Supporting Information

Three Competitive Transition States at the Glycosidic Bond of Sucrose in the Acid-Catalyzed Hydrolysis

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I. Figure S1. The neutral reaction path [I] of the mutarotation of glucose with $(H_2O)_9$. $\Delta(E_T + ZPE)$ is the B3LYP/6-311G(d,p) SCRF = PCM relative energy in kcal/mol. The distance is in Å. At the step of β form → aldehyde open form, TS1 involving the proton transfer via the water dimer and that via the trimer were obtained. The former was found to be more likely than the latter by $\Delta(E_T + ZPE)$ = +17.16 kcal/mol □ +24.79 kcal/mol. (page S2)

II. Figure S2. The H^+ containing reaction path [II] with $H_3O^+(H_2O)_8$. The acid catalyst enhances the mutarotation after the hydrolysis of sucrose. (page S3)

III. Cartesian coordinates of the optimized geometries for Scheme 3 and Figures 1, 2, 3, 5, S1, and S2. (page S4-S89)

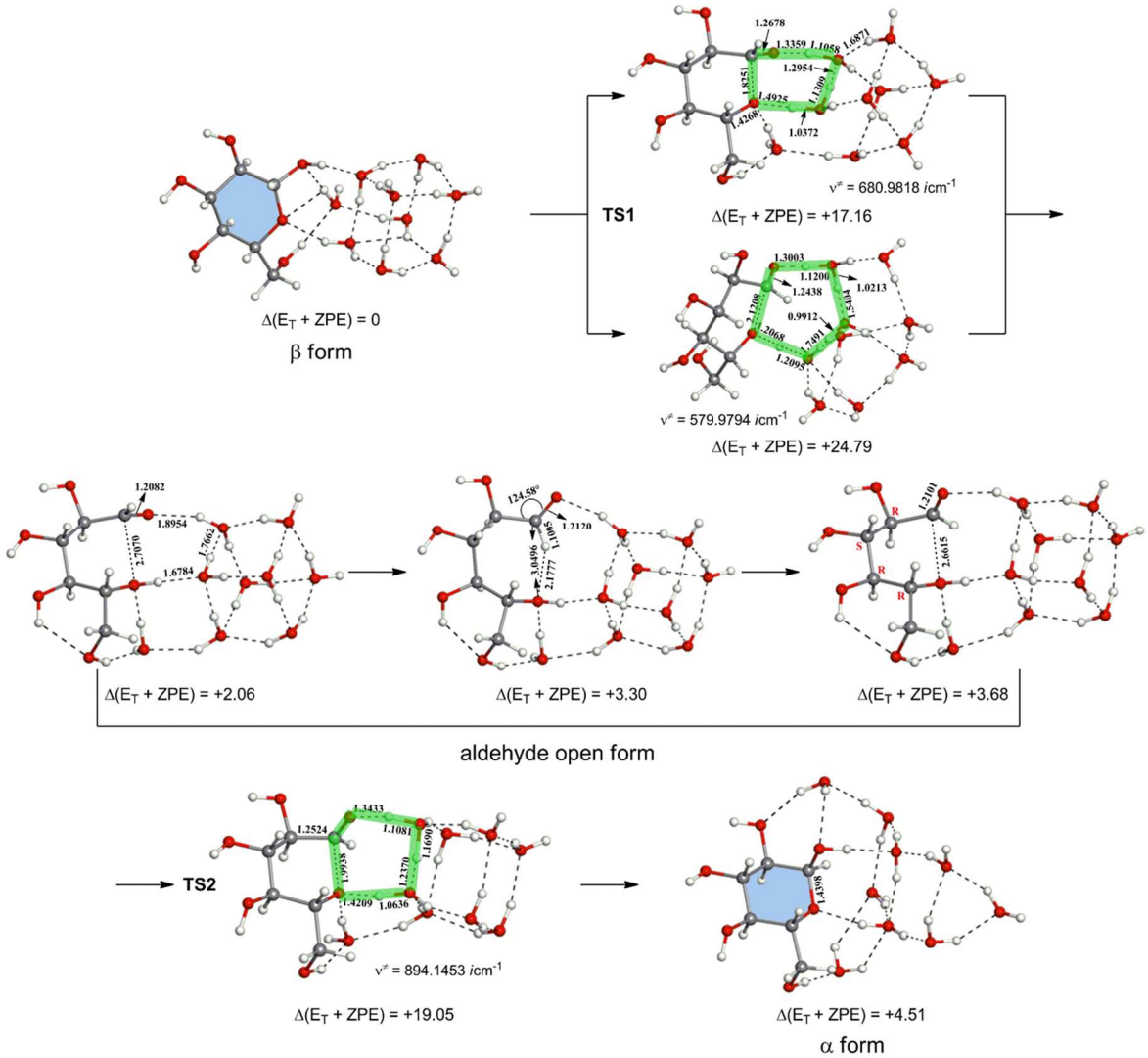


Figure S1. The neutral reaction path [I] of the mutarotation of glucose with $(H_2O)_9$. $\Delta(E_T + ZPE)$ is the B3LYP/6-311G(d,p) SCRF = PCM relative energy in kcal/mol. The distance is in Å. At the step of β form → aldehyde open form, TS1 involving the proton transfer via the water dimer and that via the trimer were obtained. The former was found to be more likely than the latter by $\Delta(E_T + ZPE)$ = +17.16 kcal/mol □ +24.79 kcal/mol.

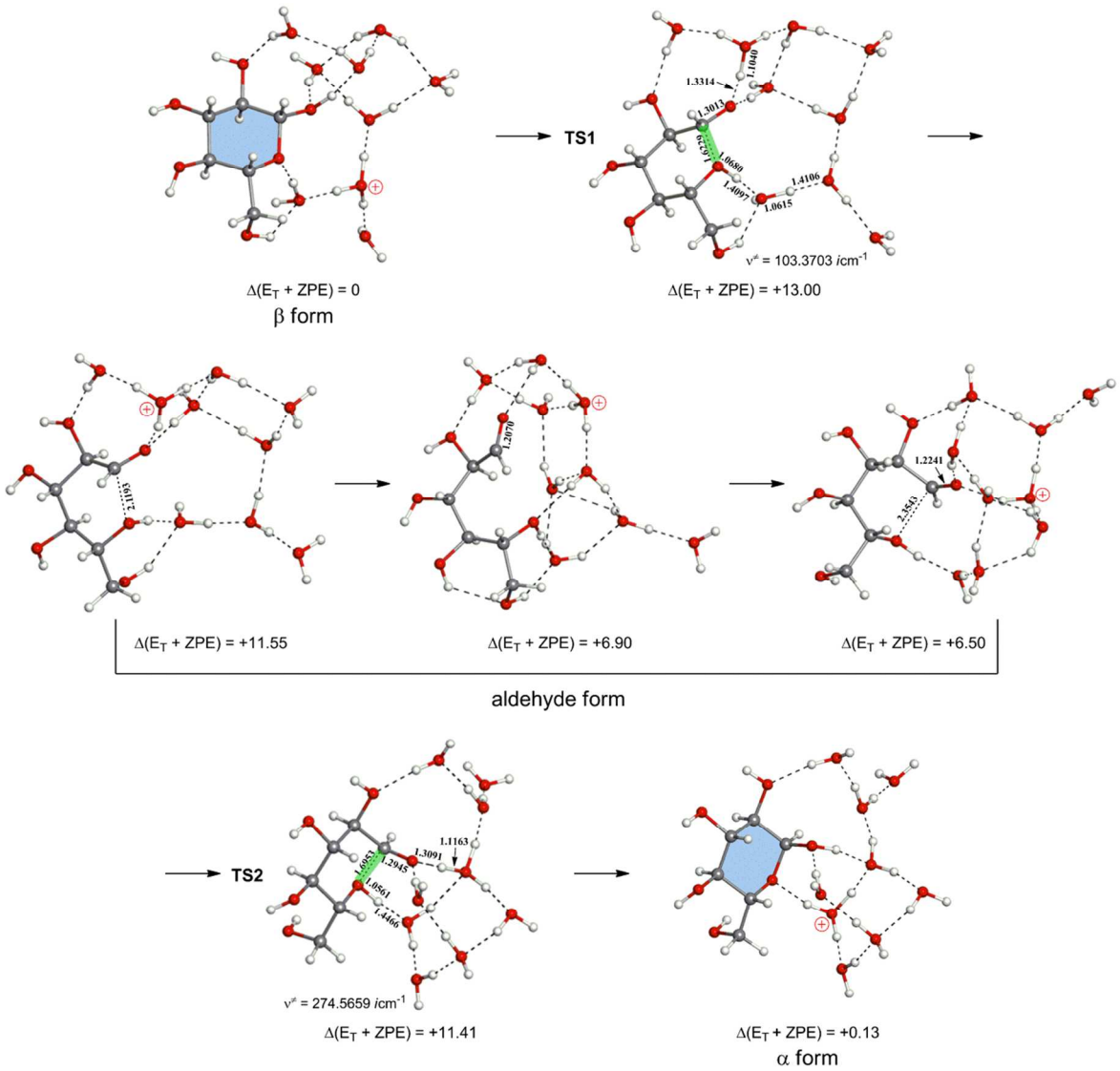


Figure S2. The H^+ containing reaction path [II] with $H_3O^+(H_2O)_8$. The acid catalyst enhances the mutarotation after the hydrolysis of sucrose.

III. Cartesian coordinates of geometries optimized by B3LYP/6-311G(d,p) and B3LYP/6-311G(d,p) SCRF=(PCM,solvent=water)

==== Scheme 3 ====

1) sucrose (a neutral molecule)
satouh00.high.chk
Stoichiometry C12H22O11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.258022	-1.321485	-0.671281
2	6	0	-3.026635	-0.010357	-0.701964
3	6	0	-1.628607	-1.555730	0.698863
4	6	0	-2.115125	1.140839	-0.277394
5	6	0	-0.790104	-0.338094	1.123081
6	8	0	-1.508576	0.860199	1.003457
7	6	0	-2.862463	2.455112	-0.084776
8	1	0	-3.413285	2.685589	-0.997079
9	1	0	-2.130773	3.253495	0.098325
10	8	0	-3.809175	2.376141	0.969534
11	1	0	-3.319795	2.079589	1.745768
12	1	0	-1.336952	1.273676	-1.038328
13	8	0	-3.489965	0.278934	-2.016291
14	1	0	-3.984418	-0.496360	-2.305862
15	1	0	-3.868528	-0.069729	-0.000398
16	8	0	-3.168607	-2.365210	-1.007841
17	1	0	-2.714896	-3.196340	-0.823047
18	1	0	-1.456891	-1.268733	-1.422600
19	8	0	-0.866848	-2.756789	0.710572
20	1	0	-0.106484	-2.632699	0.117303
21	1	0	-2.426147	-1.697664	1.433185
22	8	0	0.366154	-0.310150	0.274393
23	1	0	-0.494800	-0.390626	2.167240
24	6	0	1.690506	-0.473208	0.750708
25	8	0	2.369776	0.777237	0.767600
26	6	0	2.429132	-1.249082	-0.350045
27	6	0	1.839500	-1.075255	2.151666
28	6	0	2.652927	-0.176535	-1.411798
29	6	0	2.864568	1.095951	-0.565650
30	6	0	2.137645	2.332486	-1.076094
31	8	0	1.686009	-2.379028	-0.772751
32	1	0	2.207515	-2.852332	-1.429867

33	1	0	3.412530	-1.552828	0.029180
34	1	0	2.883194	-1.393743	2.261639
35	1	0	1.199705	-1.953381	2.247941
36	8	0	1.476370	-0.166125	3.175981
37	1	0	1.954538	0.653028	2.999529
38	8	0	3.765785	-0.555891	-2.213065
39	1	0	3.773380	-0.019016	-3.011179
40	1	0	1.745397	-0.094602	-2.020195
41	1	0	3.933370	1.302619	-0.466891
42	1	0	1.077156	2.089137	-1.223074
43	1	0	2.558690	2.632858	-2.040912
44	8	0	2.297954	3.434365	-0.202349
45	1	0	1.956542	3.150733	0.653497

SCF Done: E(RB3LYP) = -1298.30492177 A.U. after 10 cycles
Convg = 0.5083D-08 -V/T = 2.0042
Sum of electronic and zero-point Energies= -1297.935081
Sum of electronic and thermal Energies= -1297.911085
Sum of electronic and thermal Enthalpies= -1297.910141
Sum of electronic and thermal Free Energies= -1297.988380

2) sucrose protonated to O(6) on the glucose moiety, H+(A)
satouh+b.high.chk
Stoichiometry C12H23O11(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.923977	1.574294	-0.679259
2	6	0	2.895477	0.396549	-0.722297
3	6	0	1.342656	1.755429	0.727757
4	6	0	2.219753	-0.921847	-0.349032
5	6	0	0.556273	0.524117	1.176925
6	8	0	1.460439	-0.755568	0.937503
7	6	0	3.200196	-2.042870	-0.029854
8	1	0	3.981963	-2.043858	-0.792601
9	1	0	2.689907	-3.009667	-0.016419
10	8	0	3.709975	-1.708974	1.270980
11	1	0	4.248879	-2.425605	1.621854
12	1	0	1.487029	-1.234766	-1.090770
13	8	0	3.400766	0.175880	-2.021442
14	1	0	3.776185	1.010243	-2.330865
15	1	0	3.710001	0.603537	-0.013672
16	8	0	2.682741	2.706413	-1.052443

17	1	0	2.136337	3.492417	-0.927886
18	1	0	1.109118	1.397529	-1.395156
19	8	0	0.499204	2.882289	0.819519
20	1	0	-0.363249	2.671231	0.422385
21	1	0	2.167565	1.932164	1.424126
22	8	0	-0.528586	0.373349	0.401573
23	1	0	0.392792	0.448565	2.247569
24	6	0	-1.835840	-0.138897	0.860872
25	8	0	-2.046607	-1.385393	0.291930
26	6	0	-2.862700	0.789809	0.196645
27	6	0	-1.944824	-0.250560	2.377957
28	6	0	-3.065137	0.193136	-1.212205
29	6	0	-2.474657	-1.232218	-1.104678
30	6	0	-1.263192	-1.468857	-2.011623
31	8	0	-2.418180	2.132732	0.243698
32	1	0	-3.172812	2.717719	0.114417
33	1	0	-3.816363	0.671179	0.722389
34	1	0	-2.976955	-0.529421	2.610722
35	1	0	-1.753766	0.722195	2.835527
36	8	0	-1.014036	-1.171180	2.919608
37	1	0	-1.300859	-2.060307	2.683214
38	8	0	-4.454296	0.236867	-1.484931
39	1	0	-4.606852	0.085171	-2.423481
40	1	0	-2.501745	0.792801	-1.936019
41	1	0	-3.243203	-1.990188	-1.253310
42	1	0	-0.663727	-0.550799	-2.062084
43	1	0	-1.602774	-1.701384	-3.024457
44	8	0	-0.464762	-2.551990	-1.557328
45	1	0	-0.588100	-2.590877	-0.600514
46	1	0	2.125474	-0.951789	1.648440

SCF Done: E(RB3LYP) = -1298.65032515 A.U. after 10 cycles
Convg = 0.5048D-08 -V/T = 2.0042
Sum of electronic and zero-point Energies= -1298.268868
Sum of electronic and thermal Energies= -1298.244697
Sum of electronic and thermal Enthalpies= -1298.243752
Sum of electronic and thermal Free Energies= -1298.321113

3) Fructose ether oxygen protonated sucrose, H+(B)
satouh+.high.chk
Stoichiometry C12H23O11(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.368891	1.391075	0.025684
2	6	0	3.410066	0.731351	-0.873104
3	6	0	2.158611	0.526206	1.273196
4	6	0	3.053456	-0.709288	-1.243939
5	6	0	1.910818	-0.907784	0.904824
6	8	0	2.392687	-1.457793	-0.118236
7	6	0	4.248512	-1.552435	-1.633261
8	1	0	4.689251	-1.080473	-2.519639
9	1	0	3.910917	-2.561303	-1.897533
10	8	0	5.126559	-1.561663	-0.521349
11	1	0	5.936150	-2.024501	-0.758066
12	1	0	2.296990	-0.715523	-2.029586
13	8	0	3.520792	1.389495	-2.119780
14	1	0	3.822869	2.289420	-1.946479
15	1	0	4.366078	0.736298	-0.337744
16	8	0	2.901402	2.656813	0.355747
17	1	0	2.309359	3.102074	0.972430
18	1	0	1.415841	1.484036	-0.510497
19	8	0	1.243718	1.032909	2.201762
20	1	0	0.444518	1.366847	1.752015
21	1	0	3.128581	0.467507	1.800568
22	8	0	-0.304214	-0.494587	0.153701
23	1	0	1.416629	-1.591343	1.595942
24	6	0	-1.237008	-0.474665	0.936476
25	8	0	-3.486230	-1.357386	-0.331920
26	6	0	-2.152004	0.752693	0.969450
27	6	0	-1.442719	-1.536251	1.993784
28	6	0	-2.962536	0.948854	-0.327675
29	6	0	-4.092422	-0.070689	-0.445196
30	6	0	-4.862472	0.018231	-1.757797
31	8	0	-1.262012	1.853008	1.145452
32	1	0	-1.777922	2.649513	0.947251
33	1	0	-2.845084	0.690892	1.817986
34	1	0	-2.477462	-1.888995	1.928107
35	1	0	-1.323337	-1.049365	2.968930
36	8	0	-0.494756	-2.577697	1.926691
37	1	0	-0.711931	-3.144782	1.178111
38	8	0	-3.474705	2.280273	-0.235062
39	1	0	-3.517527	2.674211	-1.111506
40	1	0	-2.273003	0.852008	-1.173971
41	1	0	-4.800611	0.091472	0.378964
42	1	0	-4.160711	-0.028167	-2.602040
43	1	0	-5.426474	0.957010	-1.801767
44	8	0	-5.727166	-1.114146	-1.747855
45	1	0	-6.177306	-1.186393	-2.594787

46	1	0	-4.141586	-1.988044	-0.664569

SCF Done: E(RB3LYP) = -1298.65659064 A.U. after 10 cycles
Convg = 0.7809D-08 -V/T = 2.0042
Sum of electronic and zero-point Energies= -1298.280239
Sum of electronic and thermal Energies= -1298.253463
Sum of electronic and thermal Enthalpies= -1298.252519
Sum of electronic and thermal Free Energies= -1298.338389

4) Sucrose + H+, C(5).....O(22) cleaved, H+(C)
satouhaa.high.chk
Stoichiometry C12H23O11(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.241553	1.318060	-0.517583
2	6	0	3.277152	0.320171	-1.024815
3	6	0	1.959900	1.041261	0.966292
4	6	0	2.882316	-1.138867	-0.780163
5	6	0	1.599306	-0.394746	1.171769
6	8	0	2.044185	-1.333725	0.458974
7	6	0	4.063351	-2.068430	-0.597422
8	1	0	4.645236	-2.022520	-1.526225
9	1	0	3.704527	-3.093856	-0.453226
10	8	0	4.782464	-1.594835	0.527857
11	1	0	5.582547	-2.117383	0.640783
12	1	0	2.230404	-1.482973	-1.583320
13	8	0	3.445459	0.395853	-2.426603
14	1	0	3.791907	1.272736	-2.632491
15	1	0	4.217213	0.527894	-0.502072
16	8	0	2.816350	2.591847	-0.705778
17	1	0	2.235661	3.261022	-0.325680
18	1	0	1.305942	1.211025	-1.082255
19	8	0	1.065260	1.928335	1.568119
20	1	0	0.245435	1.994756	1.037795
21	1	0	2.915635	1.142571	1.510934
22	8	0	-0.653212	-0.355503	0.195589
23	1	0	1.024943	-0.725956	2.037722
24	6	0	-1.876813	-0.023878	0.912274
25	8	0	-2.863684	-0.952033	0.571203
26	6	0	-2.383815	1.312098	0.377380
27	6	0	-1.619593	-0.095126	2.418611
28	6	0	-3.092993	0.911408	-0.914110

29	6	0	-3.646056	-0.488217	-0.572175
30	6	0	-3.556332	-1.491681	-1.714957
31	8	0	-1.326608	2.247342	0.208451
32	1	0	-1.710006	3.107039	-0.001802
33	1	0	-3.136534	1.704798	1.071524
34	1	0	-2.570676	0.000759	2.949385
35	1	0	-0.967022	0.726455	2.717524
36	8	0	-0.941321	-1.298529	2.760392
37	1	0	-1.577724	-2.022463	2.768940
38	8	0	-4.074273	1.889082	-1.205322
39	1	0	-4.331840	1.826933	-2.130442
40	1	0	-2.346250	0.848048	-1.714419
41	1	0	-4.679927	-0.389178	-0.227519
42	1	0	-2.512221	-1.584645	-2.026556
43	1	0	-4.122538	-1.091016	-2.569799
44	8	0	-3.976595	-2.790843	-1.358577
45	1	0	-4.935305	-2.799129	-1.269852
46	1	0	-0.641472	-1.323156	0.205994

SCF Done: E(RB3LYP) = -1298.65084226 A.U. after 1 cycles
Convg = 0.3369D-08 -V/T = 2.0042
Sum of electronic and zero-point Energies= -1298.273078
Sum of electronic and thermal Energies= -1298.247068
Sum of electronic and thermal Enthalpies= -1298.246123
Sum of electronic and thermal Free Energies= -1298.330268

5) Sucrose + H+, C(24)....(22) cleaved, H+(D)
satoupc.chk
Stoichiometry C12H23O11(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.814536	-1.222189	-0.483414
2	6	0	-3.389162	0.180623	-0.364401
3	6	0	-1.830357	-1.490927	0.646781
4	6	0	-2.233787	1.189938	-0.392476
5	6	0	-0.785472	-0.372796	0.782995
6	8	0	-1.321378	0.907805	0.701654
7	6	0	-2.687194	2.630878	-0.201110
8	1	0	-3.311613	2.917129	-1.049407
9	1	0	-1.808138	3.287405	-0.195900
10	8	0	-3.474128	2.799864	0.964090
11	1	0	-2.905246	2.645155	1.726196

12	1	0	-1.701064	1.102693	-1.347654
13	8	0	-4.262866	0.360032	-1.475052
14	1	0	-4.977197	0.951336	-1.217118
15	1	0	-3.930472	0.285561	0.580490
16	8	0	-3.794856	-2.240272	-0.399637
17	1	0	-4.462215	-2.052419	-1.071149
18	1	0	-2.288541	-1.287338	-1.449134
19	8	0	-1.104023	-2.697609	0.409962
20	1	0	-1.753492	-3.386254	0.215282
21	1	0	-2.388140	-1.555776	1.586985
22	8	0	0.233302	-0.559108	-0.235059
23	1	0	-0.290524	-0.425231	1.751615
24	6	0	2.394720	-0.922854	0.487091
25	8	0	2.628946	0.235861	0.952673
26	6	0	2.829218	-1.064070	-0.942808
27	6	0	2.104804	-2.035692	1.442872
28	6	0	2.787111	0.392827	-1.442797
29	6	0	3.010016	1.200742	-0.146088
30	6	0	2.180315	2.458668	0.046018
31	8	0	2.064286	-2.013521	-1.627184
32	1	0	2.538438	-2.301311	-2.415453
33	1	0	3.893595	-1.355216	-0.898939
34	1	0	3.045007	-2.612894	1.510545
35	1	0	1.360002	-2.700710	1.001397
36	8	0	1.625025	-1.607204	2.683327
37	1	0	2.301967	-1.101428	3.147953
38	8	0	3.816494	0.585500	-2.386745
39	1	0	3.546915	1.235967	-3.042556
40	1	0	1.795363	0.588315	-1.857094
41	1	0	4.074982	1.385287	0.005540
42	1	0	1.123642	2.182465	0.082318
43	1	0	2.337505	3.089417	-0.840238
44	8	0	2.476779	3.122586	1.252307
45	1	0	3.237434	3.699389	1.127742
46	1	0	0.067094	-1.413901	-0.670086

SCF Done: E(RB3LYP) = -1298.65546244 A.U. after 1 cycles
Convg = 0.5856D-08 -V/T = 2.0042
Sum of electronic and zero-point Energies= -1298.277218
Sum of electronic and thermal Energies= -1298.251237
Sum of electronic and thermal Enthalpies= -1298.250293
Sum of electronic and thermal Free Energies= -1298.333366

===== Figure 1 =====

Geometries of H+(C) and H+(D) are included above (in Scheme 3)

TS(C -> D) for C(5).....O(22)....C(24) exchange without H2O
ishi97jbb.g03.chk
Stoichiometry C12H23O11(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.383668	-1.228235	-0.606795
2	6	0	-3.246976	0.023109	-0.718712
3	6	0	-1.770528	-1.320565	0.786237
4	6	0	-2.456663	1.277751	-0.348854
5	6	0	-1.076596	-0.019498	1.187471
6	8	0	-1.769341	1.123600	0.935367
7	6	0	-3.333081	2.510099	-0.218265
8	1	0	-3.752354	2.710273	-1.210536
9	1	0	-2.704122	3.359245	0.080531
10	8	0	-4.337272	2.242999	0.745128
11	1	0	-5.007986	2.929619	0.689716
12	1	0	-1.707168	1.461764	-1.127084
13	8	0	-3.684763	0.221650	-2.052269
14	1	0	-4.224746	-0.540091	-2.293282
15	1	0	-4.096576	-0.073427	-0.034157
16	8	0	-3.233095	-2.331005	-0.872665
17	1	0	-2.764756	-3.143313	-0.648870
18	1	0	-1.581939	-1.170789	-1.359181
19	8	0	-0.935992	-2.455274	0.941577
20	1	0	-0.279258	-2.459560	0.227181
21	1	0	-2.583365	-1.445807	1.508122
22	8	0	0.259896	0.105684	0.404665
23	1	0	-0.780327	-0.008004	2.234314
24	6	0	2.037373	-0.579199	0.824055
25	8	0	2.739942	0.521800	0.776370
26	6	0	2.306100	-1.399154	-0.418202
27	6	0	1.785233	-1.155586	2.193208
28	6	0	2.665001	-0.331267	-1.457933
29	6	0	3.337366	0.743657	-0.587595
30	6	0	3.142440	2.195510	-0.979580
31	8	0	1.274142	-2.279903	-0.767197
32	1	0	1.605530	-2.907058	-1.421754
33	1	0	3.234445	-1.952580	-0.197768

34	1	0	2.704197	-1.698337	2.463176
35	1	0	0.973865	-1.881839	2.133620
36	8	0	1.433957	-0.174129	3.133189
37	1	0	2.219749	0.302321	3.422040
38	8	0	3.526198	-0.914362	-2.406788
39	1	0	3.483903	-0.433546	-3.239904
40	1	0	1.741671	0.042903	-1.913673
41	1	0	4.400386	0.527651	-0.469676
42	1	0	2.072283	2.449856	-0.964287
43	1	0	3.484736	2.299607	-2.013884
44	8	0	3.919901	3.078286	-0.209413
45	1	0	3.532881	3.164916	0.667806
46	1	0	0.444344	1.051686	0.513623

SCF Done: E(RB+HF-LYP) = -1298.63792691 A.U. after 1 cycles
Convg = 0.4791D-08 -V/T = 2.0042
S**2 = 0.0000

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman activities (A**4/AMU), depolarization ratios for plane and unp incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1	2	3
A	A	A
Frequencies -- -130.1276	31.1096	34.7010

Sum of electronic and zero-point Energies= -1298.259809
Sum of electronic and thermal Energies= -1298.234649
Sum of electronic and thermal Enthalpies= -1298.233705
Sum of electronic and thermal Free Energies= -1298.313800

==== Figure 2 =====

I) B3LYP/6-311G(d,p)

1) precursor, reactant like complex
ishi97ib.highrev.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.328443	-1.863220	0.667590
2	6	0	1.778658	-2.496950	-0.615580
3	6	0	1.208511	-1.348935	1.581455
4	6	0	0.657781	-1.670750	-1.256077
5	6	0	0.153331	-0.540422	0.807286
6	8	0	-0.338356	-1.275701	-0.286379
7	6	0	-0.074756	-2.434209	-2.344389
8	1	0	0.665830	-2.785369	-3.068112
9	1	0	-0.774088	-1.762326	-2.856999
10	8	0	-0.771027	-3.532395	-1.753854
11	1	0	-1.249871	-4.018070	-2.455629
12	1	0	1.106488	-0.777407	-1.703529
13	8	0	2.803751	-2.609921	-1.607849
14	1	0	3.345232	-3.406024	-1.390606
15	1	0	1.392971	-3.491699	-0.371439
16	8	0	3.108709	-2.861150	1.323616
17	1	0	3.542244	-2.488745	2.123024
18	1	0	2.958396	-1.010665	0.387012
19	8	0	1.711985	-0.596219	2.681219
20	1	0	2.221012	0.166213	2.319422
21	1	0	0.695435	-2.214228	2.010814
22	8	0	0.672824	0.680979	0.277394
23	1	0	-0.709192	-0.336025	1.437738
24	6	0	0.592694	1.973952	0.912092
25	8	0	-0.014334	2.843293	-0.023740
26	6	0	2.031711	2.515172	1.045218
27	6	0	-0.229319	2.025048	2.202704
28	6	0	2.326778	2.931503	-0.403985
29	6	0	0.982328	3.522742	-0.836452
30	6	0	0.683208	3.328620	-2.318630
31	8	0	2.921412	1.573489	1.611369
32	1	0	3.748791	1.537028	1.085100
33	1	0	2.016450	3.423148	1.661018

34	1	0	-0.135951	3.038941	2.603404
35	1	0	0.175724	1.324618	2.932849
36	8	0	-1.597423	1.689110	2.004497
37	1	0	-2.025578	2.307430	1.376407
38	8	0	3.365671	3.867399	-0.557738
39	1	0	4.190707	3.358522	-0.534064
40	1	0	2.531672	2.023429	-0.984209
41	1	0	0.944079	4.585751	-0.580896
42	1	0	0.902964	2.296054	-2.608836
43	1	0	1.337435	3.988929	-2.892198
44	8	0	-0.668651	3.642575	-2.663954
45	1	0	-1.178154	2.824278	-2.556291
46	1	0	-1.078219	0.870157	-1.165100
47	8	0	-1.882016	1.180093	-1.614648
48	1	0	-2.967924	0.086195	-1.730276
49	1	0	-2.283510	1.837158	-0.986152
50	8	0	-3.125469	2.871446	0.056331
51	1	0	-2.980318	3.796768	-0.277927
52	1	0	-4.069779	2.671687	0.096594
53	8	0	-3.786040	-0.524909	-1.651724
54	1	0	-4.370293	-0.108901	-0.935767
55	1	0	-3.515187	-1.489788	-1.345940
56	8	0	4.044875	-0.185093	-2.009733
57	1	0	3.690986	-1.093102	-1.872873
58	1	0	4.199051	-0.092739	-2.954397
59	8	0	-2.805586	-4.371521	-3.297739
60	1	0	-3.135591	-5.177527	-3.705663
61	1	0	-3.432036	-4.132910	-2.600381
62	8	0	4.028198	-1.753376	3.642677
63	1	0	4.152611	-2.290515	4.431035
64	1	0	3.153136	-1.335567	3.721546
65	1	0	3.918425	-4.210067	0.341138
66	8	0	4.089312	-4.677535	-0.498972
67	1	0	5.038669	-4.825396	-0.542867
68	8	0	-3.200462	-2.831244	-0.866736
69	1	0	-3.445015	-2.936737	0.075389
70	1	0	-2.232862	-3.029036	-0.969215
71	8	0	-3.989229	-2.776944	1.805672
72	1	0	-4.887501	-2.418755	1.968034
73	1	0	-3.902257	-3.556997	2.364035
74	8	0	-2.317354	5.137611	-1.023261
75	1	0	-2.795955	5.844629	-1.465480
76	1	0	-1.669203	4.786613	-1.669098
77	1	0	5.929354	1.403029	0.070033
78	8	0	5.007484	1.540423	-0.169178
79	1	0	4.777541	0.870025	-0.855260

80	8	0	-5.016172	0.620937	0.313860
81	1	0	-4.438941	0.418269	1.092569
82	1	0	-5.883272	0.294494	0.592197
83	8	0	-3.584704	-0.069970	2.504952
84	1	0	-2.807296	0.524661	2.577395
85	1	0	-3.268363	-0.979922	2.385563
86	8	0	-6.114716	-1.104484	2.415445
87	1	0	-6.888280	-1.228961	2.975438
88	1	0	-5.488227	-0.551001	2.911838

SCF Done: E(RB+HF-LYP) = -2369.32709684 A.U. after 1 cycles
Convg = 0.3618D-08 -V/T = 2.0040
S**2 = 0.0000
Sum of electronic and zero-point Energies= -2368.583807
Sum of electronic and thermal Energies= -2368.526771
Sum of electronic and thermal Enthalpies= -2368.525827
Sum of electronic and thermal Free Energies= -2368.674002

2) TS(B)

Item	Value	Threshold	Converged?
Maximum Force	.000068	0.000450	YES
RMS Force	.00011	0.000300	YES
Maximum Displacement	.008204	0.001800	NO
RMS Displacement	.001340	0.001200	NO

3) Product(B)
ishi95a.highfor.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.543662	-1.174490	1.660881
2	6	0	-0.848677	-2.610691	1.240035
3	6	0	-1.580063	-0.254475	1.027711
4	6	0	-0.677964	-2.792529	-0.269290
5	6	0	-1.756706	-0.538253	-0.487042
6	8	0	-0.960605	-1.563084	-1.012304
7	6	0	-1.470577	-3.972913	-0.822217
8	1	0	-1.061278	-4.876870	-0.360933
9	1	0	-1.308054	-4.037967	-1.902327
10	8	0	-2.857422	-3.905561	-0.510790

11	1	0	-3.356960	-3.627862	-1.292616
12	1	0	0.382536	-2.973617	-0.459187
13	8	0	0.045206	-3.516916	1.879955
14	1	0	0.011910	-3.293535	2.821253
15	1	0	-1.880132	-2.854630	1.528565
16	8	0	-0.519163	-1.089845	3.081482
17	1	0	-1.381143	-0.789603	3.408258
18	1	0	0.464327	-0.919180	1.316758
19	8	0	-1.291339	1.129445	1.294393
20	1	0	-0.359036	1.265881	1.044453
21	1	0	-2.548345	-0.430820	1.496995
22	8	0	0.721835	1.149620	-0.489809
23	1	0	-1.482272	0.347439	-1.057518
24	6	0	1.589038	1.535206	-1.253525
25	8	0	3.589829	1.019626	0.024013
26	6	0	2.137472	2.959734	-1.162418
27	6	0	1.951490	0.721561	-2.475062
28	6	0	2.854287	3.221580	0.168890
29	6	0	4.077030	2.309942	0.320470
30	6	0	4.654181	2.385266	1.732140
31	8	0	1.014881	3.842796	-1.279256
32	1	0	1.349977	4.711151	-1.009826
33	1	0	2.837299	3.147730	-1.986256
34	1	0	3.035784	0.691135	-2.591847
35	1	0	1.542720	1.276001	-3.337559
36	8	0	1.457743	-0.597956	-2.444820
37	1	0	0.653236	-0.648150	-1.900130
38	8	0	3.168978	4.616747	0.151126
39	1	0	3.199012	4.952361	1.051668
40	1	0	2.137879	3.002815	0.971065
41	1	0	4.853195	2.622411	-0.390976
42	1	0	3.867288	2.133406	2.456758
43	1	0	5.003659	3.408026	1.922188
44	8	0	5.733728	1.458769	1.825938
45	1	0	6.303876	1.711302	2.558270
46	1	0	4.309730	0.393841	-0.293032
47	8	0	-3.157215	-0.792712	-0.689963
48	1	0	-4.319364	0.669433	-0.480401
49	1	0	-3.317874	-1.199893	-1.559825
50	8	0	-4.915917	1.341148	-0.099858
51	1	0	-5.099126	1.009676	0.826766
52	1	0	-4.540185	2.593868	-0.278558
53	8	0	-4.724522	-2.537862	-2.103300
54	1	0	-5.295813	-2.765340	-2.843645
55	1	0	-5.282629	-2.512703	-1.306860
56	8	0	-5.192304	0.158471	2.224732

57	1	0	-4.464545	0.265286	2.860804
58	1	0	-5.267134	-0.788893	2.016031
59	8	0	-4.180169	3.625750	-0.450939
60	1	0	-3.197022	3.581746	-0.673355
61	1	0	-4.694609	4.107843	-1.150009
62	8	0	-1.721779	3.035064	-0.809722
63	1	0	-0.846462	3.398621	-1.037247
64	1	0	-1.577313	2.449408	-0.046452
65	8	0	-5.537729	4.997029	-2.256115
66	1	0	-6.043505	4.613066	-2.979714
67	1	0	-6.024988	5.776262	-1.968184
68	8	0	5.280586	-0.780013	-0.835163
69	1	0	5.529480	-1.128882	0.051665
70	1	0	4.677464	-1.461397	-1.185742
71	8	0	5.315452	-1.452276	1.811112
72	1	0	5.315094	-0.505855	2.016940
73	1	0	4.378829	-1.724872	1.816341
74	8	0	3.188700	-2.554488	-1.516973
75	1	0	2.575938	-1.961695	-1.990772
76	1	0	3.354871	-3.340645	-2.072761
77	8	0	-4.982835	-2.321561	0.781334
78	1	0	-4.172541	-1.945398	0.393424
79	1	0	-4.730577	-3.226800	1.002589
80	8	0	2.659343	-2.229639	1.198868
81	1	0	2.841582	-2.454891	0.266667
82	1	0	2.023360	-2.887887	1.509900
83	8	0	-2.768292	0.664776	3.684520
84	1	0	-2.218958	1.212511	3.097395
85	1	0	-2.746379	1.078719	4.554099
86	8	0	3.834502	-4.772836	-3.052950
87	1	0	4.610002	-4.623659	-3.604480
88	1	0	4.030197	-5.574478	-2.556172

SCF Done: E(RB+HF-LYP) = -2369.28364783 A.U. after 1 cycles
Convg = 0.3450D-08 -V/T = 2.0040
Sum of electronic and zero-point Energies= -2368.547037
Sum of electronic and thermal Energies= -2368.485921
Sum of electronic and thermal Enthalpies= -2368.484977
Sum of electronic and thermal Free Energies= -2368.646577

II) B3LYP/6-311G(d,p) SCRF=(pcm,solvent=water)

1) Precursor, reactant like complex
ishi976.highrev.pcm.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.940140	2.618702	0.665518
2	6	0	-0.055307	2.694762	-0.584309
3	6	0	-0.469699	1.555937	1.668466
4	6	0	0.308220	1.312573	-1.136753
5	6	0	-0.091072	0.238123	0.976489
6	8	0	0.816305	0.450415	-0.089741
7	6	0	1.342171	1.370635	-2.245710
8	1	0	0.894900	1.910934	-3.083627
9	1	0	1.569276	0.349838	-2.573863
10	8	0	2.528032	2.036237	-1.803385
11	1	0	3.054232	2.258882	-2.600255
12	1	0	-0.595675	0.862401	-1.557647
13	8	0	-0.734929	3.372562	-1.647879
14	1	0	-0.784904	4.331556	-1.430433
15	1	0	0.865529	3.228041	-0.329933
16	8	0	-0.940302	3.920099	1.262912
17	1	0	-1.501934	3.922083	2.069497
18	1	0	-1.953706	2.352626	0.343994
19	8	0	-1.472448	1.291482	2.654954
20	1	0	-2.254190	0.905597	2.200990
21	1	0	0.402997	1.933651	2.205166
22	8	0	-1.274146	-0.331453	0.447779
23	1	0	0.412902	-0.434279	1.666184
24	6	0	-1.907967	-1.534234	0.891075
25	8	0	-1.715740	-2.543511	-0.074747
26	6	0	-3.413574	-1.210114	0.806401
27	6	0	-1.452004	-2.084909	2.242922
28	6	0	-3.632432	-1.260838	-0.711088
29	6	0	-2.671360	-2.387473	-1.154648
30	6	0	-1.936348	-2.082402	-2.458336
31	8	0	-3.729965	0.001537	1.463230
32	1	0	-4.286765	0.568217	0.875396
33	1	0	-3.980279	-2.035621	1.253919
34	1	0	-2.159017	-2.870381	2.527347
35	1	0	-1.493681	-1.295465	2.993587
36	8	0	-0.123421	-2.584224	2.226422
37	1	0	-0.023907	-3.316902	1.580506
38	8	0	-5.010126	-1.501621	-0.991036
39	1	0	-5.129995	-1.540660	-1.947288
40	1	0	-3.321732	-0.309277	-1.152280
41	1	0	-3.216148	-3.331667	-1.238865

42	1	0	-1.506382	-1.078635	-2.412402
43	1	0	-2.650768	-2.109396	-3.285523
44	8	0	-0.909047	-3.034491	-2.748213
45	1	0	-0.091527	-2.732844	-2.311644
46	1	0	1.078835	-1.400749	-0.743053
47	8	0	1.392368	-2.238258	-1.133803
48	1	0	3.001741	-2.076871	-0.880731
49	1	0	1.122909	-2.969850	-0.526419
50	8	0	0.642360	-4.402913	0.359568
51	1	0	0.004892	-4.886001	-0.228301
52	1	0	1.339305	-5.025418	0.595124
53	8	0	3.937825	-1.880246	-0.566253
54	1	0	3.881251	-1.599812	0.459131
55	1	0	4.267193	-1.028725	-1.041265
56	8	0	-3.315138	2.349857	-2.104490
57	1	0	-2.431027	2.742493	-1.946497
58	1	0	-3.230670	1.855514	-2.926700
59	8	0	4.360057	1.998761	-3.840686
60	1	0	5.011074	2.708484	-3.883447
61	1	0	4.772822	1.312832	-3.287803
62	8	0	-2.296450	3.729888	3.661098
63	1	0	-1.715630	4.084909	4.343766
64	1	0	-2.061304	2.784308	3.592839
65	1	0	-1.055088	5.383615	0.192952
66	8	0	-1.003210	5.893628	-0.641503
67	1	0	-1.903097	6.199191	-0.803534
68	8	0	4.696726	0.354904	-1.518916
69	1	0	5.442467	0.677766	-0.947143
70	1	0	3.927654	0.943597	-1.353491
71	8	0	6.708993	1.143820	0.068793
72	1	0	6.660057	0.679520	0.926791
73	1	0	7.570817	0.912974	-0.295530
74	8	0	-1.068416	-5.465246	-1.418612
75	1	0	-0.716567	-6.193271	-1.942906
76	1	0	-1.088431	-4.691298	-2.020711
77	1	0	-5.585318	0.631226	-0.733168
78	8	0	-5.220925	1.417356	-0.301185
79	1	0	-4.586822	1.794316	-0.947600
80	8	0	3.828593	-1.012359	1.742132
81	1	0	3.236553	-1.367779	2.449335
82	1	0	4.701382	-0.805640	2.128105
83	8	0	2.116987	-1.881052	3.631164
84	1	0	1.276169	-2.159542	3.210719
85	1	0	1.875300	-1.172004	4.237246
86	8	0	6.404185	-0.276181	2.481891
87	1	0	7.018991	-1.013873	2.581699

88	1	0	6.507026	0.254888	3.281656

SCF Done: E(RB3LYP) = -2369.40287964 A.U. after 1 cycles
Convg = 0.3444D-08 -V/T = 2.0041
Sum of electronic and zero-point Energies= -2368.665728
Sum of electronic and thermal Energies= -2368.607374
Sum of electronic and thermal Enthalpies= -2368.606430
Sum of electronic and thermal Free Energies= -2368.759637

2) TS(B)
ishi95a.high.pcm8.chk
Sum of electronic and zero-point Energies= -2368.603069
Sum of electronic and thermal Free Energies= -2368.698298

3) Product(B)
ishi95a.highfor.pcm.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.716999	-1.188150	1.740281
2	6	0	-0.923056	-2.573045	1.139634
3	6	0	-1.674904	-0.177298	1.108767
4	6	0	-0.617843	-2.575655	-0.355303
5	6	0	-1.972569	-0.469467	-0.383354
6	8	0	-1.092119	-1.370141	-1.021621
7	6	0	-1.117921	-3.819767	-1.086016
8	1	0	-0.626906	-4.682232	-0.627740
9	1	0	-0.790011	-3.765109	-2.130209
10	8	0	-2.518045	-4.025722	-0.991118
11	1	0	-2.950494	-3.464913	-1.654650
12	1	0	0.469367	-2.548351	-0.464170
13	8	0	-0.010289	-3.502687	1.741279
14	1	0	-0.190591	-3.476204	2.690494
15	1	0	-1.952102	-2.896956	1.325397
16	8	0	-0.902058	-1.327269	3.145254
17	1	0	-1.191759	-0.481226	3.530389
18	1	0	0.316146	-0.879625	1.527226
19	8	0	-1.200801	1.167490	1.311557
20	1	0	-0.296653	1.219663	0.947268
21	1	0	-2.623781	-0.220164	1.636102
22	8	0	0.740031	1.067364	-0.507454
23	1	0	-1.872637	0.451522	-0.958476

24	6	0	1.477628	1.521981	-1.360029
25	8	0	3.680096	0.938922	-0.274878
26	6	0	2.063701	2.927733	-1.231362
27	6	0	1.693388	0.770425	-2.650508
28	6	0	2.822757	3.099671	0.096489
29	6	0	4.085578	2.230945	0.148359
30	6	0	4.665768	2.205057	1.557563
31	8	0	0.959046	3.837840	-1.267435
32	1	0	1.304870	4.673115	-0.916231
33	1	0	2.737793	3.135274	-2.070476
34	1	0	2.756605	0.747906	-2.893131
35	1	0	1.189245	1.351281	-3.439118
36	8	0	1.212256	-0.557395	-2.598491
37	1	0	0.390046	-0.590965	-2.072277
38	8	0	3.137286	4.491440	0.199208
39	1	0	2.932940	4.796108	1.089211
40	1	0	2.140159	2.807505	0.900630
41	1	0	4.832287	2.652672	-0.537230
42	1	0	3.905009	1.837304	2.256915
43	1	0	4.957018	3.218494	1.847933
44	8	0	5.805896	1.333423	1.569445
45	1	0	6.373010	1.589635	2.304336
46	1	0	4.443221	0.370239	-0.534653
47	8	0	-3.324607	-0.925122	-0.448593
48	1	0	-4.519889	0.572487	-0.094956
49	1	0	-3.503739	-1.257392	-1.356479
50	8	0	-4.990988	1.321514	0.314172
51	1	0	-4.919896	1.162421	1.291259
52	1	0	-4.580873	2.600405	-0.181054
53	8	0	-3.788740	-2.218708	-2.812976
54	1	0	-3.321746	-1.974640	-3.621365
55	1	0	-4.701031	-2.390621	-3.076236
56	8	0	-4.737910	0.555176	2.887177
57	1	0	-3.909590	0.785283	3.347947
58	1	0	-4.697485	-0.410297	2.732970
59	8	0	-4.258699	3.533581	-0.556811
60	1	0	-3.253823	3.489162	-0.687775
61	1	0	-4.718672	3.749684	-1.428693
62	8	0	-1.759411	3.066392	-0.704817
63	1	0	-0.895751	3.454838	-0.933676
64	1	0	-1.608182	2.504013	0.076418
65	8	0	-5.417077	4.151781	-2.791205
66	1	0	-5.694469	3.405397	-3.336143
67	1	0	-6.207319	4.693513	-2.676522
68	8	0	5.400650	-1.043334	-0.984483
69	1	0	5.535951	-1.333207	-0.056942

70	1	0	4.652840	-1.594431	-1.287615
71	8	0	5.347226	-1.496394	1.759542
72	1	0	5.396123	-0.528097	1.848120
73	1	0	4.397704	-1.723165	1.791935
74	8	0	2.975084	-2.380670	-1.442705
75	1	0	2.368307	-1.761295	-1.897788
76	1	0	2.797350	-3.267706	-1.822358
77	8	0	-4.420886	-2.055366	1.937691
78	1	0	-4.172227	-1.874180	1.014325
79	1	0	-5.111671	-2.725551	1.900095
80	8	0	2.661212	-2.176611	1.320132
81	1	0	2.738068	-2.277947	0.349028
82	1	0	1.926019	-2.753246	1.579697
83	8	0	-2.121755	1.135914	3.888232
84	1	0	-1.707209	1.559711	3.114623
85	1	0	-1.921695	1.688626	4.652069
86	8	0	2.305591	-4.854582	-2.447720
87	1	0	2.712544	-5.105822	-3.284994
88	1	0	2.506486	-5.582140	-1.847606

SCF Done: E(RB3LYP) = -2369.38715071 A.U. after 1 cycles
Convg = 0.3536D-08 -V/T = 2.0041
Sum of electronic and zero-point Energies= -2368.653299
Sum of electronic and thermal Energies= -2368.591901
Sum of electronic and thermal Enthalpies= -2368.590957
Sum of electronic and thermal Free Energies= -2368.752164

==== Figure 3 ====

I) B3LYP/6-311G(d,p)

1) TS1(C)
ishi01y.highaa.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.229361	-3.354889	-0.854775
2	6	0	-1.914191	-2.597293	-1.983221
3	6	0	-1.196789	-2.469856	0.389820
4	6	0	-1.153026	-1.312605	-2.278579
5	6	0	-0.691102	-1.069269	0.091463
6	8	0	-1.039479	-0.506655	-1.046766
7	6	0	-1.805381	-0.416363	-3.320288
8	1	0	-1.675077	-0.888078	-4.296746
9	1	0	-1.298426	0.549098	-3.317721
10	8	0	-3.184986	-0.174106	-3.043569
11	1	0	-3.722985	-0.795391	-3.542923
12	1	0	-0.134417	-1.537277	-2.604907
13	8	0	-1.944480	-3.339062	-3.189788
14	1	0	-2.285874	-4.215204	-2.972200
15	1	0	-2.929160	-2.340828	-1.652944
16	8	0	-1.996005	-4.526891	-0.623639
17	1	0	-1.672050	-4.939961	0.185330
18	1	0	-0.206364	-3.619684	-1.159521
19	8	0	-0.579999	-3.086716	1.493408
20	1	0	0.341172	-3.310789	1.266814
21	1	0	-2.237999	-2.279652	0.686118
22	8	0	1.091991	-1.194840	-0.009554
23	1	0	-0.731565	-0.354017	0.904496
24	6	0	2.049462	-1.008781	1.089999
25	8	0	2.984243	-0.052310	0.673958
26	6	0	2.870772	-2.296015	1.325462
27	6	0	1.360028	-0.547971	2.380940
28	6	0	4.090587	-2.163950	0.419997
29	6	0	4.248283	-0.641656	0.245910
30	6	0	4.560435	-0.267649	-1.206210
31	8	0	2.114391	-3.472814	1.094962
32	1	0	2.603886	-4.223212	1.451794
33	1	0	3.234776	-2.272198	2.359866

34	1	0	2.154981	-0.393033	3.118976
35	1	0	0.707102	-1.346718	2.737985
36	8	0	0.555540	0.604797	2.239349
37	1	0	1.080919	1.429411	2.124262
38	8	0	5.177130	-2.815868	1.054724
39	1	0	5.864310	-3.005996	0.408353
40	1	0	3.858127	-2.638025	-0.541315
41	1	0	5.014767	-0.258731	0.923354
42	1	0	3.953388	-0.882480	-1.876168
43	1	0	5.611793	-0.508688	-1.406078
44	8	0	4.274449	1.080132	-1.536106
45	1	0	4.991113	1.678920	-1.216568
46	1	0	1.344635	-0.522557	-0.811583
47	8	0	1.597355	0.283217	-1.949936
48	1	0	0.946601	1.032721	-2.098337
49	1	0	2.479476	0.690507	-1.976156
50	8	0	1.488743	3.081084	1.927316
51	1	0	1.705959	3.651318	2.671223
52	1	0	2.166069	3.245659	1.224108
53	8	0	-0.025738	2.291554	-2.298689
54	1	0	-0.369228	2.584632	-1.424436
55	1	0	0.392930	3.096173	-2.638107
56	8	0	-4.760010	2.351269	2.146776
57	1	0	-5.282038	2.886248	2.752974
58	1	0	-4.333833	1.621451	2.691703
59	8	0	-3.167980	3.650913	0.183565
60	1	0	-3.639714	3.283247	0.950846
61	1	0	-3.558449	3.186112	-0.591047
62	8	0	-4.380305	2.105046	-1.738521
63	1	0	-4.996761	1.593926	-1.189229
64	1	0	-3.889187	1.433775	-2.236545
65	8	0	-0.590688	3.633270	-0.002541
66	1	0	-1.587427	3.683811	0.148326
67	1	0	-0.141488	3.431896	0.832981
68	8	0	1.203966	4.783693	-1.590873
69	1	0	1.180768	5.714392	-1.833522
70	1	0	0.447962	4.615180	-0.975396
71	8	0	3.096265	3.428250	-0.191968
72	1	0	3.123373	2.546581	-0.597426
73	1	0	2.540240	3.992838	-0.781172
74	8	0	5.823223	2.886068	-0.335651
75	1	0	5.042832	3.436194	-0.143562
76	1	0	6.484486	3.467718	-0.723347
77	8	0	-5.837445	0.721577	0.287738
78	1	0	-5.584580	1.383373	0.978560
79	1	0	-6.799176	0.682954	0.278627

80	8	0	-3.812352	0.270338	3.372099
81	1	0	-3.887031	-0.455480	2.727607
82	1	0	-2.917272	0.218171	3.762156
83	8	0	-4.261200	-1.407863	1.124917
84	1	0	-4.837833	-0.733424	0.705362
85	1	0	-4.827315	-2.171023	1.280080
86	8	0	-1.233020	0.193117	4.311947
87	1	0	-0.618918	0.555920	3.647851
88	1	0	-0.994667	0.580386	5.158846

SCF Done: E(RB+HF-LYP) = -2369.28088995 A.U. after 1 cycles
Convg = 0.2715D-08 -V/T = 2.0040
S**2 = 0.0000

1	2	3
A	A	A

Frequencies -- -142.5805 13.3161 24.3476
Sum of electronic and zero-point Energies= -2368.541516
Sum of electronic and thermal Energies= -2368.483635
Sum of electronic and thermal Enthalpies= -2368.482691
Sum of electronic and thermal Free Energies= -2368.634554

2) Int(C)
ishi97ibb.highfor.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.397507	1.614260	0.730655
2	6	0	-1.916356	2.320242	-0.539485
3	6	0	-1.261561	1.385931	1.743085
4	6	0	-0.645936	1.699096	-1.114751
5	6	0	0.088381	1.163022	1.136418
6	8	0	0.384196	1.456894	-0.050681
7	6	0	0.052180	2.533325	-2.164256
8	1	0	-0.660559	2.673698	-2.984802
9	1	0	0.915684	1.978662	-2.549188
10	8	0	0.439331	3.760028	-1.575533
11	1	0	0.932639	4.267322	-2.260382
12	1	0	-0.852052	0.700427	-1.500937
13	8	0	-2.894720	2.205474	-1.567505
14	1	0	-3.489756	2.986744	-1.472709
15	1	0	-1.729174	3.375861	-0.321427
16	8	0	-3.416950	2.424708	1.299183

17	1	0	-3.868171	1.924681	2.008650
18	1	0	-2.793521	0.632587	0.456509
19	8	0	-1.549017	0.422553	2.728555
20	1	0	-1.691015	-0.442643	2.261567
21	1	0	-1.104455	2.343824	2.271513
22	8	0	0.231339	-1.250588	0.546254
23	1	0	0.949118	0.928775	1.772420
24	6	0	-0.228795	-2.611678	0.565820
25	8	0	0.184348	-3.256848	-0.616373
26	6	0	-1.753200	-2.611218	0.461204
27	6	0	0.337153	-3.374772	1.762540
28	6	0	-1.956917	-2.288514	-1.031645
29	6	0	-0.758458	-2.999775	-1.687601
30	6	0	-0.092394	-2.177824	-2.800563
31	8	0	-2.336856	-1.700094	1.369518
32	1	0	-3.323857	-1.655507	1.260651
33	1	0	-2.124067	-3.626501	0.646355
34	1	0	-0.016452	-4.410395	1.712958
35	1	0	-0.048696	-2.918183	2.676224
36	8	0	1.750114	-3.322027	1.839209
37	1	0	2.174918	-3.753724	1.067646
38	8	0	-3.187230	-2.708611	-1.570872
39	1	0	-3.765387	-1.931567	-1.610384
40	1	0	-1.848878	-1.204195	-1.148432
41	1	0	-1.072327	-3.973072	-2.071707
42	1	0	-0.090263	-1.117211	-2.523647
43	1	0	-0.678102	-2.283202	-3.717249
44	8	0	1.239687	-2.582826	-3.080593
45	1	0	1.808173	-2.145678	-2.415063
46	1	0	1.141207	-1.281803	0.161113
47	8	0	2.603548	-1.447758	-0.893158
48	1	0	3.246592	-0.712469	-0.806726
49	1	0	3.048131	-2.275776	-0.619488
50	8	0	3.292646	-4.068055	-0.278675
51	1	0	2.908160	-4.550558	-1.059582
52	1	0	4.140056	-4.478643	-0.081360
53	8	0	3.998235	0.814354	-0.134277
54	1	0	3.440781	0.768927	0.673343
55	1	0	3.732194	1.647190	-0.581888
56	8	0	-4.565786	-0.124118	-1.502484
57	1	0	-4.004287	0.670191	-1.614663
58	1	0	-5.269763	-0.051401	-2.156097
59	8	0	2.294063	4.564899	-3.309025
60	1	0	2.607201	5.405525	-3.655241
61	1	0	2.975496	4.234218	-2.694839
62	8	0	-4.307423	0.739500	3.275678

63	1	0	-4.750012	0.935266	4.108301
64	1	0	-3.377931	0.528501	3.479464
65	1	0	-4.294912	3.858193	0.234505
66	8	0	-4.274250	4.262112	-0.647573
67	1	0	-5.107978	4.720131	-0.785661
68	8	0	3.249954	3.369339	-0.986584
69	1	0	3.742382	3.881178	-0.299433
70	1	0	2.304293	3.506096	-0.809141
71	8	0	4.624346	4.489960	1.041532
72	1	0	5.035196	3.716107	1.475100
73	1	0	5.327655	5.132581	0.910345
74	8	0	2.165044	-5.096472	-2.457808
75	1	0	2.659670	-5.490014	-3.182849
76	1	0	1.747621	-4.285726	-2.819227
77	1	0	-5.016394	-0.475457	1.853564
78	8	0	-4.902718	-1.124531	1.142714
79	1	0	-5.015880	-0.661477	0.295314
80	8	0	2.801039	0.834621	2.358917
81	1	0	2.916823	-0.045539	2.802274
82	1	0	3.551564	1.378436	2.644135
83	8	0	3.102109	-1.588257	3.403620
84	1	0	2.640491	-2.261911	2.856664
85	1	0	2.922175	-1.813194	4.320530
86	8	0	5.426844	1.997981	1.919633
87	1	0	5.254401	1.479761	1.105624
88	1	0	6.256564	1.680497	2.289443

SCF Done: E(RB3LYP) = -2369.29147554 A.U. after 1 cycles
Convg = 0.5382D-08 -V/T = 2.0040
Sum of electronic and zero-point Energies= -2368.550812
Sum of electronic and thermal Energies= -2368.491903
Sum of electronic and thermal Enthalpies= -2368.490958
Sum of electronic and thermal Free Energies= -2368.644351

3) TS2(C)
ishi0x.high.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.587634	-2.052053	-0.399688
2	6	0	-3.305498	-0.974532	-1.201779
3	6	0	-2.242296	-1.481985	0.979611

4	6	0	-2.432381	0.262292	-1.390716
5	6	0	-1.528221	-0.141989	0.852668
6	8	0	-1.577096	0.566976	-0.222122
7	6	0	-3.226725	1.516061	-1.738081
8	1	0	-3.713647	1.326926	-2.700163
9	1	0	-2.534989	2.353217	-1.857469
10	8	0	-4.155790	1.879499	-0.734238
11	1	0	-4.981234	1.336790	-0.784336
12	1	0	-1.709516	0.060690	-2.184180
13	8	0	-3.645595	-1.383602	-2.509998
14	1	0	-4.519436	-1.805259	-2.451906
15	1	0	-4.201323	-0.695938	-0.641881
16	8	0	-3.485946	-3.152996	-0.239654
17	1	0	-3.131672	-3.719479	0.457094
18	1	0	-1.679276	-2.380516	-0.918669
19	8	0	-1.533566	-2.394926	1.786254
20	1	0	-0.756513	-2.743204	1.309449
21	1	0	-3.190812	-1.300653	1.490188
22	8	0	0.886604	-1.378657	-0.109098
23	1	0	-0.631871	0.042026	1.434182
24	6	0	1.922001	-1.724979	0.783132
25	8	0	3.185469	-1.304200	0.271760
26	6	0	2.019135	-3.252390	0.815960
27	6	0	1.711305	-1.109610	2.174204
28	6	0	2.859021	-3.563694	-0.417354
29	6	0	3.853451	-2.384776	-0.418514
30	6	0	4.300369	-1.947243	-1.803556
31	8	0	0.729001	-3.843218	0.830442
32	1	0	0.832485	-4.790276	0.975289
33	1	0	2.591506	-3.559441	1.701027
34	1	0	2.608165	-1.291680	2.776127
35	1	0	0.871815	-1.624051	2.648318
36	8	0	1.385318	0.267891	2.128470
37	1	0	2.213423	0.776819	2.041791
38	8	0	3.453450	-4.841873	-0.264916
39	1	0	3.698968	-5.186945	-1.128416
40	1	0	2.207072	-3.526983	-1.297160
41	1	0	4.729469	-2.673673	0.176020
42	1	0	3.430608	-1.691802	-2.413496
43	1	0	4.820040	-2.788315	-2.282874
44	8	0	5.142579	-0.795389	-1.799115
45	1	0	5.728519	-0.802737	-1.022816
46	1	0	1.032728	-0.453026	-0.410020
47	8	0	1.295652	1.212074	-1.041760
48	1	0	0.996356	1.795791	-0.315687
49	1	0	2.275417	1.261871	-1.020621

50	8	0	3.805039	1.642772	1.676815
51	1	0	4.593044	1.233974	2.057157
52	1	0	3.900918	1.473434	0.709820
53	8	0	0.516669	3.469149	0.473375
54	1	0	1.334060	3.852846	0.852683
55	1	0	0.422947	3.870287	-0.408335
56	1	0	-0.970657	3.362948	1.421060
57	8	0	-1.847775	3.271545	1.852240
58	1	0	-2.482174	3.785968	1.294696
59	8	0	-2.555148	0.934185	2.168868
60	1	0	-2.255486	1.961304	2.006912
61	1	0	-2.203027	0.695537	3.037841
62	8	0	-3.501243	4.364540	0.073995
63	1	0	-4.169427	5.046450	0.185693
64	1	0	-3.960118	3.554622	-0.232752
65	8	0	3.070334	4.249926	1.214928
66	1	0	3.287261	4.940915	1.849198
67	1	0	3.445767	3.410950	1.561506
68	8	0	0.891636	3.660641	-2.297128
69	1	0	0.930149	2.687421	-2.206539
70	1	0	0.437481	3.863237	-3.121020
71	8	0	4.074853	1.553757	-0.996977
72	1	0	4.413365	0.819400	-1.552518
73	1	0	4.075624	2.442000	-1.439124
74	8	0	6.359723	0.410326	0.457282
75	1	0	5.996276	1.153070	-0.046787
76	1	0	7.298878	0.596557	0.563976
77	8	0	3.653401	4.082069	-1.628443
78	1	0	3.550404	4.383302	-0.710083
79	1	0	2.760654	4.136703	-2.010339
80	8	0	-6.321576	0.302365	-0.425278
81	1	0	-6.425692	-0.582786	-0.810376
82	1	0	-6.143020	0.147847	0.521926
83	8	0	-5.977274	-2.447239	-1.393227
84	1	0	-6.601845	-3.100638	-1.724035
85	1	0	-5.341153	-2.920642	-0.827701
86	8	0	-5.211582	-0.075950	2.091251
87	1	0	-4.416155	0.481365	2.158368
88	1	0	-5.616625	-0.084162	2.963860

SCF Done: E(RB+HF-LYP) = -2369.28755555 A.U. after 1 cycles

Convg = 0.9671D-09 -V/T = 2.0040

S**2 = 0.0000

	1	2	3
	A	A	A
Frequencies --	-183.1869	13.9859	19.3889

Sum of electronic and zero-point Energies= -2368.546606
Sum of electronic and thermal Energies= -2368.488781
Sum of electronic and thermal Enthalpies= -2368.487837
Sum of electronic and thermal Free Energies= -2368.637925

4) Product(C)
ishi0x.revhigh.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.907752	-1.999924	-0.449644
2	6	0	-3.828382	-0.943115	-1.052260
3	6	0	-2.219324	-1.484373	0.814537
4	6	0	-3.086572	0.385888	-1.219899
5	6	0	-1.546002	-0.128418	0.557759
6	8	0	-2.486202	0.784293	0.016581
7	6	0	-4.020383	1.515738	-1.642710
8	1	0	-4.502243	1.244020	-2.582812
9	1	0	-3.440893	2.428719	-1.789763
10	8	0	-5.009574	1.815349	-0.651423
11	1	0	-5.746317	1.161872	-0.676834
12	1	0	-2.315381	0.269427	-1.995507
13	8	0	-4.313085	-1.312016	-2.329520
14	1	0	-5.073886	-1.896665	-2.191026
15	1	0	-4.651647	-0.782215	-0.347130
16	8	0	-3.695405	-3.157184	-0.127117
17	1	0	-3.167761	-3.698197	0.474701
18	1	0	-2.154291	-2.276394	-1.200897
19	8	0	-1.343283	-2.468040	1.351536
20	1	0	-0.637747	-2.695747	0.722492
21	1	0	-2.980518	-1.323526	1.582939
22	8	0	1.531098	-1.293149	-0.437928
23	1	0	-0.691110	-0.234937	-0.117154
24	6	0	2.307540	-1.719145	0.634147
25	8	0	3.695630	-1.360353	0.463102
26	6	0	2.365749	-3.245615	0.559321
27	6	0	1.839078	-1.155105	1.978708
28	6	0	3.352810	-3.482265	-0.588992
29	6	0	4.349055	-2.309805	-0.425013
30	6	0	4.764053	-1.619727	-1.717392
31	8	0	1.080017	-3.800844	0.362272
32	1	0	1.152134	-4.758254	0.443995

33	1	0	2.822207	-3.631291	1.480222
34	1	0	2.603391	-1.336380	2.740653
35	1	0	0.926331	-1.678188	2.268068
36	8	0	1.505615	0.224704	1.897582
37	1	0	2.302056	0.797108	1.808867
38	8	0	3.931416	-4.767831	-0.432574
39	1	0	4.259507	-5.077623	-1.282147
40	1	0	2.804305	-3.403472	-1.532661
41	1	0	5.232875	-2.682339	0.103847
42	1	0	3.874898	-1.347777	-2.290590
43	1	0	5.360831	-2.320764	-2.315361
44	8	0	5.501174	-0.412119	-1.508458
45	1	0	5.934193	-0.411453	-0.639900
46	1	0	1.438365	-0.318306	-0.465375
47	8	0	1.144271	1.385820	-1.215018
48	1	0	0.865599	2.071697	-0.578431
49	1	0	2.123171	1.478313	-1.289477
50	8	0	3.668040	1.892795	1.420319
51	1	0	4.524252	1.568063	1.747436
52	1	0	3.764143	1.798040	0.433559
53	8	0	0.346451	3.846424	0.017133
54	1	0	1.154406	4.208304	0.436614
55	1	0	0.360626	4.155199	-0.905743
56	1	0	-1.154361	3.708277	1.007408
57	8	0	-1.765302	3.279045	1.640998
58	1	0	-3.222006	3.097915	1.496822
59	8	0	-1.135578	0.471951	1.770250
60	1	0	-1.452672	2.356741	1.671947
61	1	0	-0.151734	0.444415	1.854978
62	8	0	-4.198139	2.735138	1.588136
63	1	0	-4.097909	1.974624	2.234979
64	1	0	-4.525412	2.356791	0.691409
65	8	0	2.870158	4.498014	0.948011
66	1	0	3.098132	5.190980	1.576185
67	1	0	3.227239	3.655420	1.306800
68	8	0	0.933074	3.774104	-2.705282
69	1	0	0.890612	2.809278	-2.559743
70	1	0	0.543280	3.954620	-3.566641
71	8	0	3.825788	1.720544	-1.226013
72	1	0	4.498518	1.064233	-1.506548
73	1	0	3.989911	2.622116	-1.602210
74	8	0	5.819746	0.044867	1.401730
75	1	0	6.430098	-0.322863	2.049279
76	1	0	5.035749	-0.535220	1.378785
77	8	0	3.650851	4.285348	-1.848155
78	1	0	3.484711	4.608146	-0.947034

79	1	0	2.784919	4.305356	-2.288652
80	8	0	-7.004184	-0.048865	-0.576960
81	1	0	-6.896479	-1.004665	-0.733671
82	1	0	-7.741077	0.045859	0.033229
83	8	0	-6.317872	-2.773726	-0.985495
84	1	0	-6.809970	-3.532733	-1.313474
85	1	0	-5.536851	-3.117043	-0.509526
86	8	0	-3.549801	0.738887	3.158926
87	1	0	-2.614966	0.571597	2.932035
88	1	0	-3.619675	0.728874	4.118605

SCF Done: E(RB+HF-LYP) = -2369.33577677 A.U. after 12 cycles
Convg = 0.7464D-08 -V/T = 2.0040
Sum of electronic and zero-point Energies= -2368.591259
Sum of electronic and thermal Energies= -2368.534573
Sum of electronic and thermal Enthalpies= -2368.533629
Sum of electronic and thermal Free Energies= -2368.681023

II) B3LYP/ 6-311G(d,p) SCRF=(PCM, solvent=water)

1) TS1(C)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.033397	-3.411132	-0.933019
2	6	0	-1.732861	-2.695149	-2.082285
3	6	0	-1.157024	-2.565800	0.334122
4	6	0	-1.123508	-1.315773	-2.302765
5	6	0	-0.775477	-1.125488	0.091918
6	8	0	-1.086628	-0.553372	-1.034256
7	6	0	-1.869230	-0.429012	-3.285795
8	1	0	-1.801093	-0.884071	-4.275436
9	1	0	-1.382573	0.546882	-3.307047
10	8	0	-3.230339	-0.225612	-2.897407
11	1	0	-3.804416	-0.798486	-3.415455
12	1	0	-0.085859	-1.405729	-2.630614
13	8	0	-1.583300	-3.396248	-3.307274
14	1	0	-1.867866	-4.303946	-3.142320
15	1	0	-2.793949	-2.587103	-1.822860
16	8	0	-1.688567	-4.663317	-0.779854
17	1	0	-1.265993	-5.132295	-0.050495

18	1	0	0.024715	-3.559773	-1.183220
19	8	0	-0.550144	-3.135793	1.464960
20	1	0	0.402062	-3.280282	1.289643
21	1	0	-2.227177	-2.468839	0.573048
22	8	0	1.127717	-1.172738	0.033914
23	1	0	-0.811884	-0.434604	0.926328
24	6	0	2.074289	-0.944906	1.131844
25	8	0	2.988002	0.025318	0.710406
26	6	0	2.911357	-2.215563	1.392508
27	6	0	1.351295	-0.495584	2.407573
28	6	0	4.145371	-2.072993	0.504532
29	6	0	4.253695	-0.553739	0.267316
30	6	0	4.517697	-0.228330	-1.202913
31	8	0	2.157599	-3.394496	1.152170
32	1	0	2.588249	-4.133722	1.597809
33	1	0	3.250628	-2.185481	2.433734
34	1	0	2.123352	-0.231080	3.136132
35	1	0	0.785627	-1.343854	2.796894
36	8	0	0.427786	0.561332	2.224356
37	1	0	0.871069	1.437630	2.123439
38	8	0	5.257559	-2.643820	1.177442
39	1	0	5.947985	-2.831165	0.532231
40	1	0	3.956969	-2.596292	-0.438665
41	1	0	5.026955	-0.127410	0.909109
42	1	0	3.877216	-0.850090	-1.832596
43	1	0	5.557222	-0.488743	-1.431592
44	8	0	4.236022	1.119034	-1.558600
45	1	0	4.948523	1.724000	-1.246230
46	1	0	1.330033	-0.495469	-0.716788
47	8	0	1.546093	0.396016	-1.965216
48	1	0	0.896719	1.135727	-2.098384
49	1	0	2.425575	0.810237	-1.987917
50	8	0	1.227955	3.078828	1.919064
51	1	0	1.395190	3.605877	2.708063
52	1	0	1.984817	3.228480	1.299993
53	8	0	-0.146772	2.426313	-2.356609
54	1	0	-0.463008	2.716856	-1.472182
55	1	0	0.382853	3.190045	-2.634123
56	8	0	-4.727941	2.206931	2.171353
57	1	0	-5.307954	2.709266	2.754027
58	1	0	-4.333008	1.471039	2.723836
59	8	0	-3.361423	3.663166	0.182954
60	1	0	-3.737348	3.202644	0.956695
61	1	0	-3.696572	3.151228	-0.585469
62	8	0	-4.498990	2.073127	-1.802710
63	1	0	-5.082573	1.574574	-1.200062

64	1	0	-3.957498	1.377978	-2.215292
65	8	0	-0.703899	3.750369	-0.028158
66	1	0	-1.682531	3.762916	0.140142
67	1	0	-0.237762	3.500114	0.789944
68	8	0	1.262560	4.781388	-1.582216
69	1	0	1.377611	5.717125	-1.779444
70	1	0	0.480004	4.705878	-0.993084
71	8	0	3.039916	3.363065	-0.050860
72	1	0	3.070886	2.471972	-0.436794
73	1	0	2.517854	3.914771	-0.679533
74	8	0	5.787996	3.046736	-0.455723
75	1	0	4.948895	3.465929	-0.185718
76	1	0	6.194379	3.664652	-1.073923
77	8	0	-5.774575	0.633803	0.231705
78	1	0	-5.545442	1.253566	0.966306
79	1	0	-6.724047	0.478494	0.289442
80	8	0	-3.843865	0.075932	3.432721
81	1	0	-3.874058	-0.583553	2.712407
82	1	0	-2.922488	0.088117	3.770704
83	8	0	-4.190435	-1.482506	1.107954
84	1	0	-4.759045	-0.813683	0.668960
85	1	0	-4.761754	-2.246000	1.248156
86	8	0	-1.268859	0.198483	4.368201
87	1	0	-0.693439	0.479134	3.627685
88	1	0	-1.147035	0.861840	5.055767

SCF Done: E(RB3LYP) = -2369.36837075 A.U. after 1 cycles
Convg = 0.1784D-08 -V/T = 2.0040

1	2	3
A	A	A

Frequencies -- -110.0579 14.3329 24.8957
Sum of electronic and zero-point Energies= -2368.633598
Sum of electronic and thermal Energies= -2368.574519
Sum of electronic and thermal Enthalpies= -2368.573575
Sum of electronic and thermal Free Energies= -2368.728077

2) Int(C)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.323220	-2.349362	-0.300172

2	6	0	-3.002157	-1.337256	-1.217483
3	6	0	-2.000600	-1.661677	1.030166
4	6	0	-2.152462	-0.089429	-1.440734
5	6	0	-1.311352	-0.348918	0.828807
6	8	0	-1.501380	0.386245	-0.183571
7	6	0	-2.935684	1.096365	-1.991366
8	1	0	-3.318688	0.797223	-2.971542
9	1	0	-2.252342	1.935653	-2.130873
10	8	0	-3.967413	1.527073	-1.121622
11	1	0	-4.748847	0.925511	-1.141186
12	1	0	-1.311487	-0.314197	-2.098966
13	8	0	-3.265968	-1.857176	-2.506635
14	1	0	-4.145697	-2.273424	-2.453164
15	1	0	-3.932120	-1.038941	-0.729429
16	8	0	-3.247874	-3.414334	-0.087057
17	1	0	-2.903319	-3.978836	0.616290
18	1	0	-1.403736	-2.729813	-0.758084
19	8	0	-1.374990	-2.492571	1.970605
20	1	0	-0.568934	-2.889211	1.577122
21	1	0	-2.962947	-1.356580	1.475224
22	8	0	0.831859	-1.147051	0.136238
23	1	0	-0.740510	0.115565	1.625349
24	6	0	1.930174	-1.480699	0.988776
25	8	0	3.130377	-0.956736	0.449634
26	6	0	2.125419	-3.000070	0.939675
27	6	0	1.719775	-0.920590	2.403189
28	6	0	2.921242	-3.195430	-0.346457
29	6	0	3.823122	-1.948140	-0.357567
30	6	0	4.122544	-1.399063	-1.744078
31	8	0	0.879735	-3.684259	0.968079
32	1	0	1.042296	-4.622331	1.121367
33	1	0	2.749387	-3.307796	1.786761
34	1	0	2.648019	-1.060040	2.967126
35	1	0	0.933234	-1.504231	2.886586
36	8	0	1.296912	0.430918	2.410588
37	1	0	2.067708	1.015406	2.262012
38	8	0	3.628735	-4.425354	-0.289468
39	1	0	3.812359	-4.719767	-1.187422
40	1	0	2.225304	-3.183945	-1.191488
41	1	0	4.763417	-2.190392	0.147616
42	1	0	3.197844	-1.059762	-2.215777
43	1	0	4.541472	-2.208417	-2.355405
44	8	0	5.013721	-0.284195	-1.730152
45	1	0	5.869405	-0.578622	-1.349419
46	1	0	1.009307	-0.239233	-0.231301
47	8	0	1.197081	1.320671	-0.881314

48	1	0	0.763769	1.959917	-0.278930
49	1	0	2.166639	1.488203	-0.784731
50	8	0	3.410495	2.201509	1.965297
51	1	0	4.175195	2.122670	2.546708
52	1	0	3.724270	2.001857	1.045753
53	8	0	0.047343	3.618728	0.301458
54	1	0	0.816407	4.081809	0.698972
55	1	0	0.032843	3.912047	-0.626977
56	1	0	-1.515300	3.671780	1.220591
57	8	0	-2.366949	3.651294	1.701741
58	1	0	-3.039311	3.917285	1.038473
59	8	0	-2.859950	1.163703	2.489187
60	1	0	-2.693735	2.101387	2.186842
61	1	0	-2.649157	1.152193	3.429277
62	8	0	-4.199056	4.142452	-0.303038
63	1	0	-5.096148	4.266204	0.025833
64	1	0	-4.183903	3.229436	-0.658470
65	8	0	2.447650	4.645386	1.169773
66	1	0	2.543299	5.391403	1.771872
67	1	0	2.841648	3.863129	1.617849
68	8	0	0.759125	3.627751	-2.418035
69	1	0	0.851040	2.669812	-2.254772
70	1	0	0.348595	3.726053	-3.284118
71	8	0	3.838649	1.896190	-0.630620
72	1	0	4.352114	1.181988	-1.072986
73	1	0	3.903305	2.750081	-1.113779
74	8	0	7.288610	-1.258145	-0.558659
75	1	0	7.634198	-0.693345	0.142382
76	1	0	8.044634	-1.435524	-1.130397
77	8	0	3.372477	4.426361	-1.526952
78	1	0	3.120658	4.685954	-0.621140
79	1	0	2.519213	4.276384	-1.973607
80	8	0	-6.119305	-0.090862	-0.667328
81	1	0	-6.133722	-1.008583	-0.992258
82	1	0	-5.880919	-0.170645	0.280774
83	8	0	-5.652790	-2.820698	-1.476864
84	1	0	-6.261552	-3.484328	-1.819757
85	1	0	-5.092785	-3.268744	-0.818898
86	8	0	-5.034335	-0.329615	1.848173
87	1	0	-4.342614	0.314973	2.122911
88	1	0	-5.442684	-0.649873	2.658979

SCF Done: E(RB3LYP) = -2369.37810098 A.U. after 1 cycles
Convg = 0.4454D-08 -V/T = 2.0041
Sum of electronic and zero-point Energies= -2368.642986
Sum of electronic and thermal Energies= -2368.582571

Sum of electronic and thermal Enthalpies= -2368.581627
Sum of electronic and thermal Free Energies= -2368.738493

3) TS2(C)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.247861	-2.254610	-0.326851
2	6	0	-2.979626	-1.265315	-1.225537
3	6	0	-2.095366	-1.633051	1.066721
4	6	0	-2.215435	0.047364	-1.364698
5	6	0	-1.527874	-0.222014	0.972638
6	8	0	-1.537945	0.461045	-0.116304
7	6	0	-3.073689	1.211135	-1.846251
8	1	0	-3.398595	0.969919	-2.862884
9	1	0	-2.453433	2.108118	-1.888646
10	8	0	-4.173368	1.490537	-0.994758
11	1	0	-4.909736	0.848194	-1.123659
12	1	0	-1.387603	-0.092225	-2.062166
13	8	0	-3.157316	-1.745554	-2.546051
14	1	0	-3.990728	-2.250215	-2.539944
15	1	0	-3.949315	-1.065932	-0.764396
16	8	0	-3.051989	-3.431517	-0.243881
17	1	0	-2.678708	-4.005187	0.436893
18	1	0	-1.262831	-2.496688	-0.741743
19	8	0	-1.355367	-2.439917	1.953244
20	1	0	-0.514037	-2.721922	1.541291
21	1	0	-3.100457	-1.553104	1.486987
22	8	0	1.045102	-1.178939	0.113364
23	1	0	-0.735855	0.074677	1.652174
24	6	0	2.090959	-1.438500	1.026358
25	8	0	3.332747	-0.940797	0.545389
26	6	0	2.295762	-2.955059	1.053034
27	6	0	1.809246	-0.831014	2.408641
28	6	0	3.105742	-3.200356	-0.218361
29	6	0	3.960283	-1.917802	-0.325997
30	6	0	4.093175	-1.375901	-1.743713
31	8	0	1.046725	-3.633952	1.106905
32	1	0	1.199163	-4.548153	1.371045
33	1	0	2.914273	-3.219857	1.918243
34	1	0	2.722286	-0.896918	3.009497

35	1	0	1.037603	-1.436714	2.889330
36	8	0	1.315733	0.496768	2.351067
37	1	0	2.066127	1.111053	2.223505
38	8	0	3.865036	-4.395277	-0.078994
39	1	0	4.111673	-4.706672	-0.956022
40	1	0	2.411717	-3.280845	-1.060564
41	1	0	4.956360	-2.122153	0.077612
42	1	0	3.111520	-1.079773	-2.118699
43	1	0	4.481354	-2.173039	-2.390932
44	8	0	4.933633	-0.223977	-1.829268
45	1	0	5.835367	-0.480592	-1.539620
46	1	0	1.094392	-0.234313	-0.167360
47	8	0	1.165281	1.374637	-0.867624
48	1	0	0.724051	1.964919	-0.226178
49	1	0	2.130309	1.565238	-0.781721
50	8	0	3.406898	2.298732	1.933854
51	1	0	4.172282	2.228649	2.515352
52	1	0	3.718826	2.087911	1.016442
53	8	0	-0.047924	3.632617	0.383880
54	1	0	0.718929	4.115381	0.761263
55	1	0	-0.087537	3.911917	-0.548353
56	1	0	-1.549801	3.403846	1.277808
57	8	0	-2.391897	3.225957	1.752047
58	1	0	-3.110220	3.606276	1.194130
59	8	0	-2.849068	0.771647	2.106165
60	1	0	-2.655400	1.785603	1.944745
61	1	0	-2.636673	0.603655	3.035866
62	8	0	-4.403742	3.994331	0.089854
63	1	0	-5.244361	4.065561	0.555490
64	1	0	-4.437702	3.128484	-0.369383
65	8	0	2.359884	4.709181	1.163176
66	1	0	2.473192	5.462375	1.753160
67	1	0	2.788128	3.937500	1.598478
68	8	0	0.604744	3.663369	-2.346765
69	1	0	0.736692	2.710004	-2.174504
70	1	0	0.167060	3.736994	-3.201868
71	8	0	3.812276	1.958466	-0.660498
72	1	0	4.299949	1.238214	-1.122334
73	1	0	3.846101	2.806085	-1.156130
74	8	0	7.363297	-1.095981	-0.903224
75	1	0	7.743120	-0.521476	-0.228263
76	1	0	8.067662	-1.217850	-1.550501
77	8	0	3.245539	4.479549	-1.548048
78	1	0	3.009800	4.736411	-0.637031
79	1	0	2.383165	4.319228	-1.972913
80	8	0	-6.240907	-0.302140	-0.861069

81	1	0	-6.136398	-1.209821	-1.197676
82	1	0	-6.109685	-0.385479	0.105934
83	8	0	-5.477947	-2.972157	-1.655032
84	1	0	-6.003393	-3.676942	-2.049693
85	1	0	-4.895867	-3.392711	-0.997939
86	8	0	-5.373572	-0.483696	1.743054
87	1	0	-4.626181	0.121207	1.897235
88	1	0	-5.825310	-0.571554	2.588878

SCF Done: E(RB3LYP) = -2369.37511471 A.U. after 1 cycles
Convg = 0.3155D-08 -V/T = 2.0041

1	2	3
A	A	A

Frequencies -- -165.5967 13.3684 18.1967
Sum of electronic and zero-point Energies= -2368.639670
Sum of electronic and thermal Energies= -2368.580219
Sum of electronic and thermal Enthalpies= -2368.579275
Sum of electronic and thermal Free Energies= -2368.734573

4) Product(C)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.916430	-2.301654	0.149405
2	6	0	3.683649	-1.316374	1.026798
3	6	0	2.267193	-1.596661	-1.042872
4	6	0	2.769232	-0.151578	1.416196
5	6	0	1.496174	-0.346042	-0.604065
6	8	0	2.300655	0.486471	0.222507
7	6	0	3.461932	0.897504	2.279318
8	1	0	3.783685	0.416324	3.206185
9	1	0	2.742343	1.680276	2.525047
10	8	0	4.562413	1.548906	1.645288
11	1	0	5.298714	0.924188	1.456628
12	1	0	1.915858	-0.535877	1.994720
13	8	0	4.181569	-1.929699	2.207650
14	1	0	5.028790	-2.338273	1.962581
15	1	0	4.506798	-0.901408	0.438484
16	8	0	3.829841	-3.308854	-0.309031
17	1	0	3.377837	-3.819728	-0.992649
18	1	0	2.136807	-2.776481	0.761295

19	8	0	1.448142	-2.501896	-1.782449
20	1	0	0.697506	-2.798658	-1.237311
21	1	0	3.053850	-1.277236	-1.732058
22	8	0	-1.522452	-1.128524	0.244689
23	1	0	0.586982	-0.638658	-0.071963
24	6	0	-2.344127	-1.535063	-0.818867
25	8	0	-3.696614	-1.148364	-0.608130
26	6	0	-2.405938	-3.062521	-0.764182
27	6	0	-1.878656	-0.994345	-2.175966
28	6	0	-3.370131	-3.302550	0.400514
29	6	0	-4.301990	-2.063833	0.341089
30	6	0	-4.513592	-1.387051	1.692456
31	8	0	-1.107798	-3.625135	-0.611785
32	1	0	-1.179042	-4.577220	-0.745481
33	1	0	-2.880415	-3.430623	-1.681543
34	1	0	-2.683259	-1.121131	-2.904671
35	1	0	-1.015994	-1.580135	-2.497768
36	8	0	-1.446350	0.359982	-2.121059
37	1	0	-2.206533	0.983096	-2.128613
38	8	0	-4.037002	-4.545811	0.207760
39	1	0	-4.430502	-4.814725	1.044615
40	1	0	-2.794634	-3.317449	1.331362
41	1	0	-5.268059	-2.359061	-0.076171
42	1	0	-3.552547	-1.061350	2.092836
43	1	0	-4.948194	-2.116576	2.388409
44	8	0	-5.341740	-0.225449	1.616580
45	1	0	-6.217179	-0.491610	1.263143
46	1	0	-1.518655	-0.150322	0.330779
47	8	0	-1.413823	1.532028	0.946109
48	1	0	-0.947937	2.109479	0.314671
49	1	0	-2.376455	1.694707	0.798230
50	8	0	-3.478454	2.185715	-2.028146
51	1	0	-4.190511	2.111928	-2.673726
52	1	0	-3.874864	2.025060	-1.131872
53	8	0	-0.085988	3.801296	-0.249576
54	1	0	-0.845688	4.209537	-0.723581
55	1	0	-0.163511	4.089824	0.679614
56	1	0	1.271048	3.375442	-1.003255
57	8	0	1.993369	2.939868	-1.551288
58	1	0	2.981450	2.990394	-1.093357
59	8	0	1.169731	0.443366	-1.726309
60	1	0	1.734784	1.973788	-1.634182
61	1	0	0.188636	0.486108	-1.844864
62	8	0	4.235699	3.025673	-0.571745
63	1	0	4.896462	2.589815	-1.148420
64	1	0	4.284226	2.515980	0.278051

65	8	0	-2.460117	4.640590	-1.301879
66	1	0	-2.562782	5.365612	-1.928347
67	1	0	-2.840510	3.840076	-1.727986
68	8	0	-1.049699	3.899101	2.360303
69	1	0	-1.120793	2.931405	2.245266
70	1	0	-0.672791	4.052078	3.233809
71	8	0	-4.073715	1.929130	0.530537
72	1	0	-4.606109	1.216107	0.954517
73	1	0	-4.191073	2.797014	0.975382
74	8	0	-7.699172	-1.133094	0.540292
75	1	0	-8.030228	-0.589891	-0.184417
76	1	0	-8.448481	-1.230829	1.139353
77	8	0	-3.652969	4.513596	1.310019
78	1	0	-3.329330	4.730511	0.416202
79	1	0	-2.834257	4.423416	1.830763
80	8	0	6.711062	0.128784	0.658851
81	1	0	6.724214	-0.843375	0.594202
82	1	0	6.639232	0.461333	-0.253076
83	8	0	6.383203	-2.710142	0.650496
84	1	0	7.031386	-3.409191	0.788198
85	1	0	5.683886	-3.081928	0.080797
86	8	0	6.203263	1.489433	-1.826843
87	1	0	5.892255	0.932356	-2.551390
88	1	0	6.968104	1.961099	-2.180108

SCF Done: E(RB3LYP) = -2369.41691143 A.U. after 1 cycles
Convg = 0.5818D-08 -V/T = 2.0041
Sum of electronic and zero-point Energies= -2368.678533
Sum of electronic and thermal Energies= -2368.620720
Sum of electronic and thermal Enthalpies= -2368.619776
Sum of electronic and thermal Free Energies= -2368.770764

==== Figure 4 ====

I) B3LYP/6-311G(d,p)

1) TS1(D)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.620077	-2.088023	0.926153
2	6	0	1.070863	-2.662245	-0.385933
3	6	0	0.586464	-1.268052	1.718768
4	6	0	0.128064	-1.706418	-1.117945
5	6	0	-0.367529	-0.438389	0.857134
6	8	0	-0.856122	-1.139295	-0.216821
7	6	0	-0.635217	-2.369981	-2.248779
8	1	0	0.101793	-2.754342	-2.962569
9	1	0	-1.247660	-1.614032	-2.755142
10	8	0	-1.441555	-3.412711	-1.725582
11	1	0	-1.993432	-3.745532	-2.464581
12	1	0	0.718094	-0.890842	-1.548975
13	8	0	2.148087	-2.942251	-1.292368
14	1	0	2.529043	-3.814299	-1.026478
15	1	0	0.530438	-3.586952	-0.167182
16	8	0	2.085414	-3.189486	1.702146
17	1	0	2.488265	-2.875723	2.542146
18	1	0	2.455064	-1.429567	0.672624
19	8	0	1.182117	-0.493070	2.754660
20	1	0	1.945888	-0.027633	2.356026
21	1	0	-0.080777	-1.980561	2.213318
22	8	0	0.243364	0.826163	0.248990
23	1	0	-1.216889	-0.102066	1.447910
24	6	0	1.197386	2.238543	0.628727
25	8	0	0.875735	2.998599	-0.416263
26	6	0	2.646917	1.825098	0.448403
27	6	0	0.682538	2.737536	1.961048
28	6	0	2.697122	1.601485	-1.075985
29	6	0	1.746398	2.701391	-1.579480
30	6	0	0.894627	2.289089	-2.780357
31	8	0	3.042048	0.775121	1.275067
32	1	0	3.950707	0.440217	1.036404
33	1	0	3.230966	2.735178	0.665514

34	1	0	1.288091	3.622209	2.205478
35	1	0	0.868688	1.972578	2.713671
36	8	0	-0.693272	3.017078	1.966715
37	1	0	-0.935490	3.724788	1.328258
38	8	0	3.977616	1.697514	-1.640697
39	1	0	4.228722	0.792300	-1.884004
40	1	0	2.267308	0.619388	-1.285222
41	1	0	2.289197	3.626862	-1.776727
42	1	0	0.563850	1.253642	-2.658592
43	1	0	1.530306	2.336882	-3.668243
44	8	0	-0.233952	3.124110	-2.988776
45	1	0	-0.958669	2.734393	-2.462873
46	1	0	-0.557429	1.270895	-0.214879
47	8	0	-1.783342	1.962342	-0.959888
48	1	0	-2.611140	1.409475	-0.880003
49	1	0	-1.973702	2.831660	-0.550929
50	8	0	-1.802203	4.572528	0.070900
51	1	0	-1.269667	5.080375	-0.597923
52	1	0	-2.566888	5.109957	0.300680
53	8	0	-3.861264	0.407549	-0.360882
54	1	0	-3.546780	0.242397	0.560702
55	1	0	-3.843161	-0.479463	-0.796165
56	8	0	4.198283	-1.188921	-1.889485
57	1	0	3.442474	-1.793888	-1.681861
58	1	0	4.642677	-1.581511	-2.648716
59	8	0	-3.368035	-3.577031	-3.606912
60	1	0	-3.937534	-4.297063	-3.893111
61	1	0	-3.885320	-3.047882	-2.970936
62	8	0	2.893213	-2.202193	4.122297
63	1	0	2.744269	-2.728636	4.913918
64	1	0	2.178827	-1.545740	4.083028
65	1	0	2.779562	-4.672344	0.791188
66	8	0	2.954776	-5.148830	-0.042087
67	1	0	3.829779	-5.539343	0.036800
68	8	0	-3.943256	-2.183614	-1.256914
69	1	0	-4.605588	-2.557864	-0.629401
70	1	0	-3.080702	-2.589425	-1.047238
71	8	0	-5.827700	-2.874340	0.559176
72	1	0	-6.098538	-1.995509	0.887192
73	1	0	-6.636468	-3.336880	0.321716
74	8	0	-0.294813	5.622520	-1.850113
75	1	0	-0.508404	6.371741	-2.414388
76	1	0	-0.213788	4.839967	-2.433814
77	1	0	6.148431	0.000215	0.512045
78	8	0	5.272736	-0.396770	0.541640
79	1	0	5.103243	-0.788569	-0.337042

80	8	0	-3.333551	-0.053836	2.267799
81	1	0	-3.211814	0.754920	2.813779
82	1	0	-4.252355	-0.327994	2.401348
83	8	0	-2.775948	2.232377	3.627985
84	1	0	-1.991433	2.578331	3.164945
85	1	0	-2.543617	2.191809	4.560327
86	8	0	-6.071623	-0.205894	1.251868
87	1	0	-5.563118	0.221972	0.534895
88	1	0	-6.825595	0.360036	1.442899

SCF Done: E(RB+HF-LYP) = -2369.28501215 A.U. after 1 cycles
Convg = 0.4879D-08 -V/T = 2.0040

1	2	3
A	A	A

Frequencies -- -149.3073 17.0458 20.9189
Sum of electronic and zero-point Energies= -2368.544216
Sum of electronic and thermal Energies= -2368.486061
Sum of electronic and thermal Enthalpies= -2368.485117
Sum of electronic and thermal Free Energies= -2368.637215

2) Int(D)
ishi97ibb.highrev.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.765033	-2.054694	0.848524
2	6	0	1.174733	-2.759070	-0.374231
3	6	0	0.722263	-1.379718	1.755706
4	6	0	0.063278	-1.939179	-1.027656
5	6	0	-0.420599	-0.697067	0.979638
6	8	0	-0.900426	-1.535740	-0.044834
7	6	0	-0.681896	-2.697586	-2.112561
8	1	0	0.048937	-3.015090	-2.865531
9	1	0	-1.396386	-2.016651	-2.590455
10	8	0	-1.349199	-3.805260	-1.530430
11	1	0	-2.001205	-4.124872	-2.187393
12	1	0	0.515296	-1.054754	-1.493076
13	8	0	2.199843	-2.971122	-1.357128
14	1	0	2.643688	-3.823058	-1.134887
15	1	0	0.758250	-3.721771	-0.065287
16	8	0	2.517959	-3.036862	1.569750
17	1	0	3.069342	-2.597360	2.243176

18	1	0	2.443482	-1.272523	0.487609
19	8	0	1.354582	-0.465615	2.662987
20	1	0	1.718427	0.268732	2.134553
21	1	0	0.264405	-2.153039	2.375019
22	8	0	0.023710	0.551996	0.452083
23	1	0	-1.273844	-0.537405	1.640439
24	6	0	1.323540	2.914276	0.395986
25	8	0	0.711805	3.083067	-0.695234
26	6	0	2.662971	2.273490	0.240763
27	6	0	0.755625	3.419605	1.670145
28	6	0	2.508845	1.576883	-1.146471
29	6	0	1.490477	2.489497	-1.853386
30	6	0	0.513136	1.792004	-2.790149
31	8	0	2.966200	1.500336	1.352897
32	1	0	3.823114	0.981507	1.218943
33	1	0	3.388706	3.097633	0.094403
34	1	0	1.385021	4.296985	1.920799
35	1	0	0.979947	2.670605	2.433954
36	8	0	-0.605363	3.697529	1.686024
37	1	0	-0.933052	4.207918	0.905296
38	8	0	3.684694	1.479251	-1.883807
39	1	0	3.988636	0.549937	-1.837510
40	1	0	2.049872	0.602221	-0.965623
41	1	0	1.969118	3.352312	-2.318746
42	1	0	0.183017	0.859608	-2.329540
43	1	0	1.072098	1.548718	-3.698534
44	8	0	-0.609247	2.584414	-3.125541
45	1	0	-1.311610	2.332921	-2.483678
46	1	0	-0.760184	1.006612	0.070113
47	8	0	-2.059747	1.893847	-0.935399
48	1	0	-2.854097	1.311547	-0.805188
49	1	0	-2.276099	2.783687	-0.606477
50	8	0	-1.925109	4.719852	-0.375661
51	1	0	-1.457847	5.043782	-1.188785
52	1	0	-2.643643	5.333090	-0.190429
53	8	0	-3.962329	0.163631	-0.175540
54	1	0	-3.593177	0.136834	0.740620
55	1	0	-3.855453	-0.755197	-0.520167
56	8	0	4.295780	-1.197834	-1.431220
57	1	0	3.536287	-1.834776	-1.454966
58	1	0	4.997319	-1.600555	-1.955510
59	8	0	-3.525248	-3.973113	-3.138495
60	1	0	-4.114234	-4.713150	-3.311665
61	1	0	-3.944475	-3.444102	-2.432620
62	8	0	3.848890	-1.397202	3.362098
63	1	0	4.150412	-1.623244	4.247794

64	1	0	2.961702	-0.987374	3.438682
65	1	0	3.256511	-4.503146	0.642109
66	8	0	3.469975	-4.992203	-0.174071
67	1	0	3.140454	-5.887972	-0.052325
68	8	0	-3.846923	-2.521811	-0.785465
69	1	0	-4.433333	-2.850790	-0.064610
70	1	0	-2.949962	-2.856704	-0.605203
71	8	0	-5.551772	-3.071419	1.247524
72	1	0	-5.877967	-2.179364	1.475020
73	1	0	-6.330774	-3.624905	1.141831
74	8	0	-0.507235	5.252795	-2.572591
75	1	0	-0.692408	5.900947	-3.259133
76	1	0	-0.533156	4.368761	-2.995920
77	1	0	4.845894	-0.662883	1.886260
78	8	0	4.974180	-0.092192	1.108304
79	1	0	4.878297	-0.645647	0.312001
80	8	0	-3.318930	0.146759	2.459128
81	1	0	-3.163644	1.055131	2.794628
82	1	0	-4.236292	-0.071623	2.679120
83	8	0	-2.779791	2.731505	3.204040
84	1	0	-1.979483	3.064591	2.763920
85	1	0	-2.693036	2.971411	4.131318
86	8	0	-6.051089	-0.358668	1.581238
87	1	0	-5.585252	-0.024319	0.787288
88	1	0	-6.883736	0.118624	1.645257

SCF Done: E(RB3LYP) = -2369.30301510 A.U. after 1 cycles
Convg = 0.5431D-08 -V/T = 2.0040
Sum of electronic and zero-point Energies= -2368.561364
Sum of electronic and thermal Energies= -2368.502939
Sum of electronic and thermal Enthalpies= -2368.501995
Sum of electronic and thermal Free Energies= -2368.654115

3) TS2(D)
ishi07bb.high.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.727744	-2.256560	-0.535616
2	6	0	-4.770631	-0.749461	-0.344510
3	6	0	-4.719622	-2.981138	0.807996
4	6	0	-3.565681	-0.343343	0.507112

5	6	0	-3.590210	-2.438920	1.705408
6	8	0	-3.652368	-1.023733	1.768839
7	6	0	-3.433706	1.133593	0.816627
8	1	0	-3.206778	1.676092	-0.099972
9	1	0	-2.597925	1.251204	1.512298
10	8	0	-4.622523	1.720924	1.349902
11	1	0	-4.789495	1.323393	2.212170
12	1	0	-2.650650	-0.632731	-0.018470
13	8	0	-4.716661	-0.115380	-1.636323
14	1	0	-5.261734	-0.669671	-2.213768
15	1	0	-5.694866	-0.460599	0.166240
16	8	0	-5.844487	-2.612947	-1.339921
17	1	0	-5.880054	-3.577259	-1.370297
18	1	0	-3.798273	-2.501619	-1.072618
19	8	0	-4.605044	-4.381598	0.610295
20	1	0	-3.656999	-4.576265	0.613533
21	1	0	-5.679212	-2.806505	1.303089
22	8	0	-2.334375	-2.945143	1.311369
23	1	0	-3.731851	-2.780871	2.730048
24	6	0	2.148166	0.413419	2.042666
25	8	0	1.769822	-0.458378	1.154676
26	6	0	3.613729	0.208810	2.440758
27	6	0	1.104976	0.853854	3.044734
28	6	0	4.135912	-0.765918	1.356832
29	6	0	2.938948	-0.975045	0.407069
30	6	0	2.664021	-2.398050	-0.046440
31	8	0	3.588997	-0.343774	3.745801
32	1	0	4.454777	-0.223571	4.149381
33	1	0	4.175810	1.143611	2.410296
34	1	0	1.448552	1.790193	3.504354
35	1	0	1.127234	0.089747	3.827790
36	8	0	-0.193038	0.913816	2.537096
37	1	0	-0.232401	1.556471	1.804662
38	8	0	5.267666	-0.215170	0.706815
39	1	0	5.554938	-0.831631	-0.022331
40	1	0	4.398266	-1.706140	1.854517
41	1	0	3.027997	-0.333298	-0.468158
42	1	0	2.299847	-2.998980	0.794919
43	1	0	3.616411	-2.808165	-0.389002
44	8	0	1.778534	-2.456679	-1.153499
45	1	0	0.851341	-2.339373	-0.870761
46	1	0	-1.998326	-2.515297	0.506138
47	8	0	-0.952194	-1.910837	-1.077242
48	1	0	-1.197387	-2.359956	-1.894287
49	1	0	-0.848361	-0.957271	-1.324753
50	8	0	-0.430168	0.675039	-1.776147

51	1	0	0.419321	0.586367	-2.261451
52	1	0	-0.187307	1.768263	-0.490973
53	8	0	-0.024842	2.432899	0.229591
54	1	0	-0.546371	3.237628	0.000876
55	8	0	2.368484	1.941618	0.960833
56	1	0	1.462701	2.278223	0.649046
57	1	0	2.919386	2.671336	1.342476
58	1	0	-1.051035	1.244488	-2.301812
59	8	0	-2.031092	2.542677	-2.789449
60	1	0	-1.855105	3.312272	-2.219749
61	1	0	-3.002391	2.494128	-2.835970
62	8	0	5.676351	-1.673070	-1.430375
63	1	0	5.464832	-1.077373	-2.171415
64	1	0	6.450631	-2.203981	-1.701216
65	8	0	4.388872	3.506975	1.557481
66	1	0	4.630939	4.390957	1.849438
67	1	0	4.847720	3.330634	0.716555
68	8	0	4.754970	2.022891	-0.809604
69	1	0	5.025594	1.266674	-0.236556
70	1	0	3.791028	2.027943	-0.715892
71	8	0	-4.821963	2.532225	-2.328581
72	1	0	-5.530829	2.708542	-2.955581
73	1	0	-4.925048	1.600993	-2.031567
74	8	0	4.803734	0.455043	-3.111357
75	1	0	4.921301	1.172444	-2.453399
76	1	0	5.231232	0.744720	-3.924019
77	8	0	7.846967	-3.114033	-2.336517
78	1	0	8.733028	-3.048772	-1.966577
79	1	0	7.750763	-4.027484	-2.624317
80	8	0	2.037426	-0.066472	-2.644110
81	1	0	2.043538	-0.997207	-2.354676
82	1	0	2.909404	0.113671	-3.033407
83	8	0	-1.673927	4.398948	-0.655891
84	1	0	-2.622709	4.339637	-0.342712
85	1	0	-1.475229	5.335688	-0.752032
86	8	0	-4.232625	4.118121	-0.073278
87	1	0	-4.496938	3.533793	0.657391
88	1	0	-4.600408	3.685742	-0.866530

SCF Done: E(RB+HF-LYP) = -2369.29489258 A.U. after 1 cycles

Convg = 0.8822D-09 -V/T = 2.0040

S**2 = 0.0000

1	2	3
A	A	A

Frequencies -- -151.2608 11.5766 15.3030

Sum of electronic and zero-point Energies= -2368.553086

Sum of electronic and thermal Energies= -2368.494943
Sum of electronic and thermal Enthalpies= -2368.493999
Sum of electronic and thermal Free Energies= -2368.647761

4) Product(D)
prod.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.575349	-1.610054	-0.678401
2	6	0	-4.484917	-0.110073	-0.928880
3	6	0	-3.688049	-2.022012	0.496822
4	6	0	-3.023365	0.333261	-1.050112
5	6	0	-2.259735	-1.513627	0.295605
6	8	0	-2.263301	-0.105539	0.085444
7	6	0	-2.897171	1.849077	-1.115714
8	1	0	-3.418647	2.207385	-2.004528
9	1	0	-1.842176	2.120699	-1.183196
10	8	0	-3.418319	2.507404	0.047314
11	1	0	-4.402128	2.567869	0.009444
12	1	0	-2.600586	-0.086827	-1.970241
13	8	0	-5.141099	0.290685	-2.118972
14	1	0	-6.089484	0.331581	-1.924806
15	1	0	-4.915464	0.392498	-0.053916
16	8	0	-5.943746	-1.941221	-0.378955
17	1	0	-5.947585	-2.853395	-0.061561
18	1	0	-4.264042	-2.140607	-1.584859
19	8	0	-3.730748	-3.432359	0.684240
20	1	0	-3.146719	-3.806138	0.009639
21	1	0	-4.087624	-1.577296	1.411276
22	8	0	0.843658	-1.322405	-0.339976
23	1	0	-1.667940	-1.645618	1.206369
24	6	0	1.976255	-1.727439	0.390173
25	8	0	3.153454	-1.332108	-0.308409
26	6	0	2.011519	-3.267971	0.389990
27	6	0	2.009123	-1.082785	1.783124
28	6	0	2.733472	-3.608906	-0.930928
29	6	0	3.651263	-2.389702	-1.160857
30	6	0	5.113555	-2.570834	-0.754133
31	8	0	2.766369	-3.688435	1.519332
32	1	0	2.666309	-4.640445	1.618491
33	1	0	1.000129	-3.681437	0.388175

34	1	0	2.898417	-1.412444	2.320160
35	1	0	1.130072	-1.420383	2.336086
36	8	0	1.949819	0.337566	1.705995
37	1	0	2.852502	0.702440	1.590705
38	8	0	1.747224	-3.768058	-1.937014
39	1	0	2.168298	-4.084496	-2.742494
40	1	0	3.318405	-4.528629	-0.802718
41	8	0	5.723698	-1.275713	-0.659428
42	1	0	5.024338	-0.730247	-0.266497
43	1	0	3.578931	-2.052659	-2.199597
44	1	0	5.163292	-3.085557	0.211781
45	1	0	5.668259	-3.146068	-1.497831
46	1	0	0.973945	-0.393272	-0.633215
47	8	0	1.485838	1.257980	-1.289981
48	1	0	1.465380	1.810880	-0.485822
49	1	0	2.437975	1.093971	-1.450141
50	8	0	4.434079	1.520070	1.151860
51	1	0	5.264398	1.101251	1.472393
52	1	0	4.471542	1.443079	0.170916
53	8	0	1.273097	3.560627	0.422436
54	1	0	2.152119	3.917162	0.668651
55	1	0	1.023751	3.987152	-0.414400
56	1	0	0.351394	2.844167	1.708243
57	8	0	0.014225	2.174461	2.343597
58	1	0	-1.345335	2.054745	2.328838
59	8	0	-1.712947	-2.231775	-0.771295
60	1	0	0.607763	1.404283	2.208540
61	1	0	-0.751744	-2.058592	-0.785353
62	8	0	-2.426757	2.059609	2.340253
63	1	0	-2.807024	1.250377	2.754953
64	1	0	-2.822758	2.189219	1.402225
65	8	0	3.900991	4.180145	0.893894
66	1	0	4.246920	4.812603	1.531474
67	1	0	4.212115	3.284687	1.165402
68	8	0	1.191059	3.797355	-2.345675
69	1	0	1.155459	2.820015	-2.282912
70	1	0	0.660635	4.062264	-3.103555
71	8	0	4.286850	1.408423	-1.572237
72	1	0	4.937542	0.909738	-2.077909
73	1	0	4.311437	2.365258	-1.859063
74	8	0	6.700621	0.050004	1.620347
75	1	0	7.597544	0.369072	1.756706
76	1	0	6.737984	-0.572957	0.874440
77	8	0	4.027368	3.989965	-1.966226
78	1	0	4.091309	4.310952	-1.050618
79	1	0	3.099250	4.123292	-2.227644

80	8	0	-6.138297	2.647824	0.092839
81	1	0	-6.706918	1.876843	-0.091112
82	1	0	-6.551776	3.392099	-0.354986
83	8	0	-7.548001	0.282547	-0.635647
84	1	0	-8.459560	0.148751	-0.912533
85	1	0	-7.193498	-0.594332	-0.383954
86	8	0	-3.666150	-0.033994	3.517456
87	1	0	-3.243352	-0.720886	4.043831
88	1	0	-4.474566	0.199874	3.987049

SCF Done: E(RB+HF-LYP) = -2369.32325136 A.U. after 1 cycles
Convg = 0.3715D-08 -V/T = 2.0040
S**2 = 0.0000
Sum of electronic and zero-point Energies= -2368.582170
Sum of electronic and thermal Energies= -2368.523506
Sum of electronic and thermal Enthalpies= -2368.522562
Sum of electronic and thermal Free Energies= -2368.678647

II) B3LYP/6-311G(d,p) SCRF=(PCM, solvent=water)

1) TS1(D)
ishi976.high.pcm.chk
Stoichiometry C12H22O11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.433452	-2.556968	0.739205
2	6	0	-0.115010	-2.747639	-0.682317
3	6	0	-0.214388	-1.394105	1.513918
4	6	0	-0.452322	-1.429390	-1.379719
5	6	0	-0.601404	-0.180021	0.661905
6	8	0	-1.219599	-0.561297	-0.511523
7	6	0	-1.261972	-1.608860	-2.650088
8	1	0	-0.671314	-2.220251	-3.340273
9	1	0	-1.419132	-0.624344	-3.104454
10	8	0	-2.504251	-2.231465	-2.339264
11	1	0	-3.082909	-2.161718	-3.127286
12	1	0	0.479063	-0.926309	-1.651216
13	8	0	0.851080	-3.403564	-1.515272
14	1	0	0.916113	-4.342026	-1.221828
15	1	0	-1.023573	-3.353989	-0.619326
16	8	0	0.222790	-3.792066	1.435458
17	1	0	0.551744	-3.723477	2.359641

18	1	0	1.503199	-2.357294	0.655838
19	8	0	0.535451	-1.033886	2.669564
20	1	0	1.462466	-0.902520	2.375313
21	1	0	-1.180930	-1.753088	1.880172
22	8	0	0.537847	0.721139	0.221456
23	1	0	-1.299894	0.456771	1.202848
24	6	0	1.897002	1.544301	0.843342
25	8	0	2.070621	2.457466	-0.122118
26	6	0	3.067541	0.580192	0.743894
27	6	0	1.488759	2.126713	2.181827
28	6	0	3.245315	0.490949	-0.784066
29	6	0	2.908814	1.926176	-1.220082
30	6	0	2.151045	2.013563	-2.545773
31	8	0	2.870200	-0.616005	1.438877
32	1	0	3.616219	-1.258578	1.276769
33	1	0	3.930812	1.128457	1.150736
34	1	0	2.354714	2.699503	2.537367
35	1	0	1.304061	1.311834	2.879273
36	8	0	0.320302	2.908551	2.124166
37	1	0	0.439498	3.711008	1.568208
38	8	0	4.523394	0.076822	-1.202765
39	1	0	4.410758	-0.833138	-1.525232
40	1	0	2.492069	-0.192563	-1.177336
41	1	0	3.802999	2.550627	-1.231448
42	1	0	1.430263	1.195051	-2.617830
43	1	0	2.876669	1.893639	-3.353054
44	8	0	1.475285	3.253474	-2.730969
45	1	0	0.601382	3.146561	-2.310349
46	1	0	0.040673	1.507102	-0.272397
47	8	0	-0.661531	2.618376	-0.981329
48	1	0	-1.658543	2.467935	-0.999156
49	1	0	-0.513789	3.458904	-0.493517
50	8	0	0.167725	4.911672	0.339392
51	1	0	0.919486	5.245833	-0.216004
52	1	0	-0.410718	5.660849	0.519032
53	8	0	-3.243737	2.250792	-0.767493
54	1	0	-3.297319	2.028639	0.189450
55	1	0	-3.609569	1.456182	-1.210200
56	8	0	3.592904	-2.611900	-1.700321
57	1	0	2.638304	-2.842419	-1.676161
58	1	0	3.973485	-3.142421	-2.409764
59	8	0	-4.358645	-1.427919	-4.203632
60	1	0	-5.127897	-2.002892	-4.284714
61	1	0	-4.575351	-0.818260	-3.469035
62	8	0	0.882835	-3.402017	4.087897
63	1	0	0.139767	-3.707567	4.620824

64	1	0	0.705057	-2.458945	3.916536
65	1	0	0.755171	-5.286261	0.522116
66	8	0	1.001654	-5.818308	-0.262104
67	1	0	1.926389	-6.053234	-0.123709
68	8	0	-4.335125	-0.116198	-1.750909
69	1	0	-5.090615	-0.317910	-1.148503
70	1	0	-3.660254	-0.798284	-1.578359
71	8	0	-6.411489	-0.654691	-0.073338
72	1	0	-6.195123	-0.396824	0.843527
73	1	0	-7.191613	-0.137017	-0.301091
74	8	0	2.169147	5.550951	-1.329893
75	1	0	2.018583	6.339823	-1.862676
76	1	0	2.055686	4.795632	-1.943116
77	1	0	5.561825	-2.234310	0.812710
78	8	0	4.634449	-2.492595	0.862514
79	1	0	4.371717	-2.710779	-0.055762
80	8	0	-3.232027	1.380622	1.817689
81	1	0	-2.842076	1.862764	2.577863
82	1	0	-4.031869	0.930920	2.141136
83	8	0	-1.846363	2.652302	3.830334
84	1	0	-1.028072	2.800426	3.316034
85	1	0	-1.604321	1.999556	4.496551
86	8	0	-5.681215	0.142461	2.524022
87	1	0	-6.288225	0.793304	2.898154
88	1	0	-5.649689	-0.576086	3.167880

SCF Done: E(RB3LYP) = -2369.37070231 A.U. after 1 cycles
Convg = 0.3044D-08 -V/T = 2.0041

1	2	3
A	A	A

Frequencies -- -163.3513 15.9169 23.6444
Sum of electronic and zero-point Energies= -2368.634335
Sum of electronic and thermal Energies= -2368.575722
Sum of electronic and thermal Enthalpies= -2368.574778
Sum of electronic and thermal Free Energies= -2368.728429

2) Int(D)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.865535	-1.774272	0.773142

2	6	0	1.561709	-2.588458	-0.487101
3	6	0	0.605729	-1.351678	1.541050
4	6	0	0.409800	-1.987406	-1.296589
5	6	0	-0.537373	-0.866287	0.632088
6	8	0	-0.730776	-1.791401	-0.437685
7	6	0	-0.010845	-2.863217	-2.471080
8	1	0	0.840133	-2.909073	-3.159220
9	1	0	-0.838138	-2.368461	-2.990248
10	8	0	-0.377727	-4.169195	-2.056483
11	1	0	-1.291102	-4.330839	-2.367183
12	1	0	0.721647	-1.019560	-1.704566
13	8	0	2.712733	-2.640869	-1.341902
14	1	0	3.318920	-3.326448	-0.979326
15	1	0	1.277077	-3.604175	-0.194739
16	8	0	2.710793	-2.565104	1.618119
17	1	0	3.257648	-1.983775	2.179940
18	1	0	2.405741	-0.872994	0.467104
19	8	0	0.926265	-0.379674	2.539587
20	1	0	1.415806	0.341075	2.103016
21	1	0	0.236179	-2.227424	2.078328
22	8	0	-0.268274	0.433219	0.169762
23	1	0	-1.477260	-0.891658	1.182973
24	6	0	0.894934	3.123080	0.514887
25	8	0	0.195444	3.274428	-0.523202
26	6	0	2.262850	2.586565	0.248891
27	6	0	0.367990	3.523152	1.848360
28	6	0	2.108025	2.023351	-1.196170
29	6	0	0.962347	2.873360	-1.768532
30	6	0	0.014367	2.157792	-2.718900
31	8	0	2.626237	1.691714	1.257834
32	1	0	3.571701	1.382083	1.118091
33	1	0	2.943158	3.454547	0.194278
34	1	0	0.711351	4.568829	1.961867
35	1	0	0.902718	2.948228	2.604805
36	8	0	-1.005005	3.366016	2.038206
37	1	0	-1.545132	3.875392	1.385205
38	8	0	3.254174	2.120567	-1.989325
39	1	0	3.678838	1.238165	-1.993352
40	1	0	1.766509	0.991100	-1.100977
41	1	0	1.318892	3.821924	-2.171193
42	1	0	-0.194867	1.158167	-2.335410
43	1	0	0.547475	2.057532	-3.668130
44	8	0	-1.201226	2.858601	-2.933567
45	1	0	-1.849413	2.463617	-2.309805
46	1	0	-1.111455	0.865315	-0.097117
47	8	0	-2.519759	1.783379	-0.801301

48	1	0	-3.296685	1.186557	-0.685790
49	1	0	-2.730578	2.621194	-0.340722
50	8	0	-2.662165	4.381142	0.215123
51	1	0	-2.333555	4.885703	-0.574256
52	1	0	-3.473254	4.809336	0.510604
53	8	0	-4.392524	-0.070869	-0.091263
54	1	0	-3.969104	-0.132020	0.800234
55	1	0	-4.108255	-0.905089	-0.525052
56	8	0	4.339376	-0.413209	-1.649355
57	1	0	3.741761	-1.196400	-1.595519
58	1	0	5.045398	-0.657186	-2.259462
59	8	0	-2.995086	-4.339292	-2.910671
60	1	0	-3.399155	-5.183726	-2.682139
61	1	0	-3.318260	-3.709793	-2.229777
62	8	0	4.658684	-1.128490	2.992306
63	1	0	5.351864	-1.750396	3.246842
64	1	0	4.443928	-0.639171	3.796390
65	1	0	3.812753	-3.838340	0.852507
66	8	0	4.222687	-4.358396	0.132625
67	1	0	5.151883	-4.101383	0.135898
68	8	0	-3.421442	-2.569732	-0.852485
69	1	0	-3.833165	-3.045778	-0.090794
70	1	0	-2.476213	-2.445175	-0.642771
71	8	0	-4.814671	-3.675335	1.211263
72	1	0	-5.353842	-2.902881	1.485717
73	1	0	-5.448671	-4.311635	0.862500
74	8	0	-1.657193	5.461996	-2.028392
75	1	0	-2.284821	5.938218	-2.583589
76	1	0	-1.447381	4.639924	-2.515736
77	1	0	5.045202	-0.007669	1.558250
78	8	0	4.996661	0.667464	0.855849
79	1	0	4.911550	0.184223	0.010340
80	8	0	-3.432707	-0.559737	2.381873
81	1	0	-2.838128	0.027483	2.901403
82	1	0	-4.263222	-0.674331	2.860385
83	8	0	-1.473974	0.956789	3.501848
84	1	0	-1.414960	1.784413	2.993102
85	1	0	-0.656019	0.472745	3.286102
86	8	0	-6.132433	-1.306910	1.783540
87	1	0	-5.867873	-0.778996	1.007022
88	1	0	-7.092783	-1.254097	1.835270

SCF Done: E(RB3LYP) = -2369.39418153 A.U. after 1 cycles
Convg = 0.2595D-08 -V/T = 2.0041
Sum of electronic and zero-point Energies= -2368.656018
Sum of electronic and thermal Energies= -2368.597059

Sum of electronic and thermal Enthalpies= -2368.596115
Sum of electronic and thermal Free Energies= -2368.748725

3) TS2(D)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.449865	-2.160900	-0.841492
2	6	0	-4.918136	-0.902178	-0.129346
3	6	0	-4.039019	-3.227922	0.173476
4	6	0	-3.818815	-0.396303	0.806556
5	6	0	-3.022868	-2.673486	1.189010
6	8	0	-3.484663	-1.447546	1.734834
7	6	0	-4.232289	0.783795	1.677073
8	1	0	-4.501291	1.638857	1.056868
9	1	0	-3.368068	1.062726	2.290473
10	8	0	-5.362567	0.478592	2.489994
11	1	0	-5.123388	-0.302135	3.004372
12	1	0	-2.936790	-0.106935	0.222264
13	8	0	-5.248858	0.113831	-1.087729
14	1	0	-5.799313	-0.315051	-1.757222
15	1	0	-5.806925	-1.129063	0.469234
16	8	0	-5.527789	-2.605815	-1.663300
17	1	0	-5.224325	-3.395556	-2.127228
18	1	0	-3.592183	-1.898486	-1.474026
19	8	0	-3.539277	-4.391767	-0.476772
20	1	0	-2.591795	-4.245497	-0.607545
21	1	0	-4.935507	-3.537101	0.717688
22	8	0	-1.721752	-2.609070	0.659419
23	1	0	-2.952353	-3.348402	2.041762
24	6	0	1.750285	0.035628	1.953045
25	8	0	1.470026	-0.515037	0.826615
26	6	0	3.124847	-0.377096	2.485526
27	6	0	0.604377	0.443027	2.838527
28	6	0	3.742459	-1.130794	1.289769
29	6	0	2.707216	-0.998341	0.152752
30	6	0	2.397420	-2.268732	-0.617112
31	8	0	2.944237	-1.255819	3.583276
32	1	0	3.077506	-0.767217	4.403631
33	1	0	3.728333	0.488683	2.753752
34	1	0	0.946643	1.255769	3.489318

35	1	0	0.432015	-0.429092	3.479655
36	8	0	-0.586453	0.722798	2.162101
37	1	0	-0.458598	1.499610	1.575758
38	8	0	5.003618	-0.585571	0.952854
39	1	0	5.331814	-1.035506	0.125087
40	1	0	3.843887	-2.180621	1.584444
41	1	0	2.980047	-0.195667	-0.529565
42	1	0	1.893049	-2.987368	0.037987
43	1	0	3.358870	-2.686462	-0.921884
44	8	0	1.653632	-2.039600	-1.804932
45	1	0	0.714991	-1.857961	-1.593476
46	1	0	-1.647769	-2.016598	-0.115927
47	8	0	-0.999015	-1.225198	-1.622621
48	1	0	-1.360064	-1.529255	-2.463809
49	1	0	-0.786783	-0.262631	-1.751662
50	8	0	-0.131373	1.278339	-2.001341
51	1	0	0.733975	1.143407	-2.455341
52	1	0	-0.001014	2.120803	-0.524283
53	8	0	0.042974	2.632401	0.322981
54	1	0	-0.393716	3.491920	0.131991
55	8	0	2.360370	1.877363	1.244219
56	1	0	1.548704	2.355534	0.913822
57	1	0	2.845574	2.433106	1.901651
58	1	0	-0.677698	1.927865	-2.513411
59	8	0	-1.727373	3.202748	-2.988741
60	1	0	-1.561044	3.874328	-2.300290
61	1	0	-2.637188	2.901911	-2.802036
62	8	0	5.608468	-1.558118	-1.422815
63	1	0	5.482098	-0.772115	-1.988264
64	1	0	6.503734	-1.906758	-1.617943
65	8	0	4.312537	2.969521	2.670759
66	1	0	4.377569	3.807509	3.142170
67	1	0	4.913104	3.037394	1.912669
68	8	0	4.912745	2.022939	-0.071112
69	1	0	5.070219	1.156161	0.359905
70	1	0	3.957939	2.149321	0.057896
71	8	0	-4.315376	2.504208	-2.105932
72	1	0	-5.046092	2.751969	-2.684538
73	1	0	-4.533279	1.608178	-1.772062
74	8	0	4.924214	0.922340	-2.605357
75	1	0	5.019457	1.476832	-1.798577
76	1	0	5.461577	1.335393	-3.290637
77	8	0	8.142142	-2.516562	-1.956586
78	1	0	8.747071	-2.318927	-1.232180
79	1	0	8.163045	-3.477400	-2.035430
80	8	0	2.191438	0.421473	-3.121129

81	1	0	2.125567	-0.497567	-2.801994
82	1	0	3.125648	0.675524	-2.994766
83	8	0	-1.411395	4.733443	-0.609322
84	1	0	-2.333118	4.623642	-0.266184
85	1	0	-1.199047	5.671202	-0.552051
86	8	0	-3.911217	4.076576	0.121075
87	1	0	-4.603142	4.731273	0.263936
88	1	0	-4.179943	3.568501	-0.674209

SCF Done: E(RB3LYP) = -2369.38002089 A.U. after 1 cycles
Convg = 0.3631D-08 -V/T = 2.0041

1	2	3
A	A	A

Frequencies -- -112.9960 14.2114 16.3003
Sum of electronic and zero-point Energies= -2368.644295
Sum of electronic and thermal Energies= -2368.584577
Sum of electronic and thermal Enthalpies= -2368.583632
Sum of electronic and thermal Free Energies= -2368.742119

4) Product(D)
prod.pcm.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.422002	-1.671559	-0.789877
2	6	0	-4.376419	-0.166714	-1.024100
3	6	0	-3.593548	-2.054175	0.436571
4	6	0	-2.930802	0.338673	-1.061982
5	6	0	-2.176542	-1.488747	0.325322
6	8	0	-2.218257	-0.081706	0.110949
7	6	0	-2.854632	1.859311	-1.112510
8	1	0	-3.333049	2.207971	-2.029145
9	1	0	-1.808332	2.167148	-1.120530
10	8	0	-3.460068	2.495407	0.023021
11	1	0	-4.443830	2.474884	-0.038329
12	1	0	-2.438928	-0.053739	-1.960282
13	8	0	-4.994480	0.208242	-2.249777
14	1	0	-5.951095	0.238018	-2.080804
15	1	0	-4.881609	0.313551	-0.178799
16	8	0	-5.793480	-2.054938	-0.595079
17	1	0	-5.792596	-2.968734	-0.282653
18	1	0	-4.026060	-2.182685	-1.675469

19	8	0	-3.584555	-3.469201	0.616571
20	1	0	-2.957074	-3.815934	-0.033060
21	1	0	-4.060441	-1.632579	1.328796
22	8	0	1.026549	-1.314952	-0.286814
23	1	0	-1.642137	-1.600525	1.271861
24	6	0	2.060651	-1.742287	0.582512
25	8	0	3.320322	-1.304072	0.102163
26	6	0	2.119573	-3.273742	0.448252
27	6	0	1.878002	-1.182840	1.994918
28	6	0	2.968537	-3.475152	-0.830131
29	6	0	3.649499	-2.096137	-1.053662
30	6	0	5.162337	-2.143875	-1.188549
31	8	0	2.763189	-3.790565	1.607110
32	1	0	2.715898	-4.752028	1.569982
33	1	0	1.122688	-3.700981	0.315934
34	1	0	2.705970	-1.515433	2.623007
35	1	0	0.946851	-1.570893	2.410043
36	8	0	1.776798	0.238189	1.986172
37	1	0	2.654001	0.637267	1.793492
38	8	0	2.120879	-3.863159	-1.906255
39	1	0	2.677513	-4.102583	-2.655327
40	1	0	3.714334	-4.253345	-0.633452
41	8	0	5.737028	-0.838861	-1.321473
42	1	0	6.009962	-0.550345	-0.431300
43	1	0	3.208858	-1.637187	-1.945194
44	1	0	5.591415	-2.655617	-0.320903
45	1	0	5.419122	-2.716709	-2.084034
46	1	0	1.078769	-0.340901	-0.430750
47	8	0	1.249402	1.302728	-1.103420
48	1	0	1.208734	1.931278	-0.357846
49	1	0	2.210581	1.220769	-1.303426
50	8	0	4.118852	1.541489	1.263987
51	1	0	4.946522	1.080657	1.498797
52	1	0	4.047864	1.395259	0.289882
53	8	0	1.086646	3.677007	0.521785
54	1	0	2.007736	3.964620	0.704603
55	1	0	0.866363	4.041624	-0.353514
56	1	0	0.243709	2.829838	1.785792
57	8	0	-0.094801	2.192363	2.453394
58	1	0	-1.495251	2.051150	2.393528
59	8	0	-1.524110	-2.178226	-0.706153
60	1	0	0.467753	1.394462	2.346811
61	1	0	-0.567807	-1.975808	-0.630432
62	8	0	-2.558712	2.034870	2.376960
63	1	0	-2.918840	1.186340	2.765807
64	1	0	-2.909787	2.154785	1.426550

65	8	0	3.763830	4.189456	0.816157
66	1	0	4.130530	4.846210	1.417853
67	1	0	4.041073	3.302683	1.145819
68	8	0	1.084749	3.856666	-2.264257
69	1	0	0.963127	2.889578	-2.215558
70	1	0	0.518390	4.173182	-2.976624
71	8	0	3.939072	1.322982	-1.451900
72	1	0	4.592648	0.635224	-1.683163
73	1	0	4.171765	2.199608	-1.833110
74	8	0	6.436275	-0.027584	1.312910
75	1	0	7.302423	0.390782	1.393827
76	1	0	6.448907	-0.764730	1.935997
77	8	0	3.961042	3.978643	-2.019782
78	1	0	3.997388	4.216708	-1.074576
79	1	0	3.016046	4.055667	-2.245459
80	8	0	-6.207469	2.464246	0.116416
81	1	0	-6.717679	1.709613	-0.237212
82	1	0	-6.442583	2.504064	1.050360
83	8	0	-7.450483	0.156256	-0.920456
84	1	0	-8.331628	0.038352	-1.291095
85	1	0	-7.136672	-0.724571	-0.639342
86	8	0	-3.593693	-0.157959	3.398697
87	1	0	-2.989687	-0.756625	3.854266
88	1	0	-4.325995	-0.014432	4.010391

SCF Done: E(RB3LYP) = -2369.41599173 A.U. after 1 cycles
Convg = 0.2914D-08 -V/T = 2.0041
Sum of electronic and zero-point Energies= -2368.678307
Sum of electronic and thermal Energies= -2368.619648
Sum of electronic and thermal Enthalpies= -2368.618704
Sum of electronic and thermal Free Energies= -2368.772725

==== Figure 5 ====

Geometries of Int(C) and Int(D) arte included in Figures 3 and 4, respectively.

I) B3LYP/6-311G(d,p)

TS(C -> D)
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Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.753791	-2.038503	0.791823
2	6	0	1.103693	-2.612245	-0.468261
3	6	0	0.752824	-1.335402	1.723816
4	6	0	0.082945	-1.666845	-1.097207
5	6	0	-0.349503	-0.580271	0.999741
6	8	0	-0.844693	-1.124955	-0.091464
7	6	0	-0.768598	-2.316480	-2.166916
8	1	0	-0.090634	-2.643538	-2.962895
9	1	0	-1.453882	-1.568260	-2.582585
10	8	0	-1.474959	-3.407528	-1.602177
11	1	0	-2.047633	-3.775517	-2.310340
12	1	0	0.601879	-0.810264	-1.531734
13	8	0	2.101942	-2.848975	-1.465425
14	1	0	2.421764	-3.769346	-1.324477
15	1	0	0.604996	-3.552496	-0.218899
16	8	0	2.384927	-3.127520	1.463261
17	1	0	2.998362	-2.779891	2.137852
18	1	0	2.501189	-1.302252	0.487059
19	8	0	1.368319	-0.571142	2.740180
20	1	0	1.937528	0.094515	2.283166
21	1	0	0.177693	-2.121600	2.232827
22	8	0	0.238423	0.968984	0.312884
23	1	0	-1.136139	-0.189295	1.639260
24	6	0	1.030312	2.257466	0.551247
25	8	0	0.751411	3.023956	-0.560906
26	6	0	2.521432	1.962392	0.440354
27	6	0	0.551436	2.932131	1.828879
28	6	0	2.646123	1.659130	-1.063554
29	6	0	1.666617	2.687497	-1.658938
30	6	0	0.877836	2.170472	-2.867101

31	8	0	2.934589	0.968841	1.333369
32	1	0	3.861517	0.627732	1.166771
33	1	0	3.050681	2.905029	0.637516
34	1	0	1.120402	3.862718	1.939740
35	1	0	0.784543	2.282559	2.674120
36	8	0	-0.839976	3.161219	1.846101
37	1	0	-1.112261	3.799010	1.150531
38	8	0	3.943518	1.779280	-1.585526
39	1	0	4.291206	0.877996	-1.671192
40	1	0	2.266086	0.648371	-1.239075
41	1	0	2.191771	3.611736	-1.907057
42	1	0	0.625971	1.114644	-2.723865
43	1	0	1.515793	2.243135	-3.750891
44	8	0	-0.312203	2.905528	-3.119887
45	1	0	-1.000390	2.524283	-2.543519
46	1	0	-0.614525	1.291754	-0.150179
47	8	0	-1.877533	1.845970	-0.981748
48	1	0	-2.697399	1.301681	-0.854554
49	1	0	-2.084194	2.751657	-0.667095
50	8	0	-2.003446	4.515355	-0.186668
51	1	0	-1.484925	4.988076	-0.892827
52	1	0	-2.791698	5.038501	-0.010462
53	8	0	-3.941152	0.292907	-0.205813
54	1	0	-3.533453	0.163424	0.681750
55	1	0	-3.950299	-0.603408	-0.617125
56	8	0	4.377314	-1.153334	-1.536338
57	1	0	3.586069	-1.734892	-1.576957
58	1	0	4.988948	-1.493604	-2.198471
59	8	0	-3.451432	-3.702696	-3.391398
60	1	0	-3.980267	-4.444540	-3.698951
61	1	0	-4.000162	-3.208686	-2.754172
62	8	0	3.886582	-1.750243	3.324089
63	1	0	4.248233	-2.071914	4.156723
64	1	0	3.055289	-1.284870	3.529872
65	1	0	2.800374	-4.762770	0.466752
66	8	0	2.746379	-5.193135	-0.402474
67	1	0	3.411472	-5.885941	-0.433460
68	8	0	-4.038225	-2.334606	-1.034876
69	1	0	-4.662817	-2.705785	-0.366763
70	1	0	-3.159882	-2.716189	-0.854480
71	8	0	-5.776117	-3.026621	0.910974
72	1	0	-6.015055	-2.149297	1.267458
73	1	0	-6.603759	-3.483493	0.735217
74	8	0	-0.560701	5.482853	-2.192888
75	1	0	-0.846252	6.137931	-2.836706
76	1	0	-0.398212	4.652777	-2.687801

77	1	0	4.998039	-0.980761	1.801414
78	8	0	5.144077	-0.360971	1.069856
79	1	0	5.054252	-0.852519	0.234285
80	8	0	-3.143317	-0.079941	2.391818
81	1	0	-3.065182	0.763427	2.897118
82	1	0	-4.027695	-0.421147	2.590002
83	8	0	-2.759779	2.296356	3.604894
84	1	0	-2.048418	2.707321	3.076275
85	1	0	-2.495433	2.372329	4.526170
86	8	0	-5.952925	-0.364391	1.632622
87	1	0	-5.537659	0.077608	0.865835
88	1	0	-6.677489	0.196493	1.925828

SCF Done: E(RB3LYP) = -2369.28763292 A.U. after 14 cycles
Convg = 0.3621D-08 -V/T = 2.0040

1	2	3
A	A	A

Frequencies -- -149.2364 19.1436 25.1434
Sum of electronic and zero-point Energies= -2368.546046
Sum of electronic and thermal Energies= -2368.488416
Sum of electronic and thermal Enthalpies= -2368.487471
Sum of electronic and thermal Free Energies= -2368.636788

II) B3LYP/ 6-311G(d,p) SCRF=(PCM, solvent=water)

TS(C -> D)
ishi97ibb.highpcm.chk
Stoichiometry C12H51O25(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.820668	-1.969092	0.877048
2	6	0	1.064087	-2.602398	-0.295076
3	6	0	0.894944	-1.231907	1.856628
4	6	0	-0.002100	-1.676241	-0.880098
5	6	0	-0.267642	-0.521157	1.198104
6	8	0	-0.849740	-1.079514	0.170809
7	6	0	-0.934506	-2.342414	-1.867361
8	1	0	-0.318316	-2.689883	-2.702260
9	1	0	-1.637599	-1.591706	-2.245360
10	8	0	-1.619357	-3.421087	-1.242516
11	1	0	-2.130235	-3.878425	-1.944897
12	1	0	0.483318	-0.837394	-1.380738

13	8	0	1.959522	-2.885171	-1.372747
14	1	0	2.422927	-3.726651	-1.152144
15	1	0	0.583682	-3.525112	0.044437
16	8	0	2.521638	-3.005377	1.566187
17	1	0	3.345731	-2.640864	1.945646
18	1	0	2.532953	-1.251287	0.470788
19	8	0	1.571051	-0.436126	2.793960
20	1	0	2.201861	0.122328	2.292587
21	1	0	0.360843	-2.004571	2.430724
22	8	0	0.307310	1.041407	0.383692
23	1	0	-0.965309	-0.040045	1.877297
24	6	0	1.113787	2.295183	0.578695
25	8	0	0.729657	3.123680	-0.469838
26	6	0	2.585385	1.999037	0.290870
27	6	0	0.800542	2.933613	1.926193
28	6	0	2.533244	1.762075	-1.227893
29	6	0	1.516800	2.829396	-1.670564
30	6	0	0.601193	2.377337	-2.814212
31	8	0	3.095406	0.955620	1.076861
32	1	0	3.983979	0.636545	0.753346
33	1	0	3.140062	2.929263	0.474600
34	1	0	1.340484	3.885233	1.971225
35	1	0	1.180324	2.282831	2.714061
36	8	0	-0.582342	3.108838	2.164493
37	1	0	-0.988195	3.731229	1.521560
38	8	0	3.776624	1.865979	-1.885609
39	1	0	4.022606	0.959297	-2.132731
40	1	0	2.113691	0.769075	-1.402886
41	1	0	2.030718	3.756913	-1.931838
42	1	0	0.367682	1.313628	-2.709634
43	1	0	1.135920	2.509310	-3.757259
44	8	0	-0.613939	3.118580	-2.887468
45	1	0	-1.218189	2.705110	-2.239027
46	1	0	-0.578223	1.358606	-0.003542
47	8	0	-1.930640	1.921975	-0.713273
48	1	0	-2.726794	1.338103	-0.639163
49	1	0	-2.155014	2.780580	-0.292199
50	8	0	-2.046593	4.467629	0.334870
51	1	0	-1.653688	5.002829	-0.403110
52	1	0	-2.841971	4.926259	0.626755
53	8	0	-4.022644	0.275632	-0.218457
54	1	0	-3.727335	-0.015243	0.679307
55	1	0	-4.085524	-0.563614	-0.723681
56	8	0	4.072322	-1.022471	-2.089615
57	1	0	3.333697	-1.640152	-1.910927
58	1	0	4.557353	-1.402371	-2.831312

59	8	0	-3.473997	-4.142486	-3.125220
60	1	0	-3.901741	-5.000415	-3.025524
61	1	0	-4.029784	-3.520647	-2.615842
62	8	0	5.034859	-2.141853	2.368940
63	1	0	5.632664	-2.899026	2.409716
64	1	0	5.117413	-1.703144	3.225153
65	1	0	3.056927	-4.507302	0.560640
66	8	0	3.163386	-5.038551	-0.251956
67	1	0	4.114124	-5.068068	-0.409671
68	8	0	-4.269059	-2.343394	-1.141817
69	1	0	-5.015369	-2.582895	-0.540412
70	1	0	-3.455347	-2.709716	-0.753907
71	8	0	-6.409119	-2.722021	0.504440
72	1	0	-6.498703	-1.820232	0.877922
73	1	0	-7.199410	-2.849966	-0.031996
74	8	0	-0.933528	5.654901	-1.804389
75	1	0	-1.564432	6.135056	-2.352427
76	1	0	-0.727269	4.837193	-2.305026
77	1	0	5.361856	-0.952825	0.945879
78	8	0	5.316842	-0.235835	0.287358
79	1	0	5.034622	-0.651557	-0.550312
80	8	0	-3.644849	-0.523462	2.352169
81	1	0	-3.147390	0.138166	2.875057
82	1	0	-4.587337	-0.354663	2.504214
83	8	0	-1.982266	1.249421	3.603812
84	1	0	-1.518411	1.959609	3.111698
85	1	0	-1.372393	0.962410	4.291483
86	8	0	-6.292634	-0.099625	1.389820
87	1	0	-5.745504	0.288513	0.679561
88	1	0	-7.047627	0.485566	1.514116

SCF Done: E(RB3LYP) = -2369.37285544 A.U. after 1 cycles
Convg = 0.5395D-08 -V/T = 2.0041

1	2	3
Frequencies -- -151.5305	15.9468	24.4049

Sum of electronic and zero-point Energies= -2368.635189
Sum of electronic and thermal Energies= -2368.576835
Sum of electronic and thermal Enthalpies= -2368.575890
Sum of electronic and thermal Free Energies= -2368.727549

==== Figure S1 (neutral mutarotation in glucose and (H2O)9 ====

1) beta-glucose
glu04exta.rev.chk
Stoichiometry C6H30O15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.977690	-0.819573	-0.457290
2	6	0	-3.765311	0.671428	-0.278996
3	6	0	-2.918127	-1.592993	0.311036
4	6	0	-2.389835	1.065528	-0.823610
5	6	0	-1.506203	-1.197804	-0.119651
6	8	0	-1.357200	0.232863	-0.263203
7	6	0	-1.989422	2.492421	-0.437875
8	1	0	-2.690238	3.193000	-0.900807
9	1	0	-0.993460	2.703102	-0.848745
10	8	0	-2.035080	2.705221	0.956953
11	1	0	-1.341640	2.163372	1.375480
12	1	0	-2.407381	0.968704	-1.918886
13	8	0	-4.811463	1.335386	-0.997522
14	1	0	-4.984273	2.177929	-0.567289
15	1	0	-3.812275	0.925059	0.784098
16	8	0	-5.240595	-1.241114	0.044807
17	1	0	-5.899031	-0.669474	-0.367791
18	1	0	-3.901125	-1.067178	-1.527562
19	8	0	-3.049844	-2.987203	0.096514
20	1	0	-3.979199	-3.193867	0.251640
21	1	0	-3.018226	-1.351542	1.378710
22	8	0	-0.613867	-1.571045	0.878949
23	1	0	-1.265500	-1.683147	-1.074018
24	1	0	0.280368	-1.750404	0.506702
25	8	0	1.977367	-1.566054	0.022447
26	1	0	2.543476	-1.567626	0.843405
27	1	0	0.401875	0.823405	-0.768390
28	8	0	1.357889	0.936906	-0.652179
29	1	0	1.817116	-0.601692	-0.164012
30	1	0	1.795525	1.041994	-1.525162
31	8	0	3.663281	-1.204953	2.069718
32	1	0	4.506066	-1.139594	1.594800
33	1	0	3.394350	-0.268467	2.216825
34	8	0	3.173049	0.976833	-2.679494
35	1	0	3.758517	1.414409	-2.035122

36	1	0	3.444658	0.045347	-2.639629
37	8	0	4.570077	1.742922	-0.353202
38	1	0	5.087234	0.937927	-0.148458
39	1	0	5.101309	2.490809	-0.064802
40	8	0	3.864531	-1.736240	-1.829179
41	1	0	3.095174	-1.814859	-1.196690
42	1	0	3.893801	-2.552038	-2.337901
43	8	0	2.766227	1.387578	1.998783
44	1	0	3.016495	1.606732	1.088165
45	1	0	1.793803	1.356907	1.987258
46	8	0	5.645185	-0.787484	-0.004343
47	1	0	6.563313	-1.051537	-0.113713
48	1	0	5.132250	-1.232241	-0.718850
49	1	0	-0.299506	0.103871	1.861702
50	8	0	-0.100915	0.959110	2.290094
51	1	0	-0.223099	0.815254	3.234208

SCF Done: E(RB+HF-LYP) = -1375.62235250 A.U. after 1 cycles
Convg = 0.2710D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.192767
Sum of electronic and thermal Energies= -1375.158584
Sum of electronic and thermal Enthalpies= -1375.157640
Sum of electronic and thermal Free Energies= -1375.257212

Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.654931 a.u.
Et + ZPE = -1375.225345 a.u.

2) TS for the (beta -> aldehyde) conversion via water dimer
glu04exta.chk
Stoichiometry C6H30O15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.743918	-0.899158	0.385580
2	6	0	3.546580	0.603426	0.259891
3	6	0	2.764686	-1.696928	-0.468326
4	6	0	2.186971	1.011168	0.829036
5	6	0	1.299784	-1.521248	-0.084220
6	8	0	1.174171	0.286590	0.132589
7	6	0	1.939986	2.522760	0.716977
8	1	0	2.610988	3.031983	1.414154
9	1	0	0.911365	2.739025	1.035902
10	8	0	2.210873	3.051920	-0.569545

11	1	0	1.513971	2.750726	-1.176012
12	1	0	2.170671	0.753836	1.901142
13	8	0	4.627191	1.219986	0.974753
14	1	0	4.780482	2.084583	0.581013
15	1	0	3.586915	0.889722	-0.795389
16	8	0	5.045789	-1.278676	-0.057697
17	1	0	5.656816	-0.661789	0.364276
18	1	0	3.617750	-1.188270	1.440678
19	8	0	3.030328	-3.088217	-0.325192
20	1	0	3.990448	-3.174397	-0.379738
21	1	0	2.868001	-1.389449	-1.517314
22	8	0	0.439313	-1.811359	-0.968943
23	1	0	1.092588	-1.765957	0.969269
24	1	0	-0.854628	-1.782508	-0.637997
25	8	0	-1.891410	-1.528175	-0.349560
26	1	0	-2.448585	-1.352465	-1.162605
27	1	0	-0.214198	0.507634	0.633810
28	8	0	-1.247858	0.552099	0.707365
29	1	0	-1.618096	-0.380786	0.186130
30	1	0	-1.650295	0.564866	1.621009
31	8	0	-3.565325	-0.745485	-2.244479
32	1	0	-4.399402	-0.754772	-1.750811
33	1	0	-3.292170	0.201416	-2.244780
34	8	0	-2.870107	0.453521	2.753570
35	1	0	-3.490985	1.023710	2.260445
36	1	0	-3.214644	-0.445323	2.614493
37	8	0	-4.353308	1.703966	0.739509
38	1	0	-4.895771	0.966579	0.391329
39	1	0	-4.893675	2.497015	0.673606
40	8	0	-3.714236	-2.030589	1.506754
41	1	0	-2.972119	-2.033376	0.843419
42	1	0	-3.779147	-2.924341	1.857112
43	8	0	-2.683221	1.803706	-1.769261
44	1	0	-2.914690	1.870830	-0.831444
45	1	0	-1.708822	1.817940	-1.801308
46	8	0	-5.495196	-0.681154	-0.069961
47	1	0	-6.419493	-0.942909	-0.023142
48	1	0	-4.996330	-1.279437	0.531621
49	1	0	0.548476	0.948648	-1.382956
50	8	0	0.185100	1.599428	-2.028415
51	1	0	0.386189	1.246657	-2.901410

SCF Done: E(RB+HF-LYP) = -1375.58739717 A.U. after 1 cycles

Convg = 0.2065D-08 -V/T = 2.0039

1	2	3
A	A	A

Frequencies -- -680.9818 25.7617 33.8406
Sum of electronic and zero-point Energies= -1375.165529
Sum of electronic and thermal Energies= -1375.132685
Sum of electronic and thermal Enthalpies= -1375.131741
Sum of electronic and thermal Free Energies= -1375.228151

Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.619872 a.u.
Et + ZPE = -1375.198004 a.u.

3) TS for the (beta -> aldehyde) conversion via water trimer
glu04ext.chk
Stoichiometry C6H30O15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.061319	0.835241	-0.866676
2	6	0	3.410377	-0.467707	-0.151516
3	6	0	2.386425	1.869110	0.033272
4	6	0	2.164754	-1.301877	0.148005
5	6	0	0.945150	1.564349	0.386862
6	8	0	1.222519	-0.492486	0.823260
7	6	0	2.478603	-2.509300	1.039864
8	1	0	3.278443	-3.118799	0.608517
9	1	0	1.579489	-3.136795	1.113693
10	8	0	2.910055	-2.080336	2.321611
11	1	0	2.276262	-1.392698	2.572177
12	1	0	1.773002	-1.664834	-0.817957
13	8	0	4.300913	-1.179707	-1.035069
14	1	0	4.922586	-1.677051	-0.496670
15	1	0	3.926369	-0.237288	0.785989
16	8	0	4.253464	1.468446	-1.331644
17	1	0	4.793826	0.758544	-1.702658
18	1	0	2.406098	0.616345	-1.724005
19	8	0	2.304896	3.117986	-0.650818
20	1	0	3.133631	3.195013	-1.142357
21	1	0	2.952546	1.975469	0.966806
22	8	0	0.481308	2.032468	1.441687
23	1	0	0.282287	1.288656	-0.440578
24	1	0	-0.806315	2.048453	1.622193
25	1	0	0.121686	-0.942068	0.617408
26	8	0	-0.978507	-1.329137	0.296879
27	1	0	-1.278742	-0.626956	-0.312232
28	1	0	-2.036096	-0.812674	1.590790

29	8	0	-2.731352	-0.329496	2.106148
30	1	0	-3.557532	-0.530403	1.635070
31	1	0	-2.269897	1.136495	2.002976
32	8	0	-1.905238	2.075842	1.836790
33	1	0	-2.438141	2.491048	1.105248
34	8	0	-1.617826	0.342578	-1.894612
35	1	0	-1.491268	-0.484040	-2.387171
36	1	0	-2.567666	0.542145	-1.931293
37	8	0	-1.040011	-2.434997	-2.220095
38	1	0	-0.309567	-2.904423	-2.633413
39	1	0	-0.753091	-2.209905	-1.304865
40	8	0	-4.791722	-1.134419	0.226305
41	1	0	-4.207448	-1.909631	-0.035497
42	1	0	-5.619219	-1.504515	0.548180
43	8	0	-3.055559	-3.014086	-0.279783
44	1	0	-2.745130	-3.148290	-1.187545
45	1	0	-2.274657	-2.578211	0.134199
46	8	0	-3.462450	3.054637	-0.059882
47	1	0	-3.852861	2.354914	-0.622125
48	1	0	-4.193288	3.595788	0.251989
49	8	0	-4.396374	0.889142	-1.487818
50	1	0	-5.025820	0.897002	-2.214747
51	1	0	-4.652181	0.148336	-0.884650

SCF Done: E(RB+HF-LYP) = -1375.57340144 A.U. after 1 cycles

Convg = 0.2667D-08 -V/T = 2.0039

1 2 3

A A A

Frequencies -- -579.9794 16.6738 21.0508

Sum of electronic and zero-point Energies= -1375.153291

Sum of electronic and thermal Energies= -1375.119638

Sum of electronic and thermal Enthalpies= -1375.118694

Sum of electronic and thermal Free Energies= -1375.218552

Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.605948 a.u.

Et + ZPE = -1375.185837 a.u.

4) aldehyde form-1

glu04exta.for.chk

Stoichiometry C6H30O15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.768959	0.879959	-0.375308

2	6	0	3.413191	-0.592382	-0.116631
3	6	0	2.945107	1.931685	0.388424
4	6	0	2.142110	-1.068189	-0.833499
5	6	0	1.520162	2.156818	-0.101378
6	8	0	1.054437	-0.509756	-0.086665
7	6	0	2.077790	-2.600826	-0.918714
8	1	0	2.731043	-2.935327	-1.726641
9	1	0	1.053856	-2.902727	-1.170595
10	8	0	2.538781	-3.246089	0.263864
11	1	0	1.866614	-3.122814	0.955734
12	1	0	2.119571	-0.674078	-1.858497
13	8	0	4.546650	-1.347492	-0.551948
14	1	0	4.456349	-2.220262	-0.144523
15	1	0	3.266701	-0.738175	0.959981
16	8	0	5.106759	1.119398	0.056656
17	1	0	5.604484	0.321656	-0.170943
18	1	0	3.692768	1.082231	-1.455097
19	8	0	3.545538	3.209199	0.189956
20	1	0	4.499898	3.053432	0.221851
21	1	0	2.909566	1.674790	1.454230
22	8	0	0.627331	2.497583	0.637909
23	1	0	1.372522	2.103269	-1.197342
24	1	0	-1.243606	2.452458	0.337952
25	8	0	-2.107665	2.029593	0.184887
26	1	0	-2.413705	1.626453	1.043962
27	1	0	0.223569	-0.505153	-0.623147
28	8	0	-1.387190	-0.312067	-1.053350
29	1	0	-1.629436	0.564312	-0.677456
30	1	0	-2.082219	-0.492097	-1.742992
31	8	0	-3.152216	0.660020	2.212611
32	1	0	-4.090239	0.646140	1.955153
33	1	0	-2.840246	-0.246921	2.016369
34	8	0	-3.610864	-0.601920	-2.476800
35	1	0	-4.084973	-1.188773	-1.845539
36	1	0	-3.986199	0.276701	-2.308917
37	8	0	-4.747550	-1.958153	-0.339492
38	1	0	-5.183282	-1.222895	0.122937
39	1	0	-4.001359	-2.193170	0.236894
40	8	0	-4.365086	1.966177	-1.256534
41	1	0	-3.510305	2.177905	-0.809368
42	1	0	-4.669451	2.777946	-1.672938
43	8	0	-2.298819	-1.767131	1.124276
44	1	0	-1.960407	-1.326776	0.313805
45	1	0	-1.520996	-2.211193	1.500998
46	8	0	-5.588335	0.550104	0.762581
47	1	0	-6.489541	0.804364	0.981317

48	1	0	-5.301408	1.121969	0.017850
49	1	0	0.636298	-1.449837	1.371138
50	8	0	0.434722	-2.231078	1.933636
51	1	0	0.598274	-1.962926	2.843753

SCF Done: E(RB+HF-LYP) = -1375.62440292 A.U. after 1 cycles
Convg = 0.4331D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.195007
Sum of electronic and thermal Energies= -1375.161067
Sum of electronic and thermal Enthalpies= -1375.160122
Sum of electronic and thermal Free Energies= -1375.259466
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.651455 a.u.
Et + ZPE = -1375.222059 a.u.

5) aldehyde from-2
(an intermediate during rotation of the aldehyde group)
glu0rot.chk
Stoichiometry C6H30O15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.616527	0.986976	0.265833
2	6	0	-3.275014	-0.500913	-0.007779
3	6	0	-2.847704	2.074074	-0.534997
4	6	0	-2.078289	-1.057737	0.807157
5	6	0	-1.349892	2.091453	-0.352273
6	8	0	-0.908139	-0.906033	-0.005989
7	6	0	-2.274564	-2.529182	1.192220
8	1	0	-3.054677	-2.608932	1.950265
9	1	0	-1.341358	-2.909835	1.622747
10	8	0	-2.698144	-3.326947	0.086724
11	1	0	-1.944932	-3.442789	-0.516408
12	1	0	-1.948681	-0.481437	1.732771
13	8	0	-4.472022	-1.213508	0.310348
14	1	0	-4.335381	-2.123452	0.004459
15	1	0	-3.041115	-0.632194	-1.072175
16	8	0	-4.968733	1.239624	-0.101674
17	1	0	-5.452073	0.420285	0.077917
18	1	0	-3.483628	1.195323	1.337375
19	8	0	-3.377882	3.335537	-0.225955
20	1	0	-4.337460	3.227301	-0.251141
21	1	0	-2.999681	1.820525	-1.601883
22	8	0	-0.719378	3.036449	0.070151

23	1	0	-0.846391	1.166528	-0.671648
24	1	0	1.086753	2.568733	0.097690
25	8	0	1.891228	2.012981	0.123592
26	1	0	2.108741	1.705426	-0.796995
27	1	0	-0.101790	-0.869480	0.564445
28	8	0	1.430809	-0.503076	1.123533
29	1	0	1.543300	0.435262	0.855030
30	1	0	2.196763	-0.693847	1.731052
31	8	0	2.751571	0.845439	-2.120447
32	1	0	3.711912	0.870463	-1.962363
33	1	0	2.520466	-0.098072	-2.013991
34	8	0	3.785408	-0.760930	2.324100
35	1	0	4.255588	-1.253038	1.613714
36	1	0	4.094055	0.152593	2.216984
37	8	0	4.864329	-1.831732	0.003986
38	1	0	5.198237	-1.026747	-0.425385
39	1	0	4.078200	-2.066993	-0.517943
40	8	0	4.304013	1.939352	1.296152
41	1	0	3.395412	2.136497	0.961050
42	1	0	4.601142	2.720366	1.772431
43	8	0	2.276009	-1.770393	-1.200892
44	1	0	1.978627	-1.390968	-0.345037
45	1	0	1.584986	-2.406491	-1.448830
46	8	0	5.349317	0.817275	-0.982176
47	1	0	6.181401	1.178142	-1.301833
48	1	0	5.127295	1.297265	-0.154451
49	1	0	-0.593106	-2.090828	-1.259780
50	8	0	-0.372452	-2.952643	-1.678067
51	1	0	-0.618133	-2.878804	-2.606114

SCF Done: E(RB+HF-LYP) = -1375.62075360 A.U. after 1 cycles
Convg = 0.1727D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.191233
Sum of electronic and thermal Energies= -1375.157358
Sum of electronic and thermal Enthalpies= -1375.156413
Sum of electronic and thermal Free Energies= -1375.256234
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.649612 a.u.
Et + ZPE = -1375.220092 a.u.

6) Aldehyde-3
glu03ext.for1.chk
Stoichiometry C6H30O15

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.513681	-1.041134	-0.276239
2	6	0	-3.351889	0.486110	-0.209485
3	6	0	-2.638329	-1.825771	0.719327
4	6	0	-2.069746	1.021972	-0.855235
5	6	0	-1.170849	-1.979619	0.312695
6	8	0	-0.999640	0.661727	0.033950
7	6	0	-2.127913	2.537694	-1.076980
8	1	0	-2.789225	2.747266	-1.919733
9	1	0	-1.126375	2.897389	-1.342239
10	8	0	-2.659862	3.239894	0.041664
11	1	0	-1.992312	3.240834	0.746282
12	1	0	-1.907958	0.536991	-1.826159
13	8	0	-4.503431	1.032121	-0.862227
14	1	0	-4.602063	1.935462	-0.536519
15	1	0	-3.353999	0.791839	0.843134
16	8	0	-4.848651	-1.374620	0.100634
17	1	0	-5.412694	-0.694893	-0.292869
18	1	0	-3.309844	-1.398605	-1.293834
19	8	0	-3.113390	-3.157718	0.840542
20	1	0	-4.078114	-3.088071	0.827738
21	1	0	-2.679778	-1.316321	1.693360
22	8	0	-0.822854	-2.387947	-0.772027
23	1	0	-0.430235	-1.776376	1.106301
24	1	0	1.073955	-2.359699	-0.844726
25	8	0	1.956200	-1.967879	-0.699851
26	1	0	2.100594	-1.872117	0.279059
27	1	0	-0.145552	0.755637	-0.453367
28	8	0	1.436940	0.710262	-1.027252
29	1	0	1.624510	-0.253717	-1.015270
30	1	0	2.201939	1.106606	-1.525264
31	8	0	2.580766	-1.349530	1.829459
32	1	0	3.550773	-1.338543	1.746775
33	1	0	2.343944	-0.407749	1.944947
34	8	0	3.823509	1.376254	-1.989946
35	1	0	4.236685	1.670943	-1.147253
36	1	0	4.165049	0.476810	-2.112743
37	8	0	4.735820	1.813435	0.594494
38	1	0	5.057496	0.927094	0.828453
39	1	0	3.912829	1.904591	1.104660
40	8	0	4.412487	-1.497503	-1.674675
41	1	0	3.500156	-1.815624	-1.477266
42	1	0	4.790675	-2.113503	-2.309256
43	8	0	2.088235	1.404070	1.571341
44	1	0	1.865795	1.235023	0.629388

45	1	0	1.357968	1.953662	1.902216
46	8	0	5.239863	-0.997377	0.905136
47	1	0	6.075491	-1.392416	1.170791
48	1	0	5.094423	-1.241527	-0.034776
49	1	0	-0.796641	1.674628	1.464467
50	8	0	-0.592150	2.461064	2.017556
51	1	0	-0.963779	2.288862	2.888814

SCF Done: E(RB+HF-LYP) = -1375.62145998 A.U. after 1 cycles
Convg = 0.4715D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.191976
Sum of electronic and thermal Energies= -1375.157855
Sum of electronic and thermal Enthalpies= -1375.156910
Sum of electronic and thermal Free Energies= -1375.256861
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.648972 a.u.
Et + ZPE = -1375.219488 a.u.

7)TS for conversion form the aldehyde form to the alpha form
glu03ts1.chk
Stoichiometry C6H30O15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.502165	-0.977752	-0.345747
2	6	0	-3.410161	0.542883	-0.393218
3	6	0	-2.589829	-1.581739	0.720419
4	6	0	-2.012491	1.016754	-0.802307
5	6	0	-1.114057	-1.501105	0.346411
6	8	0	-1.061158	0.477892	0.109893
7	6	0	-1.907179	2.548212	-0.832999
8	1	0	-2.568418	2.933084	-1.614090
9	1	0	-0.881814	2.829852	-1.107535
10	8	0	-2.306775	3.165491	0.382062
11	1	0	-1.632366	2.981224	1.053256
12	1	0	-1.810430	0.649865	-1.821360
13	8	0	-4.411668	0.971983	-1.328926
14	1	0	-4.692385	1.856655	-1.076076
15	1	0	-3.638004	0.942197	0.600715
16	8	0	-4.825499	-1.375661	0.013368
17	1	0	-5.415804	-0.876904	-0.564913
18	1	0	-3.235557	-1.397666	-1.324256
19	8	0	-2.875862	-2.958080	0.910870
20	1	0	-3.837435	-3.031868	0.850828

21	1	0	-2.738631	-1.029770	1.659294
22	8	0	-0.696316	-2.057899	-0.694678
23	1	0	-0.427941	-1.362614	1.191875
24	1	0	0.646666	-2.051055	-0.721555
25	8	0	1.719858	-1.777083	-0.688530
26	1	0	2.124241	-1.959563	0.213322
27	1	0	0.264679	0.662255	-0.366533
28	8	0	1.313785	0.583673	-0.523131
29	1	0	1.575974	-0.617265	-0.661801
30	1	0	1.812167	1.161465	-1.167887
31	8	0	2.957482	-1.744605	1.638699
32	1	0	3.878154	-1.589576	1.362334
33	1	0	2.678783	-0.892790	2.032303
34	8	0	3.205180	1.701237	-1.911471
35	1	0	3.738989	1.898887	-1.107735
36	1	0	3.588973	0.878774	-2.251402
37	8	0	4.525695	1.803198	0.524262
38	1	0	4.951363	0.930512	0.559584
39	1	0	3.873655	1.778081	1.244318
40	8	0	3.994364	-1.184939	-2.147139
41	1	0	3.157693	-1.582301	-1.826616
42	1	0	4.248850	-1.675704	-2.934852
43	8	0	2.230524	0.940739	2.051993
44	1	0	1.952648	0.900005	1.115281
45	1	0	1.452383	1.340899	2.479621
46	8	0	5.310763	-0.945737	0.276068
47	1	0	6.211200	-1.279966	0.328623
48	1	0	5.007328	-1.082718	-0.645835
49	1	0	-0.785685	1.242537	1.608575
50	8	0	-0.482269	1.836463	2.342952
51	1	0	-1.068835	1.666592	3.086807

SCF Done: E(RB+HF-LYP) = -1375.58678865 A.U. after 2 cycles
Convg = 0.6890D-08 -V/T = 2.0039
1 2 3
A A A
Frequencies -- -894.1453 25.9534 32.9608
Sum of electronic and zero-point Energies= -1375.165023
Sum of electronic and thermal Energies= -1375.132406
Sum of electronic and thermal Enthalpies= -1375.131461
Sum of electronic and thermal Free Energies= -1375.227126
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.616754 a.u.
Et + ZPE = -1375.194988 a.u.

6) alpha form of glucose
glu03ext.rev.chk

Stoichiometry C6H30O15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.226686	0.303480	-0.783528
2	6	0	2.941819	-1.172667	-0.562964
3	6	0	2.412571	1.125282	0.202695
4	6	0	1.438687	-1.448685	-0.697232
5	6	0	0.918864	0.838251	0.023798
6	8	0	0.710828	-0.575146	0.202921
7	6	0	1.072868	-2.884598	-0.323686
8	1	0	1.498208	-3.545187	-1.084857
9	1	0	-0.018762	-2.999888	-0.378042
10	8	0	1.589688	-3.290086	0.923813
11	1	0	1.062460	-2.878230	1.636007
12	1	0	1.124097	-1.248199	-1.728019
13	8	0	3.697860	-1.898012	-1.537114
14	1	0	3.897653	-2.765190	-1.171288
15	1	0	3.256985	-1.452502	0.446666
16	8	0	4.595459	0.624453	-0.545985
17	1	0	5.115699	0.053396	-1.122981
18	1	0	2.944760	0.583210	-1.806409
19	8	0	2.681170	2.515014	0.056400
20	1	0	3.637664	2.594529	-0.052132
21	1	0	2.678809	0.805899	1.218530
22	8	0	0.472267	1.280767	-1.221014
23	1	0	0.345402	1.290671	0.835188
24	1	0	-2.239882	2.119149	-0.020590
25	1	0	-1.029252	-1.017529	0.578956
26	8	0	-1.934228	-0.968937	0.946971
27	1	0	-2.545155	-1.479061	0.348670
28	1	0	-2.265154	0.570612	-0.058958
29	8	0	-2.257169	1.347936	-0.652787
30	1	0	-0.509904	1.285077	-1.186711
31	8	0	-1.819148	3.163137	1.241877
32	1	0	-1.015664	3.622353	0.917523
33	1	0	-1.528960	2.569785	1.954527
34	8	0	-3.582107	-2.083987	-0.828561
35	1	0	-4.505465	-1.932266	-0.541657
36	1	0	-3.531992	-1.498752	-1.601140
37	8	0	-6.043942	-0.868358	-0.552402
38	1	0	-5.618922	-0.258701	-1.184191
39	1	0	-6.820131	-1.208388	-1.007357

40	8	0	-4.185944	0.344165	-2.253036
41	1	0	-3.545999	0.886196	-1.734256
42	1	0	-4.223547	0.733274	-3.131294
43	8	0	-1.207933	0.839780	2.902754
44	1	0	-1.714187	0.228492	2.333793
45	1	0	-1.646613	0.825046	3.759595
46	8	0	0.408092	4.116525	-0.107106
47	1	0	1.287423	3.848939	0.204686
48	1	0	0.327151	3.565180	-0.896814
49	1	0	0.095112	-1.173928	3.009658
50	8	0	-0.079095	-2.118493	2.902415
51	1	0	-0.947213	-2.120435	2.475240

SCF Done: E(RB+HF-LYP) = -1375.61906035 A.U. after 1 cycles
Convg = 0.7687D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.190134
Sum of electronic and thermal Energies= -1375.154907
Sum of electronic and thermal Enthalpies= -1375.153963
Sum of electronic and thermal Free Energies= -1375.256991
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1375.647090 a.u.
Et + ZPE = -1375.218164 a.u.

==== Figure S2 (muratotation in glucose and H3O+(H2O)8 ====

1) beta-glucose
gluh4ext.rev1.chk
Stoichiometry C6H31O15(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.070667	-0.826431	0.827478
2	6	0	-3.466324	0.520813	0.230706
3	6	0	-1.558998	-0.945769	0.942236
4	6	0	-2.736380	0.725567	-1.107732
5	6	0	-0.905511	-0.715993	-0.419177
6	8	0	-1.313235	0.582730	-0.894086
7	6	0	-2.979343	2.093007	-1.736231
8	1	0	-4.041383	2.173779	-1.978614
9	1	0	-2.418320	2.158943	-2.673933
10	8	0	-2.662502	3.165077	-0.856531
11	1	0	-1.726357	3.372806	-0.952728
12	1	0	-3.068270	-0.044677	-1.816978
13	8	0	-4.879939	0.485684	0.060447
14	1	0	-5.228849	1.378923	0.139990
15	1	0	-3.177419	1.322505	0.918250
16	8	0	-3.587399	-1.021472	2.135374
17	1	0	-4.548715	-0.962619	2.077938
18	1	0	-3.437391	-1.617739	0.156296
19	8	0	-1.180003	-2.235811	1.431227
20	1	0	-1.794263	-2.437670	2.151281
21	1	0	-1.191885	-0.173897	1.633087
22	8	0	0.473003	-0.700679	-0.315113
23	1	0	-1.237250	-1.474640	-1.137680
24	1	0	0.871530	-1.307917	-1.032372
25	1	0	-0.286894	1.840405	-0.323716
26	8	0	0.190921	2.647853	-0.012054
27	1	0	-0.195351	2.873481	0.841302
28	1	0	1.746929	2.572565	-0.087419
29	8	0	2.760204	2.556525	-0.125950
30	1	0	3.130843	3.396029	0.259361
31	1	0	3.199965	1.677032	0.318356
32	8	0	3.836991	0.608253	0.888489
33	1	0	4.432778	0.121839	0.285984
34	1	0	3.255730	-0.062547	1.317761
35	8	0	3.642642	4.824589	0.874038

36	1	0	3.939777	5.540431	0.302357
37	1	0	4.115022	4.924606	1.707075
38	8	0	1.414122	-2.473953	-1.894198
39	1	0	2.223624	-2.782413	-1.430155
40	1	0	0.745263	-3.166430	-1.735141
41	8	0	3.514673	-3.042151	-0.231203
42	1	0	4.314487	-2.523574	-0.395470
43	1	0	3.137687	-2.663797	0.579604
44	8	0	-0.751846	-3.888199	-0.892229
45	1	0	-0.889676	-3.578294	0.017947
46	1	0	-1.129831	-4.770293	-0.951119
47	8	0	5.454530	-0.926091	-0.813547
48	1	0	6.398643	-1.013906	-0.636455
49	1	0	5.373197	-0.807823	-1.767677
50	8	0	2.161055	-1.358170	1.670223
51	1	0	1.389198	-1.195064	1.077979
52	1	0	1.814784	-1.670704	2.512125

SCF Done: E(RB+HF-LYP) = -1376.00504337 A.U. after 1 cycles
Convg = 0.2126D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.568489
Sum of electronic and thermal Energies= -1375.532198
Sum of electronic and thermal Enthalpies= -1375.531254
Sum of electronic and thermal Free Energies= -1375.639565
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1376.086045 a.u.
Et + ZPE = -1375.649491 a.u.

2) TS for conversion from beta form to aldehyde form
gluh4extb.chk
Stoichiometry C6H31O15(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.276910	-0.886150	0.402945
2	6	0	-3.400999	0.598210	0.078863
3	6	0	-1.836522	-1.278205	0.709980
4	6	0	-2.529891	0.950301	-1.133026
5	6	0	-0.884619	-1.021091	-0.459342
6	8	0	-1.146840	0.531406	-0.852755
7	6	0	-2.556595	2.433698	-1.505138
8	1	0	-3.514562	2.627761	-1.991914
9	1	0	-1.767039	2.630022	-2.240348
10	8	0	-2.481251	3.293149	-0.386103

11	1	0	-1.571871	3.272114	-0.050209
12	1	0	-2.838853	0.361275	-2.000968
13	8	0	-4.772176	0.844232	-0.198861
14	1	0	-4.971595	1.761463	0.018789
15	1	0	-3.071420	1.187365	0.940648
16	8	0	-4.022785	-1.242642	1.555556
17	1	0	-4.939871	-0.985011	1.399473
18	1	0	-3.628151	-1.463343	-0.465889
19	8	0	-1.762882	-2.676693	0.991449
20	1	0	-2.517565	-2.880102	1.562266
21	1	0	-1.483926	-0.707943	1.579986
22	8	0	0.384519	-1.153664	-0.204439
23	1	0	-1.239051	-1.503733	-1.381497
24	1	0	1.052892	-1.958445	-1.027989
25	1	0	-0.615441	1.198482	-0.209945
26	8	0	0.002409	2.234013	0.520315
27	1	0	0.008023	2.166500	1.480745
28	1	0	0.987482	2.479486	0.210160
29	8	0	2.300663	2.767495	-0.216867
30	1	0	2.608375	3.659987	0.038953
31	1	0	2.958932	2.116844	0.130879
32	8	0	3.959709	0.979975	0.894267
33	1	0	4.608229	0.509744	0.348909
34	1	0	3.433342	0.285486	1.327599
35	8	0	3.028692	5.302671	0.582626
36	1	0	3.161345	6.007287	-0.059798
37	1	0	3.682045	5.454603	1.273025
38	8	0	1.584157	-2.780378	-1.538957
39	1	0	2.510119	-2.810507	-1.110971
40	1	0	1.065154	-3.579904	-1.242782
41	8	0	3.753138	-2.669583	-0.196013
42	1	0	4.479913	-2.089842	-0.480905
43	1	0	3.396469	-2.263140	0.616838
44	8	0	-0.073267	-4.471327	-0.434538
45	1	0	-0.672370	-3.955743	0.135223
46	1	0	-0.579760	-5.206864	-0.790444
47	8	0	5.722847	-0.686005	-0.739214
48	1	0	6.603288	-0.857733	-0.384215
49	1	0	5.860300	-0.393073	-1.647862
50	8	0	2.315828	-1.174361	1.690533
51	1	0	1.487302	-1.114482	1.161594
52	1	0	2.079390	-1.515439	2.558966

SCF Done: E(RB+HF-LYP) = -1375.98312371 A.U. after 1 cycles

Convg = 0.2072D-08 -V/T = 2.0039

1 2 3

A A A

Frequencies -- -103.3703 13.1349 17.8549

Sum of electronic and zero-point Energies= -1375.550334

Sum of electronic and thermal Energies= -1375.514979

Sum of electronic and thermal Enthalpies= -1375.514034

Sum of electronic and thermal Free Energies= -1375.620216

Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1376.061556 a.u.

Et + ZPE = -1375.628767 a.u.

3) Aldehyde form-1

gluh4extb.rev.chk

Stoichiometry C6H31O15(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.131364	-1.190070	-0.229005
2	6	0	3.408183	0.308010	-0.095392
3	6	0	1.665987	-1.527419	-0.499514
4	6	0	2.747672	0.897361	1.156078
5	6	0	0.737184	-1.370558	0.692242
6	8	0	1.331838	0.622134	1.100945
7	6	0	3.033249	2.392584	1.330723
8	1	0	4.068780	2.506760	1.659310
9	1	0	2.387200	2.778236	2.128739
10	8	0	2.900267	3.129099	0.128702
11	1	0	1.954880	3.174359	-0.092854
12	1	0	3.118738	0.372544	2.042164
13	8	0	4.827927	0.427981	-0.043275
14	1	0	5.067995	1.307788	-0.354573
15	1	0	3.020826	0.823565	-0.980802
16	8	0	3.828431	-1.730755	-1.344131
17	1	0	4.739138	-1.411704	-1.285125
18	1	0	3.458027	-1.696417	0.692178
19	8	0	1.560573	-2.924585	-0.830054
20	1	0	2.365465	-3.138168	-1.329199
21	1	0	1.290208	-0.923199	-1.333306
22	8	0	-0.487676	-1.338789	0.524992
23	1	0	1.148254	-1.639422	1.672574
24	1	0	-1.575251	-2.385570	1.335241
25	1	0	0.889218	1.231124	0.452967
26	8	0	0.239328	2.440474	-0.523234
27	1	0	0.191403	2.436631	-1.484032
28	1	0	-0.649527	2.811030	-0.193721

29	8	0	-2.044183	3.282897	0.280221
30	1	0	-2.291892	4.161040	-0.064284
31	1	0	-2.747863	2.659062	0.006241
32	8	0	-3.826651	1.425006	-0.680818
33	1	0	-4.464939	0.958838	-0.123130
34	1	0	-3.311264	0.725848	-1.112871
35	8	0	-2.553428	5.826856	-0.743666
36	1	0	-2.403652	6.570509	-0.150769
37	1	0	-3.336698	6.059592	-1.252353
38	8	0	-2.153267	-3.193159	1.320893
39	1	0	-3.035767	-2.908365	0.773043
40	1	0	-1.603830	-3.856287	0.772323
41	8	0	-4.037978	-2.418700	-0.051233
42	1	0	-4.690281	-1.804732	0.338953
43	1	0	-3.569143	-1.913309	-0.749644
44	8	0	-0.611697	-4.576114	-0.172835
45	1	0	0.161475	-4.061473	-0.481101
46	1	0	-0.313076	-5.475378	-0.005953
47	8	0	-5.696129	-0.341377	0.816050
48	1	0	-6.576110	-0.297948	0.422143
49	1	0	-5.818859	-0.139572	1.751545
50	8	0	-2.310879	-0.875550	-1.513904
51	1	0	-1.529613	-0.948147	-0.925642
52	1	0	-2.017472	-1.080031	-2.408092

SCF Done: E(RB+HF-LYP) = -1375.98508579 A.U. after 1 cycles
Convg = 0.4596D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.549943
Sum of electronic and thermal Energies= -1375.513012
Sum of electronic and thermal Enthalpies= -1375.512068
Sum of electronic and thermal Free Energies= -1375.622927
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1376.066236 a.u.
Et + ZPE = -1375.631093 a.u.

4) aldehyde form-2
gluhrot.chk
Stoichiometry C6H31O15(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.195710	1.986425	0.044616
2	6	0	-0.865697	2.743072	0.148641
3	6	0	-2.041168	0.446079	0.000863

4	6	0	0.110835	2.570873	-1.036573
5	6	0	-1.917780	-0.086485	-1.417953
6	8	0	0.713088	1.264144	-0.956868
7	6	0	1.167661	3.684557	-1.037151
8	1	0	0.732939	4.592603	-1.456384
9	1	0	1.999749	3.379319	-1.681665
10	8	0	1.606444	4.025960	0.274407
11	1	0	2.129208	3.294813	0.637727
12	1	0	-0.421945	2.608831	-1.991829
13	8	0	-1.246767	4.102426	0.330095
14	1	0	-0.469370	4.559175	0.683040
15	1	0	-0.358426	2.377993	1.050648
16	8	0	-2.957306	2.246615	1.216683
17	1	0	-2.908974	3.200035	1.374187
18	1	0	-2.745480	2.343104	-0.838323
19	8	0	-3.147864	-0.196301	0.627489
20	1	0	-3.495798	0.448190	1.267548
21	1	0	-1.112872	0.176304	0.524608
22	8	0	-2.368440	-1.154716	-1.753518
23	1	0	-1.369084	0.545201	-2.135609
24	1	0	-2.370057	-3.167156	-2.095299
25	1	0	1.367208	1.293970	-0.222368
26	8	0	2.551411	1.361420	1.062102
27	1	0	2.113778	0.816521	1.737360
28	1	0	3.256041	0.777033	0.725224
29	8	0	3.811120	-0.992917	0.177379
30	1	0	4.749631	-1.234698	0.006659
31	1	0	3.558076	-1.418996	1.007481
32	8	0	1.305575	-1.044268	1.777081
33	1	0	1.177839	-1.151871	0.820674
34	1	0	0.726787	-1.714251	2.168887
35	8	0	6.402130	-1.702874	-0.163713
36	1	0	7.132336	-1.114710	0.054590
37	1	0	6.731027	-2.290670	-0.851320
38	8	0	-2.138022	-3.855775	-1.454003
39	1	0	-0.800511	-3.768054	-1.131242
40	1	0	-2.625840	-3.589582	-0.643284
41	8	0	0.199406	-3.676736	-0.718930
42	1	0	0.665591	-2.828380	-0.994698
43	1	0	0.088442	-3.657790	0.274313
44	8	0	-2.995335	-2.864890	0.996663
45	1	0	-3.122889	-1.891125	0.855422
46	1	0	-3.798504	-3.188835	1.420287
47	8	0	1.442221	-1.419675	-1.088363
48	1	0	2.401949	-1.337060	-0.885699
49	1	0	1.142762	-0.549989	-1.412527

50	8	0	-0.447426	-3.378497	1.835617
51	1	0	-1.412823	-3.203083	1.735721
52	1	0	-0.351525	-4.085293	2.484251

SCF Done: E(RB+HF-LYP) = -1376.00152172 A.U. after 1 cycles
Convg = 0.2939D-08 -V/T = 2.0040
Sum of electronic and zero-point Energies= -1375.563781
Sum of electronic and thermal Energies= -1375.528209
Sum of electronic and thermal Enthalpies= -1375.527265
Sum of electronic and thermal Free Energies= -1375.632164
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1376.076229 a.u.
Et + ZPE = -1375.638488 a.u.

5) Aldehyde form-3
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Stoichiometry C6H31O15(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.847432	-1.723026	0.568137
2	6	0	3.122227	-0.952398	0.206028
3	6	0	0.975893	-2.118509	-0.634377
4	6	0	2.839424	0.487843	-0.226823
5	6	0	0.202130	-0.986292	-1.302576
6	8	0	2.108720	0.385941	-1.460037
7	6	0	4.117496	1.299967	-0.431229
8	1	0	4.603888	1.465778	0.531769
9	1	0	3.850932	2.281776	-0.844559
10	8	0	5.058135	0.622830	-1.249903
11	1	0	4.662067	0.517566	-2.122396
12	1	0	2.228534	0.983587	0.539898
13	8	0	3.929197	-0.981901	1.384427
14	1	0	4.853933	-0.940880	1.116867
15	1	0	3.633498	-1.467617	-0.613213
16	8	0	2.191217	-2.975527	1.150249
17	1	0	2.926842	-2.803275	1.754569
18	1	0	1.249099	-1.137176	1.278742
19	8	0	-0.024644	-3.051057	-0.186450
20	1	0	0.465915	-3.677843	0.369920
21	1	0	1.606680	-2.606081	-1.384618
22	8	0	-0.633100	-0.334062	-0.689942
23	1	0	0.287019	-0.899690	-2.391314
24	1	0	-1.936393	0.712490	-1.235129

25	1	0	1.596087	1.218619	-1.581369
26	8	0	0.519565	2.576207	-1.623689
27	1	0	0.327205	3.111084	-0.826187
28	1	0	0.564265	3.196367	-2.358166
29	1	0	-0.805576	-0.076459	1.143228
30	8	0	-1.051333	-0.003462	2.081166
31	1	0	-1.638935	-0.766892	2.199168
32	8	0	-0.269988	4.034975	0.592232
33	1	0	-0.529256	3.552542	1.407043
34	1	0	0.155502	4.851746	0.872420
35	8	0	-1.582893	2.563141	2.501502
36	1	0	-1.403279	1.586824	2.470454
37	1	0	-1.733986	2.797582	3.422759
38	8	0	-2.862719	1.050007	-1.239118
39	1	0	-3.472703	0.278384	-0.779863
40	1	0	-2.903445	1.926006	-0.693476
41	8	0	-4.160665	-0.702598	-0.139206
42	1	0	-4.880283	-1.170899	-0.616356
43	1	0	-3.599900	-1.363448	0.319557
44	8	0	-2.935058	3.149230	0.170461
45	1	0	-2.760655	2.929622	1.107593
46	1	0	-2.224024	3.777672	-0.032486
47	8	0	-6.169536	-2.045860	-1.359001
48	1	0	-7.071735	-1.906110	-1.052905
49	1	0	-6.234809	-2.213990	-2.304557
50	8	0	-2.385930	-2.344814	1.184503
51	1	0	-1.599769	-2.606054	0.658426
52	1	0	-2.692057	-3.141144	1.631680

SCF Done: E(RB+HF-LYP) = -1376.00240238 A.U. after 1 cycles
Convg = 0.1575D-08 -V/T = 2.0039
Sum of electronic and zero-point Energies= -1375.566233
Sum of electronic and thermal Energies= -1375.529888
Sum of electronic and thermal Enthalpies= -1375.528944
Sum of electronic and thermal Free Energies= -1375.636536
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1376.075303 a.u.
Et + ZPE = -1375.639133 a.u.

6) TS for conversion from the aldehyde form to the alpha one
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Stoichiometry C6H31O15(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.995788	-1.787970	-0.845384
2	6	0	-2.885805	-1.064598	0.160101
3	6	0	-0.664533	-2.183736	-0.216485
4	6	0	-2.200277	0.206072	0.673439
5	6	0	0.150962	-0.978184	0.246090
6	8	0	-0.946742	-0.241389	1.307380
7	6	0	-3.032691	0.970398	1.697285
8	1	0	-3.887130	1.394036	1.165996
9	1	0	-2.452944	1.808861	2.097684
10	8	0	-3.557969	0.140428	2.718120
11	1	0	-2.845646	-0.098713	3.320128
12	1	0	-1.950566	0.869372	-0.159701
13	8	0	-4.093295	-0.741459	-0.519181
14	1	0	-4.819479	-0.769519	0.112575
15	1	0	-3.084136	-1.724025	1.010051
16	8	0	-2.578727	-3.006349	-1.281085
17	1	0	-3.446455	-2.796450	-1.647195
18	1	0	-1.819356	-1.121872	-1.699543
19	8	0	0.143076	-2.884064	-1.160309
20	1	0	-0.426633	-3.560245	-1.552950
21	1	0	-0.865546	-2.822704	0.651579
22	8	0	0.543364	-0.130801	-0.650350
23	1	0	0.888565	-1.239989	1.015032
24	1	0	1.605364	0.524422	-0.254756
25	1	0	-0.399084	0.589936	1.659813
26	8	0	0.416326	1.717294	2.055642
27	1	0	0.057208	2.533348	1.624763
28	1	0	1.326943	1.618903	1.733931
29	1	0	-0.240553	0.616931	-2.027557
30	8	0	-0.704286	1.245357	-2.622274
31	1	0	-0.651856	0.881461	-3.511405
32	8	0	-0.759664	3.677896	0.701464
33	1	0	-0.499205	3.794256	-0.235638
34	1	0	-0.997640	4.545705	1.040961
35	8	0	0.107672	3.694341	-1.933951
36	1	0	-0.226584	2.825565	-2.282491
37	1	0	-0.185309	4.369923	-2.555132
38	8	0	2.505268	1.033802	0.165654
39	1	0	3.292605	0.301792	0.153197
40	1	0	2.713351	1.833921	-0.402993
41	8	0	4.172363	-0.758911	0.085058
42	1	0	4.627315	-1.047552	0.903748
43	1	0	3.791111	-1.554291	-0.355389
44	8	0	2.755234	3.115951	-1.380454
45	1	0	1.877427	3.458069	-1.646872

46	1	0	3.329898	3.872671	-1.234132
47	8	0	5.493042	-1.477690	2.370178
48	1	0	6.438203	-1.293728	2.388141
49	1	0	5.390622	-2.340950	2.784115
50	8	0	2.988318	-2.913365	-1.032523
51	1	0	2.018268	-2.954646	-1.112208
52	1	0	3.338174	-3.254705	-1.860997

SCF Done: E(RB+HF-LYP) = -1375.98867260 A.U. after 1 cycles
Convg = 0.3134D-08 -V/T = 2.0039

1	2	3
A	A	A

Frequencies -- -274.5659 10.4164 14.9129
Sum of electronic and zero-point Energies= -1375.556753
Sum of electronic and thermal Energies= -1375.520875
Sum of electronic and thermal Enthalpies= -1375.519931
Sum of electronic and thermal Free Energies= -1375.627737
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1376.063234 a.u.
Et + ZPE = -1375.631315 a.u.

7) alpha form of glucose
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Stoichiometry C6H31O15(1+)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.439014	-1.647091	-0.756086
2	6	0	-3.088816	-0.705734	0.248961
3	6	0	-1.115918	-2.154098	-0.203545
4	6	0	-2.132749	0.447436	0.586224
5	6	0	-0.183655	-0.996110	0.148454
6	8	0	-0.859521	-0.104282	1.058530
7	6	0	-2.658478	1.355367	1.689471
8	1	0	-3.563217	1.843578	1.322996
9	1	0	-1.926024	2.147355	1.893153
10	8	0	-3.023573	0.650711	2.862968
11	1	0	-2.229210	0.254153	3.236269
12	1	0	-1.954266	1.047123	-0.311727
13	8	0	-4.280327	-0.207753	-0.354966
14	1	0	-4.946681	-0.081889	0.327894
15	1	0	-3.319262	-1.258844	1.164126
16	8	0	-3.227151	-2.799272	-1.005520
17	1	0	-4.083752	-2.500939	-1.333431

18	1	0	-2.257337	-1.099966	-1.691461
19	8	0	-0.466234	-3.012012	-1.132731
20	1	0	-1.124120	-3.659916	-1.418352
21	1	0	-1.320724	-2.699089	0.726471
22	8	0	0.251177	-0.327828	-1.006938
23	1	0	0.679724	-1.360866	0.709439
24	1	0	1.146788	0.027178	-0.818239
25	1	0	0.295262	1.005873	1.651187
26	8	0	1.090109	1.591420	1.784297
27	1	0	0.816186	2.543064	1.556177
28	1	0	1.834227	1.244179	1.059576
29	1	0	-0.456766	1.019685	-2.012518
30	8	0	-0.735524	1.890582	-2.356952
31	1	0	-1.172077	1.735132	-3.200053
32	8	0	0.291557	3.890271	1.016787
33	1	0	0.464865	4.059130	0.063588
34	1	0	0.380219	4.720351	1.494564
35	8	0	0.853528	3.938322	-1.660620
36	1	0	0.260096	3.222691	-2.005553
37	1	0	0.692520	4.712294	-2.211731
38	8	0	2.553877	0.729448	0.039534
39	1	0	3.061007	-0.136722	0.248516
40	1	0	3.047581	1.388996	-0.511957
41	8	0	3.339103	-1.575103	0.585603
42	1	0	4.102754	-1.929759	1.082004
43	1	0	3.097194	-2.203628	-0.130325
44	8	0	3.376086	2.701717	-1.496360
45	1	0	2.585930	3.255247	-1.643700
46	1	0	4.128203	3.293863	-1.407500
47	8	0	5.494295	-2.552390	1.981358
48	1	0	6.303170	-2.823147	1.535428
49	1	0	5.370076	-3.181893	2.698944
50	8	0	2.332961	-3.102794	-1.402090
51	1	0	1.363540	-3.174302	-1.334049
52	1	0	2.512985	-2.895851	-2.323800

SCF Done: E(RB+HF-LYP) = -1376.00943805 A.U. after 1 cycles
Convg = 0.2769D-08 -V/T = 2.0039
S**2 = 0.0000
Sum of electronic and zero-point Energies= -1375.573495
Sum of electronic and thermal Energies= -1375.537295
Sum of electronic and thermal Enthalpies= -1375.536351
Sum of electronic and thermal Free Energies= -1375.643271
Et[B3LYP/6-311G(d,p) SCRF=PCM//B3LYP/6-311G(d,p)]= -1376.085227 a.u.
Et + ZPE = -1375.649284 a.u.