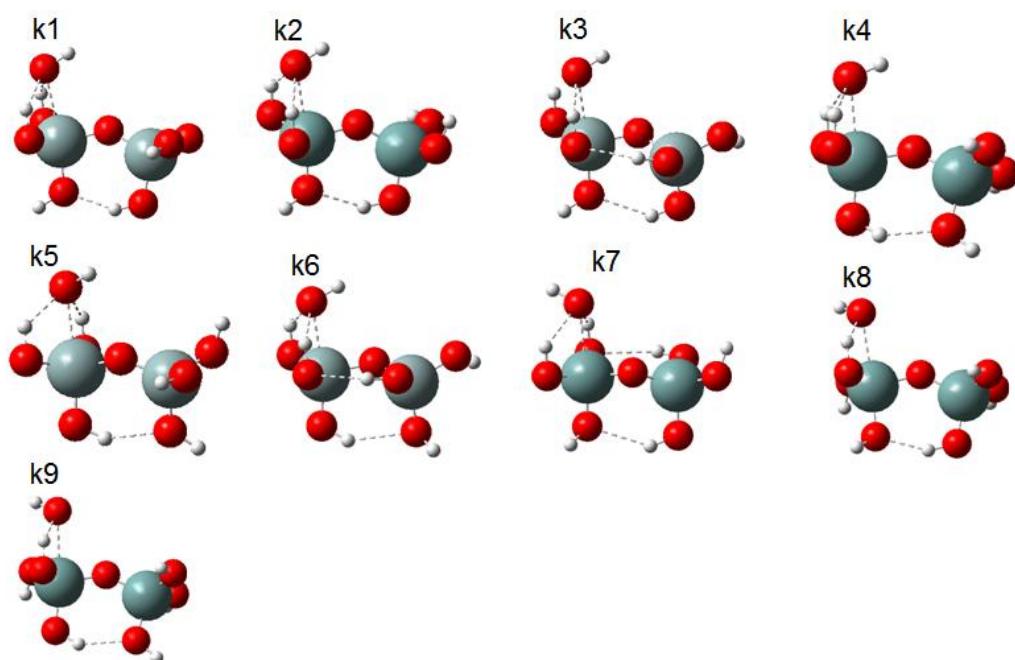


Figure S8. The geometries of the 6-center transition state (TS4) connected to IM2 for water cleavage.

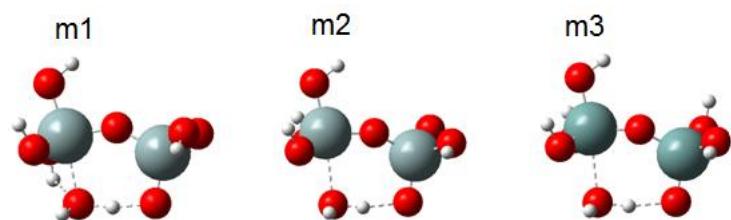


Figure S9. The geometries of the product complexes (PC-1).

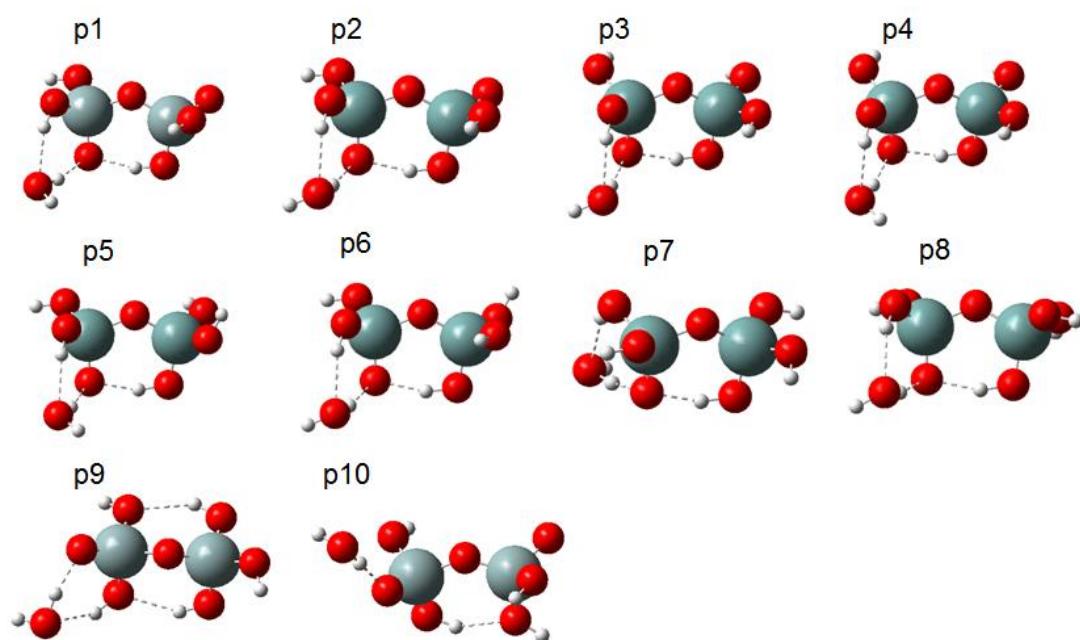


Figure S10. The geometries of the product complexes (PC-2).

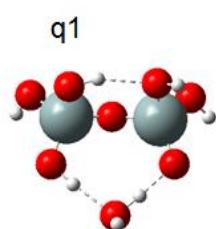


Figure S11. The geometries of the prereactive hydrogen bond complexes (RC-w) formed between $\text{Si}(\text{OH})_4$ and $\text{Si}(\text{OH})_3\text{O}^-$ in the presence of one additional water molecule as shown in tube models.

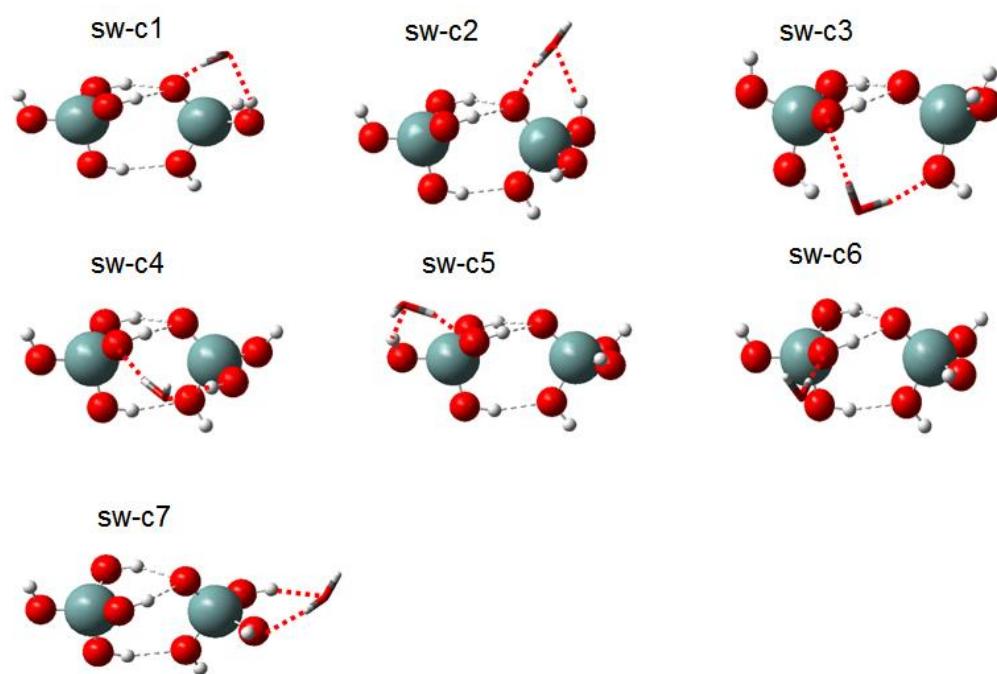


Figure S12. The geometries of the transition state (TS1-w) for the Si-O bond association path in the presence of one additional water molecule as shown in tube models.

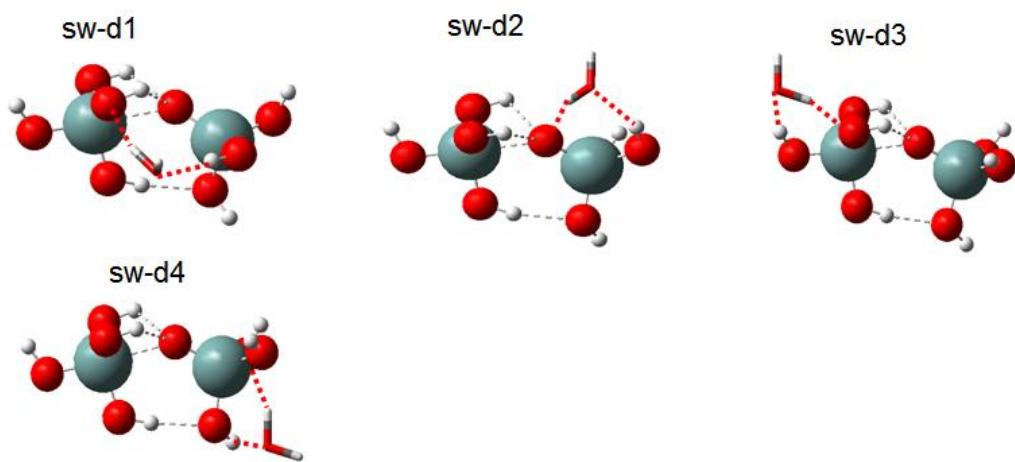


Figure S13. The geometries of the intermediates (IM1-w) with three OH groups equatorially bound to the five-coordinated silicon atom in the presence of one additional water molecule as shown in tube models.

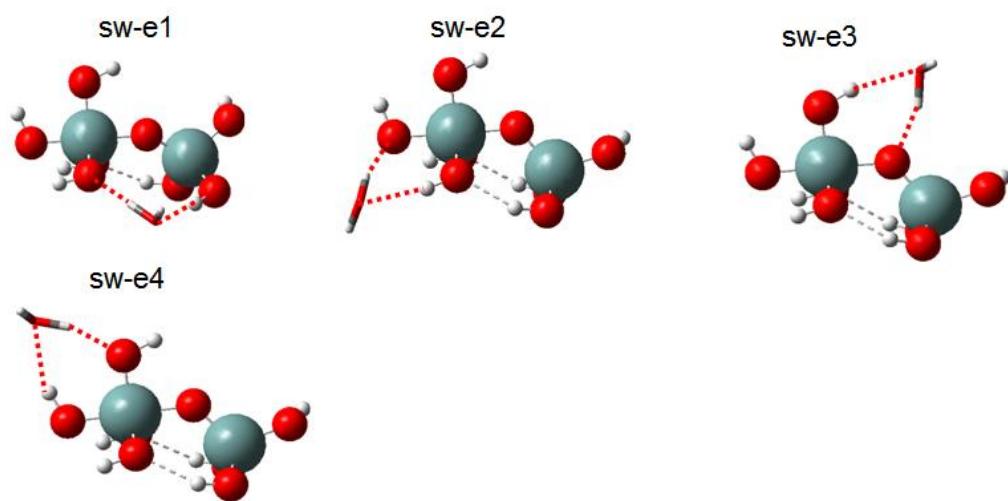


Figure S14. The geometries of the transition state (TS-iso-w) for the isomerization of IM1-w in the presence of one additional water molecule as shown in tube models.

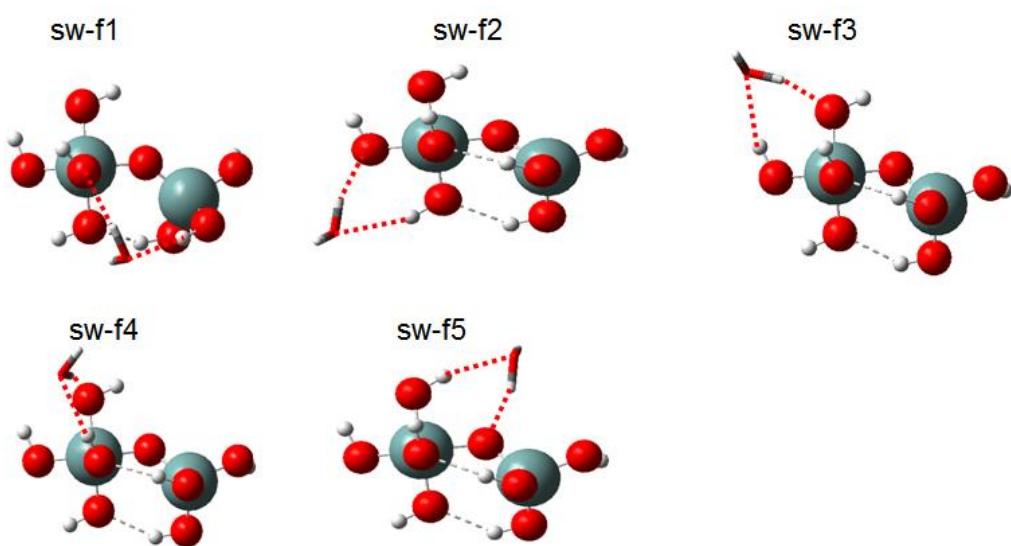


Figure S15. The geometries of the intermediate (IM2-w) with two nearly collinear SiOH bonds and the bridge oxygen atom in the apical position in the presence of one additional water molecule as shown in tube models.

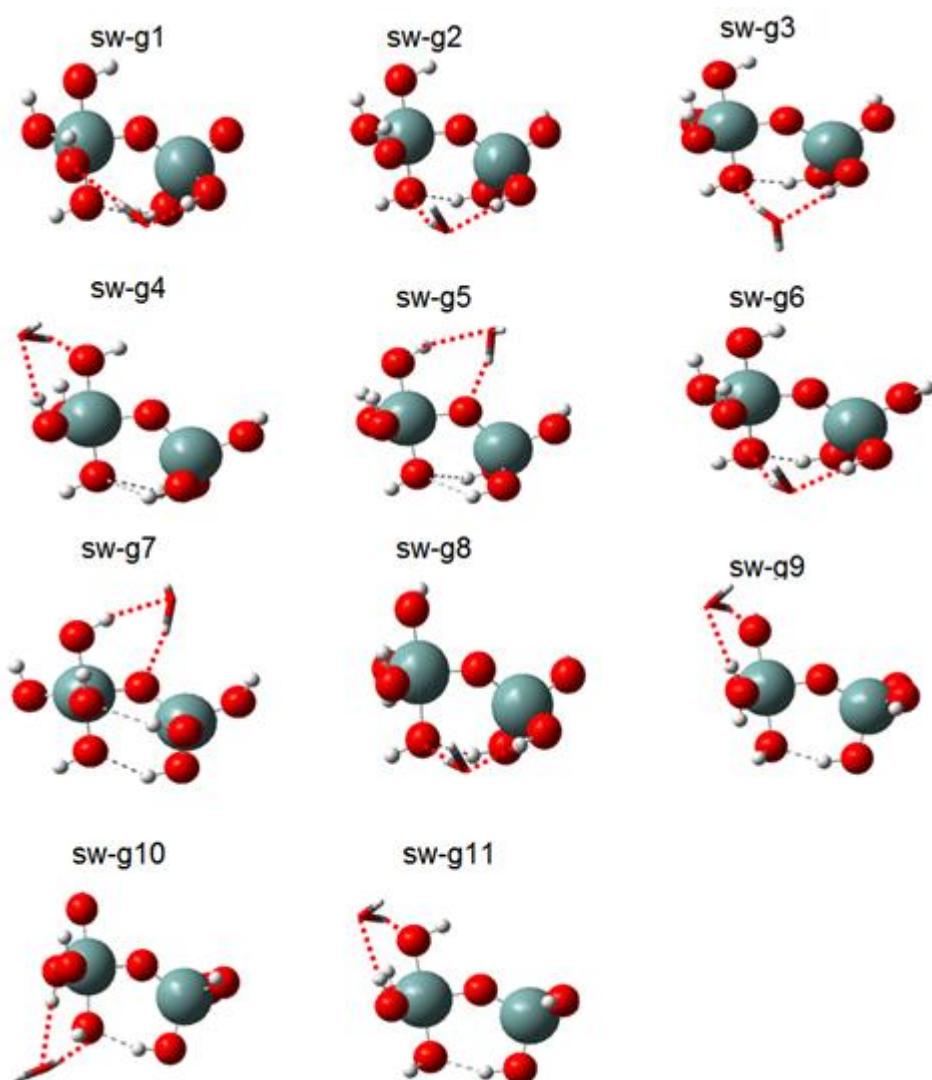


Figure S16. The geometries of the 4-center transition state (TS2-cw and TS2-sw) connected to IM1-w for water cleavage.

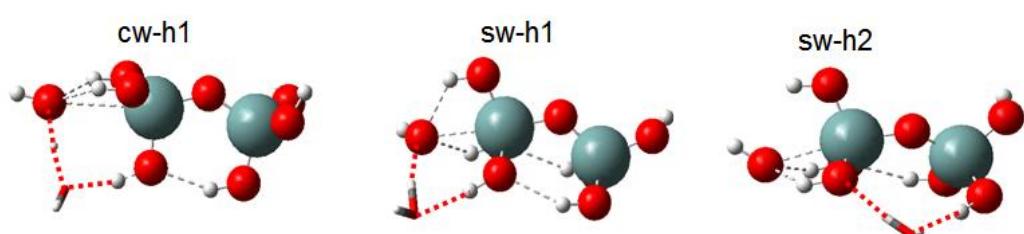


Figure S17. The geometries of the 4-center transition state (TS3-cw and TS3-sw) connected to IM2-w for water cleavage.

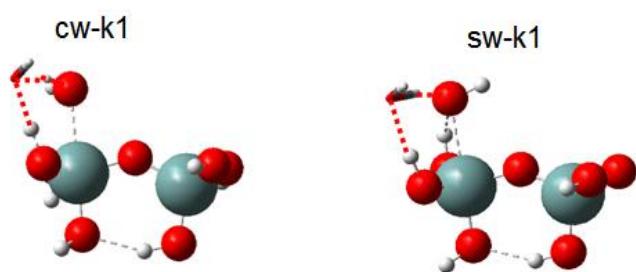


Figure S18. The geometries of the 6-center transition state (TS4-cw and TS4-sw) connected to IM2-w for water cleavage.

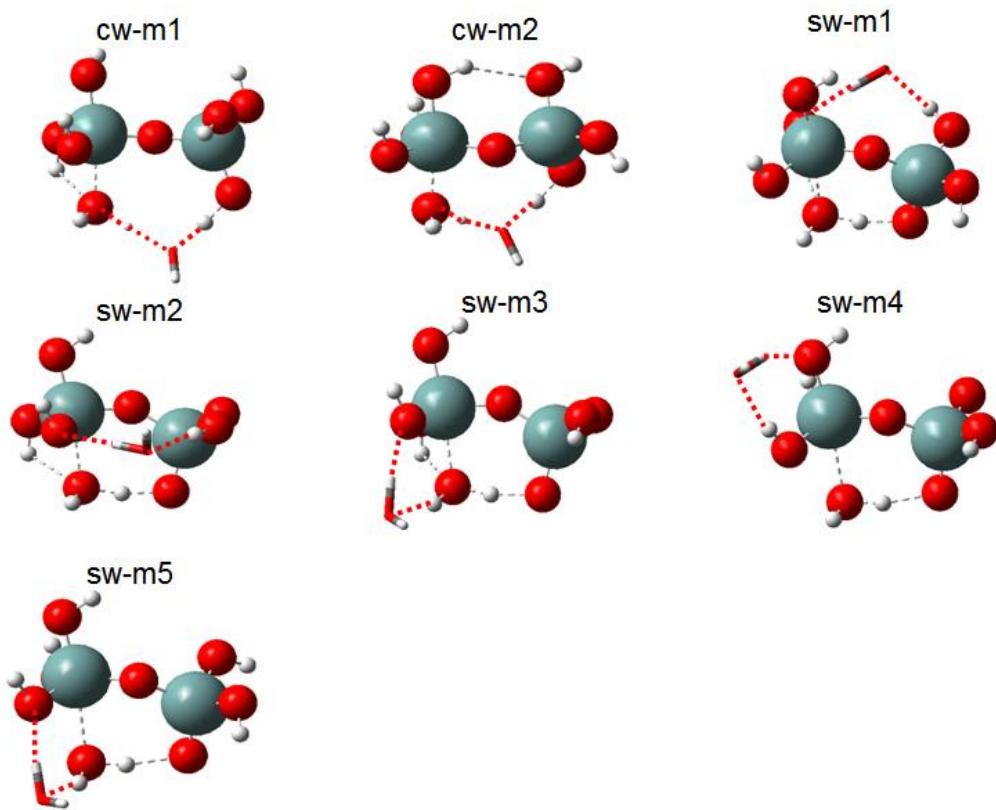


Figure S19. The geometries of the procut complexes (PC1-cw, PC1-sw, PC2-cw, and PC2-cw) formed via the 4-center water cleavage paths.

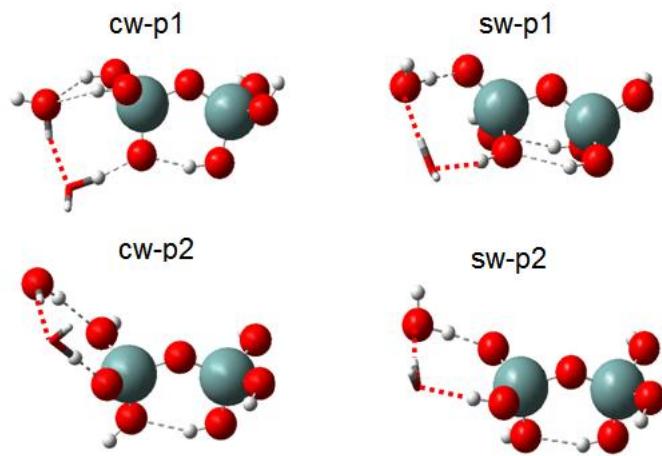


Figure S20. The geometries of the procut complexes (PC3-cw and PC3-sw) formed via the t-center water cleavage paths.

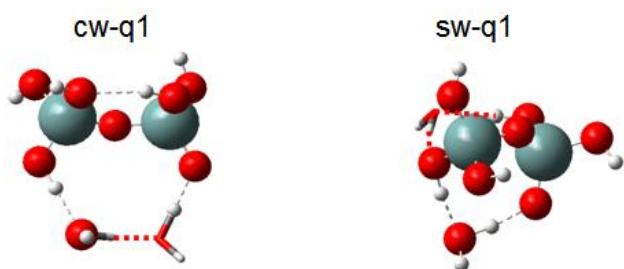


Table S1. The CAM-B3LYP/6-311++G(2d,2p)-PCM optimized Cartesian coordinates (in Ångstroms) for all the stationary points involved in the silica dimerization reaction. Total energies (HF, in Hartrees) and zero-point energies (ZPE, in Hartrees) are listed following the labels of the species.

c1: HF=-1185.6942105,ZeroPoint=0.1071672

Si,0,1.9182192422,-0.0446945181,-0.0495312725
O,0,1.1211535037,-1.423684822,-0.560643429
H,0,1.6768831069,-2.1576793472,-0.8309769059
O,0,0.8651052087,1.0361895963,0.3872167052
O,0,2.9972231949,-0.4718221235,1.137544281
H,0,2.6613414777,-0.3992002516,2.0327194115
H,0,-0.520601877,0.5456431416,1.3563887383
O,0,2.8872185618,0.3102559325,-1.3443206676
H,0,3.5523399806,0.984818586,-1.196917982
Si,0,-2.0366647166,0.0172562208,-0.0556758345
O,0,-3.6712489439,0.0406745281,-0.0677137839
H,0,-4.0942724771,0.8420681363,0.2450892989
O,0,-1.6867351932,-1.4675606198,-0.6484377615
O,0,-1.4175335331,1.2111933707,-0.9902431968
H,0,-0.4924303299,1.3615696363,-0.670602285
O,0,-1.4499366577,0.2230571843,1.4599987128
H,0,-0.725964578,-1.6218958506,-0.6881532991

c2: HF=-1185.6937649,ZeroPoint=0.1068376

Si,0,2.1424890572,0.1440564057,-0.0156211972
O,0,1.7642701917,-1.0955969572,-1.0198760627
H,0,0.8017114226,-1.2162134604,-1.1107867316
O,0,1.5962768123,1.5817078441,-0.5734275421
O,0,1.5124230651,-0.0789732749,1.4789586989
H,0,0.5926963103,0.2838429018,1.4474238327
H,0,0.6638377712,1.664862373,-0.2532910698
O,0,3.7746849897,0.1977750696,0.0627532482
H,0,4.2478297805,-0.5383497205,-0.3280733589
Si,0,-1.8120089175,0.200912878,-0.1217828017
O,0,-2.9476700924,-0.4938933531,0.8700018167
H,0,-2.6438187051,-0.6837594438,1.7594116979
O,0,-1.0387029788,-1.0153861534,-0.9711251735
O,0,-2.719826292,0.9365659932,-1.2948789858
H,0,-3.3649352184,1.5749556526,-0.9858989517
O,0,-0.7440069202,1.0771445525,0.6259049478
H,0,-1.605472366,-1.6253407569,-1.4479735172

c3: HF=-1185.6933666,ZeroPoint=0.1055095

Si,0,-2.083268663,-0.4091273043,-0.3786977485
O,0,-0.9730346785,0.1346853838,-1.5057206702
H,0,-1.2784387308,0.2056444408,-2.4123218335
O,0,-2.6259316567,-1.813911889,-1.0711449184
O,0,-1.4044849293,-0.4937183836,1.0289151493
H,0,0.0344559214,-0.461913161,1.3617792093
H,0,-3.4046069719,-2.203635804,-0.670171664
O,0,-3.4172030286,0.5796111485,-0.435354765
H,0,-3.403167821,1.3015821134,0.195486544
Si,0,2.0310030992,0.4530624533,0.7037808877
O,0,2.051759136,2.0402156453,1.1433599171
H,0,2.147992868,2.2202790193,2.0802352034
O,0,1.6769324464,0.4330833552,-0.8873799256
O,0,3.5783109027,-0.0658707132,0.9073965554
H,0,3.7216897579,-1.010801393,0.8292670244
O,0,1.0389323584,-0.4462387222,1.597672772
H,0,0.7366543699,0.3378772706,-1.1343312474

c4: HF=-1185.6944597,ZeroPoint=0.1070654

Si,0,1.861933256,0.1405867645,-0.0181422037
O,0,1.3736229889,-0.7319491526,1.3223009073
H,0,1.7774890571,-1.5963207159,1.4300742025
O,0,1.4462282368,-0.913204678,-1.2514426494
O,0,1.1485199961,1.5313816506,-0.0395628606
H,0,-0.3966553221,1.5839750613,-0.1554435383
H,0,1.7945399155,-0.6912495868,-2.1180686232
O,0,3.5146563731,0.1664976091,-0.0730954592
H,0,3.9222084175,0.9537970758,0.2925385823
Si,0,-1.9053071869,-0.0317586643,-0.005399712
O,0,-1.4438619478,-0.6372586568,1.4498831543
H,0,-0.4820641477,-0.7446643464,1.5521092059
O,0,-1.3933112615,-1.0290895649,-1.2061478863
O,0,-3.5400438771,0.0124444165,-0.0443240137
H,0,-4.0026257889,-0.8204772369,0.0603309077
O,0,-1.4083869224,1.4931872205,-0.2190297979
H,0,-0.4290243765,-1.0814645856,-1.3229383557

c5: HF=-1185.6943859,ZeroPoint=0.1070423

Si,0,-1.756862478,0.0782785817,0.1157953784
O,0,-1.1418664987,1.3779335443,-0.7374335813
H,0,-1.4556184687,1.4738626671,-1.6397649025
O,0,-1.3079742123,-1.1978532658,-0.8714079887
O,0,-1.1619254416,0.0655278224,1.5613872514

H,0,0.3707862809,-0.1191352931,1.697119003
H,0,-1.7385874212,-2.0346732976,-0.681888746
O,0,-3.406927058,0.0875522149,0.0041820871
H,0,-3.8637582265,0.4754171662,0.7528075108
Si,0,2.0135846199,-0.1314855387,0.1828574892
O,0,1.6717520018,1.324855021,-0.4959413185
H,0,0.7222659135,1.5003299754,-0.6164001688
O,0,1.5333375102,-1.3510760054,-0.8017004983
O,0,3.6402768171,-0.2997464424,0.2350505761
H,0,4.1181881677,0.275364668,0.8344995761
O,0,1.3803222155,-0.2477048577,1.670122823
H,0,0.5699368285,-1.4231489801,-0.9127162512

c6: HF=-1185.6910625,ZeroPoint=0.1040712

Si,0,2.1785761771,-0.0402658866,-0.0417560271
O,0,1.4717491077,0.4438285083,1.36810065
H,0,0.5020697322,0.4407647265,1.3631627004
O,0,3.0714109219,-1.3566063676,0.4383030842
O,0,1.1597409251,-0.2810981722,-1.2219252334
H,0,-0.1626295523,-0.5946598128,-1.076652344
H,0,3.6396511803,-1.7312237034,-0.2366864441
O,0,3.3532258271,1.073503859,-0.430120608
H,0,3.0481295303,1.7894666323,-0.9898927652
Si,0,-2.1893873585,-0.0346121487,-0.0420569017
O,0,-2.784659397,1.3796382973,-0.628630811
H,0,-3.4497733478,1.320383131,-1.3169226393
O,0,-1.352734289,0.413301547,1.3137379942
O,0,-3.5150050128,-0.933762871,0.3275116256
H,0,-3.3708445013,-1.8762648914,0.4317144892
O,0,-1.2035583753,-0.8550402609,-0.9855389773
H,0,-1.7951925677,1.010094413,1.9214532076

c7: HF=-1185.693669,ZeroPoint=0.1071349

Si,0,1.8829602976,0.087875669,0.0456235009
O,0,1.318657329,-0.7849749158,1.3551960633
H,0,1.6122457281,-1.6966960961,1.4213158075
O,0,1.4400148726,-0.9262956368,-1.21760018
O,0,1.2392951833,1.5103091006,0.0250952406
H,0,-0.2893206616,1.5968422987,-0.1737483181
H,0,1.7946310864,-0.6889049662,-2.0778409494
O,0,3.5341536328,0.1468487225,0.0732786355
H,0,3.9980767001,-0.6864084257,-0.0274308027
Si,0,-1.8904686551,0.0448924127,-0.0810357891
O,0,-1.5032717363,-0.5342736443,1.4071059974

H,0,-0.5489176557,-0.649083543,1.5555085835
O,0,-1.4061611363,-1.0027681628,-1.2453895979
O,0,-3.5210208057,0.045963798,-0.2179905745
H,0,-4.001432055,0.6834232344,0.3124438353
O,0,-1.2985312526,1.5368002291,-0.3021262624
H,0,-0.4415863117,-1.0711658543,-1.34906357

c8: HF=-1185.6929545,ZeroPoint=0.1066779

Si,0,1.8391776339,0.1894551696,-0.0098848155
O,0,1.323238359,-0.6869186677,1.3181680232
H,0,1.7090198782,-0.4139055326,2.1535160826
O,0,1.3871783414,-0.9180722135,-1.1807978452
O,0,1.1899695597,1.605074658,-0.1748444943
H,0,-0.3579079323,1.6492726446,-0.2138230421
H,0,1.6389492514,-0.6720095528,-2.0741173617
O,0,3.492805663,0.1980444196,0.0532218265
H,0,3.8850074118,1.0683760404,-0.0365812682
Si,0,-1.9406230409,0.0781427657,0.0263585982
O,0,-1.5187361747,-0.5354977655,1.4873776021
H,0,-0.5618886506,-0.6771139438,1.5835382769
O,0,-1.4610191814,-0.9432355627,-1.1678937103
O,0,-3.5760804085,0.0871570362,0.0631932716
H,0,-4.022573127,0.6011119343,-0.6112971058
O,0,-1.3743820649,1.5769808728,-0.2114899426
H,0,-0.4983538283,-1.0217151425,-1.2798331654

c9: HF=-1185.6926694,ZeroPoint=0.1068332

Si,0,1.7386096789,-0.1656002847,0.3848775347
O,0,2.1562923545,-1.4586232527,1.3312604428
H,0,2.7594230071,-2.0893553785,0.9336263164
O,0,1.2003401846,-0.840250494,-1.0545386856
O,0,0.6753296411,0.721394161,1.1246397579
H,0,-0.4764971651,1.5876881661,0.1343330495
H,0,1.6077943497,-0.4671204351,-1.8393392399
O,0,3.1127315264,0.622381844,-0.1093074422
H,0,3.3419683496,1.4032791745,0.3971674495
Si,0,-2.0961513871,0.2293764067,-0.1698670172
O,0,-1.8033700446,-0.2993914634,1.350558241
H,0,-0.87392904,-0.0384230157,1.5597102279
O,0,-1.6169339632,-0.8469586508,-1.3108250321
O,0,-3.7133943559,0.398539018,-0.337907432
H,0,-4.0906733034,0.1219821371,-1.1744408812
O,0,-1.3347728854,1.6667052023,-0.3534336191
H,0,-0.6487602273,-0.9469979646,-1.3505600105

c10: HF=-1185.6915214,ZeroPoint=0.1057282

Si,0,2.3567161467,0.0088386253,-0.1214851957
O,0,3.2320197009,-0.888004041,-1.1862328767
H,0,2.7651828879,-1.5981690568,-1.6307460257
O,0,1.379132232,1.0992148705,-0.8307004745
O,0,1.4283692841,-0.9529608867,0.8110404469
H,0,0.4822270607,-0.6357409246,0.7660619763
H,0,0.4429984491,0.9458565974,-0.5205084849
O,0,3.4981697302,0.8394991262,0.7149196681
H,0,4.3244077756,0.3838865149,0.88486451
Si,0,-2.338343534,0.0081561273,0.0583497835
O,0,-3.2569589452,-0.420419354,1.3711958129
H,0,-3.3431568782,0.2487047837,2.0523911605
O,0,-2.5191225517,-1.2805576293,-0.9684284778
O,0,-3.1516801402,1.3160026615,-0.5707144572
H,0,-2.6184594635,1.8950581212,-1.1179946152
O,0,-0.8168880882,0.2919010564,0.3333329984
H,0,-3.420443406,-1.4935111021,-1.2166236686

c11: HF=-1185.6924368,ZeroPoint=0.1072008

Si,0,2.0135678143,-0.2123814409,0.0008077512
O,0,1.482258956,-1.3852610255,-1.0355671447
H,0,1.6787265103,-2.2950064931,-0.7995933913
O,0,1.5183480841,1.2025894112,-0.6302679913
O,0,1.376055747,-0.3893478062,1.4918038735
H,0,0.4842018723,0.0484042036,1.4602199006
H,0,0.6011370284,1.3553285122,-0.2712913798
O,0,3.639408897,-0.3579865125,0.0458717963
H,0,4.1069743941,0.1487320642,0.7128320578
Si,0,-1.9288319328,0.1558090158,-0.0422874938
O,0,-2.8076795212,-0.8455989713,0.9479754793
H,0,-3.1870955124,-0.4252580711,1.7214993529
O,0,-1.4097816617,-0.8564834775,-1.243941964
O,0,-3.0906672924,1.1256768752,-0.729289319
H,0,-2.7548675891,1.9221364543,-1.1439229622
O,0,-0.7645656156,0.9535114574,0.6676819801
H,0,-0.4743934782,-1.0990930458,-1.2117332356

c12: HF=-1185.6920773,ZeroPoint=0.1068526

Si,0,2.0062470962,0.0204299871,0.0089068092
O,0,1.5797124702,-1.1175610204,-1.1110856469
H,0,1.919161348,-2.0060102914,-0.9791731299
O,0,1.3577470279,1.4215626911,-0.5040069403

O,0,1.4115653024,-0.3331606523,1.4856937165
H,0,0.4804484887,0.0176546148,1.4965873139
H,0,0.4416628921,1.4583939409,-0.1139498555
O,0,3.638938602,0.0378830073,0.0273155121
H,0,4.0653565847,0.5354428212,0.727884565
Si,0,-1.9815716497,0.041239959,0.0551638336
O,0,-3.1395710703,-0.687211449,0.9929041304
H,0,-2.8772084597,-1.5215128212,1.3847141091
O,0,-1.3703763171,-1.1920236572,-0.8714705426
O,0,-2.9391248966,0.997818339,-0.9073924865
H,0,-2.55531848,1.851174728,-1.1137822229
O,0,-0.8601053801,0.8566785425,0.8128878104
H,0,-0.4152345588,-1.1782497395,-1.0186669755

c13: HF=-1185.6899943,ZeroPoint=0.1051929

Si,0,1.836169292,0.0810662024,0.0272355155
O,0,1.4888158733,-0.4317668043,1.5725773254
H,0,0.5389324393,-0.4671989231,1.7467413435
O,0,1.4589536444,-1.1590084631,-1.0094022159
O,0,1.1395086307,1.4541208505,-0.3287603053
H,0,-0.2505922925,1.5242487728,-0.2513553942
H,0,0.5099672958,-1.2449040733,-1.1727972975
O,0,3.4883510213,0.0860006785,-0.0538049693
H,0,3.9036201027,0.9090516646,0.2069517151
Si,0,-1.9773395367,0.0726703754,-0.0141208239
O,0,-1.4639720626,-0.5848766411,1.4117603104
H,0,-1.7182099859,-1.4933891646,1.5910702222
O,0,-1.4888261848,-1.0478734162,-1.1333388045
O,0,-3.6010777329,0.2707255508,-0.0761337992
H,0,-4.1485420405,-0.516486615,-0.0578848984
O,0,-1.3189794085,1.5133461122,-0.1872932419
H,0,-1.8135323051,-0.9289958765,-2.0292976119

c14: HF=-1185.6915974,ZeroPoint=0.1068284

Si,0,1.8889916803,0.0099869893,0.0476342502
O,0,1.4147558198,-1.2792988907,-0.8797328498
H,0,1.704915095,-1.2823324193,-1.7952985251
O,0,1.3145504759,1.4169721406,-0.5361559566
O,0,1.2612105791,-0.2672283198,1.5226970882
H,0,0.3454898314,0.1252317115,1.5052178402
H,0,0.3879709601,1.4953073902,-0.1834720133
O,0,3.5172346642,0.132582214,0.0561710095
H,0,4.0245369178,-0.6809528209,0.0639297859
Si,0,-2.1039330604,0.1125738867,0.1121471061

O,0,-3.1411017642,-0.5594380392,1.2211823698
H,0,-2.7656894661,-0.6619685172,2.0968289158
O,0,-1.5291429956,-1.1001466168,-0.863983173
O,0,-3.1899501643,0.9377563055,-0.8324919593
H,0,-2.8979722921,1.1094377915,-1.7288872754
O,0,-0.9493095061,0.9646654673,0.7731830222
H,0,-0.5703660747,-1.2239265829,-0.8621202252

c15: HF=-1185.6918674,ZeroPoint=0.1071354

Si,0,1.8810598653,-0.0488100692,-0.0450705396
O,0,1.374267911,0.7745339004,1.3014396384
H,0,1.7068944648,0.4637197041,2.147198458
O,0,1.4354647436,-1.6146072599,0.0043424745
O,0,1.1569321864,0.6886399927,-1.3006082086
H,0,0.2689204357,0.2443057608,-1.3989993238
H,0,0.4981460229,-1.6378955081,-0.3229979517
O,0,3.511019623,-0.0278715768,-0.1418448294
H,0,3.9626729553,0.772114467,0.1324849143
Si,0,-2.088224406,-0.3915231554,-0.0430309452
O,0,-3.1921658712,0.6412469532,-0.7266858682
H,0,-3.7153778498,0.2670671128,-1.4374037227
O,0,-1.5566275637,0.4803490363,1.2589092553
O,0,-3.040778373,-1.6266108295,0.5367357766
H,0,-2.5778802532,-2.4534458416,0.6817392391
O,0,-0.9246541008,-0.8908560503,-0.9878953151
H,0,-0.6027052304,0.6306864038,1.3029696782

c16: HF=-1185.6917603,ZeroPoint=0.1071975

Si,0,2.0000067479,0.0022620791,0.0542398555
O,0,1.5752415226,-1.1820304158,-1.0247985842
H,0,1.8644004438,-1.0629724789,-1.932819217
O,0,1.4124227856,1.4567720112,-0.384395989
O,0,1.3417922486,-0.4484395082,1.4712927531
H,0,0.4157730228,-0.0767668408,1.4691057081
H,0,0.4778697075,1.4803310606,-0.0497157558
O,0,3.624672217,0.1514195333,0.1207573858
H,0,4.1482258656,-0.6467524316,0.031383137
Si,0,-1.9807794967,-0.0007042999,0.0176377345
O,0,-3.2142174502,-0.6601066621,0.9094282822
H,0,-2.9981079992,-1.4819956523,1.352446979
O,0,-1.3602490059,-1.2874421539,-0.8261756967
O,0,-2.8485415436,0.9521946102,-1.030280232
H,0,-2.4329230916,1.7924657638,-1.2285272317
O,0,-0.8769442375,0.8044872165,0.8112145329

H,0,-0.4004868467,-1.2892397612,-0.9446819617

c17: HF=-1185.6873411,ZeroPoint=0.1074776

Si,0,2.000265632,-0.0145146221,-0.1022521486
O,0,1.3956015538,1.4984420503,-0.2409765299
H,0,0.4207003703,1.5480003229,-0.2594931843
O,0,1.6145130604,-0.6581171733,1.350488492
O,0,1.5173313523,-0.9728507813,-1.3326905716
H,0,0.5625191928,-1.1720221496,-1.3178896145
H,0,0.6605081663,-0.6537887896,1.5578247742
O,0,3.6246475881,0.0430240173,-0.2471521491
H,0,4.1064769121,0.579372555,0.3843661097
Si,0,-1.9957235749,-0.2403353047,0.1510913853
O,0,-1.1417425812,-0.5685250036,1.5576878848
H,0,-1.5530632402,-0.2444266731,2.361839594
O,0,-1.3595676724,1.2548166556,-0.2679607408
O,0,-1.2196073699,-1.247893418,-0.9432523082
H,0,-1.6206878076,-2.1143681772,-1.0395768915
O,0,-3.5390350516,-0.3482729432,0.2261813955
H,0,-1.8578735803,1.7295033146,-0.9367634868

c18: HF=-1185.6859402,ZeroPoint=0.1061532

Si,0,2.2103308662,0.0016437605,-0.0024628781
O,0,1.6895335427,1.5559913036,0.0923563939
H,0,0.7161061507,1.4953101674,0.1076365344
O,0,1.7034309052,-0.8528473968,1.3055068037
O,0,1.7384298885,-0.7071174162,-1.4035545427
H,0,0.7657251566,-0.6983309667,-1.3823404571
H,0,0.7299903035,-0.8135294694,1.2739742134
O,0,3.8429033858,-0.020552753,-0.0621323738
H,0,4.3178873476,0.3556618961,0.6805203119
Si,0,-2.1122487399,0.0024838588,-0.0041017561
O,0,-2.791303125,-1.5010115366,-0.2374137893
H,0,-2.2556436683,-2.1004336372,-0.7597909343
O,0,-2.6880643133,1.0326961258,-1.1700891817
O,0,-2.8627351402,0.5422121781,1.3761214292
H,0,-2.7423469121,-0.0067832398,2.1527773391
O,0,-0.5421396928,-0.0068775442,-0.0012868035
H,0,-3.6419499551,1.0666716698,-1.2603673089

c19: HF=-1185.6853302,ZeroPoint=0.1079256

Si,0,-1.885067212,-0.0154594938,-0.047441458
O,0,-1.396062878,-0.2331966923,1.5195541948
H,0,-1.6887810061,-1.0431869676,1.9456237647

O,0,-1.292753951,1.4298406959,-0.4833829769
O,0,-1.3844586595,-1.249356416,-0.9786853014
H,0,-0.410913547,-1.3199871282,-1.0550205081
H,0,-0.3154348608,1.5175064996,-0.4794638326
O,0,-3.5083157439,-0.0346612862,-0.1936513711
H,0,-4.0111620237,0.5800561922,0.3436310244
Si,0,2.1535332724,-0.0733683449,0.0346525419
O,0,1.4205351421,1.3798814401,-0.4293138109
H,0,1.9036494928,2.1648553671,-0.1622930751
O,0,1.5169187789,-0.4540512721,1.512753003
O,0,1.3595500022,-1.1475964317,-0.9945423154
H,0,1.7413000068,-1.2000067211,-1.8738569287
O,0,3.7033841751,-0.0683730995,-0.026126799
H,0,0.5601745918,-0.3523219416,1.6110837385

c20: HF=-1185.6804873,ZeroPoint=0.1076767

Si,0,-1.9562173789,0.0238009395,0.0374273492
O,0,-1.3449120931,-0.6649162904,1.3981109554
H,0,-1.6518712757,-1.5467385984,1.6239036593
O,0,-1.3403089425,1.5114886528,-0.0662639701
O,0,-1.485466267,-0.9729312937,-1.1810240173
H,0,-1.8479681531,-0.8064853514,-2.0549315177
H,0,-0.3568165835,1.5839108563,-0.0890969968
O,0,-3.5820086423,0.0859374248,0.0038204086
H,0,-4.022537415,0.7551298026,0.5316557224
Si,0,2.1442327545,-0.0025505607,-0.0409685999
O,0,1.3403557627,1.4953347149,-0.1387354398
H,0,1.7506978545,2.1833221033,0.3903362565
O,0,1.5912673233,-0.6855486892,1.3739561038
O,0,1.4577947067,-0.8259795641,-1.3088046032
H,0,0.5009536912,-0.9533867161,-1.2975192237
O,0,3.6939383483,0.0900929106,-0.1027991378
H,0,0.6321449396,-0.6966513807,1.4871872011

c21: HF=-1185.6720817,ZeroPoint=0.1067852

Si,0, 1.994581512311,-0.002367340383,0.004895399156
O,0,1.376519541421,0.002133539116,1.517706929226
H,0,1.649323923322,0.706056810768,2.112232365483
O,0,1.354364949106,-1.309719742758,-0.736642675753
O,0,1.413613593240,1.323789825362,-0.745718577800
H,0,1.724969100671,1.523681378848,-1.632161909671
H,0,1.798415177382,-2.158016438163,-0.670923710151
O,0,3.616995792677,0.050610259296,-0.041234121326
H,0,4.126164330789,-0.614590486253,0.426131958385

Si,0,-2.186129964679,0.000470857870,-0.006406420254
O,0,-1.551639519457,-1.056345478317,-1.139396501087
H,0,-0.612561786026,-1.255657296198,-1.046675386597
O,0,-1.549330893865,-0.466435101906,1.470042424319
O,0,-1.522056717738,1.499617184991,-0.346572819505
H,0,-0.578339735722,1.513726075044,-0.542856159380
O,0,-3.742849518659,0.021424932266,-0.008896843676
H,0,-0.604792784772,-0.311103979580,1.587852048625

d1: HF=-1185.6845842,ZeroPoint=0.1074836

Si,0,-1.6786040752,-0.0323604382,0.0436914926
O,0,-1.1476630201,1.4694287432,-0.3795916524
H,0,-0.1921380788,1.5685248774,-0.479248383
O,0,-1.7685792976,-1.2188202066,-1.117569895
O,0,-1.5398128119,-0.5272871815,1.6251402566
H,0,-0.6426511254,-0.8534800276,1.7493210753
H,0,-0.8877031529,-1.5945837831,-1.2168483216
O,0,-3.3090270953,0.4034551976,0.070501833
H,0,-3.8921809269,-0.3224204743,0.2950276373
Si,0,1.8604457183,-0.0453357361,-0.0439186965
O,0,2.6794307859,0.1668186615,1.3749963641
H,0,3.1522831371,-0.5969780987,1.7097642428
O,0,1.6807041376,1.5023762088,-0.6237104
O,0,2.9205163726,-0.9017524983,-0.982848657
H,0,2.5176855132,-1.4154665242,-1.6851622899
O,0,0.4224032584,-0.6825766545,0.0202301705
H,0,2.4017539711,2.1191640646,-0.4875968667

d2: HF=-1185.683257,ZeroPoint=0.1072665

Si,0,1.493347227,0.728412774,0.6482976368
O,0,1.2443307761,-0.4267430139,-0.5227872531
H,0,2.0630689161,-0.8521650813,-0.7900255947
O,0,1.2014866917,2.2784208646,0.1784282577
O,0,1.1186253756,0.3175052138,2.197867001
H,0,0.1530176321,0.364056213,2.2543309169
H,0,0.2377556951,2.3719855441,0.1687810311
O,0,3.1615447454,0.669769482,0.6777249328
H,0,3.5789529166,1.0956613641,1.4275416286
Si,0,-2.0033815686,0.0234857661,-0.0397875197
O,0,-2.9857448273,-0.8801345818,0.945723841
H,0,-3.5943893689,-0.3782196749,1.4901438055
O,0,-1.379033405,-1.0996448294,-1.0768052368
O,0,-3.0955641012,0.970401302,-0.8645694219
H,0,-2.7194249948,1.7560556807,-1.2649415143

O,0,-0.8655677535,0.8581898775,0.6714579846
H,0,-0.4095489063,-1.0464801007,-1.0450961656

d3: HF=-1185.6831647,ZeroPoint=0.1072093

Si,0,1.812825822,0.0070633249,-0.0253697246
O,0,1.1036874182,-0.7955910692,-1.2977318342
H,0,1.7482047998,-1.2528243266,-1.8437793869
O,0,1.8359333285,1.6496231654,-0.1284714066
O,0,1.6012176839,-0.655494896,1.4665789722
H,0,0.6974320129,-0.4261507742,1.7281695488
H,0,0.9373511188,1.9385811365,0.0875594206
O,0,3.3981537614,-0.3905293455,-0.3638345707
H,0,4.0534823746,-0.0577549579,0.2507335503
Si,0,-1.8209122946,0.2527114383,-0.107604377
O,0,-1.6567355881,-0.7514351575,-1.4138868151
H,0,-0.7105983772,-0.9041895359,-1.573553969
O,0,-2.7129294155,1.5817971002,-0.5486366033
O,0,-2.9168387563,-0.4725347745,0.9059591282
H,0,-2.7658717816,-1.4061743248,1.0604625601
O,0,-0.4102797753,0.6060765595,0.511343828
H,0,-2.1905398615,2.3264470376,-0.8501689908

d4: HF=-1185.6832201,ZeroPoint=0.1072806

Si,0,1.8369930352,-0.0334663984,0.2183212375
O,0,1.9444862695,-1.1155498409,-1.0173294855
H,0,1.0601072554,-1.500711245,-1.1031879723
O,0,1.0877296065,1.4055262052,-0.1487918864
O,0,1.5956842636,-0.6306323475,1.7332914534
H,0,0.7063091368,-1.0137739088,1.7259774429
H,0,1.7031303973,2.143031124,-0.1539550319
O,0,3.3997438834,0.5446660806,0.3234249535
H,0,4.0487149833,-0.0679062922,0.6718881056
Si,0,-1.7582962704,-0.2703462463,-0.1752332924
O,0,-2.7302496777,-1.0382624887,-1.2837421922
H,0,-2.4716571265,-0.9265965958,-2.2001427245
O,0,-1.618898058,1.2899205829,-0.7116395397
O,0,-2.684126237,-0.3122360549,1.2010011528
H,0,-3.5866986676,-0.0037309343,1.1039244265
O,0,-0.3475707622,-0.9221594362,0.0954860809
H,0,-0.7008195715,1.5815976364,-0.5865608581

d5: HF=-1185.6829393,ZeroPoint=0.1073418

Si,0,-1.7469050181,-0.0465833696,0.0832490302
O,0,-1.0679436369,1.3520524077,-0.509367101

H,0,-1.7307369499,2.0185153453,-0.7074476156
O,0,-1.667037749,-1.3534469444,-0.9143724183
O,0,-1.6114547267,-0.3125980399,1.7023551189
H,0,-0.7001196906,-0.6082501539,1.843064822
H,0,-0.7543762375,-1.6716034147,-0.8564191985
O,0,-3.3482956807,0.4068521667,-0.0538675688
H,0,-3.984562374,-0.1773385909,0.3604281678
Si,0,1.871580742,-0.037854991,0.0391071049
O,0,2.8547920473,0.1964896548,1.3604640961
H,0,3.189251532,-0.6031077611,1.7701352472
O,0,1.6908804249,1.4966039193,-0.5427170921
O,0,2.7531766495,-0.9349751872,-1.0491661175
H,0,3.6497240292,-0.6327067627,-1.2048434406
O,0,0.4910894281,-0.7490693088,0.3160002082
H,0,0.7421700004,1.6844223302,-0.6340479629

d6: HF=-1185.6778145,ZeroPoint=0.1065438

Si,0,-1.794987617,0.0399490506,0.017771524
O,0,-1.1751024493,-1.0624833107,-1.0291227553
H,0,-0.2115292323,-1.0928170785,-1.1216884234
O,0,-1.7075162104,-0.311935244,1.6327577154
O,0,-1.7027450226,1.6332496181,-0.3967681318
H,0,-0.7707390158,1.8692903809,-0.2686230336
H,0,-2.5476811043,-0.6518082189,1.9501960992
O,0,-3.4357816133,-0.251718505,-0.196225991
H,0,-3.7026236236,-0.4063472665,-1.1030441309
Si,0,1.8710477437,0.033144039,0.0409488163
O,0,1.6378880272,-1.0611590909,-1.1967596249
H,0,2.3095145113,-1.7322347037,-1.3285841596
O,0,2.6487152757,-0.8755413644,1.1869063641
O,0,3.0170013923,1.1494195232,-0.4015994997
H,0,2.6618207544,1.9601360636,-0.7702030166
O,0,0.4739981267,0.6519180824,0.3900861782
H,0,3.1237970573,-0.3850019752,1.8596380695

d7: HF=-1185.6767758,ZeroPoint=0.106985

Si,0,1.6885861751,-0.029169102,0.0860866819
O,0,1.0549659569,-1.00827798,-1.0912151999
H,0,1.6994541656,-1.2193583116,-1.7717260575
O,0,1.1379185853,1.5232811876,-0.0717411624
O,0,1.7666659598,-0.6648474485,1.5866730349
H,0,0.8250542364,-0.7539003016,1.8422043649
H,0,1.8363028224,2.1367078117,-0.3144418503
O,0,3.2838614386,0.1388581848,-0.3534261394

H, 0, 3.914831866, -0.3522583889, 0.1749303932
Si, 0, -1.8163828925, 0.0680666747, 0.0320779964
O, 0, -1.8079514912, -0.8539216578, -1.3496009067
H, 0, -0.8976275154, -1.1344867755, -1.5167488586
O, 0, -1.7205008224, 1.6798782125, -0.3778607771
O, 0, -3.3816179926, -0.1403008211, 0.5407640029
H, 0, -3.6853080297, 0.4954362226, 1.1903567325
O, 0, -0.6545700363, -0.3338283843, 1.0146519769
H, 0, -0.7968712161, 1.9585334375, -0.3065625317

d8: HF=-1185.6768138,ZeroPoint=0.1071242

Si, 0, 1.6121002942, 0.026706945, -0.0288890895
O, 0, 0.9464624933, -0.6322038539, 1.3386430466
H, 0, 1.5545378282, -1.2262802504, 1.7863507086
O, 0, 1.0124872916, -0.6961184473, -1.3916516499
O, 0, 1.787040914, 1.6489808799, -0.0334640104
H, 0, 0.8635314572, 1.9750979952, -0.0503650765
H, 0, 1.6847701149, -1.187629443, -1.870642015
O, 0, 3.1773567247, -0.5361702778, -0.0218440049
H, 0, 3.8466077194, 0.0991518585, 0.2370782619
Si, 0, -1.8902581106, 0.1429499989, -0.1368487307
O, 0, -1.9197990335, -0.8159293056, 1.2248273612
H, 0, -1.0137172952, -0.8997026503, 1.5540516173
O, 0, -1.8667960601, -0.8206819478, -1.4896765767
O, 0, -3.4176359495, 0.7829116242, -0.231623748
H, 0, -3.7386553127, 1.1882489742, 0.5752375964
O, 0, -0.667755961, 1.1335676295, -0.0997563841
H, 0, -0.9464599549, -0.9333458395, -1.7641163563

d9: HF=-1185.6744191,ZeroPoint=0.1065892

Si, 0, 1.7722330718, 0.0139393594, 0.0307371305
O, 0, 0.998839893, -0.7119125308, -1.2481223138
H, 0, 1.6203635688, -1.1265230216, -1.8518898352
O, 0, 1.7621238949, 1.6547562069, -0.0982017687
O, 0, 1.5376633701, -0.6644135954, 1.4998046666
H, 0, 0.5913482308, -0.4770934083, 1.6781957254
H, 0, 2.6477931987, 2.0057901177, -0.2184728247
O, 0, 3.3779211512, -0.3313003976, -0.2743380232
H, 0, 3.7585750905, -1.0169437623, 0.2765093957
Si, 0, -1.948148009, 0.2083046646, 0.0114662061
O, 0, -1.7757292486, -0.6993687462, -1.3668717757
H, 0, -0.827441056, -0.8163380603, -1.5399228234
O, 0, -2.640415215, 1.6675992954, -0.3807509507
O, 0, -3.1639103815, -0.5296700715, 0.8791975548

H,0,-3.0393580514,-1.4676043793,1.0333508259
O,0,-0.5771415421,0.4210207336,0.7493212091
H,0,-3.5093676461,1.6180571857,-0.7826865987

e1: HF=-1185.6972058,ZeroPoint=0.1100517

Si,0,1.372882775,0.1366479838,0.0398195298
O,0,0.9735831085,-0.6145755595,1.5140149281
H,0,1.7340399285,-1.0989766676,1.8427695543
O,0,1.0477397356,-0.7653360885,-1.3664165249
O,0,2.0081185312,1.6968915862,-0.0242385475
H,0,1.2999287662,2.3413979693,-0.0775458675
H,0,1.8218432572,-1.2820477233,-1.6003988158
O,0,3.0025336011,-0.5220166317,0.1167500144
H,0,3.6595260088,0.1735899519,0.0849713414
Si,0,-1.6497697585,-0.0037783248,-0.0419435908
O,0,-1.7818566588,-0.8539360208,1.3620683817
H,0,-0.8881492528,-0.9653894446,1.7308015483
O,0,-1.7204762885,-0.9721925284,-1.3673209327
O,0,-2.986038037,0.9404410082,-0.1708695183
H,0,-3.2973365505,1.3411939715,0.6425148884
O,0,-0.2640570834,0.8101489351,-0.0388264302
H,0,-0.8104040826,-1.1245724168,-1.6747859589

e2: HF=-1185.6923889,ZeroPoint=0.108998

Si,0,1.3926316903,0.0617060754,0.0606267465
O,0,0.9148295538,-1.2038825689,-0.9756137354
H,0,1.6876015103,-1.5536701967,-1.4240113152
O,0,1.3781026023,1.6215794659,-0.5747356854
O,0,1.8419357183,-0.2408287066,1.6606707526
H,0,1.0730127382,-0.1994362117,2.2320691111
H,0,2.2531199774,1.8181886319,-0.9161790764
O,0,3.075490896,-0.1653428411,-0.4363073062
H,0,3.6248836029,-0.3974459815,0.3124843105
Si,0,-1.7519614396,0.0799409766,-0.0153345524
O,0,-1.75226523,-1.0544974332,-1.202307083
H,0,-0.8266236048,-1.3192796191,-1.3696402041
O,0,-2.2944538271,1.5333536831,-0.5657262752
O,0,-2.8734063806,-0.3542244329,1.1133651243
H,0,-2.8549249304,-1.2715040016,1.3921821578
O,0,-0.2880737937,0.2602772963,0.5896324728
H,0,-3.2180284232,1.5770258043,-0.8194763423

e3: HF=-1185.692243,ZeroPoint=0.1089429

Si,0,1.3790659768,0.4105721278,0.3009532573

O,0,1.3912854881,-0.7211627076,-0.9711974891
H,0,2.274379881,-1.0829794154,-1.0726034817
O,0,1.5316701634,2.0448037237,-0.0721190394
O,0,1.1589358289,-0.0370319811,1.9149051202
H,0,0.2305940824,0.0060427358,2.150892851
H,0,0.6641102155,2.4202949853,-0.2347199125
O,0,3.1025915847,0.2026873515,0.4535153541
H,0,3.4105160923,0.4110166275,1.3355726271
Si,0,-1.6382224694,-0.3477510568,-0.3736575111
O,0,-2.3965074913,-1.1652572975,0.839146264
H,0,-2.93343657,-0.640358559,1.4353828724
O,0,-1.1348184972,-1.5006931393,-1.4217937459
O,0,-2.8327215092,0.5770580453,-1.0340019607
H,0,-2.5441042181,1.2841033234,-1.6139334822
O,0,-0.4108358546,0.5590801797,0.1011902014
H,0,-0.1600737031,-1.4535389432,-1.4723189249

e4: HF=-1185.6934266,ZeroPoint=0.1102464

Si,0,1.3656994817,-0.0237398896,0.0942863151
O,0,0.9700487504,-1.3348648794,-0.9239999144
H,0,1.7218573235,-1.6265406149,-1.4419767307
O,0,0.9752094853,1.5390995954,-0.4675731103
O,0,2.0131736753,-0.2674100721,1.6238394178
H,0,1.2992674172,-0.3667936347,2.2560238961
H,0,1.7278242028,1.9732677179,-0.8722146589
O,0,3.0077839603,0.0698539314,-0.520817617
H,0,3.0614181411,0.2186409984,-1.4659872431
Si,0,-1.6730262407,0.004039266,0.0104763575
O,0,-1.7898544648,-1.1919699696,-1.1160282598
H,0,-0.8915670951,-1.5153520627,-1.3032957933
O,0,-1.7989322415,1.5008475556,-0.656516035
O,0,-2.992945907,-0.1075175024,0.9804282874
H,0,-3.2744140938,-0.9961440279,1.204594957
O,0,-0.2717444263,-0.1300507862,0.7822997735
H,0,-0.9019670885,1.8662904249,-0.7404982517

e5: HF=-1185.6935003,ZeroPoint=0.1102865

Si,0,1.3407954083,-0.0521287124,0.134229525
O,0,0.9801761521,-1.3509269573,-0.9040039158
H,0,1.7207123236,-1.5312729838,-1.4872443096
O,0,0.9918326234,1.534495411,-0.3911031225
O,0,1.9674327146,-0.3038088535,1.6767625509
H,0,2.9194703037,-0.4080901029,1.6465897886
H,0,1.6807732664,1.8684445513,-0.9683724605

O,0,2.9553514935,-0.0046105281,-0.6113739298
H,0,3.5378025691,0.6751966178,-0.2690044018
Si,0,-1.6664483159,0.0032153881,0.0339128549
O,0,-1.7778321966,-1.1584926089,-1.1284606
H,0,-0.8795270485,-1.4831164935,-1.314438612
O,0,-1.7846259353,1.520211295,-0.5871475314
O,0,-2.9917549603,-0.1335829551,0.9928574997
H,0,-3.275193309,-1.0275807419,1.1918421051
O,0,-0.2713170611,-0.1582155682,0.8111293798
H,0,-0.883097028,1.8772582423,-0.6626218204

e6: HF=-1185.6935402,ZeroPoint=0.1103222

Si,0,-1.3295216322,-0.0444780912,0.3151964756
O,0,-1.0358916337,1.6231424258,0.1541658252
H,0,-1.8164591394,2.0711426095,-0.179182828
O,0,-1.0350205306,-1.0566957694,-1.0280044191
O,0,-1.8373022536,-0.7170713546,1.7727764814
H,0,-2.787804754,-0.6448524076,1.8701045666
H,0,-1.7696673436,-1.0379034967,-1.6439516476
O,0,-2.9964597533,0.276223754,-0.2203912613
H,0,-3.558159884,-0.4983082065,-0.2774550998
Si,0,1.6620310375,0.0900400755,0.0126791177
O,0,3.0553591795,-0.2116990895,0.8264604212
H,0,3.3644736008,-1.1190095522,0.8072418228
O,0,1.7123263486,1.708235959,-0.2701642487
O,0,1.7063094317,-0.7895345294,-1.3792630527
H,0,0.7978861599,-1.0793269911,-1.5740392242
O,0,0.3292252337,-0.2770711881,0.8281614024
H,0,0.8065737927,2.0530277325,-0.1908793015

e7: HF=-1185.6920293,ZeroPoint=0.1087905

Si,0,1.4549018631,-0.0538608582,0.1201679904
O,0,0.9385605995,-1.1567992078,-1.0680832605
H,0,1.6958045968,-1.603298807,-1.4525127255
O,0,1.8578071429,1.5468484752,-0.2310800312
O,0,1.5131457797,-0.5572734378,1.7270162045
H,0,0.6746174165,-0.376647967,2.1560053623
H,0,1.084784511,2.1063767443,-0.1359022605
O,0,3.0934173872,-0.565547736,-0.1804184198
H,0,3.7327087657,0.0842368178,0.1119289906
Si,0,-1.7521778078,0.0607778564,-0.0717897291
O,0,-1.7292907703,-1.1812607974,-1.1444328909
H,0,-0.7955940278,-1.4035936104,-1.3298862387
O,0,-2.5902150493,1.3488732445,-0.6648686579

O,0,-2.7222376321,-0.3478204645,1.1952901993
H,0,-2.6011607065,-1.2323179288,1.5441601549
O,0,-0.2621575974,0.4602465352,0.3416136274
H,0,-2.1059167312,1.9189804315,-1.2641845754

e8: HF=-1185.692297,ZeroPoint=0.1090505

Si,0,-1.4236893117,0.0156751617,0.1046038191
O,0,-0.969940157,-1.3766737487,-0.7714738883
H,0,-1.7144332875,-1.6644831281,-1.3041667927
O,0,-1.9772804902,-0.1864869789,1.6795722733
O,0,-1.2437632096,1.5365150069,-0.6109494284
H,0,-0.354111669,1.8832270949,-0.5108224324
H,0,-1.2280697451,-0.2241678858,2.2771480223
O,0,-3.0581390317,-0.080745298,-0.5000488959
H,0,-3.2364851313,0.6394810995,-1.1046142377
Si,0,1.690185947,-0.0133042785,0.0519745091
O,0,2.9439157417,-0.1639084685,1.1047429233
H,0,3.079784746,-1.0362312552,1.4793345915
O,0,1.9508905069,1.4195675515,-0.7221100277
O,0,1.736167339,-1.28915636,-0.9798213532
H,0,0.8159616805,-1.5747110169,-1.1384314586
O,0,0.2615263663,0.1003817427,0.7543013507
H,0,2.7415207656,1.5011062113,-1.2582630545

e9: HF=-1185.6921702,ZeroPoint=0.1089225

Si,0,-1.4276118802,0.0591390417,-0.0675426363
O,0,-0.8695651434,1.653770584,-0.2764350019
H,0,-1.6062969072,2.2668625977,-0.2309484841
O,0,-1.9137190816,-0.9152318014,-1.3561172709
O,0,-1.4370642803,-0.5984983102,1.4842859221
H,0,-0.6047305523,-1.0395806108,1.6640202623
H,0,-1.1665748397,-1.4189204649,-1.6844751238
O,0,-3.0425176337,0.6898805404,0.1076538748
H,0,-3.7088347278,0.0321021605,-0.0915800228
Si,0,1.753263779,0.0078853471,-0.0818357998
O,0,2.3815713876,-0.3704712091,1.3936794311
H,0,2.6127370128,-1.2901696619,1.5353460081
O,0,1.8094996554,1.6420894358,-0.17084079
O,0,2.8047560998,-0.6784779997,-1.1496593601
H,0,2.4962365287,-0.7517588018,-2.0546369782
O,0,0.2647379967,-0.5221652571,-0.3212877273
H,0,0.8912253063,1.9702796495,-0.2294396432

e10: HF=-1185.6932644,ZeroPoint=0.1101828

Si,0,1.348585805,-0.0266510846,0.0946477363
O,0,0.9729587703,-1.3359279785,-0.9333238498
H,0,1.7285132128,-1.6152379175,-1.452471907
O,0,0.9762724404,1.5392053625,-0.4711821043
O,0,1.9895603377,-0.2749506179,1.6267847599
H,0,2.9478267918,-0.2699415558,1.5823762967
H,0,1.7318588286,1.9638191665,-0.8801735431
O,0,3.0102124507,0.0721279957,-0.531957317
H,0,3.0843536741,0.2191175035,-1.4761064257
Si,0,-1.6664381427,0.0033736911,0.0109068999
O,0,-1.7894974669,-1.1879321712,-1.1201796119
H,0,-0.8928893658,-1.5126405347,-1.3125364905
O,0,-1.7987268117,1.503057771,-0.6485730459
O,0,-2.980360203,-0.1132517911,0.9881850239
H,0,-3.2562267573,-1.0028291124,1.2155216952
O,0,-0.2626011126,-0.1335091619,0.7754705716
H,0,-0.9028933413,1.8700449251,-0.737069318

e11: HF=-1185.6861375,ZeroPoint=0.1081805

Si,0,-1.5475573112,-0.0579122081,0.0127481341
O,0,-1.4751445841,-0.6310124797,1.5928267635
H,0,-0.6002471094,-0.9776378353,1.7723486434
O,0,-1.1585192534,1.5346832825,-0.3511428077
O,0,-3.2169587212,0.3168258405,0.2504578501
H,0,-3.5856254985,0.7630712093,-0.5123475858
H,0,-0.2272455017,1.688346976,-0.5411681844
O,0,-1.8764377272,-1.0977819216,-1.2729210638
H,0,-1.0547387131,-1.4661425921,-1.6032893873
Si,0,1.7326603726,-0.0330737611,-0.0226621835
O,0,2.8176842667,-0.9776128543,-0.8233834865
H,0,2.4903297494,-1.4202241727,-1.6086176773
O,0,2.3263905006,0.0808354177,1.5073908538
O,0,1.7319872624,1.51923732,-0.5893788141
H,0,2.4768318308,2.0805175389,-0.3670683318
O,0,0.2544341196,-0.5792623899,-0.1760961717
H,0,2.6805263176,-0.7222093701,1.8936744489

e12: HF=-1185.6861558,ZeroPoint=0.1082653

Si,0,1.5056630114,-0.0256742727,-0.0257899259
O,0,1.0944907491,1.5725703887,-0.3036071682
H,0,0.1547321636,1.7621233976,-0.2209004204
O,0,1.8800959482,-0.5697249668,1.5257307367
O,0,1.4200042499,-1.1674136337,-1.265039879
H,0,0.559564199,-1.5904027187,-1.2655143069

H, 0, 1.0804752679, -0.8768719128, 1.9572805749
O, 0, 3.1547731789, 0.3495194511, -0.3779687897
H, 0, 3.7116832843, -0.4258344936, -0.3024694758
Si, 0, -1.7781002409, -0.0361039593, 0.064440943
O, 0, -2.4158632339, -0.6001115653, -1.3431606769
H, 0, -2.7779473718, -1.4878407818, -1.3275366807
O, 0, -1.7934508458, 1.6087632637, -0.0960713785
O, 0, -2.8214683284, -0.5492590176, 1.23008212
H, 0, -2.464755313, -0.6038278585, 2.1185859877
O, 0, -0.284787597, -0.4491808574, 0.3890104014
H, 0, -2.5538310715, 2.014439257, -0.5161219616

e13: HF=-1185.6858219,ZeroPoint=0.1081452

Si, 0, -1.5321211879, 0.0095084354, 0.0607806242
O, 0, -1.1374491555, 1.5095776716, -0.5705505408
H, 0, -0.1955647701, 1.7051828035, -0.564766511
O, 0, -1.4739949168, -1.3676722482, -0.9132237001
O, 0, -1.8653574771, -0.1949262957, 1.7019744085
H, 0, -1.0542362098, -0.4068912388, 2.1680401543
H, 0, -0.6101696131, -1.7804258551, -0.8560355503
O, 0, -3.1926320851, 0.3064816294, -0.3130856644
H, 0, -3.7513231964, -0.4073873592, -0.0044556524
Si, 0, 1.7343503628, -0.0494132889, -0.0130579703
O, 0, 1.7696858991, 1.5231350674, -0.5321225301
H, 0, 2.5325644954, 1.8285019326, -1.0260187238
O, 0, 2.1046282237, -1.0870190429, -1.2333524157
O, 0, 2.9180387789, -0.2913046356, 1.1036874393
H, 0, 2.9659495254, 0.3375005189, 1.8261900063
O, 0, 0.2651550258, -0.308702601, 0.5099786501
H, 0, 3.0327543007, -1.2275664933, -1.4285450239

e14: HF=-1185.6853242,ZeroPoint=0.1080013

Si, 0, -1.4562733646, 0.0074846565, -0.0311588015
O, 0, -1.1144578524, -0.7246564678, 1.4409254342
H, 0, -0.1736414412, -0.8558618776, 1.597374383
O, 0, -1.3365416053, 1.6903505446, -0.1056589971
O, 0, -1.8431261087, -0.9236607835, -1.3920798766
H, 0, -1.0441073474, -1.1422960718, -1.874555292
H, 0, -2.2053547447, 2.0546955616, 0.0770423175
O, 0, -3.1616999455, 0.1037532841, 0.3685624576
H, 0, -3.684293993, -0.3800951728, -0.2704824857
Si, 0, 1.7681292486, 0.0120222422, -0.0420437246
O, 0, 1.7819842358, -0.7426374938, 1.4327945777
H, 0, 2.5625243684, -0.6581752485, 1.9829521892

O,0,2.2841283243,1.5656568184,0.0910367311
O,0,2.8766733646,-0.6907183288,-1.0358291746
H,0,2.8193356428,-1.6421015455,-1.1417493608
O,0,0.2811594633,-0.0834231592,-0.5688526969
H,0,3.2321275449,1.7091483816,0.0831616793

f1: HF=-1185.6871121,ZeroPoint=0.1082925

Si,0,1.3634680633,0.0238635825,-0.1170900188
O,0,2.4007687792,1.113769921,-0.87671337
H,0,2.9469955291,0.6322827858,-1.5021959561
O,0,1.8049641954,-0.6672587382,1.3650889929
O,0,2.0982686668,-1.310665106,-1.0161513673
H,0,1.4226870868,-1.8622432723,-1.410562188
H,0,2.2796859842,-1.4846359734,1.1994345808
O,0,0.5931386285,1.3504708699,0.7730246231
H,0,1.082664487,1.5847129111,1.5621824118
Si,0,-1.5934588258,-0.0167991774,-0.1059651998
O,0,-1.9366068853,1.5879310206,-0.1584619685
H,0,-1.1476965067,2.0557021251,0.1572685599
O,0,-1.6925719236,-0.6622887984,1.402502979
O,0,-2.8136065568,-0.7723015447,-0.8982715023
H,0,-3.1530964175,-0.3323469182,-1.6792441958
O,0,-0.1579610681,-0.3555035953,-0.7788443301
H,0,-0.8743777866,-0.5836187123,1.9018587792

f2: HF=-1185.6860345,ZeroPoint=0.1087251

Si,0,-1.3322775003,0.0528809438,0.152604116
O,0,-0.9444584866,1.5902374733,-0.4698425469
H,0,-1.7025747609,1.9340792815,-0.9486095255
O,0,-1.016587207,-1.3734072455,-0.7166871573
O,0,-2.0292386088,-0.1769749764,1.6743946745
H,0,-2.2417836544,0.6240243915,2.1540221925
H,0,-1.7674915132,-1.5642296131,-1.2836401378
O,0,-2.9180688055,0.1999185458,-0.6451520323
H,0,-3.6141662849,-0.0965627556,-0.0585797828
Si,0,1.6810016792,-0.0034324483,0.0047833238
O,0,1.8084858622,1.4261651329,-0.8049087487
H,0,0.9167205532,1.8082549132,-0.8763096429
O,0,1.7563127269,-1.2982256652,-1.0056819834
O,0,3.0224967501,-0.1542647627,0.9400702088
H,0,3.3287983442,0.6486628364,1.3650672615
O,0,0.2991319014,-0.0320778406,0.8194115984
H,0,0.8500824044,-1.6249767113,-1.1373692479

f3: HF=-1185.6867337,ZeroPoint=0.1095559

Si,0,1.3605729291,-0.018757151,-0.1127251322
O,0,2.9543296499,0.6371475657,-0.2074637294
H,0,3.5745491948,-0.0219116623,-0.5219602181
O,0,1.1981719046,-0.5522085411,1.4956265272
O,0,1.9529494008,-1.3914366275,-0.9637097754
H,0,1.2212850666,-1.9338989487,-1.2616188977
H,0,1.5949318667,-1.414685562,1.6318249333
O,0,0.7986475217,1.6104108814,0.0401268637
H,0,1.5311470294,2.2006356164,0.2253165522
Si,0,-1.6389550227,-0.0057169195,-0.0507135976
O,0,-1.9323293286,1.6011107787,-0.2441218089
H,0,-1.0705003864,2.049357068,-0.2039767894
O,0,-1.6083445767,-0.4545571751,1.5283913657
O,0,-2.927525613,-0.7965604299,-0.6866935104
H,0,-3.3141574978,-0.4111486099,-1.474780371
O,0,-0.2344919705,-0.4097986957,-0.7328608648
H,0,-0.684312168,-0.5854765876,1.8074994529

f4: HF=-1185.6859647,ZeroPoint=0.108927

Si,0,1.4025292687,0.0027931565,0.2709272792
O,0,1.0536585666,-1.2973871969,-0.7659078985
H,0,1.837924581,-1.5165366475,-1.2737912925
O,0,1.0785488359,1.5273264467,-0.452883495
O,0,1.9318437135,-0.1536832231,1.8579778244
H,0,1.170997503,-0.2686387529,2.4310135425
H,0,1.1568129595,2.2672834743,0.1524604407
O,0,3.0758380329,0.0303108887,-0.2493587751
H,0,3.1940266381,0.6769621786,-0.9452764894
Si,0,-1.6290650935,-0.1193334017,0.0156785807
O,0,-1.7203126962,-1.4984036966,-0.8816937971
H,0,-0.8126826252,-1.7873876686,-1.0704490458
O,0,-1.6741584561,1.229168165,-0.924476306
O,0,-3.0085682675,-0.0460943735,0.9033419137
H,0,-3.322503715,-0.8770718757,1.2637939622
O,0,-0.2811052847,-0.1144270564,0.8867508567
H,0,-0.7754453012,1.6008932232,-0.9570267007

f5: HF=-1185.6829334,ZeroPoint=0.1080025

Si,0,1.4457947284,0.030593029,0.0915452848
O,0,0.8666110794,-1.4726924215,-0.5663729214
H,0,1.5793481361,-1.9217222207,-1.024318088
O,0,1.8347172824,1.6978713536,-0.0447178388
O,0,1.839094587,-0.3384029117,1.6849786425

H, 0, 1.3258643266, -1.0666241399, 2.0365390276
H, 0, 1.0875013201, 2.2315174735, 0.2285646403
O, 0, 2.9118312742, -0.2946384688, -0.7746545232
H, 0, 3.4470264069, 0.497097364, -0.8388517507
Si, 0, -1.7403409742, 0.0901105339, -0.0741128751
O, 0, -2.7181270497, 0.0491070516, 1.2484493197
H, 0, -2.5440153874, -0.6528300439, 1.8775061923
O, 0, -1.7500482592, -1.3588948955, -0.8371884097
O, 0, -2.5249092395, 1.2321014191, -0.9615801099
H, 0, -2.0834763803, 1.5193315398, -1.7624823293
O, 0, -0.2348218513, 0.510586874, 0.2728908888
H, 0, -0.8162499994, -1.6596595366, -0.8915881498

f6: HF=-1185.682303,ZeroPoint=0.1093803

Si, 0, 1.5740802886, -0.050384736, -0.1482773023
O, 0, 2.7915985942, -0.2321957904, -1.2229141204
H, 0, 3.0166409285, -1.1294144033, -1.4749042127
O, 0, 1.7353876991, -1.1950058294, 1.0187753554
O, 0, 1.7678439027, 1.4663075585, 0.4424797229
H, 0, 0.9039488529, 1.7639650128, 0.7821119642
H, 0, 0.8646310959, -1.3192148002, 1.4399666809
O, 0, 0.1026075796, -0.1856034442, -0.8136105228
Si, 0, -1.3443831652, 0.0089934046, 0.0419912255
O, 0, -2.2847296667, -1.3612238677, -0.43695556
H, 0, -2.7809497558, -1.2854959257, -1.2505692888
O, 0, -2.2695511341, 1.0811194288, -0.9499515983
H, 0, -2.7704291434, 0.6909217558, -1.664967159
O, 0, -0.9853805489, 1.4197259779, 1.0037706563
H, 0, -1.3359252179, 2.1912532443, 0.5541560051
O, 0, -1.0151865092, -0.892469006, 1.4987558329
H, 0, -1.3799838002, -1.7741075799, 1.3980003211

g1: HF=-1185.6878042,ZeroPoint=0.108198

Si, 0, 1.3514486679, 0.0311067296, -0.0320198569
O, 0, 2.1360079204, -0.359362204, 1.4140945758
H, 0, 2.6920930245, 0.3775439396, 1.6759090759
O, 0, 2.0992080838, -0.4138956595, -1.4779564803
O, 0, 2.138201684, 1.6141469027, -0.0477340855
H, 0, 1.4913942177, 2.310746632, -0.1587461638
H, 0, 2.647209083, 0.3151517483, -1.7766138524
O, 0, 0.4960418044, -1.5215235825, 0.0364486225
H, 0, 1.0628080482, -2.2427677777, 0.3119468047
Si, 0, -1.6233993237, 0.0735117741, -0.012355314
O, 0, -1.8558498826, -0.6354327696, 1.4552112509

H,0,-1.1219470911,-1.2272209831,1.654803511
O,0,-1.8922645226,-0.9515755587,-1.2655507496
O,0,-2.8250964182,1.1732155893,-0.1920008315
H,0,-2.8941376242,1.852769016,0.4803571883
O,0,-0.1718347417,0.7905062385,-0.0957755434
H,0,-1.1547369298,-1.5736670352,-1.3123021519

g2: HF=-1185.688948,ZeroPoint=0.1083621

Si,0,-1.4216200049,-0.0186310339,0.0450052445
O,0,-0.8838096563,1.5709422419,-0.6301437532
H,0,-1.2330525635,1.6740964012,-1.5167183759
O,0,-2.1487720162,-1.4942966259,0.6252285147
O,0,-1.9542646206,0.8000634645,1.4267958925
H,0,-1.7523136591,1.734319488,1.3465207613
H,0,-2.1170294439,-1.5555475927,1.580207517
O,0,-2.2064049031,-0.2616748246,-1.4370233134
H,0,-2.7237567151,-1.068773068,-1.4035888431
Si,0,1.6835744072,-0.1294217552,-0.0036895302
O,0,2.5825561478,-0.3296689157,1.3555268771
H,0,2.4662311044,0.332679392,2.0386641451
O,0,1.7134311943,1.4316583516,-0.4749530371
O,0,2.4845840148,-1.1231763915,-1.0376207074
H,0,2.0261749682,-1.3480859734,-1.8489304481
O,0,0.1557603521,-0.6086491424,0.1791594755
H,0,0.7699443939,1.7072019841,-0.6178084193

g3: HF=-1185.6885433,ZeroPoint=0.1082574

Si,0,-1.4100526937,-0.0314337915,0.0124270042
O,0,-0.857052809,1.6583997421,-0.0220660048
H,0,-1.3458639422,2.1485718702,-0.6840404995
O,0,-2.0094846288,-1.7009680437,-0.0265405973
O,0,-2.1321666053,0.2394572226,1.5114076861
H,0,-2.5317518554,-0.5818546176,1.8057708338
H,0,-1.2849688801,-2.3180510518,0.0744627193
O,0,-2.2513565373,0.2869236199,-1.4228078776
H,0,-2.6855396063,-0.517048582,-1.7152661141
Si,0,1.7126798519,-0.0969755294,-0.025850232
O,0,2.6199557797,-0.6836735114,1.2093987077
H,0,2.4552024984,-0.3039611224,2.0740236211
O,0,1.7335983639,1.5325597761,-0.0463163834
O,0,2.5066157409,-0.7521700247,-1.3050062569
H,0,2.0972871724,-0.6366714581,-2.1641430271
O,0,0.1842182929,-0.6115433322,0.0402160041
H,0,0.7854354478,1.8284116639,-0.0597418337

g4: HF=-1185.6885664,ZeroPoint=0.1083851

Si,0,-1.4034755754,-0.0152442352,0.0474994825
O,0,-0.8535462985,1.6750937707,0.086617156
H,0,-1.3718642719,2.2032779034,-0.5215915077
O,0,-1.9835918174,-1.6877619313,-0.0710920556
O,0,-2.1823251905,0.1987067668,1.5273553455
H,0,-2.593668926,-0.632356549,1.7745276809
H,0,-1.2603636981,-2.3030181724,0.0481761788
O,0,-2.2098299682,0.348035645,-1.3966898375
H,0,-2.6325673182,-0.4476588184,-1.7263864615
Si,0,1.7129206461,-0.0516252974,-0.0190706135
O,0,2.6439301861,-0.7023876484,1.1700395973
H,0,2.2823790081,-0.6798194894,2.0580493204
O,0,1.7398001919,1.5745820427,-0.0116814318
O,0,2.4358180043,-0.5331344828,-1.41157697
H,0,2.673493231,-1.4597915098,-1.4763759926
O,0,0.194900452,-0.5816786702,0.119368165
H,0,0.7922054747,1.8692471959,0.0075650938

g5: HF=-1185.6884163,ZeroPoint=0.1084611

Si,0,1.236249597,0.1193408727,-0.1973822606
O,0,1.8581489028,-0.5955439142,-1.5914321641
H,0,2.3716212332,-1.3637380693,-1.3323865362
O,0,2.06649542,1.3814663935,0.5686097846
O,0,2.0880738625,-1.0443194873,0.8363994287
H,0,1.4661169658,-1.6445911957,1.2472210459
H,0,2.6296396713,1.0148075103,1.253328047
O,0,0.4273931643,1.3518741721,-1.1916329507
H,0,0.8593912779,2.1990743202,-1.0776760827
Si,0,-1.8256558042,-0.1732465136,0.2810042163
O,0,-2.1183865905,0.9946336738,-0.8181367605
H,0,-1.2323720781,1.3374977001,-1.1048743178
O,0,-2.2875148778,0.2309356541,1.8038401766
O,0,-2.7217580191,-1.5020355312,-0.0863808754
H,0,-2.7823829149,-1.7272090001,-1.0166542859
O,0,-0.248545926,-0.4892800515,0.3537070551
H,0,-3.2299152842,0.2946726459,1.9684460399

g6: HF=-1185.6885974,ZeroPoint=0.1085442

Si,0,-1.3768081029,0.1448080039,0.128745737
O,0,-0.586860528,1.5462202213,0.9558456235
H,0,-0.9033612611,2.3640493002,0.5692303048
O,0,-2.3299217233,-1.0974124694,-0.6405403165

O,0,-1.7998093122,-0.4593234695,1.6515503477
H,0,-1.4530359696,0.1165578635,2.3357763017
H,0,-2.3297860515,-1.9100920674,-0.1342881699
O,0,-2.1687854392,1.2936951649,-0.8321166877
H,0,-2.8072910103,0.8587900843,-1.4007549078
Si,0,1.6661455676,-0.1814840694,-0.3276941703
O,0,1.9627749772,1.0580612919,0.6850579943
H,0,1.0803144387,1.4476266855,0.9175597838
O,0,2.1946685796,0.096292805,-1.8621019922
O,0,2.4977971099,-1.4572628396,0.2944367788
H,0,2.6038228723,-2.2201505914,-0.2767163969
O,0,0.0882631112,-0.4619248084,-0.4542096446
H,0,3.1418017416,0.1860698947,-1.9825835857

g7: HF=-1185.6881055,ZeroPoint=0.1085342

Si,0,1.3183493463,0.0328662801,-0.2128430823
O,0,1.9128209343,-0.8417426287,-1.5253244956
H,0,2.4201718658,-1.5833489499,-1.1885189043
O,0,2.1756169749,1.360412378,0.3969994001
O,0,2.1684832697,-1.0195999332,0.9353057279
H,0,1.5449255961,-1.5635887381,1.4160700237
H,0,2.7417536995,1.0642873265,1.1127001193
O,0,0.5119078331,1.1579118535,-1.3290514442
H,0,0.9567355981,2.0060170221,-1.3166682363
Si,0,-1.739787729,-0.1601329751,0.3136735495
O,0,-2.0376904766,0.888199568,-0.894365918
H,0,-1.1517861265,1.1833293825,-1.2289951855
O,0,-2.1776361071,0.41387869,1.7929247424
O,0,-2.6410491327,-1.4921785346,-0.0275777465
H,0,-2.7604987638,-2.1240513435,0.6837034144
O,0,-0.1670245334,-0.4875548391,0.4207938259
H,0,-3.1117132888,0.5774116216,1.9354871995

g8: HF=-1185.6881055,ZeroPoint=0.108528

Si,0,-1.2647155433,-0.0845641211,0.2944189721
O,0,-0.5305059146,1.0275393745,1.4720309218
H,0,-1.0360701012,1.8399882687,1.5129718594
O,0,-2.048299592,-1.1257662046,-0.9099305971
O,0,-1.7776221427,-1.0789957822,1.5548972924
H,0,-2.2320128058,-1.8348510642,1.1766856243
H,0,-1.3918255405,-1.589790327,-1.4291579648
O,0,-2.224509448,1.2103898692,-0.2263535405
H,0,-2.7764491941,0.9170656654,-0.9541887348
Si,0,1.7925805661,-0.0157077178,-0.2663436322

O,0,2.0267191041,0.9762111222,1.0018582762
H,0,1.1253696707,1.183032913,1.3608768574
O,0,2.1674753088,0.6791948084,-1.7107288693
O,0,2.7951351206,-1.2943232115,-0.015432856
H,0,2.9506865744,-1.8722240374,-0.7646252126
O,0,0.2474313198,-0.4535217542,-0.3808847307
H,0,3.0844954476,0.9230469986,-1.8492630757

g9: HF=-1185.6886031,ZeroPoint=0.1095444

Si,0,1.3280904119,-0.0007390376,-0.0906830819
O,0,0.6952942346,1.5944868487,0.3170436639
H,0,1.3812541118,2.1844076837,0.631365695
O,0,1.3455522781,-0.4496851833,1.5529795767
O,0,2.6831739716,0.753711459,-0.763386098
H,0,3.2602400953,0.0907083811,-1.1488329656
H,0,1.7145425596,-1.3324666114,1.6341927266
O,0,1.9789008155,-1.5448553081,-0.6306742265
H,0,1.2735096223,-2.1588096558,-0.8363634528
Si,0,-1.606249455,-0.01783275,-0.097475235
O,0,-2.8679718643,-0.7669214401,-0.8233258163
H,0,-2.9739209155,-1.7017373723,-0.6390933852
O,0,-1.96844871,1.5708575226,-0.2631196175
O,0,-1.550233465,-0.5042523095,1.4724046277
H,0,-0.6359702783,-0.5470772438,1.7993715269
O,0,-0.1834505735,-0.373111837,-0.7907909938
H,0,-1.1390228392,2.0542138537,-0.1066039442

g10: HF=-1185.6884708,ZeroPoint=0.1095441

Si,0,1.3171840408,-0.0152685801,-0.0630401594
O,0,2.6800187184,0.7511835967,-0.7067283223
H,0,3.2497321389,0.0981954548,-1.1192096387
O,0,1.332181697,-0.5299903616,1.5612610381
O,0,1.9512115929,-1.5424691358,-0.6673301363
H,0,1.2388310544,-2.1404948071,-0.8948307866
H,0,1.6932361404,-1.4186406815,1.6062554816
O,0,0.703473083,1.5699836057,0.4070326705
H,0,1.3995449366,2.1440577363,0.7283378303
Si,0,-1.6184493901,-0.0174533523,-0.0546757946
O,0,-1.9601984183,1.5846413144,-0.1530731674
H,0,-1.1222540807,2.0525068376,0.0086962142
O,0,-1.5667667171,-0.5713667671,1.4891189415
O,0,-2.8721134561,-0.8142308858,-0.742788651
H,0,-3.2833374765,-0.3926354459,-1.4993082424
O,0,-0.2006564281,-0.3464177834,-0.7702378509

H,0,-0.6520124355,-0.6352457451,1.8105535731

g11: HF=-1185.6850915,ZeroPoint=0.1091011

Si,0,-1.3347730254,0.0225415469,0.2176036006
O,0,-0.6238472303,1.2310789779,1.3236882103
H,0,-0.8756723334,2.1093164425,1.0343204309
O,0,-2.1170379082,-1.1509449415,-0.8574029415
O,0,-1.6719019037,-0.9109528883,1.5848715981
H,0,-2.0078607121,-1.7680668953,1.3169565494
H,0,-3.0558474172,-1.2429130104,-0.6843032746
O,0,-2.3022723041,1.2825169485,-0.382708728
H,0,-2.816077039,0.988495439,-1.1364913
Si,0,1.6949002109,-0.0668309964,-0.2947108674
O,0,1.9352343389,0.7697828407,1.0808547711
H,0,1.0419435871,1.0902443422,1.3723314931
O,0,2.2593120573,0.7037957691,-1.6353494892
O,0,2.5323712133,-1.4684474804,-0.0970383202
H,0,2.6607448047,-2.0053819093,-0.8811043163
O,0,0.1257698299,-0.2977952158,-0.5622025852
H,0,3.2089974612,0.8202929506,-1.6986186212

g12: HF=-1185.6844552,ZeroPoint=0.1097292

Si,0,1.611689915,-0.0012401681,-0.1617268568
O,0,2.8642196394,-0.5828153585,-1.0374932436
H,0,3.0027794464,-1.5311872962,-1.0137913935
O,0,1.6471326179,-0.6986003577,1.3279577839
O,0,1.895093573,1.6104376393,-0.102234804
H,0,1.0485585993,2.0122255436,0.1659412661
H,0,0.7541637332,-0.7918823811,1.6977668106
O,0,0.1703564832,-0.3121034984,-0.833110844
Si,0,-1.3061638071,-0.0450814534,-0.0516340548
O,0,-1.9153292918,-1.5722694837,-0.6974113265
H,0,-2.829342581,-1.7483491313,-0.4666967922
O,0,-2.5601926867,0.8182018459,-0.8007298326
H,0,-3.0739516642,0.261830274,-1.3879578979
O,0,-0.7666458961,1.5085663139,0.6180663509
H,0,-1.327532523,2.210873063,0.2870723166
O,0,-1.2615399016,-0.6698750595,1.5361146573
H,0,-1.4982736558,-1.5999674917,1.5119398605

g13: HF=-1185.6795893,ZeroPoint=0.107744

Si,0,1.3451009087,-0.0607568282,0.035629655
O,0,2.2325182619,-0.4694335978,1.4136063828
H,0,2.7432699096,0.299793785,1.6732229047

O,0,1.9163075631,-0.3482766237,-1.5327326516
O,0,2.1421879453,1.5417849108,0.0425767482
H,0,1.4852923891,2.2359661346,-0.0074167446
H,0,2.3726854124,0.4392162553,-1.8367835107
O,0,0.6303265645,-1.6454825936,0.1069296109
H,0,0.0455977281,-1.806698116,-0.6357255406
Si,0,-1.7004035317,0.2801659279,0.1440227892
O,0,-2.0791281848,-0.28618322,1.6338794259
H,0,-2.9964032788,-0.5220013568,1.7850882702
O,0,-2.0820095673,-0.8968419274,-0.9384499793
O,0,-2.6528479887,1.5533769822,-0.2770346896
H,0,-2.3743236258,2.4183152226,0.0295999339
O,0,-0.1658788844,0.7425401185,0.1491755121
H,0,-2.2944305312,-0.6035736332,-1.8268411266

g14: HF=-1185.6805212,ZeroPoint=0.1094136

Si,0,1.337498652,0.1100071732,-0.0707617914
O,0,0.9291068077,1.7556523384,0.2951562219
H,0,-0.0023233991,1.9639066941,0.2087325421
O,0,1.2622504614,-0.3551900854,1.5720893147
O,0,2.7919932137,0.6829916775,-0.7130221989
H,0,3.2853348907,-0.0619453591,-1.0628074212
H,0,1.5781409891,-1.2597406532,1.6433985219
O,0,1.8538477927,-1.5146870614,-0.5735724926
H,0,1.0993240401,-2.0519305868,-0.8153146776
Si,0,-1.6334573501,-0.1085228572,-0.1153104417
O,0,-2.7561829008,-1.0599897915,-0.8295146194
H,0,-3.1765232238,-0.7204148448,-1.6216118751
O,0,-2.0945103552,1.4736406813,-0.1888006705
O,0,-1.5497863769,-0.6439551296,1.4273530421
H,0,-0.6383120177,-0.5899597253,1.7686489636
O,0,-0.1910086926,-0.1742715945,-0.8247183128
H,0,-2.8737117413,1.7315018742,0.3080393949

h1: HF=-1185.6727255,ZeroPoint=0.106182

Si,0,1.0790035605,-0.0224746682,0.0329381019
O,0,1.0064870923,-1.2557568552,-1.0552076986
H,0,1.8087675415,-1.0901452621,-1.6080703785
O,0,1.0180577529,1.4619622303,-0.6753410899
O,0,2.2201640017,-0.191279898,1.1941748055
H,0,3.101228649,-0.1415840558,0.8098844252
H,0,1.8192233665,1.4452594209,-1.2547351487
O,0,3.0061505722,0.2057840942,-1.6448416491
H,0,3.9619330708,0.1985169503,-1.580137227

Si,0,-1.8032662944,-0.0046156188,0.1065878542
O,0,-1.9236931779,-1.2200303289,-0.9840961635
H,0,-1.0598044559,-1.5230701825,-1.2992012762
O,0,-1.9170357244,1.4814825424,-0.56363624
O,0,-3.0579120365,-0.0982856299,1.1367432985
H,0,-3.3528831949,-0.9747856833,1.3909362507
O,0,-0.3514067287,-0.1286833082,0.8445326613
H,0,-1.0512615648,1.8476669429,-0.793741966

h2: HF=-1185.6694576,ZeroPoint=0.105725

Si,0,1.1664572697,0.1318312706,-0.2363004312
O,0,1.0496523532,-0.8450707231,1.0884894776
H,0,2.0116549488,-1.0488654941,1.2359049464
O,0,1.7895930541,-0.5337835713,-1.5973624224
O,0,1.7442882064,1.6426633821,0.0864440362
H,0,1.0740388104,2.327358,0.0339773305
H,0,2.6996091692,-0.7588149917,-1.30906554
O,0,3.4252876123,-0.6981361934,0.35893097
H,0,4.0104538754,-0.0036467286,0.6652909732
Si,0,-1.855149721,-0.1508562651,-0.1163882473
O,0,-1.6636327454,-0.9971431591,1.2670379264
H,0,-0.7258238703,-1.1669075883,1.4665269948
O,0,-2.4703961288,-1.0411078702,-1.34213991
O,0,-2.9373629195,1.0500728703,0.1405951983
H,0,-2.8696823605,1.5233228306,0.9722058691
O,0,-0.4242157822,0.3995428943,-0.6322010538
H,0,-3.3829193917,-1.3259005431,-1.2657766777

h3: HF=-1185.6694612,ZeroPoint=0.1060568

Si,0,1.1619712257,-0.0736800623,0.4238352497
O,0,1.2138881224,-1.3092905915,-0.6630559186
H,0,2.0866357269,-1.1379291924,-1.0985181463
O,0,1.2087616919,1.4358320707,-0.232227526
O,0,2.1118232223,-0.2822098037,1.7453647895
H,0,1.6287967898,-0.3947045378,2.5670252948
H,0,2.0808368803,1.411279889,-0.6992726244
O,0,3.2453917389,0.1481327978,-0.9798581433
H,0,4.0796950481,0.0730461798,-0.5145325523
Si,0,-1.7043048741,-0.0072934628,0.0299762264
O,0,-1.6672345662,-1.2114974094,-1.0802866029
H,0,-0.7665290846,-1.5297452809,-1.2416873255
O,0,-1.6824219291,1.486632853,-0.6343714703
O,0,-3.1155045882,-0.0862401853,0.8368288403
H,0,-3.4658670405,-0.9597356812,1.0211953041

O,0,-0.3967621245,-0.1638530402,0.992593813
H,0,-0.7826900092,1.839082287,-0.6977350782

h4: HF=-1185.66501,ZeroPoint=0.1055997

Si,0,1.2110444058,-0.2847120195,0.1201270067
O,0,1.1236216357,1.2575845652,-0.4549767199
H,0,2.1021876523,1.4260641702,-0.575147549
O,0,1.7962443661,-0.4176786068,1.6558742544
O,0,1.7151351971,-1.4841799588,-0.8834615829
H,0,2.6568656807,-1.3337788539,-1.0348317955
H,0,1.1167294123,-0.6473961029,2.2930303426
O,0,3.4725479769,0.4980444857,-0.3606784006
H,0,3.8306587936,0.4470683768,-1.2507295944
Si,0,-1.8120362132,0.050027442,0.0058569847
O,0,-2.5275803483,-0.8052934222,-1.1909185794
H,0,-3.4446245407,-0.6052285934,-1.3872868668
O,0,-1.5685585497,1.6193568518,-0.3764189029
O,0,-2.842278664,-0.0322414873,1.2762758543
H,0,-2.7102282474,0.6048256402,1.9810719789
O,0,-0.3985769345,-0.6762241853,0.2985643368
H,0,-0.6249798525,1.8133090681,-0.521349427

h5: HF=-1185.6647953,ZeroPoint=0.105962

Si,0,1.1049733315,0.3085869693,-0.0076285037
O,0,1.1188111073,-0.5020013314,1.4209015872
H,0,2.0360339165,-0.9027001889,1.3528642704
O,0,1.1316551733,-0.605553294,-1.3841414727
O,0,2.0312237091,1.6612018605,-0.0656802155
H,0,1.5230221207,2.4729857893,-0.1265000113
H,0,1.9864245168,-1.0571862342,-1.4015235463
O,0,3.2748903881,-0.862943261,0.2497156131
H,0,3.4342271197,-1.7801638864,0.013179154
Si,0,-1.7780007476,-0.0707987535,-0.0006835517
O,0,-1.7318248935,-0.9128586036,1.4035420038
H,0,-0.8261021493,-1.0028952825,1.7382306197
O,0,-1.798864833,-1.0297228001,-1.3263583973
O,0,-3.17863089,0.7567188328,-0.0686418615
H,0,-3.504210097,1.1316410025,0.7518133333
O,0,-0.4583381319,0.8811868217,-0.0685633574
H,0,-0.9142759505,-1.1680458605,-1.6905569543

h6: HF=-1185.6609312,ZeroPoint=0.1032681

Si,0,1.02454715,-0.2542520186,0.0826672232
O,0,0.8395322559,1.2425391942,0.7144424354

H, 0, 1.894157212, 1.3453076808, 0.9011764034
O, 0, 1.3931741112, -1.4750650563, 1.1308497339
O, 0, 1.8348709874, -0.3659678786, -1.3537660677
H, 0, 1.2648567264, -0.6520024339, -2.0713275761
H, 0, 0.6735701116, -2.104377413, 1.21661249
O, 0, 3.1203604325, 0.6809313031, 0.8476881262
H, 0, 3.5942367188, 0.9404106752, 0.0551171475
Si, 0, -1.9830090573, 0.0624178928, -0.3160127963
O, 0, -3.0816820945, -0.850884519, 0.4826231757
H, 0, -2.8632041864, -1.1043076306, 1.3810816294
O, 0, -2.6897781911, 0.163191797, -1.7887133497
O, 0, -1.8015818443, 1.5386145415, 0.3558970057
H, 0, -0.8662418654, 1.7016042359, 0.5982263549
O, 0, -0.5377449641, -0.6696726094, -0.3776370778
H, 0, -2.3086383127, 0.787628399, -2.4083267777

h7: HF=-1185.6608593,ZeroPoint=0.1033746

Si, 0, 1.1854609666, -0.2860727981, 0.1000149275
O, 0, 1.0170674982, 1.2791655502, -0.341539292
H, 0, 2.0791325567, 1.4161141332, -0.4385534247
O, 0, 1.7821628498, -0.5781551841, 1.6112492048
O, 0, 1.7668287106, -1.332915142, -1.0395277911
H, 0, 1.1059651456, -1.9723398439, -1.3152695645
H, 0, 1.1215430571, -0.9647376419, 2.1903943054
O, 0, 3.3206136351, 0.7998615363, -0.2604939857
H, 0, 3.6372835077, 0.4644265386, -1.1014659909
Si, 0, -1.849163017, -0.1072637209, 0.0898788578
O, 0, -2.8587787725, -0.944794188, -0.8932196133
H, 0, -2.7458887551, -0.8149568669, -1.8368652456
O, 0, -1.6632077595, 1.40563578, -0.4938568478
O, 0, -2.5530214135, -0.1532027095, 1.567076284
H, 0, -3.4863881873, 0.0610560818, 1.615739131
O, 0, -0.4032299541, -0.8121807325, 0.2559622625
H, 0, -0.7160609486, 1.6529931978, -0.5242792175

h8: HF=-1185.6608928,ZeroPoint=0.1034765

Si, 0, -1.2608906555, -0.2790680884, 0.0250034057
O, 0, -1.0790693089, 1.3370918159, -0.1468649127
H, 0, -2.134697808, 1.5145090548, -0.0715717164
O, 0, -1.9185584215, -1.1072996723, -1.2422313975
O, 0, -1.790516523, -0.8214978339, 1.4936769347
H, 0, -1.1179999815, -1.3233700359, 1.9600995433
H, 0, -1.2773840393, -1.6809497953, -1.667758343
O, 0, -3.3836815702, 0.8881974405, 0.029191494

H,0,-3.6742379121,0.893931939,0.9433319237
Si,0,1.7743306361,-0.1336888873,-0.0760644132
O,0,2.5257155314,-0.4711177321,1.3387534339
H,0,3.4641706511,-0.2820869836,1.3933301036
O,0,1.5958439785,1.4653169698,-0.3507812104
O,0,2.7362975177,-0.7766035589,-1.2370976689
H,0,2.5990065622,-0.4620504061,-2.1327437663
O,0,0.3227874839,-0.842226552,0.003683743
H,0,0.652652579,1.7239549657,-0.2990225135

h9: HF=-1185.6566479,ZeroPoint=0.1045473

Si,0,-1.1517129922,0.1091662532,-0.0669034194
O,0,-1.1168327483,-1.2212829478,-1.037910465
H,0,-0.2184254594,-1.4910484576,-1.2692007188
O,0,-1.579266034,-0.120290916,1.4859111862
O,0,-1.7873335514,1.4413136055,-0.8120617285
H,0,-1.1089686068,2.0689585045,-1.0715314815
H,0,-2.5728640103,-0.3041366475,1.2891686181
O,0,-3.5816807512,-0.4664823686,0.1693393022
H,0,-4.0401677956,0.3629485686,0.0218285463
Si,0,1.9216040968,-0.1068905919,-0.0732182482
O,0,1.7429545823,-1.3479900832,-1.1347015814
H,0,2.4594409488,-1.9778329882,-1.2345848064
O,0,2.5062785292,-0.7600468839,1.3032293844
O,0,3.0183902009,1.0080407088,-0.5464421852
H,0,2.7379847118,1.6583513372,-1.1934659679
O,0,0.4654572672,0.558870676,0.0450134886
H,0,2.8841432421,-0.1649417791,1.9537258166

k1: HF=-1185.6683167,ZeroPoint=0.1054353

Si,0,1.3140397214,0.3243562066,-0.0346481023
O,0,2.2096926388,0.1709615116,-1.3990696579
H,0,2.5531265979,-0.7439787942,-1.297973162
O,0,2.0725111514,0.2615402698,1.4181200068
O,0,2.4115163998,-1.8634778556,0.0981459901
H,0,1.7753571447,-2.5804018551,0.1039019853
H,0,2.4321689374,-0.6545316331,1.398440073
O,0,0.7854373069,1.9175659372,-0.0962052195
H,0,1.3773155046,2.5675945069,0.286107734
Si,0,-1.7045494264,-0.1337055872,0.0167239505
O,0,-2.5455971163,-0.7490954859,-1.2412636533
H,0,-2.3165521268,-0.4315052134,-2.1164601389
O,0,-1.893767354,1.481938456,0.1513902681
O,0,-2.3974468746,-0.9234915149,1.2675266214

H,0,-2.1238095195,-0.6682901253,2.1502788342
O,0,-0.122923369,-0.4715094217,-0.1163040155
H,0,-1.0391306562,1.9470522186,0.1050959661

k2: HF=-1185.6683463,ZeroPoint=0.1057196

Si,0,1.362894996,-0.160049392,-0.1767608032
O,0,2.441554434,-0.4388834836,1.0255223328
H,0,2.7328687235,0.4763870388,1.2332597942
O,0,1.8996671798,0.4991716944,-1.5791497571
O,0,2.3474223044,2.0136489072,0.3926279612
H,0,1.6871174475,2.6164794852,0.7380552235
H,0,2.2239126838,1.3721037591,-1.2605286216
O,0,0.9050585406,-1.7034451936,-0.6549249362
H,0,1.4549236553,-2.1112695333,-1.3260290072
Si,0,-1.6470663977,0.0470500402,0.2318428844
O,0,-2.3871791385,0.2044342561,1.6824772506
H,0,-1.959816152,-0.1979187159,2.4411602737
O,0,-1.8030598707,-1.4518311195,-0.3862058262
O,0,-2.4467472304,1.0556797243,-0.773999318
H,0,-2.6339023552,1.9399800863,-0.453440276
O,0,-0.0743071523,0.418904008,0.3768085454
H,0,-0.9372988781,-1.832357412,-0.6176475402

k3: HF=-1185.6674797,ZeroPoint=0.1065735

Si,0,-1.1723746921,-0.0155887492,-0.3348291956
O,0,-2.3832698335,0.4549952326,-1.3268603199
H,0,-2.605805224,1.3367102118,-0.9549948894
O,0,-1.4328301132,-0.2261917187,1.283558389
O,0,-1.9660026011,2.1080968878,0.5284538048
H,0,-1.2812920032,2.7779005961,0.4923456987
H,0,-1.7129532165,0.6876591907,1.5309735277
O,0,-0.8174556982,-1.5718750306,-0.8457854444
H,0,-1.4489698327,-2.2528756521,-0.6080509492
Si,0,1.6984287117,0.1110844811,-0.02215807
O,0,2.070499608,-1.2897650975,-0.7845418574
H,0,1.2709155997,-1.787443985,-1.0064205733
O,0,1.533619275,-0.0619994724,1.5960818502
O,0,2.9442864083,1.1392028378,-0.2192801224
H,0,3.4066672324,1.1130160072,-1.0590490346
O,0,0.2951163951,0.6834044819,-0.6257118287
H,0,0.6114767242,-0.1665810516,1.8714830247

k4: HF=-1185.664823,ZeroPoint=0.1059515

Si,0,1.3598402952,0.3286046388,-0.0298809484

O,0,2.4200100565,0.2248718039,-1.2811592316
H,0,2.7004499345,-0.710946939,-1.2183662311
O,0,1.8995609154,0.1410137443,1.5158401082
O,0,2.2249718146,-1.8987650594,0.0616069721
H,0,1.5112532095,-2.5169226826,-0.1032511152
H,0,2.1713948006,-0.7986311407,1.5154380031
O,0,1.0052904871,1.9554388446,-0.0932275556
H,0,0.1016266925,2.1631498701,0.1663580818
Si,0,-1.667104699,-0.1375327187,-0.0253979408
O,0,-2.6017861568,-0.5109656105,-1.3086826128
H,0,-2.4048352296,-0.0767620903,-2.1406626294
O,0,-1.770780773,1.4500556558,0.3939441376
O,0,-2.2895852674,-1.1158073461,1.1228302919
H,0,-1.8854406183,-1.0889900676,1.992106603
O,0,-0.1065262468,-0.3969003606,-0.3130436572
H,0,-2.6277084448,1.800549368,0.6453953045

k5: HF=-1185.6647868,ZeroPoint=0.1059971

Si,0,1.3011248286,0.3547174544,-0.1005151941
O,0,2.384008525,0.2147871603,-1.3282953462
H,0,2.6897248004,-0.7076530793,-1.2094627663
O,0,1.8186396829,0.2695538258,1.461561661
O,0,2.2282478213,-1.8370598835,0.1262765468
H,0,1.533998153,-2.482203191,-0.0168537308
H,0,2.1161907702,-0.6601376824,1.5195689981
O,0,0.8998864244,1.9646178722,-0.2587804077
H,0,-0.0117924981,2.1605585727,-0.0195617016
Si,0,-1.6969341086,-0.209389126,-0.0282255922
O,0,-2.6253164986,-0.7930006913,-1.2396215642
H,0,-2.3218618824,-0.6495059703,-2.1383248598
O,0,-1.8820206429,1.4010398898,0.2254376074
O,0,-2.2047197317,-0.9549269667,1.33136403
H,0,-2.3745712469,-1.8978784688,1.2860605309
O,0,-0.1403519247,-0.425157606,-0.3706626726
H,0,-2.7335800319,1.7246302002,0.5257112512

k6: HF=-1185.6651978,ZeroPoint=0.1068452

Si,0,1.2245842818,0.3998398217,-0.1087165319
O,0,2.5494924525,0.4851054056,-1.0672319842
H,0,2.8276369633,-0.4533038853,-1.1029630661
O,0,1.3283056589,-0.0956066851,1.4712818663
O,0,2.0911639139,-1.8176102169,-0.183366385
H,0,1.452330293,-2.402334358,-0.5940907355
H,0,1.6574866932,-1.0137605541,1.3432336443

O,0,0.8793938337,2.0243024454,0.0463941203
H,0,-0.0605140348,2.2240378767,0.0799784195
Si,0,-1.6206246324,-0.2387940616,-0.10999841
O,0,-2.109987778,1.3319070515,-0.114489294
H,0,-2.9025148441,1.5586447737,0.3768552903
O,0,-1.5222754316,-0.8524955504,1.3995163428
O,0,-2.6740604491,-1.2061820822,-0.8876886455
H,0,-3.0992688535,-0.860760013,-1.6748074782
O,0,-0.1592666147,-0.2010849373,-0.8081771131
H,0,-0.6538669421,-0.6972415808,1.8005506702

k7: HF=-1185.6626614,ZeroPoint=0.1064692

Si,0,-1.8250678087,0.3556014126,0.0769181974
O,0,-3.1620579093,0.3484072164,1.0038729221
H,0,-3.5440019463,-0.5050541573,1.2172676347
O,0,-1.985488191,-0.7939198466,-1.0809271063
O,0,-1.7543882741,1.8691626363,-0.5385769222
H,0,-0.841695012,2.125413789,-0.7311100211
H,0,-1.1368714711,-1.1522335207,-1.3745814844
O,0,-0.4594827467,0.0623279357,0.9135741705
Si,0,1.046616309,-0.0358068506,0.2395048392
O,0,1.1686937956,-2.224741748,1.2704594379
H,0,1.9867872382,-2.7267636504,1.2173323166
O,0,2.2619327153,0.1342650417,1.3233826627
H,0,2.2479544935,-0.7073735235,1.8127516173
O,0,1.1638253902,1.3940055273,-0.6293028211
H,0,1.6883086796,2.0767242499,-0.2071011731
O,0,1.0201122761,-1.1146862586,-1.007108825
H,0,1.0221442718,-1.9563681132,-0.4935374253

k8: HF=-1185.6584438,ZeroPoint=0.1042577

Si,0,-1.3109571061,-0.0759193082,0.1011217218
O,0,-1.023726265,1.592409096,0.056451063
H,0,-1.5894483611,2.0666388713,-0.5562282044
O,0,-1.9684063414,-2.4537032141,-0.1610215922
O,0,-2.0785271986,-0.2566539491,1.5511617124
H,0,-2.1750906139,0.5799052461,2.012592789
H,0,-2.6848587135,-2.6012333169,0.4594158241
O,0,-2.1503844593,-0.3277423838,-1.2670374974
H,0,-2.3082166643,-1.3371782171,-1.0944277907
Si,0,1.7356063567,-0.1042587578,-0.0238938962
O,0,2.7238451292,-0.5793620022,1.1867105925
H,0,2.6164216395,-0.1406660738,2.0323771011
O,0,1.6944340667,1.5232561297,-0.1422917212

O,0,2.4579598127,-0.8061541271,-1.3108656083
H,0,1.9942619126,-0.7626337732,-2.1489602482
O,0,0.2237339657,-0.6564103642,0.1763449426
H,0,0.77762397,1.8541938745,-0.1109958178

k9: HF=-1185.654643,ZeroPoint=0.1049921

Si,0,-1.2868868453,0.3509631585,0.0730543692
O,0,-0.8732175943,1.9661551314,-0.0608231427
H,0,0.0362499304,2.1163773438,-0.3404476203
O,0,-2.1453638433,-1.9610998299,0.0583742909
O,0,-2.2388832407,0.4122394825,1.422800998
H,0,-2.2028938621,1.2834819858,1.8260136063
H,0,-2.9218937614,-1.9430797441,0.6209883573
O,0,-2.0013406652,0.0091439536,-1.3542778286
H,0,-2.2829090083,-0.936996905,-1.1179596615
Si,0,1.7274885064,-0.2021771514,0.0095315879
O,0,2.6782827852,-0.4481176396,1.3116687584
H,0,2.5427450148,0.1223023418,2.0706008928
O,0,1.8598469851,1.3279456794,-0.5808143795
O,0,2.3029615967,-1.3198226467,-1.0298629206
H,0,1.8414480407,-1.4278944787,-1.8635621319
O,0,0.1663813799,-0.3905236821,0.3425740251
H,0,2.7225142616,1.6345382407,-0.8675103807

m1: HF=-1185.6785809,ZeroPoint=0.1055095

Si,0,-1.4830650573,-0.0970379036,0.0902859888
O,0,-2.1027371312,0.3060873959,1.574345578
H,0,-1.8620795009,1.2036821733,1.8145995737
O,0,-2.2369263132,-1.6083063611,-0.05602469
O,0,-0.7189952148,1.912381024,0.1937642679
H,0,-1.0423050401,2.3484421684,-0.5987775986
H,0,-1.6693144083,-2.3388245283,0.1903265867
O,0,0.07624674,-0.6108946403,0.0496842749
O,0,-2.1770386336,0.5624556666,-1.2743463176
Si,0,1.6358195381,-0.0782059153,0.013721976
O,0,2.3734291943,-0.7128089407,-1.3246060486
O,0,1.670505885,1.5017813851,0.0981208624
H,0,0.3699071825,1.8401241028,0.1364330564
O,0,2.4483834239,-0.9031510343,1.19575913
H,0,2.0915589412,-0.8135789152,2.0807734269
H,0,2.3618365087,-0.1414400553,-2.0938307713
H,0,-2.6971613043,-0.0986569121,-1.7371931856

m2: HF=-1185.6748079,ZeroPoint=0.1065067

Si,0,-1.4349772352,-0.2065762117,-0.0501795067
O,0,-1.7947656917,0.1110661966,1.5294858913
H,0,-2.1735110428,-0.6644626808,1.9506246947
O,0,-2.0992860027,-1.7431107329,-0.2292375476
O,0,-0.7398642279,2.0585167764,0.1737791478
H,0,-0.9286477702,2.4095241443,-0.6998408322
H,0,-1.4510565774,-2.4318292204,-0.3814016163
O,0,0.1258291572,-0.4783172352,-0.4095023084
O,0,-2.3279485164,0.6070687626,-1.1803122979
Si,0,1.660402404,-0.020121597,0.0221551392
O,0,2.6185649941,-0.5574731647,-1.2211385942
O,0,1.731026512,1.5101592222,0.3733084112
H,0,0.2730655592,1.963919711,0.2482862697
O,0,2.1531544344,-1.0379846286,1.2369104006
H,0,2.2149609794,-0.6141062225,2.0939910847
H,0,2.4253821325,-0.1767012787,-2.0791897646
H,0,-2.8793329686,0.0008709093,-1.6809992111

m3: HF=-1185.6748185,ZeroPoint=0.106585

Si,0,1.4272565856,-0.2709430416,-0.0210997273
O,0,1.7929445425,0.3504991934,-1.5056830294
H,0,2.1647553735,-0.3298941861,-2.0723768301
O,0,2.088171035,-1.8134053934,-0.151279511
O,0,0.7321781898,2.0009602188,0.2060715852
H,0,0.9615555388,2.1783264216,1.1214815854
H,0,1.4436822348,-2.5195418203,-0.0911514447
O,0,-0.13289606,-0.6073753982,0.2797081891
O,0,2.3193883523,0.3082143859,1.2461830973
Si,0,-1.6766883624,-0.05729359,0.0221764784
O,0,-2.597158919,-0.839915745,1.1635135212
O,0,-1.7518353819,1.5097521432,0.014115099
H,0,-0.2836649572,1.9252600595,0.1591918737
O,0,-2.2137109647,-0.7162777769,-1.4005687077
H,0,-2.2096472658,-1.6740118897,-1.4450831398
H,0,-2.4331929437,-0.581548859,2.0720235247
H,0,2.8766253824,-0.3810293523,1.615740506

p1: HF=-1185.6983265,ZeroPoint=0.1071801

Si,0,-1.0969043749,0.7879228007,0.0647920803
O,0,-1.4266232395,-0.3146689985,-1.0250326662
O,0,-2.0834740968,0.6557433875,1.3857092683
O,0,-1.1644156136,2.3710976971,-0.4094508741
H,0,-2.0393337011,2.7033632986,-0.6174856588
H,0,-2.6183362723,-0.1512688708,1.3412311714

Si,0,1.6304214078,-0.3743545752,0.0697860703
O,0,0.9839588941,-1.3220233887,-1.0827613838
H,0,0.0196253359,-1.0758061664,-1.2116335955
O,0,2.2495244094,-1.219244754,1.3287012194
O,0,2.9715534522,0.4074852293,-0.4507320239
H,0,2.8967896411,0.881544372,-1.2806663856
O,0,0.4784411929,0.6641201047,0.5722225865
H,0,1.6308512208,-1.7388166528,1.844889984
H,0,-2.5910974831,-1.2810550785,-0.347416622
O,0,-3.2972432848,-1.6817288641,0.2339884467
H,0,-2.9833938879,-2.5550775009,0.479520143

p2: HF=-1185.698308,ZeroPoint=0.1071856

Si,0,-1.5669927921,-0.0641604027,-0.2089904347
O,0,-1.5783279598,-0.4582773531,1.3261744362
O,0,-2.4691863513,1.2916762159,-0.4979776085
O,0,-2.078858507,-1.2053961916,-1.2915391375
H,0,-3.0135146372,-1.416327246,-1.2589520523
H,0,-2.7683098051,1.6936367787,0.3316770073
Si,0,1.3766997214,0.1001896153,0.1007062972
O,0,1.0182006878,-0.3836877564,1.6111752804
H,0,0.0228518732,-0.4738463306,1.7026682798
O,0,2.2091596712,1.5097757131,0.0546750884
O,0,2.4456615314,-0.8991560686,-0.6337992128
H,0,2.2368129173,-1.8347442571,-0.6212512156
O,0,-0.0182541328,0.2159804317,-0.7352612867
H,0,1.7647721192,2.284115355,0.4041276548
H,0,-3.7466083162,1.3395259164,2.6803247168
O,0,-2.8885348725,1.593960901,2.3334357095
H,0,-2.4158161174,0.747229829,2.0951954879

p3: HF=-1185.6982171,ZeroPoint=0.1071253

Si,0,-0.0659851819,0.1123410179,0.0728024977
O,0,-0.0258321265,0.0549444754,1.6562096807
O,0,1.4386714206,0.2210262255,-0.5949323507
O,0,-0.8606965851,1.3869127434,-0.6197956525
H,0,-1.8132015539,1.3934286478,-0.5117812858
H,0,2.12431211,0.1844554635,0.0889096543
Si,0,-1.3803826316,-2.5455262798,0.2795069006
O,0,-1.2024612511,-2.2612632415,1.8702949444
H,0,-0.7473775585,-1.3742149604,1.9953857803
O,0,-0.6524654197,-3.9271896276,-0.215089406
O,0,-2.9341087009,-2.8691054048,-0.1242516101
H,0,-3.5963244368,-2.2505216203,0.1885760019

O,0,-0.8033336265,-1.2530311257,-0.5302630713
H,0,0.3001171113,-3.9711990207,-0.1158003492
H,0,2.891779248,0.8679239538,2.4470246056
O,0,2.585554016,0.0547353984,2.0391015882
H,0,1.5884568265,0.087566925,2.0550135818

p4: HF=-1185.6981888,ZeroPoint=0.1071242

Si,0,1.1729985146,-0.6084229436,-0.0417386423
O,0,1.2506345853,0.4900893241,-1.1816267174
H,0,2.3044382978,1.6425525659,-0.6067102459
O,0,2.1578108785,-0.2648646062,1.2364762911
O,0,1.6264368265,-2.1483380068,-0.4395616976
H,0,1.041625202,-2.6138383989,-1.0397868603
H,0,2.5833360646,0.5983905766,1.1236980514
O,0,2.9765483395,2.1580157327,-0.079339685
H,0,2.5562620194,2.9875813366,0.1588867041
Si,0,-1.7063068374,0.1192863531,0.0885483509
O,0,-1.2745667318,1.1330519848,-1.106957516
H,0,-0.292062928,1.0259130521,-1.2879203627
O,0,-2.3661048514,0.884058772,1.3782049343
O,0,-2.9482477398,-0.8565801962,-0.3439491265
H,0,-2.8596928665,-1.3187522829,-1.1791767102
O,0,-0.387977817,-0.7361332184,0.5234257104
H,0,-1.7989929561,1.4931079549,1.8542605215

p5: HF=-1185.6982261,ZeroPoint=0.1072336

Si,0,1.0319034799,0.7790404932,0.0008971202
O,0,2.0468955032,0.4678134785,-1.2673749109
H,0,2.5058996955,-0.3771681794,-1.1461273968
O,0,1.2207631071,-0.2704293377,1.1735090566
O,0,3.0107459939,-1.8758000989,0.0913527518
H,0,2.6297948487,-2.733593472,-0.1101458236
H,0,2.3213008772,-1.3765327968,0.6134739769
O,0,1.2287481836,2.3790806377,0.3716606782
H,0,2.1238889809,2.6461669314,0.5873453258
Si,0,-1.7760181565,-0.1571781256,-0.0491747098
O,0,-3.060827226,0.7940064987,0.3198109556
H,0,-2.8917136754,1.5550034634,0.8786854623
O,0,-1.2688470856,-1.0708854253,1.192341405
O,0,-2.3272062893,-1.161700981,-1.2182162804
H,0,-2.88051633,-0.775646332,-1.899640164
O,0,-0.5310699454,0.7637621033,-0.557650386
H,0,-0.2930559617,-0.8979498573,1.3487099393

p6: HF=-1185.6981616,ZeroPoint=0.1072265

Si,0,-1.0053079945,0.7628354547,0.0901620485
O,0,-1.2500044448,-0.2846524993,-1.0738332522
O,0,-2.0364149374,0.5171845014,1.359831618
O,0,-1.1123173395,2.3679809402,-0.2949951531
H,0,-1.9901779942,2.6822008601,-0.5180696276
H,0,-2.5510843983,-0.2949049016,1.2372759789
Si,0,1.7668551892,-0.2746758965,0.1057003412
O,0,1.1975476896,-1.207403866,-1.0940281113
H,0,0.2300324511,-0.9907156126,-1.2463426529
O,0,2.4212011373,-1.1233896344,1.3479962751
O,0,3.0115215976,0.6019662371,-0.4962197615
H,0,3.6062985484,1.0056846287,0.1384269764
O,0,0.5519102124,0.6622589356,0.655974714
H,0,1.8116062489,-1.5633787444,1.9435551
H,0,-3.9004665693,-1.7776097429,-0.3663781469
O,0,-3.0433026134,-1.8458958383,0.0602150068
H,0,-2.402610363,-1.3293012517,-0.5055491534

p7: HF=-1185.6980933,ZeroPoint=0.1071947

Si,0,0.9667235885,0.9089777342,0.097366469
O,0,1.4006372579,-0.2229924941,-0.9235269887
H,0,2.5138769918,-1.1505938175,-0.1186646943
O,0,1.055243354,2.477360299,-0.4203569673
O,0,1.8385504876,0.8329700299,1.500674984
H,0,2.3832979502,0.031839945,1.5287268863
H,0,1.9407414849,2.8173567548,-0.5597063512
O,0,3.1723349203,-1.5234548834,0.5330466195
H,0,2.8453576622,-2.3908187612,0.782656928
Si,0,-1.7237876657,-0.3020119187,-0.083988316
O,0,-2.2673822051,-1.1129759045,1.2309721441
H,0,-3.0747627227,-1.6200558243,1.1296486189
O,0,-0.9936858223,-1.2414021115,-1.1928105354
O,0,-3.0578763892,0.4057495703,-0.7245055779
H,0,-2.9869093309,0.7107501984,-1.6311238849
O,0,-0.6451928369,0.7800864046,0.4723079296
H,0,-0.0199017246,-1.003684221,-1.2320362638

p8: HF=-1185.6980253,ZeroPoint=0.107213

Si,0,-1.0014038816,0.7648429103,0.0545847814
O,0,-1.2599183905,-0.3031004834,-1.087576334
O,0,-1.9777338853,0.5061827575,1.3642452651
O,0,-1.1669953088,2.3618271787,-0.3433658218
H,0,-2.0619663107,2.6510554152,-0.5290368034

H,0,-2.473414051,-0.3213758366,1.2701548152
Si,0,1.779520335,-0.2360288105,0.0205532444
O,0,1.2202375649,-1.1237059305,-1.2220666156
H,0,0.2374651338,-0.9532526316,-1.3289231246
O,0,2.269084356,-1.1176955632,1.3109427831
O,0,3.105593887,0.614285855,-0.4372846039
H,0,3.0891067342,0.9903741868,-1.3194945936
O,0,0.5785755867,0.7177312347,0.5609448293
H,0,3.1151699804,-1.5632865436,1.2413121683
H,0,-3.8431147099,-1.8555484268,-0.2676848948
O,0,-2.9692867681,-1.8976164928,0.1273091783
H,0,-2.363408842,-1.3710869493,-0.4667986836

p9: HF=-1185.6931905,ZeroPoint=0.1080727

Si,0,-0.9390050106,0.220432857,-0.5495118084
O,0,-2.2147928418,-0.1533723417,-1.3694492161
O,0,-1.0740784815,-0.2051004279,1.0641005996
O,0,-0.4470966581,1.8169843444,-0.5497163711
H,0,-1.08200875,2.4588113548,-0.2265534216
H,0,-1.8905686821,-0.7060704607,1.2198979286
Si,0,1.9053835053,-0.3488288837,-0.263578088
O,0,3.1083781445,-1.2029832451,-0.9539075438
H,0,3.1606146481,-2.1354654608,-0.7361555061
O,0,1.6984778597,-0.8726158627,1.2749274289
O,0,2.4067781444,1.2064635432,-0.351476155
H,0,1.6583825729,1.8154511949,-0.4183084999
O,0,0.4821962697,-0.4871236633,-1.0422366984
H,0,0.7692939575,-0.812282116,1.5496404843
H,0,-4.367958388,-0.9840575284,0.6970728653
O,0,-3.5701624539,-1.4575557356,0.4509111118
H,0,-3.1761442361,-0.9663052783,-0.3304275101

p10: HF=-1185.6866863,ZeroPoint=0.1054502

Si,0,-1.1435610802,0.3994693371,0.0838845506
O,0,-0.8222487977,1.9293622834,-0.4781224426
H,0,0.0990147173,2.066843771,-0.7279007943
O,0,-3.2449429585,-2.7460426201,-0.5764948549
O,0,-1.9978259007,0.6100166592,1.4925649202
H,0,-1.6194125666,1.239344921,2.109107259
H,0,-4.0421665092,-2.5287747553,-0.0896426049
O,0,-1.9123251412,-0.5399064115,-0.8973620704
H,0,-2.7389407191,-1.8829760562,-0.6711472109
Si,0,1.9052572406,0.0051970619,0.2185103494
O,0,2.835854651,0.0962317195,1.5563365086

H, 0, 2.6320623474, 0.788982569, 2.187295398
O, 0, 1.9685918223, 1.3847999143, -0.678763853
O, 0, 2.5799270448, -1.2648110929, -0.5537057063
H, 0, 2.1544303924, -1.5682904292, -1.3577619217
O, 0, 0.3483588475, -0.1983601941, 0.5540485375
H, 0, 2.8199516102, 1.6767003229, -1.0106870642

q1: HF=-1185.7002685,ZeroPoint=0.1073285

Si, 0, 1.5086223794, -0.7559723403, 0.1165769344
O, 0, 2.3328034476, 0.5670361215, -0.3414059224
H, 0, 1.8006498973, 1.3917280128, -0.4619554161
O, 0, 2.3701994744, -2.0585797486, -0.3735243994
O, 0, 0.7424601622, 2.6959117442, -0.692463262
H, 0, 0.8409310193, 3.3782090369, -0.0243454711
H, 0, 2.8586326427, -1.9614806918, -1.1928466591
O, 0, 0.0082336932, -0.7586539383, -0.5154193628
O, 0, 1.3728063464, -0.9091167611, 1.7415617002
Si, 0, -1.4000751009, -0.0336511354, -0.0285611763
O, 0, -1.3988661203, -0.4419437356, 1.596581299
O, 0, -1.4909492182, 1.5004922861, -0.3327337974
H, 0, -0.1688724161, 2.2640662582, -0.5371447074
O, 0, -2.6134540319, -0.936797907, -0.7035731136
H, 0, -3.1085449478, -0.4784952463, -1.3843811
H, 0, -1.9574296357, 0.1015770625, 2.1554649819
H, 0, 0.4547564085, -0.7961860177, 2.035029472

sw-c1: HF=-1262.1497152,ZeroPoint=0.1326179

Si, 0, -1.596757559, 0.5079576764, 0.1164469359
O, 0, -0.6360820992, 1.8331288638, -0.2057324726
H, 0, -1.0727150328, 2.5707626439, -0.6378042221
O, 0, -0.6939275252, -0.6915833876, 0.6189506096
O, 0, -2.7452681152, 0.9174528639, 1.2311424083
H, 0, -2.6911276781, 0.3620489863, 2.0238551176
H, 0, 0.8764641794, -0.3475188705, 1.4698678496
O, 0, -2.3877128707, 0.297020093, -1.3216803715
H, 0, -3.1862778812, -0.2324527207, -1.286071989
Si, 0, 2.3102152843, -0.1013338012, -0.1047120253
O, 0, 3.9165616536, -0.3514589573, -0.2587615203
H, 0, 4.248392816, -1.2143872616, -0.0050001446
O, 0, 2.1054690028, 1.3985840668, -0.7234625106
O, 0, 1.4600603593, -1.2348941133, -0.9264202045
H, 0, 0.5565432683, -1.2662031075, -0.5347174481
O, 0, 1.842952317, -0.1692768218, 1.4649639361
H, 0, 1.1894754199, 1.7113732876, -0.6205317113

O,0,-1.9630973733,-1.2671595868,2.8996917731
H,0,-1.3843747723,-1.1870096825,2.098628769
H,0,-1.3927337536,-1.1347539309,3.6606643307

sw-c2: HF=-1262.1495902,ZeroPoint=0.1327652

Si,0,1.9704556531,-0.2845539,0.0784412978
O,0,1.1017380579,-0.8056745249,1.4088278593
H,0,1.5919994131,-0.869685893,2.2315609563
O,0,0.9730508395,-0.0211961606,-1.1220864642
O,0,2.8731605188,1.0072590654,0.5865327179
H,0,2.3808058438,1.7560183694,0.9279622475
H,0,-0.3761582351,1.1180937522,-0.8403863445
O,0,3.1091360833,-1.4215383896,-0.2772759693
H,0,3.0879353852,-1.6657390749,-1.2148306337
Si,0,-1.9981620958,-0.0734068361,-0.0902448907
O,0,-3.6260938483,0.0491405419,-0.132029362
H,0,-4.0216527449,0.3015385819,-0.9680712688
O,0,-1.6930645682,-0.4427603246,1.4733768253
O,0,-1.4638757794,-1.2483082023,-1.100572721
H,0,-0.5191224885,-1.0581537036,-1.2920263491
O,0,-1.2914068435,1.3328034307,-0.5444443167
H,0,-0.7461103982,-0.6070090501,1.6281773222
O,0,2.2173922705,-1.4592182515,-3.003402333
H,0,1.6830175807,-0.8327836372,-2.4524359548
H,0,2.6847276461,-0.923350143,-3.6486268684

sw-c3: HF=-1262.1486258,ZeroPoint=0.1327977

Si,0,-2.2161121526,-0.2486310341,-0.0191438911
O,0,-1.8835832466,1.2872067177,-0.5824457193
H,0,-2.6386310483,1.7942245216,-0.8887783626
O,0,-0.8955592914,-0.9328670826,0.4898897057
O,0,-3.4065675684,-0.1421344309,1.1315239512
H,0,-3.0909663791,-0.0977071638,2.035852572
H,0,0.4106144133,-0.2208064509,1.1760248959
O,0,-2.9766841506,-0.9495076155,-1.3103892411
H,0,-3.4037937159,-1.7908162072,-1.140220722
Si,0,2.2303660978,-0.3132441159,-0.0104777072
O,0,3.692034246,-0.9413755204,0.3785866652
H,0,3.6922048864,-1.8436974689,0.7032194325
O,0,2.6330733319,1.0120099201,-0.8810653797
O,0,1.344050353,-1.409511306,-0.8334158583
H,0,0.4070971404,-1.3783809311,-0.5024656938
O,0,1.340222867,0.1354726188,1.2938782723
H,0,1.9589569715,1.7109798805,-0.8187840583

O,0,0.5124810389,2.6041503142,0.0591107861
H,0,-0.340101335,2.2376031354,-0.2400842507
H,0,0.7617615417,2.018789219,0.7904036032

sw-c4: HF=-1262.1487527,ZeroPoint=0.1329849

Si,0,2.0024907379,-0.5307274829,0.0477503437
O,0,1.2749394862,-0.028240453,1.4725201975
H,0,1.8342123938,0.4871477696,2.0583070505
O,0,0.9270444708,-1.2789863262,-0.8312958086
O,0,2.685918971,0.7886360898,-0.6692110876
H,0,2.05346796,1.3979147605,-1.0914982359
H,0,-0.1969517792,-0.3027369635,-1.4460214082
O,0,3.2823741243,-1.4368411479,0.5756353424
H,0,3.8696700695,-1.7732405,-0.1032695601
Si,0,-1.8611597695,-0.1590911847,-0.1174526115
O,0,-3.4567514008,0.1438036408,-0.2718618717
H,0,-3.9041409502,-0.2441721928,-1.0258994678
O,0,-1.4288665621,0.7383957206,1.177739135
O,0,-1.5650236517,-1.7521186617,0.1208050498
H,0,-0.6265178751,-1.9111442609,-0.1330832726
O,0,-1.0278222062,0.2736474145,-1.4685305426
H,0,-0.501856476,0.5822309519,1.4339351901
O,0,0.6620070413,2.4333016012,-1.7206823038
H,0,-0.0656677933,1.7794719119,-1.6882672679
H,0,0.7360958792,2.7059903127,-2.6389563505

sw-c5: HF=-1262.1461568,ZeroPoint=0.1324706

Si,0,2.0053192683,-0.2994956632,0.0069813931
O,0,1.1974445479,0.4964637379,1.235699397
H,0,1.740514022,1.0120913486,1.8356108018
O,0,0.9636187072,-1.0592948625,-0.8924960668
O,0,2.9437227568,0.800492433,-0.8072185201
H,0,2.5295830292,1.1946243636,-1.5769864476
H,0,-0.4493699936,-0.2953754108,-1.4527583322
O,0,3.1074013717,-1.2164010299,0.8335217754
H,0,3.7864863969,-1.6355837214,0.3021417813
Si,0,-1.9420382689,-0.5779075381,0.0717076281
O,0,-3.5655701059,-0.6998186384,0.0148865134
H,0,-3.9148320864,-0.7397028533,-0.8910404147
O,0,-1.6126261735,0.4535682802,1.2974247487
O,0,-1.2256122191,-2.0291727711,0.3230013206
H,0,-0.3121937061,-1.9584736346,-0.0469704895
O,0,-1.4018558494,-0.0125314697,-1.3810576333
H,0,-0.65449794,0.5539542831,1.4413366398

O,0,-3.7143238996,-0.574825348,-2.7947250583
H,0,-4.1515982604,0.169363637,-3.2167456929
H,0,-2.8081008372,-0.2796446223,-2.5892543039

sw-c6: HF=-1262.1442015,ZeroPoint=0.131033

Si,0,2.130754473,0.0378182164,0.3314948392
O,0,1.4151894746,1.5469674674,0.2547467488
H,0,2.0065593623,2.300275481,0.3150196036
O,0,1.0262678952,-1.0673993916,0.1520958395
O,0,3.3540033468,-0.0231729036,-0.7869692272
H,0,3.0992812381,-0.3577774624,-1.6487719685
H,0,-0.1618552734,-0.876843249,-0.9910637512
O,0,2.9272748399,0.0835314127,1.7804472021
H,0,3.5344424894,-0.6389497662,1.9496465377
Si,0,-1.7946303916,0.189740421,-0.0944654603
O,0,-3.4126634177,0.2411952165,-0.2999867184
H,0,-3.8765345704,-0.5975628252,-0.3226028519
O,0,-1.3724530672,1.7665942061,-0.0292604951
O,0,-1.3879944298,-0.6213967386,1.267690942
H,0,-0.4594728255,-0.9329246417,1.1469324604
O,0,-1.052276707,-0.5813707671,-1.3424850388
H,0,-0.4099651491,1.879865659,0.06916103
O,0,-1.274944955,-0.3271347648,-4.0871871402
H,0,-1.2131529855,-0.4249818784,-3.1175084479
H,0,-1.734242597,-1.1112343112,-4.3962275237

sw-c7: HF=-1262.1458016,ZeroPoint=0.1327929

Si,0,1.8206793333,-0.4895651503,-0.2391417868
O,0,1.1991541816,0.2320269195,1.1365863363
H,0,1.8377296898,0.4402217102,1.8220283527
O,0,0.6294597766,-0.9224144384,-1.1648358376
O,0,2.8807187918,0.5903091138,-0.9594606321
H,0,2.4949206564,1.1532250024,-1.6337263428
H,0,-0.6997601934,0.1956449949,-1.4469951543
O,0,2.8384801653,-1.6596168965,0.316396309
H,0,3.7049693198,-1.6843333532,-0.1178402395
Si,0,-2.1209627623,-0.2162836241,0.0952322696
O,0,-3.7452949634,-0.1023892243,0.2389756739
H,0,-4.2693168054,-0.4573748163,-0.4810348569
O,0,-1.579561609,0.4696081982,1.4788702415
O,0,-1.6449245287,-1.7776729428,-0.0408171361
H,0,-0.7492462699,-1.7593058707,-0.4603145594
O,0,-1.5848966366,0.5809794728,-1.2317064518
H,0,-0.6066202325,0.4675771726,1.5240022658

O,0,5.1864658641,-0.938248989,-1.0891029637
H,0,5.4024913774,-1.3257844321,-1.9413272311

sw-d1: HF=-1262.1387758,ZeroPoint=0.133665

Si,0,-1.5983884221,0.0441800322,-0.0551560553
O,0,-0.9932275866,1.4119417329,-0.7353522056
H,0,-0.0769014464,1.6325638731,-0.5173462826
O,0,-1.2436149945,-1.4408782443,-0.7470873336
O,0,-1.9243652237,0.0248913175,1.5674450611
H,0,-1.0894436226,-0.114400759,2.0285093384
H,0,-0.4472007156,-1.745813218,-0.2905090413
O,0,-3.1496316941,0.2375831795,-0.6659828881
H,0,-3.7251206384,-0.5108637645,-0.5040724816
Si,0,1.8848289789,0.1232901717,0.266009283
O,0,3.0903685459,0.0538001205,1.3933520945
H,0,3.3824869656,-0.82360867,1.6460860615
O,0,1.760074158,1.7439103942,-0.1106247196
O,0,2.4758301561,-0.6855501264,-1.0404533477
H,0,1.8276419107,-0.9068396908,-1.7342337739
O,0,0.4561605947,-0.3358344658,0.7587955278
H,0,2.4236670361,2.099347653,-0.7047248441
O,0,0.4739202139,-1.2368261962,-2.922142663
H,0,-0.273811723,-1.3377325016,-2.3012681019
H,0,0.5321429972,-2.0629233179,-3.4095343979

sw-d2: HF=-1262.138018,ZeroPoint=0.1330857

Si,0,-2.0618908411,0.12302528,-0.0157353676
O,0,-1.3578093682,1.5992835698,-0.2626822197
H,0,-0.4338290495,1.5912472184,-0.5392852124
O,0,-2.4491734953,-0.7863391844,-1.3583202595
O,0,-1.991955737,-0.6436407828,1.4652620519
H,0,-1.1719423555,-1.138592889,1.5315134829
H,0,-1.6823065507,-1.2432867077,-1.70783222
O,0,-3.6050296334,0.7873045034,0.2282458911
H,0,-4.2060652375,0.1761110808,0.6549972918
Si,0,1.3421381796,-0.2430693633,-0.1160092235
O,0,1.8860872978,0.054490245,1.4122806966
H,0,2.2521619276,-0.6933478529,1.8876326356
O,0,1.424906818,1.244034499,-0.8410281864
O,0,2.3861087558,-1.3069060633,-0.8093115257
H,0,1.9453778548,-2.0903295873,-1.1723172077
O,0,-0.1587313621,-0.7565014497,-0.2561510241
H,0,2.1042238687,1.8436903851,-0.5262501335
O,0,0.295369677,-3.1389551209,-1.4232130712

H,0,-0.0243112968,-2.3696435642,-0.8972078727
H,0,0.1637991379,-3.9188067362,-0.8782126057

sw-d3: HF=-1262.1362367,ZeroPoint=0.1327425

Si,0,-1.7327352722,0.1621953762,-0.1284783738
O,0,-1.0727302033,1.5597145245,-0.6956340194
H,0,-0.1076676464,1.605879233,-0.6957140678
O,0,-1.8271464879,-1.1778676104,-1.1313025002
O,0,-1.7005940082,-0.1150859432,1.5084392695
H,0,-0.8265590783,-0.4501545334,1.7323511407
H,0,-0.9739087844,-1.6255829545,-1.106101189
O,0,-3.3338120164,0.6475647159,-0.2829945627
H,0,-3.9477115405,-0.0845914848,-0.408660238
Si,0,1.7937544927,-0.099012672,0.0187464997
O,0,2.5421759612,0.1585172232,1.4682738755
H,0,2.9338530591,-0.6102310918,1.8862264417
O,0,1.75794761,1.4102664928,-0.6759467045
O,0,2.8392584842,-1.0927021637,-0.7912990955
H,0,2.444726467,-1.6188446032,-1.4891334643
O,0,0.3108054796,-0.6287616833,0.0409239418
H,0,2.5172080083,1.9817448191,-0.5505087593
O,0,-4.4462620158,-1.9392020427,-1.163699287
H,0,-4.6511735499,-2.6358851235,-0.5352619756
H,0,-3.4711587887,-1.896239378,-1.2115247916

sw-d4: HF=-1262.136419,ZeroPoint=0.1329555

Si,0,-1.181246843,-0.4918511192,-0.0066260934
O,0,-0.4107631053,-0.8474882507,1.4061279722
H,0,0.4988272719,-0.528284464,1.488480977
O,0,-1.7896334755,1.0389182961,-0.2380620248
O,0,-0.8493804277,-1.3918839633,-1.3658784589
H,0,-0.0487815826,-1.0360732173,-1.7640395129
H,0,-1.0649966331,1.5984808749,-0.5352893446
O,0,-2.6229010289,-1.2546335627,0.4316917841
H,0,-3.2999842936,-1.2017572526,-0.2436602756
Si,0,2.1339345068,0.6653562942,-0.1517994219
O,0,3.278326333,-0.3122459607,-0.8677620447
H,0,3.5989298053,-0.0379511396,-1.7291800615
O,0,2.2205210116,0.1986351317,1.4340927833
O,0,2.7433272533,2.1896282783,-0.3522274273
H,0,2.0837282973,2.8799467714,-0.4397337145
O,0,0.647932778,0.5280418971,-0.6517437353
H,0,3.0351083254,-0.2652258603,1.689990582
O,0,4.5967620759,-1.281139361,1.3809697905

H, 0, 4.4311265908, -1.0539073906, 0.4497519381
H, 0, 5.4423412406, -0.8848809917, 1.6076932583

sw-e1: HF=-1262.1526825,ZeroPoint=0.1351252

Si, 0, 1.0534036313, -0.3600241451, 0.0496100363
O, 0, 0.2908184854, -1.5980952454, -0.8303017496
H, 0, 0.9533185862, -2.1845525265, -1.2016179552
O, 0, 1.4261349106, 1.0694133844, -0.7953404798
O, 0, 1.4417118166, -0.5251985078, 1.6823347756
H, 0, 0.7150094564, -0.2219519967, 2.2295597386
H, 0, 2.3170117224, 0.9988257872, -1.1470629009
O, 0, 2.6309222698, -1.0250732044, -0.3793068876
H, 0, 3.1463543825, -1.221342975, 0.4031763503
Si, 0, -2.0255681595, 0.3608065793, -0.0390247445
O, 0, -2.2878858316, -0.8860232893, -1.0791990493
H, 0, -1.4484580106, -1.3691309096, -1.1999669127
O, 0, -2.4098244108, 1.7983507303, -0.7120593649
O, 0, -3.1262774944, 0.24530843, 1.1843227536
H, 0, -3.2566573825, -0.6361113412, 1.537993665
O, 0, -0.5098276592, 0.3169605615, 0.4833006996
H, 0, -1.649319203, 2.3118353446, -1.0543045087
O, 0, -0.1618036528, 3.06288371, -1.6050665061
H, 0, 0.4665196275, 2.3705636241, -1.286392422
H, 0, 0.0492966957, 3.8633206495, -1.1179290776

sw-e2: HF=-1262.1511175,ZeroPoint=0.1353874

Si, 0, 1.3396222401, -0.0983166118, 0.4108771591
O, 0, 1.0984120865, -1.0078598321, -1.0047621224
H, 0, 1.9125863357, -1.0503422446, -1.5105968476
O, 0, 1.0368800793, 1.5599038575, 0.2832758814
O, 0, 1.8434932961, -0.8160509736, 1.8487948754
H, 0, 1.0843425664, -1.1047337312, 2.3589349034
H, 0, 1.8002001293, 2.0906086726, 0.0188015563
O, 0, 3.0612500911, 0.1262578231, -0.0177536624
H, 0, 3.6227370883, -0.3367586782, 0.6059035114
Si, 0, -1.6519285333, 0.0376855735, 0.0244830116
O, 0, -1.6385173962, -0.750752804, -1.4209824277
H, 0, -0.7231680399, -1.0174478401, -1.6132318939
O, 0, -1.6979578236, 1.669632425, -0.1528465605
O, 0, -3.0694257786, -0.3242556995, 0.7672449834
H, 0, -3.3752259152, -1.2280421273, 0.6735939281
O, 0, -0.3437912864, -0.3754605094, 0.8634889867
H, 0, -0.7899721161, 2.0022797403, -0.0402669958
O, 0, 3.6093693226, 2.6731528735, -0.4782525116

H, 0, 3.5957840208, 1.6906280338, -0.3755231745
H, 0, 3.7400536129, 2.8461514025, -1.4136574803

sw-e3: HF=-1262.1493458,ZeroPoint=0.1348472

Si, 0, 0.9508726877, -0.4165527152, 0.145171669
O, 0, 0.2989069955, -1.6965086312, -0.7656439975
H, 0, 0.9911105576, -2.0835755719, -1.3064365734
O, 0, 0.8572004308, 1.1317919861, -0.5522010471
O, 0, 1.5911157601, -0.6576799813, 1.6721109937
H, 0, 0.9645024224, -0.5850004775, 2.4024607316
H, 0, 1.6585645019, 1.3016080384, -1.0525691696
O, 0, 2.5324322668, -0.6754672503, -0.5764336286
H, 0, 3.1910059771, -0.8486032658, 0.0964662331
Si, 0, -2.0321163973, 0.1978351052, -0.0046620616
O, 0, -2.3583395439, -1.0431164155, -1.0306492054
H, 0, -1.5345003833, -1.5433891553, -1.1710533409
O, 0, -1.8431500625, 1.6293847985, -0.7814739032
O, 0, -3.34796721, 0.4211235762, 0.9477238842
H, 0, -3.8205002556, -0.3713541484, 1.2086149325
O, 0, -0.6924443039, -0.1436742096, 0.8333131726
H, 0, -0.8886876627, 1.7914589624, -0.8822737339
O, 0, -0.6451482618, -0.4097373566, 3.5142810769
H, 0, -0.7249816211, 0.4298110908, 3.9738751356
H, 0, -0.8764041177, -0.2315699989, 2.5781183622

sw-e4: HF=-1262.1489262,ZeroPoint=0.1350784

Si, 0, 0.9148636991, -0.2165948949, -0.0141263543
O, 0, 0.4281217673, -0.7724826961, 1.5174714133
H, 0, 1.0812511877, -1.3891812106, 1.8553483788
O, 0, 0.3771188291, -1.112800845, -1.3542948998
O, 0, 1.8166003787, 1.2149044777, -0.1747284373
H, 0, 1.2346813043, 1.975944169, -0.2273734469
H, 0, 1.0335331819, -1.7744453235, -1.5834423232
O, 0, 2.3840670363, -1.1612747685, 0.0487297612
H, 0, 3.1917719574, -0.6464906147, 0.1319408676
Si, 0, -2.0773330246, 0.2385903889, -0.0299072192
O, 0, -2.3293354606, -0.4823634509, 1.4286480812
H, 0, -1.4645611882, -0.7406389182, 1.792013372
O, 0, -2.3786106119, -0.7742970831, -1.287637525
O, 0, -3.2034446016, 1.4208005256, -0.1943523135
H, 0, -3.4056397724, 1.9225554361, 0.5971780458
O, 0, -0.558637875, 0.7606351485, -0.1065536729
H, 0, -1.527267408, -1.1215153216, -1.6040317362
O, 0, 4.4792917831, 1.0232598534, 0.2156746568

H, 0, 4.9736000698, 1.165296601, -0.5951518559
H, 0, 3.5569997477, 1.2889945269, 0.0208532074

sw-f1: HF=-1262.1407711,ZeroPoint=0.1348671

Si, 0, -1.3914812328, -0.1282640427, -0.1150779613
O, 0, -2.8668344085, -0.9847536329, -0.3790016512
H, 0, -3.4174139201, -0.5221048842, -1.0121559976
O, 0, -1.6599909587, 0.7806149023, 1.2885022892
O, 0, -1.858632247, 0.9125874373, -1.4043207404
H, 0, -1.1221561672, 1.4656389082, -1.6682279865
H, 0, -2.4536271609, 1.3158110811, 1.2551402056
O, 0, -0.7952883848, -1.6265421001, 0.5823698124
H, 0, -1.5229226215, -2.2486234658, 0.6537542935
Si, 0, 1.7297554656, -0.2811460708, -0.1141880558
O, 0, 1.7624507273, -1.9095552646, -0.3527184217
H, 0, 0.8834720828, -2.2523250113, -0.1198766803
O, 0, 2.2290955387, 0.1401525961, 1.3854292703
O, 0, 2.8851350853, 0.3861061201, -1.0700395851
H, 0, 2.8663668059, 0.1349969789, -1.9949246673
O, 0, 0.2590065366, 0.2843846894, -0.4463218137
H, 0, 1.5537747072, -0.0078730783, 2.0766880622
O, 0, 0.0709458951, -0.4859263031, 3.013030314
H, 0, -0.16140502, -1.1927614533, 2.385493312
H, 0, -0.549201993, 0.2053971837, 2.7219683619

sw-f2: HF=-1262.1396194,ZeroPoint=0.1346877

Si, 0, 1.3348482941, 0.0282597451, -0.1853572766
O, 0, 2.9039319433, 0.707310998, -0.5017109916
H, 0, 3.5279211776, 0.0260276508, -0.7572511447
O, 0, 1.2814214809, -0.2782487139, 1.4850162671
O, 0, 1.969965274, -1.4430319421, -0.8217904476
H, 0, 1.2576197983, -2.0546081601, -1.0129110064
H, 0, 1.6823370953, -1.1215991051, 1.7051191271
O, 0, 0.7129168305, 1.6374742636, -0.1882968895
H, 0, 1.3778733027, 2.3194580824, -0.0417812921
Si, 0, -1.6449451832, -0.0511441608, -0.0426893955
O, 0, -2.0133013339, 1.4973388951, -0.4528591092
H, 0, -1.1701953196, 1.981450616, -0.4794136351
O, 0, -1.5486543349, -0.2707974477, 1.5814061542
O, 0, -2.9126401052, -0.9764565039, -0.5168452878
H, 0, -3.3399933897, -0.7223897833, -1.3365734224
O, 0, -0.2436021737, -0.4983293535, -0.7098208224
H, 0, -0.6153365216, -0.3204918246, 1.8526423615
O, 0, 3.1835236339, 3.31228498, -0.0271922135

H, 0, 3.2981480865, 2.3493284575, -0.1889794384
H, 0, 3.5390784547, 3.4803288565, 0.848725163

sw-f3: HF=-1262.1390681,ZeroPoint=0.1343291

Si, 0, 0.9433178187, -0.6143966711, -0.1601988465
O, 0, 2.6547080806, -0.4874308715, -0.2578687452
H, 0, 3.1051196591, -1.2935763005, -0.5272005852
O, 0, 0.6477819449, -1.0565208141, 1.4543829426
O, 0, 1.0549643807, -2.1116494458, -1.0273311742
H, 0, 0.1847779504, -2.400631701, -1.30713029
H, 0, 0.8729790663, -1.9694117449, 1.641681095
O, 0, 0.9017665218, 1.1074158945, -0.0736119727
H, 0, 1.7826257493, 1.4509037845, 0.0869707634
Si, 0, -1.9281141239, 0.2672474654, -0.0375776443
O, 0, -1.7295972398, 1.8886031747, -0.2271833063
H, 0, -0.7722439959, 2.0586894121, -0.2280088601
O, 0, -2.014577214, -0.1771337447, 1.5404838015
O, 0, -3.4004306438, -0.103775134, -0.6570848479
H, 0, -3.6619139026, 0.376676793, -1.4444534085
O, 0, -0.7137141485, -0.5312536757, -0.7358871639
H, 0, -1.1680481081, -0.576613826, 1.8084601798
O, 0, 3.4816355728, -3.1702156284, -1.400748953
H, 0, 2.5237657043, -2.9681382036, -1.3218029467
H, 0, 3.6566410875, -3.8799950728, -0.7783353077

sw-f4: HF=-1262.1396206,ZeroPoint=0.1350141

Si, 0, 0.8426307733, -0.6971135882, -0.0718683803
O, 0, 2.5700915675, -0.6990368156, -0.1100416655
H, 0, 2.9226674119, -1.5409659296, -0.3994460073
O, 0, 0.487334691, -1.0335703682, 1.5494009738
O, 0, 0.9064824, -2.2438550173, -0.8657702861
H, 0, 0.0348306597, -2.4590724651, -1.2052525246
H, 0, 0.7234654996, -1.9392917513, 1.7936605052
O, 0, 0.9200151635, 1.0221657314, -0.123663809
H, 0, 1.8184952423, 1.3208934874, 0.0286919679
Si, 0, -1.9760325124, 0.3330733386, -0.0499368444
O, 0, -1.6722075282, 1.9321173253, -0.2853924176
H, 0, -0.7057584893, 2.0411168738, -0.2928139051
O, 0, -2.1213979949, -0.0551472231, 1.5380394676
O, 0, -3.4530880551, 0.0286454191, -0.693386464
H, 0, -3.6675834524, 0.4974366496, -1.5017056539
O, 0, -0.793032495, -0.554981065, -0.692972311
H, 0, -1.2965452439, -0.4823607193, 1.8350231967
O, 0, 1.348362155, -3.7892864307, 1.3647801568

H, 0, 1.1990154291, -3.433569926, 0.4642007969
H, 0, 0.7109063583, -4.4980126858, 1.4825979939

sw-f5: HF=-1262.1374157 ZeroPoint=0.1345592

Si, 0, 0.8869365727, -0.6628007528, -0.1127071651
O, 0, 2.5860223672, -0.4849821286, -0.3079033287
H, 0, 2.9715828983, -1.3054807602, -0.6188288832
O, 0, 0.5944204814, -1.0872310542, 1.5072495055
O, 0, 1.0276483291, -2.1898160042, -0.8790158071
H, 0, 0.204860299, -2.5675374634, -1.2044495678
H, 0, 0.6155491046, -2.0381500127, 1.6326744457
O, 0, 0.8292194468, 1.0623050366, 0.0740062736
H, 0, 1.7047008077, 1.406120651, 0.2589807712
Si, 0, -1.9179860725, 0.3939441681, -0.054250637
O, 0, -1.6902309523, 1.9845085304, -0.3872399015
H, 0, -0.7345501656, 2.1474254239, -0.3270860536
O, 0, -1.9583285307, 0.0690894031, 1.5507144705
O, 0, -3.4119231058, 0.0141396638, -0.6115052356
H, 0, -3.6958200994, 0.4611633149, -1.4108410483
O, 0, -0.7645840096, -0.5254380888, -0.7389756621
H, 0, -1.1348844665, -0.3748372036, 1.8239013206
O, 0, -1.6163631669, -2.7564295315, -2.0800943999
H, 0, -1.4800641932, -1.8610543523, -1.7117801769
H, 0, -1.5584148642, -2.6631350197, -3.0341961502

sw-g1: HF=-1262.1470648,ZeroPoint=0.1345547

Si, 0, 1.3743107109, -0.0348395049, 0.1852754236
O, 0, 2.2766393721, -0.0577262761, 1.6131223151
H, 0, 2.815061229, 0.7352133013, 1.6606086111
O, 0, 2.0256581261, -0.7827256219, -1.2050634563
O, 0, 2.1269268663, 1.5049350804, -0.2401052738
H, 0, 1.4808127183, 2.1060688119, -0.6110261969
H, 0, 2.5361288898, -0.1273118033, -1.6882740801
O, 0, 0.6413688948, -1.5672702194, 0.6651570046
H, 0, 1.2675908485, -2.1222972034, 1.1315791762
Si, 0, -1.6903773593, 0.1170730308, -0.0796336831
O, 0, -1.9180670324, -1.0188325471, 1.0796739726
H, 0, -1.0512347976, -1.4622747104, 1.1985824366
O, 0, -2.0685517692, -0.3963920209, -1.5800751539
O, 0, -2.763994631, 1.3307732495, 0.1765543125
H, 0, -2.8710743387, 1.6143663531, 1.0860142566
O, 0, -0.1592247189, 0.6477310081, -0.0186358572
H, 0, -1.3601880935, -0.8825958824, -2.051185622
O, 0, 0.005345082, -1.7563928445, -2.7449194732

H, 0, 0.7823005724, -1.4463394844, -2.2240128367
H, 0, 0.1891971803, -1.5311166863, -3.6605245456

sw-g2: HF=-1262.1470331,ZeroPoint=0.1350331

Si, 0, 1.3940227892, -0.0755170501, 0.0662538642
O, 0, 2.2062489347, -0.1872847428, 1.5412111859
H, 0, 2.7276498031, 0.6065691546, 1.6781238774
O, 0, 2.1066663184, -0.741082927, -1.3167832349
O, 0, 2.1248232943, 1.4992194731, -0.2213304316
H, 0, 1.4773616146, 2.1220862457, -0.5516755133
H, 0, 2.6153265913, -0.0578562063, -1.7593311227
O, 0, 0.6566509151, -1.6745664375, 0.4409949573
H, 0, 1.2697459346, -2.2150719878, 0.9430036894
Si, 0, -1.6745163711, 0.0255163845, -0.1114459575
O, 0, -1.8713036617, -0.967243357, 1.1818956083
H, 0, -1.0410545979, -1.4648228724, 1.2878910491
O, 0, -2.0799439429, -0.6786366638, -1.5265918846
O, 0, -2.7572599948, 1.2480232935, 0.0137729324
H, 0, -2.7937523974, 1.7024978072, 0.8570242949
O, 0, -0.1507678891, 0.5769131378, -0.1386356548
H, 0, -1.4283802476, -1.3352473579, -1.8478307849
O, 0, -0.056256607, -2.4872009281, -2.0389256184
H, 0, 0.1937454632, -2.4015845444, -1.0902186834
H, 0, 0.654088211, -1.9792704611, -2.4511332927

sw-g3: HF=-1262.145914,ZeroPoint=0.1344127

Si, 0, 1.7162077065, 2.0059908789, 0.2197493586
O, 0, 2.4633659747, 2.0274137321, 1.7330834416
H, 0, 3.0277155468, 2.8014644675, 1.7908638954
O, 0, 2.4412875791, 1.1436408454, -1.032337403
O, 0, 2.5478115994, 3.4913595717, -0.2388764186
H, 0, 1.9248910003, 4.1487826596, -0.5483023052
H, 0, 2.998983981, 1.7417775575, -1.5346920224
O, 0, 0.8680516825, 0.5019139059, 0.7349231062
H, 0, 1.4691372833, -0.067972655, 1.2192375481
Si, 0, -1.3378762992, 2.4054415025, 0.2449265209
O, 0, -1.4418418557, 1.6065807598, 1.6762460011
H, 0, -0.6629255873, 1.0251366918, 1.7401605264
O, 0, -2.0509131517, 1.5962031564, -0.9794870619
O, 0, -2.2312749629, 3.7751204884, 0.3367603399
H, 0, -1.9810820397, 4.4073318168, 1.012513068
O, 0, 0.2174948754, 2.7313466288, -0.069909502
H, 0, -1.6340868877, 0.731901759, -1.1708583416
O, 0, -0.5568998647, -0.7038379681, -1.2044044954

H,0,-0.9750307874,-1.491930392,-0.8482627293
H,0,0.0497276973,-0.368793427,-0.4980323868

sw-g4: HF=-1262.1416162,ZeroPoint=0.1333978

Si,0,1.3999404631,0.0460523682,0.0771363091
O,0,2.1034401197,-0.2870565345,1.5711273127
H,0,2.6484693107,0.4564438078,1.8370969004
O,0,2.2185893042,-0.4443713477,-1.3045526533
O,0,2.1949263172,1.6587768988,0.036153152
H,0,1.5364951877,2.3481489943,0.1318594536
H,0,2.8368610076,0.2096931706,-1.6516188769
O,0,0.5226206849,-1.4883459098,0.1052621533
H,0,1.0777023389,-2.2339851434,-0.1253235717
Si,0,-1.5705677598,0.1519363149,-0.0212160124
O,0,-1.8577124779,-0.7572132888,1.3185274026
H,0,-1.1230659309,-1.3735158072,1.4380860119
O,0,-1.8250850867,-0.6708320343,-1.4190335936
O,0,-2.7407607383,1.2969799275,-0.0804087086
H,0,-2.8197738276,1.8759420756,0.679316786
O,0,-0.1027242744,0.840069767,0.0360009995
H,0,-1.1320047127,-1.3258992247,-1.551835791
O,0,3.9895413128,1.8491926595,-1.8954269733
H,0,3.6906030954,2.4084986442,-2.6162735101
H,0,3.3360980262,1.968327552,-1.1623643002

sw-g5: HF=-1262.1385048,ZeroPoint=0.1335011

Si,0,1.3458446599,0.0279493906,0.0472463362
O,0,2.1077331381,-0.6881594449,1.3763165152
H,0,2.6846971709,-0.0464857443,1.7960025138
O,0,2.0443915114,-0.1210533574,-1.4802340561
O,0,2.1826567279,1.5283726413,0.3922292973
H,0,1.6886265453,2.3237988848,0.1746107946
H,0,2.6354999689,0.6208454931,-1.6244351602
O,0,0.4432943383,-1.4835586584,-0.1879753474
H,0,0.9414634017,-2.2492044315,0.1000454723
Si,0,-1.6336406969,0.077930511,0.1203937278
O,0,-1.8388912036,-0.8313473577,1.4738748976
H,0,-1.1189275568,-1.4607049195,1.5819761823
O,0,-1.9500060846,-0.7215735264,-1.2743434395
O,0,-2.8161139978,1.212763407,0.1502033642
H,0,-2.92223506,1.7084126442,0.9637261863
O,0,-0.1802051915,0.8184366254,0.1102867491
H,0,-1.2211929077,-1.3312540827,-1.4489361364
O,0,0.0414756492,3.5521757818,-0.08944515

H,0,-0.1503992765,3.8633228111,-0.9775635976
H,0,-0.2267325462,2.6132882525,-0.0704201795

sw-g6: HF=-1262.1468761,ZeroPoint=0.1348486

Si,0,-1.4832787319,-0.0974506869,0.0580278806
O,0,-0.9378600562,-1.8130718501,0.0772378486
H,0,-1.643083006,-2.3911756152,-0.2203343463
O,0,-2.134578011,-0.2977063244,1.6070920706
O,0,-2.4309584484,-0.4892380756,-1.2820541348
H,0,-2.8835147874,0.2980868674,-1.5920910394
H,0,-2.5329044879,0.5313934802,1.8815904802
O,0,-2.0286672428,1.5731948737,-0.0359973342
H,0,-1.2934155103,2.1786410151,0.0593299915
Si,0,1.5803214114,-0.3220529191,-0.0133126445
O,0,2.7393410215,0.6567253728,-0.6309143776
H,0,3.1349038523,1.2876840335,-0.0274466889
O,0,1.5612358069,-1.6136856713,-1.0223570997
O,0,2.0422325437,-0.6963465174,1.5096951844
H,0,1.3565767746,-1.1466850219,2.0450903841
O,0,0.1293211915,0.399683181,-0.0134889714
H,0,0.6854875313,-2.0284801178,-0.9343339109
O,0,-0.0928453273,-2.0324286297,2.6365924444
H,0,-0.7105941411,-1.3560198618,2.9419563613
H,0,-0.417968873,-2.1656814125,1.7163809421

sw-g7: HF=-1262.1384115,ZeroPoint=0.1341392

Si,0,1.2843906248,-0.0541594301,-0.0306077348
O,0,0.6353678649,1.5689852831,0.1999877042
H,0,1.3213206884,2.1965329436,0.4303133133
O,0,1.319682004,-0.313851794,1.6511422085
O,0,2.6259763393,0.6471084366,-0.7854945778
H,0,3.2087957015,-0.0473699852,-1.1004619259
H,0,1.6690920266,-1.1904863036,1.8287472669
O,0,1.9389678158,-1.6276031081,-0.4131927784
H,0,1.2889269237,-2.2911140434,-0.6578105145
Si,0,-1.6575518254,0.0194868658,0.0319271566
O,0,-2.9424573076,-0.8264547907,-0.5265088341
H,0,-3.0694164922,-1.7054164195,-0.1651793144
O,0,-2.0087563294,1.5562506111,-0.402812706
O,0,-1.549201988,-0.2019431664,1.6536862914
H,0,-0.6239698627,-0.2374449985,1.9522037308
O,0,-0.2653721983,-0.4989141282,-0.6489335379
H,0,-1.1805142067,2.0576369651,-0.3224774607
O,0,-0.3914060113,-3.075725406,-1.6400204547

H,0,-0.2607410977,-3.1451087346,-2.5889717114
H,0,-0.4842563399,-2.1236163069,-1.4498681613

sw-g8: HF=-1262.1443227,ZeroPoint=0.1347251

Si,0,-1.4633720065,-0.3562492728,0.0324251189
O,0,-0.6103192611,1.1399887342,-0.6014595547
H,0,-1.2385578879,1.8027578829,-0.8979654109
O,0,-2.3472841409,-1.766761865,0.5286193879
O,0,-2.0768275832,0.5325060128,1.3296787166
H,0,-1.6873088634,1.4069323027,1.3776971742
H,0,-2.2515988988,-1.9472983568,1.4641771263
O,0,-2.196625109,-0.4574814929,-1.4850828316
H,0,-2.8119061011,-1.1943241431,-1.4967902598
Si,0,1.59912451,-0.6364877934,0.2444559303
O,0,2.5123134198,-1.5568685005,1.246167849
H,0,2.3847580036,-1.4219065821,2.1865873611
O,0,1.7468082874,0.9294924516,0.7185240719
O,0,2.2626705492,-0.9248586751,-1.2192036107
H,0,1.7176798928,-0.5933984167,-1.9606868699
O,0,0.0410767541,-1.0713497475,0.2739993085
H,0,0.9761535761,1.4199926529,0.381332316
O,0,0.4711825167,0.2655778116,-2.9427581259
H,0,-0.1805774125,-0.3514043233,-3.288411388
H,0,0.0307578047,0.6499652904,-2.1474241093

sw-g9: HF=-1262.1427728,ZeroPoint=0.1333925

Si,0,-1.3868327144,-0.0610019206,-0.0818811491
O,0,-0.90187867,1.6748485537,-0.1050320816
H,0,-1.2396184481,2.0867187576,-0.9018952518
O,0,-2.0408634696,-1.7044614229,-0.0526511404
O,0,-2.0097685141,0.1717334167,1.4724195473
H,0,-1.8630638098,1.0790996867,1.7466801079
H,0,-2.1111115371,-2.0396899547,0.8416723063
O,0,-2.1245855913,0.2106987588,-1.5701206994
H,0,-2.636882052,-0.5338294893,-1.9074390446
Si,0,1.7174337934,-0.0681601091,-0.033081526
O,0,2.5431622191,-0.755277337,1.2081242093
H,0,2.1530639487,-0.6663855862,2.0792742159
O,0,1.6975469147,1.5587684473,0.0768529682
O,0,2.627927807,-0.5758811499,-1.3011977306
H,0,2.4285354367,-0.1817279123,-2.1519692107
O,0,0.2035695657,-0.6179160556,-0.112500718
H,0,0.7485013879,1.8424532894,0.0137175111
O,0,-3.6126399773,-2.2917486333,-2.0824104935

H, 0, -3.1919128346, -2.9209595846, -2.6730310434
H, 0, -3.0577129548, -2.2652819446, -1.2652992068

sw-g10: HF=-1262.1413233,ZeroPoint=0.1336461

Si, 0, -1.2366673036, 0.2501458981, -0.1314165836
O, 0, -0.4154499574, 1.7742558455, -0.7621466392
H, 0, -0.7343096984, 1.9348237412, -1.6530489324
O, 0, -2.1948985631, -1.1239757974, 0.3435341709
O, 0, -1.6821233262, 1.0729201886, 1.2639845916
H, 0, -1.3637639802, 1.9807695875, 1.3242075996
H, 0, -2.2409694058, -1.2110128289, 1.295860785
O, 0, -1.9983672093, 0.217884458, -1.6427385432
H, 0, -2.6427032349, -0.492533644, -1.6657208461
Si, 0, 1.8200678787, -0.3819343616, -0.1520597322
O, 0, 2.6345037482, -0.6924696999, 1.2382252965
H, 0, 2.6099727172, -0.0052736325, 1.9061630702
O, 0, 2.1417257999, 1.1299091015, -0.6767724321
O, 0, 2.4567696865, -1.5338012794, -1.1324844822
H, 0, 2.0097462916, -1.67638459, -1.968453632
O, 0, 0.228360291, -0.5711158069, 0.0016929948
H, 0, 1.2758981562, 1.5863597499, -0.8054062654
O, 0, -0.5520756839, 3.7923303924, 0.9815338471
H, 0, -1.2074613649, 4.4541927622, 0.7480869123
H, 0, -0.4667981716, 3.1998566857, 0.1992607304

sw-g11: HF=-1262.1423386,ZeroPoint=0.1333438

Si, 0, -1.4153681966, -0.0088030506, 0.0305946271
O, 0, -0.8700646603, 1.6756700696, 0.11865546
H, 0, -1.3772368944, 2.2131137837, -0.490789472
O, 0, -1.9854509954, -1.7178346917, -0.0917407165
O, 0, -2.1124501098, 0.1272922562, 1.5566515445
H, 0, -2.500798879, -0.7167648245, 1.7961195546
H, 0, -1.2440797302, -2.3134841769, 0.0242810165
O, 0, -2.2859637934, 0.3980584087, -1.3497190085
H, 0, -2.7731176525, -0.3328976645, -1.7482904245
Si, 0, 1.7043506196, -0.0711785499, -0.0377416107
O, 0, 2.5964116995, -0.7287364638, 1.1720874908
H, 0, 2.4381609711, -0.3823645207, 2.0518317877
O, 0, 1.7222826692, 1.5564914122, 0.0342558073
O, 0, 2.5095465991, -0.6519689134, -1.3445069328
H, 0, 2.1115244521, -0.4849220635, -2.200505839
O, 0, 0.1746061196, -0.5895231505, -0.0175139617
H, 0, 0.7748978175, 1.8521224594, 0.0564971003
O, 0, -3.6432897977, -2.1052337254, -2.1081054315

H,0,-3.2302023225,-2.5827762817,-2.8313709286
H,0,-3.012090876,-2.1532384128,-1.3471493132

cw-h1: HF=-1262.1405248,ZeroPoint=0.1272365

Si,0,-0.6119378248,-0.5135877178,0.1338921905
O,0,-1.3084145837,-1.1144567703,1.4879581336
H,0,-2.2676577464,-1.2101017215,1.3084258483
O,0,-0.8306901007,1.0990875293,0.0002830768
O,0,-1.2060094468,-1.3194248,-1.1621475457
H,0,-2.1735658452,-1.4092265125,-1.0450274244
H,0,-1.8170884056,1.3622591467,-0.0790547087
O,0,-3.6126630152,-0.9304993738,0.0591756556
H,0,-4.5187174543,-1.2376541146,0.1111528793
Si,0,2.3058153811,0.2188401683,0.1465770673
O,0,3.2924526796,-0.0882902135,1.4113686303
H,0,2.8997313945,-0.1209347883,2.286034995
O,0,1.8134499481,1.7673282626,0.0891739272
O,0,3.2009416479,-0.0548113959,-1.1884755697
H,0,3.7594083517,-0.8344174998,-1.197438481
O,0,0.9982118552,-0.7555111101,0.2178291773
H,0,0.8432961366,1.8522037467,0.0371395866
O,0,-3.3523825939,1.4592820634,-0.1245568089
H,0,-3.652067064,1.7735354773,-0.980084315
H,0,-3.5790136241,0.261141634,-0.0537336843

sw-h1: HF=-1262.1336957,ZeroPoint=0.1318467

Si,0,-0.7120379166,-0.5835977509,-0.2453400011
O,0,-0.6032808423,-0.9750329327,1.3624804612
H,0,-1.4724152165,-0.9051931078,1.7701848062
O,0,-0.9788239697,1.0125739042,-0.5328827036
O,0,-1.3708056159,-1.6665969698,-1.280453524
H,0,-2.3184339204,-1.6518892359,-1.0529364344
H,0,-1.848114346,1.400083863,-0.2977535104
O,0,-3.0874061433,-0.6142869431,0.3091761252
H,0,-3.5217927542,-1.1886044413,0.9428054947
Si,0,2.0876423462,0.2068269849,0.0099132064
O,0,2.1799428197,-0.1480283674,1.6086073193
H,0,1.3390993803,-0.4824604096,1.9512862247
O,0,1.7783845886,1.7863165907,-0.2816533383
O,0,3.5498061695,-0.0638230633,-0.6569188914
H,0,4.0426780697,-0.8196561053,-0.3322338101
O,0,0.9006587674,-0.6867025342,-0.6488509866
H,0,0.8308669943,1.9292702892,-0.4288602294
O,0,-3.4623218888,1.8529654731,0.2323025241

H, 0, -4.0492812564, 2.0870692888, -0.4901238569
H, 0, -3.4776062658, 0.8250804675, 0.3115791241

sw-h2: HF=-1262.1316879,ZeroPoint=0.1321343

Si, 0, 1.1897329881, 0.1901766186, -0.1735966875
O, 0, 1.0971958196, -0.3907765679, 1.3695909687
H, 0, 2.0242022046, -0.640214405, 1.5686804679
O, 0, 1.6419366362, -0.9193726613, -1.3120183398
O, 0, 1.8631818068, 1.6766071695, -0.345926305
H, 0, 2.807977866, 1.6328329318, -0.1732702099
H, 0, 2.5612553604, -1.1347891879, -1.0310372166
O, 0, 3.4311852413, -0.5701654271, 0.4105664245
H, 0, 4.2622063243, -0.0960933437, 0.4667998092
Si, 0, -1.8153209521, -0.1450916273, -0.0759158994
O, 0, -1.6483447059, -0.7390582127, 1.4413871439
H, 0, -0.7207479115, -0.7782031269, 1.7260463177
O, 0, -2.3328639739, -1.2510568244, -1.1451236424
O, 0, -3.0047832896, 0.9778555184, -0.075162158
H, 0, -3.0279738082, 1.573966738, 0.6755550803
O, 0, -0.3888352287, 0.4837897181, -0.5454170362
H, 0, -1.6376779874, -1.7305500999, -1.6441122479
O, 0, -0.2731141743, -2.4931270193, -2.4273962331
H, 0, -0.2761608353, -2.3920581366, -3.3828464265
H, 0, 0.4872961798, -1.9671905743, -2.0970817699

cw-k1: HF=-1262.1214732,ZeroPoint=0.130194

Si, 0, -0.9202423187, 0.6578208996, 0.0104328369
O, 0, -1.4292599376, 1.4229357119, 1.3920539536
H, 0, -1.2060965425, 2.3564753759, 1.3707297462
O, 0, -1.9500748718, 0.2818930675, -1.1728759174
O, 0, 0.363199616, -0.3422138444, 0.2663300612
H, 0, -2.6630110713, -0.4618272973, -1.0441984786
O, 0, -2.0256546919, -1.0329155031, 1.1792427861
H, 0, -2.461547813, -0.5434966961, 1.8813541381
O, 0, -3.64803598, -1.4872416211, -0.6657114413
H, 0, -3.4827795883, -2.3174872159, -1.1163532324
H, 0, -2.7589725641, -1.3314300883, 0.5100070318
O, 0, -0.1237789702, 1.9799564798, -0.7260088133
H, 0, -0.5297948167, 2.2306471982, -1.5580429765
Si, 0, 1.958590274, -0.3704849657, -0.0168331983
O, 0, 2.8202559624, -0.6860381265, 1.3358875167
H, 0, 2.9126720076, 0.0301730168, 1.9664050719
O, 0, 2.4104980172, 1.0539839081, -0.671817118
H, 0, 1.6270112158, 1.618606253, -0.8268569547

O,0,2.3627185183,-1.6524571838,-0.9481408907
H,0,1.8759106748,-1.7665884185,-1.7661128915

sw-k1: HF=-1262.1278624,ZeroPoint=0.1303768

Si,0,-0.8602531171,0.7909107354,0.0456508195
O,0,-1.4996344499,1.4326628916,1.411940724
H,0,-1.9580875318,0.6634379524,1.8094579559
O,0,-1.8237523903,0.4528503825,-1.2248072659
O,0,-2.1658061342,-0.988789649,1.1752262246
H,0,-1.5063528605,-1.6347173483,1.4332400506
H,0,-2.4754152246,-0.273317764,-1.1384230142
O,0,-0.0132504773,2.1098754467,-0.5791245406
H,0,-0.4643658685,2.5672335356,-1.2907850193
Si,0,1.959401303,-0.3832885169,-0.0223360325
O,0,2.8336570219,-0.7437336199,1.3097221224
H,0,2.9085187196,-0.0607324963,1.9783816776
O,0,2.4632064294,1.0074375896,-0.7110477343
O,0,2.2716947897,-1.6860369485,-0.9581476681
H,0,1.8357103022,-1.72486943,-1.8111641176
O,0,0.377027917,-0.2607291723,0.3164566414
H,0,1.7224115538,1.6351296421,-0.8099402231
O,0,-3.6057953376,-1.565569085,-0.7610079835
H,0,-3.3556863771,-2.3978018706,-1.168274707
H,0,-3.0316467678,-1.4634051051,0.1063806803

cw-m1: HF=-1262.1236557,ZeroPoint=0.1263919

Si,0,1.469259294,-0.3601424767,-0.0674155976
O,0,2.4501428822,0.0012047577,-1.3673592122
H,0,2.4949893045,0.9450995358,-1.5323331754
O,0,1.7495960748,-2.0447837216,-0.0707472413
O,0,1.3649421195,1.7239692115,0.1149416048
H,0,1.7273884577,1.9583323647,0.9738299442
H,0,1.5346922701,-2.4922508678,-0.8898898236
O,0,-0.1398116469,-0.313600159,-0.4031600252
O,0,1.9888317365,-0.1729962524,1.515845415
Si,0,-1.7242016687,-0.3611982009,0.0072464343
O,0,-1.9007890666,-1.2709966954,1.3920384941
O,0,-2.3484418821,1.1065086175,0.117291383
H,0,0.4447216971,2.2387101352,-0.0071863949
O,0,-2.5453640597,-1.2264572308,-1.1448628416
H,0,-2.2843486227,-2.1406255541,-1.2692387462
H,0,-1.5361725247,-0.9059318744,2.2001566393
H,0,2.2714072837,-1.010203453,1.8909477105
O,0,-0.7894345085,2.9030149615,-0.2168621328

H,0,-0.9220475253,3.6074528388,0.4208707443
H,0,-1.6263156148,2.0085470634,-0.0316881787

cw-m2: HF=-1262.1257151, ZeroPoint=0.1284024

Si,0,1.4861900722,-0.270008387,0.0564005362
O,0,1.6806559518,0.3585855302,-1.4799954488
H,0,1.7197902327,-0.3567088399,-2.117985162
O,0,1.5277276175,-1.9252876503,-0.4244221463
O,0,1.6082608723,1.6150337079,0.5563068062
H,0,1.6540505239,1.6817769017,1.514402557
H,0,0.6565066053,-2.23280615,-0.6921962813
O,0,-0.0392362646,-0.2811737257,0.7154288328
O,0,2.7540605319,-0.433011379,1.1265672653
Si,0,-1.5395400747,-0.3231838291,0.0847679998
O,0,-2.5830331008,-0.8464430744,1.2570364448
O,0,-1.9938539441,1.0740153637,-0.5254191351
H,0,0.7473025158,2.1729470719,0.2252687861
O,0,-1.4486082785,-1.5723858753,-1.0028994782
H,0,-2.2272137504,-1.7477075609,-1.5338295868
H,0,-3.0996078928,-0.1525836296,1.6699749036
H,0,2.9959897149,-1.3577061134,1.2129953955
O,0,-0.3694072985,2.8325073879,-0.2697731066
H,0,-0.6869067433,3.4794882728,0.3640033312
H,0,-1.2125247905,1.9719854287,-0.3978524732

sw-m1: HF=-1262.1338424,ZeroPoint=0.1317035

Si,0,-0.9018664967,-0.8500870407,-0.0876913907
O,0,-0.9741941963,-1.3699316106,1.4985907757
H,0,-1.1205800908,-0.6223451306,2.0863913907
O,0,-1.0096619945,-2.3649234739,-0.8224232217
O,0,-0.9982781386,1.0917480249,0.9381406869
H,0,-1.6037842709,1.6374088519,0.4307266917
H,0,-0.173431036,-2.6839189012,-1.1627720008
O,0,0.5736480447,-0.3970550552,-0.6251890051
O,0,-2.2684293604,-0.1976524721,-0.7649063985
Si,0,1.8622082129,0.5230599491,-0.1306489634
O,0,2.7112233451,0.9570378085,-1.4844370719
O,0,1.3344575081,1.7515202611,0.7185356682
H,0,0.0053959412,1.4983963522,0.8701058431
O,0,2.9190185514,-0.4999676555,0.6062843757
H,0,2.5081484286,-1.1547403818,1.1989754779
H,0,2.4689208819,1.8120522167,-1.8432195627
H,0,-2.6478533231,-0.8012982949,-1.4083148924
O,0,1.5437244917,-2.3671915276,2.1742263391

H,0,0.6179504748,-2.0897351627,2.0287366338
H,0,1.686024277,-2.3377470573,3.1239681746

sw-m2: HF=-1262.1330019,ZeroPoint=0.1312575

Si,0,1.4100563391,0.0200658291,-0.1814805501
O,0,2.3061169712,1.0948798565,0.6938957269
H,0,2.1417165752,0.9777720752,1.6329499078
O,0,2.1073986398,0.4332831564,-1.6629240461
O,0,0.7414121839,-0.5153446103,1.8404304648
H,0,0.9959110082,-1.4265651328,2.0046042206
H,0,1.5041425333,0.3442877946,-2.401625938
O,0,-0.1602657482,0.3144200584,-0.5205163703
O,0,1.8346887474,-1.6083268739,-0.1524785642
Si,0,-1.6899776059,-0.0375154391,0.0112432759
O,0,-2.2507107962,-1.2745387536,-0.9178903113
O,0,-1.6518303414,-0.2904238152,1.5765904364
H,0,-0.3632578814,-0.4490645756,1.828016893
O,0,-2.6797611856,1.1994592398,-0.4605742827
H,0,-2.752144151,1.9169740679,0.1705869452
H,0,-1.6729366807,-2.05826037,-0.8946940092
H,0,2.4282429735,-1.8001300521,-0.8845344096
O,0,-0.354414588,-3.3126610283,-0.6151158717
H,0,0.4505833462,-2.7827818032,-0.4566638387
H,0,-0.1568420495,-3.8783649339,-1.3662847186

sw-m3: HF=-1262.1302878,ZeroPoint=0.1315476

Si,0,1.469848493,-0.2042572815,-0.0544862642
O,0,2.1356602001,0.199213224,-1.5156823174
H,0,1.9625606566,1.1192424479,-1.7281156071
O,0,2.0984787902,-1.778586443,0.0184805453
O,0,0.8522908858,1.8416607811,-0.1041734459
H,0,1.2136469241,2.3744386434,0.621892207
H,0,1.4228567883,-2.4507025596,-0.0714306201
O,0,-0.1192040113,-0.5982951899,0.0039062404
O,0,2.2464390444,0.3196106666,1.3383739237
Si,0,-1.6457486124,0.0296046884,0.0704557678
O,0,-2.3942994239,-0.5982603485,1.4074726437
O,0,-1.5906756255,1.606193737,0.0136666167
H,0,-0.2086274291,1.8559548712,-0.0425288742
O,0,-2.5143662064,-0.7316204016,-1.1164807273
H,0,-2.1793561561,-0.6183032489,-2.0072753023
H,0,-2.3553127739,-0.0372260731,2.1833163276
H,0,2.7190404991,-0.4153951849,1.7380913513
O,0,2.2496995756,2.9102639087,2.1389920527

H, 0, 2.362999216, 1.9414918924, 2.0886562239
H, 0, 1.7409930755, 3.0808808305, 2.9358197485

sw-m4: HF=-1262.1273279,ZeroPoint=0.1319402

Si, 0, 1.4596268414, 0.0997271382, -0.032790195
O, 0, 1.7627671246, -0.2317690041, 1.5548788075
H, 0, 2.0870709482, 0.5458252177, 2.0153649537
O, 0, 1.9922972694, 1.7098776789, -0.1390826669
O, 0, 0.9255572078, -2.243468757, 0.0956934664
H, 0, 1.1882267492, -2.5213331302, -0.7850667973
H, 0, 1.2827442682, 2.3544286307, -0.1093120921
O, 0, -0.1025948276, 0.2606588911, -0.4401988118
O, 0, 2.4588501547, -0.5967845021, -1.1337571416
Si, 0, -1.6101360085, -0.3182605137, -0.0560444637
O, 0, -2.5889287875, 0.2436693356, -1.2719590017
O, 0, -1.5912666421, -1.8694870891, 0.1914435533
H, 0, -0.0914562305, -2.2225335436, 0.1154603709
O, 0, -2.1692442799, 0.5866013819, 1.2181517421
H, 0, -2.2160315095, 0.1025544229, 2.0437233095
H, 0, -2.3707986279, -0.0704572289, -2.1507657209
H, 0, 3.0185436538, 0.0401288447, -1.6081944215
O, 0, 3.9220786994, 1.6310301235, -2.066691872
H, 0, 3.2642824493, 1.9660471817, -1.4277582635
H, 0, 3.6944025675, 2.0174696517, -2.9163266054

sw-m5: HF=-1262.1261116,ZeroPoint=0.1320728

Si, 0, -1.5297311781, -0.2448041499, 0.054995294
O, 0, -1.7809979682, 0.1538692567, 1.6329892297
H, 0, -2.0790738597, -0.611112892, 2.1316618451
O, 0, -2.1443920248, -1.8080175132, 0.0204299117
O, 0, -0.8871427378, 2.0748084292, 0.1404496852
H, 0, -1.0616822116, 2.4950920879, -0.7132377467
H, 0, -1.5095033494, -2.4742604062, -0.2457116806
O, 0, -0.0033189049, -0.4592926955, -0.4448580288
O, 0, -2.5619989484, 0.4602678641, -1.0431332758
Si, 0, 1.5356574548, 0.0186978615, -0.0591351563
O, 0, 2.4674730761, -0.3981578488, -1.3723952793
O, 0, 1.6219454256, 1.5329180029, 0.3438975742
H, 0, 0.1150620133, 1.9921388621, 0.2292486848
O, 0, 1.9642511325, -1.0930490448, 1.0969348438
H, 0, 2.7926697649, -0.9135955719, 1.5446287333
H, 0, 2.6132542982, 0.3200417883, -1.9903298601
H, 0, -3.1550148755, -0.2001148992, -1.4127573509
O, 0, -2.0501057772, 2.796800396, -2.392581

H,0,-2.3237443903,1.9106505473,-2.0902006018
H,0,-1.5564271995,2.6601946057,-3.2051079217

cw-p1: HF=-1262.1516247,ZeroPoint=0.131976

Si,0,0.5409481317,-0.44396433,0.0218910749
O,0,1.1889039622,-1.2776474083,-1.2549594659
H,0,2.1527184782,-1.3113616499,-1.1927592861
O,0,0.6786880891,1.1327638736,-0.0874014761
O,0,1.1922657413,-1.0935246594,1.400510291
H,0,2.1548964051,-1.145961872,1.3407559391
H,0,2.1629306487,1.6826770585,-0.1260344536
O,0,3.7283393307,-0.7312811882,0.0244586166
H,0,4.6507946569,-0.9955097191,-0.0032143454
Si,0,-2.3712480534,0.083137683,0.016260062
O,0,-3.3821905745,-0.4021344941,-1.1806483442
H,0,-2.9934678852,-0.5574504117,-2.0436894494
O,0,-1.8832244764,1.6231754955,-0.1293988005
O,0,-3.2616048239,-0.0317222511,1.3845104775
H,0,-3.8196158612,-0.8057729947,1.4792476758
O,0,-1.0546486477,-0.8799456403,0.0516393574
H,0,-0.880718751,1.6518334276,-0.131247701
O,0,3.1482080215,1.9027209805,-0.176155
H,0,3.3491561915,2.4389334366,0.5945016928
H,0,3.7019906664,0.2520781236,-0.0335446952

sw-p1: HF=-1262.1497389,ZeroPoint=0.1326852

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O,0,-0.0408135251,-0.5107600978,2.002476838
H,0,-0.2846409723,-1.3017097634,2.4870204385
O,0,-0.7903606395,1.0515692971,0.0229437441
O,0,-1.5796582668,-1.5884889045,0.0324310337
H,0,-3.0631027061,-1.2294373594,-0.1711453274
H,0,-1.7218205901,1.3453275503,0.0802642522
O,0,-4.0311945484,-0.9270471273,-0.2601914804
H,0,-4.3149208069,-1.1670289177,-1.1452709194
Si,0,2.2738406412,0.2069257486,-0.2128041251
O,0,2.7186665062,0.1624378785,1.3653051655
H,0,1.9741882382,-0.0808660945,1.9361877451
O,0,1.8908693253,1.7110519926,-0.7290896677
O,0,3.549643372,-0.2326976675,-1.1258075219
H,0,4.1080097497,-0.9333657788,-0.783817996
O,0,0.9762836802,-0.7567714015,-0.3990248953
H,0,0.9412883833,1.8776235609,-0.6242980779
O,0,-3.4659432121,1.6668172812,0.143922408

H, 0, -3.7748926629, 2.2324022244, -0.5683737888
H, 0, -3.7869978745, 0.7551588086, -0.0634475513

cw-p2: HF=-1262.1464144,ZeroPoint=0.131493

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H, 0, 0.9462641773, -1.9888061338, 1.1277300914
O, 0, 1.6148980639, 0.6829342806, -1.0637581903
O, 0, -0.6340878193, 0.2084112072, 0.4180688811
H, 0, 3.0099886572, 1.2525755628, -0.6527518692
O, 0, 4.1232130979, -0.5617045508, 1.4043670118
H, 0, 3.2376908575, -0.9162120029, 1.2293611559
O, 0, 3.9350461147, 1.5659451217, -0.3914128547
H, 0, 3.8235622718, 2.4303157179, 0.010352192
H, 0, 4.1685886204, 0.2276159197, 0.8318178067
O, 0, -0.0972065831, -1.3790282508, -1.5367845864
H, 0, 0.3737338025, -1.5048285638, -2.3627428146
Si, 0, -2.2463655424, 0.2768276262, 0.2607476637
O, 0, -3.0076045744, -0.197344301, 1.626489487
H, 0, -2.9282524569, -1.1210190899, 1.8708450627
O, 0, -2.6901472923, -0.6353312446, -1.0194634763
H, 0, -1.9240233525, -1.0517994473, -1.4511654778
O, 0, -2.7836901451, 1.8141980733, 0.127971249
H, 0, -2.4576984208, 2.3291062091, -0.6121800916

sw-p2: HF=-1262.1489961,ZeroPoint=0.1318389

Si, 0, 0.6576413411, 0.0339393166, 0.2369606938
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H, 0, 3.0109343542, 1.3944082987, -0.2224774041
O, 0, 1.3576328681, -1.3773759991, -0.2343599612
O, 0, 4.0238574135, 1.3795459434, -0.3636726305
H, 0, 4.189785105, 1.7824118281, -1.2189284836
H, 0, 2.3335116022, -1.391548517, -0.2409952797
O, 0, 0.1595657013, -0.1728196756, 1.8349098974
H, 0, 0.578514412, 0.4389428084, 2.4433970481
Si, 0, -2.3643617546, 0.0033332268, -0.2272057387
O, 0, -3.1374473848, 1.3341338347, -0.7807544074
H, 0, -2.8901282634, 2.1735124825, -0.3889843091
O, 0, -2.5412401744, -0.1658013146, 1.3881913007
O, 0, -3.1570556112, -1.168770407, -1.0466138836
H, 0, -2.8734045921, -2.0719100863, -0.8946146865
O, 0, -0.7854052981, 0.0184696287, -0.5818562274
H, 0, -1.6764403456, -0.189168644, 1.8377990259
O, 0, 4.1327679159, -1.2968556452, -0.2741091217

H, 0, 4.5120911618, -1.6811508111, -1.0684235145
H, 0, 4.2106216175, -0.3163129805, -0.3739929677

cw-q1: HF=-1262.149845,ZeroPoint=0.1313601

Si, 0, 1.5754018862, -0.4937838132, -0.1741669944
O, 0, 2.2661063996, 0.967892529, -0.2536766959
H, 0, 1.7372944582, 1.7599994786, 0.0035918366
O, 0, 2.4896243578, -1.5071822819, -1.0785676198
O, 0, 0.8801937037, 3.1581163057, 0.4021686705
H, 0, 0.8830652716, 3.3278633582, 1.3475938719
H, 0, 2.8711746825, -1.1459835603, -1.8807931904
O, 0, 0.0340479375, -0.4764914825, -0.6438533267
O, 0, 1.5419128516, -1.1295923841, 1.3461778328
Si, 0, -1.5020496145, -0.71409823, -0.0432203151
O, 0, -1.2816244732, -1.2965309925, 1.4953260171
O, 0, -2.4118296909, 0.5542755393, -0.1529979253
H, 0, -0.0746273013, 3.0950165111, 0.1316735886
O, 0, -2.1625316615, -1.9550772176, -0.9289582335
H, 0, -1.7505510072, -2.8111672815, -0.8000098285
H, 0, -0.3557787648, -1.3626427522, 1.7601689274
H, 0, 2.3600731107, -1.1592585577, 1.8453640816
O, 0, -1.6244289135, 2.9360007928, -0.4307058464
H, 0, -2.2547990757, 3.5028259257, 0.0192116112
H, 0, -1.9524601566, 1.9682431131, -0.3073864618

sw-q1: HF=-1262.1500669,ZeroPoint=0.13169

Si, 0, 1.4928886001, -0.0891729588, -0.7502467791
O, 0, 1.665852229, 0.7220122715, 0.6570669572
H, 0, 1.3640291937, 0.2307407235, 1.4718394773
O, 0, 2.2211716761, 0.7728247793, -1.9365507763
O, 0, 0.6049439488, -0.5771302382, 2.6776595002
H, 0, 1.0668537138, -1.3724472865, 2.9529273396
H, 0, 1.6761565396, 1.4047152728, -2.4088747662
O, 0, -0.0567889802, -0.3163102684, -1.1470057639
O, 0, 2.3146385787, -1.4941441502, -0.5785467101
Si, 0, -1.4800419263, -0.4646792769, -0.2789556777
O, 0, -2.5316195852, -1.2503243152, -1.2910225121
O, 0, -1.2622122534, -1.1858771101, 1.1008875743
H, 0, -0.179158678, -0.873930947, 2.0756813859
O, 0, -2.1250887213, 1.0533080638, -0.2411923156
H, 0, -1.5237518069, 1.7410062282, 0.0931751527
H, 0, -2.6482182741, -2.1789875467, -1.0857613618
H, 0, 2.1950184446, -2.1580222939, -1.2603598168
O, 0, -0.1514730113, 2.8522398339, 0.6590765716

H, 0, 0.574471037, 2.2052842266, 0.7463909912
 H, 0, -0.2700881046, 3.2416777922, 1.5294289196

Table S2. Dependence of the energetic reaction path on the theoretical methods with the 6-311++G(2d,2p) basis set. The relative energies ΔE (in kcal/mol) are calculated using the respective optimized geometries. No ZPE corrections are included for the purpose of comparison. It is evident that the CAM-B3LYP data are in good agreement with the MP2 data while the M06-2X data show significant deviations.

Species	ΔE		
	CAM-B3LYP	M06-2X	MP2
RC	0.0	0.0	0.0
TS1	6.0	4.3	5.2
IM1	-1.9	-5.6	-2.5
TS-iso	4.7	0.7	3.9
IM2	4.0	-0.4	2.8
TS2	13.5	12.3	13.2
TS4	9.8	7.6	9.4
PC1	-2.6	-2.0	-2.7
PC2	-3.8	-3.2	-3.5

Table S3. Dependence of the energetic reaction path on the basis sets using the CAM-B3LYP method. The relative energies ΔE (in kcal/mol) are calculated using the respective optimized geometries. No ZPE corrections are included for the purpose of comparison. It is evident that 6-311++G(2d,2p) is a good basis set in the present calculations in the consideration of accuracy and efficiency.

Species	ΔE		
	6-311++G(2d,2p)	6-311++G(3df,3pd)	Aug-cc-pVT(+d) Z
RC	0.0	0.0	0.0
TS1	6.0	6.0	6.4
IM1	-1.9	-2.3	-1.7
TS-iso	4.7	4.2	4.9
IM2	4.0	3.5	4.2
TS2	13.5	13.0	13.3
TS4	9.8	8.9	9.4
PC1	-2.6	-3.1	-2.8
PC2	-3.8	-4.6	-4.3

Table S4. The relative energies (in kcal/mol, with the Gibbs Free Energy ΔG and ZPE corrected ΔE) of the most stable conformations of the stationary points involved in the silica dimerization reaction.

Species	CAM-B3LYP/6-311++G(2d, 2p)		CBS-QB3
	ΔG	ΔE	ΔE
H₄SiO₄+H₃SiO₄⁻	5.5	18.0	19.8
RC	0.0	0.0	0.0
TS1	6.9	6.2	5.0
IM1	2.1	-0.1	-2.3
TS-iso	7.4	6.2	3.7
IM2	5.6	4.7	1.7
TS2	14.4	12.9	12.1
TS4	15.0	15.2	14.3
PC1	9.8	8.8	7.8
PC2	-2.5	-2.6	-3.1
RC	-2.9	-3.7	-3.8

Table S5. The relative energies (in kcal/mol, with the Gibbs Free Energy ΔG and ZPE corrected ΔE) of the most stable conformations of the stationary points involved in the water-mediated silica dimerization reaction.

Species	CAM-B3LYP/6-311++G(2d, 2p)		CBS-QB3
	ΔG	ΔE	ΔE
H₄SiO₄+H₃SiO₄⁻+H₂O	5.5	18.0	19.8
RC+H₂O	0.0	0.0	0.0
RC-w	2.5	-6.5	-6.7
TS1-w	11.7	1.1	-0.6
IM1-w	3.9	-6.8	-8.6
TS-iso-w	12.3	0.6	-2.6
IM2-w	7.1	-3.6	-5.9
TS2-cw	5.9	-4.1	-2.0
TS2-sw	13.9	3.1	3.3
TS3-cw	19.8	9.7	10.6
TS3-sw	14.8	5.8	6.1
TS4-cw	15.3	6.0	6.0
TS4-sw	13.8	2.9	1.8
PC1-cw	0.9	-8.1	-8.7
PC1-sw	2.3	-6.4	-6.1
PC2-cw	1.8	-5.1	-5.4
PC2-sw	1.1	-6.5	-5.9
PC3-cw	0.6	-7.3	-6.6
PC3-sw	1.9	-7.3	-8.1

Table S6. Comparison of the CBS-QB3 calculated energies (in kcal/mol) with the explicitly correlated CCSD(T)-F12/VDZ-F12 results. The CAM-B3LYP/6-311++G(2d,2p) optimized geometrical parameters, zero-point energies, and solvation energies were used for the CCSD(T)-F12 calculations. Evidently, the CBS-QB3 data are in very good agreement with the CCSD(T)-F12 data.

Species	CBS-QB3	CCSD (T) -F12/VDZ-F12
RC	0.0	0.0
TS1	5.0	4.8
IM1	-2.3	-2.3
TS-iso	3.7	3.9
IM2	1.7	2.0
TS2	12.1	12.2
TS4	7.8	7.8
PC1	-3.1	-2.9
PC2	-3.8	-3.7