Supplementary Information for the article

Multi-step mechanisms of early phospholipid hydrolysis and mineralisation unveiled through combined quantum chemical calculations and experimental analysis

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Stationary structures in all the reactions investigated. E stands for potential energy, Gcorr stands for Gibbs free energy correction. The energies are in hartress, the coordinates in angstroms.

I. Structures of molecules and transition states (TS) related to PS6 + 2 H_2O (R1) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

1. PS6+2H_2O, R1, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	-3.326888	-3.844871	-0.200719
2	C	-2.469079	-2.667382	0.214645
3	O	-2.509581	-2.128950	1.302775
4	O	-1.625080	-2.297935	-0.780944
5	C	-0.768636	-1.154565	-0.556549
6	C	-1.375127	0.051736	-1.270069
7	O	-2.726341	0.294122	-0.839189
8	C	-3.052877	1.097651	0.208648
9	O	-4.225295	1.131595	0.530324
10	C	-1.986613	1.941182	0.877042
11	C	-1.679767	3.252570	0.114310
12	C	0.591275	-1.538645	-1.143650
13	O	1.468317	-0.399233	-1.083456
14	P	2.758981	-0.387751	-0.101170
15	O	3.150837	1.083017	0.055738
16	O	2.585028	-1.260094	1.109598
17	O	3.879063	-1.041493	-1.130274
18	C	5.156470	-1.439095	-0.638751
19	C	5.925857	-0.256299	-0.003903
20	C	7.430253	-0.477664	0.084943
21	O	7.709168	-1.687900	0.569777
22	O	8.244524	0.362539	-0.230631
23	N	5.667423	1.006667	-0.757626
24	H	-2.839092	-4.743411	0.198907
25	H	-3.313645	-3.934388	-1.290410
26	H	5.766556	0.879781	-1.767916
27	H	4.660228	1.286735	-0.531657
28	H	6.335458	1.728835	-0.473595
29	H	8.676864	-1.785423	0.629623
30	H	5.553713	-0.081199	1.010048
31	H	5.070107	-2.232074	0.108092
32	H	5.701050	-1.825656	-1.503185
33	H	1.001109	-2.383493	-0.585915
34	H	0.488879	-1.819661	-2.195964
35	H	-0.675954	-0.967389	0.515632
36	H	-0.736979	0.924429	-1.134125
37	H	-1.458401	-0.153725	-2.340555
38	H	-1.352917	3.027984	-0.908981
39	H	-0.821817	3.717694	0.612765
40	H	-2.382566	2.187205	1.865913
41	H	-1.068953	1.369700	1.033767
42	C	-2.853813	4.237576	0.065990
43	C	-2.513060	5.537750	-0.672358
44	H	-3.168839	4.473530	1.092134
45	C	-3.680150	6.528701	-0.715128
46	H	-1.647358	6.011168	-0.189703
47	H	-2.197318	5.299536	-1.697150
48	H	-4.549276	6.094402	-1.222322
49	H	-3.995340	6.812571	0.295453
50	H	-3.719315	3.763338	-0.415292
51	C	-4.760897	-3.742415	0.339672
52	C	-5.569554	-2.599798	-0.287921

53	H	-5.620236	-2.747710	-1.376217
54	H	-5.045996	-1.647538	-0.131375
55	H	-4.716800	-3.611344	1.426971
56	C	-6.991514	-2.482809	0.273967
57	C	-7.781021	-1.321560	-0.338133
58	H	-6.938505	-2.354180	1.363600
59	H	-7.275259	-0.365852	-0.159149
60	H	-7.885155	-1.441808	-1.422630
61	H	-7.530108	-3.425132	0.104452
62	H	-5.267809	-4.697301	0.156566
63	H	-8.787601	-1.252085	0.087186
64	H	-3.407042	7.445119	-1.248424
65	O	0.459978	0.040382	2.514030
66	H	0.797285	0.950124	2.380079
67	H	1.184186	-0.511452	2.162164
68	O	1.587181	2.543686	1.806258
69	H	2.178662	2.112265	1.148243
70	H	2.179954	2.815751	2.519620

E[B3LYP/6-31G(d,p)] = -2007.840185 h, E[APFD/6-311+G(2d,p)] = -2007.017383 h
Gcorr[B3LYP/6-31G(d,p)] = 0.510935 h

2. PS6+2H_2O, R1, 1st step, TS

Center No.	Atom	X	Y	Z
1	C	-2.675166	-4.152124	0.021728
2	C	-2.145521	-2.845637	0.574030
3	O	-2.467512	-2.365072	1.642667
4	O	-1.251359	-2.274417	-0.271982
5	C	-0.725758	-0.974824	0.078529
6	C	-1.390837	0.061235	-0.820645
7	O	-2.814753	0.090289	-0.607210
8	C	-3.405109	0.847077	0.355262
9	O	-4.591553	0.669099	0.550838
10	C	-2.603642	1.916215	1.074473
11	C	-2.540607	3.242518	0.277221
12	C	0.788222	-1.033039	-0.119211
13	O	1.273755	0.248835	0.292455
14	P	2.857785	0.602857	0.586499
15	O	3.487448	1.591148	-0.521745
16	O	3.529152	0.312600	1.911150
17	O	3.366983	-0.789318	-0.328727
18	C	4.574805	-1.432798	-0.019641
19	C	5.790335	-0.526579	-0.348605
20	C	7.098482	-1.276907	-0.506013
21	O	7.353906	-2.026973	0.570355
22	O	7.808813	-1.197362	-1.486425
23	N	5.506889	0.234730	-1.601812
24	H	-2.139420	-4.956207	0.541966
25	H	-2.419040	-4.227695	-1.038349
26	H	5.255583	-0.387748	-2.373188
27	H	4.682861	0.873185	-1.378043
28	H	6.323036	0.773922	-1.899087
29	H	8.197984	-2.491609	0.427173
30	H	5.896646	0.215771	0.446936
31	H	4.649229	-1.707898	1.035854
32	H	4.620726	-2.342030	-0.630171
33	H	1.200853	-1.837927	0.493269
34	H	1.040529	-1.232450	-1.164796
35	H	-0.952421	-0.774730	1.127680
36	H	-0.932502	1.038832	-0.672453
37	H	-1.269023	-0.225283	-1.867909
38	H	-2.064516	3.070525	-0.696479
39	H	-1.876879	3.920210	0.826818
40	H	-3.114100	2.086834	2.025421
41	H	-1.589645	1.577699	1.301623
42	C	-3.901613	3.917822	0.070061
43	C	-3.797025	5.244563	-0.692155
44	H	-4.368439	4.095412	1.048889
45	C	-5.152639	5.927499	-0.896494
46	H	-3.123285	5.921646	-0.149903

47	H	-3.326734	5.064510	-1.668312
48	H	-5.836416	5.287018	-1.465179
49	H	-5.631436	6.151617	0.063544
50	H	-4.576442	3.241544	-0.470014
51	C	-4.188266	-4.300398	0.248245
52	C	-5.026120	-3.284162	-0.538386
53	H	-4.827380	-3.404593	-1.612930
54	H	-4.708735	-2.265069	-0.280242
55	H	-4.392963	-4.197829	1.320088
56	C	-6.532716	-3.412914	-0.283572
57	C	-7.356491	-2.367662	-1.042060
58	H	-6.724771	-3.317427	0.793754
59	H	-7.057883	-1.352088	-0.758024
60	H	-7.216028	-2.462416	-2.124968
61	H	-6.866225	-4.421210	-0.564252
62	H	-4.480987	-5.318763	-0.033511
63	H	-8.426542	-2.472177	-0.834802
64	H	-5.046502	6.869868	-1.443664
65	O	2.008250	2.222945	1.399575
66	H	2.516031	3.213115	0.876621
67	H	2.348370	2.131679	2.301082
68	O	3.127218	3.883964	0.106472
69	H	3.413896	2.724885	-0.318595
70	H	3.902790	4.225689	0.573391

E[B3LYP/6-31G(d,p)] = -2007.78104 h, E[APFD/6-311+G(2d,p)] = -2006.954908 h
Gcorr[B3LYP/6-31G(d,p)] = 0.505808 h

3. PS6+2H_2O, R1, first step, products

Center No.	Atom	X	Y	Z
1	C	-2.541586	-4.120055	0.008084
2	C	-2.071033	-2.793006	0.565724
3	O	-2.432674	-2.319452	1.624989
4	O	-1.174225	-2.198876	-0.260021
5	C	-0.682823	-0.889012	0.105224
6	C	-1.387150	0.141650	-0.770909
7	O	-2.815714	0.080802	-0.596404
8	C	-3.480625	0.768102	0.368504
9	O	-4.659884	0.513732	0.519063
10	C	-2.769460	1.858826	1.146969
11	C	-2.759164	3.211853	0.393876
12	C	0.829528	-0.910036	-0.117385
13	O	1.301000	0.375308	0.288545
14	P	2.889493	0.787174	0.551450
15	O	3.558766	1.633969	-0.726375
16	O	3.650198	0.447331	1.822665
17	O	3.374176	-0.654334	-0.386571
18	C	4.502825	-1.389746	-0.022412
19	C	5.805037	-0.582081	-0.279038
20	C	7.054910	-1.433842	-0.335780
21	O	7.228813	-2.109806	0.804941
22	O	7.787758	-1.497865	-1.301435
23	N	5.666996	0.162202	-1.568458
24	H	-1.960665	-4.899058	0.518359
25	H	-2.287640	-4.176059	-1.053879
26	H	5.508163	-0.473066	-2.354130
27	H	4.837332	0.806322	-1.459463
28	H	6.509737	0.700160	-1.780981
29	H	8.032377	-2.653364	0.717694
30	H	5.899653	0.168288	0.509466
31	H	4.512084	-1.673516	1.033889
32	H	4.515583	-2.299880	-0.636563
33	H	1.267185	-1.711675	0.482015
34	H	1.062768	-1.103999	-1.168364
35	H	-0.902588	-0.712213	1.160059
36	H	-0.989311	1.137239	-0.574659
37	H	-1.224362	-0.096246	-1.824880
38	H	-2.234644	3.102261	-0.563770
39	H	-2.162718	3.911376	0.991218
40	H	-3.319947	1.968004	2.084527

41	H	-1.745855	1.570813	1.398825
42	C	-4.151341	3.806938	0.150865
43	C	-4.102105	5.164906	-0.560151
44	H	-4.668834	3.918196	1.113882
45	C	-5.489849	5.766893	-0.800278
46	H	-3.497274	5.863092	0.034093
47	H	-3.580833	5.051671	-1.520327
48	H	-6.105778	5.105827	-1.420589
49	H	-6.022097	5.923644	0.144873
50	H	-4.757844	3.109489	-0.440863
51	C	-4.042749	-4.349078	0.242067
52	C	-4.938569	-3.387787	-0.549777
53	H	-4.735345	-3.505293	-1.623858
54	H	-4.679480	-2.350453	-0.299898
55	H	-4.249092	-4.249233	1.313870
56	C	-6.434857	-3.601381	-0.290919
57	C	-7.319976	-2.616376	-1.060888
58	H	-6.631295	-3.504275	0.785486
59	H	-7.082871	-1.581233	-0.789801
60	H	-7.174717	-2.715821	-2.142748
61	H	-6.708780	-4.630940	-0.558736
62	H	-4.280236	-5.384279	-0.030375
63	H	-8.381763	-2.782183	-0.851038
64	H	-5.422925	6.734029	-1.309093
65	O	2.241349	2.320836	1.157977
66	H	2.766357	3.824635	0.435356
67	H	2.478472	2.290443	2.094735
68	O	3.275801	4.315931	-0.254918
69	H	3.523833	2.617661	-0.613028
70	H	4.073013	4.615371	0.203833

E[B3LYP/6-31G(d,p)] = -2007.792743 h, E[APFD/6-311+G(2d,p)] = -2006.966007 h
Gcorr[B3LYP/6-31G(d,p)] = 0.510379 h

4. PS6+2H_2O, R1, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	C	-2.263395	-4.126173	-0.608086
2	C	-1.637224	-2.829471	-0.138172
3	O	-1.606173	-2.454783	1.017672
4	O	-1.093205	-2.140082	-1.170595
5	C	-0.512990	-0.844777	-0.890047
6	C	-1.479623	0.226726	-1.381360
7	O	-2.759183	0.101330	-0.730624
8	C	-3.070093	0.724992	0.435408
9	O	-4.111439	0.404539	0.975885
10	C	-2.173869	1.828805	0.961177
11	C	-2.467147	3.194215	0.292169
12	C	0.830580	-0.794349	-1.623844
13	O	1.446274	0.476251	-1.426969
14	P	2.369316	0.785048	-0.083455
15	O	3.638815	1.742262	-0.492304
16	O	2.113853	0.197428	1.291339
17	O	3.444571	-0.593378	-0.667389
18	C	4.283313	-1.234095	0.243845
19	C	5.612584	-0.413829	0.394390
20	C	6.772599	-1.269458	0.852688
21	O	6.653928	-1.595721	2.141082
22	O	7.661890	-1.645408	0.114369
23	N	5.924588	0.127889	-0.961839
24	H	-1.520295	-4.915254	-0.434587
25	H	-2.427951	-4.076341	-1.687941
26	H	6.560004	-0.509663	-1.455141
27	H	4.995783	0.192488	-1.429701
28	H	6.349148	1.055240	-0.933084
29	H	7.387777	-2.190979	2.377842
30	H	5.452506	0.429433	1.065091
31	H	3.832057	-1.330457	1.234096
32	H	4.527359	-2.231852	-0.145301
33	H	1.472417	-1.606552	-1.277085
34	H	0.675819	-0.908087	-2.701981

35	H	-0.350386	-0.755718	0.186097
36	H	-1.037856	1.213313	-1.244574
37	H	-1.689894	0.078870	-2.443648
38	H	-2.314852	3.117357	-0.791929
39	H	-1.713958	3.902733	0.656516
40	H	-2.374073	1.896707	2.033366
41	H	-1.116502	1.586801	0.832344
42	C	-3.869221	3.746547	0.574852
43	C	-4.114487	5.112971	-0.076908
44	H	-4.011227	3.830273	1.661375
45	C	-5.511585	5.671942	0.208609
46	H	-3.355667	5.824150	0.276495
47	H	-3.969098	5.027157	-1.162280
48	H	-6.291055	4.997740	-0.164312
49	H	-5.673658	5.800983	1.284829
50	H	-4.628429	3.035939	0.223613
51	C	-3.560789	-4.452496	0.146502
52	C	-4.704303	-3.475134	-0.154510
53	H	-4.920757	-3.491896	-1.232308
54	H	-4.384938	-2.450854	0.078558
55	H	-3.349069	-4.453885	1.221892
56	C	-5.988091	-3.784370	0.624979
57	C	-7.112803	-2.783331	0.343122
58	H	-5.764003	-3.788459	1.700356
59	H	-6.805503	-1.764211	0.604379
60	H	-7.386374	-2.783669	-0.718285
61	H	-6.328115	-4.800048	0.380969
62	H	-3.866913	-5.471856	-0.117069
63	H	-8.013721	-3.018996	0.919091
64	H	-5.657411	6.646163	-0.269278
65	O	1.352176	2.232538	0.188395
66	H	2.061128	3.815167	-0.133450
67	H	1.175211	2.176536	1.137830
68	O	2.844586	4.376670	-0.350120
69	H	3.439969	2.707273	-0.406289
70	H	3.121183	4.738056	0.503394

E[B3LYP/6-31G(d,p)] = -2007.79019 h, E[APFD/6-311+G(2d,p)] = -2006.964815 h
Gcorr[B3LYP/6-31G(d,p)] = 0.511156 h

5. PS6+2H_2O, R1, 2nd step, TS

Center No.	Atom	X	Y	Z
1	C	2.281190	-4.151550	0.281931
2	C	1.721727	-2.817559	-0.165891
3	O	1.830210	-2.361456	-1.286943
4	O	1.061034	-2.194095	0.841686
5	C	0.522600	-0.877471	0.583661
6	C	1.431743	0.148395	1.252019
7	O	2.774727	0.052347	0.742406
8	C	3.222569	0.753842	-0.332156
9	O	4.315654	0.454430	-0.772325
10	C	2.404231	1.909435	-0.873737
11	C	2.627831	3.216698	-0.074245
12	C	-0.893957	-0.864809	1.163317
13	O	-1.494042	0.419241	0.960948
14	P	-2.321678	0.728961	-0.419930
15	O	-3.550664	1.721073	-0.069429
16	O	-2.208795	-0.127149	-1.650136
17	O	-3.631583	-0.672457	0.423294
18	C	-4.681647	-1.117199	-0.380863
19	C	-5.953729	-0.235783	0.006148
20	C	-7.226421	-1.045281	0.052337
21	O	-7.627866	-1.388009	-1.177563
22	O	-7.786272	-1.381076	1.077968
23	N	-5.616859	0.276389	1.351917
24	H	1.566995	-4.917711	-0.046338
25	H	2.304213	-4.184710	1.374590
26	H	-6.163552	-0.205420	2.069470
27	H	-4.494545	-0.032141	1.294395
28	H	-5.728415	1.282617	1.442952

29	H	-8.419419	-1.949045	-1.094028
30	H	-6.051573	0.597981	-0.687321
31	H	-4.467329	-0.998370	-1.445523
32	H	-4.902175	-2.176173	-0.181522
33	H	-1.494637	-1.650811	0.704017
34	H	-0.865878	-1.032220	2.244240
35	H	0.485555	-0.718598	-0.496219
36	H	1.014045	1.148377	1.136689
37	H	1.518560	-0.073316	2.318686
38	H	2.333431	3.068586	0.972514
39	H	1.940265	3.967261	-0.481659
40	H	2.732650	2.053102	-1.906053
41	H	1.336880	1.676715	-0.893684
42	C	4.062948	3.753558	-0.131806
43	C	4.237840	5.069688	0.635845
44	H	4.350094	3.903322	-1.181927
45	C	5.668474	5.613418	0.576519
46	H	3.543669	5.819150	0.232252
47	H	3.946665	4.918342	1.684087
48	H	6.381106	4.899062	1.004326
49	H	5.975479	5.807220	-0.457582
50	H	4.758299	3.005008	0.269302
51	C	3.665807	-4.432442	-0.321227
52	C	4.760045	-3.491465	0.199007
53	H	4.834015	-3.591134	1.291407
54	H	4.473494	-2.449577	0.004442
55	H	3.595288	-4.350863	-1.411971
56	C	6.134692	-3.753331	-0.427913
57	C	7.212977	-2.788682	0.075367
58	H	6.053365	-3.672430	-1.520389
59	H	6.942433	-1.749218	-0.142857
60	H	7.345702	-2.874358	1.160011
61	H	6.439583	-4.788209	-0.221032
62	H	3.935237	-5.471645	-0.098408
63	H	8.181326	-2.988089	-0.395208
64	H	5.762581	6.551529	1.133138
65	O	-1.252737	2.011256	-0.861255
66	H	-1.954189	3.749220	-0.798391
67	H	-0.995564	1.807920	-1.772168
68	O	-2.781519	4.245700	-0.626025
69	H	-3.351875	2.671244	-0.295850
70	H	-3.097296	4.503040	-1.503757

E[B3LYP/6-31G(d,p)] = -2007.787253 h, E[APFD/6-311+G(2d,p)] = -2006.957321 h
Gcorr[B3LYP/6-31G(d,p)] = 0.507482 h

6. PS6+2H_2O, R1, 2nd step, products

Center No.	Atom	X	Y	Z
1	C	2.495822	-4.055991	0.005292
2	C	1.927916	-2.724908	-0.438156
3	O	2.153024	-2.191788	-1.505909
4	O	1.104596	-2.199886	0.506649
5	C	0.526452	-0.902526	0.249476
6	C	1.285332	0.133708	1.075406
7	O	2.689723	0.098786	0.767059
8	C	3.271122	0.853209	-0.204343
9	O	4.431250	0.609325	-0.472161
10	C	2.500183	1.992449	-0.841062
11	C	2.532734	3.281593	0.016479
12	C	-0.944614	-1.018201	0.654466
13	O	-1.624021	0.243950	0.497149
14	P	-2.244897	0.673175	-0.927410
15	O	-3.358840	1.707406	-0.496698
16	O	-2.676907	-0.444707	-1.803215
17	O	-4.077979	-2.178174	1.172991
18	C	-5.154247	-1.841007	0.317451
19	C	-5.879052	-0.591598	0.879734
20	C	-7.129545	-0.289782	0.065087
21	O	-6.828784	0.115537	-1.183969
22	O	-8.268641	-0.425994	0.465360

23	N	-6.150140	-0.826437	2.295840
24	H	1.849718	-4.830554	-0.427970
25	H	2.406870	-4.140874	1.091827
26	H	-7.035731	-1.322252	2.387295
27	H	-4.432093	-1.993164	2.064587
28	H	-6.268401	0.056630	2.784466
29	H	-7.666817	0.253132	-1.660104
30	H	-5.195412	0.257894	0.784258
31	H	-4.751461	-1.631778	-0.675297
32	H	-5.876626	-2.670958	0.239719
33	H	-1.439675	-1.790486	0.064136
34	H	-1.032529	-1.275149	1.711913
35	H	0.618939	-0.683623	-0.816656
36	H	0.852881	1.123801	0.929432
37	H	1.223260	-0.119598	2.136651
38	H	2.083289	3.089691	0.999090
39	H	1.886086	4.016584	-0.477289
40	H	2.986317	2.182864	-1.801058
41	H	1.464007	1.713166	-1.046857
42	C	3.933550	3.877416	0.201353
43	C	3.926605	5.172849	1.022182
44	H	4.374344	4.073877	-0.785904
45	C	5.322538	5.777145	1.201240
46	H	3.269341	5.906121	0.535594
47	H	3.484174	4.974172	2.007695
48	H	5.992758	5.079107	1.715720
49	H	5.776374	6.018206	0.233208
50	H	4.590529	3.144148	0.686559
51	C	3.944909	-4.258103	-0.461337
52	C	4.943837	-3.316324	0.223287
53	H	4.905493	-3.477016	1.310239
54	H	4.643324	-2.273615	0.055966
55	H	3.986377	-4.116406	-1.547399
56	C	6.385275	-3.502795	-0.265534
57	C	7.372684	-2.544932	0.408267
58	H	6.418261	-3.355831	-1.353646
59	H	7.094009	-1.500846	0.225500
60	H	7.392385	-2.695939	1.493720
61	H	6.699421	-4.540506	-0.088809
62	H	4.227207	-5.299643	-0.267331
63	H	8.391317	-2.689617	0.033612
64	H	5.285830	6.699121	1.790573
65	O	-1.048364	1.581666	-1.560592
66	H	-1.653478	3.987832	-1.183240
67	H	-0.989683	1.460461	-2.521356
68	O	-2.531595	4.149342	-0.804641
69	H	-3.089513	2.678462	-0.595732
70	H	-3.023350	4.603089	-1.504771

E[B3LYP/6-31G(d,p)] = -2007.82265 h, E[APFD/6-311+G(2d,p)] = -2006.993431 h
Gcorr[B3LYP/6-31G(d,p)] = 0.498406 h

7. PS6+2H_2O, R1, 3rd step, reactants (hydrolysed serine neglected)

Center No.	Atom	X	Y	Z
1	C	-1.926997	-3.780349	-0.521422
2	C	-0.998051	-2.644470	-0.150783
3	O	-0.812013	-2.237312	0.978053
4	O	-0.372128	-2.138731	-1.246197
5	C	0.504010	-1.007860	-1.056773
6	C	-0.218961	0.248325	-1.536559
7	O	-1.457367	0.423257	-0.827172
8	C	-1.568394	1.121299	0.335855
9	O	-2.634433	1.059130	0.915984
10	C	-0.420261	1.990273	0.810293
11	C	-0.394509	3.372886	0.112960
12	C	1.758067	-1.312318	-1.880072
13	O	2.687042	-0.209182	-1.827408
14	P	3.747064	-0.101286	-0.616115
15	O	4.738053	1.039038	-1.161307
16	O	4.401111	-1.405932	-0.284936

17	H	-1.380505	-4.710227	-0.317749
18	H	-2.120004	-3.752668	-1.597199
19	H	2.231708	-2.227204	-1.515707
20	H	1.502553	-1.441118	-2.934051
21	H	0.750379	-0.924865	0.003487
22	H	0.434303	1.116626	-1.449555
23	H	-0.507231	0.134245	-2.584484
24	H	-0.267567	3.245246	-0.969512
25	H	0.501397	3.897110	0.465852
26	H	-0.575511	2.128856	1.883119
27	H	0.544167	1.492524	0.680174
28	C	-1.631620	4.237488	0.383950
29	C	-1.554014	5.614833	-0.286187
30	H	-1.751115	4.366131	1.468729
31	C	-2.784603	6.484975	-0.013574
32	H	-0.651905	6.136158	0.061441
33	H	-1.431178	5.483370	-1.369767
34	H	-3.698282	6.004200	-0.381292
35	H	-2.913728	6.662273	1.060222
36	H	-2.534411	3.717338	0.038568
37	C	-3.232839	-3.751933	0.287715
38	C	-4.133449	-2.556255	-0.047898
39	H	-4.382722	-2.580615	-1.118425
40	H	-3.583558	-1.620529	0.118542
41	H	-2.983625	-3.740745	1.355055
42	C	-5.428552	-2.523829	0.772648
43	C	-6.310404	-1.314115	0.447984
44	H	-5.177368	-2.516413	1.841997
45	H	-5.776531	-0.376269	0.639145
46	H	-6.609980	-1.314372	-0.606372
47	H	-5.993974	-3.449530	0.599065
48	H	-3.774388	-4.686433	0.099185
49	H	-7.222864	-1.308771	1.053199
50	H	-2.700772	7.460070	-0.504371
51	O	2.959091	0.620604	0.537415
52	H	4.635747	0.891384	3.026126
53	H	3.355584	0.506525	1.492800
54	O	3.911018	0.274962	2.850368
55	H	5.378432	0.700191	-1.806131
56	H	4.333455	-0.628886	2.787523
57	O	4.961291	-2.106436	2.301418
58	H	4.331459	-2.797420	2.548860
59	H	4.822231	-1.975770	1.334669

E[B3LYP/6-31G(d,p)] = -1685.290635 h, E[APFD/6-311+G(2d,p)] = -1684.602217 h
Gcorr[B3LYP/6-31G(d,p)] = 0.426268 h

8. PS6+2H_2O, R1, 3rd step, TS

Center No.	Atom	X	Y	Z
1	C	2.057009	-3.764995	0.440274
2	C	1.157131	-2.624246	0.011945
3	O	1.076317	-2.193231	-1.121784
4	O	0.427903	-2.153549	1.052929
5	C	-0.446915	-1.025608	0.812062
6	C	0.215086	0.221889	1.386942
7	O	1.515698	0.433037	0.804839
8	C	1.723473	1.141827	-0.335451
9	O	2.841639	1.107990	-0.812371
10	C	0.608065	1.991979	-0.911662
11	C	0.490985	3.368745	-0.212511
12	C	-1.769995	-1.355611	1.512771
13	O	-2.694774	-0.276952	1.425036
14	P	-3.805628	-0.146408	0.164662
15	O	-4.641673	0.956307	1.029681
16	O	-4.254708	-1.618963	0.068667
17	H	1.513356	-4.692617	0.218342
18	H	2.190933	-3.729195	1.525032
19	H	-2.190748	-2.269319	1.084754
20	H	-1.581662	-1.529713	2.577856
21	H	-0.597730	-0.918511	-0.262134

22	H	-0.439753	1.083912	1.260877
23	H	0.407140	0.083936	2.454055
24	H	0.273927	3.229734	0.854165
25	H	-0.382609	3.876312	-0.638429
26	H	0.859081	2.140756	-1.964904
27	H	-0.353554	1.474380	-0.871122
28	C	1.726803	4.262775	-0.370618
29	C	1.560911	5.632318	0.299317
30	H	1.935466	4.403327	-1.440366
31	C	2.789387	6.532636	0.137541
32	H	0.679492	6.135982	-0.120092
33	H	1.349938	5.489106	1.367735
34	H	3.679843	6.069587	0.577824
35	H	3.004386	6.722132	-0.920307
36	H	2.608368	3.759451	0.046898
37	C	3.404370	-3.756718	-0.296128
38	C	4.299330	-2.569139	0.081006
39	H	4.497853	-2.594732	1.162092
40	H	3.765754	-1.629059	-0.111237
41	H	3.213559	-3.748315	-1.375402
42	C	5.631625	-2.548428	-0.677958
43	C	6.507888	-1.346111	-0.313163
44	H	5.430621	-2.539725	-1.757873
45	H	5.990940	-0.403790	-0.527784
46	H	6.759425	-1.348812	0.753672
47	H	6.180392	-3.478829	-0.477958
48	H	3.925037	-4.695844	-0.074240
49	H	7.446859	-1.348127	-0.876423
50	H	2.641729	7.501309	0.626011
51	O	-2.671980	0.419382	-0.864045
52	H	-5.606355	1.091999	-0.913343
53	H	-3.124392	0.676474	-1.685151
54	O	-5.044213	0.373055	-1.236195
55	H	-4.223389	1.024702	1.903757
56	H	-5.723224	-0.679943	-1.562536
57	O	-6.029683	-1.775273	-1.539607
58	H	-5.759504	-2.199227	-2.368181
59	H	-5.213893	-1.903527	-0.778912

E[B3LYP/6-31G(d,p)] = -1685.244185 h, E[APFD/6-311+G(2d,p)] = -1684.551348 h
Gcorr[B3LYP/6-31G(d,p)] = 0.426608 h

9. PS6+2H_2O, R1, 3rd step, products

Center No.	Atom	X	Y	Z
1	C	-1.926997	-3.780349	-0.521422
2	C	-0.998051	-2.644470	-0.150783
3	O	-0.812013	-2.237312	0.978053
4	O	-0.372128	-2.138731	-1.246197
5	C	0.504010	-1.007860	-1.056773
6	C	-0.218961	0.248325	-1.536559
7	O	-1.457367	0.423257	-0.827172
8	C	-1.568394	1.121299	0.335855
9	O	-2.634433	1.059130	0.915984
10	C	-0.420261	1.990273	0.810293
11	C	-0.394509	3.372886	0.112960
12	C	1.758067	-1.312318	-1.880072
13	O	2.687042	-0.209182	-1.827408
14	P	3.747064	-0.101286	-0.616115
15	O	4.738053	1.039038	-1.161307
16	O	4.401111	-1.405932	-0.284936
17	H	-1.380505	-4.710227	-0.317749
18	H	-2.120004	-3.752668	-1.597199
19	H	2.231708	-2.227204	-1.515707
20	H	1.502553	-1.441118	-2.934051
21	H	0.750379	-0.924865	0.003487
22	H	0.434303	1.116626	-1.449555
23	H	-0.507231	0.134245	-2.584484
24	H	-0.267567	3.245246	-0.969512
25	H	0.501397	3.897110	0.465852
26	H	-0.575511	2.128856	1.883119

27	H	0.544167	1.492524	0.680174
28	C	-1.631620	4.237488	0.383950
29	C	-1.554014	5.614833	-0.286187
30	H	-1.751115	4.366131	1.468729
31	C	-2.784603	6.484975	-0.013574
32	H	-0.651905	6.136158	0.061441
33	H	-1.431178	5.483370	-1.369767
34	H	-3.698282	6.004200	-0.381292
35	H	-2.913728	6.662273	1.060222
36	H	-2.534411	3.717338	0.038568
37	C	-3.232839	-3.751933	0.287715
38	C	-4.133449	-2.556255	-0.047898
39	H	-4.382722	-2.580615	-1.118425
40	H	-3.583558	-1.620529	0.118542
41	H	-2.983625	-3.740745	1.355055
42	C	-5.428552	-2.523829	0.772648
43	C	-6.310404	-1.314115	0.447984
44	H	-5.177368	-2.516413	1.841997
45	H	-5.776531	-0.376269	0.639145
46	H	-6.609980	-1.314372	-0.606372
47	H	-5.993974	-3.449530	0.599065
48	H	-3.774388	-4.686433	0.099185
49	H	-7.222864	-1.308771	1.053199
50	H	-2.700772	7.460070	-0.504371
51	O	2.959091	0.620604	0.537415
52	H	4.635747	0.891384	3.026126
53	H	3.355584	0.506525	1.492800
54	O	3.911018	0.274962	2.850368
55	H	5.378432	0.700191	-1.806131
56	H	4.333455	-0.628886	2.787523
57	O	4.961291	-2.106436	2.301418
58	H	4.331459	-2.797420	2.548860
59	H	4.822231	-1.975770	1.334669

E[B3LYP/6-31G(d,p)] = -1685.260267 h, E[APFD/6-311+G(2d,p)] = -1684.567746 h
Gcorr[B3LYP/6-31G(d,p)] = 0.430120 h

10. PS6+2H_2O, R1, 4th step, reactants

Center No.	Atom	X	Y	Z
1	C	2.621000	-3.515946	0.258747
2	C	1.577193	-2.535432	-0.234463
3	O	1.550954	-2.058463	-1.352389
4	O	0.658449	-2.265265	0.724554
5	C	-0.374001	-1.296271	0.419812
6	C	-0.020396	0.010854	1.119939
7	O	1.269668	0.493251	0.697927
8	C	1.455468	1.260044	-0.408250
9	O	2.603189	1.472062	-0.749313
10	C	0.261398	1.875990	-1.112387
11	C	-0.205827	3.192314	-0.443672
12	C	-1.685924	-1.902436	0.933291
13	O	-2.765297	-0.971594	0.865530
14	P	-3.874341	-0.947016	-0.445065
15	O	-4.703063	0.236627	0.261478
16	O	-4.240292	-2.511412	-0.152627
17	H	2.327242	-4.504156	-0.118020
18	H	2.582572	-3.565911	1.350320
19	H	-1.905290	-2.814048	0.371854
20	H	-1.564057	-2.180158	1.986440
21	H	-0.416872	-1.154120	-0.658598
22	H	-0.806720	0.748257	0.957916
23	H	0.084293	-0.155147	2.195166
24	H	-0.505482	2.998984	0.594193
25	H	-1.111660	3.519290	-0.967729
26	H	0.590815	2.085308	-2.133160
27	H	-0.575302	1.175698	-1.174317
28	C	0.834877	4.318113	-0.474188
29	C	0.325013	5.617790	0.160620
30	H	1.126157	4.511273	-1.516048
31	C	1.357952	6.748137	0.125759

32	H	-0.588430	5.939703	-0.357491
33	H	0.031884	5.421501	1.200858
34	H	2.269703	6.467517	0.665315
35	H	1.644720	6.990322	-0.903932
36	H	1.748654	3.996668	0.041819
37	C	4.030208	-3.162420	-0.240767
38	C	4.575909	-1.855812	0.349349
39	H	4.607224	-1.938924	1.445223
40	H	3.885674	-1.032452	0.122985
41	H	4.006416	-3.093245	-1.334413
42	C	5.971392	-1.490454	-0.170909
43	C	6.493933	-0.169151	0.401502
44	H	5.941679	-1.427123	-1.267179
45	H	5.820849	0.659397	0.153183
46	H	6.572438	-0.214554	1.493838
47	H	6.674337	-2.300021	0.068359
48	H	4.703458	-3.990939	0.009355
49	H	7.485434	0.075408	0.006464
50	H	0.966399	7.661209	0.585869
51	O	-2.637381	-0.627884	-1.469243
52	H	-5.678039	-0.296485	-1.584754
53	H	-3.015507	-0.530444	-2.358576
54	O	-4.962170	-0.919060	-1.768751
55	H	-4.387624	0.503838	1.171513
56	H	-3.160235	0.103634	2.499053
57	O	-3.816248	0.793261	2.708091
58	H	-3.311024	1.618812	2.714754
59	H	-4.900242	-2.777939	-0.812646

E[B3LYP/6-31G(d,p)] = -1685.259086 h, E[APFD/6-311+G(2d,p)] = -1684.568998 h
Gcorr[B3LYP/6-31G(d,p)] = 0.430512 h

11. PS6+2H_2O, R1, 4th step, TS

Center No.	Atom	X	Y	Z
1	C	2.563946	-3.523661	0.336277
2	C	1.529644	-2.532197	-0.154998
3	O	1.491508	-2.070686	-1.278858
4	O	0.630098	-2.235434	0.814703
5	C	-0.390627	-1.253904	0.514103
6	C	-0.006849	0.055623	1.194295
7	O	1.289574	0.506118	0.757791
8	C	1.483905	1.272564	-0.347388
9	O	2.633321	1.453001	-0.700898
10	C	0.299382	1.924625	-1.034145
11	C	-0.126629	3.247407	-0.350799
12	C	-1.704432	-1.830438	1.053118
13	O	-2.777548	-0.903066	0.915243
14	P	-3.967555	-0.804729	-0.546606
15	O	-4.852005	0.177619	0.251105
16	O	-4.110917	-2.419748	-0.359716
17	H	2.218781	-4.517696	0.023295
18	H	2.573341	-3.521559	1.429775
19	H	-1.937310	-2.759040	0.527799
20	H	-1.592368	-2.061619	2.118822
21	H	-0.449511	-1.122341	-0.565491
22	H	-0.780432	0.805214	1.026697
23	H	0.101161	-0.098624	2.270986
24	H	-0.420522	3.053855	0.688662
25	H	-1.029147	3.601611	-0.862809
26	H	0.623888	2.133402	-2.056646
27	H	-0.556002	1.246972	-1.091624
28	C	0.942412	4.346229	-0.383924
29	C	0.472694	5.654227	0.264614
30	H	1.228576	4.539146	-1.427259
31	C	1.534186	6.757724	0.227265
32	H	-0.437006	6.003293	-0.242394
33	H	0.184507	5.458355	1.306309
34	H	2.443439	6.449984	0.756144
35	H	1.817368	6.999469	-0.803525
36	H	1.852498	3.997536	0.120869

37	C	3.959383	-3.245942	-0.241462
38	C	4.583644	-1.941230	0.270191
39	H	4.666452	-1.984992	1.365665
40	H	3.915418	-1.099354	0.045808
41	H	3.886414	-3.217278	-1.334724
42	C	5.964679	-1.653472	-0.330822
43	C	6.569668	-0.336868	0.166321
44	H	5.882263	-1.627117	-1.425894
45	H	5.919856	0.511129	-0.078441
46	H	6.701828	-0.347896	1.254367
47	H	6.645065	-2.483554	-0.096671
48	H	4.611796	-4.090555	0.010069
49	H	7.549016	-0.149068	-0.285943
50	H	1.170785	7.677449	0.697126
51	O	-2.646759	-0.308405	-1.377295
52	H	-5.677741	-0.264774	-1.818487
53	H	-2.936667	-0.161221	-2.292749
54	O	-4.902308	-0.822721	-1.968233
55	H	-4.578164	0.364311	1.558268
56	H	-3.283704	-0.351838	1.930852
57	O	-4.064061	0.255916	2.527364
58	H	-3.682564	1.111783	2.775259
59	H	-4.695241	-2.728938	-1.070555

E[B3LYP/6-31G(d,p)] = -1685.240795 h, E[APFD/6-311+G(2d,p)] = -1684.55153 h
Gcorr[B3LYP/6-31G(d,p)] = 0.425881 h

12. PS6+2H_2O, R1, 4th step, products

Center No.	Atom	X	Y	Z
1	C	-1.814573	-3.697750	1.120027
2	C	-1.757403	-2.214139	0.855108
3	O	-2.363054	-1.684560	-0.073486
4	O	-0.950332	-1.567883	1.699742
5	C	-0.628801	-0.164340	1.476866
6	C	0.863751	-0.018991	1.728727
7	O	1.635748	-0.670549	0.701323
8	C	2.074394	-0.031160	-0.415694
9	O	2.632839	-0.706143	-1.258768
10	C	1.911783	1.472221	-0.542516
11	C	3.054719	2.255498	0.148916
12	C	-1.449930	0.713465	2.430155
13	O	-1.075717	2.060705	2.224334
14	P	-3.104498	1.706073	-1.436944
15	O	-3.497622	3.093837	-1.055336
16	O	-3.484813	0.658978	-0.319345
17	H	-2.869005	-3.989050	1.107926
18	H	-1.404106	-3.908782	2.110243
19	H	-2.514426	0.546015	2.232777
20	H	-1.250056	0.402405	3.466788
21	H	-0.863603	0.094933	0.443662
22	H	1.110917	1.037494	1.819268
23	H	1.136494	-0.523933	2.658337
24	H	3.070668	2.026995	1.222083
25	H	2.812928	3.321705	0.067001
26	H	1.926022	1.683247	-1.614739
27	H	0.945278	1.803871	-0.155143
28	C	4.443830	2.000101	-0.448366
29	C	5.544933	2.820222	0.235077
30	H	4.424558	2.238045	-1.521012
31	C	6.934135	2.573533	-0.360832
32	H	5.299046	3.888237	0.162318
33	H	5.559216	2.583459	1.307565
34	H	7.221303	1.519625	-0.271579
35	H	6.960127	2.834107	-1.425057
36	H	4.690386	0.932949	-0.378499
37	C	-1.047420	-4.483505	0.031303
38	C	0.465500	-4.234361	0.042276
39	H	0.874366	-4.541936	1.015066
40	H	0.669924	-3.159547	-0.043030
41	H	-1.465300	-4.221178	-0.948156

42	C	1.210415	-4.968969	-1.078800
43	C	2.714364	-4.675709	-1.078960
44	H	0.781189	-4.676906	-2.046842
45	H	2.902382	-3.601622	-1.186374
46	H	3.180202	-5.002061	-0.141859
47	H	1.041895	-6.050243	-0.984193
48	H	-1.250171	-5.549768	0.183635
49	H	3.222760	-5.192045	-1.899924
50	H	7.698193	3.171037	0.147015
51	O	-1.541193	1.412084	-1.664330
52	H	-4.585017	1.654157	-3.021385
53	H	-1.154900	1.909613	-2.402031
54	O	-3.729577	1.232901	-2.843643
55	H	-3.427718	3.424632	0.694995
56	H	-1.883479	2.592574	2.025503
57	O	-3.298029	3.527725	1.665166
58	H	-3.027035	4.448999	1.777780
59	H	-3.009758	-0.221602	-0.312955

E[B3LYP/6-31G(d,p)] = -1685.285332 h, E[APFD/6-311+G(2d,p)] = -1684.599598 h
Gcorr[B3LYP/6-31G(d,p)] = 0.425076 h

II. Structures of molecules and transition states (TS) related to PS6 + 2 H_2O (R2) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

13. PS6+2H_2O, R2, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	-3.274244	-3.866636	-0.238605
2	C	-2.337291	-2.708059	0.031224
3	O	-2.132569	-2.221680	1.125583
4	O	-1.732749	-2.285179	-1.108098
5	C	-0.852153	-1.141974	-1.019637
6	C	-1.587643	0.072707	-1.577118
7	O	-2.802412	0.315406	-0.844674
8	C	-2.853775	1.059529	0.292945
9	O	-3.901801	1.053861	0.908963
10	C	-1.664557	1.909823	0.695706
11	C	-1.621480	3.262046	-0.058174
12	C	0.386001	-1.508825	-1.843005
13	O	1.295907	-0.401005	-1.966473
14	P	2.297385	0.003677	-0.753609
15	O	3.153901	1.152075	-1.269110
16	O	1.568227	0.130144	0.561083
17	O	3.244123	-1.355063	-0.753184
18	C	4.236257	-1.546882	0.254193
19	C	5.356186	-0.479549	0.162902
20	C	6.688328	-0.935692	0.730344
21	O	6.528491	-1.527794	1.916146
22	O	7.751314	-0.748793	0.176644
23	N	5.561201	-0.060961	-1.258762
24	H	-2.722521	-4.781374	0.013825
25	H	-3.493512	-3.911779	-1.308812
26	H	5.619583	-0.857837	-1.897393
27	H	4.719867	0.528848	-1.519231
28	H	6.434233	0.467213	-1.344052
29	H	7.404910	-1.782263	2.257180
30	H	5.064018	0.444253	0.688029
31	H	3.802077	-1.513528	1.256860
32	H	4.643123	-2.545438	0.080766
33	H	0.885241	-2.371733	-1.393265
34	H	0.094013	-1.770420	-2.863312
35	H	-0.577877	-0.980185	0.022511
36	H	-0.931581	0.943164	-1.583748
37	H	-1.913329	-0.123683	-2.601632
38	H	-1.535819	3.087587	-1.138213
39	H	-0.698770	3.772108	0.242709
40	H	-1.781689	2.096863	1.766132
41	H	-0.719672	1.376862	0.557861
42	C	-2.821938	4.175611	0.217335
43	C	-2.727727	5.519965	-0.514740

44	H	-2.898541	4.353991	1.298968
45	C	-3.921524	6.438939	-0.238724
46	H	-1.798767	6.027430	-0.221571
47	H	-2.647485	5.338485	-1.595107
48	H	-4.861545	5.971512	-0.553479
49	H	-4.007124	6.666082	0.830028
50	H	-3.751628	3.669510	-0.073334
51	C	-4.559688	-3.781765	0.598238
52	C	-5.467210	-2.608824	0.205671
53	H	-5.749888	-2.708229	-0.852140
54	H	-4.909175	-1.666808	0.287532
55	H	-4.283767	-3.698896	1.655727
56	C	-6.735565	-2.509812	1.061793
57	C	-7.620633	-1.318950	0.680893
58	H	-6.450446	-2.429370	2.119572
59	H	-7.075021	-0.374387	0.787573
60	H	-7.954838	-1.391193	-0.360500
61	H	-7.311133	-3.441120	0.971510
62	H	-5.106714	-4.725474	0.487084
63	H	-8.512569	-1.263190	1.313547
64	H	-3.826377	7.389020	-0.774490
65	O	4.416768	2.433380	0.974011
66	H	3.906012	2.251736	0.163792
67	H	3.780796	2.203279	1.686838
68	O	2.487185	1.474665	2.750920
69	H	2.945687	0.807647	3.279183
70	H	2.091906	0.962867	2.006559

E[B3LYP/6-31G(d,p)] = -2007.841824 h, E[APFD/6-311+G(2d,p)] = -2007.017948 h
Gcorr[B3LYP/6-31G(d,p)] = 0.512146 h

14. PS6+2H_2O, R2, 1st step, TS

Center No.	Atom	X	Y	Z
1	C	-2.924788	-3.964727	-0.321590
2	C	-2.165731	-2.727224	0.111709
3	O	-2.210701	-2.245373	1.227216
4	O	-1.411689	-2.229944	-0.897453
5	C	-0.677523	-1.003903	-0.655602
6	C	-1.403333	0.129476	-1.369932
7	O	-2.760448	0.251746	-0.898977
8	C	-3.107353	0.976240	0.196345
9	O	-4.253606	0.872281	0.589882
10	C	-2.104595	1.924840	0.825105
11	C	-2.045719	3.290332	0.097070
12	C	0.733983	-1.234444	-1.207989
13	O	1.512453	-0.042516	-1.212580
14	P	2.467720	0.384625	0.101467
15	O	3.014547	1.703100	-0.621388
16	O	1.314847	0.415824	1.147475
17	O	3.412288	-0.925697	-0.106489
18	C	4.778128	-1.161031	0.261036
19	C	5.766229	-0.066474	-0.222783
20	C	7.165089	-0.653992	-0.391798
21	O	7.537761	-1.355498	0.693178
22	O	7.867584	-0.492633	-1.367290
23	N	5.299742	0.613039	-1.438008
24	H	-2.343115	-4.828561	0.025300
25	H	-2.944808	-4.011853	-1.413822
26	H	5.136836	-0.062963	-2.183725
27	H	3.918415	1.433443	-1.039650
28	H	6.040029	1.225872	-1.775560
29	H	8.435957	-1.697913	0.536998
30	H	5.833059	0.686090	0.567330
31	H	4.877750	-1.276067	1.339297
32	H	5.005514	-2.115416	-0.221146
33	H	1.214976	-2.036391	-0.638451
34	H	0.658077	-1.567255	-2.249540
35	H	-0.639218	-0.819017	0.416109
36	H	-0.845314	1.059217	-1.262094
37	H	-1.499322	-0.096733	-2.434790

38	H	-1.745424	3.144313	-0.948285
39	H	-1.245320	3.874719	0.566169
40	H	-2.441021	2.077336	1.853737
41	H	-1.104898	1.484816	0.867050
42	C	-3.354541	4.087861	0.146537
43	C	-3.248564	5.450310	-0.549508
44	H	-3.646651	4.236299	1.195489
45	C	-4.551044	6.254472	-0.496746
46	H	-2.439838	6.031525	-0.086229
47	H	-2.953521	5.299405	-1.596752
48	H	-5.370355	5.712687	-0.982941
49	H	-4.853166	6.450701	0.538340
50	H	-4.163846	3.507236	-0.314529
51	C	-4.340943	-4.014367	0.271450
52	C	-5.269059	-2.920354	-0.272007
53	H	-5.349898	-3.023636	-1.363634
54	H	-4.823689	-1.933542	-0.088961
55	H	-4.266463	-3.928531	1.361606
56	C	-6.672447	-2.953401	0.345147
57	C	-7.581292	-1.837616	-0.179856
58	H	-6.587288	-2.871339	1.437266
59	H	-7.151488	-0.851158	0.028366
60	H	-7.717887	-1.915801	-1.264599
61	H	-7.135477	-3.929974	0.148418
62	H	-4.769855	-5.001186	0.060365
63	H	-8.572448	-1.875402	0.283966
64	H	-4.444865	7.220298	-1.001382
65	O	3.723514	0.890279	1.610254
66	H	3.894623	1.832293	1.469709
67	H	3.056333	0.780184	2.707665
68	O	2.141323	0.654329	3.378621
69	H	2.201333	-0.202701	3.825274
70	H	1.586322	0.505182	2.322580

E[B3LYP/6-31G(d,p)] = -2007.78096 h, E[APFD/6-311+G(2d,p)] = -2006.945853 h
Gcorr[B3LYP/6-31G(d,p)] = 0.50582 h

15. PS6+2H_2O, R2, 1st step, products

Center No.	Atom	X	Y	Z
1	C	-2.934861	-3.939888	-0.351251
2	C	-2.214505	-2.695283	0.125704
3	O	-2.320489	-2.222528	1.241143
4	O	-1.420557	-2.179985	-0.842384
5	C	-0.713739	-0.946918	-0.556885
6	C	-1.426775	0.185065	-1.285352
7	O	-2.798688	0.298017	-0.855636
8	C	-3.180499	1.007493	0.237233
9	O	-4.338114	0.898942	0.594068
10	C	-2.198634	1.948707	0.909702
11	C	-2.111840	3.321400	0.198611
12	C	0.724141	-1.140642	-1.050002
13	O	1.463103	0.069695	-0.963859
14	P	2.583307	0.339827	0.285311
15	O	2.924207	1.795199	-0.329038
16	O	1.396630	0.137356	1.368453
17	O	3.483883	-0.901237	-0.297560
18	C	4.868931	-1.171214	-0.039403
19	C	5.820279	0.023188	-0.332225
20	C	7.211302	-0.491714	-0.695639
21	O	7.657842	-1.381965	0.208862
22	O	7.851301	-0.132808	-1.661629
23	N	5.281573	0.933942	-1.349185
24	H	-2.372373	-4.798285	0.037929
25	H	-2.883516	-3.991838	-1.442176
26	H	5.090496	0.424184	-2.211127
27	H	3.839870	1.675248	-0.759446
28	H	5.998799	1.616948	-1.586908
29	H	8.547255	-1.668310	-0.065397
30	H	5.929854	0.595232	0.592873
31	H	5.021216	-1.501688	0.987895

32	H	5.092033	-2.003572	-0.712311
33	H	1.184595	-1.955938	-0.483061
34	H	0.704051	-1.443953	-2.104477
35	H	-0.719829	-0.777500	0.518632
36	H	-0.877228	1.117275	-1.156499
37	H	-1.489461	-0.036382	-2.353672
38	H	-1.772723	3.185918	-0.836136
39	H	-1.329637	3.900534	0.703427
40	H	-2.568342	2.090267	1.928259
41	H	-1.202218	1.505228	0.980953
42	C	-3.421698	4.118796	0.206786
43	C	-3.289612	5.486505	-0.474349
44	H	-3.752242	4.259006	1.245373
45	C	-4.593290	6.290384	-0.465168
46	H	-2.499113	6.064106	0.023577
47	H	-2.955065	5.343323	-1.510736
48	H	-5.393382	5.752327	-0.986250
49	H	-4.934653	6.479061	0.559058
50	H	-4.213521	3.542335	-0.288574
51	C	-4.386734	-3.996128	0.148259
52	C	-5.283407	-2.909195	-0.458431
53	H	-5.290918	-3.015156	-1.552745
54	H	-4.856909	-1.919359	-0.248684
55	H	-4.384061	-3.906444	1.240667
56	C	-6.724408	-2.949251	0.064368
57	C	-7.602990	-1.840396	-0.523088
58	H	-6.712421	-2.863961	1.159483
59	H	-7.194165	-0.850709	-0.289382
60	H	-7.666538	-1.921939	-1.614296
61	H	-7.167534	-3.929109	-0.159881
62	H	-4.795364	-4.986084	-0.086968
63	H	-8.622591	-1.883279	-0.126212
64	H	-4.468035	7.259855	-0.958299
65	O	3.742836	0.573370	1.593226
66	H	3.856698	1.527067	1.709038
67	H	3.231721	0.018328	3.329839
68	O	2.424187	-0.124885	3.864757
69	H	2.416558	-1.074122	4.052283
70	H	1.708988	0.097567	2.312162

E[B3LYP/6-31G(d,p)] = -2007.79499 h, E[APFD/6-311+G(2d,p)] = -2006.960089 h
Gcorr[B3LYP/6-31G(d,p)] = 0.509487 h

16. PS6+2H_2O, R2, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	C	-0.914470	4.338090	1.085009
2	C	-0.370665	2.986530	0.678918
3	O	0.275495	2.786925	-0.335039
4	O	-0.727706	2.017648	1.550329
5	C	-0.396940	0.641005	1.232317
6	C	-1.642377	-0.188745	1.499557
7	O	-2.689496	0.116558	0.555580
8	C	-2.839799	-0.539090	-0.624515
9	O	-3.698644	-0.130910	-1.382720
10	C	-1.994961	-1.763343	-0.925316
11	C	-2.588892	-3.062216	-0.327058
12	C	0.783634	0.213086	2.112476
13	O	1.091308	-1.161520	1.880052
14	P	2.472460	-1.628259	0.983198
15	O	3.454141	-1.285846	2.261375
16	O	1.799438	-3.081623	0.848142
17	O	2.081855	-0.524080	-0.151425
18	C	2.917854	0.026621	-1.180257
19	C	3.949552	1.024063	-0.625307
20	C	4.707630	1.669268	-1.792593
21	O	5.276271	0.749240	-2.597798
22	O	4.817477	2.864824	-1.968977
23	N	3.331024	1.991406	0.266585
24	H	-0.085871	5.051293	1.033828
25	H	-1.274523	4.299152	2.116083

26	H	2.508256	2.400882	-0.174557
27	H	2.911326	-1.088308	3.039375
28	H	3.981818	2.756109	0.430074
29	H	5.752249	1.225699	-3.301029
30	H	4.699363	0.448698	-0.066996
31	H	3.420596	-0.759031	-1.739487
32	H	2.215917	0.548712	-1.837490
33	H	1.630465	0.873616	1.899613
34	H	0.509060	0.320709	3.169339
35	H	-0.103080	0.581797	0.184432
36	H	-1.385217	-1.247179	1.494939
37	H	-2.059940	0.064118	2.476997
38	H	-2.657888	-2.975094	0.764627
39	H	-1.871645	-3.867537	-0.524492
40	H	-1.966841	-1.846495	-2.014568
41	H	-0.966636	-1.633680	-0.578874
42	C	-3.959598	-3.447694	-0.896340
43	C	-4.500857	-4.756393	-0.307851
44	H	-3.882775	-3.543171	-1.988376
45	C	-5.866874	-5.150844	-0.877329
46	H	-3.779061	-5.563035	-0.494263
47	H	-4.573457	-4.659126	0.783824
48	H	-6.617437	-4.378000	-0.675997
49	H	-5.817852	-5.288870	-1.963472
50	H	-4.680873	-2.641320	-0.712004
51	C	-2.041457	4.785495	0.127980
52	C	-3.296201	3.906752	0.202358
53	H	-3.707088	3.949361	1.221029
54	H	-3.027335	2.856565	0.030972
55	H	-1.647028	4.788205	-0.895523
56	C	-4.382561	4.308850	-0.802348
57	C	-5.604643	3.385869	-0.753574
58	H	-3.957272	4.297469	-1.815141
59	H	-5.318748	2.348706	-0.961571
60	H	-6.077258	3.407654	0.235268
61	H	-4.691658	5.345819	-0.613302
62	H	-2.299876	5.823602	0.367636
63	H	-6.359847	3.681621	-1.489290
64	H	-6.227008	-6.087087	-0.438626
65	O	3.901726	-2.082104	0.136835
66	H	4.636329	-2.131529	0.763853
67	H	3.875281	-3.810076	-0.742947
68	O	3.351653	-4.634123	-0.708825
69	H	2.921911	-4.689828	-1.574096
70	H	2.351173	-3.720102	0.319139

E[B3LYP/6-31G(d,p)] = -2007.798597 h, E[APFD/6-311+G(2d,p)] = -2006.966199 h
Gcorr[B3LYP/6-31G(d,p)] = 0.511078 h

17. PS6+2H_2O, R2, 2nd step, TS

Center No.	Atom	X	Y	Z
1	C	0.035413	4.420086	0.994285
2	C	0.330524	2.966294	0.698103
3	O	1.049766	2.587072	-0.210807
4	O	-0.337772	2.138287	1.527775
5	C	-0.257909	0.706669	1.291810
6	C	-1.642867	0.139303	1.552436
7	O	-2.597070	0.615276	0.580107
8	C	-2.903085	-0.053816	-0.560708
9	O	-3.646399	0.500795	-1.348615
10	C	-2.374861	-1.457999	-0.784036
11	C	-3.247915	-2.538779	-0.100525
12	C	0.796613	0.115028	2.234395
13	O	0.869941	-1.292618	2.079107
14	P	2.077800	-2.216239	0.648102
15	O	2.798268	-2.438741	2.032250
16	O	0.762094	-3.031477	0.283536
17	O	2.091489	-0.786877	-0.084998
18	C	3.090464	-0.310000	-1.010852
19	C	4.298314	0.302095	-0.285698

20	C	5.296499	0.830807	-1.327713
21	O	5.655202	-0.119375	-2.213260
22	O	5.743069	1.958422	-1.341829
23	N	3.889166	1.306929	0.680518
24	H	0.989420	4.955621	0.979815
25	H	-0.401488	4.514887	1.991680
26	H	3.210741	1.938646	0.256922
27	H	1.937425	-1.846896	2.531248
28	H	4.696171	1.872351	0.933698
29	H	6.302252	0.273789	-2.825562
30	H	4.826606	-0.508553	0.236495
31	H	3.411152	-1.110738	-1.673719
32	H	2.570219	0.459843	-1.585389
33	H	1.756431	0.603317	2.026303
34	H	0.511354	0.338583	3.272374
35	H	0.044825	0.539743	0.257519
36	H	-1.587643	-0.948000	1.577029
37	H	-2.019350	0.491580	2.515952
38	H	-3.277500	-2.366328	0.982759
39	H	-2.742857	-3.501478	-0.242737
40	H	-2.390258	-1.612870	-1.865857
41	H	-1.339130	-1.559369	-0.451027
42	C	-4.679150	-2.626936	-0.643762
43	C	-5.505850	-3.728713	0.030475
44	H	-4.642730	-2.809760	-1.726803
45	C	-6.933827	-3.826468	-0.514705
46	H	-4.997126	-4.693552	-0.098982
47	H	-5.538845	-3.544930	1.112900
48	H	-7.478277	-2.886603	-0.368369
49	H	-6.933158	-4.044026	-1.588883
50	H	-5.187082	-1.662367	-0.515936
51	C	-0.909500	5.018173	-0.072427
52	C	-2.320612	4.417971	-0.052113
53	H	-2.781843	4.615324	0.926016
54	H	-2.263717	3.325900	-0.141394
55	H	-0.454915	4.873261	-1.060312
56	C	-3.229896	4.958576	-1.162111
57	C	-4.620375	4.314639	-1.152870
58	H	-2.752339	4.781886	-2.135541
59	H	-4.547498	3.227079	-1.265380
60	H	-5.142325	4.516370	-0.210175
61	H	-3.323678	6.048495	-1.062226
62	H	-0.964447	6.100900	0.091047
63	H	-5.244943	4.698134	-1.966548
64	H	-7.498799	-4.619881	-0.014667
65	O	3.162741	-3.021568	-0.314785
66	H	3.892196	-3.356461	0.227227
67	H	2.295734	-4.551595	-1.519730
68	O	1.372070	-4.855214	-1.503782
69	H	1.015532	-4.613362	-2.370902
70	H	0.939650	-3.757290	-0.395499

E[B3LYP/6-31G(d,p)] = -2007.77489 h, E[APFD/6-311+G(2d,p)] = -2006.942432 h
Gcorr[B3LYP/6-31G(d,p)] = 0.503743 h

18. PS6+2H_2O, R2, 2nd step, products

Center No.	Atom	X	Y	Z
1	C	1.886214	-3.954493	1.024663
2	C	1.123524	-2.663187	0.806957
3	O	0.699938	-2.288388	-0.272180
4	O	0.947545	-1.993271	1.965301
5	C	0.279285	-0.705556	1.932271
6	C	1.343656	0.381161	2.036426
7	O	2.346320	0.232679	1.011197
8	C	2.259807	0.794916	-0.220477
9	O	3.094108	0.463745	-1.041832
10	C	1.207667	1.849220	-0.501915
11	C	1.625946	3.257469	-0.013290
12	C	-0.679682	-0.682998	3.130697
13	O	-1.277134	0.587854	3.304894

14	P	-3.204816	1.584100	0.363086
15	O	-3.511953	0.963122	1.684936
16	O	-2.256436	2.837943	0.495398
17	O	-2.423783	0.680406	-0.709656
18	C	-3.061263	-0.375306	-1.461557
19	C	-3.515180	-1.561597	-0.593877
20	C	-4.173839	-2.614429	-1.500225
21	O	-5.197666	-2.100787	-2.210830
22	O	-3.840188	-3.778840	-1.557320
23	N	-2.429761	-2.086313	0.210046
24	H	1.133154	-4.744901	1.141205
25	H	2.430334	-3.895117	1.971410
26	H	-1.628149	-2.325562	-0.371060
27	H	-2.068056	0.651458	2.729287
28	H	-2.728417	-2.950995	0.654137
29	H	-5.577648	-2.819564	-2.746727
30	H	-4.310890	-1.209364	0.076044
31	H	-3.910578	0.033478	-2.010357
32	H	-2.299751	-0.700060	-2.174701
33	H	-1.422163	-1.477272	2.985899
34	H	-0.111627	-0.913964	4.040231
35	H	-0.281762	-0.624549	0.999936
36	H	0.872994	1.363934	2.019464
37	H	1.893440	0.277146	2.975417
38	H	1.757457	3.251909	1.076102
39	H	0.786527	3.930291	-0.221630
40	H	1.086036	1.864790	-1.587920
41	H	0.241397	1.580310	-0.069105
42	C	2.894886	3.803753	-0.678842
43	C	3.253672	5.217582	-0.204988
44	H	2.757078	3.809005	-1.769142
45	C	4.516985	5.771536	-0.870570
46	H	2.409058	5.891125	-0.403495
47	H	3.387288	5.210351	0.885261
48	H	5.385300	5.136421	-0.661148
49	H	4.400481	5.823266	-1.959128
50	H	3.740199	3.131361	-0.483297
51	C	2.822123	-4.289595	-0.145249
52	C	4.009847	-3.326902	-0.273244
53	H	4.598788	-3.354386	0.654829
54	H	3.642311	-2.297155	-0.373773
55	H	2.238643	-4.283080	-1.073041
56	C	4.923565	-3.648405	-1.462044
57	C	6.098357	-2.674256	-1.594268
58	H	4.330319	-3.632819	-2.386469
59	H	5.743276	-1.645201	-1.721040
60	H	6.733329	-2.696456	-0.701103
61	H	5.304806	-4.673890	-1.362541
62	H	3.190818	-5.313476	-0.010623
63	H	6.727775	-2.919213	-2.456134
64	H	4.747925	6.779993	-0.512164
65	O	-4.521830	2.010584	-0.466418
66	H	-5.281361	2.175041	0.113286
67	H	-2.235076	4.701394	-1.983087
68	O	-1.565279	4.068650	-1.685883
69	H	-1.434064	3.468987	-2.434209
70	H	-2.011184	3.296405	-0.370863

E[B3LYP/6-31G(d,p)] = -2007.829094 h, E[APFD/6-311+G(2d,p)] = -2007.00141 h
Gcorr[B3LYP/6-31G(d,p)] = 0.504247 h

19. PS6+2H_2O, R2, 3rd step, reactants (hydrolysed glycerol + carbon chains neglected)

Center No.	Atom	X	Y	Z
1	P	1.143955	-0.849021	0.160453
2	O	0.337637	-2.015142	0.858769
3	O	2.473581	-1.265765	-0.385448
4	O	0.195027	-0.366570	-1.070429
5	C	-0.960200	0.473126	-0.916168
6	C	-1.970452	-0.046481	0.132784
7	C	-3.312658	0.669291	-0.015926

8	O	-3.159708	2.003473	-0.030358
9	O	-4.382363	0.104793	-0.092837
10	N	-2.103060	-1.506234	0.072289
11	H	-2.357592	-1.806907	-0.867630
12	H	-0.658838	-1.986858	0.568867
13	H	-2.863456	-1.802504	0.681640
14	H	-4.041251	2.408426	-0.117083
15	H	-1.590725	0.208630	1.129511
16	H	-0.657720	1.487253	-0.647543
17	H	-1.419876	0.495417	-1.907246
18	O	1.167376	0.337171	1.211718
19	H	1.903894	1.037094	1.073766
20	H	3.594099	1.652858	0.155849
21	O	3.028530	2.073940	0.861631
22	H	3.582571	2.089060	1.654633
23	O	4.307980	0.638928	-0.992783
24	H	4.080927	0.965708	-1.874094
25	H	3.705445	-0.131463	-0.849725

E[B3LYP/6-31G(d,p)] = -1119.620075 h, E[APFD/6-311+G(2d,p)] = -1119.258008 h
Gcorr[B3LYP/6-31G(d,p)] = 0.143502 h

20. PS6+2H_2O, R2, 3rd step, TS

Center No.	Atom	X	Y	Z
1	P	-1.321708	-0.078096	-0.114556
2	O	-0.864468	1.286841	0.587792
3	O	-2.422663	-0.044406	-1.203103
4	O	-0.055705	-0.211429	-1.198490
5	C	1.250883	-0.666052	-0.877951
6	C	1.970725	0.207125	0.182384
7	C	3.468191	-0.082150	0.182224
8	O	3.717360	-1.385047	0.404128
9	O	4.332009	0.751448	0.008574
10	N	1.664198	1.623493	-0.030002
11	H	1.932754	1.910672	-0.969699
12	H	0.077132	1.570854	0.276672
13	H	2.205178	2.197581	0.613383
14	H	4.682725	-1.512035	0.389276
15	H	1.594149	-0.069342	1.174322
16	H	1.240709	-1.702041	-0.530657
17	H	1.807618	-0.622736	-1.819974
18	O	-0.956789	-1.469873	0.642637
19	H	-1.580979	-1.537979	1.387479
20	H	-3.868341	0.087388	0.704888
21	O	-2.768474	-0.038505	1.331592
22	H	-2.586160	0.745089	1.868816
23	O	-4.581343	0.180959	-0.196059
24	H	-5.090150	-0.639659	-0.267663
25	H	-3.576591	0.065762	-0.834995

E[B3LYP/6-31G(d,p)] = -1119.571013 h, E[APFD/6-311+G(2d,p)] = -1119.206162 h
Gcorr[B3LYP/6-31G(d,p)] = 0.143352 h

21. PS6+2H_2O, R2, 3rd step, products

Center No.	Atom	X	Y	Z
1	P	1.337972	-0.059263	-0.028184
2	O	0.802961	1.300225	-0.711777
3	O	2.366434	0.007388	1.208880
4	O	0.084448	-0.120686	1.124343
5	C	-1.222367	-0.600050	0.881216
6	C	-2.001062	0.217912	-0.184238
7	C	-3.487518	-0.113833	-0.123425
8	O	-3.710436	-1.422823	-0.343165
9	O	-4.368399	0.691238	0.096479
10	N	-1.725981	1.646202	-0.020857
11	H	-1.987908	1.953610	0.914148
12	H	-0.114320	1.584498	-0.362027
13	H	-2.288990	2.189251	-0.671876

14	H	-4.670239	-1.575581	-0.283031
15	H	-1.647208	-0.079878	-1.178270
16	H	-1.223919	-1.651084	0.580789
17	H	-1.745714	-0.516869	1.841209
18	O	0.891739	-1.525263	-0.607266
19	H	1.481370	-1.724360	-1.351794
20	H	4.370435	0.038480	-0.549021
21	O	2.653279	-0.058009	-1.201388
22	H	2.487624	0.663666	-1.823399
23	O	4.905063	0.140286	0.267699
24	H	5.300509	-0.730948	0.411596
25	H	3.315619	0.091718	0.928671

E[B3LYP/6-31G(d,p)] = -1119.586115 h, E[APFD/6-311+G(2d,p)] = -1119.221108 h
Gcorr[B3LYP/6-31G(d,p)] = 0.148559 h

22. PS6+2H_2O, R2, 4th step, reactants

Center No.	Atom	X	Y	Z
1	P	1.337995	-0.059410	-0.028138
2	O	0.803099	1.299851	-0.712294
3	O	2.366409	0.007696	1.208945
4	O	0.084377	-0.120221	1.124326
5	C	-1.222443	-0.599644	0.881393
6	C	-2.001093	0.217881	-0.184446
7	C	-3.487542	-0.113787	-0.123302
8	O	-3.710590	-1.422695	-0.343397
9	O	-4.368312	0.691242	0.097214
10	N	-1.725896	1.646229	-0.021759
11	H	-1.987960	1.954159	0.913037
12	H	-0.114128	1.584307	-0.362593
13	H	-2.288722	2.188996	-0.673173
14	H	-4.670374	-1.575433	-0.282930
15	H	-1.647290	-0.080422	-1.178332
16	H	-1.224051	-1.650814	0.581436
17	H	-1.745807	-0.516000	1.841336
18	O	0.891730	-1.525652	-0.606579
19	H	1.481399	-1.725122	-1.350977
20	H	4.370347	0.038417	-0.548917
21	O	2.653307	-0.058740	-1.201344
22	H	2.487722	0.662756	-1.823584
23	O	4.905022	0.140807	0.267685
24	H	5.300726	-0.730239	0.412004
25	H	3.315612	0.091952	0.928744

E[B3LYP/6-31G(d,p)] = -1119.586114 h, E[APFD/6-311+G(2d,p)] = -1119.221108 h
Gcorr[B3LYP/6-31G(d,p)] = 0.148552 h

23. PS6+2H_2O, R2, 4th step, TS

Center No.	Atom	X	Y	Z
1	P	1.537201	0.163909	-0.156517
2	O	1.117198	1.645343	-0.463101
3	O	2.355842	-0.216102	1.157208
4	O	-0.009832	0.484198	1.044947
5	C	-1.269943	-0.164683	1.030297
6	C	-2.147654	0.279923	-0.163306
7	C	-3.483312	-0.462379	-0.109491
8	O	-3.338161	-1.783496	-0.337441
9	O	-4.555667	0.055852	0.128872
10	N	-2.292322	1.729398	-0.169946
11	H	-2.971503	1.994663	0.542157
12	H	0.202708	1.464340	0.327816
13	H	-2.698413	2.024739	-1.054683
14	H	-4.217783	-2.194128	-0.262052
15	H	-1.637811	-0.031163	-1.080356
16	H	-1.130146	-1.247784	0.999530
17	H	-1.784947	0.090304	1.966835
18	O	0.698211	-1.084497	-0.764834
19	H	1.181091	-1.429064	-1.533351

20	H	4.596684	-0.452888	-0.448274
21	O	2.799868	0.043754	-1.258461
22	H	2.831226	0.859226	-1.780109
23	O	4.882082	-0.601572	0.471382
24	H	5.093843	-1.545078	0.516201
25	H	3.332406	-0.362594	0.970082

E[B3LYP/6-31G(d,p)] = -1119.547719 h, E[APFD/6-311+G(2d,p)] = -1119.184476 h
Gcorr[B3LYP/6-31G(d,p)] = 0.140518 h

24. PS6+2H_2O, R2, 4th step, products

Center No.	Atom	X	Y	Z
1	P	-1.993789	0.378872	0.179254
2	O	-1.277437	1.529144	0.819333
3	O	-3.360572	0.822923	-0.500046
4	O	1.110515	2.019565	-0.393608
5	C	2.102882	1.260759	0.253647
6	C	2.400138	-0.063471	-0.495909
7	C	3.689604	-0.686270	0.030483
8	O	4.772179	0.025419	-0.327689
9	O	3.738507	-1.688360	0.715345
10	N	1.282084	-1.015174	-0.392573
11	H	1.297856	-1.431426	0.539965
12	H	0.250422	1.866789	0.057568
13	H	1.445918	-1.795221	-1.028820
14	H	5.553293	-0.399576	0.068975
15	H	2.545471	0.191178	-1.549716
16	H	3.031610	1.841389	0.277399
17	H	1.830894	1.028151	1.293276
18	O	-1.196871	-0.408873	-0.921597
19	H	-0.182444	-0.575643	-0.699978
20	H	-4.440566	-1.736287	0.308914
21	O	-2.396276	-0.785457	1.247534
22	H	-2.615381	-0.408196	2.113770
23	O	-4.910372	-1.312397	-0.426579
24	H	-4.767374	-1.902372	-1.180758
25	H	-4.010585	0.062548	-0.572270

E[B3LYP/6-31G(d,p)] = -1119.617626 h, E[APFD/6-311+G(2d,p)] = -1119.25711 h
Gcorr[B3LYP/6-31G(d,p)] = 0.140608 h

III. Structures of molecules and transition states (TS) related to PC6 + 2 H_2O (R1) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

25. PC6+2H_2O, R1, 1st step, reactants

Center No.	Atom	X	Y	Z
1	P	-2.872582	0.390485	-0.480574
2	O	-2.749584	0.527700	1.017755
3	O	-3.887219	-0.882972	-0.810078
4	O	-2.237355	4.020415	-0.783516
5	H	-3.022605	4.575495	-0.686990
6	H	-2.599342	3.133767	-1.038552
7	O	-1.725199	3.036723	1.837377
8	H	-2.054927	2.134839	1.644699
9	H	-1.869013	3.491870	0.982665
10	O	-1.515175	-0.230732	-1.148697
11	O	-3.258261	1.571066	-1.339553
12	C	-5.128466	-0.938723	-0.110130
13	H	-5.855992	-0.270673	-0.584328
14	H	-4.985074	-0.626663	0.928297
15	C	-5.551496	-2.404460	-0.209770
16	H	-4.816413	-3.029931	0.299158
17	H	-5.595446	-2.701725	-1.258909
18	C	-6.955856	-2.371103	1.855877
19	H	-6.897684	-1.289387	1.956077
20	H	-7.898057	-2.727713	2.269805
21	H	-6.118547	-2.845344	2.366355
22	C	-7.105035	-4.234312	0.268089

23	H	-8.080456	-4.489874	0.679759
24	H	-7.058204	-4.507100	-0.785269
25	H	-6.317517	-4.740640	0.824542
26	C	-8.019419	-2.042085	-0.343260
27	H	-7.922392	-0.967043	-0.209512
28	H	-7.955516	-2.299340	-1.399746
29	H	-8.969486	-2.379705	0.068208
30	N	-6.905796	-2.743016	0.394696
31	C	-0.764247	-1.236881	-0.461949
32	H	-1.057585	-1.279336	0.591240
33	H	-0.955772	-2.210034	-0.927723
34	C	0.716007	-0.889616	-0.577435
35	H	0.980369	-0.726592	-1.624426
36	C	1.599189	-1.966883	0.025542
37	H	1.454953	-2.039895	1.107373
38	H	1.377576	-2.940947	-0.420029
39	C	1.259568	1.458958	-0.544291
40	C	1.358213	2.641581	0.389718
41	H	2.157582	2.424352	1.111029
42	H	0.425997	2.683077	0.970527
43	C	1.609544	3.967397	-0.330902
44	H	0.773247	4.162407	-1.013169
45	H	2.507753	3.884982	-0.954855
46	C	1.759296	5.142231	0.642528
47	H	0.857570	5.214253	1.266683
48	H	2.591535	4.941726	1.332627
49	O	0.942740	0.336276	0.151446
50	O	1.432587	1.483403	-1.746752
51	C	1.997981	6.484575	-0.059314
52	H	1.165710	6.684777	-0.747660
53	H	2.898122	6.409937	-0.684572
54	C	3.913053	-2.460419	0.189536
55	C	5.298918	-1.961733	-0.155526
56	H	5.330096	-1.787507	-1.238281
57	H	5.416929	-0.972102	0.304116
58	C	6.415563	-2.909344	0.284917
59	H	6.343024	-3.073661	1.366701
60	H	6.263102	-3.889221	-0.183615
61	C	7.810223	-2.379321	-0.066507
62	H	7.956031	-1.395809	0.402394
63	H	7.875013	-2.211824	-1.151015
64	C	8.941249	-3.319298	0.368147
65	H	8.875287	-3.486230	1.451781
66	H	8.794091	-4.301721	-0.100547
67	O	2.965437	-1.604484	-0.255781
68	O	3.650566	-3.486137	0.786575
69	C	2.148398	7.656951	0.914784
70	H	2.316913	8.599740	0.383952
71	H	1.249571	7.777466	1.530392
72	H	2.994731	7.501249	1.593692
73	C	10.334336	-2.788808	0.016512
74	H	11.118936	-3.481075	0.339019
75	H	10.441423	-2.644351	-1.064677
76	H	10.523375	-1.822981	0.498941

E[B3LYP/6-31G(d,p)] = -1937.194810 h, E[APFD/6-311+G(2d,p)] = -1936.364952 h
Gcorr[B3LYP/6-31G(d,p)] = 0.574051 h

26. PC6+2H_2O, R1, 1st step, TS

Center No.	Atom	X	Y	Z
1	P	3.004629	0.819304	0.081089
2	O	3.278308	0.973680	-1.392262
3	O	3.644050	-0.728237	0.417352
4	O	3.554648	4.034277	1.205676
5	H	4.225605	4.389507	0.606489
6	H	3.797837	2.571576	1.266367
7	O	1.963933	2.777765	-0.088325
8	H	2.140901	2.869818	-1.033700
9	H	2.743358	3.601880	0.533981
10	O	1.537146	0.365786	0.649334

11	O	3.842648	1.531353	1.230001
12	C	4.979398	-0.977052	0.026679
13	H	5.679024	-0.506478	0.729541
14	H	5.166936	-0.572431	-0.973635
15	C	5.102149	-2.501765	0.040256
16	H	4.445992	-2.925949	-0.721558
17	H	4.795863	-2.885129	1.015257
18	C	7.026362	-2.583839	-1.550668
19	H	7.176909	-1.507287	-1.510058
20	H	7.976208	-3.082053	-1.740479
21	H	6.308013	-2.836747	-2.329547
22	C	6.380539	-4.568028	-0.262185
23	H	7.371647	-4.987585	-0.429094
24	H	5.981806	-4.911336	0.691408
25	H	5.710776	-4.849603	-1.073560
26	C	7.451122	-2.679843	0.873698
27	H	7.579932	-1.599910	0.880715
28	H	7.044431	-3.018481	1.825808
29	H	8.407167	-3.164926	0.680805
30	N	6.492400	-3.063952	-0.225268
31	C	0.877480	-0.757013	0.057204
32	H	1.094869	-0.811827	-1.015178
33	H	1.214336	-1.686050	0.528816
34	C	-0.620168	-0.569003	0.276239
35	H	-0.832845	-0.457990	1.341644
36	C	-1.423195	-1.721162	-0.298381
37	H	-1.358429	-1.744523	-1.390118
38	H	-1.059417	-2.676533	0.090518
39	C	-1.367675	1.713820	0.355542
40	C	-1.421629	2.964218	-0.486380
41	H	-1.766852	2.702875	-1.492343
42	H	-0.366781	3.265008	-0.580527
43	C	-2.260385	4.087274	0.127434
44	H	-1.894771	4.293237	1.140094
45	H	-3.299380	3.750499	0.239583
46	C	-2.226148	5.372441	-0.707298
47	H	-1.184579	5.705988	-0.818735
48	H	-2.586961	5.158822	-1.723583
49	O	-1.013096	0.643934	-0.400264
50	O	-1.572386	1.658793	1.552457
51	C	-3.059969	6.509406	-0.104252
52	H	-2.698885	6.722011	0.911119
53	H	-4.100179	6.174353	0.007035
54	C	-3.668465	-2.484688	-0.286135
55	C	-5.069054	-2.161400	0.185448
56	H	-5.026153	-2.001733	1.270018
57	H	-5.345069	-1.189435	-0.243235
58	C	-6.097946	-3.233860	-0.175279
59	H	-6.105440	-3.375379	-1.262736
60	H	-5.785464	-4.193014	0.255272
61	C	-7.508466	-2.883447	0.311742
62	H	-7.815291	-1.920148	-0.119939
63	H	-7.492969	-2.737360	1.401166
64	C	-8.552088	-3.950532	-0.040178
65	H	-8.566903	-4.095593	-1.128851
66	H	-8.243779	-4.912668	0.390795
67	O	-2.794920	-1.527186	0.099342
68	O	-3.337900	-3.463182	-0.927138
69	C	-3.023430	7.793106	-0.938924
70	H	-3.627493	8.584406	-0.482953
71	H	-1.999504	8.171297	-1.038393
72	H	-3.410550	7.619130	-1.949503
73	C	-9.960766	-3.599812	0.448076
74	H	-10.681874	-4.379595	0.182025
75	H	-9.984074	-3.482309	1.537556
76	H	-10.309650	-2.659029	0.007049

E[B3LYP/6-31G(d,p)] = -1937.134679 h, E[APFD/6-311+G(2d,p)] = -1936.303045 h
Gcorr[B3LYP/6-31G(d,p)] = 0.573956 h

27. PC6+2H_2O, R1, 1st step, products

Center No.	Atom	X	Y	Z
1	P	-3.201568	1.156159	-0.493876
2	O	-3.660351	1.669902	0.864168
3	O	-3.603316	-0.548826	-0.241553
4	O	-4.233768	3.658216	-2.974939
5	H	-4.969303	4.096223	-2.525410
6	H	-4.254530	1.947257	-2.269561
7	O	-2.639859	2.771101	-1.062208
8	H	-2.663981	3.282783	-0.242502
9	H	-3.540130	3.569885	-2.269974
10	O	-1.626498	0.681675	-0.769741
11	O	-4.171192	1.076754	-1.823898
12	C	-4.901475	-0.833442	0.204986
13	H	-5.648429	-0.585366	-0.562531
14	H	-5.137508	-0.255743	1.107055
15	C	-4.888808	-2.337109	0.492355
16	H	-4.141260	-2.555184	1.257145
17	H	-4.626931	-2.883689	-0.415582
18	C	-6.631273	-2.297598	2.283066
19	H	-6.864283	-1.250349	2.104461
20	H	-7.516604	-2.817530	2.647168
21	H	-5.820754	-2.385136	3.005744
22	C	-5.968060	-4.410576	1.233451
23	H	-6.897354	-4.856563	1.585618
24	H	-5.658860	-4.875261	0.298131
25	H	-5.187934	-4.524374	1.984986
26	C	-7.289423	-2.786323	-0.037052
27	H	-7.502510	-1.729654	-0.181017
28	H	-6.954333	-3.234038	-0.971871
29	H	-8.179955	-3.298077	0.326122
30	N	-6.198059	-2.940279	0.990652
31	C	-1.044027	-0.523065	-0.282965
32	H	-1.281637	-0.679115	0.773979
33	H	-1.405357	-1.391341	-0.842004
34	C	0.464156	-0.394771	-0.464965
35	H	0.697694	-0.134686	-1.499278
36	C	1.184248	-1.671030	-0.067064
37	H	1.074866	-1.871206	1.002571
38	H	0.786236	-2.525559	-0.621893
39	C	1.538374	1.743549	-0.173965
40	C	1.932564	2.749009	0.886843
41	H	2.561453	2.228404	1.619944
42	H	1.020822	3.029581	1.429350
43	C	2.641997	3.982774	0.327513
44	H	1.991469	4.469550	-0.409018
45	H	3.538470	3.666484	-0.219530
46	C	3.029187	4.986496	1.419345
47	H	2.127686	5.297266	1.966368
48	H	3.677311	4.492422	2.157146
49	O	0.940773	0.670057	0.393163
50	O	1.728101	1.869573	-1.367532
51	C	3.741945	6.229321	0.872487
52	H	3.093695	6.721609	0.134987
53	H	4.642311	5.917599	0.325964
54	C	3.395689	-2.526895	-0.063047
55	C	4.827906	-2.224645	-0.445408
56	H	4.847519	-2.036592	-1.526590
57	H	5.104323	-1.271811	0.022849
58	C	5.808032	-3.334518	-0.062503
59	H	5.757039	-3.502935	1.020090
60	H	5.491183	-4.273299	-0.532492
61	C	7.250670	-3.012768	-0.468245
62	H	7.560617	-2.068450	0.001440
63	H	7.295592	-2.841949	-1.553256
64	C	8.245356	-4.116451	-0.088463
65	H	8.198981	-4.286369	0.995733
66	H	7.934288	-5.059574	-0.557762
67	O	2.580006	-1.497341	-0.383605
68	O	2.997069	-3.549574	0.459508

69	C	4.128070	7.232216	1.963759
70	H	4.634605	8.106638	1.542237
71	H	3.243855	7.588228	2.504822
72	H	4.803420	6.777814	2.697764
73	C	9.686735	-3.794643	-0.494159
74	H	10.371508	-4.600273	-0.209748
75	H	9.770604	-3.653232	-1.577794
76	H	10.037133	-2.874305	-0.013012

E[B3LYP/6-31G(d,p)] = -1937.143668 h, E[APFD/6-311+G(2d,p)] = -1936.310478 h
Gcorr[B3LYP/6-31G(d,p)] = 0.574926 h

28. PC6+2H_2O, R1, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	P	3.716146	-2.205339	-0.930630
2	O	4.130932	-3.271310	0.069622
3	O	4.207812	-0.774885	0.193464
4	O	6.067627	0.751729	-0.901011
5	H	5.580842	1.511158	-1.249561
6	H	3.213115	-4.124620	-1.789565
7	O	4.693083	-1.471782	-2.022653
8	H	5.176413	-0.698871	-1.663389
9	H	5.436155	0.339258	-0.260396
10	O	2.194905	-1.499415	-0.807476
11	O	3.226982	-3.251598	-2.202479
12	C	3.756512	-0.802395	1.521604
13	H	4.596349	-0.957513	2.215115
14	H	3.050989	-1.624115	1.675952
15	C	3.084969	0.555453	1.762849
16	H	2.267676	0.676657	1.053228
17	H	3.809472	1.359468	1.615381
18	C	1.377126	-0.199532	3.420175
19	H	1.796562	-1.202656	3.457314
20	H	0.923722	0.045405	4.380283
21	H	0.642812	-0.117568	2.619924
22	C	1.883593	2.178071	3.155238
23	H	1.436430	2.360270	4.132408
24	H	2.678601	2.899328	2.968148
25	H	1.127842	2.229742	2.372220
26	C	3.526695	0.699709	4.221104
27	H	3.916194	-0.315478	4.260045
28	H	4.327743	1.401185	3.989776
29	H	3.069227	0.956578	5.176093
30	N	2.478342	0.791907	3.146393
31	C	1.021014	-2.195056	-1.221825
32	H	0.970461	-2.268958	-2.311441
33	H	0.995055	-3.212262	-0.814474
34	C	-0.184027	-1.431838	-0.687474
35	H	-0.077253	-1.257776	0.383888
36	C	-1.483853	-2.165238	-0.971320
37	H	-1.669957	-2.243165	-2.046192
38	H	-1.454551	-3.173978	-0.549752
39	C	-0.196461	0.984509	-0.636445
40	C	-0.318388	2.196479	-1.533204
41	H	-1.259307	2.096422	-2.088882
42	H	0.475330	2.127376	-2.287592
43	C	-0.258127	3.530150	-0.787939
44	H	0.693628	3.600407	-0.247575
45	H	-1.046412	3.554344	-0.026019
46	C	-0.408249	4.732897	-1.726661
47	H	0.380274	4.699871	-2.491802
48	H	-1.361532	4.656100	-2.268598
49	O	-0.252911	-0.148069	-1.360974
50	O	-0.065994	1.017950	0.576341
51	C	-0.348659	6.080336	-0.996998
52	H	0.604029	6.155794	-0.455550
53	H	-1.136635	6.111830	-0.232430
54	C	-3.795610	-1.898155	-0.512117
55	C	-4.812694	-1.015462	0.176826
56	H	-4.532561	-0.953503	1.236114

57	H	-4.691944	0.001028	-0.218209
58	C	-6.253158	-1.503211	0.015677
59	H	-6.496780	-1.562530	-1.052012
60	H	-6.333358	-2.525461	0.404488
61	C	-7.264373	-0.597310	0.727204
62	H	-7.175623	0.426525	0.336935
63	H	-7.013461	-0.538335	1.795851
64	C	-8.714229	-1.072799	0.573785
65	H	-8.963347	-1.132021	-0.494343
66	H	-8.801546	-2.095925	0.963720
67	O	-2.543827	-1.411146	-0.351274
68	O	-4.034889	-2.915321	-1.132755
69	C	-0.499278	7.280815	-1.936119
70	H	-0.452471	8.226636	-1.386543
71	H	0.295076	7.294603	-2.691152
72	H	-1.458130	7.250661	-2.466178
73	C	-9.723985	-0.166835	1.284661
74	H	-10.748197	-0.532133	1.156739
75	H	-9.520663	-0.115341	2.360447
76	H	-9.683515	0.855539	0.891697

E[B3LYP/6-31G(d,p)] = -1937.147896 h, E[APFD/6-311+G(2d,p)] = -1936.317414 h
Gcorr[B3LYP/6-31G(d,p)] = 0.577364 h

29. PC6+2H_2O, R1, 2nd step, TS

Center No.	Atom	X	Y	Z
1	P	3.743665	-2.271571	-0.963322
2	O	4.160359	-3.116788	0.205316
3	O	4.128958	-0.416517	0.350492
4	O	6.297906	0.276227	-0.586053
5	H	6.151760	1.142007	-0.991212
6	H	3.468267	-4.256283	-1.756898
7	O	4.766445	-1.465501	-1.894476
8	H	5.345025	-0.788703	-1.433796
9	H	5.453716	0.117674	-0.000108
10	O	2.273175	-1.529232	-0.936001
11	O	3.377695	-3.381409	-2.157738
12	C	3.654361	-0.474454	1.645621
13	H	4.450847	-0.641800	2.396637
14	H	2.934669	-1.298800	1.769332
15	C	2.958883	0.874639	1.907069
16	H	2.182660	1.016036	1.155936
17	H	3.686695	1.685297	1.824655
18	C	1.196312	0.035229	3.468016
19	H	1.663049	-0.944224	3.547219
20	H	0.662499	0.265973	4.389935
21	H	0.518288	0.068635	2.616024
22	C	1.607815	2.433597	3.241489
23	H	1.113749	2.600530	4.198815
24	H	2.374871	3.190452	3.079946
25	H	0.881881	2.450367	2.429119
26	C	3.256608	1.020817	4.385453
27	H	3.708182	0.031323	4.414290
28	H	4.022832	1.776590	4.215198
29	H	2.737002	1.220106	5.322526
30	N	2.263301	1.077433	3.259083
31	C	1.091971	-2.275218	-1.257213
32	H	1.011012	-2.415528	-2.338876
33	H	1.103305	-3.262497	-0.783776
34	C	-0.104065	-1.497042	-0.727217
35	H	0.027800	-1.280673	0.333733
36	C	-1.402881	-2.253836	-0.952464
37	H	-1.609019	-2.378374	-2.019213
38	H	-1.355678	-3.243887	-0.489899
39	C	-0.192781	0.915971	-0.761404
40	C	-0.314652	2.091669	-1.704782
41	H	-1.228860	1.943677	-2.293350
42	H	0.510883	2.021675	-2.424159
43	C	-0.324029	3.450954	-1.004703
44	H	0.601486	3.567723	-0.428070

45	H	-1.144454	3.477353	-0.277531
46	C	-0.468467	4.616520	-1.989998
47	H	0.352902	4.582074	-2.719680
48	H	-1.394954	4.492810	-2.568486
49	O	-0.190513	-0.243648	-1.449200
50	O	-0.107771	0.993283	0.452419
51	C	-0.479324	5.988557	-1.305168
52	H	0.446574	6.110633	-0.727003
53	H	-1.300096	6.021372	-0.575968
54	C	-3.708473	-1.980119	-0.472758
55	C	-4.721149	-1.076754	0.195150
56	H	-4.429360	-0.974849	1.248167
57	H	-4.609114	-0.075054	-0.238389
58	C	-6.161170	-1.575814	0.068021
59	H	-6.415540	-1.676804	-0.994004
60	H	-6.233048	-2.582750	0.496416
61	C	-7.168902	-0.647356	0.754950
62	H	-7.088585	0.361158	0.324992
63	H	-6.907447	-0.546676	1.817929
64	C	-8.618107	-1.134224	0.634565
65	H	-8.877614	-1.235214	-0.427943
66	H	-8.696957	-2.142055	1.064117
67	O	-2.456335	-1.483144	-0.343760
68	O	-3.949951	-3.019600	-1.054009
69	C	-0.623930	7.152274	-2.290357
70	H	-0.628312	8.116685	-1.771991
71	H	0.201573	7.165266	-3.011209
72	H	-1.557718	7.075519	-2.859052
73	C	-9.624746	-0.205896	1.320557
74	H	-10.648519	-0.580074	1.217138
75	H	-9.410880	-0.112449	2.391456
76	H	-9.592850	0.800839	0.888386

E[B3LYP/6-31G(d,p)] = -1937.143962 h, E[APFD/6-311+G(2d,p)] = -1936.311906 h
Gcorr[B3LYP/6-31G(d,p)] = 0.576771 h

30. PC6+2H_2O, R1, 2nd step, products

Center No.	Atom	X	Y	Z
1	P	3.249977	-2.296584	-1.019039
2	O	2.477834	-2.279174	0.274974
3	O	4.732269	0.733704	2.324840
4	O	6.192520	-0.969374	0.832209
5	H	6.890364	-0.453915	0.406398
6	H	3.065324	-4.438751	-0.805249
7	O	4.573465	-1.580259	-1.166873
8	H	5.579698	-1.225258	0.085948
9	H	5.294061	0.136021	1.769449
10	O	2.353615	-1.705841	-2.274584
11	O	3.441808	-3.867785	-1.489556
12	C	3.638250	-0.030505	2.791793
13	H	3.810327	-0.379343	3.822020
14	H	3.460047	-0.907571	2.158925
15	C	2.433986	0.913728	2.726711
16	H	2.187711	1.121981	1.684589
17	H	2.679669	1.851971	3.228805
18	C	0.765328	-0.933786	2.791749
19	H	1.498104	-1.678020	3.095533
20	H	-0.218455	-1.200364	3.177526
21	H	0.753496	-0.850627	1.706965
22	C	0.055955	1.398221	3.067187
23	H	-0.864488	1.053433	3.537645
24	H	0.344091	2.366503	3.475604
25	H	-0.063215	1.457269	1.986342
26	C	1.298412	0.290673	4.863719
27	H	2.068415	-0.441008	5.097601
28	H	1.571967	1.266377	5.264093
29	H	0.345081	-0.031286	5.281543
30	N	1.150000	0.404711	3.370535
31	C	1.042523	-2.222270	-2.499385
32	H	0.843946	-2.125182	-3.571444

33	H	0.988351	-3.285485	-2.238759
34	C	-0.003818	-1.446181	-1.704327
35	H	0.282030	-1.432238	-0.652998
36	C	-1.396104	-2.024843	-1.877931
37	H	-1.739934	-1.934378	-2.912427
38	H	-1.408554	-3.082708	-1.600126
39	C	0.231942	0.935163	-1.367030
40	C	0.194784	2.254809	-2.105607
41	H	-0.767281	2.312981	-2.629475
42	H	0.955511	2.205741	-2.895258
43	C	0.411802	3.474196	-1.209089
44	H	1.371684	3.373867	-0.688641
45	H	-0.359676	3.492607	-0.429604
46	C	0.383694	4.790796	-1.993910
47	H	1.155663	4.765812	-2.776072
48	H	-0.577973	4.883193	-2.518345
49	O	-0.018987	-0.085569	-2.209082
50	O	0.459591	0.800692	-0.177149
51	C	0.598549	6.025965	-1.110905
52	H	1.559555	5.932470	-0.587306
53	H	-0.172918	6.049606	-0.329367
54	C	-3.578506	-1.665431	-1.020295
55	C	-4.399072	-0.810822	-0.079627
56	H	-3.936570	-0.872530	0.913451
57	H	-4.280645	0.233947	-0.393921
58	C	-5.875452	-1.206161	-0.026452
59	H	-6.301907	-1.144749	-1.034920
60	H	-5.956723	-2.257261	0.275940
61	C	-6.686046	-0.327539	0.932928
62	H	-6.598354	0.724712	0.627132
63	H	-6.250841	-0.388820	1.940544
64	C	-8.168871	-0.713047	0.998545
65	H	-8.602406	-0.652194	-0.008822
66	H	-8.255017	-1.764643	1.303821
67	O	-2.280097	-1.286346	-1.010941
68	O	-3.996653	-2.577656	-1.706043
69	C	0.570322	7.340240	-1.896825
70	H	0.726052	8.202310	-1.240014
71	H	1.353477	7.359730	-2.663348
72	H	-0.391567	7.477370	-2.404042
73	C	-8.978092	0.165460	1.957240
74	H	-10.030832	-0.134437	1.982131
75	H	-8.588472	0.098628	2.979514
76	H	-8.938883	1.218891	1.657163

E[B3LYP/6-31G(d,p)] = -1937.19478 h, E[APFD/6-311+G(2d,p)] = -1936.364043 h
Gcorr[B3LYP/6-31G(d,p)] = 0.575076 h

31. PC6+2H_2O, R1, 3rd step, reactants (hydrolised choline neglected)

Center No.	Atom	X	Y	Z
1	P	-3.885771	-1.185424	-1.067560
2	O	-2.986954	-1.041962	-2.263404
3	O	-6.754358	-0.341803	0.922995
4	H	-6.261489	0.013009	1.675385
5	H	-5.581699	-2.892003	0.360918
6	O	-5.093775	-0.116260	-1.177023
7	H	-5.723646	-0.173659	-0.405385
8	O	-3.152521	-0.562927	0.298504
9	O	-4.397716	-2.577261	-0.707008
10	C	-2.101628	-1.329655	0.878667
11	H	-2.138456	-1.171897	1.962218
12	H	-2.250436	-2.398573	0.685628
13	C	-0.737388	-0.891473	0.349674
14	H	-0.757718	-0.865080	-0.740740
15	C	0.378179	-1.793682	0.847275
16	H	0.467639	-1.752298	1.936820
17	H	0.191500	-2.831069	0.554686
18	C	-0.201948	1.433646	-0.035518
19	C	0.011627	2.742986	0.694677
20	H	0.805636	2.582657	1.434951

21	H	-0.895256	2.947289	1.277783
22	C	0.347941	3.914161	-0.229021
23	H	-0.458107	4.038913	-0.962123
24	H	1.249367	3.672338	-0.805058
25	C	0.558936	5.225295	0.536605
26	H	-0.345847	5.459984	1.115252
27	H	1.364590	5.092915	1.272794
28	O	-0.486761	0.447807	0.845790
29	O	-0.131145	1.279539	-1.238637
30	C	0.897349	6.411270	-0.374733
31	H	0.091859	6.542836	-1.109817
32	H	1.801212	6.175831	-0.952761
33	C	2.728815	-2.003193	0.602483
34	C	3.945522	-1.417966	-0.080339
35	H	3.755917	-1.425799	-1.160987
36	H	4.003320	-0.358322	0.199410
37	C	5.245981	-2.148302	0.257576
38	H	5.396294	-2.133137	1.343775
39	H	5.149968	-3.204335	-0.022550
40	C	6.464165	-1.535645	-0.442532
41	H	6.552903	-0.476696	-0.161089
42	H	6.305547	-1.548951	-1.530224
43	C	7.776727	-2.257526	-0.114301
44	H	7.933573	-2.244571	0.972772
45	H	7.686967	-3.315344	-0.396155
46	O	1.607424	-1.336763	0.247813
47	O	2.725297	-2.944231	1.372130
48	C	1.107827	7.719965	0.392652
49	H	1.347525	8.546544	-0.284237
50	H	0.208333	7.998862	0.953422
51	H	1.930091	7.629179	1.111682
52	C	8.993250	-1.643653	-0.813598
53	H	9.913354	-2.180144	-0.559748
54	H	8.880091	-1.673595	-1.903371
55	H	9.128483	-0.595121	-0.524450
56	O	-6.354674	-2.994814	0.994219
57	H	-6.704415	-1.330203	1.036914
58	H	-7.051214	-3.396174	0.457239

E[B3LYP/6-31G(d,p)] = -1684.788393 h, E[APFD/6-311+G(2d,p)] = -1684.158671 h
Gcorr[B3LYP/6-31G(d,p)] = 0.409829 h

32. PC6+2H_2O, R1, 3rd step, TS

Center No.	Atom	X	Y	Z
1	P	3.797928	-1.721101	0.130362
2	O	2.727426	-2.107632	1.123842
3	O	6.639749	-0.795877	2.180414
4	H	7.465059	-0.819072	1.677068
5	H	4.982911	-3.341532	-0.303056
6	O	4.711647	-0.399901	0.313660
7	H	5.416314	-0.491848	1.007684
8	O	2.945733	-0.931794	-1.104836
9	O	4.401898	-2.834784	-0.914149
10	C	1.761953	-1.547145	-1.576652
11	H	1.688420	-1.345886	-2.653054
12	H	1.780997	-2.635455	-1.443714
13	C	0.523175	-0.987311	-0.876933
14	H	0.661994	-1.059788	0.201103
15	C	-0.748868	-1.692886	-1.307100
16	H	-0.961700	-1.526393	-2.367436
17	H	-0.666766	-2.770075	-1.135954
18	C	0.478583	1.351962	-0.279773
19	C	0.343346	2.736231	-0.880422
20	H	-0.588776	2.758000	-1.458724
21	H	1.148004	2.854540	-1.617406
22	C	0.377298	3.861208	0.154662
23	H	1.314492	3.801843	0.720981
24	H	-0.428657	3.706611	0.882412
25	C	0.241985	5.250224	-0.479286
26	H	1.049431	5.398342	-1.210487

27	H	-0.696941	5.302195	-1.048801
28	O	0.394155	0.411485	-1.244877
29	O	0.639568	1.113631	0.901665
30	C	0.274118	6.389579	0.546647
31	H	1.212626	6.336978	1.114909
32	H	-0.532475	6.240153	1.277148
33	C	-3.053103	-1.691215	-0.732963
34	C	-4.092166	-1.045580	0.157965
35	H	-3.744708	-1.137988	1.194515
36	H	-4.088757	0.030637	-0.057360
37	C	-5.493205	-1.635305	-0.009468
38	H	-5.803937	-1.535764	-1.056483
39	H	-5.458731	-2.711865	0.197543
40	C	-6.526438	-0.965943	0.903758
41	H	-6.554044	0.113023	0.695028
42	H	-6.206848	-1.064935	1.950902
43	C	-7.937151	-1.546979	0.749036
44	H	-8.255911	-1.446934	-0.297327
45	H	-7.907970	-2.625239	0.956402
46	O	-1.830434	-1.160787	-0.512625
47	O	-3.258884	-2.570677	-1.547122
48	C	0.138063	7.776758	-0.088202
49	H	0.164455	8.567466	0.668754
50	H	0.950651	7.968337	-0.798367
51	H	-0.807186	7.870683	-0.635063
52	C	-8.967869	-0.878425	1.663620
53	H	-9.963400	-1.314211	1.529977
54	H	-8.693394	-0.992192	2.718625
55	H	-9.043615	0.195144	1.456182
56	O	5.234943	-2.720179	1.332949
57	H	6.194969	-1.694218	1.981566
58	H	4.639856	-3.092951	1.996324

E[B3LYP/6-31G(d,p)] = -1684.791584 h, E[APFD/6-311+G(2d,p)] = -1684.10603 h
Gcorr[B3LYP/6-31G(d,p)] = 0.41218 h

33. PC6+2H_2O, R1, 3rd step, products

Center No.	Atom	X	Y	Z
1	P	3.835931	-1.766540	0.161817
2	O	2.732564	-2.229007	1.100311
3	O	6.768041	-0.684020	2.101233
4	H	7.533443	-0.693085	1.510387
5	H	5.075603	-3.329434	-0.508532
6	O	4.621197	-0.342300	0.331077
7	H	5.361758	-0.399506	0.975037
8	O	2.903422	-0.979693	-1.061122
9	O	4.455046	-2.770211	-1.006557
10	C	1.730318	-1.623497	-1.499475
11	H	1.630044	-1.455942	-2.581557
12	H	1.759067	-2.707627	-1.334608
13	C	0.492168	-1.062021	-0.797359
14	H	0.644337	-1.120009	0.279423
15	C	-0.782491	-1.774149	-1.205831
16	H	-1.001497	-1.629028	-2.267930
17	H	-0.699781	-2.847905	-1.013585
18	C	0.481357	1.288530	-0.241240
19	C	0.367850	2.663260	-0.868915
20	H	-0.561016	2.689438	-1.451937
21	H	1.177820	2.753372	-1.604361
22	C	0.418711	3.808685	0.142615
23	H	1.347550	3.737391	0.721057
24	H	-0.399190	3.690806	0.864036
25	C	0.326778	5.186565	-0.522734
26	H	1.145552	5.296698	-1.248077
27	H	-0.604290	5.250784	-1.103794
28	O	0.353250	0.332182	-1.183282
29	O	0.662727	1.072963	0.942079
30	C	0.378967	6.347667	0.477591
31	H	1.309049	6.282002	1.058225
32	H	-0.439855	6.237664	1.201455

33	C	-3.094207	-1.721258	-0.658574
34	C	-4.127640	-1.054219	0.223542
35	H	-3.822042	-1.208765	1.266171
36	H	-4.057989	0.027859	0.055451
37	C	-5.551977	-1.558036	-0.013183
38	H	-5.819082	-1.403540	-1.065660
39	H	-5.584186	-2.641496	0.153769
40	C	-6.579123	-0.864097	0.888538
41	H	-6.538643	0.221472	0.720024
42	H	-6.304354	-1.018681	1.941663
43	C	-8.013577	-1.357141	0.662903
44	H	-8.286568	-1.203394	-0.389880
45	H	-8.053229	-2.441687	0.832205
46	O	-1.861476	-1.226193	-0.417062
47	O	-3.313529	-2.588900	-1.482136
48	C	0.289503	7.723111	-0.190269
49	H	0.329265	8.530133	0.548671
50	H	1.115500	7.875381	-0.894473
51	H	-0.646169	7.830710	-0.750916
52	C	-9.038594	-0.661307	1.563453
53	H	-10.051392	-1.034296	1.379120
54	H	-8.810763	-0.825745	2.622868
55	H	-9.045928	0.421163	1.391582
56	O	5.182029	-2.574649	1.254697
57	H	6.308671	-1.552968	1.918771
58	H	4.634926	-2.967610	1.947884

E[B3LYP/6-31G(d,p)] = -1684.792319 h, E[APFD/6-311+G(2d,p)] = -1684.108239 h
Gcorr[B3LYP/6-31G(d,p)] = 0.412643 h

34. PC6+2H_2O, R1, 4th step, reactants

Center No.	Atom	X	Y	Z
1	P	3.742828	-2.141052	-0.051880
2	O	3.155817	-3.516984	-0.327678
3	O	4.374406	-2.016772	3.743563
4	H	3.660356	-1.432110	3.456420
5	H	5.798492	-1.831509	-0.361181
6	O	3.201787	-1.179050	1.176364
7	H	2.580144	-0.509846	0.827033
8	O	2.772802	-1.196463	-1.205980
9	O	5.038801	-1.514507	-0.876332
10	C	1.532354	-1.673985	-1.658555
11	H	1.433411	-1.441814	-2.730054
12	H	1.462999	-2.760206	-1.532601
13	C	0.355167	-1.019747	-0.927161
14	H	0.460000	-1.147047	0.152690
15	C	-0.983097	-1.565238	-1.384257
16	H	-1.181441	-1.309566	-2.429031
17	H	-1.002014	-2.654024	-1.284716
18	C	0.881483	1.268664	-0.351821
19	C	0.723755	2.695179	-0.830122
20	H	-0.344884	2.868549	-1.007830
21	H	1.199083	2.760876	-1.817208
22	C	1.302059	3.736663	0.128685
23	H	2.364911	3.523835	0.294566
24	H	0.814517	3.638302	1.106083
25	C	1.135390	5.169094	-0.391086
26	H	1.621728	5.260331	-1.372708
27	H	0.068801	5.375047	-0.559693
28	O	0.337305	0.407518	-1.221771
29	O	1.423780	0.945536	0.695018
30	C	1.710620	6.227138	0.558268
31	H	2.776057	6.019802	0.726444
32	H	1.224217	6.134805	1.538754
33	C	-3.274848	-1.364345	-0.798644
34	C	-4.240974	-0.691253	0.151685
35	H	-3.927252	-0.940130	1.173390
36	H	-4.098207	0.392630	0.057281
37	C	-5.701419	-1.077793	-0.085627
38	H	-5.978628	-0.825356	-1.116293

39	H	-5.805058	-2.166213	0.000321
40	C	-6.658628	-0.387285	0.892407
41	H	-6.547136	0.702805	0.804422
42	H	-6.372220	-0.639931	1.923246
43	C	-8.128139	-0.764629	0.669464
44	H	-8.413452	-0.511782	-0.360660
45	H	-8.238202	-1.853987	0.756984
46	O	-2.003014	-0.985619	-0.543728
47	O	-3.570389	-2.146193	-1.681621
48	C	1.544253	7.657919	0.037739
49	H	1.964224	8.388920	0.736381
50	H	2.049668	7.789618	-0.925857
51	H	0.486514	7.905658	-0.107667
52	C	-9.082548	-0.074169	1.648346
53	H	-10.122432	-0.363217	1.464125
54	H	-8.842940	-0.335602	2.685439
55	H	-9.019302	1.016467	1.559836
56	O	4.964732	-2.760559	1.145215
57	H	4.679077	-2.334810	2.863176
58	H	4.845772	-3.717260	1.076784

E[B3LYP/6-31G(d,p)] = -1684.788393 h, E[APFD/6-311+G(2d,p)] = -1684.107194 h
Gcorr[B3LYP/6-31G(d,p)] = 0.415116 h

35. PC6+2H_2O, R1, 4th step, TS

Center No.	Atom	X	Y	Z
1	P	4.026899	-1.999926	1.023331
2	O	2.716810	-2.687974	1.280081
3	O	4.863545	-1.292334	-2.345677
4	H	3.988144	-1.028408	-1.766417
5	H	5.022129	-2.083310	-0.988450
6	O	4.210684	-0.394754	1.314211
7	H	4.732795	-0.352865	2.131755
8	O	3.012146	-0.992637	-0.800176
9	O	5.072520	-2.516321	-0.070747
10	C	1.866713	-1.616913	-1.278074
11	H	1.790773	-1.522350	-2.378858
12	H	1.840489	-2.695044	-1.045291
13	C	0.594981	-1.014937	-0.666639
14	H	0.658108	-1.073001	0.419809
15	C	-0.668293	-1.687479	-1.164194
16	H	-0.821551	-1.509405	-2.232697
17	H	-0.615991	-2.767412	-0.998638
18	C	0.626236	1.333589	-0.102672
19	C	0.630799	2.713075	-0.731930
20	H	-0.200155	2.762027	-1.445774
21	H	1.543487	2.788763	-1.337930
22	C	0.557496	3.853378	0.284204
23	H	1.392741	3.762125	0.988587
24	H	-0.357010	3.747361	0.881082
25	C	0.584400	5.236459	-0.376027
26	H	1.501359	5.337825	-0.974018
27	H	-0.251394	5.319564	-1.085382
28	O	0.519360	0.385690	-1.051706
29	O	0.707164	1.114123	1.092077
30	C	0.508103	6.390141	0.631414
31	H	1.343517	6.306463	1.339670
32	H	-0.408125	6.287617	1.228582
33	C	-3.006481	-1.629081	-0.743323
34	C	-4.085759	-0.969874	0.089069
35	H	-3.818079	-1.100642	1.145018
36	H	-4.030694	0.110674	-0.095313
37	C	-5.490142	-1.504506	-0.194828
38	H	-5.717398	-1.373865	-1.259720
39	H	-5.509349	-2.585389	-0.009414
40	C	-6.565966	-0.815736	0.652356
41	H	-6.540173	0.267321	0.465700
42	H	-6.331015	-0.946213	1.718301
43	C	-7.980018	-1.342224	0.378428
44	H	-8.213395	-1.211897	-0.686970

45	H	-8.004477	-2.424404	0.564956
46	O	-1.787754	-1.144228	-0.426944
47	O	-3.184751	-2.482657	-1.591724
48	C	0.535028	7.771405	-0.029820
49	H	0.479234	8.572544	0.714487
50	H	1.455827	7.916170	-0.606473
51	H	-0.308611	7.897054	-0.718198
52	C	-9.054488	-0.653303	1.224982
53	H	-10.051202	-1.050544	1.006722
54	H	-8.866342	-0.795462	2.295357
55	H	-9.076940	0.425789	1.034236
56	O	4.971977	-2.473287	2.333168
57	H	5.457759	-0.532311	-2.279385
58	H	4.382800	-2.958825	2.926508

E[B3LYP/6-31G(d,p)] = -1684.783045 h, E[APFD/6-311+G(2d,p)] = -1684.102077 h
Gcorr[B3LYP/6-31G(d,p)] = 0.410444 h

36. PC6+2H_2O, R1, 4th step, products

Center No.	Atom	X	Y	Z
1	P	5.770552	-1.685491	0.438680
2	O	4.490387	-2.471027	0.334884
3	O	5.106844	1.296895	-1.469208
4	H	3.589212	1.125279	-0.640276
5	H	5.587886	0.457846	-1.209497
6	O	5.642668	-0.615384	1.688753
7	H	4.876641	-0.861511	2.226321
8	O	2.733082	0.987287	-0.166540
9	O	6.348073	-0.912043	-0.728730
10	C	2.067491	-0.087620	-0.798650
11	H	2.058348	0.025928	-1.894783
12	H	2.544197	-1.051903	-0.565861
13	C	0.628322	-0.122135	-0.299942
14	H	0.616104	-0.139062	0.791912
15	C	-0.147033	-1.302961	-0.852692
16	H	-0.271396	-1.225378	-1.936501
17	H	0.370945	-2.240082	-0.629619
18	C	-0.444496	1.985095	0.179738
19	C	-1.037773	3.203596	-0.496202
20	H	-1.804320	2.855999	-1.199703
21	H	-0.249186	3.647424	-1.117649
22	C	-1.608069	4.231886	0.481225
23	H	-0.820834	4.540917	1.179233
24	H	-2.386925	3.757644	1.090900
25	C	-2.184495	5.462702	-0.227574
26	H	-1.400791	5.932173	-0.839115
27	H	-2.969090	5.146436	-0.929667
28	O	-0.037793	1.087315	-0.743862
29	O	-0.345048	1.827983	1.381197
30	C	-2.761652	6.503313	0.739734
31	H	-1.977183	6.817851	1.441301
32	H	-3.544848	6.033485	1.349977
33	C	-2.301454	-2.270753	-0.615826
34	C	-3.623118	-2.153638	0.111562
35	H	-3.413122	-2.177462	1.188252
36	H	-4.021835	-1.150683	-0.087189
37	C	-4.632462	-3.234376	-0.278223
38	H	-4.804826	-3.193085	-1.360472
39	H	-4.200129	-4.221798	-0.075744
40	C	-5.965606	-3.090434	0.464386
41	H	-6.391071	-2.097246	0.261788
42	H	-5.786355	-3.129090	1.548274
43	C	-6.989752	-4.166170	0.082780
44	H	-7.167318	-4.127100	-1.000474
45	H	-6.563821	-5.158091	0.285646
46	O	-1.443527	-1.305117	-0.219397
47	O	-2.018434	-3.108370	-1.450473
48	C	-3.335643	7.733214	0.030034
49	H	-3.739392	8.456267	0.746319
50	H	-2.566624	8.243783	-0.560948

51	H	-4.145620	7.453620	-0.653425
52	C	-8.321724	-4.020317	0.824631
53	H	-9.030634	-4.801400	0.531011
54	H	-8.180224	-4.089590	1.909292
55	H	-8.787981	-3.051044	0.613810
56	O	6.994474	-2.676832	0.926338
57	H	5.571772	1.992940	-0.985965
58	H	6.629124	-3.404782	1.449096

E[B3LYP/6-31G(d,p)] = -1684.829415 h, E[APFD/6-311+G(2d,p)] = -1684.149438 h
Gcorr[B3LYP/6-31G(d,p)] = 0.405936 h

IV. Structures of molecules and transition states (TS) related to PC6 + 2 H_2O (R2) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

37. PC6+2H_2O, R2, 1st step, reactants

Center No.	Atom	X	Y	Z
1	P	3.356054	-1.594826	-1.607767
2	O	3.394585	-3.023066	-2.053447
3	O	2.994972	-1.658752	0.021723
4	O	6.614492	-0.767346	-0.144153
5	H	6.612870	0.076764	0.325515
6	H	5.876842	-0.690056	-0.803904
7	O	5.437492	-2.787186	1.384873
8	H	4.608305	-2.825949	0.885317
9	H	5.930747	-2.077131	0.916549
10	O	2.044947	-0.806664	-2.224120
11	O	4.504801	-0.632294	-1.810018
12	C	3.002680	-0.436127	0.769190
13	H	2.146076	0.178591	0.479546
14	H	3.925854	0.110959	0.563395
15	C	2.933338	-0.879342	2.230985
16	H	3.849385	-1.421380	2.477552
17	H	2.078245	-1.542030	2.376339
18	C	3.834422	1.305496	3.037565
19	H	3.655547	1.814741	2.092780
20	H	3.767005	2.019684	3.857186
21	H	4.814681	0.829574	3.034006
22	C	2.951202	-0.344992	4.619169
23	H	2.794353	0.440341	5.357469
24	H	2.216734	-1.138094	4.752754
25	H	3.959279	-0.747414	4.705104
26	C	1.410077	0.871499	3.150851
27	H	1.250983	1.275493	2.153541
28	H	0.667622	0.101986	3.359690
29	H	1.345755	1.663984	3.895609
30	N	2.780912	0.246930	3.241958
31	C	0.836230	-1.525387	-2.486791
32	H	0.570140	-1.358488	-3.536234
33	H	0.984587	-2.598704	-2.335879
34	C	-0.284530	-1.019476	-1.585854
35	H	0.024474	-1.064473	-0.540296
36	C	-1.572357	-1.798803	-1.788164
37	H	-1.966995	-1.659478	-2.798488
38	H	-1.404477	-2.867408	-1.625353
39	C	-0.359977	1.324044	-1.005192
40	C	-0.693671	2.685902	-1.571909
41	H	-1.727548	2.645674	-1.937258
42	H	-0.072883	2.830167	-2.465156
43	C	-0.503540	3.830937	-0.576366
44	H	0.535868	3.836464	-0.226640
45	H	-1.123642	3.646466	0.309146
46	C	-0.853591	5.196380	-1.178672
47	H	-0.232985	5.372853	-2.068636
48	H	-1.894696	5.184063	-1.531251
49	O	-0.550114	0.363414	-1.932862
50	O	0.025872	1.109283	0.130022
51	C	-0.666924	6.357028	-0.193962
52	H	0.373489	6.367749	0.158035
53	H	-1.287200	6.179408	0.694968

54	C	-3.760742	-1.850387	-0.874823
55	C	-4.662187	-1.245833	0.178642
56	H	-4.184114	-1.405134	1.153570
57	H	-4.666260	-0.158966	0.028215
58	C	-6.083234	-1.810964	0.163142
59	H	-6.526967	-1.644337	-0.825867
60	H	-6.040548	-2.898286	0.299426
61	C	-6.975515	-1.187789	1.242499
62	H	-7.009778	-0.097836	1.103666
63	H	-6.523870	-1.354476	2.230769
64	C	-8.405065	-1.742776	1.239941
65	H	-8.855073	-1.576042	0.251944
66	H	-8.369580	-2.831842	1.378250
67	O	-2.523570	-1.304701	-0.825144
68	O	-4.071235	-2.712763	-1.672718
69	C	-1.016478	7.720745	-0.797149
70	H	-0.872942	8.527680	-0.071159
71	H	-0.388595	7.940697	-1.668157
72	H	-2.061223	7.751406	-1.127064
73	C	-9.295344	-1.119165	2.318963
74	H	-10.307814	-1.535055	2.291477
75	H	-8.888360	-1.299346	3.320567
76	H	-9.377190	-0.034286	2.186104

E[B3LYP/6-31G(d,p)] = -1937.192777 h, E[APFD/6-311+G(2d,p)] = -1936.366317 h
Gcorr[B3LYP/6-31G(d,p)] = 0.575085 h

38. PC6+2H_2O, R2, 1st step, TS

Center No.	Atom	X	Y	Z
1	P	3.321347	-2.413333	-0.116348
2	O	2.943795	-3.511621	0.837316
3	O	4.051055	-1.024523	0.440930
4	O	5.639672	-4.033148	-2.013273
5	H	6.239471	-3.491476	-2.544751
6	H	4.412761	-3.272009	-1.908328
7	O	5.401169	-3.003962	0.138446
8	H	5.889796	-2.170387	0.146574
9	H	5.678712	-3.567787	-0.909101
10	O	1.863014	-1.589011	-0.375384
11	O	3.569774	-2.683389	-1.668513
12	C	3.352526	0.199912	0.681637
13	H	2.410827	0.022879	1.198189
14	H	3.131875	0.698250	-0.266336
15	C	4.328597	1.005480	1.540075
16	H	5.282175	1.120056	1.021532
17	H	4.504407	0.481957	2.481416
18	C	3.754169	3.274934	0.674122
19	H	2.982649	2.879236	0.017753
20	H	3.489721	4.283897	0.987916
21	H	4.717770	3.280969	0.166083
22	C	4.888181	3.010757	2.828997
23	H	4.579424	4.025862	3.074902
24	H	4.943746	2.405336	3.732572
25	H	5.852817	3.023266	2.323419
26	C	2.528044	2.372653	2.612457
27	H	1.752496	2.031991	1.927291
28	H	2.607585	1.698989	3.465220
29	H	2.302109	3.381384	2.956400
30	N	3.860723	2.407623	1.902937
31	C	0.703970	-2.338951	-0.676987
32	H	0.664098	-2.575295	-1.750014
33	H	0.695467	-3.280002	-0.114455
34	C	-0.518943	-1.519493	-0.279274
35	H	-0.447805	-1.237747	0.772831
36	C	-1.815113	-2.263256	-0.541314
37	H	-1.975266	-2.420112	-1.611719
38	H	-1.802851	-3.238438	-0.046242
39	C	-0.278898	0.874172	-0.485648
40	C	-0.312772	2.000419	-1.496602
41	H	-1.033178	1.744574	-2.279659

42	H	0.672524	2.014736	-1.983761
43	C	-0.618257	3.368342	-0.879067
44	H	0.109080	3.577604	-0.086646
45	H	-1.601261	3.333292	-0.392156
46	C	-0.598184	4.497964	-1.914904
47	H	0.386871	4.527833	-2.402072
48	H	-1.324309	4.277936	-2.710162
49	O	-0.553920	-0.305970	-1.075631
50	O	-0.026616	1.006267	0.699498
51	C	-0.908038	5.874603	-1.314517
52	H	-0.182641	6.093174	-0.519216
53	H	-1.892406	5.842994	-0.828261
54	C	-4.135663	-1.957151	-0.154693
55	C	-5.164964	-1.018989	0.436408
56	H	-4.894959	-0.849347	1.486351
57	H	-5.047566	-0.045974	-0.057336
58	C	-6.600818	-1.530304	0.311485
59	H	-6.831419	-1.703140	-0.746655
60	H	-6.680391	-2.506657	0.804659
61	C	-7.625058	-0.561406	0.912862
62	H	-7.537611	0.416137	0.417663
63	H	-7.386479	-0.388335	1.971896
64	C	-9.070483	-1.059986	0.795247
65	H	-9.307235	-1.233602	-0.263189
66	H	-9.156703	-2.036608	1.290462
67	O	-2.886792	-1.460985	-0.005881
68	O	-4.365763	-3.020294	-0.697339
69	C	-0.885907	7.002181	-2.350801
70	H	-1.110785	7.970801	-1.892545
71	H	0.096880	7.080313	-2.829676
72	H	-1.625191	6.827830	-3.140933
73	C	-10.093060	-0.090468	1.395347
74	H	-11.113800	-0.473964	1.296092
75	H	-9.902071	0.076081	2.461691
76	H	-10.053705	0.884757	0.896638

E[B3LYP/6-31G(d,p)] = -1937.131755 h, E[APFD/6-311+G(2d,p)] = -1936.30415 h
Gcorr[B3LYP/6-31G(d,p)] = 0.571674 h

39. PC6+2H_2O, R2, 1st step, products

Center No.	Atom	X	Y	Z
1	P	3.428990	-2.428249	-0.041878
2	O	2.936349	-3.508241	0.899044
3	O	4.064841	-0.953821	0.500724
4	O	5.700582	-4.389040	-2.092177
5	H	6.357493	-3.875268	-2.581524
6	H	4.233618	-3.238334	-1.925717
7	O	5.163601	-2.928007	0.061771
8	H	5.704155	-2.130273	-0.019227
9	H	5.698629	-3.976905	-1.189069
10	O	1.924541	-1.572912	-0.296730
11	O	3.469677	-2.675669	-1.675669
12	C	3.320424	0.228074	0.769201
13	H	2.425022	0.010803	1.349942
14	H	3.005271	0.703566	-0.163683
15	C	4.304277	1.099610	1.554456
16	H	5.233246	1.217704	0.993651
17	H	4.533415	0.625299	2.510381
18	C	3.698679	3.331251	0.617833
19	H	2.955981	2.887936	-0.041086
20	H	3.393281	4.339575	0.894385
21	H	4.671559	3.355730	0.128419
22	C	4.822161	3.154824	2.785894
23	H	4.502481	4.176442	2.987658
24	H	4.872319	2.587192	3.714010
25	H	5.792516	3.155270	2.291044
26	C	2.475551	2.467743	2.576137
27	H	1.710277	2.096189	1.895305
28	H	2.560615	1.817221	3.446235
29	H	2.230857	3.480986	2.893221

30	N	3.811412	2.505140	1.874004
31	C	0.777220	-2.315226	-0.616749
32	H	0.743795	-2.556581	-1.691053
33	H	0.753005	-3.259070	-0.056424
34	C	-0.460007	-1.504448	-0.240484
35	H	-0.403256	-1.208124	0.808334
36	C	-1.746902	-2.262624	-0.505587
37	H	-1.894780	-2.436074	-1.575255
38	H	-1.731441	-3.230563	0.003232
39	C	-0.282926	0.894540	-0.469859
40	C	-0.323033	2.008003	-1.496076
41	H	-1.035098	1.732112	-2.280261
42	H	0.664286	2.028957	-1.978865
43	C	-0.651638	3.379330	-0.898952
44	H	0.067711	3.609645	-0.105055
45	H	-1.636687	3.336379	-0.416814
46	C	-0.642094	4.496341	-1.948503
47	H	0.344893	4.534298	-2.431225
48	H	-1.361033	4.256656	-2.744639
49	O	-0.504036	-0.298425	-1.051826
50	O	-0.070057	1.051245	0.720480
51	C	-0.974134	5.875633	-1.366222
52	H	-0.255731	6.113791	-0.570170
53	H	-1.960266	5.835918	-0.884118
54	C	-4.075435	-1.978256	-0.142713
55	C	-5.120891	-1.043408	0.425526
56	H	-4.856596	-0.846650	1.472147
57	H	-5.017223	-0.079644	-0.089100
58	C	-6.548413	-1.579202	0.308205
59	H	-6.773827	-1.777302	-0.746615
60	H	-6.614031	-2.546452	0.821029
61	C	-7.588768	-0.614308	0.887971
62	H	-7.515570	0.354227	0.373131
63	H	-7.354795	-0.416003	1.943616
64	C	-9.026128	-1.137444	0.778594
65	H	-9.258820	-1.335243	-0.276495
66	H	-9.097846	-2.105488	1.292619
67	O	-2.834638	-1.464647	0.006769
68	O	-4.289870	-3.052961	-0.669346
69	C	-0.962899	6.991257	-2.415523
70	H	-1.203429	7.961923	-1.969678
71	H	0.020939	7.077598	-2.890824
72	H	-1.695964	6.797380	-3.206900
73	C	-10.064366	-0.172473	1.358822
74	H	-11.078951	-0.573504	1.265933
75	H	-9.877369	0.017465	2.421965
76	H	-10.039375	0.793501	0.841525

E[B3LYP/6-31G(d,p)] = -1937.142307 h, E[APFD/6-311+G(2d,p)] = -1936.311933 h
Gcorr[B3LYP/6-31G(d,p)] = 0.57788 h

40. PC6+2H_2O, R2, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	P	3.724421	-2.458655	-0.776546
2	O	2.937789	-3.722532	-0.532788
3	O	3.988851	-1.353008	0.449197
4	O	2.701308	0.488428	-2.941321
5	H	3.347188	1.071582	-2.519799
6	H	3.627985	-1.251002	-2.616753
7	O	5.275150	-3.091668	-0.509164
8	H	5.933632	-2.450966	-0.810467
9	H	2.344550	-0.060563	-2.191667
10	O	2.125136	-1.400769	-1.179813
11	O	4.250655	-1.898819	-2.236589
12	C	2.956660	-0.690715	1.170394
13	H	2.109910	-1.358019	1.338754
14	H	2.594004	0.179851	0.624732
15	C	3.623931	-0.305334	2.492671
16	H	4.548100	0.241779	2.297631
17	H	3.865425	-1.201658	3.066904

18	C	2.571103	1.944204	2.788433
19	H	1.939893	1.848089	1.906896
20	H	2.075927	2.574042	3.526934
21	H	3.542701	2.365269	2.532424
22	C	3.528049	0.745180	4.702172
23	H	2.946948	1.393353	5.356684
24	H	3.657683	-0.233818	5.161602
25	H	4.498643	1.194436	4.494856
26	C	1.438125	-0.047304	3.677940
27	H	0.851728	-0.045350	2.760771
28	H	1.591447	-1.063475	4.039879
29	H	0.934275	0.547353	4.439286
30	N	2.782359	0.580682	3.401991
31	C	0.917265	-2.038107	-1.499841
32	H	0.760083	-2.080333	-2.593052
33	H	0.922172	-3.067446	-1.124831
34	C	-0.266713	-1.296143	-0.874211
35	H	-0.135055	-1.216428	0.205994
36	C	-1.593763	-1.957245	-1.192236
37	H	-1.815063	-1.911970	-2.262329
38	H	-1.578006	-3.007323	-0.886640
39	C	-0.023976	1.103268	-0.648213
40	C	0.037784	2.367339	-1.476932
41	H	-0.865751	2.406015	-2.097213
42	H	0.872909	2.227400	-2.176801
43	C	0.203950	3.647425	-0.657842
44	H	1.124016	3.581804	-0.064618
45	H	-0.619762	3.729102	0.062130
46	C	0.248233	4.903713	-1.535556
47	H	1.069837	4.813620	-2.260315
48	H	-0.674902	4.967167	-2.128984
49	O	-0.310418	0.047421	-1.429335
50	O	0.175168	1.038233	0.554833
51	C	0.422405	6.197927	-0.731679
52	H	1.345261	6.133456	-0.139430
53	H	-0.398471	6.285912	-0.007125
54	C	-3.886643	-1.694857	-0.635855
55	C	-4.863789	-0.874044	0.177390
56	H	-4.542410	-0.918713	1.225642
57	H	-4.744025	0.175077	-0.121372
58	C	-6.316397	-1.327657	0.026137
59	H	-6.599522	-1.283731	-1.032474
60	H	-6.397718	-2.381108	0.320092
61	C	-7.287217	-0.481522	0.857403
62	H	-7.197244	0.573537	0.562070
63	H	-6.996549	-0.526644	1.916633
64	C	-8.748826	-0.923256	0.715093
65	H	-9.037803	-0.878305	-0.343654
66	H	-8.837491	-1.977569	1.010115
67	O	-2.620923	-1.256159	-0.459209
68	O	-4.170300	-2.629550	-1.359902
69	C	0.465479	7.451989	-1.609891
70	H	0.590736	8.357822	-1.007695
71	H	1.297385	7.407850	-2.322133
72	H	-0.458916	7.561825	-2.188433
73	C	-9.717915	-0.076754	1.545795
74	H	-10.751639	-0.416080	1.422891
75	H	-9.474666	-0.129735	2.613196
76	H	-9.676078	0.977686	1.249614

E[B3LYP/6-31G(d,p)] = -1937.144018 h, E[APFD/6-311+G(2d,p)] = -1936.313016 h
Gcorr[B3LYP/6-31G(d,p)] = 0.578953 h

41. PC6+2H_2O, R2, 2nd step, TS

Center No.	Atom	X	Y	Z
1	P	3.770036	-2.607358	-0.809946
2	O	2.985119	-3.782674	-1.310045
3	O	3.578846	-2.048988	0.737117
4	O	2.902413	0.542748	-2.677413
5	H	3.178694	1.243432	-2.071345

6	H	3.916356	-0.821343	-2.145184
7	O	5.201178	-3.366393	-0.406422
8	H	5.812042	-2.730776	-0.008126
9	H	2.363715	-0.112452	-2.099774
10	O	2.023971	-1.341251	-1.258435
11	O	4.504500	-1.501480	-1.735418
12	C	2.970209	-0.824509	1.135270
13	H	1.885912	-0.898865	1.099162
14	H	3.269289	-0.009986	0.473257
15	C	3.496716	-0.611906	2.556776
16	H	4.564766	-0.387803	2.538184
17	H	3.341987	-1.518379	3.144789
18	C	2.924711	1.819751	2.567379
19	H	2.281992	1.764603	1.690060
20	H	2.583795	2.621000	3.222254
21	H	3.963959	1.985635	2.285061
22	C	3.551726	0.663249	4.642819
23	H	3.064686	1.446304	5.222353
24	H	3.501305	-0.285196	5.176199
25	H	4.589582	0.930169	4.447677
26	C	1.377783	0.209590	3.599551
27	H	0.832006	0.193257	2.658647
28	H	1.315492	-0.753289	4.105448
29	H	0.980765	0.994980	4.241888
30	N	2.830439	0.519065	3.326813
31	C	0.816272	-1.948020	-1.577026
32	H	0.633458	-1.974470	-2.670529
33	H	0.795370	-2.993384	-1.237473
34	C	-0.370316	-1.215067	-0.932608
35	H	-0.246128	-1.169968	0.150858
36	C	-1.704619	-1.844493	-1.277332
37	H	-1.926503	-1.749803	-2.344137
38	H	-1.700046	-2.907162	-1.018713
39	C	0.002566	1.163258	-0.666337
40	C	0.079165	2.443747	-1.470450
41	H	-0.842501	2.527807	-2.058214
42	H	0.885059	2.294636	-2.201801
43	C	0.319407	3.698985	-0.631359
44	H	1.257713	3.589596	-0.074411
45	H	-0.474156	3.791221	0.120546
46	C	0.373611	4.972928	-1.482589
47	H	1.164713	4.872821	-2.239282
48	H	-0.567967	5.080148	-2.039611
49	O	-0.397037	0.146697	-1.445979
50	O	0.273451	1.063578	0.520365
51	C	0.620155	6.241866	-0.657594
52	H	1.561329	6.133735	-0.101645
53	H	-0.170369	6.339687	0.098754
54	C	-3.992558	-1.605928	-0.685745
55	C	-4.962669	-0.811525	0.161925
56	H	-4.622212	-0.874076	1.203151
57	H	-4.858191	0.244589	-0.117563
58	C	-6.413589	-1.275577	0.027137
59	H	-6.716029	-1.212448	-1.025128
60	H	-6.479991	-2.335674	0.300309
61	C	-7.376930	-0.456346	0.893331
62	H	-7.302589	0.605397	0.618269
63	H	-7.066180	-0.520212	1.945883
64	C	-8.836669	-0.909561	0.769096
65	H	-9.146104	-0.845390	-0.282854
66	H	-8.909617	-1.970641	1.043450
67	O	-2.727027	-1.167146	-0.513393
68	O	-4.283134	-2.521543	-1.431519
69	C	0.672939	7.513866	-1.509058
70	H	0.849788	8.401002	-0.892149
71	H	1.476615	7.459407	-2.252316
72	H	-0.267642	7.666829	-2.050525
73	C	-9.797888	-0.090352	1.635548
74	H	-10.830469	-0.437335	1.525008
75	H	-9.533861	-0.163232	2.696825
76	H	-9.771809	0.970427	1.360977

E[B3LYP/6-31G(d,p)] = -1937.141958 h, E[APFD/6-311+G(2d,p)] = -1936.310286 h
Gcorr[B3LYP/6-31G(d,p)] = 0.578566 h

42. PC6+2H_2O, R2, 2nd step, products

Center No.	Atom	X	Y	Z
1	P	5.922631	-0.304528	-1.446512
2	O	5.994857	-1.603441	-2.189812
3	O	5.672304	-0.593367	0.178184
4	O	2.354292	0.948350	-1.540568
5	H	2.300885	1.582104	-0.813526
6	H	3.335951	0.868617	-1.718456
7	O	7.431755	0.315469	-1.325612
8	H	7.387558	1.253553	-1.090557
9	H	1.720575	-0.589022	-1.068145
10	O	1.457105	-1.478866	-0.722795
11	O	4.968928	0.796401	-1.878412
12	C	4.360288	-1.028032	0.529448
13	H	4.049799	-1.862763	-0.106468
14	H	3.645642	-0.212764	0.392766
15	C	4.464621	-1.446994	1.992893
16	H	4.802279	-0.599967	2.593089
17	H	5.189412	-2.256638	2.094578
18	C	2.097776	-0.876661	2.576470
19	H	1.754937	-0.757706	1.550335
20	H	1.268187	-1.209495	3.199341
21	H	2.508646	0.052808	2.969792
22	C	3.468083	-2.270255	4.065287
23	H	2.556397	-2.642711	4.530105
24	H	4.245258	-3.032849	4.098654
25	H	3.804388	-1.366275	4.571826
26	C	2.667648	-3.178822	1.926554
27	H	2.364389	-2.912481	0.915179
28	H	3.463547	-3.923022	1.919281
29	H	1.810049	-3.555065	2.483593
30	N	3.171764	-1.938561	2.624710
31	C	0.266123	-1.907291	-1.353399
32	H	0.288247	-1.699345	-2.432406
33	H	0.193624	-2.992982	-1.224973
34	C	-0.978570	-1.263629	-0.737744
35	H	-0.970261	-1.406742	0.344587
36	C	-2.265985	-1.804093	-1.331045
37	H	-2.359975	-1.539801	-2.388247
38	H	-2.300889	-2.893784	-1.242146
39	C	-0.757768	1.022498	0.013022
40	C	-0.745858	2.447364	-0.497965
41	H	-1.691675	2.615677	-1.028227
42	H	0.035114	2.509982	-1.266389
43	C	-0.534541	3.492345	0.598281
44	H	0.411299	3.288771	1.115266
45	H	-1.322854	3.387238	1.353428
46	C	-0.527727	4.924747	0.052570
47	H	0.260265	5.022376	-0.707657
48	H	-1.476647	5.122397	-0.465978
49	O	-0.934901	0.159187	-1.012865
50	O	-0.625648	0.687664	1.174708
51	C	-0.315469	5.985026	1.139940
52	H	0.632926	5.786459	1.657277
53	H	-1.102864	5.885688	1.899315
54	C	-4.602363	-1.589957	-0.974002
55	C	-5.653514	-0.905065	-0.128409
56	H	-5.437665	-1.137611	0.921974
57	H	-5.502014	0.177470	-0.226051
58	C	-7.085195	-1.295908	-0.497475
59	H	-7.260900	-1.064825	-1.554999
60	H	-7.199651	-2.382225	-0.399088
61	C	-8.131165	-0.585163	0.368735
62	H	-8.009257	0.502843	0.269639
63	H	-7.947203	-0.816654	1.427516
64	C	-9.572654	-0.967019	0.010997
65	H	-9.755264	-0.735356	-1.047043

66	H	-9.692854	-2.054369	0.109493
67	O	-3.358721	-1.223116	-0.590471
68	O	-4.812338	-2.369527	-1.882761
69	C	-0.309811	7.415863	0.593656
70	H	-0.156269	8.148347	1.392860
71	H	0.489263	7.554778	-0.143549
72	H	-1.259055	7.654901	0.100617
73	C	-10.616939	-0.256777	0.877466
74	H	-11.634299	-0.549828	0.598312
75	H	-10.480393	-0.496786	1.938158
76	H	-10.543423	0.831808	0.773182

E[B3LYP/6-31G(d,p)] = -1937.194465 h, E[APFD/6-311+G(2d,p)] = -1936.362517 h
Gcorr[B3LYP/6-31G(d,p)] = 0.575104 h

43. PC6+2H_2O, R2, 3rd step, reactants (hydrolised glycerol + carbon chains neglected)

Center No.	Atom	X	Y	Z
1	P	-1.395393	-0.420989	0.058231
2	O	-1.128246	0.703830	-0.930620
3	O	-0.128532	-1.497723	0.038541
4	O	-4.740342	0.034815	-0.577426
5	H	-3.362686	-1.004748	-0.603761
6	H	-2.836715	1.559798	1.082770
7	O	-2.486055	-1.471396	-0.523802
8	H	-5.279783	-0.256381	0.170535
9	O	-1.697997	-0.020963	1.490298
10	C	1.099403	-1.045600	0.599255
11	H	1.631665	-1.931303	0.954242
12	H	0.907607	-0.390973	1.455792
13	C	1.876300	-0.330449	-0.514926
14	H	1.260282	0.479653	-0.909041
15	H	2.086999	-1.037084	-1.319694
16	C	3.022944	1.375608	0.902483
17	H	2.622028	0.955856	1.822529
18	H	3.990632	1.835659	1.099100
19	H	2.333003	2.111868	0.492255
20	C	3.846116	0.860740	-1.348379
21	H	4.798497	1.313087	-1.074712
22	H	4.003345	0.062635	-2.072586
23	H	3.175098	1.614296	-1.758387
24	C	4.135830	-0.775128	0.456566
25	H	3.720801	-1.155941	1.387467
26	H	4.239332	-1.580490	-0.269574
27	H	5.104911	-0.316747	0.648566
28	N	3.214295	0.274363	-0.110057
29	O	-3.199920	2.103452	0.351727
30	H	-2.491631	1.939194	-0.309360
31	H	-4.307376	0.868768	-0.258953

E[B3LYP/6-31G(d,p)] = -1048.954493 h, E[APFD/6-311+G(2d,p)] = -1048.601217 h
Gcorr[B3LYP/6-31G(d,p)] = 0.214882 h

44. PC6+2H_2O, R2, 3rd step, TS

Center No.	Atom	X	Y	Z
1	P	-1.483935	-0.157972	0.033393
2	O	-0.841872	1.042491	0.686097
3	O	-0.251670	-0.819293	-0.929055
4	O	-4.831982	0.938074	-0.642443
5	H	-3.326420	0.355919	-1.089254
6	H	-2.443615	-1.276904	1.444104
7	O	-2.418606	-0.021857	-1.269254
8	H	-5.446985	0.207296	-0.793882
9	O	-1.679757	-1.545009	0.876253
10	C	1.010065	-1.020497	-0.320086
11	H	1.462956	-1.899520	-0.789938
12	H	0.912356	-1.224964	0.751133
13	C	1.844581	0.241547	-0.576877
14	H	1.310451	1.088105	-0.144115

15	H	1.956557	0.391689	-1.652323
16	C	3.209114	0.142020	1.510617
17	H	2.836186	-0.840386	1.792033
18	H	4.218787	0.276270	1.896749
19	H	2.550878	0.919473	1.896317
20	C	3.897643	1.562582	-0.361220
21	H	4.906888	1.584477	0.048542
22	H	3.931022	1.643405	-1.446765
23	H	3.303176	2.373179	0.057993
24	C	4.082022	-0.874174	-0.555611
25	H	3.656140	-1.826615	-0.246828
26	H	4.084724	-0.796628	-1.642346
27	H	5.097069	-0.783444	-0.170867
28	N	3.252959	0.250276	0.007832
29	O	-3.282895	0.214612	1.198285
30	H	-2.961647	0.939562	1.749937
31	H	-4.366506	0.705720	0.243780

E[B3LYP/6-31G(d,p)] = -1048.910596 h, E[APFD/6-311+G(2d,p)] = -1048.553979 h
Gcorr[B3LYP/6-31G(d,p)] = 0.217201 h

45. PC6+2H_2O, R2, 3rd step, products

Center No.	Atom	X	Y	Z
1	P	1.524960	0.121923	0.110906
2	O	0.737936	-1.030440	0.721747
3	O	0.285047	0.815608	-0.903045
4	O	4.980306	-0.858883	-0.614531
5	H	3.304378	-0.351495	-1.099670
6	H	2.345907	1.448555	1.531992
7	O	2.395449	-0.013945	-1.265526
8	H	5.505032	-0.052293	-0.710197
9	O	1.644928	1.590236	0.874255
10	C	-0.977480	1.023686	-0.318037
11	H	-1.416952	1.922875	-0.767706
12	H	-0.905763	1.194280	0.761963
13	C	-1.831567	-0.215574	-0.623798
14	H	-1.295298	-1.080490	-0.232459
15	H	-1.963284	-0.316568	-1.702978
16	C	-3.161713	-0.212273	1.487224
17	H	-2.789232	0.757174	1.810384
18	H	-4.162526	-0.373749	1.886192
19	H	-2.488614	-1.001475	1.819611
20	C	-3.895293	-1.529758	-0.440864
21	H	-4.900813	-1.562654	-0.022315
22	H	-3.940585	-1.558779	-1.528648
23	H	-3.304668	-2.365430	-0.067695
24	C	-4.058873	0.914939	-0.508510
25	H	-3.609494	1.845942	-0.168788
26	H	-4.088562	0.887137	-1.597291
27	H	-5.066085	0.822112	-0.103634
28	N	-3.232989	-0.244024	-0.017651
29	O	3.066058	-0.308251	1.094558
30	H	2.759112	-1.070462	1.603928
31	H	4.445738	-0.706069	0.211530

E[B3LYP/6-31G(d,p)] = -1048.912643 h, E[APFD/6-311+G(2d,p)] = -1048.55679 h
Gcorr[B3LYP/6-31G(d,p)] = 0.219769 h

46. PC6+2H_2O, R2, 4th step, reactants

Center No.	Atom	X	Y	Z
1	P	-2.073511	-0.484600	0.152231
2	O	-2.789923	-0.129450	1.433438
3	O	-0.628933	0.661425	0.573488
4	O	-2.320142	0.439633	-1.198111
5	H	-2.080282	1.373702	-1.007425
6	H	-1.315501	-2.435959	-0.277615
7	O	-3.119330	-1.678892	-0.541331
8	H	-1.254259	2.236571	0.387377

9	O	-0.892722	-1.655523	0.113279
10	C	0.535009	0.643856	-0.222420
11	H	0.815786	1.673901	-0.484666
12	H	0.379327	0.094742	-1.157380
13	C	1.630173	-0.017335	0.623395
14	H	1.316021	-1.033206	0.861952
15	H	1.763436	0.545009	1.549554
16	C	2.962182	-0.937675	-1.278162
17	H	2.366984	-0.407497	-2.018402
18	H	3.977766	-1.072237	-1.648646
19	H	2.511150	-1.903940	-1.055565
20	C	3.922418	-0.823740	0.973544
21	H	4.916799	-0.909648	0.536476
22	H	3.964235	-0.233545	1.888097
23	H	3.516327	-1.812392	1.183049
24	C	3.585255	1.235711	-0.306365
25	H	2.972515	1.726743	-1.059100
26	H	3.591125	1.818736	0.613843
27	H	4.601727	1.114016	-0.679022
28	N	3.017185	-0.127080	-0.009713
29	O	-1.693873	2.968554	-0.121055
30	H	-3.805795	-1.215570	-1.037647
31	H	-2.505819	3.148259	0.372026

E[B3LYP/6-31G(d,p)] = -1048.906623 h, E[APFD/6-311+G(2d,p)] = -1048.554591 h
Gcorr[B3LYP/6-31G(d,p)] = 0.218461 h

47. PC6+2H_2O, R2, 4th step, TS

Center No.	Atom	X	Y	Z
1	P	-2.231919	-0.528805	0.134152
2	O	-2.758719	-0.153508	1.484350
3	O	-0.485330	0.871483	0.596377
4	O	-2.434469	0.480249	-1.106630
5	H	-2.208775	1.428237	-0.859047
6	H	-1.274321	-2.347827	-0.411589
7	O	-3.251937	-1.701565	-0.503930
8	H	-1.141852	2.145251	0.278970
9	O	-0.947782	-1.541058	0.018358
10	C	0.651170	0.789373	-0.200896
11	H	1.020814	1.791312	-0.485048
12	H	0.469040	0.240438	-1.139337
13	C	1.715463	0.057399	0.632506
14	H	1.330783	-0.929164	0.892375
15	H	1.906293	0.621232	1.547772
16	C	2.954190	-1.019258	-1.251219
17	H	2.378896	-0.475257	-1.996964
18	H	3.951132	-1.234538	-1.634715
19	H	2.444215	-1.945222	-0.988180
20	C	3.955740	-0.900855	0.980009
21	H	4.934811	-1.073452	0.533297
22	H	4.054675	-0.285960	1.873779
23	H	3.483939	-1.850491	1.229563
24	C	3.741127	1.134515	-0.362256
25	H	3.147347	1.642906	-1.118612
26	H	3.802618	1.744433	0.538435
27	H	4.740137	0.933284	-0.747979
28	N	3.086411	-0.174499	-0.012404
29	O	-1.730216	2.863432	-0.201948
30	H	-3.986988	-1.266821	-0.957005
31	H	-2.417374	3.095894	0.437363

E[B3LYP/6-31G(d,p)] = -1048.903624 h, E[APFD/6-311+G(2d,p)] = -1048.550937 h
Gcorr[B3LYP/6-31G(d,p)] = 0.215184 h

48. PC6+2H_2O, R2, 4th step, products

Center No.	Atom	X	Y	Z
1	P	2.337724	-0.547109	0.078266
2	O	1.000984	-1.205596	0.285541

3	O	-1.108102	2.634028	0.800614
4	O	2.510211	0.961139	0.070871
5	H	1.534243	2.125474	-0.601333
6	H	4.034943	-0.490937	1.423291
7	O	2.935545	-1.144874	-1.334753
8	H	-0.414800	2.825128	0.121960
9	O	3.354790	-1.150185	1.223380
10	C	-1.199285	1.223935	0.867496
11	H	-1.252717	0.920428	1.919834
12	H	-0.321563	0.737549	0.432976
13	C	-2.488845	0.804991	0.142288
14	H	-2.538543	1.302875	-0.827745
15	H	-3.359147	1.106275	0.728762
16	C	-1.765503	-1.104085	-1.290356
17	H	-0.721659	-0.984395	-0.994947
18	H	-1.968882	-2.152609	-1.509282
19	H	-2.016595	-0.490944	-2.155525
20	C	-4.085333	-0.946629	-0.501767
21	H	-4.195219	-1.996147	-0.772794
22	H	-4.714524	-0.713565	0.356510
23	H	-4.351920	-0.311921	-1.346332
24	C	-2.282968	-1.509547	1.073850
25	H	-1.207718	-1.431640	1.232345
26	H	-2.841823	-1.138577	1.932654
27	H	-2.553702	-2.546635	0.875772
28	N	-2.647975	-0.688165	-0.137530
29	O	0.935631	2.840415	-0.955044
30	H	3.608042	-0.541585	-1.682964
31	H	0.650691	2.513607	-1.818401

E[B3LYP/6-31G(d,p)] = -1048.953123 h, E[APFD/6-311+G(2d,p)] = -1048.598445 h
Gcorr[B3LYP/6-31G(d,p)] = 0.213537 h

V. Structures of molecules and transition states (TS) related to PS6Ca + 4 H_2O (R1) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

49. PS6Ca+4H_2O, R1, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	3.271897	-4.208873	-0.684245
2	C	2.350420	-3.121613	-1.188028
3	O	2.003600	-2.990377	-2.344342
4	O	1.976527	-2.276240	-0.189924
5	C	1.175747	-1.127285	-0.542502
6	C	1.846665	0.098152	0.056329
7	O	3.107621	0.266481	-0.613951
8	C	3.736246	1.464168	-0.756151
9	O	4.811886	1.457369	-1.322449
10	C	3.103740	2.725640	-0.201192
11	C	3.266217	2.877258	1.329653
12	C	-0.224688	-1.375881	0.016385
13	O	-1.115820	-0.380705	-0.539602
14	P	-2.592621	-0.180416	0.100052
15	O	-2.504952	0.094355	1.597106
16	O	-3.318049	0.801089	-0.781231
17	O	-3.185492	-1.696445	-0.082070
18	C	-4.562567	-2.011320	0.139505
19	C	-5.033338	-1.631803	1.559983
20	C	-6.319128	-2.332789	1.986645
21	O	-7.233416	-2.289990	1.019171
22	O	-6.464689	-2.829625	3.081769
23	N	-3.975925	-1.922416	2.574668
24	H	2.846356	-5.165359	-1.004745
25	H	3.301561	-4.194851	0.407989
26	H	-3.551822	-2.844390	2.443750
27	H	-3.234443	-1.177776	2.459071
28	H	-4.383381	-1.905965	3.515159
29	H	-8.046588	-2.725210	1.334297
30	H	-5.210694	-0.553719	1.616771
31	H	-5.203639	-1.503060	-0.584479
32	H	-4.641822	-3.089058	-0.014726

33	H	-0.562699	-2.368350	-0.290825
34	H	-0.231097	-1.315859	1.109193
35	H	1.129640	-1.044001	-1.630234
36	H	1.202392	0.966839	-0.079529
37	H	2.024061	-0.057474	1.125264
38	H	2.722387	2.080415	1.850466
39	H	2.771835	3.813717	1.614035
40	H	3.616721	3.550217	-0.702241
41	H	2.043842	2.784093	-0.467948
42	C	4.723676	2.904493	1.805641
43	C	4.854305	3.116194	3.318890
44	H	5.261926	3.703906	1.277714
45	C	6.308759	3.143994	3.798062
46	H	4.358545	4.056226	3.596283
47	H	4.310848	2.318874	3.843704
48	H	6.820214	2.203275	3.564343
49	H	6.868827	3.953209	3.315758
50	H	5.224781	1.967281	1.528478
51	C	4.688948	-4.049269	-1.275271
52	C	5.418841	-2.792959	-0.784747
53	H	5.522753	-2.841050	0.308576
54	H	4.810221	-1.903052	-0.991495
55	H	4.609692	-4.034118	-2.369090
56	C	6.802238	-2.606135	-1.419275
57	C	7.514874	-1.342364	-0.926597
58	H	6.693471	-2.562906	-2.511531
59	H	6.913979	-0.448937	-1.130028
60	H	7.689153	-1.384592	0.154891
61	H	7.423321	-3.487645	-1.209696
62	H	5.269705	-4.941704	-1.014400
63	H	8.486892	-1.214860	-1.414523
64	H	6.369669	3.296050	4.880584
65	O	-0.487659	2.735432	-0.573838
66	H	-0.602741	2.615362	0.407048
67	H	-0.684217	1.861587	-0.944909
68	O	-0.859685	2.266298	2.067567
69	H	-1.458598	1.485717	2.044371
70	H	-1.391510	2.975722	2.453372
71	Ca	-4.307834	2.522948	-1.997823
72	O	-5.207530	3.075697	-4.207466
73	H	-5.728988	3.880257	-4.333182
74	H	-4.647405	3.007597	-4.992828
75	O	-2.617488	4.147257	-1.399129
76	H	-2.832206	4.815972	-0.735855
77	H	-1.779422	3.709371	-1.087255

E[B3LYP/6-31G(d,p)] = -2838.189814 h, E[APFD/6-311+G(2d,p)] = -2837.250385 h
Gcorr[B3LYP/6-31G(d,p)] = 0.549315 h

50. PS6Ca+4H_2O, R1, 1st step, TS

Center No.	Atom	X	Y	Z
1	C	-3.324097	-4.118949	0.354067
2	C	-2.736725	-2.774768	0.728331
3	O	-2.968526	-2.178906	1.761503
4	O	-1.894790	-2.317684	-0.233334
5	C	-1.306607	-1.011349	-0.050697
6	C	-2.040846	-0.027831	-0.957061
7	O	-3.445222	0.012638	-0.643593
8	C	-3.976894	0.828655	0.304514
9	O	-5.147139	0.661614	0.587017
10	C	-3.137653	1.942498	0.901168
11	C	-3.135991	3.217319	0.021959
12	C	0.171587	-1.150004	-0.411731
13	O	0.753842	0.136785	-0.163919
14	P	2.319265	0.552165	-0.442269
15	O	2.635718	1.103372	-1.906047
16	O	3.340462	0.669684	0.702459
17	O	2.691084	-1.078567	-0.906640
18	C	3.985416	-1.609144	-0.802258
19	C	4.966919	-0.915336	-1.781919

20	C	6.224801	-1.715126	-2.065993
21	O	6.843723	-2.055345	-0.931053
22	O	6.605962	-1.996962	-3.182113
23	N	4.260628	-0.637276	-3.066963
24	H	-2.730101	-4.878143	0.879018
25	H	-3.184018	-4.288421	-0.716919
26	H	3.826805	-1.479102	-3.452691
27	H	3.506840	0.077780	-2.829298
28	H	4.907240	-0.276599	-3.771983
29	H	7.642871	-2.564835	-1.156689
30	H	5.252550	0.057836	-1.373239
31	H	4.401394	-1.515421	0.204731
32	H	3.913185	-2.673838	-1.051618
33	H	0.628472	-1.919389	0.213492
34	H	0.289027	-1.439939	-1.459244
35	H	-1.409922	-0.720662	0.996929
36	H	-1.576606	0.956806	-0.900765
37	H	-1.994937	-0.374854	-1.992141
38	H	-2.726976	2.986460	-0.969872
39	H	-2.440185	3.928574	0.482266
40	H	-3.584616	2.170103	1.871920
41	H	-2.109667	1.618636	1.081136
42	C	-4.512036	3.876461	-0.131232
43	C	-4.467793	5.156681	-0.974517
44	H	-4.912367	4.110044	0.865137
45	C	-5.838316	5.823898	-1.123979
46	H	-3.762520	5.865494	-0.519952
47	H	-4.064558	4.921132	-1.968683
48	H	-6.555541	5.150412	-1.606807
49	H	-6.251596	6.101791	-0.147699
50	H	-5.217742	3.168143	-0.583554
51	C	-4.801944	-4.239574	0.756290
52	C	-5.728517	-3.308213	-0.035835
53	H	-5.637812	-3.533769	-1.108026
54	H	-5.400366	-2.267713	0.088025
55	H	-4.891461	-4.027580	1.827926
56	C	-7.199852	-3.417807	0.381986
57	C	-8.112385	-2.461579	-0.392213
58	H	-7.284915	-3.213053	1.457860
59	H	-7.804998	-1.419982	-0.244505
60	H	-8.078312	-2.666344	-1.468461
61	H	-7.543540	-4.451530	0.240601
62	H	-5.114120	-5.280756	0.612644
63	H	-9.154680	-2.551700	-0.069132
64	H	-5.775489	6.733489	-1.730089
65	O	1.641179	2.293228	0.037499
66	H	1.719237	3.060951	-0.980258
67	H	2.272812	2.590749	0.707379
68	O	1.923229	3.377604	-2.069128
69	H	2.347487	2.277567	-2.148940
70	H	2.665610	3.999353	-2.073359
71	Ca	4.136212	0.638182	2.855487
72	O	5.287251	-0.890396	4.396813
73	H	6.227799	-0.783965	4.593980
74	H	4.876152	-1.150579	5.232413
75	O	4.131099	2.950969	3.618386
76	H	4.717262	3.620863	3.241332
77	H	3.317299	3.417572	3.852106

E[B3LYP/6-31G(d,p)] = -2838.124014 h, E[APFD/6-311+G(2d,p)] = -2837.186159 h
Gcorr[B3LYP/6-31G(d,p)] = 0.544521 h

51. PS6Ca+4H_2O, R1, 1st step, products

Center No.	Atom	X	Y	Z
1	C	-3.289194	-4.131126	0.174192
2	C	-2.708478	-2.790507	0.571362
3	O	-2.913540	-2.231461	1.630597
4	O	-1.906312	-2.290623	-0.402440
5	C	-1.332545	-0.980422	-0.199092
6	C	-2.113104	0.017201	-1.049514

7	O	-3.506229	0.026163	-0.685243
8	C	-4.012479	0.796073	0.313833
9	O	-5.170016	0.603315	0.630582
10	C	-3.164741	1.894299	0.927660
11	C	-3.213159	3.208223	0.109508
12	C	0.136676	-1.083839	-0.607934
13	O	0.696787	0.213586	-0.375047
14	P	2.282903	0.645711	-0.498074
15	O	2.750622	1.180125	-1.993719
16	O	3.267850	0.581262	0.688172
17	O	2.647104	-0.965230	-1.106493
18	C	3.868543	-1.605185	-0.871303
19	C	5.029665	-0.911945	-1.628805
20	C	6.287881	-1.752282	-1.731918
21	O	6.726145	-2.110334	-0.520830
22	O	6.812430	-2.054509	-2.782764
23	N	4.570186	-0.557662	-3.006886
24	H	-2.661268	-4.897538	0.646569
25	H	-3.191038	-4.260568	-0.907021
26	H	4.237960	-1.378192	-3.519901
27	H	3.783986	0.128344	-2.889741
28	H	5.326149	-0.142790	-3.556714
29	H	7.527665	-2.652787	-0.632224
30	H	5.265199	0.030874	-1.128904
31	H	4.143883	-1.634434	0.186715
32	H	3.766477	-2.636161	-1.232168
33	H	0.627226	-1.847823	-0.002288
34	H	0.228415	-1.365642	-1.660391
35	H	-1.407702	-0.723437	0.859641
36	H	-1.662635	1.007364	-0.980201
37	H	-2.099933	-0.298175	-2.095555
38	H	-2.835311	3.030613	-0.905364
39	H	-2.512416	3.908590	0.578977
40	H	-3.576288	2.070889	1.924369
41	H	-2.126397	1.577893	1.052891
42	C	-4.603169	3.851212	0.034719
43	C	-4.606255	5.173465	-0.742279
44	H	-4.973929	4.027026	1.054145
45	C	-5.990836	5.824522	-0.812127
46	H	-3.896907	5.869729	-0.274812
47	H	-4.233007	4.996055	-1.759950
48	H	-6.713646	5.164902	-1.305637
49	H	-6.375330	6.044877	0.190257
50	H	-5.312514	3.155026	-0.430556
51	C	-4.746683	-4.292093	0.632401
52	C	-5.721500	-3.353596	-0.090442
53	H	-5.674906	-3.546379	-1.171809
54	H	-5.404135	-2.311850	0.049751
55	H	-4.795226	-4.115627	1.713080
56	C	-7.171028	-3.499373	0.388156
57	C	-8.131350	-2.535936	-0.316152
58	H	-7.211156	-3.327445	1.472361
59	H	-7.833103	-1.494240	-0.151325
60	H	-8.142461	-2.708769	-1.398461
61	H	-7.505171	-4.533995	0.231304
62	H	-5.046611	-5.333840	0.468206
63	H	-9.156699	-2.652146	0.049966
64	H	-5.961955	6.765036	-1.371842
65	O	1.736502	2.263087	-0.111610
66	H	1.958551	3.590874	-1.318249
67	H	2.177093	2.486914	0.718195
68	O	2.317300	3.834716	-2.201434
69	H	2.661933	2.163060	-2.126797
70	H	3.131897	4.319606	-2.008342
71	Ca	4.067388	0.540443	2.834189
72	O	5.219273	-0.991530	4.371688
73	H	6.157555	-0.879964	4.576555
74	H	4.804557	-1.265040	5.201204
75	O	4.061465	2.849829	3.607695
76	H	4.656408	3.520338	3.245863
77	H	3.247680	3.318615	3.836912

E[B3LYP/6-31G(d,p)] = -2838.136896 h, E[APFD/6-311+G(2d,p)] = -2837.198649 h
Gcorr[B3LYP/6-31G(d,p)] = 0.549495 h

52. PS6Ca+4H_2O, R1, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	C	-2.911872	-4.007027	-0.772606
2	C	-2.420981	-2.759437	-0.069424
3	O	-2.664770	-2.474290	1.086430
4	O	-1.655136	-1.995657	-0.889316
5	C	-1.172210	-0.733258	-0.379080
6	C	-1.994414	0.380426	-1.019270
7	O	-3.391946	0.229852	-0.708818
8	C	-3.977613	0.767796	0.393614
9	O	-5.121431	0.433964	0.632719
10	C	-3.232263	1.800203	1.217981
11	C	-3.317183	3.221330	0.609261
12	C	0.309344	-0.650636	-0.745136
13	O	0.796119	0.563118	-0.158907
14	P	2.393189	0.877263	0.173403
15	O	3.182342	2.085798	-0.599717
16	O	3.136913	-0.025739	1.165971
17	O	2.780531	-0.110324	-1.279038
18	C	4.057901	-0.652324	-1.457815
19	C	4.998410	0.396517	-2.140681
20	C	6.136618	-0.257096	-2.897167
21	O	7.027657	-0.789968	-2.060052
22	O	6.188102	-0.316507	-4.109362
23	N	4.161376	1.158755	-3.115932
24	H	-2.269842	-4.831165	-0.436496
25	H	-2.759708	-3.899452	-1.849791
26	H	4.252412	0.746702	-4.052428
27	H	3.190554	1.083619	-2.758215
28	H	4.417580	2.145648	-3.168470
29	H	7.714366	-1.241274	-2.583457
30	H	5.370793	1.100476	-1.398816
31	H	4.519528	-0.962788	-0.517341
32	H	3.963564	-1.526511	-2.113848
33	H	0.828566	-1.523145	-0.340856
34	H	0.446003	-0.638684	-1.829216
35	H	-1.289765	-0.723350	0.706510
36	H	-1.606826	1.354635	-0.720911
37	H	-1.937849	0.302680	-2.107683
38	H	-2.861237	3.229119	-0.388710
39	H	-2.700489	3.879210	1.232778
40	H	-3.705198	1.796411	2.202880
41	H	-2.184679	1.519839	1.356501
42	C	-4.740796	3.785155	0.525017
43	C	-4.783015	5.208278	-0.045225
44	H	-5.191266	3.780005	1.527258
45	C	-6.201757	5.778986	-0.130040
46	H	-4.159613	5.865683	0.575715
47	H	-4.326947	5.210836	-1.044467
48	H	-6.838986	5.160673	-0.772493
49	H	-6.671350	5.820762	0.859322
50	H	-5.367003	3.128900	-0.092993
51	C	-4.379511	-4.318195	-0.438596
52	C	-5.364274	-3.280637	-0.992631
53	H	-5.261941	-3.232282	-2.086177
54	H	-5.101281	-2.283465	-0.615417
55	H	-4.483990	-4.383836	0.650552
56	C	-6.824958	-3.577995	-0.632897
57	C	-7.797222	-2.520641	-1.165087
58	H	-6.920198	-3.644920	0.459399
59	H	-7.554216	-1.528757	-0.767344
60	H	-7.753861	-2.457648	-2.258494
61	H	-7.103640	-4.565954	-1.023999
62	H	-4.621637	-5.309372	-0.839858
63	H	-8.830944	-2.749135	-0.885639
64	H	-6.199669	6.793848	-0.540789
65	O	1.799769	2.048421	1.312699

66	H	2.249595	3.810816	1.209833
67	H	0.973422	1.726056	1.694251
68	O	2.806802	4.450820	0.717266
69	H	3.110284	2.967108	-0.150088
70	H	3.561863	4.612667	1.299868
71	Ca	3.583217	-1.351663	2.962540
72	O	3.788420	-3.787314	2.995041
73	H	4.652894	-4.211990	3.079817
74	H	3.180398	-4.333055	3.512096
75	O	4.083768	-0.124340	5.038519
76	H	4.837975	0.478845	5.086011
77	H	3.378188	0.303943	5.542072

E[B3LYP/6-31G(d,p)] = -2838.13577 h, E[APFD/6-311+G(2d,p)] = -2837.195781 h
Gcorr[B3LYP/6-31G(d,p)] = 0.54391 h

53. PS6Ca+4H_2O, R1, 2nd step, TS

Center No.	Atom	X	Y	Z
1	C	-2.664391	-3.960174	-0.938920
2	C	-2.210842	-2.705406	-0.224262
3	O	-2.433097	-2.453350	0.943437
4	O	-1.505529	-1.890083	-1.050100
5	C	-1.067652	-0.616590	-0.528731
6	C	-1.939641	0.470975	-1.148296
7	O	-3.325125	0.257553	-0.822810
8	C	-3.917687	0.750272	0.297703
9	O	-5.043159	0.364240	0.544334
10	C	-3.205495	1.797360	1.132463
11	C	-3.382099	3.227678	0.566040
12	C	0.407321	-0.481161	-0.904062
13	O	0.861292	0.767028	-0.350554
14	P	2.318380	0.962522	0.364311
15	O	3.296716	2.094921	-0.228601
16	O	2.835318	-0.171649	1.232084
17	O	2.987586	-0.027569	-1.291511
18	C	4.330173	-0.457509	-1.308655
19	C	5.109627	0.582296	-2.224216
20	C	6.077852	-0.103354	-3.163085
21	O	7.106590	-0.633937	-2.490731
22	O	5.918889	-0.192788	-4.363801
23	N	4.040338	1.264235	-2.975680
24	H	-1.987970	-4.764277	-0.622544
25	H	-2.531571	-3.832077	-2.016327
26	H	4.040732	0.969905	-3.954102
27	H	3.147335	0.776886	-2.259582
28	H	4.093052	2.277266	-2.920537
29	H	7.678093	-1.101689	-3.125548
30	H	5.638139	1.299639	-1.597650
31	H	4.763809	-0.476544	-0.308243
32	H	4.391232	-1.463188	-1.741410
33	H	0.966655	-1.320501	-0.488954
34	H	0.540847	-0.473461	-1.988493
35	H	-1.175521	-0.623704	0.558057
36	H	-1.590353	1.457876	-0.843516
37	H	-1.892801	0.407565	-2.238050
38	H	-2.964572	3.282989	-0.447246
39	H	-2.775283	3.899181	1.184653
40	H	-3.651100	1.742073	2.128532
41	H	-2.141374	1.570870	1.236976
42	C	-4.833800	3.721369	0.550157
43	C	-4.968603	5.155652	0.024069
44	H	-5.244287	3.666398	1.567990
45	C	-6.415921	5.656605	0.013146
46	H	-4.353040	5.826075	0.638882
47	H	-4.554917	5.208594	-0.992045
48	H	-7.048252	5.025105	-0.621261
49	H	-6.845402	5.647275	1.021410
50	H	-5.450234	3.051224	-0.062558
51	C	-4.114913	-4.330788	-0.589857
52	C	-5.146302	-3.325821	-1.118576

53	H	-5.056380	-3.256546	-2.212076
54	H	-4.921430	-2.324353	-0.728158
55	H	-4.202214	-4.413888	0.499622
56	C	-6.590046	-3.689318	-0.751054
57	C	-7.610828	-2.667278	-1.260951
58	H	-6.673006	-3.775025	0.340928
59	H	-7.407432	-1.671349	-0.851340
60	H	-7.579126	-2.587657	-2.353672
61	H	-6.830029	-4.682811	-1.153625
62	H	-4.323870	-5.325586	-1.000616
63	H	-8.631493	-2.943742	-0.976913
64	H	-6.480693	6.681300	-0.366931
65	O	1.671873	2.031642	1.496765
66	H	2.369079	3.864568	1.662890
67	H	0.889426	1.648273	1.915879
68	O	3.067012	4.347217	1.182659
69	H	3.259966	2.957527	0.280306
70	H	3.794329	4.424460	1.816519
71	Ca	3.234089	-1.569213	3.014378
72	O	3.484087	-3.951212	3.502231
73	H	4.343411	-4.341073	3.712482
74	H	2.842671	-4.425720	4.048140
75	O	3.722566	-0.328875	5.080144
76	H	4.492554	0.251673	5.149889
77	H	3.020511	0.109333	5.579930

E[B3LYP/6-31G(d,p)] = -2838.127806 h, E[APFD/6-311+G(2d,p)] = -2837.185025 h
Gcorr[B3LYP/6-31G(d,p)] = 0.540187 h

54. PS6Ca+4H_2O, R1, 2nd step, products

Center No.	Atom	X	Y	Z
1	C	-3.475114	-3.755055	-0.737802
2	C	-2.800540	-2.566960	-0.087684
3	O	-2.933822	-2.237267	1.073043
4	O	-1.996258	-1.910151	-0.967711
5	C	-1.345371	-0.709162	-0.507531
6	C	-2.072355	0.490990	-1.109499
7	O	-3.457606	0.482175	-0.727856
8	C	-3.942634	1.110820	0.377915
9	O	-5.099766	0.889603	0.674176
10	C	-3.071601	2.097438	1.130895
11	C	-3.028394	3.490440	0.456026
12	C	0.106272	-0.811045	-0.979926
13	O	0.853188	0.359789	-0.569569
14	P	1.594673	0.432574	0.845552
15	O	2.436327	1.737951	0.628745
16	O	2.323621	-0.823176	1.225840
17	O	4.697887	-1.175397	-1.127720
18	C	5.887203	-0.379201	-1.112822
19	C	5.437193	1.101857	-0.990472
20	C	6.592106	2.043292	-1.302051
21	O	7.587844	1.912464	-0.408260
22	O	6.630686	2.796162	-2.252905
23	N	4.286441	1.285430	-1.869400
24	H	-2.874100	-4.636228	-0.478478
25	H	-3.427897	-3.646235	-1.824657
26	H	4.582264	1.698401	-2.751424
27	H	4.067725	-0.584572	-1.613659
28	H	3.603086	1.900921	-1.439374
29	H	8.310441	2.509175	-0.673047
30	H	5.122445	1.271095	0.043528
31	H	6.508230	-0.681146	-0.268618
32	H	6.447390	-0.536784	-2.042827
33	H	0.569050	-1.721916	-0.592819
34	H	0.160449	-0.826264	-2.070137
35	H	-1.393184	-0.678840	0.582788
36	H	-1.570695	1.418360	-0.832180
37	H	-2.076589	0.412142	-2.199389
38	H	-2.603117	3.406986	-0.551924
39	H	-2.330433	4.109016	1.032266

40	H	-3.516429	2.188703	2.124679
41	H	-2.055545	1.715753	1.262839
42	C	-4.389329	4.192893	0.378651
43	C	-4.304539	5.584287	-0.260929
44	H	-4.808250	4.281234	1.390625
45	C	-5.660149	6.292794	-0.338718
46	H	-3.599498	6.202911	0.310543
47	H	-3.880725	5.492860	-1.270133
48	H	-6.375722	5.713284	-0.933064
49	H	-6.093084	6.429477	0.658767
50	H	-5.096849	3.575940	-0.190394
51	C	-4.919824	-3.943133	-0.250123
52	C	-5.870002	-2.829033	-0.707961
53	H	-5.880531	-2.791768	-1.806668
54	H	-5.489662	-1.855471	-0.371452
55	H	-4.915590	-4.000554	0.844392
56	C	-7.303544	-3.007217	-0.193290
57	C	-8.241780	-1.880829	-0.637587
58	H	-7.288277	-3.058622	0.903885
59	H	-7.882758	-0.907805	-0.283458
60	H	-8.309368	-1.829898	-1.730381
61	H	-7.697675	-3.972935	-0.537889
62	H	-5.282750	-4.910821	-0.615949
63	H	-9.254736	-2.025473	-0.247890
64	H	-5.567713	7.281410	-0.799981
65	O	0.466549	0.800170	1.933106
66	H	2.560214	3.250378	3.274743
67	H	0.430065	0.160763	2.661821
68	O	3.283242	2.955447	2.701913
69	H	2.766211	2.205944	1.478596
70	H	3.848949	2.409253	3.266985
71	Ca	3.818511	-2.577830	0.659619
72	O	2.209667	-4.015300	-0.514308
73	H	2.411829	-4.456785	-1.350345
74	H	1.613817	-4.610717	-0.039840
75	O	5.346390	-3.718062	2.204763
76	H	6.277247	-3.858940	1.985040
77	H	5.327210	-3.546573	3.156000

E[B3LYP/6-31G(d,p)] = -2838.173603 h, E[APFD/6-311+G(2d,p)] = -2837.226481 h
Gcorr[B3LYP/6-31G(d,p)] = 0.540862 h

55. PS6Ca+4H_2O, R1, 3rd step, reactants (two extra waters around hydrolised serine)

Center No.	Atom	X	Y	Z
1	C	-4.025130	-3.804364	-0.205127
2	C	-3.220074	-2.605943	0.250496
3	O	-3.319355	-2.075035	1.338480
4	O	-2.348809	-2.199908	-0.709814
5	C	-1.563045	-1.016190	-0.446371
6	C	-2.153441	0.139700	-1.249177
7	O	-3.528680	0.360814	-0.887172
8	C	-3.911087	1.149192	0.153861
9	O	-5.090712	1.142500	0.446661
10	C	-2.896245	2.040261	0.844043
11	C	-2.681200	3.382433	0.101828
12	C	-0.133561	-1.364448	-0.872910
13	O	0.716494	-0.201483	-0.843046
14	P	1.501889	0.309509	0.505182
15	O	1.959099	1.711716	0.192586
16	O	2.616055	-0.693942	0.847694
17	O	4.859633	-1.009857	-1.140768
18	C	6.084681	-0.341093	-0.888214
19	C	5.896462	1.011631	-0.179759
20	C	5.343982	2.150053	-1.043830
21	O	5.773756	2.057075	-2.304885
22	O	4.662849	3.049297	-0.605916
23	N	5.023792	0.867940	1.026485
24	H	-3.529710	-4.691740	0.209675
25	H	-3.965447	-3.886068	-1.293799
26	H	4.651412	1.779284	1.385629

27	H	4.284419	-0.541278	-1.808048
28	H	5.533126	0.417914	1.789838
29	H	5.444176	2.829480	-2.798308
30	H	6.880666	1.350536	0.162254
31	H	6.676465	-0.996381	-0.244738
32	H	6.649895	-0.169344	-1.807742
33	H	0.254648	-2.160266	-0.230730
34	H	-0.127037	-1.719289	-1.906165
35	H	-1.596540	-0.798924	0.620605
36	H	-1.547756	1.037423	-1.125713
37	H	-2.181190	-0.115872	-2.311203
38	H	-2.322200	3.194394	-0.918046
39	H	-1.871899	3.912332	0.617824
40	H	-3.302316	2.239119	1.839029
41	H	-1.937699	1.532886	0.978172
42	C	-3.925019	4.277703	0.051064
43	C	-3.667287	5.616575	-0.651138
44	H	-4.274664	4.465427	1.075829
45	C	-4.902824	6.520820	-0.690685
46	H	-2.846409	6.139770	-0.142308
47	H	-3.318865	5.426907	-1.675404
48	H	-5.730067	6.037423	-1.222777
49	H	-5.253140	6.756014	0.320808
50	H	-4.743540	3.752356	-0.457488
51	C	-5.482177	-3.742718	0.277914
52	C	-6.292239	-2.611447	-0.368355
53	H	-6.300289	-2.749478	-1.459050
54	H	-5.795857	-1.649537	-0.184064
55	H	-5.485052	-3.624632	1.367531
56	C	-7.735731	-2.530871	0.143002
57	C	-8.528861	-1.381838	-0.487280
58	H	-7.724376	-2.410956	1.234860
59	H	-8.051142	-0.416824	-0.283225
60	H	-8.592586	-1.494975	-1.575642
61	H	-8.246741	-3.483242	-0.053426
62	H	-5.957478	-4.707090	0.063098
63	H	-9.550901	-1.338267	-0.096852
64	H	-4.688773	7.467456	-1.197411
65	O	0.350841	0.249291	1.622417
66	H	2.907628	-0.372319	-3.551883
67	H	0.664833	0.713271	2.462109
68	O	3.035333	0.098606	-2.716877
69	H	4.174856	0.284486	0.831819
70	H	2.187901	0.017187	-2.241827
71	Ca	3.618099	-2.723066	0.154421
72	O	2.593109	-4.458344	-1.217162
73	H	3.117235	-5.020461	-1.803830
74	H	1.880175	-5.020890	-0.885414
75	O	4.964249	-3.745766	1.904288
76	H	5.927403	-3.821664	1.887348
77	H	4.712197	-3.773802	2.836761
78	O	1.370691	1.533873	3.688815
79	H	2.094245	2.077670	3.298705
80	H	1.815178	0.917810	4.287346
81	O	3.326332	2.772015	2.160754
82	H	2.772790	2.567987	1.354047
83	H	3.485283	3.725724	2.155649

E[B3LYP/6-31G(d,p)] = -2991.083581 h, E[APFD/6-311+G(2d,p)] = -2990.096161 h
Gcorr[B3LYP/6-31G(d,p)] = 0.597262 h

56. PS6Ca+4H_2O, R1, 3rd step, TS

Center No.	Atom	X	Y	Z
1	C	-3.916336	-3.831246	-0.136870
2	C	-3.207276	-2.605961	0.399868
3	O	-3.445170	-2.079484	1.468582
4	O	-2.251340	-2.169414	-0.459878
5	C	-1.531066	-0.964873	-0.114050
6	C	-2.082216	0.183366	-0.954454
7	O	-3.491745	0.360884	-0.722561

8	C	-3.993794	1.120087	0.287620
9	O	-5.195358	1.080093	0.465480
10	C	-3.073711	2.024555	1.085403
11	C	-2.818897	3.381434	0.384091
12	C	-0.059173	-1.256603	-0.418819
13	O	0.735339	-0.069222	-0.286449
14	P	1.592542	0.278704	1.108852
15	O	1.703124	1.816394	0.731880
16	O	2.851576	-0.585322	0.975499
17	O	4.680625	-0.900523	-1.386226
18	C	5.895125	-0.166952	-1.405497
19	C	5.765279	1.201333	-0.710009
20	C	4.926839	2.227608	-1.473800
21	O	5.283979	2.267888	-2.760757
22	O	4.089550	2.934133	-0.960420
23	N	5.190239	1.039109	0.658350
24	H	-3.474592	-4.698000	0.371208
25	H	-3.697913	-3.938131	-1.202736
26	H	4.830026	1.925450	1.097561
27	H	3.954582	-0.447387	-1.906233
28	H	5.884979	0.639545	1.292706
29	H	4.747898	2.948822	-3.204801
30	H	6.767614	1.628849	-0.607500
31	H	6.640594	-0.765840	-0.877284
32	H	6.250522	-0.000256	-2.425736
33	H	0.291047	-2.060013	0.236030
34	H	0.043105	-1.591641	-1.455244
35	H	-1.662898	-0.765510	0.949198
36	H	-1.516241	1.095749	-0.766055
37	H	-2.003668	-0.059272	-2.016990
38	H	-2.344174	3.216078	-0.591322
39	H	-2.087996	3.928342	0.991169
40	H	-3.577716	2.198026	2.039310
41	H	-2.120889	1.535837	1.303747
42	C	-4.075965	4.240527	0.202121
43	C	-3.781261	5.593244	-0.457791
44	H	-4.543582	4.407289	1.182441
45	C	-5.032059	6.458970	-0.636053
46	H	-3.041913	6.136908	0.145699
47	H	-3.310711	5.423706	-1.435718
48	H	-5.775780	5.954949	-1.263727
49	H	-5.505153	6.673961	0.328872
50	H	-4.816326	3.697327	-0.399041
51	C	-5.429574	-3.785354	0.127036
52	C	-6.152528	-2.683954	-0.658821
53	H	-5.993273	-2.842941	-1.734959
54	H	-5.706493	-1.708735	-0.423061
55	H	-5.592646	-3.642121	1.201429
56	C	-7.657817	-2.622678	-0.372872
57	C	-8.363170	-1.495060	-1.132804
58	H	-7.814058	-2.489011	0.706178
59	H	-7.938174	-0.519619	-0.869900
60	H	-8.256415	-1.620591	-2.216442
61	H	-8.118324	-3.586191	-0.630307
62	H	-5.854235	-4.762943	-0.130002
63	H	-9.433744	-1.465870	-0.905012
64	H	-4.790737	7.416347	-1.109220
65	O	0.428833	-0.139014	2.137280
66	H	2.200840	-0.169526	-3.242399
67	H	0.843990	0.156692	2.994517
68	O	2.576327	0.253734	-2.458537
69	H	4.366166	0.394796	0.654729
70	H	1.880584	0.210198	-1.769974
71	Ca	3.682453	-2.630627	0.044920
72	O	2.668345	-4.376560	-1.317964
73	H	3.173149	-4.876881	-1.973386
74	H	2.010838	-4.993025	-0.968261
75	O	5.217497	-3.760425	1.585411
76	H	6.180074	-3.741404	1.500257
77	H	5.037835	-3.866496	2.529178
78	O	2.371704	0.891952	3.122978
79	H	3.196668	2.009883	2.788679

80	H	2.982315	0.175940	3.348266
81	O	3.682740	2.721373	2.169330
82	H	2.422788	2.319583	1.224967
83	H	3.680565	3.592823	2.584552

E[B3LYP/6-31G(d,p)] = -2991.037155 h, E[APFD/6-311+G(2d,p)] = -2990.047808 h
Gcorr[B3LYP/6-31G(d,p)] = 0.597038 h

57. PS6Ca+4H_2O, R1, 3rd step, products

Center No.	Atom	X	Y	Z
1	C	-3.702680	-3.840828	-0.198564
2	C	-3.083162	-2.578879	0.365798
3	O	-3.393998	-2.068869	1.424700
4	O	-2.116008	-2.095105	-0.450925
5	C	-1.464363	-0.857484	-0.074570
6	C	-2.029268	0.261869	-0.941252
7	O	-3.455833	0.380491	-0.773123
8	C	-4.030765	1.088018	0.233880
9	O	-5.235464	0.988437	0.365339
10	C	-3.185645	2.016514	1.085413
11	C	-2.993124	3.406326	0.430237
12	C	0.035382	-1.071458	-0.302331
13	O	0.755373	0.142480	-0.132549
14	P	1.700515	0.456786	1.315701
15	O	1.741433	1.988202	0.790664
16	O	2.861603	-0.518746	0.962416
17	O	4.498545	-1.018640	-1.473700
18	C	5.721492	-0.317236	-1.622656
19	C	5.698041	1.079414	-0.971658
20	C	4.860818	2.130985	-1.702312
21	O	5.093041	2.098570	-3.016876
22	O	4.137642	2.921201	-1.139217
23	N	5.219011	1.001348	0.441950
24	H	-3.191695	-4.683927	0.284329
25	H	-3.479676	-3.904488	-1.267193
26	H	4.972146	1.930271	0.852067
27	H	3.729955	-0.524908	-1.895355
28	H	5.933295	0.579517	1.039516
29	H	4.567797	2.802908	-3.436511
30	H	6.724384	1.460721	-0.955998
31	H	6.497872	-0.917741	-1.142338
32	H	5.992044	-0.192376	-2.675032
33	H	0.375322	-1.859434	0.377193
34	H	0.195871	-1.421129	-1.329979
35	H	-1.656105	-0.664582	0.980196
36	H	-1.510912	1.197303	-0.730327
37	H	-1.895551	0.021925	-1.998983
38	H	-2.498542	3.295099	-0.543090
39	H	-2.299297	3.971478	1.063614
40	H	-3.722865	2.131578	2.030096
41	H	-2.211524	1.577693	1.313902
42	C	-4.291345	4.204145	0.258280
43	C	-4.061972	5.590278	-0.356523
44	H	-4.777057	4.315957	1.237690
45	C	-5.354805	6.395170	-0.519601
46	H	-3.356822	6.152356	0.270612
47	H	-3.575426	5.476294	-1.334671
48	H	-6.066342	5.873259	-1.169578
49	H	-5.845974	6.554589	0.447093
50	H	-4.995873	3.641415	-0.367295
51	C	-5.213066	-3.921127	0.068260
52	C	-6.025092	-2.865202	-0.692679
53	H	-5.853315	-2.984917	-1.771996
54	H	-5.661413	-1.862332	-0.432826
55	H	-5.385075	-3.814646	1.145463
56	C	-7.530250	-2.936960	-0.408552
57	C	-8.329989	-1.863095	-1.152625
58	H	-7.697976	-2.834250	0.672170
59	H	-7.990084	-0.858356	-0.876519
60	H	-8.213967	-1.964064	-2.237863

61	H	-7.906177	-3.932329	-0.681796
62	H	-5.559513	-4.923609	-0.209755
63	H	-9.398921	-1.928739	-0.924680
64	H	-5.160257	7.378308	-0.960388
65	O	0.405866	-0.023736	2.202829
66	H	1.925835	0.015775	-3.055818
67	H	0.633688	0.134245	3.133153
68	O	2.423121	0.326067	-2.288129
69	H	4.351581	0.414938	0.532091
70	H	1.791634	0.332817	-1.524575
71	Ca	3.675197	-2.603960	0.229910
72	O	2.670379	-4.377759	-1.106843
73	H	3.176816	-4.892075	-1.749964
74	H	2.001640	-4.981910	-0.757104
75	O	5.217427	-3.736158	1.764523
76	H	6.179318	-3.717998	1.671205
77	H	5.046330	-3.821812	2.711986
78	O	2.478995	0.962260	2.856015
79	H	3.607749	2.321429	2.697437
80	H	3.054236	0.227967	3.115255
81	O	4.023408	2.941180	2.051847
82	H	2.437086	2.519162	1.236155
83	H	4.205518	3.774907	2.503985

E[B3LYP/6-31G(d,p)] = -2991.044657 h, E[APFD/6-311+G(2d,p)] = -2990.055267 h
Gcorr[B3LYP/6-31G(d,p)] = 0.600943 h

58. PS6Ca+4H_2O, R1, 4th step, reactants

Center No.	Atom	X	Y	Z
1	C	-4.060219	-3.795085	0.179897
2	C	-3.322034	-2.571714	0.682687
3	O	-3.598556	-1.971657	1.703198
4	O	-2.304735	-2.227853	-0.144266
5	C	-1.564786	-1.020057	0.155662
6	C	-2.029450	0.071466	-0.801904
7	O	-3.436835	0.340699	-0.648964
8	C	-3.932980	1.220425	0.259170
9	O	-5.141288	1.265602	0.386150
10	C	-2.992594	2.144251	1.010604
11	C	-2.625477	3.411393	0.200019
12	C	-0.079374	-1.344670	-0.032365
13	O	0.697444	-0.164624	0.123220
14	P	1.658621	0.164961	1.552279
15	O	1.636204	1.704181	1.037126
16	O	2.848954	-0.761094	1.173166
17	O	4.401896	-0.824185	-1.379883
18	C	5.662905	-0.186430	-1.472846
19	C	5.731558	1.113261	-0.630500
20	C	4.986524	2.264960	-1.294615
21	O	5.632912	2.661120	-2.391221
22	O	3.940481	2.732913	-0.893499
23	N	5.173407	0.877631	0.735155
24	H	-3.751951	-4.635541	0.814211
25	H	-3.737651	-4.021627	-0.839680
26	H	4.894838	1.754187	1.242233
27	H	3.638754	-0.255062	-1.713597
28	H	5.862330	0.393573	1.315767
29	H	5.117787	3.369010	-2.818996
30	H	6.778548	1.406682	-0.528254
31	H	6.408060	-0.890296	-1.095479
32	H	5.922784	0.063960	-2.505997
33	H	0.205953	-2.129479	0.675457
34	H	0.082694	-1.728863	-1.047362
35	H	-1.753123	-0.736919	1.191092
36	H	-1.422899	0.966709	-0.668719
37	H	-1.923314	-0.269853	-1.834683
38	H	-2.122949	3.126815	-0.732975
39	H	-1.886538	3.969266	0.787148
40	H	-3.522475	2.436163	1.920594
41	H	-2.080827	1.624256	1.314703

42	C	-3.816815	4.322682	-0.118506
43	C	-3.408838	5.586066	-0.886568
44	H	-4.312051	4.610128	0.819386
45	C	-4.591994	6.506263	-1.201259
46	H	-2.660115	6.138380	-0.302756
47	H	-2.911710	5.295688	-1.822024
48	H	-5.341645	5.991688	-1.813095
49	H	-5.087938	6.841010	-0.283062
50	H	-4.565369	3.769949	-0.700517
51	C	-5.585721	-3.615488	0.259585
52	C	-6.123031	-2.532646	-0.684888
53	H	-5.859069	-2.790794	-1.720465
54	H	-5.626227	-1.577395	-0.470603
55	H	-5.854452	-3.370878	1.293770
56	C	-7.640205	-2.334378	-0.582687
57	C	-8.156379	-1.215035	-1.492376
58	H	-7.904161	-2.108108	0.459336
59	H	-7.681839	-0.258895	-1.243892
60	H	-7.938786	-1.428195	-2.545314
61	H	-8.150046	-3.275796	-0.828583
62	H	-6.058875	-4.577299	0.028807
63	H	-9.239445	-1.086340	-1.395839
64	H	-4.269548	7.397493	-1.749415
65	O	0.403187	-0.367512	2.463861
66	H	2.424052	1.494921	-1.783410
67	H	0.645660	-0.208583	3.390084
68	O	2.254317	0.562131	-1.987646
69	H	4.314132	0.275634	0.722787
70	H	1.645053	0.279648	-1.258592
71	Ca	3.609314	-2.688201	0.039081
72	O	2.292238	-4.002981	-1.593526
73	H	2.894280	-4.736628	-1.794783
74	H	1.442205	-4.410309	-1.378413
75	O	2.448264	0.695430	3.082720
76	H	3.498497	2.092556	2.944533
77	H	3.051783	-0.020387	3.329263
78	O	3.905465	2.738769	2.316461
79	H	2.307751	2.260504	1.483974
80	H	4.120515	3.546326	2.800692
81	O	4.955628	-4.607272	-0.814846
82	H	5.227461	-5.316492	-0.215664
83	H	5.709273	-4.465562	-1.404627

E[B3LYP/6-31G(d,p)] = -2991.044667 h, E[APFD/6-311+G(2d,p)] = -2990.055383 h
Gcorr[B3LYP/6-31G(d,p)] = 0.603705 h

59. PS6Ca+4H_2O, R1, 4th step, TS

Center No.	Atom	X	Y	Z
1	C	-3.993736	-3.729438	-0.121183
2	C	-3.285793	-2.502909	0.415718
3	O	-3.567801	-1.939675	1.455207
4	O	-2.274838	-2.117027	-0.402005
5	C	-1.552439	-0.911199	-0.057136
6	C	-2.027888	0.208643	-0.975636
7	O	-3.444364	0.428643	-0.833820
8	C	-3.982285	1.230136	0.122662
9	O	-5.191597	1.211481	0.245958
10	C	-3.087734	2.154519	0.927015
11	C	-2.768291	3.471970	0.178719
12	C	-0.065730	-1.223936	-0.242751
13	O	0.721938	-0.056127	-0.011667
14	P	1.632569	0.218289	1.650384
15	O	1.995756	1.614407	0.923803
16	O	2.472384	-1.047917	1.479067
17	O	4.378879	-0.741893	-0.961287
18	C	5.618516	-0.336214	-1.451315
19	C	6.028955	1.023312	-0.763659
20	C	5.312422	2.188312	-1.416518
21	O	5.934750	2.562576	-2.534802
22	O	4.277425	2.674880	-1.000786

23	N	5.571218	0.901631	0.652186
24	H	-3.527969	-4.598049	0.362429
25	H	-3.793699	-3.819301	-1.192569
26	H	5.221506	1.767642	1.107646
27	H	3.274051	-0.080512	-1.439955
28	H	6.296563	0.492505	1.244177
29	H	5.410174	3.264156	-2.961364
30	H	7.106676	1.179100	-0.799046
31	H	6.401536	-1.070187	-1.215598
32	H	5.628998	-0.176941	-2.537576
33	H	0.221008	-2.031809	0.437567
34	H	0.114745	-1.565001	-1.269061
35	H	-1.751536	-0.665923	0.985032
36	H	-1.450204	1.114461	-0.791323
37	H	-1.895656	-0.081549	-2.020938
38	H	-2.243107	3.252463	-0.759436
39	H	-2.062055	4.035421	0.799848
40	H	-3.638856	2.382048	1.842786
41	H	-2.157995	1.659537	1.218788
42	C	-3.996173	4.342634	-0.114263
43	C	-3.638586	5.657510	-0.818056
44	H	-4.514972	4.563492	0.828937
45	C	-4.859954	6.535552	-1.106384
46	H	-2.923258	6.216174	-0.199464
47	H	-3.117827	5.434014	-1.758996
48	H	-5.577716	6.015438	-1.750923
49	H	-5.381417	6.804256	-0.180633
50	H	-4.711999	3.784286	-0.731140
51	C	-5.500627	-3.708724	0.173488
52	C	-6.258134	-2.614706	-0.590163
53	H	-6.126054	-2.769719	-1.670561
54	H	-5.818250	-1.634372	-0.364362
55	H	-5.644394	-3.573896	1.251629
56	C	-7.755831	-2.573972	-0.263390
57	C	-8.499347	-1.460718	-1.007888
58	H	-7.884273	-2.438174	0.819085
59	H	-8.081359	-0.477572	-0.762966
60	H	-8.422716	-1.590719	-2.093526
61	H	-8.208894	-3.545308	-0.504211
62	H	-5.916049	-4.691083	-0.080655
63	H	-9.563084	-1.445655	-0.748756
64	H	-4.573612	7.465077	-1.609082
65	O	0.132633	0.141228	2.293067
66	H	2.540821	1.373589	-1.577704
67	H	0.218507	0.322343	3.242847
68	O	2.352106	0.431579	-1.726925
69	H	4.774269	0.229972	0.587810
70	H	1.527755	0.172955	-0.906933
71	Ca	3.583693	-2.661456	0.187744
72	O	2.343930	-4.051489	-1.450574
73	H	2.976840	-4.773009	-1.594122
74	H	1.496111	-4.473180	-1.256186
75	O	2.317678	0.730718	3.157194
76	H	3.680718	2.056042	3.013551
77	H	2.752605	-0.043727	3.542907
78	O	4.095222	2.615273	2.323280
79	H	2.687755	2.129104	1.404558
80	H	4.138673	3.517942	2.666551
81	O	4.982634	-4.568541	-0.665227
82	H	5.291096	-5.253605	-0.055671
83	H	5.727678	-4.398927	-1.258747

E[B3LYP/6-31G(d,p)] = -2991.030647 h, E[APFD/6-311+G(2d,p)] = -2990.036376 h
Gcorr[B3LYP/6-31G(d,p)] = 0.600943 h

60. PS6Ca+4H_2O, R1, 4th step, products

Center No.	Atom	X	Y	Z
1	C	-4.035214	-3.548840	-1.427894
2	C	-2.745617	-2.970118	-0.902812
3	O	-1.955766	-3.596218	-0.209094

4	O	-2.584590	-1.677425	-1.237801
5	C	-1.469671	-0.957710	-0.656012
6	C	-1.905017	0.483261	-0.479632
7	O	-2.911976	0.506528	0.550412
8	C	-3.555003	1.648256	0.910011
9	O	-4.353674	1.575857	1.823403
10	C	-3.291629	2.927562	0.140923
11	C	-4.216420	3.081460	-1.092677
12	C	-0.242180	-1.083547	-1.566205
13	O	0.895322	-0.637047	-0.839322
14	P	2.217546	1.862572	1.775929
15	O	2.853758	2.663018	0.570509
16	O	2.475890	0.391886	1.854335
17	O	4.146721	-0.961716	-0.487330
18	C	5.305627	-1.515062	-1.008321
19	C	6.504452	-0.515758	-0.707495
20	C	6.644802	0.542016	-1.784447
21	O	7.098993	0.000441	-2.912276
22	O	6.370312	1.724332	-1.667301
23	N	6.120654	0.115099	0.585852
24	H	-3.810598	-4.551156	-1.803116
25	H	-4.401748	-2.937971	-2.256589
26	H	6.258816	1.133257	0.640141
27	H	3.406710	0.224486	-1.407384
28	H	6.571923	-0.330283	1.385229
29	H	7.151909	0.695579	-3.592794
30	H	7.452099	-1.046558	-0.612724
31	H	5.565852	-2.475213	-0.535516
32	H	5.270580	-1.678472	-2.093342
33	H	-0.123165	-2.132265	-1.858862
34	H	-0.378477	-0.491155	-2.477421
35	H	-1.241278	-1.395901	0.318771
36	H	-1.034754	1.069716	-0.173308
37	H	-2.303346	0.872289	-1.420678
38	H	-4.065119	2.240410	-1.781024
39	H	-3.889363	3.978560	-1.631245
40	H	-3.480486	3.746961	0.839102
41	H	-2.246860	2.993001	-0.172794
42	C	-5.706957	3.203825	-0.755117
43	C	-6.583437	3.385612	-2.000608
44	H	-5.854824	4.055955	-0.077260
45	C	-8.073872	3.513597	-1.672114
46	H	-6.251323	4.276454	-2.550634
47	H	-6.429663	2.534740	-2.678022
48	H	-8.441896	2.622367	-1.151096
49	H	-8.263640	4.377068	-1.024422
50	H	-6.039322	2.315277	-0.203781
51	C	-5.100456	-3.641496	-0.309605
52	C	-5.611547	-2.280488	0.178376
53	H	-6.068160	-1.745490	-0.666279
54	H	-4.770583	-1.658272	0.510193
55	H	-4.679563	-4.209983	0.528843
56	C	-6.629293	-2.391947	1.320157
57	C	-7.156721	-1.029170	1.780785
58	H	-6.162230	-2.910774	2.168271
59	H	-6.336962	-0.374049	2.095910
60	H	-7.691294	-0.520096	0.970196
61	H	-7.468879	-3.024331	1.001139
62	H	-5.938385	-4.231937	-0.697663
63	H	-7.850509	-1.132363	2.621692
64	H	-8.673113	3.640012	-2.579659
65	O	0.645616	2.115224	1.624296
66	H	2.770923	1.639275	-1.274800
67	H	0.399779	3.051406	1.553040
68	O	2.762249	0.854009	-1.846084
69	H	5.067774	-0.095344	0.580857
70	H	1.466897	-0.002082	-1.365792
71	Ca	2.327770	-1.759376	0.793673
72	O	0.771022	-3.566696	0.354901
73	H	0.996158	-4.346999	0.878856
74	H	-0.196167	-3.587355	0.206015
75	O	2.749286	2.669305	3.054676

76	H	5.793180	3.778638	0.928418
77	H	2.676634	2.161406	3.878453
78	O	5.414361	2.960250	0.576896
79	H	3.855802	2.830342	0.624091
80	H	5.732505	2.863966	-0.343360
81	O	3.226146	-3.856942	1.806074
82	H	3.391817	-3.902939	2.757934
83	H	3.978771	-4.304090	1.394836

E[B3LYP/6-31G(d,p)] = -2991.076874 h, E[APFD/6-311+G(2d,p)] = -2990.067029 h
Gcorr[B3LYP/6-31G(d,p)] = 0.597145 h

VI. Structures of molecules and transition states (TS) related to PS6Ca + 4 H_2O (R2) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

61. PS6Ca+4H_2O, R2, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	-4.162592	-3.820047	-0.138860
2	C	-3.338575	-2.645729	0.342299
3	O	-3.513715	-2.048671	1.384915
4	O	-2.344777	-2.347068	-0.537345
5	C	-1.507384	-1.212606	-0.239125
6	C	-1.941995	-0.046589	-1.124432
7	O	-3.327209	0.270390	-0.905595
8	C	-3.758330	1.129309	0.057571
9	O	-4.956488	1.192749	0.246488
10	C	-2.761930	2.012220	0.784435
11	C	-2.398380	3.286074	-0.017358
12	C	-0.074935	-1.658746	-0.516170
13	O	0.785049	-0.542329	-0.200088
14	P	2.348051	-0.778253	0.120158
15	O	2.897242	0.598638	0.527385
16	O	2.568035	-1.919035	1.087138
17	O	2.880807	-1.114129	-1.383368
18	C	4.221278	-1.506996	-1.698898
19	C	5.221483	-0.356277	-1.449404
20	C	6.487542	-0.448784	-2.286656
21	O	6.969278	-1.691154	-2.291450
22	O	6.986956	0.507756	-2.839706
23	N	4.584422	0.973404	-1.720123
24	H	-3.736538	-4.714162	0.334751
25	H	-4.024145	-3.937721	-1.217147
26	H	4.068176	0.990755	-2.604475
27	H	3.920291	1.182906	-0.945115
28	H	5.312997	1.692983	-1.779161
29	H	7.791664	-1.707827	-2.813973
30	H	5.524518	-0.329434	-0.390047
31	H	4.529825	-2.378240	-1.117575
32	H	4.195586	-1.779335	-2.755102
33	H	0.170046	-2.517370	0.113708
34	H	0.058233	-1.931105	-1.567766
35	H	-1.618341	-0.957599	0.817046
36	H	-1.291432	0.814451	-0.967277
37	H	-1.882533	-0.338201	-2.175692
38	H	-1.942944	3.008093	-0.976199
39	H	-1.623004	3.815868	0.549136
40	H	-3.242759	2.297477	1.723190
41	H	-1.851500	1.462715	1.037452
42	C	-3.581485	4.229089	-0.267444
43	C	-3.179711	5.499369	-1.027060
44	H	-4.030973	4.506929	0.695942
45	C	-4.356850	6.447525	-1.274204
46	H	-2.396928	6.025520	-0.464071
47	H	-2.727677	5.218437	-1.987876
48	H	-5.140674	5.959258	-1.864328
49	H	-4.808078	6.772488	-0.329829
50	H	-4.365030	3.704005	-0.828607
51	C	-5.647044	-3.685416	0.230165
52	C	-6.363313	-2.553248	-0.517439
53	H	-6.290499	-2.731989	-1.599756

54	H	-5.849550	-1.601464	-0.327961
55	H	-5.726827	-3.524482	1.311320
56	C	-7.838950	-2.408748	-0.126096
57	C	-8.543098	-1.264465	-0.861704
58	H	-7.909625	-2.244765	0.957765
59	H	-8.054090	-0.305273	-0.656600
60	H	-8.523167	-1.419782	-1.946526
61	H	-8.363305	-3.353104	-0.325942
62	H	-6.142311	-4.639690	0.015514
63	H	-9.591209	-1.176991	-0.557262
64	H	-4.040070	7.343529	-1.817740
65	Ca	2.039258	1.884401	2.411053
66	O	3.415481	3.629842	1.398417
67	H	4.360306	3.474162	1.263030
68	H	3.346063	4.551445	1.683214
69	O	2.051795	-0.379134	3.399000
70	H	2.240153	-1.085620	2.742966
71	H	2.632687	-0.550876	4.152126
72	O	4.975286	-2.635198	2.280142
73	H	5.488203	-3.232950	1.719782
74	H	4.110698	-2.546714	1.827477
75	O	5.640503	-0.017895	1.639537
76	H	4.733312	0.288324	1.484792
77	H	5.513243	-0.946419	1.942780

E[B3LYP/6-31G(d,p)] = -2838.180221 h, E[APFD/6-311+G(2d,p)] = -2837.251023 h
Gcorr[B3LYP/6-31G(d,p)] = 0.55417 h

62. PS6Ca+4H_2O, R2, 1st step, TS

Center No.	Atom	X	Y	Z
1	C	4.011807	-3.571807	0.553282
2	C	3.188956	-2.550884	-0.203602
3	O	3.526928	-2.018558	-1.242946
4	O	2.004253	-2.314735	0.412978
5	C	1.118350	-1.335568	-0.173822
6	C	1.263650	-0.025808	0.599873
7	O	2.635668	0.403939	0.675931
8	C	3.246084	1.147479	-0.283778
9	O	4.431894	1.372146	-0.141992
10	C	2.434989	1.708528	-1.435196
11	C	1.781184	3.072469	-1.104963
12	C	-0.288274	-1.923513	-0.054451
13	O	-1.224904	-0.996797	-0.598092
14	P	-2.951633	-1.207430	-0.293224
15	O	-3.274333	0.032342	-1.175630
16	O	-2.935836	-2.695203	-0.781964
17	O	-2.657847	-0.898509	1.299757
18	C	-3.555972	-0.381649	2.280980
19	C	-4.192452	0.956424	1.846746
20	C	-4.660383	1.827790	3.004963
21	O	-5.320407	1.109347	3.911441
22	O	-4.466370	3.023823	3.051877
23	N	-3.245487	1.765721	1.015160
24	H	3.881140	-4.527205	0.029101
25	H	3.597277	-3.697853	1.556990
26	H	-2.299084	1.768219	1.405814
27	H	-3.203250	1.347729	0.051471
28	H	-3.565348	2.740056	0.986539
29	H	-5.626204	1.702478	4.621681
30	H	-5.054446	0.746039	1.210804
31	H	-4.358382	-1.080791	2.512702
32	H	-2.935048	-0.236084	3.168218
33	H	-0.324640	-2.878694	-0.589262
34	H	-0.511206	-2.112083	1.001369
35	H	1.391380	-1.201713	-1.223069
36	H	0.620109	0.741413	0.168647
37	H	0.966687	-0.179644	1.640034
38	H	1.111610	2.967645	-0.241560
39	H	1.145342	3.341650	-1.957028
40	H	3.134778	1.833336	-2.265283

41	H	1.669867	0.998693	-1.756131
42	C	2.782393	4.203907	-0.843074
43	C	2.099569	5.549144	-0.567380
44	H	3.446737	4.304037	-1.712569
45	C	3.094133	6.687321	-0.320277
46	H	1.451907	5.806512	-1.416446
47	H	1.436180	5.446802	0.302075
48	H	3.733569	6.473421	0.543648
49	H	3.748205	6.835882	-1.186989
50	H	3.428011	3.942334	0.004688
51	C	5.502703	-3.202810	0.602180
52	C	5.798093	-1.962720	1.455543
53	H	5.438780	-2.135157	2.480225
54	H	5.230944	-1.105128	1.070403
55	H	5.857765	-3.042121	-0.422345
56	C	7.286712	-1.596373	1.496369
57	C	7.571187	-0.343854	2.331226
58	H	7.647833	-1.441334	0.470593
59	H	7.032683	0.523903	1.933738
60	H	7.254264	-0.481132	3.371491
61	H	7.860100	-2.443805	1.896165
62	H	6.056455	-4.062743	0.997210
63	H	8.638685	-0.100286	2.338092
64	H	2.577903	7.633174	-0.126675
65	Ca	-1.465736	0.181378	-2.798218
66	O	-2.816155	2.187917	-3.147390
67	H	-3.727774	2.075831	-2.843495
68	H	-2.873773	2.681921	-3.976369
69	O	-1.834923	-2.198940	-3.279436
70	H	-2.213849	-2.595676	-2.461567
71	H	-2.413953	-2.473873	-4.002725
72	O	-5.045241	-3.703964	-0.233560
73	H	-5.016230	-4.240364	0.573357
74	H	-4.002770	-3.426242	-0.532359
75	O	-4.822133	-1.353369	0.132180
76	H	-5.256719	-0.852853	-0.574484
77	H	-5.169040	-2.616413	0.036971

E[B3LYP/6-31G(d,p)] = -2838.13275 h, E[APFD/6-311+G(2d,p)] = -2837.195527 h
Gcorr[B3LYP/6-31G(d,p)] = 0.555626 h

63. PS6Ca+4H_2O, R2, 1st step, products

Center No.	Atom	X	Y	Z
1	C	3.992346	-3.564226	0.557586
2	C	3.169704	-2.557057	-0.217710
3	O	3.514655	-2.032360	-1.258745
4	O	1.977203	-2.324179	0.384238
5	C	1.084674	-1.364605	-0.225326
6	C	1.196287	-0.045236	0.536469
7	O	2.560702	0.405891	0.626444
8	C	3.176914	1.133194	-0.341676
9	O	4.360357	1.366207	-0.193348
10	C	2.372867	1.672679	-1.508470
11	C	1.707713	3.035926	-1.198156
12	C	-0.313032	-1.977099	-0.121551
13	O	-1.263959	-1.070419	-0.671987
14	P	-2.986285	-1.165310	-0.224121
15	O	-3.287373	0.020956	-1.185277
16	O	-2.922355	-2.723314	-0.703610
17	O	-2.497105	-0.782759	1.309956
18	C	-3.329869	-0.257366	2.345071
19	C	-4.034050	1.048576	1.913478
20	C	-4.422711	1.962036	3.069056
21	O	-4.973444	1.270691	4.064816
22	O	-4.264256	3.163978	3.041885
23	N	-3.181365	1.842216	0.969290
24	H	3.879278	-4.524275	0.037848
25	H	3.564978	-3.688061	1.556157
26	H	-2.204106	1.876711	1.273228
27	H	-3.209065	1.395587	0.020186

28	H	-3.524190	2.808844	0.935976
29	H	-5.231920	1.888720	4.772697
30	H	-4.941096	0.794237	1.362213
31	H	-4.092813	-0.967979	2.660623
32	H	-2.647370	-0.066553	3.176215
33	H	-0.322878	-2.932026	-0.658766
34	H	-0.537968	-2.174595	0.931467
35	H	1.373341	-1.236572	-1.270869
36	H	0.547138	0.706681	0.086404
37	H	0.886145	-0.191421	1.573699
38	H	1.025033	2.933275	-0.344775
39	H	1.084498	3.297032	-2.061961
40	H	3.079795	1.792998	-2.333108
41	H	1.615076	0.954032	-1.828821
42	C	2.699516	4.173437	-0.926467
43	C	2.006726	5.516597	-0.666017
44	H	3.376543	4.273158	-1.786154
45	C	2.992654	6.658761	-0.403028
46	H	1.373427	5.770043	-1.526987
47	H	1.328361	5.413436	0.191721
48	H	3.616854	6.448616	0.472893
49	H	3.662060	6.808012	-1.257824
50	H	3.333542	3.918570	-0.068002
51	C	5.478378	-3.179164	0.625325
52	C	5.747422	-1.928530	1.471866
53	H	5.370755	-2.094312	2.491408
54	H	5.180052	-1.079743	1.067882
55	H	5.847191	-3.023708	-0.395149
56	C	7.231730	-1.548626	1.536626
57	C	7.489135	-0.284892	2.363276
58	H	7.610874	-1.401208	0.516252
59	H	6.950742	0.573726	1.946172
60	H	7.153348	-0.414051	3.398655
61	H	7.804749	-2.386658	1.956266
62	H	6.035003	-4.029695	1.036363
63	H	8.554110	-0.031678	2.388068
64	H	2.469747	7.603174	-0.220659
65	Ca	-1.531102	0.124075	-2.840648
66	O	-2.871568	2.138277	-3.196641
67	H	-3.780834	2.033702	-2.883197
68	H	-2.934536	2.625455	-4.029256
69	O	-1.941408	-2.244921	-3.328644
70	H	-2.272311	-2.663936	-2.508908
71	H	-2.539119	-2.527919	-4.033461
72	O	-5.139223	-4.019757	0.007965
73	H	-4.927042	-4.588597	0.761723
74	H	-3.748459	-3.250039	-0.494867
75	O	-4.634654	-1.346892	0.302111
76	H	-5.181585	-0.925636	-0.376517
77	H	-5.360482	-3.152319	0.399514

E[B3LYP/6-31G(d,p)] = -2838.147367 h, E[APFD/6-311+G(2d,p)] = -2837.210756 h
Gcorr[B3LYP/6-31G(d,p)] = 0.557909 h

64. PS6Ca+4H_2O, R2, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	C	-3.804925	-3.013161	-1.999297
2	C	-2.590486	-2.744761	-1.146361
3	O	-2.126080	-3.561599	-0.361754
4	O	-2.109670	-1.502213	-1.311973
5	C	-1.000862	-1.064651	-0.479913
6	C	-1.234128	0.409365	-0.207652
7	O	-2.402904	0.514727	0.625651
8	C	-2.676498	1.598257	1.401367
9	O	-3.707789	1.571289	2.043981
10	C	-1.726233	2.779850	1.415199
11	C	-1.924763	3.733028	0.212281
12	C	0.301897	-1.355794	-1.241551
13	O	1.411113	-1.397764	-0.340745
14	P	3.114737	-1.331165	-0.982966

15	O	3.642844	-1.811708	0.390819
16	O	2.593609	-2.331286	-2.167159
17	O	2.821167	0.290997	-1.142963
18	C	3.800518	1.307494	-1.382086
19	C	4.935917	1.324361	-0.330766
20	C	5.591227	2.690675	-0.169538
21	O	5.818851	3.260804	-1.352363
22	O	5.886095	3.162254	0.908466
23	N	4.465848	0.883663	1.019060
24	H	-3.698504	-4.023578	-2.403733
25	H	-3.834788	-2.304001	-2.830151
26	H	3.478716	1.187517	1.238455
27	H	4.440523	-0.152869	1.060145
28	H	5.097626	1.263887	1.731684
29	H	6.258296	4.118343	-1.207665
30	H	5.708553	0.619404	-0.642573
31	H	4.251983	1.204675	-2.368296
32	H	3.232526	2.239197	-1.342463
33	H	0.191628	-2.319381	-1.745692
34	H	0.461338	-0.591463	-2.010705
35	H	-1.027341	-1.619620	0.458730
36	H	-0.359561	0.823945	0.292992
37	H	-1.401538	0.943229	-1.148066
38	H	-1.718793	3.205267	-0.726616
39	H	-1.162740	4.517136	0.292279
40	H	-1.940306	3.317916	2.341934
41	H	-0.684760	2.448143	1.459750
42	C	-3.315065	4.376539	0.145764
43	C	-3.465908	5.347257	-1.031982
44	H	-3.511615	4.910187	1.085992
45	C	-4.851838	5.995329	-1.102362
46	H	-2.698571	6.129482	-0.956462
47	H	-3.263867	4.812007	-1.969616
48	H	-5.637104	5.238781	-1.212468
49	H	-5.068309	6.566352	-0.192323
50	H	-4.084823	3.597062	0.072584
51	C	-5.102872	-2.923754	-1.162166
52	C	-5.431909	-1.507579	-0.674431
53	H	-5.556968	-0.848736	-1.545319
54	H	-4.587251	-1.098151	-0.105921
55	H	-5.016528	-3.607062	-0.308321
56	C	-6.693412	-1.445804	0.195264
57	C	-7.017050	-0.025003	0.668646
58	H	-6.561788	-2.101703	1.066565
59	H	-6.179007	0.403225	1.229801
60	H	-7.217268	0.637056	-0.181797
61	H	-7.545656	-1.852214	-0.366071
62	H	-5.924373	-3.300945	-1.782019
63	H	-7.900320	-0.010308	1.315688
64	H	-4.928893	6.681311	-1.952160
65	Ca	1.903006	-2.767119	1.720322
66	O	1.649874	-0.949077	3.478297
67	H	2.380291	-0.838937	4.105499
68	H	0.846298	-0.968367	4.019459
69	O	-0.335972	-3.720986	1.711028
70	H	-0.893711	-3.678237	2.498877
71	H	-0.952256	-3.700992	0.945703
72	O	1.763285	1.111332	1.450487
73	H	1.620414	0.582565	2.260041
74	H	3.335192	-2.446152	-2.783031
75	O	4.640555	-1.194115	-1.756179
76	H	5.262013	-1.763920	-1.281717
77	H	1.627685	0.473044	0.724390

E[B3LYP/6-31G(d,p)] = -2838.159392 h, E[APFD/6-311+G(2d,p)] = -2837.215235 h
Gcorr[B3LYP/6-31G(d,p)] = 0.563276 h

65. PS6Ca+4H_2O, R2, 2nd step, TS

Center No.	Atom	X	Y	Z
1	C	-3.848639	-3.437605	-1.632128

2	C	-2.775292	-2.813137	-0.774403
3	O	-2.462925	-3.250452	0.326746
4	O	-2.245350	-1.714732	-1.326896
5	C	-1.267505	-0.945860	-0.566394
6	C	-1.473828	0.498566	-0.993948
7	O	-2.790756	0.951632	-0.620580
8	C	-3.056245	1.754783	0.441080
9	O	-4.224908	1.967795	0.699886
10	C	-1.920634	2.395741	1.215461
11	C	-1.368934	3.671283	0.533942
12	C	0.140832	-1.494084	-0.877846
13	O	1.090650	-1.141683	0.100382
14	P	3.222291	-1.908036	-0.219262
15	O	3.349491	-1.554868	1.252650
16	O	2.368616	-3.192651	-0.677561
17	O	3.137126	-0.703915	-1.297192
18	C	4.275474	0.021653	-1.794803
19	C	5.131238	0.630716	-0.665298
20	C	6.007700	1.785032	-1.148216
21	O	6.628282	1.477943	-2.284315
22	O	6.117447	2.827525	-0.538782
23	N	4.299668	1.140069	0.468632
24	H	-3.682791	-4.518670	-1.620970
25	H	-3.753784	-3.079577	-2.660210
26	H	3.284007	1.373585	0.206198
27	H	4.219788	0.419302	1.197124
28	H	4.753429	1.980226	0.848784
29	H	7.187746	2.229283	-2.553399
30	H	5.797010	-0.138544	-0.266643
31	H	4.910924	-0.616431	-2.408326
32	H	3.838153	0.805071	-2.415394
33	H	0.047720	-2.584211	-0.949959
34	H	0.447134	-1.135984	-1.873778
35	H	-1.486866	-1.062722	0.496994
36	H	-0.683692	1.127509	-0.585939
37	H	-1.437438	0.568771	-2.084125
38	H	-0.961518	3.424996	-0.454267
39	H	-0.522847	4.022977	1.136155
40	H	-2.336315	2.656352	2.191602
41	H	-1.111759	1.681067	1.387822
42	C	-2.398444	4.799937	0.398916
43	C	-1.812610	6.066894	-0.236279
44	H	-2.799919	5.042365	1.392577
45	C	-2.834577	7.200539	-0.363616
46	H	-0.957496	6.409473	0.361890
47	H	-1.411503	5.821609	-1.228899
48	H	-3.685693	6.897966	-0.984189
49	H	-3.227490	7.490844	0.617427
50	H	-3.252924	4.457114	-0.198675
51	C	-5.256194	-3.123394	-1.073520
52	C	-5.657239	-1.648639	-1.200562
53	H	-5.682258	-1.374466	-2.264654
54	H	-4.891151	-1.008917	-0.744538
55	H	-5.292224	-3.435538	-0.022487
56	C	-7.014421	-1.332112	-0.560792
57	C	-7.401844	0.144363	-0.693911
58	H	-6.983217	-1.608343	0.501994
59	H	-6.639390	0.791363	-0.246164
60	H	-7.502686	0.431699	-1.746948
61	H	-7.790517	-1.961953	-1.016399
62	H	-5.977632	-3.750206	-1.610140
63	H	-8.356516	0.353553	-0.199985
64	H	-2.388847	8.090079	-0.820374
65	Ca	1.238255	-1.546711	2.453663
66	O	1.085842	0.071197	4.289732
67	H	1.796812	0.158196	4.939205
68	H	0.265932	0.202881	4.784775
69	O	-0.901789	-2.690545	2.500296
70	H	-1.546695	-2.506785	3.195721
71	H	-1.429340	-2.905538	1.698874
72	O	1.667317	1.432783	0.074787
73	H	1.345833	1.780100	0.918699

74	H	2.978305	-3.848920	-1.055866
75	O	4.717073	-2.459448	-0.645652
76	H	5.203545	-2.767890	0.133470
77	H	1.417070	0.449897	0.064149

E[B3LYP/6-31G(d,p)] = -2838.147972 h, E[APFD/6-311+G(2d,p)] = -2837.206257 h
Gcorr[B3LYP/6-31G(d,p)] = 0.555795 h

66. PS6Ca+4H_2O, R2, 2nd step, products

Center No.	Atom	X	Y	Z
1	C	-3.550112	-3.783045	-1.596452
2	C	-2.563627	-3.017863	-0.750944
3	O	-2.063406	-3.462207	0.274090
4	O	-2.335369	-1.779685	-1.221706
5	C	-1.509232	-0.886412	-0.434571
6	C	-2.040816	0.519372	-0.650430
7	O	-3.367567	0.614865	-0.105096
8	C	-3.752934	1.506713	0.846198
9	O	-4.904646	1.442371	1.228089
10	C	-2.776237	2.549077	1.356224
11	C	-2.606294	3.750683	0.396772
12	C	-0.045075	-1.042393	-0.869985
13	O	0.813169	-0.430674	0.088691
14	P	4.183625	-1.773541	-0.408913
15	O	3.773134	-1.450383	0.994218
16	O	3.169643	-2.829798	-1.035843
17	O	4.154648	-0.578537	-1.452892
18	C	5.179587	0.441390	-1.593587
19	C	5.493622	1.149989	-0.264968
20	C	6.447683	2.319792	-0.505336
21	O	7.475628	1.971037	-1.290095
22	O	6.298820	3.422455	-0.023370
23	N	4.278439	1.635662	0.396102
24	H	-3.199025	-4.817109	-1.648661
25	H	-3.567916	-3.365972	-2.606513
26	H	2.790013	1.734254	-0.533212
27	H	4.012419	0.981871	1.128265
28	H	4.488057	2.530697	0.836734
29	H	8.055843	2.746254	-1.395137
30	H	6.049023	0.448702	0.374638
31	H	6.077562	-0.015618	-2.009587
32	H	4.753770	1.142366	-2.311903
33	H	0.190777	-2.108489	-0.938599
34	H	0.114815	-0.599231	-1.858674
35	H	-1.599947	-1.154703	0.619746
36	H	-1.353218	1.224956	-0.185747
37	H	-2.111037	0.742374	-1.719025
38	H	-2.207150	3.412258	-0.567346
39	H	-1.842364	4.406638	0.830402
40	H	-3.189658	2.897122	2.305607
41	H	-1.802147	2.100609	1.572754
42	C	-3.894404	4.550391	0.166246
43	C	-3.685203	5.764905	-0.746572
44	H	-4.288792	4.886437	1.135202
45	C	-4.965762	6.574301	-0.971699
46	H	-2.912740	6.414001	-0.312570
47	H	-3.290519	5.426547	-1.714105
48	H	-5.745726	5.960021	-1.435775
49	H	-5.364646	6.955141	-0.024622
50	H	-4.665854	3.900298	-0.267134
51	C	-4.965837	-3.746311	-0.971512
52	C	-5.619449	-2.359189	-0.988330
53	H	-5.715589	-2.020230	-2.029494
54	H	-4.967312	-1.628831	-0.493904
55	H	-4.904340	-4.121979	0.057375
56	C	-6.996818	-2.330531	-0.314718
57	C	-7.626139	-0.933422	-0.317242
58	H	-6.898250	-2.685405	0.720240
59	H	-6.976363	-0.209944	0.187757
60	H	-7.787205	-0.575742	-1.340891

61	H	-7.666662	-3.040861	-0.817972
62	H	-5.590419	-4.456294	-1.525798
63	H	-8.595836	-0.930520	0.191485
64	H	-4.784785	7.433128	-1.626129
65	Ca	1.641829	-1.438226	2.146491
66	O	1.455904	0.408224	3.758751
67	H	2.133250	0.543918	4.435443
68	H	0.614224	0.600644	4.194087
69	O	-0.405268	-2.726790	2.363875
70	H	-1.001764	-2.574092	3.108560
71	H	-0.976168	-3.016643	1.619201
72	O	1.892020	1.669757	-0.975351
73	H	1.432516	2.490281	-0.750314
74	H	3.336704	-3.049792	-1.966852
75	O	5.680254	-2.321581	-0.535948
76	H	5.968316	-2.855584	0.222077
77	H	1.214705	0.409389	-0.302320

E[B3LYP/6-31G(d,p)] = -2838.180643 h, E[APFD/6-311+G(2d,p)] = -2837.230844 h
Gcorr[B3LYP/6-31G(d,p)] = 0.550637 h

67. PS6Ca+4H_2O, R2, 3rd step, reactants (extra water between Ca and serine)

Center No.	Atom	X	Y	Z
1	C	-4.163352	-3.746912	-1.406343
2	C	-3.278051	-2.632745	-0.891127
3	O	-2.940752	-2.490057	0.267310
4	O	-2.881005	-1.810889	-1.897207
5	C	-2.074663	-0.666129	-1.552209
6	C	-2.964237	0.575157	-1.588149
7	O	-4.093370	0.422564	-0.710787
8	C	-4.084114	0.776503	0.602574
9	O	-5.050698	0.458587	1.266946
10	C	-2.938427	1.598609	1.157264
11	C	-3.116395	3.116097	0.906917
12	C	-0.947244	-0.610349	-2.579452
13	O	-0.056055	0.439978	-2.190453
14	P	5.245383	0.922834	-0.672402
15	O	3.974698	0.851366	0.179600
16	O	5.748803	2.245676	-1.164570
17	O	6.452176	0.239137	0.196911
18	C	6.462961	-1.140561	0.576558
19	C	5.279060	-1.510111	1.498008
20	C	5.523022	-2.755049	2.341884
21	O	6.043035	-3.737589	1.608135
22	O	5.242834	-2.819394	3.519289
23	N	4.951517	-0.375643	2.416390
24	H	-3.520299	-4.629329	-1.518728
25	H	-4.526104	-3.487035	-2.404383
26	H	5.783998	0.043471	2.840371
27	H	4.463017	0.341567	1.831673
28	H	4.351917	-0.706532	3.179171
29	H	6.164015	-4.522569	2.172897
30	H	4.369256	-1.676979	0.912396
31	H	6.438038	-1.792960	-0.298714
32	H	7.411185	-1.286977	1.097127
33	H	-0.434776	-1.579004	-2.596015
34	H	-1.351920	-0.413970	-3.578378
35	H	-1.659736	-0.814560	-0.552045
36	H	-2.380884	1.467865	-1.360304
37	H	-3.397110	0.689466	-2.584927
38	H	-3.181424	3.312387	-0.170911
39	H	-2.199604	3.607075	1.253350
40	H	-2.925712	1.408050	2.233387
41	H	-1.974410	1.277211	0.757382
42	C	-4.328016	3.733037	1.615345
43	C	-4.446357	5.244806	1.386171
44	H	-4.254801	3.532883	2.693396
45	C	-5.648414	5.867507	2.102508
46	H	-3.523585	5.735277	1.724463
47	H	-4.519099	5.442899	0.308262

48	H	-6.588365	5.419985	1.760028
49	H	-5.585491	5.715307	3.186037
50	H	-5.248899	3.241183	1.276807
51	C	-5.322840	-4.062259	-0.448979
52	C	-6.358976	-2.935140	-0.352315
53	H	-6.771868	-2.737340	-1.351868
54	H	-5.867531	-2.006441	-0.033472
55	H	-4.909980	-4.273883	0.544074
56	C	-7.506056	-3.248300	0.616083
57	C	-8.525251	-2.109636	0.722165
58	H	-7.090258	-3.460439	1.610467
59	H	-8.047265	-1.185331	1.066015
60	H	-8.987403	-1.900504	-0.249464
61	H	-8.013366	-4.168445	0.295601
62	H	-5.809928	-4.982938	-0.791255
63	H	-9.327284	-2.353477	1.426560
64	H	-5.707032	6.945513	1.920555
65	Ca	1.645866	0.650564	-0.353412
66	O	0.513041	2.186329	1.195111
67	H	0.608118	3.146449	1.130904
68	H	0.394395	1.996718	2.135751
69	O	1.874173	-1.625710	0.613680
70	H	1.551800	-1.846678	1.498499
71	H	1.718720	-2.415407	0.077108
72	O	2.480078	1.180755	-2.650576
73	H	0.592485	0.622095	-2.895098
74	H	3.214021	0.567771	-2.823709
75	O	4.979278	-0.137555	-1.893153
76	H	5.684230	-0.105570	-2.559830
77	H	2.889066	2.090227	-2.726694
78	O	3.791829	3.502964	-2.626850
79	H	4.566227	3.176824	-2.108260
80	H	3.344513	4.125392	-2.037200

E[B3LYP/6-31G(d,p)] = -2914.635637 h, E[APFD/6-311+G(2d,p)] = -2913.662387 h
Gcorr[B3LYP/6-31G(d,p)] = 0.575044 h

68. PS6Ca+4H_2O, R2, 3rd step, TS

Center No.	Atom	X	Y	Z
1	C	5.429393	-3.457322	-0.452201
2	C	4.277153	-2.488405	-0.607195
3	O	4.004432	-1.888667	-1.627907
4	O	3.560461	-2.382951	0.542082
5	C	2.458025	-1.453236	0.564562
6	C	2.900787	-0.195579	1.310346
7	O	4.082749	0.369199	0.716833
8	C	4.059447	1.270481	-0.301808
9	O	5.126941	1.567387	-0.800833
10	C	2.750598	1.910997	-0.716899
11	C	2.377201	3.130534	0.160746
12	C	1.310799	-2.174485	1.267629
13	O	0.176924	-1.301790	1.267866
14	P	-4.579646	-0.649746	1.335434
15	O	-3.837313	0.175938	0.278393
16	O	-4.650515	-0.198258	2.842555
17	O	-6.174245	-0.198334	1.074937
18	C	-6.880675	-0.407547	-0.140471
19	C	-6.297120	0.394810	-1.328590
20	C	-7.302535	0.673169	-2.438413
21	O	-7.983219	-0.427621	-2.755802
22	O	-7.426595	1.759393	-2.961578
23	N	-5.744921	1.697046	-0.851358
24	H	5.106824	-4.401066	-0.910295
25	H	5.594164	-3.656413	0.610010
26	H	-6.374390	2.168956	-0.196843
27	H	-4.852972	1.455615	-0.355830
28	H	-5.585981	2.328559	-1.642349
29	H	-8.600604	-0.217812	-3.480032
30	H	-5.451145	-0.142753	-1.764355
31	H	-6.914737	-1.461043	-0.434263

32	H	-7.903926	-0.081079	0.059443
33	H	1.094604	-3.106438	0.732966
34	H	1.597913	-2.421578	2.295637
35	H	2.178366	-1.212551	-0.464023
36	H	2.081581	0.522150	1.362292
37	H	3.197548	-0.456251	2.329157
38	H	2.290762	2.824561	1.211257
39	H	1.375782	3.452411	-0.147963
40	H	2.891505	2.238525	-1.750064
41	H	1.926233	1.195013	-0.712125
42	C	3.351607	4.308781	0.048172
43	C	2.927318	5.515797	0.893762
44	H	3.429225	4.611611	-1.005323
45	C	3.889789	6.701049	0.772767
46	H	1.918623	5.830703	0.593837
47	H	2.851030	5.211514	1.946405
48	H	4.899552	6.425453	1.097539
49	H	3.959666	7.049419	-0.264006
50	H	4.358314	3.990555	0.347821
51	C	6.710378	-2.955216	-1.137025
52	C	7.322522	-1.722050	-0.460347
53	H	7.548920	-1.960635	0.588744
54	H	6.586662	-0.907455	-0.438916
55	H	6.481794	-2.729344	-2.185012
56	C	8.596760	-1.221577	-1.151594
57	C	9.188335	0.023394	-0.483268
58	H	8.372444	-0.999650	-2.203793
59	H	8.467924	0.849226	-0.483978
60	H	9.458650	-0.178007	0.559696
61	H	9.345752	-2.025090	-1.162847
62	H	7.439948	-3.773624	-1.142028
63	H	10.090466	0.366115	-1.000578
64	H	3.561489	7.546111	1.386559
65	Ca	-1.621056	-0.560494	-0.297231
66	O	-0.644394	1.468239	-1.322186
67	H	-0.970210	2.358523	-1.132930
68	H	-0.335564	1.491948	-2.238084
69	O	-1.689623	-2.172321	-2.141281
70	H	-2.345036	-2.122232	-2.850144
71	H	-1.515464	-3.114554	-2.013001
72	O	-2.532022	-1.433951	1.770972
73	H	-0.523866	-1.642418	1.855944
74	H	-2.697371	-2.380498	1.881437
75	O	-4.765126	-2.241867	1.051168
76	H	-5.685487	-2.509374	1.206655
77	H	-2.206749	-0.826233	3.253932
78	O	-2.432623	-0.336566	4.101729
79	H	-3.786930	-0.210186	3.390885
80	H	-1.970405	0.511854	4.044550

E[B3LYP/6-31G(d,p)] = -2914.589204 h, E[APFD/6-311+G(2d,p)] = -2913.613127 h
Gcorr[B3LYP/6-31G(d,p)] = 0.573759 h

69. PS6Ca+4H_2O, R2, 3rd step, products

Center No.	Atom	X	Y	Z
1	C	-4.474551	-3.841848	-1.029649
2	C	-3.559197	-2.724597	-0.578199
3	O	-3.253487	-2.497241	0.575202
4	O	-3.095712	-2.005869	-1.634819
5	C	-2.248751	-0.871839	-1.357115
6	C	-3.076993	0.399511	-1.527975
7	O	-4.238138	0.374085	-0.681365
8	C	-4.246757	0.819105	0.605197
9	O	-5.251530	0.607243	1.254394
10	C	-3.069256	1.606386	1.143280
11	C	-3.136692	3.109038	0.776379
12	C	-1.080618	-0.968185	-2.343016
13	O	-0.110356	0.063670	-2.095033
14	P	4.726178	0.628490	-1.169437
15	O	3.920918	0.485651	0.158424

16	O	5.293773	2.060277	-1.628585
17	O	6.296074	0.343507	-0.470543
18	C	6.692419	-0.856597	0.155276
19	C	5.946132	-1.135174	1.489950
20	C	6.742583	-1.977099	2.472189
21	O	7.223084	-3.075336	1.883080
22	O	6.897686	-1.681484	3.637899
23	N	5.581230	0.158573	2.128825
24	H	-3.867949	-4.756540	-1.041056
25	H	-4.790957	-3.655464	-2.059384
26	H	6.368488	0.809965	2.157630
27	H	4.820402	0.541993	1.480701
28	H	5.252687	0.018000	3.086792
29	H	7.718440	-3.590881	2.544896
30	H	4.999268	-1.642155	1.287573
31	H	6.566854	-1.745181	-0.475148
32	H	7.762496	-0.750907	0.359340
33	H	-0.582582	-1.930463	-2.205995
34	H	-1.436061	-0.908695	-3.375366
35	H	-1.879231	-0.950913	-0.331980
36	H	-2.460030	1.281958	-1.349860
37	H	-3.473052	0.452235	-2.545140
38	H	-3.144779	3.228930	-0.314483
39	H	-2.204771	3.567002	1.128149
40	H	-3.108673	1.497307	2.230009
41	H	-2.114671	1.193425	0.809831
42	C	-4.333027	3.852275	1.382090
43	C	-4.344188	5.345863	1.034094
44	H	-4.315693	3.732714	2.474276
45	C	-5.531662	6.095380	1.645559
46	H	-3.406185	5.803942	1.375881
47	H	-4.360095	5.462771	-0.057935
48	H	-6.483800	5.680604	1.295624
49	H	-5.522795	6.025493	2.739244
50	H	-5.269546	3.392890	1.040809
51	C	-5.678945	-4.023628	-0.092953
52	C	-6.667001	-2.850905	-0.133950
53	H	-7.037013	-2.725923	-1.161651
54	H	-6.146058	-1.918467	0.120731
55	H	-5.309895	-4.162928	0.929691
56	C	-7.858435	-3.029458	0.814924
57	C	-8.828527	-1.844364	0.784494
58	H	-7.485661	-3.170319	1.838585
59	H	-8.321323	-0.914332	1.065231
60	H	-9.247995	-1.701968	-0.218073
61	H	-8.395438	-3.952324	0.556750
62	H	-6.194111	-4.950304	-0.372026
63	H	-9.663851	-1.991841	1.476859
64	H	-5.513101	7.157234	1.379554
65	Ca	1.563264	0.287174	-0.272487
66	O	0.425023	1.824814	1.273977
67	H	0.537170	2.784387	1.237773
68	H	0.283397	1.612680	2.206655
69	O	1.544004	-1.937251	0.790707
70	H	1.954422	-2.101865	1.650253
71	H	1.680820	-2.745288	0.278003
72	O	3.141065	0.887268	-2.037218
73	H	-0.229492	0.787549	-2.723299
74	H	3.183051	0.491912	-2.919696
75	O	4.915935	-0.616633	-2.232921
76	H	5.846195	-0.883624	-2.272867
77	H	2.810215	2.719663	-2.473360
78	O	3.279206	3.570635	-2.585120
79	H	4.600216	2.655429	-2.022092
80	H	2.974578	4.121583	-1.850015

E[B3LYP/6-31G(d,p)] = -2914.595371 h, E[APFD/6-311+G(2d,p)] = -2913.62158 h
Gcorr[B3LYP/6-31G(d,p)] = 0.573357 h

70. PS6Ca+4H_2O, R2, 4th step, reactants

Center No.	Atom	X	Y	Z
1	C	-4.974488	-3.704550	-0.344537
2	C	-3.955528	-2.605164	-0.136814
3	O	-3.564823	-2.209187	0.942932
4	O	-3.500531	-2.123606	-1.323942
5	C	-2.549875	-1.039617	-1.288654
6	C	-3.283756	0.251191	-1.647530
7	O	-4.409428	0.457448	-0.778509
8	C	-4.345160	1.125751	0.405778
9	O	-5.334237	1.092916	1.110426
10	C	-3.109285	1.928363	0.758169
11	C	-3.103808	3.333010	0.106762
12	C	-1.448562	-1.410574	-2.286529
13	O	-0.347359	-0.489302	-2.207421
14	P	4.514563	-0.509677	-1.107576
15	O	3.679015	-0.671690	0.173851
16	O	5.361108	0.873878	-1.342133
17	O	5.981942	-1.267898	-0.543688
18	C	6.333291	-1.313533	0.817365
19	C	6.743822	0.083166	1.341655
20	C	7.532630	0.053662	2.639622
21	O	6.892182	-0.654695	3.571835
22	O	8.598590	0.612371	2.788506
23	N	7.560422	0.784824	0.302796
24	H	-4.418159	-4.650839	-0.322229
25	H	-5.400027	-3.613684	-1.347808
26	H	8.344696	0.211789	-0.019072
27	H	6.924963	0.974185	-0.504152
28	H	7.951675	1.655856	0.671291
29	H	7.424918	-0.647256	4.387572
30	H	5.847279	0.691757	1.488340
31	H	5.520555	-1.677921	1.450173
32	H	7.182409	-2.000263	0.901767
33	H	-1.064374	-2.399994	-2.029753
34	H	-1.836185	-1.446389	-3.308401
35	H	-2.127612	-0.971229	-0.283110
36	H	-2.595407	1.098224	-1.635222
37	H	-3.713739	0.168736	-2.648842
38	H	-3.127343	3.240526	-0.986474
39	H	-2.143309	3.800190	0.354478
40	H	-3.123513	2.034546	1.845761
41	H	-2.190593	1.397916	0.496931
42	C	-4.247960	4.243501	0.568390
43	C	-4.186964	5.641691	-0.058688
44	H	-4.217075	4.333399	1.663119
45	C	-5.322171	6.557945	0.407770
46	H	-3.220150	6.104207	0.181783
47	H	-4.216738	5.549187	-1.152759
48	H	-6.300976	6.137165	0.150946
49	H	-5.297049	6.696842	1.494595
50	H	-5.213782	3.780478	0.328648
51	C	-6.065447	-3.708436	0.735637
52	C	-7.006044	-2.498929	0.658632
53	H	-7.497632	-2.486185	-0.324682
54	H	-6.422777	-1.570836	0.722377
55	H	-5.584543	-3.742947	1.719920
56	C	-8.074360	-2.492199	1.758822
57	C	-9.001365	-1.275058	1.684341
58	H	-7.580922	-2.516403	2.739956
59	H	-8.433081	-0.341963	1.771179
60	H	-9.539977	-1.245697	0.730204
61	H	-8.669757	-3.413149	1.694771
62	H	-6.645823	-4.633128	0.635033
63	H	-9.746275	-1.288577	2.486729
64	H	-5.252810	7.547202	-0.056114
65	Ca	1.313090	-0.300604	-0.371475
66	O	0.421434	1.530926	0.979190
67	H	0.579309	2.469102	0.808456
68	H	0.256996	1.458929	1.929185

69	O	1.764271	-2.500857	0.714811
70	H	2.719446	-2.295134	0.682662
71	H	1.651089	-3.325123	0.222549
72	O	3.077016	0.200975	-1.979729
73	H	-0.431447	0.191286	-2.887679
74	H	3.083930	-0.072727	-2.908361
75	O	4.546544	-1.582957	-2.348180
76	H	5.299281	-2.178338	-2.199919
77	H	3.110043	2.115060	-2.144624
78	O	3.746817	2.855537	-2.090370
79	H	4.813783	1.659019	-1.635480
80	H	3.487350	3.353457	-1.301954

E[B3LYP/6-31G(d,p)] = -2914.600362 h, E[APFD/6-311+G(2d,p)] = -2913.623999 h
Gcorr[B3LYP/6-31G(d,p)] = 0.577907 h

71. PS6Ca+4H_2O, R2, 4th step, TS

Center No.	Atom	X	Y	Z
1	C	-5.002327	-3.831598	-0.465216
2	C	-4.038351	-2.722148	-0.105023
3	O	-3.763834	-2.377664	1.026837
4	O	-3.490761	-2.161529	-1.215897
5	C	-2.585213	-1.053950	-1.034650
6	C	-3.320561	0.233735	-1.398722
7	O	-4.519486	0.373068	-0.619582
8	C	-4.577068	1.011599	0.581337
9	O	-5.615218	0.917111	1.205011
10	C	-3.409987	1.858358	1.048841
11	C	-3.394433	3.265862	0.404041
12	C	-1.387182	-1.339020	-1.944626
13	O	-0.362311	-0.344237	-1.774484
14	P	4.323791	-0.140831	-1.114198
15	O	3.719813	-0.462361	0.244835
16	O	5.209935	1.175253	-1.308102
17	O	6.130128	-0.968116	-0.560707
18	C	6.487749	-1.114931	0.804539
19	C	7.496840	0.069794	1.093748
20	C	8.621267	-0.357197	2.014335
21	O	8.170686	-0.579494	3.254729
22	O	9.771000	-0.514343	1.658066
23	N	8.003214	0.441380	-0.238093
24	H	-4.454648	-4.773993	-0.336062
25	H	-5.261861	-3.755169	-1.524431
26	H	8.955260	0.096067	-0.370501
27	H	7.060023	-0.224068	-0.820501
28	H	7.978536	1.441376	-0.414390
29	H	8.914683	-0.894290	3.798723
30	H	6.958032	0.910434	1.532550
31	H	5.611510	-1.044446	1.446278
32	H	6.978101	-2.083807	0.947641
33	H	-0.956715	-2.304253	-1.669744
34	H	-1.695268	-1.385384	-2.992779
35	H	-2.263836	-1.026585	0.009506
36	H	-2.656134	1.092265	-1.288420
37	H	-3.660883	0.188817	-2.436384
38	H	-3.290264	3.180458	-0.684949
39	H	-2.489875	3.773500	0.759582
40	H	-3.531356	1.957581	2.130279
41	H	-2.451598	1.362176	0.875750
42	C	-4.623376	4.121785	0.733511
43	C	-4.554551	5.524518	0.117301
44	H	-4.721979	4.207024	1.824561
45	C	-5.778943	6.384286	0.445014
46	H	-3.645808	6.030606	0.470136
47	H	-4.450378	5.435935	-0.972558
48	H	-6.699359	5.919360	0.073854
49	H	-5.889734	6.518977	1.526982
50	H	-5.533981	3.617867	0.384408
51	C	-6.254955	-3.828158	0.424602
52	C	-7.167274	-2.617130	0.191308

53	H	-7.480621	-2.598839	-0.862365
54	H	-6.603824	-1.689926	0.360647
55	H	-5.939685	-3.859626	1.473918
56	C	-8.410539	-2.614697	1.089008
57	C	-9.308824	-1.394832	0.861980
58	H	-8.095477	-2.646053	2.140865
59	H	-8.763586	-0.463849	1.054407
60	H	-9.671360	-1.357467	-0.171744
61	H	-8.986822	-3.533836	0.916302
62	H	-6.813223	-4.752430	0.234572
63	H	-10.183202	-1.412494	1.520788
64	H	-5.701599	7.377914	-0.008145
65	Ca	1.289895	-0.103265	0.061192
66	O	0.142439	1.447046	1.570651
67	H	0.230105	2.408800	1.529161
68	H	-0.045801	1.239070	2.495847
69	O	1.848994	-2.319881	0.993060
70	H	2.807119	-2.212804	0.856395
71	H	1.605945	-3.148254	0.558002
72	O	2.877405	0.458409	-1.825370
73	H	-0.428472	0.323835	-2.469088
74	H	2.799909	0.211646	-2.759148
75	O	4.470890	-1.255822	-2.281628
76	H	5.266226	-1.785906	-2.099036
77	H	2.907949	2.684490	-2.121777
78	O	3.732047	3.197250	-2.106430
79	H	4.674349	1.967251	-1.626489
80	H	3.614900	3.840971	-1.392727

E[B3LYP/6-31G(d,p)] = -2914.584821 h, E[APFD/6-311+G(2d,p)] = -2913.604918 h
Gcorr[B3LYP/6-31G(d,p)] = 0.565354 h

72. PS6Ca+4H_2O, R2, 4th step, products

Center No.	Atom	X	Y	Z
1	C	4.886144	-4.014404	0.358439
2	C	4.049424	-2.770310	0.153899
3	O	3.680613	-2.348740	-0.923886
4	O	3.739511	-2.180169	1.338607
5	C	2.980950	-0.953841	1.303185
6	C	3.932483	0.209762	1.572942
7	O	5.015492	0.215962	0.628244
8	C	4.967708	0.849885	-0.575704
9	O	5.896973	0.659621	-1.334699
10	C	3.831389	1.802631	-0.889657
11	C	4.070668	3.224013	-0.323853
12	C	1.894688	-1.109764	2.371703
13	O	1.019165	0.031302	2.390004
14	P	-4.399858	0.383126	1.204509
15	O	-3.055909	1.047043	1.235158
16	O	-5.518941	1.095551	0.346086
17	O	-6.331496	-2.212487	-0.386110
18	C	-6.991081	-1.568337	-1.483478
19	C	-8.184054	-0.762019	-0.905538
20	C	-9.131350	-0.334220	-2.018477
21	O	-8.532187	0.509848	-2.876818
22	O	-10.273785	-0.724453	-2.140112
23	N	-8.817503	-1.591712	0.115728
24	H	4.207349	-4.869177	0.245067
25	H	5.260659	-4.034617	1.385188
26	H	-9.556755	-2.152099	-0.305005
27	H	-7.077057	-2.362061	0.250462
28	H	-9.252775	-1.017642	0.830999
29	H	-9.168749	0.722394	-3.582426
30	H	-7.775228	0.135138	-0.431679
31	H	-6.278979	-0.917280	-1.991156
32	H	-7.343283	-2.332798	-2.186452
33	H	1.290570	-1.987609	2.132697
34	H	2.339848	-1.256720	3.359145
35	H	2.524123	-0.850202	0.315776
36	H	3.387084	1.154846	1.574937

37	H	4.410647	0.082575	2.547331
38	H	4.174262	3.180904	0.767874
39	H	3.163607	3.806841	-0.523543
40	H	3.777491	1.852452	-1.980102
41	H	2.869620	1.424967	-0.535214
42	C	5.283318	3.944037	-0.925725
43	C	5.465395	5.364779	-0.377854
44	H	5.170663	3.986493	-2.017965
45	C	6.669365	6.091347	-0.984849
46	H	4.552726	5.945666	-0.567783
47	H	5.576520	5.320192	0.713981
48	H	7.600939	5.550872	-0.782031
49	H	6.569704	6.181374	-2.072547
50	H	6.194739	3.362557	-0.736706
51	C	6.031539	-4.117993	-0.661375
52	C	7.110699	-3.043379	-0.478165
53	H	7.531147	-3.122365	0.534594
54	H	6.655569	-2.046371	-0.545172
55	H	5.608824	-4.052486	-1.670602
56	C	8.244350	-3.141772	-1.506205
57	C	9.303401	-2.048701	-1.332798
58	H	7.819696	-3.081853	-2.517507
59	H	8.858349	-1.051965	-1.430165
60	H	9.772736	-2.105690	-0.343922
61	H	8.718605	-4.129924	-1.433107
62	H	6.482111	-5.113422	-0.571398
63	H	10.096228	-2.135698	-2.082954
64	H	6.774221	7.101256	-0.575315
65	Ca	-0.775376	0.666655	0.806841
66	O	0.258908	2.028202	-0.932319
67	H	0.214534	2.993430	-0.959287
68	H	0.344608	1.741787	-1.851634
69	O	-1.612881	-1.468424	-0.046097
70	H	-2.581729	-1.516535	0.084970
71	H	-1.258040	-2.295123	0.307346
72	O	-4.920520	0.285351	2.722670
73	H	1.248113	0.614655	3.125111
74	H	-5.820359	-0.066283	2.810824
75	O	-4.311204	-1.072679	0.590357
76	H	-5.170869	-1.504802	0.205431
77	H	-6.234752	3.665500	1.888438
78	O	-6.044547	3.547968	0.946361
79	H	-5.713829	2.061435	0.596036
80	H	-5.298742	4.137949	0.764424

E[B3LYP/6-31G(d,p)] = -2914.624193 h, E[APFD/6-311+G(2d,p)] = -2913.647921 h
Gcorr[B3LYP/6-31G(d,p)] = 0.563265 h

VII. Structures of molecules and transition states (TS) related to PC6Ca + 4 H_2O (R1) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

73. PC6Ca+4H_2O, R1, 1st step, reactants

Center No.	Atom	X	Y	Z
1	P	3.057239	0.199418	0.290905
2	O	3.760342	-1.148565	0.342166
3	O	2.177663	0.239942	1.672686
4	O	5.534905	1.758767	-1.917591
5	H	5.054715	2.250435	-2.597552
6	H	4.907978	1.711120	-1.148168
7	O	5.708713	-0.789155	-2.583752
8	H	5.147833	-0.937278	-3.355643
9	H	5.661092	0.193284	-2.389566
10	O	1.940819	0.188793	-0.901344
11	O	3.839823	1.474424	0.132865
12	C	1.524490	1.465923	2.037861
13	H	0.669224	1.635298	1.378667
14	H	2.227917	2.296342	1.942531
15	C	1.098080	1.247960	3.489321
16	H	1.978031	1.198081	4.132717
17	H	0.549936	0.308214	3.574355

18	C	0.803386	3.696748	3.880865
19	H	0.827770	3.943600	2.821389
20	H	0.185387	4.419216	4.411916
21	H	1.811142	3.690089	4.294810
22	C	0.034918	2.062052	5.538787
23	H	-0.657074	2.796143	5.948856
24	H	-0.361171	1.056163	5.671551
25	H	1.007970	2.152266	6.019242
26	C	-1.170238	2.290804	3.417152
27	H	-1.082371	2.455164	2.345472
28	H	-1.613099	1.314073	3.608845
29	H	-1.779765	3.071904	3.869905
30	N	0.195002	2.328949	4.061921
31	C	1.178897	-0.992856	-1.196401
32	H	1.260088	-1.166513	-2.273502
33	H	1.591412	-1.859966	-0.673223
34	C	-0.281388	-0.791467	-0.809546
35	H	-0.355836	-0.483538	0.234688
36	C	-1.106143	-2.045967	-1.043128
37	H	-1.152129	-2.299594	-2.106020
38	H	-0.677354	-2.894034	-0.501555
39	C	-1.284894	1.389339	-1.067020
40	C	-1.819425	2.342015	-2.111898
41	H	-2.602467	1.812267	-2.668972
42	H	-1.014253	2.519143	-2.835976
43	C	-2.344602	3.657808	-1.536327
44	H	-1.542248	4.152946	-0.976206
45	H	-3.138247	3.443689	-0.810515
46	C	-2.876078	4.600714	-2.621845
47	H	-2.077847	4.807267	-3.348812
48	H	-3.676058	4.097345	-3.183057
49	O	-0.825655	0.258534	-1.645260
50	O	-1.264855	1.596499	0.132774
51	C	-3.407126	5.926642	-2.063858
52	H	-2.607015	6.428500	-1.503124
53	H	-4.204160	5.718998	-1.337198
54	C	-3.325907	-2.786302	-0.660988
55	C	-4.677334	-2.374888	-0.121268
56	H	-4.531538	-2.026297	0.908837
57	H	-5.003619	-1.492319	-0.686104
58	C	-5.724318	-3.487844	-0.185035
59	H	-5.834993	-3.819987	-1.224272
60	H	-5.361205	-4.357140	0.376498
61	C	-7.085049	-3.046945	0.365910
62	H	-7.442074	-2.173776	-0.198466
63	H	-6.966376	-2.709565	1.405394
64	C	-8.146315	-4.152562	0.311424
65	H	-8.263813	-4.489025	-0.727527
66	H	-7.788077	-5.024616	0.875025
67	O	-2.432280	-1.775113	-0.551823
68	O	-3.042979	-3.868403	-1.135570
69	C	-3.937763	6.867168	-3.149949
70	H	-4.309190	7.803656	-2.721235
71	H	-3.153282	7.119612	-3.872533
72	H	-4.761931	6.405042	-3.705319
73	C	-9.505305	-3.710795	0.862550
74	H	-10.240251	-4.520689	0.810418
75	H	-9.425346	-3.400574	1.910732
76	H	-9.904803	-2.861559	0.296438
77	Ca	5.551332	-2.289412	-0.707186
78	O	7.779268	-3.345703	-0.705111
79	H	8.414966	-3.153630	-0.002409
80	H	7.880033	-4.288604	-0.893635
81	O	4.117349	-3.829083	0.638609
82	H	3.598487	-3.084304	0.991974
83	H	4.471145	-4.295305	1.408183

E[B3LYP/6-31G(d,p)] = -2767.554377 h, E[APFD/6-311+G(2d,p)] = -2766.601405 h
Gcorr[B3LYP/6-31G(d,p)] = 0.614343 h

74. PC6Ca+4H_2O, R1, 1st step, TS

Center No.	Atom	X	Y	Z
1	P	2.912573	-0.915560	-0.700514
2	O	3.473381	-2.217823	-0.127835
3	O	3.078447	0.001513	0.715316
4	O	4.068835	-0.759421	-3.857801
5	H	3.551847	-0.251886	-4.498857
6	H	3.918569	-0.189866	-2.653215
7	O	2.595375	-2.034953	-2.485459
8	H	2.951854	-2.897940	-2.237787
9	H	3.320597	-1.513959	-3.330031
10	O	1.295240	-0.695687	-0.741504
11	O	3.719146	0.090543	-1.605761
12	C	2.544074	1.315204	0.768403
13	H	1.451660	1.282004	0.710288
14	H	2.922974	1.918201	-0.064263
15	C	3.017776	1.874152	2.110860
16	H	4.096675	2.038848	2.092187
17	H	2.787093	1.159756	2.903027
18	C	2.568683	4.241793	1.456978
19	H	2.006697	3.954875	0.570650
20	H	2.196192	5.191875	1.837651
21	H	3.630006	4.322257	1.224294
22	C	3.071627	3.663155	3.784977
23	H	2.602611	4.589648	4.113710
24	H	2.962574	2.894953	4.549440
25	H	4.125527	3.831108	3.568020
26	C	0.912721	3.024002	2.817383
27	H	0.387559	2.702875	1.919653
28	H	0.801618	2.277437	3.603218
29	H	0.521162	3.982116	3.157318
30	N	2.384410	3.195516	2.526061
31	C	0.328995	-1.709904	-1.024938
32	H	0.278085	-1.887003	-2.100018
33	H	0.600881	-2.648186	-0.530126
34	C	-1.005362	-1.214164	-0.481158
35	H	-0.908237	-0.942719	0.571523
36	C	-2.102106	-2.248173	-0.664399
37	H	-2.306093	-2.426569	-1.723692
38	H	-1.816523	-3.197051	-0.201068
39	C	-1.384044	1.167474	-0.610688
40	C	-1.817258	2.255623	-1.568246
41	H	-2.781805	1.954229	-1.995018
42	H	-1.111244	2.250677	-2.408619
43	C	-1.903725	3.642914	-0.930995
44	H	-0.925043	3.912385	-0.515922
45	H	-2.597589	3.608555	-0.082335
46	C	-2.355632	4.718186	-1.925779
47	H	-1.659630	4.744526	-2.776232
48	H	-3.334663	4.441951	-2.342256
49	O	-1.396248	-0.034497	-1.227091
50	O	-1.069132	1.334205	0.553736
51	C	-2.447259	6.116887	-1.303820
52	H	-1.468699	6.391430	-0.887208
53	H	-3.142829	6.089099	-0.454197
54	C	-4.400686	-2.487293	-0.132903
55	C	-5.568828	-1.831897	0.569861
56	H	-5.290695	-1.705958	1.624139
57	H	-5.669680	-0.815346	0.169904
58	C	-6.877585	-2.611655	0.435384
59	H	-7.117312	-2.732893	-0.627989
60	H	-6.737486	-3.623522	0.834143
61	C	-8.046487	-1.928766	1.154296
62	H	-8.177810	-0.913000	0.755082
63	H	-7.800416	-1.807855	2.218846
64	C	-9.367233	-2.697253	1.024704
65	H	-9.611500	-2.817752	-0.039381
66	H	-9.234818	-3.712173	1.423280
67	O	-3.283972	-1.731002	-0.023781
68	O	-4.424878	-3.549274	-0.723311

69	C	-2.898326	7.190190	-2.298956
70	H	-2.953928	8.175978	-1.825755
71	H	-2.202969	7.264508	-3.142893
72	H	-3.889236	6.960135	-2.706874
73	C	-10.534888	-2.014269	1.742909
74	H	-11.461999	-2.586042	1.631773
75	H	-10.333866	-1.910875	2.815381
76	H	-10.712968	-1.009847	1.342010
77	Ca	5.532148	-2.881929	0.684180
78	O	7.160839	-3.076042	-1.146414
79	H	7.971009	-2.548137	-1.148423
80	H	7.421578	-3.948211	-1.472521
81	O	5.988628	-2.283927	3.011585
82	H	5.431567	-2.611977	3.730485
83	H	6.234259	-1.383616	3.263651

E[B3LYP/6-31G(d,p)] = -2767.482461 h, E[APFD/6-311+G(2d,p)] = -2766.538455 h
Gcorr[B3LYP/6-31G(d,p)] = 0.610176 h

75. PC6Ca+4H_2O, R1, 1st step, products

Center No.	Atom	X	Y	Z
1	P	2.854066	-1.515900	-1.227748
2	O	3.811107	-2.620204	-0.736337
3	O	3.342764	-0.496397	0.213095
4	O	2.875968	-0.869813	-4.772416
5	H	2.070502	-0.410458	-5.048228
6	H	3.187310	-0.415167	-3.114663
7	O	2.333838	-2.404533	-2.632824
8	H	2.697831	-3.293859	-2.529273
9	H	2.554610	-1.657686	-4.282578
10	O	1.324236	-1.382972	-0.625906
11	O	3.315527	-0.257492	-2.144890
12	C	2.740281	0.767616	0.429027
13	H	1.672464	0.645230	0.632757
14	H	2.853816	1.391535	-0.463654
15	C	3.460124	1.397577	1.624013
16	H	4.508609	1.579107	1.377743
17	H	3.414192	0.723980	2.482324
18	C	2.898667	3.746611	0.988810
19	H	2.194853	3.440419	0.218422
20	H	2.599813	4.709564	1.400674
21	H	3.904945	3.811489	0.576370
22	C	3.775184	3.231067	3.220015
23	H	3.369467	4.173618	3.585427
24	H	3.780274	2.491223	4.019424
25	H	4.784023	3.378929	2.836724
26	C	1.492105	2.563865	2.634082
27	H	0.824748	2.237628	1.838269
28	H	1.514635	1.824231	3.433953
29	H	1.162742	3.525342	3.026591
30	N	2.895137	2.729595	2.101565
31	C	0.183321	-2.130146	-1.062214
32	H	0.113636	-2.147228	-2.149802
33	H	0.255581	-3.162413	-0.701238
34	C	-1.047031	-1.463188	-0.461807
35	H	-0.880316	-1.233594	0.592239
36	C	-2.286849	-2.326239	-0.624841
37	H	-2.535314	-2.471181	-1.679847
38	H	-2.133834	-3.307257	-0.166099
39	C	-1.189258	0.950643	-0.515155
40	C	-1.521499	2.101928	-1.439083
41	H	-2.457025	1.853672	-1.954012
42	H	-0.752038	2.121798	-2.222179
43	C	-1.619827	3.455949	-0.735048
44	H	-0.666451	3.680233	-0.242406
45	H	-2.370097	3.395205	0.062807
46	C	-1.981155	4.592200	-1.698656
47	H	-1.229678	4.645026	-2.499211
48	H	-2.935984	4.362332	-2.192272
49	O	-1.287286	-0.223694	-1.174322

50	O	-0.872892	1.050638	0.656623
51	C	-2.083995	5.958635	-1.010280
52	H	-1.129340	6.187357	-0.517526
53	H	-2.834203	5.903854	-0.209899
54	C	-4.584756	-2.230350	-0.049869
55	C	-5.633186	-1.415153	0.673845
56	H	-5.310292	-1.313515	1.717806
57	H	-5.608878	-0.399602	0.259265
58	C	-7.037706	-2.014134	0.587217
59	H	-7.322677	-2.114010	-0.467127
60	H	-7.021775	-3.031280	0.996811
61	C	-8.083319	-1.173214	1.328125
62	H	-8.090321	-0.153748	0.916955
63	H	-7.791531	-1.073722	2.383301
64	C	-9.497746	-1.760293	1.247780
65	H	-9.787402	-1.860185	0.192994
66	H	-9.489531	-2.778847	1.658794
67	O	-3.368243	-1.643969	0.038019
68	O	-4.772880	-3.276025	-0.639677
69	C	-2.446400	7.092592	-1.973869
70	H	-2.511810	8.053699	-1.453516
71	H	-1.696166	7.193250	-2.766515
72	H	-3.413299	6.908291	-2.455899
73	C	-10.542386	-0.919059	1.987202
74	H	-11.540081	-1.363660	1.911455
75	H	-10.297377	-0.830048	3.051789
76	H	-10.597504	0.095068	1.575132
77	Ca	5.042068	-1.975672	1.140967
78	O	7.366377	-1.976312	0.383526
79	H	8.028279	-1.357290	0.719814
80	H	7.841022	-2.803531	0.225240
81	O	5.102869	-1.810305	3.584790
82	H	4.475394	-2.277804	4.152326
83	H	5.337382	-1.004031	4.063257

E[B3LYP/6-31G(d,p)] = -2767.50801 h, E[APFD/6-311+G(2d,p)] = -2766.555816 h
Gcorr[B3LYP/6-31G(d,p)] = 0.618164 h

76. PC6Ca+4H_2O, R1, 2nd step, products (choline hydrolsis following H migration after turning 180 degrees, no TS)

Center No.	Atomic No.	X	Y	Z
1	P	2.577896	-2.513092	-1.001736
2	O	3.662628	-2.114944	-0.016614
3	O	3.790498	1.154394	0.046428
4	O	2.858103	0.813412	-2.372232
5	H	3.416437	1.041537	-3.127226
6	H	2.714821	-0.173825	-2.418003
7	O	2.672458	-4.108091	-1.325677
8	H	2.857123	-4.621645	-0.524883
9	H	3.513042	1.107663	-0.918753
10	O	1.196056	-2.362210	-0.135595
11	O	2.469411	-1.818501	-2.336078
12	C	2.575286	1.214918	0.799145
13	H	2.165201	0.208567	0.929540
14	H	1.840983	1.815682	0.257713
15	C	2.931516	1.855775	2.139396
16	H	3.316811	2.864060	1.976038
17	H	3.704078	1.268490	2.640508
18	C	0.708815	2.910536	2.579782
19	H	0.232582	2.441508	1.720192
20	H	-0.029749	3.072091	3.364137
21	H	1.172580	3.857225	2.304437
22	C	2.327049	2.569755	4.397528
23	H	1.509864	2.689166	5.107564
24	H	3.076170	1.888055	4.798467
25	H	2.777021	3.536793	4.176822
26	C	1.156630	0.644174	3.423406
27	H	0.635888	0.281740	2.539162
28	H	1.945297	-0.045556	3.722282
29	H	0.446918	0.774582	4.239553
30	N	1.775060	1.987726	3.119901

31	C	-0.033086	-2.890629	-0.652523
32	H	0.030275	-3.055306	-1.732501
33	H	-0.238083	-3.847984	-0.161934
34	C	-1.153581	-1.904669	-0.352761
35	H	-1.062452	-1.534412	0.670243
36	C	-2.524387	-2.523764	-0.565117
37	H	-2.690268	-2.772715	-1.617466
38	H	-2.627777	-3.436345	0.027846
39	C	-0.781271	0.447721	-0.790876
40	C	-0.651606	1.439709	-1.923772
41	H	-1.293104	1.107773	-2.746044
42	H	0.383753	1.358192	-2.286756
43	C	-0.968051	2.883524	-1.520481
44	H	-0.289397	3.197550	-0.719054
45	H	-1.981284	2.930825	-1.101675
46	C	-0.854170	3.858079	-2.698446
47	H	0.160745	3.807222	-3.117401
48	H	-1.532185	3.538949	-3.502458
49	O	-1.025917	-0.789400	-1.268461
50	O	-0.659430	0.707770	0.394802
51	C	-1.172747	5.308167	-2.314342
52	H	-0.493045	5.627153	-1.512633
53	H	-2.185341	5.354961	-1.891368
54	C	-4.789003	-1.968638	-0.145976
55	C	-5.715651	-0.871631	0.328211
56	H	-5.326774	-0.494342	1.281802
57	H	-5.624525	-0.035956	-0.377867
58	C	-7.171289	-1.322052	0.461479
59	H	-7.523541	-1.695106	-0.507531
60	H	-7.223047	-2.171937	1.152962
61	C	-8.093723	-0.200838	0.952555
62	H	-8.039430	0.648787	0.257158
63	H	-7.730290	0.173888	1.919986
64	C	-9.554861	-0.643085	1.098738
65	H	-9.917771	-1.015356	0.131200
66	H	-9.606139	-1.494478	1.790843
67	O	-3.499899	-1.554930	-0.136717
68	O	-5.121296	-3.083719	-0.496247
69	C	-1.066018	6.280958	-3.492462
70	H	-1.298823	7.306077	-3.186344
71	H	-0.054967	6.281031	-3.915548
72	H	-1.760030	6.007374	-4.295392
73	C	-10.476634	0.474786	1.594988
74	H	-11.510811	0.127738	1.689009
75	H	-10.158425	0.843246	2.576971
76	H	-10.472560	1.326655	0.905383
77	Ca	5.444268	-0.685307	0.315640
78	O	7.425856	-1.477726	-0.852663
79	H	8.098581	-0.886595	-1.216353
80	H	7.891778	-2.290166	-0.613634
81	O	5.976978	0.206010	2.537579
82	H	6.143029	-0.363438	3.301278
83	H	6.534749	0.985712	2.664637

E[B3LYP/6-31G(d,p)] = -2767.55508 h, E[APFD/6-311+G(2d,p)] = -2766.6039 h
Gcorr[B3LYP/6-31G(d,p)] = 0.616472 h

77. PC6Ca+4H_2O, R1, 3rd step, reactants (extra water around Ca)

Center No.	Atom	X	Y	Z
1	P	3.129416	-0.786787	-2.080413
2	O	3.473085	-2.111651	-1.414723
3	O	3.675234	-0.401574	1.294101
4	H	3.876906	0.024570	0.425074
5	O	3.284969	-0.683099	-3.577110
6	H	3.506456	0.752674	-4.454269
7	O	1.605174	-0.351855	-1.635062
8	O	3.951027	0.357265	-1.277992
9	C	2.457615	0.184398	1.776362
10	H	1.597827	-0.226849	1.241511
11	H	2.479061	1.263718	1.602492

12	C	2.418338	-0.129758	3.270230
13	H	3.199486	0.427128	3.790001
14	H	2.584190	-1.197799	3.419448
15	C	0.728604	1.644112	3.773086
16	H	0.462847	1.805644	2.729462
17	H	-0.131736	1.857713	4.406520
18	H	1.571069	2.269230	4.067775
19	C	1.298328	-0.070490	5.439515
20	H	0.359292	0.127442	5.954063
21	H	1.586456	-1.112474	5.572827
22	H	2.079223	0.588506	5.816676
23	C	-0.008935	-0.684635	3.453224
24	H	-0.239021	-0.409124	2.426089
25	H	0.314426	-1.722981	3.514703
26	H	-0.884846	-0.522644	4.080419
27	N	1.106845	0.195794	3.966848
28	C	0.501372	-1.006860	-2.266665
29	H	0.425793	-0.688559	-3.312195
30	H	0.628905	-2.095650	-2.238469
31	C	-0.760241	-0.638739	-1.497472
32	H	-0.648483	-0.914455	-0.447414
33	C	-1.994237	-1.301003	-2.083313
34	H	-2.221119	-0.906595	-3.077936
35	H	-1.849231	-2.381882	-2.163499
36	C	-0.792100	1.550087	-0.476882
37	C	-0.996032	3.011833	-0.804887
38	H	-1.972934	3.103324	-1.295632
39	H	-0.257725	3.278390	-1.572181
40	C	-0.895544	3.943239	0.403347
41	H	0.095633	3.837881	0.860974
42	H	-1.621257	3.629796	1.163422
43	C	-1.137627	5.410805	0.031439
44	H	-0.412010	5.717830	-0.734999
45	H	-2.129704	5.510607	-0.431168
46	O	-0.947411	0.794139	-1.583295
47	O	-0.529847	1.103090	0.626164
48	C	-1.040670	6.362310	1.230007
49	H	-0.048900	6.262081	1.691308
50	H	-1.765246	6.053365	1.995500
51	C	-4.272143	-1.600406	-1.499153
52	C	-5.337289	-1.229700	-0.491615
53	H	-4.945056	-1.456039	0.507463
54	H	-5.452770	-0.138469	-0.521562
55	C	-6.674981	-1.930582	-0.733801
56	H	-7.031464	-1.688607	-1.742100
57	H	-6.521190	-3.016437	-0.716757
58	C	-7.738203	-1.542622	0.299846
59	H	-7.886507	-0.453583	0.280435
60	H	-7.371767	-1.781858	1.308289
61	C	-9.084672	-2.240609	0.072894
62	H	-9.450397	-2.000371	-0.934539
63	H	-8.934492	-3.328549	0.090664
64	O	-3.088132	-1.021852	-1.189083
65	O	-4.422439	-2.317135	-2.468716
66	C	-1.285113	7.827379	0.856398
67	H	-1.208990	8.481020	1.731438
68	H	-0.554435	8.174306	0.116809
69	H	-2.282928	7.964210	0.424113
70	C	-10.145588	-1.854183	1.107717
71	H	-11.093747	-2.368259	0.919282
72	H	-9.821837	-2.113797	2.122172
73	H	-10.341882	-0.776035	1.089564
74	Ca	4.011755	-2.836338	0.728365
75	O	6.234204	-3.700738	1.243262
76	H	6.794256	-3.341131	1.944092
77	H	6.455298	-4.639945	1.186567
78	O	2.314717	-3.455462	2.415187
79	H	1.493124	-3.867128	2.111568
80	H	2.579187	-3.957200	3.199561
81	O	3.663848	1.659979	-4.826590
82	H	4.566948	1.628697	-5.170699
83	H	3.724507	2.439495	-3.332105

84	O	3.736839	2.689829	-2.365544
85	H	2.860171	3.058123	-2.188576
86	H	3.858904	1.293723	-1.671681

E[B3LYP/6-31G(d,p)] = -2843.999284 h, E[APFD/6-311+G(2d,p)] = -2843.025124 h
Gcorr[B3LYP/6-31G(d,p)] = 0.642358 h

78. PC6Ca+4H_2O, R1, 3rd step, TS

Center No.	Atom	X	Y	Z
1	P	3.334482	-0.707543	-1.955527
2	O	3.525885	-1.965698	-1.113067
3	O	3.266375	0.214720	1.302784
4	H	3.475959	0.580531	0.414115
5	O	3.223698	-0.811178	-3.560252
6	H	4.181371	-0.991427	-3.776381
7	O	1.742035	-0.299231	-1.705626
8	O	3.835582	0.695196	-1.339476
9	C	1.943229	0.641081	1.656286
10	H	1.244256	-0.187258	1.525100
11	H	1.629114	1.456173	1.003597
12	C	2.021393	1.072353	3.119445
13	H	2.713202	1.909248	3.228082
14	H	2.382568	0.233655	3.716793
15	C	0.187955	2.769505	3.089242
16	H	-0.079417	2.556120	2.055595
17	H	-0.696112	3.095550	3.636380
18	H	0.963792	3.532326	3.145860
19	C	0.957631	1.781918	5.202349
20	H	0.030401	2.127365	5.656963
21	H	1.289011	0.860719	5.679700
22	H	1.726126	2.549167	5.287439
23	C	-0.339470	0.423024	3.619273
24	H	-0.651380	0.343930	2.579527
25	H	0.091794	-0.515269	3.967015
26	H	-1.191706	0.699578	4.238800
27	N	0.703562	1.508593	3.740609
28	C	0.741734	-1.236161	-2.094588
29	H	0.611361	-1.218781	-3.183166
30	H	1.022619	-2.252486	-1.793321
31	C	-0.564039	-0.868856	-1.402335
32	H	-0.419713	-0.834881	-0.321471
33	C	-1.676503	-1.842098	-1.751624
34	H	-1.936724	-1.782217	-2.812076
35	H	-1.373147	-2.868562	-1.526422
36	C	-1.084713	1.445830	-0.956208
37	C	-1.506291	2.726491	-1.640672
38	H	-2.436258	2.514374	-2.183050
39	H	-0.759773	2.944735	-2.414627
40	C	-1.680497	3.912109	-0.691177
41	H	-0.733110	4.103199	-0.172636
42	H	-2.409241	3.649905	0.085189
43	C	-2.134472	5.182924	-1.418828
44	H	-1.403688	5.437854	-2.199319
45	H	-3.081345	4.985575	-1.941075
46	O	-0.969070	0.446854	-1.853747
47	O	-0.878784	1.318317	0.238909
48	C	-2.314335	6.383992	-0.482547
49	H	-1.367605	6.580466	0.038574
50	H	-3.043746	6.127329	0.297544
51	C	-3.926626	-2.247171	-1.126139
52	C	-5.054972	-1.775854	-0.236167
53	H	-4.692942	-1.804383	0.799440
54	H	-5.230835	-0.715374	-0.456182
55	C	-6.337989	-2.593176	-0.394172
56	H	-6.667920	-2.548339	-1.439092
57	H	-6.121232	-3.648162	-0.187501
58	C	-7.463354	-2.105803	0.525325
59	H	-7.673733	-1.047331	0.316163
60	H	-7.125271	-2.148043	1.570505
61	C	-8.756663	-2.916794	0.379314

62	H	-9.093387	-2.874008	-0.665289
63	H	-8.544808	-3.974246	0.587613
64	O	-2.820278	-1.487099	-0.951316
65	O	-3.969966	-3.180405	-1.903086
66	C	-2.769632	7.652061	-1.210877
67	H	-2.888600	8.490597	-0.517000
68	H	-2.043073	7.952132	-1.974621
69	H	-3.731274	7.496240	-1.713075
70	C	-9.880366	-2.429784	1.298985
71	H	-10.788637	-3.027786	1.171577
72	H	-9.584914	-2.493150	2.352556
73	H	-10.137516	-1.384955	1.090457
74	Ca	3.955408	-2.206696	1.179875
75	O	6.167825	-3.079377	1.724526
76	H	6.755860	-2.654320	2.363180
77	H	6.353291	-4.026007	1.786740
78	O	2.300740	-2.365383	3.022120
79	H	1.517360	-2.918989	2.894059
80	H	2.615434	-2.571283	3.913840
81	O	5.424445	-0.966635	-2.659906
82	H	5.645719	-1.843842	-2.320967
83	H	6.213348	0.108367	-2.001119
84	O	6.368504	0.954987	-1.421179
85	H	6.635127	1.654498	-2.033761
86	H	4.851031	0.874271	-1.373893

E[B3LYP/6-31G(d,p)] = -2843.948107 h, E[APFD/6-311+G(2d,p)] = -2842.971025 h
Gcorr[B3LYP/6-31G(d,p)] = 0.641103 h

79. PC6Ca+4H_2O, R1, 3rd step, products

Center No.	Atom	X	Y	Z
1	P	3.503158	-0.694866	-1.996257
2	O	3.619624	-2.018452	-1.204724
3	O	3.207432	0.109906	1.305831
4	H	3.448748	0.467949	0.416236
5	O	3.090696	-0.640711	-3.587215
6	H	3.913748	-0.802922	-4.076217
7	O	1.866276	-0.336209	-1.593441
8	O	3.859278	0.731193	-1.243893
9	C	1.933652	0.656186	1.665757
10	H	1.139043	-0.051381	1.422492
11	H	1.751354	1.570109	1.098242
12	C	2.004191	0.926601	3.166969
13	H	2.749702	1.695315	3.376744
14	H	2.287235	0.007335	3.682180
15	C	0.244197	2.700036	3.208568
16	H	-0.051202	2.536399	2.173356
17	H	-0.611881	3.051831	3.783405
18	H	1.059660	3.419538	3.275536
19	C	0.966088	1.586710	5.277090
20	H	0.046662	1.926319	5.751612
21	H	1.281373	0.636323	5.705979
22	H	1.749529	2.333727	5.398388
23	C	-0.384189	0.357723	3.634750
24	H	-0.686096	0.326244	2.589768
25	H	0.001287	-0.609137	3.956217
26	H	-1.230874	0.651794	4.253800
27	N	0.704149	1.391472	3.804534
28	C	0.868986	-1.250452	-1.999822
29	H	0.739001	-1.231244	-3.090024
30	H	1.129033	-2.277729	-1.708190
31	C	-0.448027	-0.883650	-1.325299
32	H	-0.323863	-0.855834	-0.241979
33	C	-1.561822	-1.846609	-1.697113
34	H	-1.802553	-1.781926	-2.761736
35	H	-1.270868	-2.876161	-1.469108
36	C	-1.019757	1.421823	-0.875982
37	C	-1.409001	2.710694	-1.566130
38	H	-2.324941	2.509872	-2.136432
39	H	-0.638796	2.927647	-2.316542

40	C	-1.602200	3.891348	-0.614083
41	H	-0.669498	4.069402	-0.064915
42	H	-2.356584	3.630084	0.137624
43	C	-2.020957	5.172815	-1.344024
44	H	-1.264853	5.426334	-2.100509
45	H	-2.954198	4.990484	-1.895478
46	O	-0.841783	0.438250	-1.776509
47	O	-0.888206	1.282707	0.328956
48	C	-2.214885	6.367737	-0.402584
49	H	-1.281810	6.548310	0.148124
50	H	-2.969921	6.112687	0.353297
51	C	-3.843024	-2.203323	-1.149756
52	C	-4.981441	-1.724766	-0.276057
53	H	-4.661626	-1.830617	0.768587
54	H	-5.096214	-0.646036	-0.439552
55	C	-6.296053	-2.465228	-0.525879
56	H	-6.584123	-2.344369	-1.577237
57	H	-6.139198	-3.539867	-0.373974
58	C	-7.429645	-1.973100	0.380965
59	H	-7.577149	-0.894438	0.228909
60	H	-7.134491	-2.094392	1.432958
61	C	-8.756608	-2.703272	0.140870
62	H	-9.050505	-2.581159	-0.910380
63	H	-8.608008	-3.781012	0.292050
64	O	-2.719573	-1.486503	-0.917374
65	O	-3.894320	-3.109072	-1.958462
66	C	-2.633655	7.647776	-1.131843
67	H	-2.763385	8.481206	-0.433730
68	H	-1.881313	7.946296	-1.870839
69	H	-3.581725	7.508122	-1.663720
70	C	-9.887893	-2.210899	1.048357
71	H	-10.820525	-2.750207	0.853082
72	H	-9.636761	-2.351965	2.105881
73	H	-10.082117	-1.143210	0.894715
74	Ca	3.601126	-2.352494	1.104133
75	O	5.801586	-3.241838	1.675116
76	H	6.377992	-2.837329	2.337233
77	H	5.986234	-4.190003	1.710930
78	O	2.046681	-2.530105	3.023690
79	H	1.235273	-3.047508	2.921536
80	H	2.400142	-2.778162	3.889844
81	O	5.219948	-0.800560	-2.578238
82	H	5.524860	-1.658002	-2.251515
83	H	6.333506	0.462339	-2.069945
84	O	6.486051	1.276861	-1.532182
85	H	6.586757	1.988703	-2.179463
86	H	4.817741	0.990186	-1.318772

E[B3LYP/6-31G(d,p)] = -2843.954161 h, E[APFD/6-311+G(2d,p)] = -2842.977666 h
Gcorr[B3LYP/6-31G(d,p)] = 0.642358 h

80. PC6Ca+4H_2O, R1, 4th step, reactants

Center No.	Atom	X	Y	Z
1	P	3.235220	-0.915530	-2.089296
2	O	3.384246	-2.304199	-1.432292
3	O	2.098581	-1.205624	1.156526
4	H	1.912711	-0.850586	0.232672
5	O	2.513951	-0.728252	-3.552356
6	H	3.219687	-0.843004	-4.208320
7	O	1.643884	-0.564662	-1.348101
8	O	3.688303	0.465480	-1.309152
9	C	1.964076	-0.154228	2.109540
10	H	1.852827	-0.620523	3.090613
11	H	1.060452	0.419099	1.887173
12	C	3.226265	0.719819	2.052526
13	H	3.462479	0.951933	1.011767
14	H	4.071537	0.187028	2.493020
15	C	2.217922	2.999091	2.030440
16	H	1.234651	2.551456	1.898803
17	H	2.139868	3.924087	2.600516

18	H	2.665366	3.196535	1.057064
19	C	4.500890	2.658026	2.852659
20	H	4.424895	3.647189	3.302264
21	H	5.136540	2.016024	3.460918
22	H	4.898718	2.733958	1.841593
23	C	2.604288	1.862982	4.187501
24	H	1.571718	1.521917	4.148456
25	H	3.228298	1.129283	4.697001
26	H	2.654839	2.819702	4.705711
27	N	3.121256	2.052428	2.784410
28	C	0.533875	-1.376656	-1.707137
29	H	0.385261	-1.355351	-2.791165
30	H	0.692357	-2.419826	-1.401632
31	C	-0.715056	-0.844412	-1.010469
32	H	-0.556321	-0.782562	0.067641
33	C	-1.929037	-1.706239	-1.306663
34	H	-2.200113	-1.658201	-2.365051
35	H	-1.729110	-2.749582	-1.046708
36	C	-0.833422	1.545870	-0.689200
37	C	-1.155677	2.832119	-1.417688
38	H	-2.134801	2.705039	-1.895080
39	H	-0.437457	2.926427	-2.242573
40	C	-1.132193	4.074008	-0.525881
41	H	-0.137949	4.178181	-0.075361
42	H	-1.833310	3.935432	0.306109
43	C	-1.486645	5.353388	-1.292506
44	H	-0.784153	5.485420	-2.127618
45	H	-2.481666	5.242970	-1.746389
46	O	-0.995228	0.487313	-1.508764
47	O	-0.483278	1.464930	0.475117
48	C	-1.468853	6.609412	-0.412899
49	H	-0.473971	6.719183	0.039500
50	H	-2.169786	6.475025	0.422038
51	C	-4.193403	-1.867458	-0.625450
52	C	-5.256990	-1.247892	0.253717
53	H	-4.867395	-1.220705	1.279023
54	H	-5.363962	-0.197924	-0.047425
55	C	-6.599291	-1.978166	0.191042
56	H	-6.950959	-1.996855	-0.847487
57	H	-6.454013	-3.025393	0.482834
58	C	-7.663439	-1.334508	1.086841
59	H	-7.802708	-0.284620	0.792332
60	H	-7.303439	-1.314073	2.125313
61	C	-9.014524	-2.058082	1.034202
62	H	-9.372707	-2.078130	-0.003943
63	H	-8.873512	-3.107124	1.327670
64	O	-3.018369	-1.207783	-0.505487
65	O	-4.340298	-2.828755	-1.354592
66	C	-1.825709	7.886587	-1.179182
67	H	-1.804464	8.764332	-0.525036
68	H	-1.121568	8.065537	-1.999803
69	H	-2.829480	7.819528	-1.614141
70	C	-10.077990	-1.415390	1.929529
71	H	-11.029367	-1.954036	1.869910
72	H	-9.762288	-1.412123	2.979114
73	H	-10.265104	-0.375613	1.637758
74	Ca	3.503695	-3.227579	0.688169
75	O	5.726722	-3.211263	1.752487
76	H	5.880186	-2.802699	2.615026
77	H	6.528298	-3.042538	1.239228
78	O	1.194169	-3.904703	1.144804
79	H	0.897638	-4.660873	1.668466
80	H	0.777758	-3.121029	1.533337
81	O	4.789376	-0.933992	-2.885091
82	H	5.183055	-1.792314	-2.679928
83	H	4.622492	0.590373	-1.540342

E[B3LYP/6-31G(d,p)] = -2767.514699 h, E[APFD/6-311+G(2d,p)] = -2766.562305 h
Gcorr[B3LYP/6-31G(d,p)] = 0.620433 h

81. PC6Ca+4H_2O, R1, 4th step, TS

Center No.	Atom	X	Y	Z
1	P	3.373045	-0.696986	-2.258560
2	O	3.648668	-2.054939	-1.637545
3	O	2.254809	-1.327679	1.088254
4	H	1.885965	-0.876444	-0.136057
5	O	2.323313	-0.529652	-3.480850
6	H	2.839864	-0.505981	-4.302761
7	O	1.586981	-0.610262	-1.157945
8	O	3.580794	0.667195	-1.397661
9	C	1.995167	-0.361343	2.075404
10	H	1.861621	-0.840964	3.054596
11	H	1.069792	0.183779	1.846457
12	C	3.189744	0.607509	2.127012
13	H	3.438612	0.924183	1.112515
14	H	4.057091	0.106388	2.562708
15	C	2.037086	2.817270	2.215800
16	H	1.085352	2.319385	2.040264
17	H	1.892581	3.703975	2.832302
18	H	2.489406	3.094274	1.264047
19	C	4.313909	2.575166	3.083369
20	H	4.163005	3.524690	3.596057
21	H	4.977648	1.936040	3.664126
22	H	4.729865	2.746077	2.091178
23	C	2.439973	1.575366	4.306440
24	H	1.435225	1.168597	4.211628
25	H	3.098277	0.852729	4.787745
26	H	2.411036	2.497985	4.884851
27	N	2.981206	1.886598	2.936067
28	C	0.493372	-1.456794	-1.506472
29	H	0.385124	-1.447607	-2.592010
30	H	0.677444	-2.488326	-1.179851
31	C	-0.788586	-0.944736	-0.851083
32	H	-0.658225	-0.865010	0.229838
33	C	-1.979904	-1.831685	-1.165243
34	H	-2.221601	-1.808255	-2.231568
35	H	-1.774311	-2.867083	-0.878614
36	C	-0.969259	1.445135	-0.566523
37	C	-1.269016	2.716437	-1.330007
38	H	-2.230721	2.577912	-1.838834
39	H	-0.522812	2.796706	-2.131117
40	C	-1.278476	3.975289	-0.462132
41	H	-0.304970	4.082652	0.031026
42	H	-2.017198	3.857060	0.339873
43	C	-1.589242	5.240869	-1.269548
44	H	-0.849773	5.350150	-2.075556
45	H	-2.564249	5.128139	-1.764459
46	O	-1.074646	0.372726	-1.379445
47	O	-0.678215	1.383060	0.614363
48	C	-1.599385	6.515295	-0.416772
49	H	-0.625174	6.625848	0.078420
50	H	-2.339076	6.405430	0.387731
51	C	-4.270531	-1.981748	-0.564526
52	C	-5.359879	-1.345735	0.270387
53	H	-5.010967	-1.322667	1.310370
54	H	-5.438161	-0.294754	-0.035870
55	C	-6.710502	-2.053871	0.156024
56	H	-7.018376	-2.075169	-0.896266
57	H	-6.596551	-3.100862	0.462186
58	C	-7.799367	-1.382805	1.000827
59	H	-7.905878	-0.333187	0.691955
60	H	-7.483048	-1.359518	2.053366
61	C	-9.161050	-2.080511	0.897650
62	H	-9.475305	-2.104609	-0.154542
63	H	-9.053785	-3.128876	1.207295
64	O	-3.096179	-1.329585	-0.404577
65	O	-4.397768	-2.946534	-1.292609
66	C	-1.907707	7.778693	-1.225808
67	H	-1.907676	8.670303	-0.590345
68	H	-1.164694	7.933173	-2.016600

69	H	-2.890985	7.711379	-1.705259
70	C	-10.248272	-1.407162	1.740469
71	H	-11.206880	-1.927766	1.646413
72	H	-9.976957	-1.398082	2.802364
73	H	-10.402157	-0.367293	1.430151
74	Ca	3.977738	-2.917782	0.537117
75	O	6.200984	-2.890535	1.603162
76	H	6.353629	-2.443654	2.446691
77	H	7.002057	-2.741438	1.082952
78	O	1.750206	-3.911694	1.087067
79	H	1.625107	-4.402906	1.909996
80	H	1.540236	-2.966576	1.289153
81	O	4.729619	-0.461623	-3.209545
82	H	5.298241	-1.241281	-3.137715
83	H	4.446508	1.028027	-1.650193

E[B3LYP/6-31G(d,p)] = -2767.506074 h, E[APFD/6-311+G(2d,p)] = -2766.550389 h
Gcorr[B3LYP/6-31G(d,p)] = 0.618014 h

82. PC6Ca+4H_2O, R1, 4th step, products

Center No.	Atom	X	Y	Z
1	P	5.039648	-1.612828	-2.374793
2	O	4.927048	-2.212836	-1.012837
3	O	2.173907	-0.806946	1.519247
4	H	1.683076	-0.610611	-0.026259
5	O	3.911630	-1.982403	-3.436514
6	H	3.927336	-2.908376	-3.727783
7	O	1.408339	-0.566802	-0.989501
8	O	4.937851	-0.027606	-2.283051
9	C	1.676612	0.232276	2.304622
10	H	1.472860	-0.102368	3.334521
11	H	0.730537	0.621606	1.899033
12	C	2.734111	1.351684	2.336854
13	H	3.044784	1.579648	1.315202
14	H	3.608126	1.016607	2.900135
15	C	1.342101	3.398514	2.035591
16	H	0.479529	2.766150	1.833619
17	H	1.030077	4.324386	2.518111
18	H	1.861093	3.621729	1.103932
19	C	3.528529	3.541431	3.131005
20	H	3.221343	4.518984	3.501274
21	H	4.192269	3.060051	3.848104
22	H	4.026527	3.644582	2.167531
23	C	1.658682	2.471784	4.297113
24	H	0.719133	1.939123	4.165768
25	H	2.337382	1.894409	4.924118
26	H	1.471319	3.446031	4.747566
27	N	2.302989	2.683136	2.952492
28	C	0.381035	-1.511049	-1.185105
29	H	0.311910	-1.721785	-2.259363
30	H	0.593589	-2.461279	-0.672168
31	C	-0.979415	-1.002274	-0.691651
32	H	-0.923146	-0.751373	0.369743
33	C	-2.091395	-2.004102	-0.934431
34	H	-2.268444	-2.147873	-2.004150
35	H	-1.836747	-2.972219	-0.493431
36	C	-1.286424	1.390185	-0.797822
37	C	-1.595416	2.509206	-1.769383
38	H	-2.521059	2.244786	-2.295074
39	H	-0.810115	2.499041	-2.536374
40	C	-1.705267	3.887612	-1.117089
41	H	-0.762927	4.123777	-0.608322
42	H	-2.475816	3.858945	-0.337055
43	C	-2.035109	4.989953	-2.130120
44	H	-1.262935	5.009806	-2.912323
45	H	-2.978029	4.746464	-2.640006
46	O	-1.309352	0.200589	-1.430526
47	O	-1.057988	1.532892	0.390289
48	C	-2.148356	6.381632	-1.496289
49	H	-1.205552	6.624552	-0.987729

50	H	-2.919339	6.360355	-0.714242
51	C	-4.398251	-2.251799	-0.437930
52	C	-5.581645	-1.601764	0.244909
53	H	-5.309753	-1.439578	1.295662
54	H	-5.702555	-0.599309	-0.184601
55	C	-6.873772	-2.411517	0.128231
56	H	-7.105381	-2.569652	-0.932013
57	H	-6.715198	-3.408045	0.557784
58	C	-8.060198	-1.732142	0.821254
59	H	-8.211246	-0.732071	0.390588
60	H	-7.821818	-1.573488	1.882604
61	C	-9.363631	-2.532431	0.709999
62	H	-9.600122	-2.690905	-0.350865
63	H	-9.211429	-3.531535	1.140244
64	O	-3.288145	-1.490339	-0.313543
65	O	-4.409806	-3.315127	-1.027185
66	C	-2.479657	7.480023	-2.510987
67	H	-2.553597	8.460477	-2.029282
68	H	-1.708597	7.547426	-3.287032
69	H	-3.434618	7.281659	-3.010955
70	C	-10.549151	-1.853107	1.401916
71	H	-11.463211	-2.447962	1.304651
72	H	-10.355569	-1.712406	2.471511
73	H	-10.746869	-0.865590	0.969461
74	Ca	4.116840	-2.102730	1.209982
75	O	5.659008	-1.326641	2.961336
76	H	5.437541	-1.378699	3.900851
77	H	6.189212	-0.524420	2.862461
78	O	2.008710	-3.366583	1.613664
79	H	1.871522	-3.818305	2.456724
80	H	1.703352	-2.422818	1.739675
81	O	6.383656	-2.016198	-3.141695
82	H	7.137379	-2.151103	-2.545053
83	H	5.002579	0.435540	-3.133589

E[B3LYP/6-31G(d,p)] = -2767.519269 h, E[APFD/6-311+G(2d,p)] = -2766.560705 h
Gcorr[B3LYP/6-31G(d,p)] = 0.608779 h

VIII. Structures of molecules and transition states (TS) related to PC6Ca + 4 H_2O (R2) as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

83. PC6Ca+4H_2O, R2, 1st step, reactants

Center No.	Atom	X	Y	Z
1	P	2.631613	-1.020868	-0.492416
2	O	3.503681	-2.248439	-0.348629
3	O	3.215081	0.039232	0.629218
4	O	4.793294	0.786149	-2.724384
5	H	5.169298	0.178584	-3.375572
6	H	3.915408	0.392518	-2.495438
7	O	5.994011	0.327502	-0.319420
8	H	5.185315	0.220009	0.209416
9	H	5.646442	0.552305	-1.220722
10	O	1.174535	-1.274567	0.191882
11	O	2.482678	-0.362759	-1.839766
12	C	2.540216	1.301355	0.780288
13	H	1.469480	1.127586	0.905386
14	H	2.706578	1.911203	-0.111471
15	C	3.164828	1.920653	2.029176
16	H	4.221978	2.130645	1.855718
17	H	3.079284	1.221301	2.862366
18	C	2.595101	4.269574	1.401894
19	H	1.969694	3.964078	0.565873
20	H	2.227817	5.209933	1.810336
21	H	3.630556	4.378580	1.081567
22	C	3.316916	3.716756	3.679664
23	H	2.869844	4.646476	4.027749
24	H	3.273826	2.961739	4.463405
25	H	4.348354	3.886658	3.374094
26	C	1.096078	3.013429	2.910152
27	H	0.497378	2.686965	2.061196

28	H	1.075940	2.259058	3.695948
29	H	0.713712	3.959179	3.292364
30	N	2.531458	3.223848	2.487404
31	C	0.152371	-2.002664	-0.504062
32	H	0.337127	-2.001025	-1.582707
33	H	0.149426	-3.036138	-0.142382
34	C	-1.189392	-1.343077	-0.210678
35	H	-1.239135	-1.068578	0.845206
36	C	-2.355950	-2.244466	-0.575629
37	H	-2.402442	-2.419692	-1.654520
38	H	-2.265073	-3.209871	-0.070880
39	C	-1.224019	1.068025	-0.414479
40	C	-1.382518	2.172643	-1.435477
41	H	-2.135874	1.856975	-2.164802
42	H	-0.435325	2.227440	-1.989899
43	C	-1.730368	3.533037	-0.826663
44	H	-0.955917	3.818024	-0.105528
45	H	-2.663732	3.445867	-0.256466
46	C	-1.876135	4.628940	-1.888607
47	H	-0.939975	4.710852	-2.458945
48	H	-2.649172	4.335309	-2.612653
49	O	-1.306103	-0.141583	-1.011097
50	O	-1.031109	1.226774	0.777716
51	C	-2.231057	5.998934	-1.298103
52	H	-1.457938	6.291713	-0.574892
53	H	-3.165621	5.914576	-0.727259
54	C	-4.706158	-2.282116	-0.278118
55	C	-5.893438	-1.481365	0.207845
56	H	-5.648839	-1.085793	1.200860
57	H	-5.984436	-0.603055	-0.444816
58	C	-7.196761	-2.281655	0.232900
59	H	-7.399832	-2.670735	-0.771801
60	H	-7.068813	-3.158237	0.879886
61	C	-8.389537	-1.451271	0.719649
62	H	-8.514560	-0.574347	0.068669
63	H	-8.175359	-1.057283	1.723277
64	C	-9.701436	-2.244543	0.757730
65	H	-9.915219	-2.636776	-0.245704
66	H	-9.573602	-3.121714	1.406371
67	O	-3.556700	-1.580419	-0.139547
68	O	-4.741766	-3.405266	-0.740600
69	C	-2.378039	7.092370	-2.360425
70	H	-2.631503	8.056947	-1.908666
71	H	-1.447887	7.223075	-2.925218
72	H	-3.167872	6.842892	-3.078162
73	C	-10.892871	-1.416226	1.247626
74	H	-11.812763	-2.009815	1.263598
75	H	-10.722064	-1.039329	2.262555
76	H	-11.066518	-0.550211	0.598671
77	Ca	5.238660	-3.768955	-0.408108
78	O	6.980048	-2.118157	-0.419190
79	H	6.654707	-1.168981	-0.385612
80	H	7.708139	-2.174526	0.212412
81	O	4.504208	-5.615960	1.047676
82	H	3.653072	-6.045663	0.886541
83	H	4.566617	-5.523583	2.008239

E[B3LYP/6-31G(d,p)] = -2767.550592 h, E[APFD/6-311+G(2d,p)] = -2766.605000 h
Gcorr[B3LYP/6-31G(d,p)] = 0.618023 h

84. PC6Ca+4H_2O, R2, 1st step, TS

Center No.	Atom	X	Y	Z
1	P	2.958632	-0.888281	-0.426005
2	O	3.129185	-2.328992	0.001989
3	O	3.428362	0.269302	0.625900
4	O	5.285059	-0.562132	-3.132277
5	H	5.413911	-1.423012	-3.553946
6	H	3.861352	-0.532883	-2.464796
7	O	5.238900	-0.906572	-0.645358
8	H	5.536511	-0.133499	-0.148039

9	H	5.518175	-0.703899	-2.144914
10	O	1.346112	-0.598390	-0.198679
11	O	2.981670	-0.470915	-1.957798
12	C	2.658711	1.468992	0.835938
13	H	1.622178	1.220315	1.055717
14	H	2.697083	2.084314	-0.067413
15	C	3.357247	2.141661	2.015969
16	H	4.391597	2.377641	1.760460
17	H	3.353771	1.465280	2.872403
18	C	2.752065	4.482707	1.393511
19	H	2.118326	4.167145	0.567601
20	H	2.379086	5.419752	1.804233
21	H	3.781143	4.603681	1.057542
22	C	3.516137	3.942051	3.660934
23	H	3.074648	4.875799	4.005477
24	H	3.479760	3.194460	4.452124
25	H	4.544842	4.106618	3.343324
26	C	1.289391	3.219663	2.927104
27	H	0.676558	2.910747	2.081512
28	H	1.283176	2.451480	3.699666
29	H	0.914160	4.158387	3.333363
30	N	2.716577	3.439200	2.482529
31	C	0.376016	-1.500420	-0.716246
32	H	0.467431	-1.584254	-1.806099
33	H	0.508688	-2.494153	-0.273735
34	C	-0.997791	-0.953289	-0.350215
35	H	-1.022040	-0.706835	0.713363
36	C	-2.106433	-1.932373	-0.690567
37	H	-2.190746	-2.078952	-1.771381
38	H	-1.916233	-2.902137	-0.222990
39	C	-1.156703	1.454628	-0.495043
40	C	-1.450265	2.567101	-1.477643
41	H	-2.384042	2.313531	-1.993653
42	H	-0.670469	2.531831	-2.249714
43	C	-1.529669	3.956015	-0.843374
44	H	-0.576824	4.186708	-0.352114
45	H	-2.289146	3.950222	-0.052076
46	C	-1.858788	5.047122	-1.868831
47	H	-1.097661	5.044096	-2.661955
48	H	-2.812064	4.808316	-2.361275
49	O	-1.241646	0.254842	-1.111090
50	O	-0.885522	1.600508	0.682914
51	C	-1.944676	6.449860	-1.255539
52	H	-0.991348	6.688704	-0.765061
53	H	-2.704101	6.450907	-0.462010
54	C	-4.433197	-2.161975	-0.306239
55	C	-5.657225	-1.474098	0.255864
56	H	-5.416431	-1.138899	1.272052
57	H	-5.814457	-0.556887	-0.326600
58	C	-6.908528	-2.353534	0.242570
59	H	-7.106297	-2.682714	-0.784446
60	H	-6.715436	-3.264012	0.823058
61	C	-8.140593	-1.634668	0.803414
62	H	-8.329289	-0.723125	0.218702
63	H	-7.933352	-1.300339	1.829894
64	C	-9.401730	-2.507212	0.801133
65	H	-9.607165	-2.841765	-0.224694
66	H	-9.211577	-3.417496	1.385695
67	O	-3.335399	-1.381032	-0.179985
68	O	-4.403605	-3.266088	-0.813348
69	C	-2.277378	7.535927	-2.282976
70	H	-2.331752	8.524808	-1.816172
71	H	-1.517322	7.580983	-3.071379
72	H	-3.242193	7.341736	-2.765337
73	C	-10.632985	-1.788461	1.360682
74	H	-11.515283	-2.436638	1.345880
75	H	-10.469455	-1.472118	2.397257
76	H	-10.868129	-0.892303	0.775132
77	Ca	4.250785	-4.353497	-0.131975
78	O	6.248366	-3.071689	0.126437
79	H	5.892532	-2.125710	-0.146771
80	H	6.596463	-2.981570	1.022720

81	O	2.809828	-5.969406	1.037923
82	H	1.889674	-6.077141	0.760912
83	H	2.788413	-5.981041	2.004652

E[B3LYP/6-31G(d,p)] = -2767.500841 h, E[APFD/6-311+G(2d,p)] = -2766.550423 h
Gcorr[B3LYP/6-31G(d,p)] = 0.618805 h

85. PC6Ca+4H_2O, R2, 1st step, products

Center No.	Atom	X	Y	Z
1	P	3.205517	-0.807576	-0.742714
2	O	3.186521	-2.231069	-0.173242
3	O	3.528785	0.530837	0.198567
4	O	5.517245	-1.382594	-3.448468
5	H	5.414698	-2.327137	-3.629998
6	H	3.963835	-0.816266	-2.822204
7	O	5.059233	-0.846662	-0.849075
8	H	5.384554	0.059197	-0.740811
9	H	5.672533	-1.329008	-2.478057
10	O	1.543932	-0.463523	-0.605259
11	O	3.128903	-0.574871	-2.350641
12	C	2.555726	1.472485	0.662125
13	H	1.753374	0.970181	1.198457
14	H	2.118453	2.006843	-0.184178
15	C	3.362319	2.397833	1.574128
16	H	4.209690	2.820041	1.031227
17	H	3.742009	1.832341	2.426748
18	C	2.202976	4.547352	1.057789
19	H	1.527695	4.063106	0.356060
20	H	1.706016	5.400189	1.518283
21	H	3.109343	4.872383	0.548759
22	C	3.474817	4.280436	3.134532
23	H	2.938732	5.141774	3.530425
24	H	3.721559	3.589201	3.939281
25	H	4.380141	4.603259	2.621985
26	C	1.335801	3.107491	2.860346
27	H	0.634000	2.685076	2.141813
28	H	1.620995	2.362255	3.602399
29	H	0.887946	3.969558	3.353291
30	N	2.581703	3.572945	2.144941
31	C	0.588611	-1.377861	-1.099162
32	H	0.601382	-1.404714	-2.197482
33	H	0.790437	-2.389965	-0.727638
34	C	-0.785910	-0.936254	-0.608906
35	H	-0.762688	-0.792661	0.473034
36	C	-1.873447	-1.925844	-0.983540
37	H	-2.013391	-1.974381	-2.067393
38	H	-1.620983	-2.926111	-0.621338
39	C	-1.125434	1.453169	-0.486608
40	C	-1.455231	2.657846	-1.342036
41	H	-2.168717	2.348321	-2.112499
42	H	-0.533663	2.926703	-1.877427
43	C	-1.978808	3.855977	-0.545758
44	H	-1.244620	4.132399	0.219520
45	H	-2.887988	3.561871	-0.006118
46	C	-2.279059	5.065670	-1.438091
47	H	-1.366608	5.355182	-1.978580
48	H	-3.010253	4.779467	-2.207235
49	O	-1.124906	0.329728	-1.232087
50	O	-0.881801	1.484764	0.706951
51	C	-2.811757	6.274935	-0.660025
52	H	-2.080729	6.560663	0.108369
53	H	-3.722864	5.983780	-0.120088
54	C	-4.170645	-2.282262	-0.509860
55	C	-5.384048	-1.696583	0.178095
56	H	-5.101124	-1.459885	1.211067
57	H	-5.595744	-0.729872	-0.297123
58	C	-6.610664	-2.609000	0.134381
59	H	-6.854657	-2.835297	-0.910410
60	H	-6.363549	-3.568453	0.605103
61	C	-7.828951	-1.991072	0.829673

62	H	-8.071682	-1.029638	0.355167
63	H	-7.575341	-1.759455	1.873938
64	C	-9.066150	-2.896656	0.799244
65	H	-9.318506	-3.127926	-0.244439
66	H	-8.821941	-3.856990	1.273185
67	O	-3.093646	-1.478589	-0.359330
68	O	-4.134273	-3.329602	-1.125822
69	C	-3.111385	7.481461	-1.554651
70	H	-3.489924	8.327342	-0.971598
71	H	-2.210801	7.816599	-2.081828
72	H	-3.864632	7.235077	-2.311722
73	C	-10.282754	-2.278360	1.494461
74	H	-11.148121	-2.948059	1.456431
75	H	-10.071051	-2.067274	2.548949
76	H	-10.571742	-1.333466	1.020182
77	Ca	4.213395	-4.091907	0.697174
78	O	6.075984	-2.552865	0.885383
79	H	5.758738	-1.827602	0.269868
80	H	6.224476	-2.129594	1.741020
81	O	2.595648	-5.526530	1.867844
82	H	1.748711	-5.737576	1.451606
83	H	2.390382	-5.367107	2.799256

E[B3LYP/6-31G(d,p)] = -2767.506678 h, E[APFD/6-311+G(2d,p)] = -2766.557129 h
Gcorr[B3LYP/6-31G(d,p)] = 0.618353 h

86. PC6Ca+4H_2O, R2, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	P	3.661756	-0.114270	-0.805984
2	O	3.653967	-1.625500	-1.061150
3	O	3.450493	0.531438	0.716533
4	O	1.642578	2.255948	-2.795603
5	H	1.732709	3.060594	-2.265698
6	H	3.183021	1.377242	-2.372059
7	O	5.367066	-0.116533	-0.423509
8	H	5.644189	0.755934	-0.111137
9	H	1.391612	1.561104	-2.149101
10	O	1.903702	0.103277	-1.142978
11	O	3.987449	0.996433	-1.952613
12	C	2.221282	1.001587	1.269479
13	H	1.510447	0.182309	1.381042
14	H	1.771492	1.763047	0.633339
15	C	2.635546	1.569112	2.628295
16	H	3.396105	2.339224	2.490765
17	H	3.051493	0.777082	3.253427
18	C	0.934775	3.402079	2.700879
19	H	0.392168	3.058898	1.821983
20	H	0.249515	3.911399	3.377400
21	H	1.749914	4.069591	2.423472
22	C	2.092287	2.675192	4.740081
23	H	1.298590	3.134333	5.327609
24	H	2.501104	1.814556	5.267767
25	H	2.878263	3.401961	4.538014
26	C	0.405144	1.219794	3.704816
27	H	-0.090683	0.968509	2.769125
28	H	0.836224	0.333571	4.169588
29	H	-0.307345	1.687429	4.383376
30	N	1.510596	2.209940	3.427891
31	C	1.046893	-0.981208	-1.452340
32	H	0.976486	-1.115590	-2.542424
33	H	1.428799	-1.912506	-1.028366
34	C	-0.347276	-0.723860	-0.884797
35	H	-0.300033	-0.583594	0.195826
36	C	-1.303100	-1.855609	-1.217461
37	H	-1.490411	-1.913312	-2.293482
38	H	-0.891493	-2.812961	-0.885494
39	C	-1.175897	1.542897	-0.688327
40	C	-1.724679	2.681605	-1.518138
41	H	-2.573829	2.289356	-2.091377
42	H	-0.956501	2.928904	-2.262203

43	C	-2.129063	3.910292	-0.703257
44	H	-1.254816	4.291706	-0.161809
45	H	-2.858375	3.614634	0.060551
46	C	-2.718211	5.022762	-1.578316
47	H	-1.985748	5.310169	-2.345897
48	H	-3.591637	4.634939	-2.121445
49	O	-0.881270	0.488812	-1.478341
50	O	-1.004021	1.563430	0.518592
51	C	-3.130168	6.266058	-0.780944
52	H	-2.256615	6.653817	-0.239634
53	H	-3.860279	5.976572	-0.013094
54	C	-3.503811	-2.535321	-0.654347
55	C	-4.749316	-2.145485	0.110279
56	H	-4.452887	-1.938790	1.146146
57	H	-5.096911	-1.185470	-0.292504
58	C	-5.855368	-3.200139	0.051266
59	H	-6.119219	-3.387857	-0.996461
60	H	-5.469728	-4.149032	0.443550
61	C	-7.106217	-2.787288	0.835034
62	H	-7.488164	-1.835455	0.439413
63	H	-6.833908	-2.594073	1.882405
64	C	-8.221833	-3.838478	0.788598
65	H	-8.493134	-4.030677	-0.258249
66	H	-7.838120	-4.789164	1.182882
67	O	-2.540197	-1.594218	-0.525603
68	O	-3.353726	-3.549735	-1.306716
69	C	-3.722005	7.374071	-1.657185
70	H	-4.005872	8.247028	-1.060423
71	H	-3.002209	7.707285	-2.413567
72	H	-4.617424	7.025538	-2.184442
73	C	-9.471119	-3.426893	1.573165
74	H	-10.247551	-4.197115	1.521106
75	H	-9.237191	-3.260793	2.630994
76	H	-9.897337	-2.497117	1.179305
77	Ca	4.774280	-3.625200	-0.830079
78	O	6.207486	-2.352240	0.659026
79	H	5.949892	-1.427480	0.375158
80	H	6.037686	-2.399001	1.608816
81	O	3.639889	-5.251420	0.609561
82	H	2.676687	-5.332758	0.619377
83	H	3.920403	-5.390042	1.524229

E[B3LYP/6-31G(d,p)] = -2767.505663 h, E[APFD/6-311+G(2d,p)] = -2766.558009 h
Gcorr[B3LYP/6-31G(d,p)] = 0.620935 h

87. PC6Ca+4H_2O, R2, 2nd step, TS

Center No.	Atom	X	Y	Z
1	P	3.875310	-0.454370	-0.491128
2	O	3.599029	-1.864562	-0.959664
3	O	3.365852	-0.001656	0.989535
4	O	2.173044	1.592506	-2.740401
5	H	1.970053	2.477729	-2.407526
6	H	3.354569	1.150812	-2.050243
7	O	5.461357	-0.659365	0.007891
8	H	5.796749	0.112239	0.486370
9	H	1.743631	0.876774	-2.028015
10	O	1.677590	-0.047406	-1.055732
11	O	4.137095	0.758737	-1.457383
12	C	2.418879	1.040357	1.261260
13	H	1.407373	0.649794	1.193427
14	H	2.519865	1.841850	0.527804
15	C	2.789568	1.511527	2.668495
16	H	3.725790	2.071957	2.651904
17	H	2.913326	0.647464	3.323495
18	C	1.420463	3.588948	2.447846
19	H	0.863328	3.235366	1.581286
20	H	0.803327	4.278685	3.022454
21	H	2.346902	4.078155	2.148661
22	C	2.345417	2.909494	4.624289
23	H	1.601663	3.521050	5.132939

24	H	2.612652	2.052477	5.241564
25	H	3.230933	3.503023	4.401257
26	C	0.487377	1.646884	3.634927
27	H	0.014650	1.346210	2.702375
28	H	0.740043	0.779854	4.244173
29	H	-0.179279	2.308877	4.186692
30	N	1.754891	2.409703	3.329173
31	C	0.788350	-1.095129	-1.269483
32	H	0.671131	-1.331273	-2.344365
33	H	1.137588	-2.017723	-0.782537
34	C	-0.601910	-0.763741	-0.704000
35	H	-0.536598	-0.571977	0.368691
36	C	-1.623936	-1.847616	-0.979443
37	H	-1.829055	-1.939006	-2.049643
38	H	-1.261679	-2.813006	-0.613241
39	C	-1.042673	1.613518	-0.694067
40	C	-1.420633	2.752238	-1.617737
41	H	-2.366621	2.485202	-2.104393
42	H	-0.673203	2.768529	-2.422035
43	C	-1.517699	4.113054	-0.928070
44	H	-0.552256	4.356429	-0.468113
45	H	-2.242138	4.052198	-0.106833
46	C	-1.922639	5.233244	-1.893264
47	H	-1.198461	5.283382	-2.718776
48	H	-2.890682	4.987492	-2.352329
49	O	-1.076413	0.445295	-1.356040
50	O	-0.752117	1.734931	0.485379
51	C	-2.016739	6.607359	-1.219044
52	H	-1.048905	6.851247	-0.760391
53	H	-2.740052	6.555753	-0.394042
54	C	-3.888446	-2.329386	-0.450400
55	C	-5.097614	-1.839051	0.316075
56	H	-4.814341	-1.776683	1.374669
57	H	-5.292578	-0.805571	0.003646
58	C	-6.336976	-2.715367	0.129419
59	H	-6.583485	-2.768614	-0.937985
60	H	-6.104189	-3.740992	0.440155
61	C	-7.547205	-2.197155	0.914518
62	H	-7.770583	-1.166913	0.602814
63	H	-7.293881	-2.143375	1.982897
64	C	-8.800705	-3.062105	0.735049
65	H	-9.052033	-3.115818	-0.332853
66	H	-8.576930	-4.091184	1.047115
67	O	-2.839707	-1.493582	-0.285785
68	O	-3.834699	-3.336166	-1.130089
69	C	-2.421007	7.725734	-2.184197
70	H	-2.478769	8.692703	-1.673865
71	H	-1.697712	7.823283	-3.001879
72	H	-3.401141	7.526539	-2.632394
73	C	-10.009144	-2.541397	1.518849
74	H	-10.887003	-3.178631	1.370179
75	H	-9.799364	-2.508974	2.594143
76	H	-10.277269	-1.526337	1.204086
77	Ca	4.257213	-4.092339	-1.008149
78	O	6.102304	-3.262500	0.354214
79	H	5.991560	-2.282419	0.350525
80	H	6.157759	-3.522288	1.283094
81	O	2.705001	-5.609105	0.140794
82	H	1.749160	-5.473071	0.089875
83	H	2.874951	-5.912282	1.042977

E[B3LYP/6-31G(d,p)] = -2767.494971 h, E[APFD/6-311+G(2d,p)] = -2766.549889 h
Gcorr[B3LYP/6-31G(d,p)] = 0.613967 h

88. PC6Ca+4H_2O, R2, 2nd step, products

Center No.	Atom	X	Y	Z
1	P	4.118610	0.538562	-0.354313
2	O	4.488009	-0.703896	-1.137721
3	O	3.663958	0.123016	1.165596
4	O	1.720719	0.393702	-2.960914

5	H	0.992682	0.975133	-3.214104
6	H	2.236512	0.892514	-2.279480
7	O	5.562123	1.241862	-0.010590
8	H	5.478702	2.044351	0.526143
9	H	1.150494	-0.926791	-1.997327
10	O	0.869833	-1.706672	-1.459322
11	O	3.134052	1.516452	-0.939639
12	C	2.265812	0.061009	1.491580
13	H	1.755894	-0.670625	0.857515
14	H	1.805174	1.038104	1.334754
15	C	2.276723	-0.348392	2.964638
16	H	2.880886	0.364947	3.528042
17	H	2.723216	-1.338927	3.068156
18	C	0.248107	0.943003	3.642479
19	H	-0.038849	1.192568	2.622915
20	H	-0.641162	0.879322	4.268419
21	H	0.938541	1.680030	4.051205
22	C	1.162878	-0.819503	5.084173
23	H	0.202387	-0.869345	5.595068
24	H	1.645333	-1.795897	5.094385
25	H	1.802624	-0.077307	5.559774
26	C	0.024702	-1.423417	2.991278
27	H	-0.236211	-1.068196	1.996444
28	H	0.549136	-2.377372	2.946092
29	H	-0.876960	-1.522631	3.594789
30	N	0.924302	-0.407553	3.652433
31	C	-0.393993	-2.121567	-1.931720
32	H	-0.472578	-2.007657	-3.022685
33	H	-0.516478	-3.186445	-1.701501
34	C	-1.540899	-1.360447	-1.259715
35	H	-1.469855	-1.468692	-0.176489
36	C	-2.903257	-1.817676	-1.742655
37	H	-3.063221	-1.551214	-2.791391
38	H	-2.998468	-2.902748	-1.643318
39	C	-1.104239	0.930355	-0.618677
40	C	-1.119952	2.349738	-1.141476
41	H	-2.161372	2.693767	-1.068147
42	H	-0.884804	2.336211	-2.210152
43	C	-0.192516	3.296341	-0.372501
44	H	0.839524	2.933505	-0.455995
45	H	-0.452937	3.263483	0.691600
46	C	-0.276708	4.740550	-0.879686
47	H	-0.023583	4.769108	-1.948926
48	H	-1.314507	5.094892	-0.802511
49	O	-1.412601	0.049972	-1.589570
50	O	-0.876274	0.619539	0.538426
51	C	0.643979	5.700750	-0.116586
52	H	1.680437	5.345951	-0.195581
53	H	0.391890	5.668913	0.952037
54	C	-5.181857	-1.515986	-1.155397
55	C	-6.121794	-0.771643	-0.233110
56	H	-5.773979	-0.929576	0.795237
57	H	-5.991883	0.301221	-0.425435
58	C	-7.585566	-1.185545	-0.392043
59	H	-7.897057	-1.018306	-1.430051
60	H	-7.675879	-2.264437	-0.216509
61	C	-8.518541	-0.427326	0.558755
62	H	-8.422603	0.653203	0.380827
63	H	-8.196613	-0.594532	1.596487
64	C	-9.989792	-0.835120	0.414506
65	H	-10.311387	-0.665476	-0.621936
66	H	-10.083334	-1.915515	0.589126
67	O	-3.895574	-1.167875	-0.922246
68	O	-5.504810	-2.324997	-2.003003
69	C	0.557916	7.144989	-0.619022
70	H	1.225485	7.804762	-0.055221
71	H	0.837163	7.213389	-1.676644
72	H	-0.460375	7.538176	-0.520252
73	C	-10.920499	-0.080866	1.368757
74	H	-11.962050	-0.393705	1.241842
75	H	-10.644167	-0.259400	2.414270
76	H	-10.873891	1.000290	1.194942

77	Ca	6.003371	-2.460408	-1.216005
78	O	7.429706	-0.842168	-0.058002
79	H	6.937055	-0.003670	0.055497
80	H	7.804824	-1.048871	0.808152
81	O	5.232648	-4.288498	0.243565
82	H	4.289855	-4.400008	0.426531
83	H	5.682361	-4.482868	1.077065

E[B3LYP/6-31G(d,p)] = -2767.545388 h, E[APFD/6-311+G(2d,p)] = -2766.602499 h
Gcorr[B3LYP/6-31G(d,p)] = 0.614123 h

89. PC6Ca+4H_2O, R2, 3rd step, reactants (hydrolised glycerol + carbon chains neglected)

Center No.	Atom	X	Y	Z
1	P	-0.557151	-0.368778	0.628096
2	O	-1.307926	0.485361	-0.377068
3	O	0.952707	0.252593	0.831940
4	O	-1.183398	-0.002504	2.081173
5	H	-0.842601	-0.587911	2.774085
6	O	-0.449774	-1.857148	0.400381
7	C	1.975113	-0.137229	-0.088275
8	H	1.732642	0.220171	-1.094524
9	H	2.059213	-1.227254	-0.109132
10	C	3.232482	0.535385	0.462456
11	H	3.395887	0.208528	1.490610
12	H	3.098872	1.618307	0.458334
13	C	4.871273	-1.215410	-0.234218
14	H	4.121319	-1.791740	-0.771376
15	H	5.844907	-1.353026	-0.702287
16	H	4.909464	-1.523846	0.809753
17	C	5.623258	1.036055	0.378336
18	H	6.557053	0.835736	-0.144652
19	H	5.380906	2.096356	0.323662
20	H	5.697131	0.718440	1.417512
21	C	4.420849	0.692906	-1.730966
22	H	3.672178	0.093224	-2.244173
23	H	4.145462	1.746604	-1.755230
24	H	5.392486	0.548308	-2.201082
25	N	4.520583	0.251101	-0.292003
26	Ca	-3.476272	1.043365	-0.956977
27	O	-4.424694	-1.173590	-0.900935
28	H	-3.811311	-1.925191	-0.649680
29	H	-5.238194	-1.318804	-0.401308
30	O	-4.230698	2.820588	0.574676
31	H	-3.607382	3.201700	1.208135
32	H	-5.059780	2.716756	1.061289
33	O	-2.737755	-3.110942	-0.236363
34	H	-3.023775	-3.486128	0.607478
35	H	-1.871391	-2.668656	-0.029725

E[B3LYP/6-31G(d,p)] = -1802.864588 h, E[APFD/6-311+G(2d,p)] = -1802.421535 h
Gcorr[B3LYP/6-31G(d,p)] = 0.231235 h

90. PC6Ca+4H_2O, R2, 3rd step, TS

Center No.	Atom	X	Y	Z
1	P	-0.720029	-1.101269	0.302565
2	O	-1.188146	0.181753	-0.345937
3	O	0.842613	-0.818206	0.783215
4	O	-1.233074	-1.426106	1.804162
5	H	-0.489158	-1.303346	2.417656
6	O	-0.442024	-2.382099	-0.613118
7	C	1.806825	-0.420710	-0.189723
8	H	1.380203	0.338374	-0.851721
9	H	2.107474	-1.286876	-0.787788
10	C	2.961059	0.142165	0.640339
11	H	3.272503	-0.598106	1.379191
12	H	2.627448	1.039081	1.164451
13	C	4.876880	-0.689238	-0.727813
14	H	4.207216	-1.160785	-1.443443

15	H	5.789113	-0.372723	-1.231564
16	H	5.115369	-1.380402	0.079312
17	C	5.163899	1.186290	0.827792
18	H	6.080113	1.436224	0.295031
19	H	4.698912	2.089916	1.219470
20	H	5.376467	0.489946	1.637777
21	C	3.880891	1.508256	-1.239116
22	H	3.271326	1.015629	-1.994002
23	H	3.344441	2.352773	-0.808298
24	H	4.814416	1.846932	-1.686145
25	N	4.207830	0.528843	-0.139256
26	Ca	-3.025836	1.572185	-0.746881
27	O	-4.360366	-0.365610	-1.047933
28	H	-3.743418	-1.138405	-0.684852
29	H	-5.206803	-0.448706	-0.591807
30	O	-3.529109	2.826531	1.319878
31	H	-2.839835	2.949787	1.986734
32	H	-4.335926	2.636299	1.817576
33	O	-2.748662	-2.056667	-0.184707
34	H	-3.057076	-2.514893	0.608332
35	H	-1.417630	-2.654630	-0.745312

E[B3LYP/6-31G(d,p)] = -1802.817969 h, E[APFD/6-311+G(2d,p)] = -1802.369854 h
Gcorr[B3LYP/6-31G(d,p)] = 0.233253 h

91. PC6Ca+4H_2O, R2, 3rd step, products

Center No.	Atom	X	Y	Z
1	P	-0.921149	-1.363855	0.179417
2	O	-1.228823	0.058711	-0.300915
3	O	0.722243	-1.082019	0.694937
4	O	-1.194906	-1.856054	1.728372
5	H	-0.367079	-1.741451	2.221514
6	O	-0.341695	-2.461709	-0.903233
7	C	1.638208	-0.509752	-0.211304
8	H	1.171612	0.320075	-0.753487
9	H	1.977853	-1.255086	-0.941735
10	C	2.792350	-0.016299	0.664602
11	H	3.183489	-0.844860	1.257933
12	H	2.430657	0.757257	1.344046
13	C	4.657849	-0.450632	-0.941025
14	H	3.973604	-0.768832	-1.724176
15	H	5.544308	-0.000393	-1.385715
16	H	4.940385	-1.299396	-0.319369
17	C	4.969109	1.070596	0.956739
18	H	5.832108	1.491046	0.442010
19	H	4.487656	1.832484	1.568338
20	H	5.273710	0.228649	1.576671
21	C	3.556956	1.752017	-0.926773
22	H	2.913035	1.399362	-1.729591
23	H	3.024516	2.466577	-0.299940
24	H	4.449371	2.214221	-1.346842
25	N	3.982063	0.582743	-0.075097
26	Ca	-2.716499	1.750293	-0.758681
27	O	-4.309181	-0.059812	-0.639819
28	H	-3.720194	-0.844115	-0.434151
29	H	-4.996788	-0.053894	0.038157
30	O	-3.016019	3.086604	1.264057
31	H	-2.305273	3.161494	1.915285
32	H	-3.831983	3.028516	1.779572
33	O	-2.565083	-1.974372	-0.169589
34	H	-2.809897	-2.635367	0.493197
35	H	-1.117435	-2.849880	-1.337567

E[B3LYP/6-31G(d,p)] = -1802.82951 h, E[APFD/6-311+G(2d,p)] = -1802.380746 h
Gcorr[B3LYP/6-31G(d,p)] = 0.236926 h

92. PC6Ca+4H_2O, R2, 4th step, reactants

Center No.	Atom	X	Y	Z

1	P	-1.331822	0.882257	0.373470
2	O	-1.001150	-0.588328	0.077681
3	O	0.293968	1.512018	0.039771
4	O	-1.906262	1.903539	-0.754268
5	H	-1.221496	2.470845	-1.191404
6	O	-1.141526	1.448309	1.909372
7	C	1.404330	0.899324	0.665502
8	H	1.091733	0.307570	1.529494
9	H	2.076434	1.688115	1.021203
10	C	2.084193	0.019822	-0.391375
11	H	2.332515	0.623374	-1.266288
12	H	1.389032	-0.766381	-0.686292
13	C	4.444946	0.344531	0.368258
14	H	4.138013	0.918381	1.239721
15	H	5.370171	-0.187592	0.586113
16	H	4.584854	1.003850	-0.487608
17	C	3.857456	-1.503896	-1.128572
18	H	4.785578	-1.998493	-0.844853
19	H	3.093910	-2.243938	-1.363897
20	H	4.025307	-0.851384	-1.984449
21	C	3.146958	-1.568507	1.216842
22	H	2.876807	-0.966536	2.081818
23	H	2.343704	-2.263574	0.974833
24	H	4.067029	-2.114403	1.422017
25	N	3.379181	-0.667135	0.031570
26	Ca	-1.775860	-2.647156	-0.612658
27	O	-3.950379	-1.750165	-0.098378
28	H	-3.697947	-0.840414	0.244393
29	H	-4.570529	-1.599782	-0.823673
30	O	-3.044844	0.544045	0.782593
31	H	-3.578485	1.302261	0.504882
32	H	-1.966601	1.236570	2.374155
33	O	0.070811	3.463888	-1.802574
34	H	-0.025375	4.330439	-1.383079
35	H	0.533371	2.916223	-1.134481

E[B3LYP/6-31G(d,p)] = -1802.827433 h, E[APFD/6-311+G(2d,p)] = -1802.384806 h
Gcorr[B3LYP/6-31G(d,p)] = 0.239257 h

93. PC6Ca+4H_2O, R2, 4th step, TS

Center No.	Atom	X	Y	Z
1	P	1.545943	-0.873476	0.318429
2	O	1.495414	0.637366	0.184963
3	O	-0.497645	-0.881264	-0.468334
4	O	1.819649	-1.852843	-0.874376
5	H	0.941554	-2.431580	-1.297315
6	O	0.764967	-1.533197	1.591239
7	C	-1.561772	-0.495791	0.353862
8	H	-1.205003	0.207651	1.114837
9	H	-2.007601	-1.352651	0.880747
10	C	-2.591138	0.184768	-0.562179
11	H	-2.891456	-0.502522	-1.355768
12	H	-2.137339	1.065266	-1.020640
13	C	-4.679590	-0.502280	0.626533
14	H	-4.116563	-0.990460	1.418715
15	H	-5.623082	-0.126813	1.021057
16	H	-4.865621	-1.200515	-0.188668
17	C	-4.707806	1.366879	-0.956734
18	H	-5.640543	1.702787	-0.505042
19	H	-4.142242	2.219755	-1.329613
20	H	-4.912709	0.668498	-1.766970
21	C	-3.598867	1.629730	1.212298
22	H	-3.068244	1.112642	2.008728
23	H	-2.992701	2.446803	0.822490
24	H	-4.546342	2.013693	1.588515
25	N	-3.886182	0.662834	0.093359
26	Ca	2.652493	2.466038	-0.640928
27	O	4.489761	1.197210	0.302554
28	H	4.090566	0.347201	0.614348
29	H	5.248440	0.952465	-0.243023

30	O	3.098550	-1.021402	1.021859
31	H	3.496182	-1.858441	0.739162
32	H	1.426649	-1.672210	2.287781
33	O	-0.207033	-2.907910	-1.663432
34	H	-0.386243	-3.685780	-1.116513
35	H	-0.577699	-1.977767	-1.082701

E[B3LYP/6-31G(d,p)] = -1802.810761 h, E[APFD/6-311+G(2d,p)] = -1802.371951 h
Gcorr[B3LYP/6-31G(d,p)] = 0.231319 h

94. PC6Ca+4H_2O, R2, 4th step, products

Center No.	Atom	X	Y	Z
1	P	1.263945	1.441648	-0.032937
2	O	1.584617	0.299318	-0.981059
3	O	-0.835748	-2.589558	0.071381
4	O	0.348422	1.226019	1.145776
5	H	0.400864	-0.334025	1.840368
6	O	0.661803	2.699280	-0.864612
7	C	-1.522118	-1.530149	-0.572507
8	H	-1.989885	-1.944880	-1.469829
9	H	-0.828091	-0.740020	-0.879931
10	C	-2.574785	-0.988672	0.406157
11	H	-2.066363	-0.619551	1.298279
12	H	-3.255271	-1.791340	0.695509
13	C	-2.594065	1.326173	-0.532130
14	H	-2.089542	1.066489	-1.460660
15	H	-3.247807	2.181476	-0.698735
16	H	-1.856378	1.539909	0.241472
17	C	-4.313996	0.604197	1.061215
18	H	-4.970541	1.401893	0.716254
19	H	-4.902721	-0.245752	1.404082
20	H	-3.672758	0.966391	1.863681
21	C	-4.328488	-0.284833	-1.223101
22	H	-3.708746	-0.590033	-2.063649
23	H	-4.942090	-1.118788	-0.883906
24	H	-4.961131	0.552034	-1.517207
25	N	-3.444393	0.160554	-0.088298
26	Ca	2.669839	-1.757443	-0.818421
27	O	4.302204	-0.360304	0.351086
28	H	3.920582	0.531826	0.487583
29	H	4.660417	-0.631665	1.206537
30	O	2.746707	1.960215	0.478960
31	H	2.680923	2.539495	1.253678
32	H	1.118227	2.824124	-1.710433
33	O	0.420700	-1.287663	2.110527
34	H	-0.001324	-1.329940	2.978470
35	H	-0.362520	-2.196126	0.844721

E[B3LYP/6-31G(d,p)] = -1802.862974 h, E[APFD/6-311+G(2d,p)] = -1802.426943 h
Gcorr[B3LYP/6-31G(d,p)] = 0.236911 h

IX. Structures of molecules and transition states (TS) related to 2PS6Ca + 4 H_2O, where the hydrolysis proceeds in the sequence ser1:ser2;gly1;gly2, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

95. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	9.053402	-1.576671	-1.760627
2	C	7.617531	-1.224871	-2.085183
3	O	7.256168	-0.594108	-3.058132
4	O	6.764143	-1.729401	-1.156044
5	C	5.357293	-1.448025	-1.310649
6	C	4.976060	-0.338331	-0.330840
7	O	5.813258	0.817790	-0.516207
8	C	5.551129	1.810573	-1.407567
9	O	6.418641	2.644752	-1.576825
10	C	4.193155	1.894880	-2.076152
11	C	3.160491	2.661594	-1.213304
12	C	4.636068	-2.762401	-1.018371

13	O	3.230784	-2.567358	-1.256919
14	P	2.151923	-3.130198	-0.169873
15	O	1.896604	-4.604985	-0.352263
16	O	2.486038	-2.577613	1.200423
17	O	0.822775	-2.287891	-0.680469
18	C	-0.029047	-2.832545	-1.704397
19	C	-1.241651	-3.528183	-1.065897
20	C	-2.176619	-4.135765	-2.110687
21	O	-2.477242	-3.268919	-3.076011
22	O	-2.593695	-5.274292	-2.042706
23	N	-0.840362	-4.619231	-0.127773
24	H	9.289835	-2.479897	-2.338149
25	H	9.126973	-1.848662	-0.704063
26	H	-1.410941	-5.447032	-0.337729
27	H	0.176952	-4.851707	-0.240657
28	H	-0.968174	-4.342803	0.897430
29	H	-3.080769	-3.703980	-3.705082
30	H	-1.809629	-2.775273	-0.511918
31	H	-0.390569	-1.998023	-2.302892
32	H	0.530268	-3.523558	-2.339797
33	H	5.010030	-3.540446	-1.689227
34	H	4.821401	-3.067908	0.016171
35	H	5.168838	-1.136968	-2.340594
36	H	3.914358	-0.099483	-0.409424
37	H	5.179411	-0.665491	0.691750
38	H	3.011451	2.134420	-0.263273
39	H	2.201641	2.616852	-1.743779
40	H	4.352579	2.430753	-3.015027
41	H	3.801963	0.905783	-2.325252
42	C	3.523314	4.126723	-0.943717
43	C	2.461911	4.860386	-0.114522
44	H	3.659507	4.646101	-1.902429
45	C	2.811898	6.329463	0.142054
46	H	1.493975	4.800022	-0.630459
47	H	2.329953	4.344714	0.846323
48	H	3.760063	6.421306	0.683935
49	H	2.913740	6.882473	-0.798595
50	H	4.489824	4.184323	-0.427602
51	C	10.031140	-0.449648	-2.123828
52	C	9.882173	0.796738	-1.241823
53	H	10.045463	0.517029	-0.191106
54	H	8.852730	1.173629	-1.303891
55	H	9.880703	-0.180300	-3.175556
56	C	10.848973	1.925201	-1.620796
57	C	10.683800	3.172388	-0.746857
58	H	10.693334	2.194109	-2.674411
59	H	9.666535	3.573210	-0.822046
60	H	10.871356	2.943674	0.308593
61	H	11.882448	1.559676	-1.549426
62	H	11.052278	-0.840138	-2.040613
63	H	11.378126	3.965227	-1.043886
64	H	2.038787	6.826048	0.737819
65	C	-2.611361	1.761555	-1.545900
66	C	-3.011587	0.457876	-0.891838
67	O	-2.497077	-0.616888	-1.140340
68	O	-4.033555	0.625081	-0.021198
69	C	-4.590623	-0.542010	0.626168
70	C	-6.100377	-0.484908	0.447612
71	O	-6.350415	-0.646736	-0.960030
72	C	-7.602788	-0.594186	-1.488778
73	O	-7.711519	-0.800086	-2.681149
74	C	-8.776569	-0.240260	-0.598097
75	C	-9.023006	1.287480	-0.519566
76	C	-4.188030	-0.531819	2.093146
77	O	-2.758344	-0.674570	2.140834
78	P	-1.999492	-0.820848	3.570323
79	O	-2.771285	-1.638731	4.560994
80	O	-0.571637	-1.194442	3.194020
81	O	-2.020181	0.722730	4.164643
82	C	-1.461085	1.783490	3.392548
83	C	-0.796503	2.766411	4.379854
84	H	-1.545252	1.909628	-1.343184

85	H	-3.162476	2.588321	-1.091318
86	H	-1.563837	3.311152	4.931061
87	H	-0.730257	1.404646	2.674422
88	H	-2.243150	2.317623	2.848046
89	H	-4.487301	0.408608	2.568725
90	H	-4.663688	-1.364310	2.620091
91	H	-4.192803	-1.434953	0.140584
92	H	-6.564879	-1.298967	1.012083
93	H	-6.491160	0.471994	0.803662
94	H	-8.133780	1.790171	-0.118492
95	H	-9.821190	1.447640	0.214614
96	H	-9.650755	-0.725109	-1.040061
97	H	-8.648003	-0.644498	0.408830
98	C	-9.418722	1.932895	-1.852736
99	C	-9.697244	3.435729	-1.725463
100	H	-10.312118	1.428576	-2.246462
101	C	-10.094193	4.086145	-3.054065
102	H	-10.493847	3.595405	-0.986343
103	H	-8.805324	3.936333	-1.324910
104	H	-9.301712	3.971821	-3.802556
105	H	-11.002746	3.629197	-3.462519
106	H	-8.626863	1.772312	-2.594930
107	C	-2.843523	1.714310	-3.070013
108	C	-4.324021	1.634679	-3.461478
109	H	-4.848207	2.518064	-3.070156
110	H	-4.791166	0.766128	-2.978048
111	H	-2.301083	0.853361	-3.478715
112	C	-4.546455	1.540564	-4.975712
113	C	-6.028762	1.474483	-5.356771
114	H	-4.028926	0.651252	-5.360199
115	H	-6.520642	0.622223	-4.875078
116	H	-6.557482	2.381651	-5.041231
117	H	-4.076507	2.403008	-5.467632
118	H	-2.391796	2.609997	-3.511950
119	H	-6.160130	1.373601	-6.439170
120	H	-10.285675	5.157274	-2.932828
121	O	2.385303	1.069493	4.123666
122	H	2.439925	1.951011	3.707976
123	H	3.145234	0.998139	4.721040
124	Ca	1.737026	-0.941179	2.702674
125	O	1.290519	0.168754	0.557018
126	H	0.967930	-0.487984	-0.090236
127	H	0.880531	1.013264	0.334115
128	O	-3.064024	-4.302346	4.056713
129	H	-3.844601	-4.374572	3.490823
130	H	-3.045540	-3.354468	4.329825
131	O	-0.882230	-3.994098	2.468309
132	H	-0.719210	-3.050586	2.658672
133	H	-1.674891	-4.223217	3.017369
134	C	0.104475	3.740933	3.627170
135	O	1.304769	3.594333	3.493687
136	O	-0.610365	4.725936	3.101592
137	H	-0.026248	5.301129	2.573458
138	N	0.004777	1.998172	5.383520
139	H	0.249650	2.574205	6.193149
140	H	-0.574526	1.214364	5.708885
141	H	0.888832	1.605083	4.986647

E[B3LYP/6-31G(d,p)] = -4693.181925 h, E[APFD/6-311+G(2d,p)] = -4691.468972 h
Gcorr[B3LYP/6-31G(d,p)] = 1.053991 h

96. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 1st step, TS

Center No.	Atom	X	Y	Z
1	C	9.450792	-1.779102	-0.484187
2	C	8.274465	-1.111475	-1.163420
3	O	8.356405	-0.319089	-2.080148
4	O	7.094670	-1.526347	-0.631036
5	C	5.882938	-0.937576	-1.147230
6	C	5.389229	0.108831	-0.150362
7	O	6.390366	1.115348	0.087215

8	C	6.547757	2.217928	-0.693503
9	O	7.507528	2.926181	-0.461507
10	C	5.513835	2.558022	-1.749866
11	C	4.323393	3.372379	-1.186390
12	C	4.889423	-2.084168	-1.320084
13	O	3.706158	-1.537103	-1.926251
14	P	2.245579	-2.193242	-1.609949
15	O	1.898530	-3.332300	-2.518756
16	O	2.113862	-2.369508	-0.095339
17	O	1.325844	-0.869593	-1.977109
18	C	0.430650	-0.872748	-3.103748
19	C	-0.966114	-1.350403	-2.689012
20	C	-2.024595	-1.118452	-3.768179
21	O	-1.860466	0.039079	-4.412795
22	O	-2.937372	-1.893734	-3.974711
23	N	-0.986606	-2.778786	-2.288406
24	H	9.723707	-2.640445	-1.107551
25	H	9.130118	-2.176636	0.482669
26	H	-1.877164	-3.179849	-2.593331
27	H	-0.224964	-3.286133	-2.751950
28	H	-0.821298	-3.019667	-1.025828
29	H	-2.597295	0.145753	-5.040989
30	H	-1.301428	-0.748470	-1.836247
31	H	0.368329	0.156839	-3.453221
32	H	0.837011	-1.499427	-3.901344
33	H	5.322561	-2.848688	-1.971853
34	H	4.651605	-2.534098	-0.350981
35	H	6.097186	-0.480830	-2.115751
36	H	4.441803	0.538370	-0.476849
37	H	5.235997	-0.360799	0.824986
38	H	3.786315	2.776945	-0.438269
39	H	3.620988	3.526030	-2.014359
40	H	6.039377	3.155077	-2.499233
41	H	5.138961	1.661579	-2.249079
42	C	4.710118	4.731204	-0.591010
43	C	3.497172	5.528958	-0.096322
44	H	5.247196	5.318031	-1.349031
45	C	3.874356	6.891592	0.492511
46	H	2.793835	5.671056	-0.927899
47	H	2.960078	4.939473	0.659487
48	H	4.550870	6.779634	1.347434
49	H	4.382063	7.516448	-0.251013
50	H	5.414406	4.590368	0.238743
51	C	10.653052	-0.834739	-0.336897
52	C	10.405436	0.319349	0.642899
53	H	10.165951	-0.092394	1.633819
54	H	9.522619	0.889614	0.325222
55	H	10.907164	-0.434140	-1.324920
56	C	11.596757	1.276916	0.766580
57	C	11.329305	2.440864	1.725778
58	H	11.845254	1.672593	-0.227537
59	H	10.465256	3.029691	1.397191
60	H	11.116318	2.078663	2.738131
61	H	12.481127	0.718207	1.101846
62	H	11.515208	-1.424141	-0.003251
63	H	12.189461	3.115497	1.787807
64	H	2.989462	7.436559	0.836981
65	C	-3.650559	2.419271	0.307818
66	C	-3.636215	1.096256	-0.425815
67	O	-3.023653	0.894030	-1.457639
68	O	-4.402614	0.167760	0.193382
69	C	-4.564271	-1.125046	-0.434452
70	C	-6.057537	-1.368528	-0.603055
71	O	-6.525205	-0.381540	-1.539338
72	C	-7.837068	-0.262291	-1.879099
73	O	-8.119974	0.568536	-2.719010
74	C	-8.872524	-1.116744	-1.176263
75	C	-9.410720	-0.453562	0.116457
76	C	-3.917250	-2.178788	0.450591
77	O	-2.494915	-1.944774	0.437993
78	P	-1.530836	-2.498399	1.636182
79	O	-1.844979	-3.964158	2.174436

80	O	-0.261914	-1.717758	1.944212
81	O	-2.512526	-1.886878	2.916507
82	C	-2.471121	-0.502084	3.195491
83	C	-2.102267	-0.336168	4.696515
84	H	-2.621979	2.616769	0.630795
85	H	-4.274469	2.340623	1.201397
86	H	-2.960328	-0.592722	5.318599
87	H	-1.728466	0.012265	2.580337
88	H	-3.450574	-0.044543	3.032539
89	H	-4.302032	-2.117897	1.470623
90	H	-4.118411	-3.176531	0.047621
91	H	-4.083158	-1.105015	-1.413699
92	H	-6.221154	-2.375361	-0.999048
93	H	-6.571427	-1.267328	0.356558
94	H	-8.586399	-0.281295	0.820092
95	H	-10.076178	-1.179498	0.598084
96	H	-9.693923	-1.244384	-1.885921
97	H	-8.478431	-2.109109	-0.944452
98	C	-10.168954	0.858631	-0.115580
99	C	-10.720139	1.463659	1.181481
100	H	-10.997425	0.677571	-0.814406
101	C	-11.480815	2.773646	0.955473
102	H	-11.381508	0.734884	1.669203
103	H	-9.890801	1.637710	1.880393
104	H	-10.834710	3.532319	0.499062
105	H	-12.336906	2.623925	0.287803
106	H	-9.511905	1.587994	-0.605564
107	C	-4.133309	3.561002	-0.607906
108	C	-5.608633	3.437946	-1.008219
109	H	-6.230387	3.451697	-0.101795
110	H	-5.785266	2.463207	-1.482820
111	H	-3.502287	3.578850	-1.504286
112	C	-6.074441	4.545253	-1.961119
113	C	-7.553126	4.419727	-2.341414
114	H	-5.458432	4.519399	-2.870172
115	H	-7.759037	3.446952	-2.801444
116	H	-8.196122	4.509002	-1.457891
117	H	-5.893738	5.524968	-1.498327
118	H	-3.969203	4.511406	-0.086956
119	H	-7.852516	5.199221	-3.049765
120	H	-11.860585	3.182614	1.897387
121	O	1.524960	-0.260296	4.175900
122	H	1.110128	0.591643	4.419168
123	H	2.210508	-0.427855	4.839844
124	Ca	1.928934	-0.924180	1.788035
125	O	1.892167	0.859055	0.122484
126	H	1.599960	0.513429	-0.745019
127	H	1.518654	1.744597	0.215809
128	O	-0.887864	-5.954350	0.730527
129	H	-1.610637	-6.383036	0.250477
130	H	-1.487707	-4.734953	1.639299
131	O	-0.545529	-3.363765	0.103628
132	H	0.402929	-3.127793	0.202302
133	H	-0.595320	-5.218908	0.150894
134	C	-1.652845	1.086691	4.988526
135	O	-0.492716	1.455615	5.024364
136	O	-2.702815	1.885051	5.140091
137	H	-2.390708	2.801275	5.257676
138	N	-1.017492	-1.311199	5.023704
139	H	-0.944773	-1.484472	6.028855
140	H	-1.275205	-2.188256	4.549181
141	H	-0.079926	-1.019195	4.673732

E[B3LYP/6-31G(d,p)] = -4693.138141 h, E[APFD/6-311+G(2d,p)] = -4691.419423 h
Gcorr[B3LYP/6-31G(d,p)] = 1.049247 h

97. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 1st step, products

Center No.	Atom	X	Y	Z
1	C	9.425414	-1.755502	-0.436450
2	C	8.234960	-1.138189	-1.137941

3	O	8.295762	-0.390096	-2.092494
4	O	7.066306	-1.550088	-0.578701
5	C	5.839929	-1.019119	-1.120913
6	C	5.324740	0.072277	-0.184048
7	O	6.318996	1.092206	0.018916
8	C	6.471040	2.170345	-0.796516
9	O	7.432647	2.884721	-0.593330
10	C	5.427232	2.479446	-1.852369
11	C	4.222149	3.274414	-1.292351
12	C	4.877018	-2.200581	-1.216457
13	O	3.662025	-1.723098	-1.822858
14	P	2.216738	-2.286040	-1.334875
15	O	1.779435	-3.500293	-2.108782
16	O	2.169760	-2.308833	0.187861
17	O	1.283205	-0.996888	-1.786416
18	C	0.462337	-1.060323	-2.964339
19	C	-0.942662	-1.561656	-2.608683
20	C	-1.923241	-1.509992	-3.779214
21	O	-1.813944	-0.382508	-4.476300
22	O	-2.722240	-2.397029	-4.003533
23	N	-0.928747	-2.968794	-2.096352
24	H	9.665602	-2.675917	-0.984772
25	H	9.128982	-2.059357	0.571513
26	H	-1.719648	-3.473344	-2.515097
27	H	-0.025457	-3.435385	-2.330817
28	H	-0.984237	-3.022767	-1.042152
29	H	-2.488241	-0.384377	-5.179560
30	H	-1.370037	-0.921223	-1.831039
31	H	0.383490	-0.045969	-3.353174
32	H	0.927413	-1.698322	-3.719373
33	H	5.314795	-2.982555	-1.842924
34	H	4.675523	-2.608985	-0.221626
35	H	6.038604	-0.614405	-2.115635
36	H	4.382102	0.481350	-0.547754
37	H	5.155955	-0.349479	0.810035
38	H	3.687987	2.669306	-0.550106
39	H	3.522783	3.423002	-2.123808
40	H	5.938745	3.079732	-2.608651
41	H	5.070870	1.569781	-2.342123
42	C	4.587214	4.635034	-0.687039
43	C	3.361521	5.409510	-0.186747
44	H	5.116212	5.236166	-1.439456
45	C	3.717117	6.770821	0.418385
46	H	2.657826	5.550287	-1.018210
47	H	2.831865	4.803655	0.561444
48	H	4.392997	6.659019	1.273840
49	H	4.217472	7.411531	-0.316560
50	H	5.292323	4.499128	0.143038
51	C	10.644098	-0.822688	-0.411416
52	C	10.452254	0.409924	0.481646
53	H	10.245476	0.082040	1.510516
54	H	9.566572	0.969712	0.153240
55	H	10.865393	-0.506416	-1.437183
56	C	11.663647	1.350013	0.484083
57	C	11.459927	2.585467	1.366424
58	H	11.875312	1.667257	-0.546017
59	H	10.593083	3.167856	1.033708
60	H	11.285717	2.301605	2.410701
61	H	12.551966	0.798888	0.821540
62	H	11.510576	-1.397707	-0.064073
63	H	12.334145	3.244261	1.342112
64	H	2.823426	7.298730	0.766680
65	C	-3.544659	2.380652	0.009033
66	C	-3.567406	0.992449	-0.591634
67	O	-2.981362	0.682494	-1.613389
68	O	-4.327307	0.140193	0.131626
69	C	-4.517317	-1.208664	-0.358533
70	C	-6.016524	-1.436052	-0.491425
71	O	-6.474055	-0.532143	-1.513494
72	C	-7.785660	-0.416407	-1.853720
73	O	-8.059202	0.344537	-2.760541
74	C	-8.831488	-1.187514	-1.074170

75	C	-9.349335	-0.405506	0.158997
76	C	-3.878903	-2.181150	0.622203
77	O	-2.456477	-1.994795	0.573078
78	P	-1.453273	-2.447827	1.816895
79	O	-1.855269	-3.808820	2.584983
80	O	-0.246700	-1.569244	2.186387
81	O	-2.531207	-1.666462	3.015587
82	C	-2.546705	-0.264027	3.077034
83	C	-2.232134	0.145710	4.550582
84	H	-2.505585	2.587861	0.289827
85	H	-4.148529	2.400111	0.919462
86	H	-3.113446	-0.017353	5.171682
87	H	-1.799539	0.183269	2.415205
88	H	-3.532421	0.138171	2.822194
89	H	-4.252074	-2.013297	1.633839
90	H	-4.116624	-3.207651	0.320514
91	H	-4.047295	-1.293985	-1.339547
92	H	-6.204066	-2.472191	-0.788719
93	H	-6.518857	-1.233681	0.458338
94	H	-8.516952	-0.186624	0.839770
95	H	-10.022927	-1.075417	0.706065
96	H	-9.659740	-1.361504	-1.765805
97	H	-8.452874	-2.162819	-0.759136
98	C	-10.087731	0.894183	-0.181759
99	C	-10.622280	1.616875	1.060906
100	H	-10.922694	0.667580	-0.859241
101	C	-11.362351	2.915521	0.726888
102	H	-11.293123	0.943523	1.611317
103	H	-9.786668	1.835755	1.739446
104	H	-10.705921	3.621878	0.205830
105	H	-12.223797	2.724136	0.076982
106	H	-9.421619	1.568005	-0.734933
107	C	-4.027420	3.439456	-1.001125
108	C	-5.514262	3.312402	-1.354832
109	H	-6.112889	3.419090	-0.439044
110	H	-5.721513	2.303837	-1.737506
111	H	-3.418025	3.358590	-1.908932
112	C	-5.981324	4.342705	-2.390047
113	C	-7.470596	4.216865	-2.726217
114	H	-5.387328	4.225896	-3.306587
115	H	-7.705474	3.214429	-3.100670
116	H	-8.090874	4.391082	-1.839129
117	H	-5.771000	5.354510	-2.017630
118	H	-3.832018	4.431221	-0.576983
119	H	-7.771858	4.942063	-3.489326
120	H	-11.731097	3.409150	1.631903
121	O	1.422177	0.237953	4.241371
122	H	0.943662	1.087043	4.337403
123	H	2.069314	0.206546	4.961172
124	Ca	1.942106	-0.791595	2.019699
125	O	1.802805	0.865241	0.222415
126	H	1.509821	0.462591	-0.618420
127	H	1.417764	1.749791	0.262387
128	O	-0.810027	-5.950422	1.310259
129	H	-1.530498	-6.404259	0.850838
130	H	-1.474559	-4.627741	2.169811
131	O	-0.535424	-3.356375	0.574816
132	H	0.404133	-3.093601	0.636170
133	H	-0.555418	-5.214852	0.714293
134	C	-1.803538	1.598022	4.632658
135	O	-0.651643	1.991564	4.698863
136	O	-2.861667	2.398628	4.557138
137	H	-2.556071	3.324116	4.537825
138	N	-1.166728	-0.772213	5.050580
139	H	-1.171843	-0.862650	6.068160
140	H	-1.393724	-1.682198	4.611384
141	H	-0.210230	-0.502444	4.744591

E[B3LYP/6-31G(d,p)] = -4693.144041 h, E[APFD/6-311+G(2d,p)] = -4691.426449 h
Gcorr[B3LYP/6-31G(d,p)] = 1.051111 h

98. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	C	9.462292	-1.920803	-0.269808
2	C	8.261151	-1.397588	-1.027115
3	O	8.309408	-0.775374	-2.068823
4	O	7.099881	-1.732162	-0.404374
5	C	5.867475	-1.262017	-0.987625
6	C	5.381399	-0.055514	-0.186260
7	O	6.383101	0.976227	-0.142379
8	C	6.526850	1.928831	-1.103280
9	O	7.496701	2.655737	-1.018706
10	C	5.465591	2.099026	-2.173296
11	C	4.285841	2.990510	-1.713668
12	C	4.892349	-2.435202	-0.916396
13	O	3.676392	-2.033028	-1.574450
14	P	2.231361	-2.476278	-0.973791
15	O	1.778106	-3.817634	-1.483824
16	O	2.199792	-2.194223	0.523237
17	O	1.304215	-1.295662	-1.668788
18	C	0.447419	-1.594078	-2.783342
19	C	-0.949479	-1.996944	-2.294461
20	C	-1.964311	-2.169552	-3.424184
21	O	-1.865693	-1.209540	-4.339203
22	O	-2.775618	-3.073491	-3.442032
23	N	-0.930980	-3.273138	-1.510500
24	H	9.736454	-2.873622	-0.741098
25	H	9.168172	-2.149031	0.758328
26	H	-1.732905	-3.844118	-1.804636
27	H	-0.035121	-3.784917	-1.665192
28	H	-0.966836	-3.115597	-0.465214
29	H	-2.558443	-1.345464	-5.010808
30	H	-1.350379	-1.209158	-1.649356
31	H	0.361785	-0.681324	-3.371360
32	H	0.887461	-2.378992	-3.402501
33	H	5.317669	-3.298341	-1.435394
34	H	4.697145	-2.704345	0.125969
35	H	6.049855	-0.988648	-2.029132
36	H	4.430852	0.310061	-0.576168
37	H	5.239272	-0.345748	0.858057
38	H	3.756609	2.509248	-0.882749
39	H	3.572681	3.030163	-2.545774
40	H	5.970363	2.572182	-3.019051
41	H	5.083025	1.135047	-2.517589
42	C	4.683628	4.417314	-1.318042
43	C	3.479315	5.276011	-0.912124
44	H	5.205706	4.894721	-2.158738
45	C	3.865898	6.703553	-0.514107
46	H	2.761138	5.308497	-1.742483
47	H	2.956480	4.791743	-0.075692
48	H	4.557430	6.703629	0.336130
49	H	4.360018	7.224560	-1.341982
50	H	5.403345	4.390067	-0.489915
51	C	10.651751	-0.950394	-0.315684
52	C	10.411434	0.349061	0.463670
53	H	10.198354	0.106051	1.514585
54	H	9.515878	0.852886	0.076463
55	H	10.875085	-0.718644	-1.363398
56	C	11.595800	1.320996	0.399140
57	C	11.341019	2.624619	1.162095
58	H	11.816677	1.550121	-0.652192
59	H	10.464740	3.148426	0.763389
60	H	11.154949	2.431363	2.224865
61	H	12.493278	0.829466	0.798692
62	H	11.531264	-1.465313	0.088519
63	H	12.196786	3.304077	1.092334
64	H	2.986847	7.290440	-0.228628
65	C	-3.612967	2.360360	-0.518227
66	C	-3.622793	0.874939	-0.804348
67	O	-3.051249	0.359277	-1.748094
68	O	-4.355125	0.189059	0.101895

69	C	-4.528470	-1.236114	-0.082930
70	C	-6.024679	-1.513782	-0.115876
71	O	-6.537890	-0.852519	-1.286048
72	C	-7.859891	-0.859109	-1.605316
73	O	-8.185771	-0.302968	-2.635165
74	C	-8.854239	-1.505446	-0.661906
75	C	-9.389499	-0.518059	0.405372
76	C	-3.845723	-1.968484	1.063001
77	O	-2.428449	-1.776373	0.938751
78	P	-1.398592	-1.972050	2.227186
79	O	-1.790002	-3.142990	3.264337
80	O	-0.180110	-1.047186	2.384784
81	O	-2.441541	-0.946539	3.259366
82	C	-2.473193	0.431409	2.989948
83	C	-2.126366	1.178348	4.314102
84	H	-2.570337	2.640607	-0.329602
85	H	-4.186422	2.567492	0.388561
86	H	-2.978353	1.133642	4.992651
87	H	-1.748118	0.715676	2.221447
88	H	-3.469734	0.756428	2.674268
89	H	-4.198235	-1.595538	2.026308
90	H	-4.071100	-3.038803	0.992354
91	H	-4.082629	-1.520893	-1.037070
92	H	-6.192204	-2.592689	-0.184287
93	H	-6.505532	-1.128575	0.787424
94	H	-8.557569	-0.128330	1.005630
95	H	-10.017186	-1.096368	1.093353
96	H	-9.684331	-1.849594	-1.284165
97	H	-8.424144	-2.381218	-0.170120
98	C	-10.201013	0.650586	-0.165814
99	C	-10.747769	1.581855	0.923262
100	H	-11.036433	0.253384	-0.758974
101	C	-11.562630	2.749815	0.359695
102	H	-11.370462	1.001382	1.617316
103	H	-9.911344	1.972483	1.518548
104	H	-10.955675	3.367744	-0.311916
105	H	-12.425918	2.390552	-0.211938
106	H	-9.582109	1.229970	-0.862265
107	C	-4.155124	3.166675	-1.714604
108	C	-5.649347	2.941478	-1.976091
109	H	-6.219513	3.233516	-1.082780
110	H	-5.844505	1.870772	-2.124385
111	H	-3.574339	2.900659	-2.605672
112	C	-6.175635	3.716014	-3.190369
113	C	-7.671535	3.494845	-3.435718
114	H	-5.609252	3.414572	-4.081931
115	H	-7.893273	2.431383	-3.577369
116	H	-8.266566	3.845098	-2.584102
117	H	-5.978525	4.787820	-3.052255
118	H	-3.969628	4.229885	-1.522687
119	H	-8.015669	4.033466	-4.324798
120	H	-11.938386	3.396881	1.158945
121	O	1.526849	1.314399	3.835118
122	H	1.005751	2.134157	3.712922
123	H	2.185664	1.508395	4.517803
124	Ca	2.001953	-0.354634	2.029517
125	O	1.770314	0.909841	-0.032090
126	H	1.498663	0.355226	-0.789241
127	H	1.428648	1.798768	-0.188905
128	O	-0.797473	-5.509714	2.426714
129	H	-1.532645	-6.034661	2.080034
130	H	-1.426131	-4.034441	3.016169
131	O	-0.508585	-3.121899	1.176776
132	H	0.434062	-2.864119	1.168327
133	H	-0.544340	-4.914016	1.690403
134	C	-1.754855	2.623784	4.041071
135	O	-0.618628	3.046150	3.912543
136	O	-2.847366	3.365155	3.891302
137	H	-2.582316	4.270310	3.644674
138	N	-1.006240	0.435442	4.965472
139	H	-0.070756	0.671941	4.579177
140	H	-0.985033	0.568541	5.978322

141	H	-1.197988	-0.557529	4.744093

E[B3LYP/6-31G(d,p)] = -4693.143993 h, E[APFD/6-311+G(2d,p)] = -4691.426449 h
Gcorr[B3LYP/6-31G(d,p)] = 1.051671 h

99. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 2nd step, TS

Center No.	Atom	X	Y	Z
1	C	9.404212	-2.387782	0.074208
2	C	8.255282	-1.862551	-0.758872
3	O	8.355456	-1.407294	-1.880061
4	O	7.071703	-1.986365	-0.100909
5	C	5.887179	-1.488730	-0.755307
6	C	5.524257	-0.136421	-0.143477
7	O	6.624174	0.785965	-0.234658
8	C	6.854161	1.581178	-1.314495
9	O	7.890004	2.216048	-1.321348
10	C	5.809429	1.703759	-2.407008
11	C	4.712174	2.745717	-2.078728
12	C	4.804742	-2.539407	-0.519127
13	O	3.621246	-2.106843	-1.218812
14	P	2.152079	-2.423185	-0.606589
15	O	1.655923	-3.800895	-0.956575
16	O	2.100984	-1.967168	0.850113
17	O	1.278892	-1.304990	-1.452498
18	C	0.438245	-1.706398	-2.548208
19	C	-0.980380	-2.020353	-2.054081
20	C	-1.967773	-2.306991	-3.186048
21	O	-1.851884	-1.433253	-4.180632
22	O	-2.764791	-3.222179	-3.142390
23	N	-1.010447	-3.203924	-1.132841
24	H	9.554014	-3.432833	-0.227162
25	H	9.107083	-2.402994	1.126534
26	H	-1.797389	-3.806040	-1.408508
27	H	-0.104305	-3.727992	-1.174990
28	H	-1.108896	-2.924713	-0.132797
29	H	-2.526044	-1.634172	-4.854686
30	H	-1.381113	-1.159605	-1.511283
31	H	0.388244	-0.862544	-3.234914
32	H	0.870593	-2.565391	-3.066271
33	H	5.132522	-3.503296	-0.917397
34	H	4.601850	-2.643810	0.551136
35	H	6.087867	-1.389947	-1.824255
36	H	4.614767	0.259505	-0.596087
37	H	5.352129	-0.255599	0.929492
38	H	4.137757	2.419204	-1.203756
39	H	4.009633	2.745355	-2.920738
40	H	6.352264	2.017468	-3.301865
41	H	5.344356	0.739632	-2.627000
42	C	5.235045	4.169328	-1.853986
43	C	4.110931	5.177317	-1.584198
44	H	5.807952	4.488987	-2.735392
45	C	4.623837	6.602144	-1.354946
46	H	3.409033	5.171628	-2.428948
47	H	3.535162	4.850129	-0.707347
48	H	5.301699	6.644953	-0.494837
49	H	5.174631	6.969259	-2.228360
50	H	5.940181	4.181081	-1.012927
51	C	10.697563	-1.587983	-0.137678
52	C	10.630096	-0.157926	0.413848
53	H	10.417000	-0.196004	1.491809
54	H	9.789553	0.377421	-0.047256
55	H	10.922047	-1.561619	-1.210118
56	C	11.917583	0.641731	0.180535
57	C	11.837361	2.073815	0.718180
58	H	12.135679	0.667086	-0.895746
59	H	11.017612	2.626148	0.244732
60	H	11.659074	2.081121	1.799659
61	H	12.761826	0.118715	0.650021
62	H	11.519828	-2.130088	0.344054
63	H	12.764324	2.625374	0.530074

64	H	3.799773	7.297371	-1.164608
65	C	-4.135888	2.228601	-1.073540
66	C	-4.000189	0.723187	-1.014832
67	O	-3.409182	0.058507	-1.846046
68	O	-4.628854	0.200202	0.062627
69	C	-4.664772	-1.238560	0.212209
70	C	-6.125498	-1.643769	0.350950
71	O	-6.755849	-1.329801	-0.903484
72	C	-8.091991	-1.486477	-1.106177
73	O	-8.517497	-1.244868	-2.218066
74	C	-8.979960	-1.898778	0.050477
75	C	-9.498211	-0.685559	0.863086
76	C	-3.856145	-1.625813	1.440877
77	O	-2.473978	-1.333397	1.161331
78	P	-1.323351	-1.332714	2.323889
79	O	-1.718012	-2.115933	3.662052
80	O	-0.208155	-0.302341	2.237642
81	O	-2.462062	0.076221	3.252113
82	C	-2.548988	1.349036	2.651839
83	C	-2.097700	2.364611	3.785831
84	H	-3.124037	2.642679	-0.997543
85	H	-4.709430	2.582515	-0.213453
86	H	-2.975645	2.706416	4.334490
87	H	-1.875996	1.429578	1.792710
88	H	-3.570176	1.578244	2.339775
89	H	-4.181756	-1.065419	2.318701
90	H	-3.969114	-2.698224	1.630988
91	H	-4.239000	-1.694199	-0.683507
92	H	-6.190262	-2.717815	0.549292
93	H	-6.595460	-1.094191	1.170627
94	H	-8.651968	-0.121365	1.275110
95	H	-10.046933	-1.084815	1.724059
96	H	-9.828743	-2.427240	-0.390923
97	H	-8.466097	-2.596156	0.716525
98	C	-10.408048	0.261820	0.072362
99	C	-10.932527	1.426822	0.920826
100	H	-11.257346	-0.306747	-0.331230
101	C	-11.843166	2.376650	0.137039
102	H	-11.477318	1.027831	1.787076
103	H	-10.081521	1.988891	1.328766
104	H	-11.314327	2.817295	-0.715894
105	H	-12.720803	1.849981	-0.254697
106	H	-9.868144	0.659548	-0.796027
107	C	-4.783651	2.682328	-2.396185
108	C	-6.253079	2.263637	-2.528066
109	H	-6.828173	2.703276	-1.700825
110	H	-6.341082	1.174685	-2.413814
111	H	-4.200209	2.272318	-3.228985
112	C	-6.885992	2.676272	-3.862244
113	C	-8.359177	2.270704	-3.972858
114	H	-6.317483	2.222709	-4.685385
115	H	-8.480162	1.189249	-3.845417
116	H	-8.962120	2.762671	-3.200565
117	H	-6.791902	3.763288	-3.989592
118	H	-4.702798	3.773604	-2.460738
119	H	-8.778576	2.545391	-4.946319
120	H	-12.201016	3.197407	0.767111
121	O	1.639488	1.830416	3.788081
122	H	1.167322	2.654460	3.538379
123	H	2.264086	2.067172	4.487158
124	Ca	2.091927	0.116641	2.057901
125	O	2.015710	1.086314	-0.179838
126	H	1.665799	0.470941	-0.851867
127	H	1.745885	1.976182	-0.439640
128	O	-0.778301	-4.588187	3.540000
129	H	-1.506058	-5.223959	3.485305
130	H	-1.367598	-3.056417	3.679718
131	O	-0.522606	-2.650605	1.579617
132	H	0.434415	-2.443372	1.471676
133	H	-0.555150	-4.374953	2.615269
134	C	-1.390763	3.563141	3.195393
135	O	-0.184401	3.748369	3.165541

136	O	-2.269606	4.398895	2.644953
137	H	-1.782884	5.129673	2.222047
138	N	-1.276622	1.537721	4.687500
139	H	-0.271996	1.564895	4.478895
140	H	-1.427957	1.738837	5.672449
141	H	-1.765358	0.496100	4.244256

E[B3LYP/6-31G(d,p)] = -4693.136596 h, E[APFD/6-311+G(2d,p)] = -4691.415396 h
Gcorr[B3LYP/6-31G(d,p)] = 1.046751 h

100. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 2nd step, products

Center No.	Atom	X	Y	Z
1	C	9.121811	-1.450104	0.905095
2	C	8.012681	-1.249483	-0.104360
3	O	8.170686	-0.957532	-1.271963
4	O	6.792341	-1.468877	0.456333
5	C	5.631837	-1.291373	-0.378865
6	C	4.991420	0.057922	-0.050039
7	O	5.953033	1.120698	-0.157266
8	C	6.209041	1.799882	-1.309038
9	O	7.154721	2.561688	-1.302166
10	C	5.279466	1.653106	-2.497372
11	C	4.026703	2.555351	-2.383018
12	C	4.711680	-2.466414	-0.057297
13	O	3.554670	-2.374402	-0.919175
14	P	2.088636	-2.694710	-0.322018
15	O	1.818540	-4.163657	-0.128217
16	O	1.813793	-1.764328	0.866227
17	O	1.154378	-2.140468	-1.557453
18	C	0.622700	-3.069901	-2.522807
19	C	-0.795211	-3.510843	-2.124738
20	C	-1.417867	-4.433586	-3.173237
21	O	-1.411499	-3.874308	-4.379389
22	O	-1.862514	-5.530660	-2.904985
23	N	-0.820751	-4.255563	-0.817903
24	H	9.422322	-2.503445	0.828548
25	H	8.717630	-1.313051	1.912145
26	H	-1.270206	-5.167864	-0.986070
27	H	0.157802	-4.403511	-0.447394
28	H	-1.362370	-3.750885	-0.102402
29	H	-1.818618	-4.489992	-5.015622
30	H	-1.431942	-2.625085	-2.031546
31	H	0.563543	-2.541935	-3.473599
32	H	1.288152	-3.928797	-2.629725
33	H	5.227752	-3.408151	-0.256727
34	H	4.415695	-2.435680	0.995600
35	H	5.938409	-1.326799	-1.426603
36	H	4.117464	0.223942	-0.681290
37	H	4.672081	0.073204	0.995629
38	H	3.444195	2.270782	-1.497358
39	H	3.395053	2.342346	-3.253799
40	H	5.862370	1.948884	-3.372701
41	H	4.975037	0.613645	-2.643525
42	C	4.329494	4.057559	-2.331513
43	C	3.060839	4.914975	-2.244873
44	H	4.901622	4.340614	-3.225639
45	C	3.353583	6.417613	-2.199368
46	H	2.414414	4.692856	-3.104611
47	H	2.490443	4.626105	-1.351109
48	H	3.970668	6.674155	-1.330794
49	H	3.893327	6.742325	-3.096093
50	H	4.976119	4.279910	-1.473143
51	C	10.327806	-0.536099	0.648831
52	C	10.041099	0.946062	0.922080
53	H	9.733573	1.066684	1.970755
54	H	9.190474	1.277218	0.311941
55	H	10.652378	-0.665843	-0.389938
56	C	11.242350	1.856324	0.639222
57	C	10.947477	3.335936	0.904087
58	H	11.553798	1.727054	-0.406195

59	H	10.116063	3.688904	0.283293
60	H	10.671376	3.503094	1.951576
61	H	12.095192	1.535440	1.252776
62	H	11.155988	-0.873496	1.283102
63	H	11.817529	3.963598	0.685162
64	H	2.430052	7.002116	-2.136444
65	C	-2.542353	1.372830	-1.314328
66	C	-2.966727	-0.073556	-1.212341
67	O	-2.689306	-0.925527	-2.037961
68	O	-3.693789	-0.315547	-0.097658
69	C	-4.244366	-1.637520	0.096868
70	C	-5.762778	-1.506044	0.135718
71	O	-6.163744	-1.028186	-1.158949
72	C	-7.451246	-0.688263	-1.441974
73	O	-7.694171	-0.334493	-2.578140
74	C	-8.492010	-0.720558	-0.341102
75	C	-8.581698	0.618893	0.432742
76	C	-3.716007	-2.194466	1.408766
77	O	-2.289263	-2.458002	1.292849
78	P	-1.232095	-1.842621	2.361048
79	O	-1.895087	-1.947707	3.783453
80	O	-0.813388	-0.433119	2.045136
81	O	-4.125966	0.275774	3.773389
82	C	-3.670115	1.477824	3.177472
83	C	-2.791541	2.269337	4.178982
84	H	-1.449871	1.378151	-1.223501
85	H	-2.956937	1.939450	-0.476863
86	H	-3.433955	2.591948	5.005669
87	H	-3.083677	1.270712	2.270971
88	H	-4.544603	2.068209	2.894770
89	H	-3.908870	-1.493915	2.225865
90	H	-4.198380	-3.149646	1.630424
91	H	-3.950595	-2.268659	-0.743387
92	H	-6.210172	-2.484754	0.334765
93	H	-6.059896	-0.804470	0.919509
94	H	-7.613370	0.850602	0.894132
95	H	-9.284789	0.466192	1.259826
96	H	-9.448030	-0.918715	-0.832413
97	H	-8.304341	-1.538089	0.359119
98	C	-9.042185	1.810016	-0.415429
99	C	-9.156759	3.106550	0.395930
100	H	-10.015659	1.575752	-0.868093
101	C	-9.619918	4.300482	-0.444113
102	H	-9.854811	2.951889	1.229703
103	H	-8.183857	3.335047	0.851856
104	H	-8.922631	4.500057	-1.265923
105	H	-10.605930	4.115223	-0.885155
106	H	-8.347672	1.964726	-1.250560
107	C	-2.951648	1.993636	-2.663532
108	C	-4.468018	2.146479	-2.832610
109	H	-4.858881	2.779826	-2.023539
110	H	-4.955533	1.168990	-2.717205
111	H	-2.545659	1.373297	-3.471152
112	C	-4.870190	2.745851	-4.185545
113	C	-6.385664	2.909837	-4.337686
114	H	-4.487979	2.104185	-4.990975
115	H	-6.898706	1.949893	-4.213420
116	H	-6.785350	3.597343	-3.582915
117	H	-4.378780	3.720017	-4.312958
118	H	-2.470190	2.975005	-2.746974
119	H	-6.648952	3.309119	-5.322701
120	H	-9.691175	5.210429	0.160539
121	O	1.123417	2.157464	3.110436
122	H	0.340709	2.741594	3.233210
123	H	1.529855	2.048466	3.979428
124	Ca	1.242823	0.570499	1.301741
125	O	1.023574	0.620082	-1.114157
126	H	0.994127	-0.245225	-1.562880
127	H	1.179321	1.292485	-1.788147
128	O	-2.460845	-4.285238	4.676581
129	H	-3.140328	-4.732109	4.151092
130	H	-2.113858	-2.886038	4.119765

131	O	-0.057549	-2.898994	2.278491
132	H	0.750814	-2.516730	1.808462
133	H	-1.697128	-4.880555	4.661802
134	C	-2.260381	3.533071	3.508282
135	O	-1.097225	3.744267	3.194843
136	O	-3.232623	4.417154	3.263718
137	H	-2.841747	5.187969	2.813689
138	N	-1.776302	1.375359	4.705044
139	H	-1.099781	1.121095	3.988689
140	H	-1.273192	1.800288	5.477988
141	H	-3.349395	-0.092569	4.233871

E[B3LYP/6-31G(d,p)] = -4693.173335 h, E[APFD/6-311+G(2d,p)] = -4691.45566 h
Gcorr[B3LYP/6-31G(d,p)] = 1.043508 h

101. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 3rd step, reactants (hydrolised serine neglected)

Center No.	Atom	X	Y	Z
1	C	-8.968415	-2.061553	0.302402
2	C	-7.715121	-1.453031	0.892781
3	O	-7.656499	-0.866595	1.954251
4	O	-6.637845	-1.662071	0.088916
5	C	-5.381869	-1.083123	0.495108
6	C	-5.127545	0.162285	-0.351072
7	O	-6.185590	1.122361	-0.195101
8	C	-6.197356	2.076252	0.774328
9	O	-7.209576	2.738267	0.886906
10	C	-4.955969	2.321537	1.611986
11	C	-3.905699	3.208383	0.900387
12	C	-4.320305	-2.153858	0.257640
13	O	-3.085667	-1.655503	0.842518
14	P	-1.662341	-1.935102	0.155147
15	O	-1.473251	-3.376720	-0.264282
16	O	-1.364213	-0.868642	-0.915756
17	O	-0.651851	-1.591168	1.393807
18	C	-0.149861	-2.638463	2.247394
19	C	1.238043	-3.081772	1.759968
20	C	1.899541	-4.066581	2.729165
21	O	2.009583	-3.545915	3.945655
22	O	2.265492	-5.172342	2.390749
23	N	1.176949	-3.761417	0.419772
24	H	-9.071329	-3.059463	0.748202
25	H	-8.824721	-2.208745	-0.771576
26	H	1.552992	-4.715116	0.533440
27	H	0.189875	-3.808312	0.062104
28	H	1.742202	-3.267500	-0.285195
29	H	2.430357	-4.198348	4.534815
30	H	1.874858	-2.197293	1.669822
31	H	-0.050065	-2.214804	3.245752
32	H	-0.846278	-3.479092	2.282116
33	H	-4.595695	-3.078240	0.768817
34	H	-4.199839	-2.337362	-0.813327
35	H	-5.433127	-0.833822	1.557214
36	H	-4.151052	0.585183	-0.111604
37	H	-5.134844	-0.109506	-1.408806
38	H	-3.532647	2.701830	0.001087
39	H	-3.049555	3.300820	1.579645
40	H	-5.303720	2.826213	2.516314
41	H	-4.494382	1.379948	1.920637
42	C	-4.408759	4.606508	0.521497
43	C	-3.318735	5.474903	-0.119376
44	H	-4.795244	5.108366	1.419167
45	C	-3.819786	6.864381	-0.524633
46	H	-2.481570	5.579034	0.584574
47	H	-2.914768	4.957588	-1.000102
48	H	-4.634370	6.793553	-1.254363
49	H	-4.199849	7.416415	0.342455
50	H	-5.257435	4.522560	-0.169754
51	C	-10.219020	-1.220797	0.597306
52	C	-10.227013	0.134441	-0.121754
53	H	-10.177982	-0.031783	-1.207381

54	H	-9.323090	0.698770	0.143363
55	H	-10.289750	-1.066181	1.680043
56	C	-11.459070	0.986568	0.205548
57	C	-11.447213	2.347872	-0.496621
58	H	-11.514616	1.136461	1.292316
59	H	-10.561243	2.927978	-0.214012
60	H	-11.431465	2.231036	-1.586327
61	H	-12.367920	0.435920	-0.072742
62	H	-11.101553	-1.800410	0.302128
63	H	-12.331016	2.940250	-0.238095
64	H	-3.020069	7.461275	-0.974963
65	C	3.755511	2.330268	-0.212413
66	C	3.721184	0.844415	0.054156
67	O	3.048597	0.308303	0.924982
68	O	4.546977	0.165642	-0.762656
69	C	4.731859	-1.256399	-0.570384
70	C	6.234120	-1.504309	-0.494169
71	O	6.689686	-0.841178	0.695509
72	C	8.009652	-0.765890	1.025676
73	O	8.286150	-0.236016	2.082263
74	C	9.052342	-1.290528	0.059623
75	C	9.500767	-0.223880	-0.971099
76	C	4.107126	-2.006768	-1.738449
77	O	2.654647	-2.021211	-1.640589
78	P	1.675504	-1.065786	-2.500408
79	O	2.291414	-0.966233	-3.965567
80	O	1.475776	0.301623	-1.927085
81	H	2.741029	2.635902	-0.488353
82	H	4.406640	2.529641	-1.066579
83	H	4.405364	-1.569226	-2.693254
84	H	4.408842	-3.055033	-1.715879
85	H	4.262537	-1.552684	0.368829
86	H	6.423361	-2.579836	-0.426852
87	H	6.730904	-1.102249	-1.380879
88	H	8.641367	0.105854	-1.568533
89	H	10.184862	-0.719805	-1.669496
90	H	9.909433	-1.586108	0.669930
91	H	8.696290	-2.181368	-0.463597
92	C	10.194769	0.997447	-0.356787
93	C	10.654496	2.010909	-1.412301
94	H	11.061377	0.663111	0.230218
95	C	11.349530	3.233880	-0.806521
96	H	11.333789	1.515463	-2.119010
97	H	9.787055	2.337453	-2.001783
98	H	10.682280	3.768526	-0.120738
99	H	12.241014	2.942173	-0.239778
100	H	9.520140	1.493453	0.352281
101	C	4.216089	3.120885	1.029436
102	C	5.688052	2.890754	1.392381
103	H	6.317747	3.187721	0.541851
104	H	5.873400	1.819382	1.547928
105	H	3.573427	2.854840	1.877266
106	C	6.127659	3.660605	2.643621
107	C	7.608629	3.458262	2.978687
108	H	5.511391	3.343590	3.495772
109	H	7.838868	2.396661	3.119512
110	H	8.249270	3.829868	2.170288
111	H	5.924422	4.730760	2.501955
112	H	4.048043	4.185478	0.830478
113	H	7.887936	3.989897	3.894272
114	H	11.664143	3.939297	-1.582460
115	O	-1.204345	3.191734	-2.545608
116	H	-0.747192	4.037818	-2.643178
117	H	-1.610475	3.011446	-3.404124
118	Ca	-0.456394	1.436782	-1.000008
119	O	0.388425	1.062864	1.262801
120	H	0.006125	0.228537	1.586263
121	H	1.357868	0.908720	1.276666
122	H	2.316329	-1.796610	-4.469263
123	O	0.362550	-1.943455	-2.573579
124	H	-0.372718	-1.552258	-2.001048
125	O	-3.487833	-1.482094	-2.929716

126	H	-2.841323	-0.995907	-2.396671
127	H	-3.029730	-2.335348	-3.093971
128	O	-1.973117	-3.847828	-3.018047
129	H	-1.828661	-3.878193	-2.051585
130	H	-1.106325	-3.592779	-3.365619

E[B3LYP/6-31G(d,p)] = -4370.614597 h, E[APFD/6-311+G(2d,p)] = -4369.04926 h
Gcorr[B3LYP/6-31G(d,p)] = 0.968434 h

102. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 3rd step, TS

Center No.	Atom	X	Y	Z
1	C	-8.527268	0.887118	-0.331732
2	C	-7.177477	0.650864	0.311597
3	O	-6.903863	0.900306	1.468517
4	O	-6.302087	0.097131	-0.566844
5	C	-4.952239	-0.139230	-0.112100
6	C	-4.053928	0.955459	-0.683687
7	O	-4.513666	2.261460	-0.288762
8	C	-4.157148	2.863112	0.876490
9	O	-4.718453	3.904754	1.154984
10	C	-3.052241	2.273948	1.732619
11	C	-1.639380	2.723244	1.285730
12	C	-4.572597	-1.529619	-0.619994
13	O	-3.250629	-1.777873	-0.115495
14	P	-2.309185	-3.094429	-0.364097
15	O	-2.408688	-4.285626	0.654388
16	O	-1.330268	-3.124853	-1.597442
17	O	-1.069328	-2.243742	0.578971
18	C	-1.136802	-2.172127	1.991504
19	C	0.016358	-3.026716	2.557021
20	C	-0.019378	-3.199348	4.069220
21	O	-0.104701	-2.023313	4.689263
22	O	0.033889	-4.280897	4.618584
23	N	-0.028299	-4.392533	1.940950
24	H	-9.147860	0.016079	-0.084075
25	H	-8.410919	0.893698	-1.419025
26	H	0.194949	-5.094510	2.656314
27	H	-0.990340	-4.560062	1.540327
28	H	0.620491	-4.467407	1.148055
29	H	-0.114325	-2.177309	5.651280
30	H	0.970017	-2.568719	2.281886
31	H	-0.999381	-1.140320	2.325625
32	H	-2.096034	-2.535032	2.371155
33	H	-5.284193	-2.265442	-0.240201
34	H	-4.585181	-1.561964	-1.711377
35	H	-4.939418	-0.121350	0.979583
36	H	-3.011862	0.782469	-0.412512
37	H	-4.129876	0.955585	-1.774361
38	H	-1.430349	2.348718	0.276759
39	H	-0.921551	2.224403	1.948112
40	H	-3.242079	2.629641	2.748306
41	H	-3.098396	1.182478	1.753003
42	C	-1.409532	4.238095	1.339586
43	C	0.017635	4.635208	0.942325
44	H	-1.619099	4.600688	2.355539
45	C	0.258885	6.146623	0.998182
46	H	0.732366	4.125114	1.602051
47	H	0.225023	4.268841	-0.072591
48	H	-0.419608	6.680922	0.323409
49	H	0.094138	6.536206	2.009215
50	H	-2.123863	4.749451	0.681792
51	C	-9.199251	2.172354	0.173056
52	C	-8.478200	3.452531	-0.268276
53	H	-8.444468	3.488325	-1.366615
54	H	-7.434208	3.424113	0.070636
55	H	-9.250588	2.134589	1.267211
56	C	-9.137331	4.732306	0.260058
57	C	-8.397156	6.004187	-0.165220
58	H	-9.184771	4.686515	1.356544
59	H	-7.361477	5.994291	0.193276

60	H	-8.367687	6.098723	-1.256832
61	H	-10.178219	4.777456	-0.088127
62	H	-10.233107	2.186764	-0.191733
63	H	-8.880446	6.902091	0.233625
64	H	1.284164	6.398203	0.707478
65	C	3.210350	1.015110	-2.348672
66	C	3.064217	0.330696	-1.010954
67	O	2.137180	0.510363	-0.235555
68	O	4.096905	-0.492894	-0.747847
69	C	4.153735	-1.161668	0.534312
70	C	5.484430	-0.796559	1.179779
71	O	5.442801	0.621475	1.410204
72	C	6.494266	1.305117	1.940730
73	O	6.337465	2.491979	2.144251
74	C	7.799663	0.582082	2.202314
75	C	8.743110	0.598493	0.973271
76	C	4.025488	-2.661541	0.310567
77	O	2.645010	-3.020367	0.061647
78	P	2.032443	-3.404590	-1.374342
79	O	3.109827	-4.339946	-2.100927
80	O	1.707222	-2.249971	-2.274881
81	H	2.372252	0.683812	-2.970558
82	H	4.132944	0.681339	-2.829322
83	H	4.659727	-2.991144	-0.515648
84	H	4.312073	-3.201890	1.214854
85	H	3.329959	-0.805941	1.155831
86	H	5.586609	-1.334192	2.127143
87	H	6.315996	-1.059732	0.520246
88	H	8.254300	0.111848	0.119792
89	H	9.609718	-0.024169	1.224214
90	H	8.277815	1.107895	3.032668
91	H	7.626458	-0.448998	2.519484
92	C	9.220092	1.996430	0.562464
93	C	10.179022	1.969236	-0.634165
94	H	9.718077	2.473173	1.418149
95	C	10.661673	3.363061	-1.046587
96	H	11.044630	1.338369	-0.391028
97	H	9.680631	1.487311	-1.486170
98	H	9.819620	4.005919	-1.327665
99	H	11.194179	3.856357	-0.225502
100	H	8.357063	2.629626	0.321602
101	C	3.182980	2.549533	-2.205807
102	C	4.404526	3.113871	-1.470015
103	H	5.314859	2.836307	-2.019994
104	H	4.492741	2.645721	-0.480283
105	H	2.263375	2.838419	-1.682853
106	C	4.359912	4.636816	-1.297725
107	C	5.596929	5.191356	-0.584200
108	H	3.457825	4.908500	-0.732681
109	H	5.722859	4.728606	0.400757
110	H	6.507248	4.990953	-1.161353
111	H	4.257463	5.112243	-2.282638
112	H	3.123871	2.983107	-3.210716
113	H	5.525559	6.274740	-0.442452
114	H	11.342521	3.312808	-1.902500
115	O	-0.929041	-0.089066	-5.044023
116	H	-1.013751	0.873947	-5.026676
117	H	-0.472613	-0.292373	-5.871899
118	Ca	-0.420148	-1.341879	-2.983086
119	O	-0.528477	-0.017388	-0.923408
120	H	-0.726126	-0.709089	-0.247659
121	H	0.342335	0.350349	-0.671747
122	H	3.296016	-5.175519	-1.643015
123	O	0.793751	-4.278466	-0.952926
124	H	-0.120640	-3.827466	-1.237160
125	O	-3.637559	-3.836838	-1.434510
126	H	-3.221711	-3.972048	-2.298301
127	H	-4.073291	-4.973876	-0.899870
128	O	-4.155815	-5.761265	-0.112694
129	H	-3.333539	-5.249468	0.399800
130	H	-3.838576	-6.608058	-0.463048

E[B3LYP/6-31G(d,p)] = -4370.572367 h, E[APFD/6-311+G(2d,p)] = -4368.999759 h
Gcorr[B3LYP/6-31G(d,p)] = 0.959513 h

103. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 3rd step, products

Center No.	Atom	X	Y	Z
1	C	-8.507914	1.019113	-0.394889
2	C	-7.163319	0.750812	0.246453
3	O	-6.888204	0.973745	1.408378
4	O	-6.294859	0.199763	-0.640738
5	C	-4.951341	-0.069942	-0.186187
6	C	-4.028933	1.009443	-0.747925
7	O	-4.460390	2.319750	-0.336221
8	C	-4.091014	2.898120	0.837017
9	O	-4.644320	3.937043	1.140016
10	C	-2.977663	2.289179	1.667670
11	C	-1.569946	2.726711	1.193790
12	C	-4.600594	-1.465114	-0.699550
13	O	-3.296374	-1.757755	-0.167433
14	P	-2.409105	-3.099258	-0.489029
15	O	-2.500772	-4.311614	0.597674
16	O	-1.337292	-3.146726	-1.643058
17	O	-1.167144	-2.345461	0.545591
18	C	-1.297375	-2.218577	1.948955
19	C	-0.129839	-3.003300	2.580634
20	C	-0.209626	-3.151455	4.093997
21	O	-0.406297	-1.975292	4.686912
22	O	-0.091593	-4.216619	4.664359
23	N	-0.082730	-4.382488	1.992143
24	H	-9.133403	0.141285	-0.186281
25	H	-8.384450	1.067157	-1.480429
26	H	0.238427	-5.047886	2.704959
27	H	-1.027568	-4.651821	1.656625
28	H	0.522774	-4.412965	1.159067
29	H	-0.436859	-2.112408	5.651210
30	H	0.814077	-2.511565	2.329580
31	H	-1.214268	-1.171146	2.252400
32	H	-2.254142	-2.606991	2.308810
33	H	-5.339587	-2.184109	-0.340816
34	H	-4.590879	-1.489880	-1.791327
35	H	-4.940088	-0.059317	0.905667
36	H	-2.990848	0.808511	-0.479359
37	H	-4.106058	1.023848	-1.838337
38	H	-1.390480	2.366738	0.173661
39	H	-0.841786	2.209422	1.829976
40	H	-3.142458	2.639179	2.689612
41	H	-3.037470	1.198188	1.680888
42	C	-1.322523	4.238165	1.265165
43	C	0.094562	4.629748	0.828771
44	H	-1.495977	4.584647	2.293460
45	C	0.353285	6.137126	0.910424
46	H	0.825855	4.097626	1.451927
47	H	0.262893	4.285112	-0.200851
48	H	-0.342377	6.693179	0.271673
49	H	0.227368	6.504892	1.935093
50	H	-2.052566	4.767532	0.639672
51	C	-9.177434	2.286239	0.155735
52	C	-8.451611	3.580018	-0.235373
53	H	-8.418341	3.658777	-1.331470
54	H	-7.407422	3.534308	0.101248
55	H	-9.231749	2.207729	1.247562
56	C	-9.106384	4.840070	0.343346
57	C	-8.364704	6.126058	-0.034034
58	H	-9.151807	4.752006	1.437333
59	H	-7.328492	6.101193	0.322253
60	H	-8.336724	6.262299	-1.121258
61	H	-10.147877	4.900758	-0.000661
62	H	-10.210246	2.317716	-0.210875
63	H	-8.846041	7.008717	0.399676
64	H	1.370526	6.385524	0.590237
65	C	3.183487	1.028935	-2.233663

66	C	3.055687	0.318641	-0.907827
67	O	2.125992	0.467462	-0.128540
68	O	4.105760	-0.486663	-0.658471
69	C	4.183157	-1.166442	0.617312
70	C	5.535607	-0.823210	1.228794
71	O	5.515348	0.591267	1.482164
72	C	6.597210	1.259026	1.970354
73	O	6.458652	2.442468	2.204348
74	C	7.910071	0.524399	2.148476
75	C	8.785771	0.558548	0.870493
76	C	4.030891	-2.664097	0.392028
77	O	2.642927	-3.001008	0.151048
78	P	2.032972	-3.415619	-1.275844
79	O	3.091281	-4.398599	-1.966047
80	O	1.741083	-2.282854	-2.213577
81	H	2.317400	0.739271	-2.837034
82	H	4.082985	0.683992	-2.748795
83	H	4.655128	-3.003029	-0.437981
84	H	4.315358	-3.208378	1.294662
85	H	3.379383	-0.803833	1.260678
86	H	5.662753	-1.375646	2.164525
87	H	6.343409	-1.084551	0.539760
88	H	8.248202	0.091039	0.035834
89	H	9.660602	-0.073553	1.062336
90	H	8.435545	1.032541	2.961020
91	H	7.747388	-0.511265	2.456303
92	C	9.248836	1.961276	0.459831
93	C	10.139769	1.951016	-0.788567
94	H	9.796545	2.419153	1.295176
95	C	10.605388	3.349875	-1.203570
96	H	11.014473	1.312658	-0.604845
97	H	9.592410	1.485905	-1.619609
98	H	9.751991	4.000551	-1.426541
99	H	11.184909	3.827162	-0.405183
100	H	8.378122	2.603717	0.278729
101	C	3.198123	2.561095	-2.058167
102	C	4.451807	3.087332	-1.349385
103	H	5.340742	2.791740	-1.924390
104	H	4.553298	2.610244	-0.365356
105	H	2.300323	2.859842	-1.503823
106	C	4.447597	4.610064	-1.167992
107	C	5.714055	5.133101	-0.483169
108	H	3.566311	4.899403	-0.579378
109	H	5.852813	4.664425	0.497126
110	H	6.605195	4.913593	-1.082969
111	H	4.331454	5.092794	-2.147834
112	H	3.119376	3.014552	-3.052945
113	H	5.671323	6.217450	-0.337127
114	H	11.237363	3.311761	-2.096783
115	O	-0.854658	-0.157593	-5.098298
116	H	-0.943945	0.804968	-5.078862
117	H	-0.391179	-0.356249	-5.923380
118	Ca	-0.347675	-1.411583	-3.037505
119	O	-0.481503	-0.151327	-0.955391
120	H	-0.717473	-0.840015	-0.289637
121	H	0.366538	0.229874	-0.652330
122	H	3.251666	-5.225450	-1.483429
123	O	0.767562	-4.244499	-0.838120
124	H	-0.134494	-3.805619	-1.179630
125	O	-3.647146	-3.788709	-1.458223
126	H	-3.262087	-3.951622	-2.330056
127	H	-4.527647	-5.389120	-0.813328
128	O	-4.419575	-6.000546	-0.058288
129	H	-3.197088	-5.006517	0.388842
130	H	-4.054730	-6.809501	-0.444833

E[B3LYP/6-31G(d,p)] = -4370.585978 h, E[APFD/6-311+G(2d,p)] = -4369.014533 h
Gcorr[B3LYP/6-31G(d,p)] = 0.960159 h

104. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 4th step, reactants

Center No.	Atom	X	Y	Z
1	C	-8.182692	1.722544	-1.108606
2	C	-7.033645	1.226864	-0.257545
3	O	-6.947644	1.366769	0.945886
4	O	-6.101957	0.582590	-1.008533
5	C	-4.913449	0.112174	-0.338862
6	C	-3.769355	1.073025	-0.650692
7	O	-4.066674	2.410494	-0.209491
8	C	-3.830131	2.850501	1.054709
9	O	-4.198889	3.976263	1.325762
10	C	-3.092271	1.969211	2.046446
11	C	-1.550872	2.056290	1.935152
12	C	-4.650837	-1.294488	-0.873455
13	O	-3.485979	-1.766194	-0.165394
14	P	-2.784289	-3.231083	-0.320194
15	O	-3.188324	-4.372992	0.723300
16	O	-1.538155	-3.516128	-1.356725
17	O	-1.556961	-2.631202	0.768232
18	C	-1.750968	-2.446703	2.156607
19	C	-0.341898	-2.346284	2.763947
20	C	-0.378904	-2.209384	4.280679
21	O	-0.890619	-1.031348	4.640887
22	O	-0.007238	-3.080150	5.037359
23	N	0.451341	-3.566558	2.422509
24	H	-8.983997	0.977729	-1.019222
25	H	-7.875061	1.735399	-2.157712
26	H	0.166298	-4.353833	3.013392
27	H	0.365817	-3.829256	1.400883
28	H	1.449933	-3.414597	2.587355
29	H	-0.928579	-0.989887	5.613690
30	H	0.180366	-1.490742	2.330136
31	H	-2.292801	-1.521224	2.376907
32	H	-2.297308	-3.288905	2.591133
33	H	-5.513705	-1.932081	-0.674096
34	H	-4.462745	-1.280884	-1.948897
35	H	-5.108123	0.071880	0.734505
36	H	-2.831337	0.702364	-0.238195
37	H	-3.654492	1.160160	-1.734188
38	H	-1.218640	1.656617	0.969327
39	H	-1.142333	1.384175	2.699816
40	H	-3.401830	2.318716	3.034410
41	H	-3.404376	0.925815	1.956906
42	C	-0.976498	3.463717	2.133426
43	C	0.557238	3.480889	2.127066
44	H	-1.341680	3.876235	3.084039
45	C	1.143366	4.887606	2.278366
46	H	0.927810	2.839829	2.938311
47	H	0.921596	3.029068	1.194374
48	H	0.819087	5.541288	1.460570
49	H	0.822602	5.351107	3.218324
50	H	-1.350322	4.133525	1.348098
51	C	-8.690463	3.098248	-0.650902
52	C	-7.674913	4.226928	-0.870240
53	H	-7.430119	4.291282	-1.940098
54	H	-6.736288	3.983922	-0.354645
55	H	-8.953657	3.038348	0.411322
56	C	-8.170372	5.592758	-0.380246
57	C	-7.135246	6.705615	-0.571026
58	H	-8.435510	5.518960	0.683162
59	H	-6.209346	6.476695	-0.030994
60	H	-6.878186	6.830053	-1.629252
61	H	-9.097250	5.855894	-0.907783
62	H	-9.615961	3.322465	-1.194177
63	H	-7.507713	7.667442	-0.203629
64	H	2.238050	4.866570	2.274371
65	C	2.890556	0.879713	-2.317472
66	C	2.892604	0.155061	-0.991700
67	O	1.997894	0.226268	-0.159180
68	O	4.018375	-0.551221	-0.804176

69	C	4.236759	-1.220284	0.463694
70	C	5.637366	-0.840899	0.924496
71	O	5.612307	0.575664	1.170589
72	C	6.712940	1.264839	1.578288
73	O	6.568450	2.445171	1.825564
74	C	8.051066	0.558570	1.654267
75	C	8.825893	0.614520	0.313545
76	C	4.079693	-2.725021	0.277378
77	O	2.687019	-3.090499	0.340063
78	P	1.861580	-3.741836	-0.901024
79	O	2.818712	-4.903709	-1.490754
80	O	1.630805	-2.763431	-2.030654
81	H	1.993890	0.571462	-2.864079
82	H	3.762388	0.574228	-2.900678
83	H	4.529098	-3.045665	-0.665742
84	H	4.576902	-3.253150	1.095362
85	H	3.499682	-0.860789	1.184057
86	H	5.872405	-1.381948	1.845622
87	H	6.375854	-1.090224	0.157598
88	H	8.236044	0.137742	-0.479580
89	H	9.725931	0.000706	0.435553
90	H	8.625744	1.076504	2.426328
91	H	7.935144	-0.481053	1.969548
92	C	9.227124	2.028049	-0.124220
93	C	10.026581	2.040833	-1.433013
94	H	9.823064	2.496135	0.671556
95	C	10.431001	3.450821	-1.873754
96	H	10.925805	1.421339	-1.314781
97	H	9.431649	1.566170	-2.225016
98	H	9.550028	4.083297	-2.032491
99	H	11.055394	3.938285	-1.116380
100	H	8.331770	2.651423	-0.240022
101	C	2.867089	2.411040	-2.124672
102	C	4.155050	2.975597	-1.513685
103	H	5.001766	2.726275	-2.168736
104	H	4.360857	2.486586	-0.552281
105	H	2.005788	2.673477	-1.498540
106	C	4.106300	4.493647	-1.301545
107	C	5.410493	5.057973	-0.729373
108	H	3.274364	4.735554	-0.626255
109	H	5.663912	4.576309	0.221243
110	H	6.247297	4.889705	-1.417498
111	H	3.877730	4.987439	-2.255817
112	H	2.693317	2.869449	-3.105021
113	H	5.336881	6.136365	-0.554230
114	H	10.998501	3.429338	-2.809785
115	O	-0.869769	-0.588226	-4.953007
116	H	-0.697436	0.361759	-5.005460
117	H	-0.633647	-0.941316	-5.821750
118	Ca	-0.366525	-1.845062	-2.896712
119	O	-0.581943	-0.513658	-0.854554
120	H	-0.888975	-1.107877	-0.138811
121	H	0.271982	-0.135044	-0.556447
122	H	2.919706	-5.650648	-0.880394
123	O	0.618764	-4.323277	-0.220751
124	H	-0.702778	-3.842672	-0.855273
125	O	-3.880192	-3.695015	-1.527828
126	H	-3.416282	-4.236040	-2.182032
127	H	-5.349647	-5.050677	-0.890689
128	O	-5.372818	-5.603543	-0.089772
129	H	-3.993490	-4.907488	0.445294
130	H	-5.202051	-6.502978	-0.404526

E[B3LYP/6-31G(d,p)] = -4370.586367 h, E[APFD/6-311+G(2d,p)] = -4369.021695 h
Gcorr[B3LYP/6-31G(d,p)] = 0.965633 h

105. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 4th step, TS

Center No.	Atom	X	Y	Z
1	C	-8.437810	1.103839	-0.820962
2	C	-7.176921	0.774200	-0.051854

3	O	-7.002386	0.984344	1.131280
4	O	-6.255035	0.176041	-0.852638
5	C	-4.987212	-0.178822	-0.263582
6	C	-3.949136	0.870494	-0.662323
7	O	-4.399663	2.196513	-0.330937
8	C	-4.210337	2.780420	0.882163
9	O	-4.742579	3.857930	1.064096
10	C	-3.314111	2.126707	1.915710
11	C	-1.818998	2.489285	1.738079
12	C	-4.662568	-1.564131	-0.816794
13	O	-3.407018	-1.959215	-0.211895
14	P	-2.601538	-3.276602	-0.664214
15	O	-2.439562	-4.322478	0.506954
16	O	-1.433153	-3.065879	-1.631855
17	O	-1.058356	-2.185358	0.794090
18	C	-1.349456	-2.047775	2.143286
19	C	-0.102558	-2.604206	2.955137
20	C	-0.495197	-3.215297	4.278622
21	O	-0.821108	-2.274534	5.169577
22	O	-0.556008	-4.412990	4.477800
23	N	0.464832	-3.651809	2.069667
24	H	-9.111256	0.246278	-0.692054
25	H	-8.202081	1.159747	-1.887457
26	H	0.145247	-4.579540	2.366059
27	H	0.023359	-3.349009	1.135614
28	H	1.482409	-3.646355	2.002121
29	H	-1.123441	-2.714845	5.984073
30	H	0.638165	-1.816356	3.090692
31	H	-1.504788	-1.007739	2.458603
32	H	-2.238032	-2.629962	2.428890
33	H	-5.452162	-2.266896	-0.545769
34	H	-4.573585	-1.532203	-1.905610
35	H	-5.100559	-0.222605	0.821502
36	H	-2.975517	0.641023	-0.227447
37	H	-3.844190	0.882906	-1.750624
38	H	-1.444668	2.076612	0.794043
39	H	-1.270476	1.969706	2.533393
40	H	-3.664296	2.493851	2.883648
41	H	-3.429058	1.040170	1.915857
42	C	-1.515869	3.990439	1.813664
43	C	-0.017742	4.298309	1.698637
44	H	-1.898663	4.391914	2.762270
45	C	0.296311	5.795612	1.769061
46	H	0.522844	3.772126	2.496858
47	H	0.362876	3.889017	0.752640
48	H	-0.204711	6.343384	0.962790
49	H	-0.039452	6.226004	2.719386
50	H	-2.055860	4.522293	1.019834
51	C	-9.116900	2.387362	-0.323241
52	C	-8.318203	3.660692	-0.630287
53	H	-8.172048	3.741818	-1.716981
54	H	-7.315478	3.584083	-0.189609
55	H	-9.279627	2.302945	0.757334
56	C	-8.993192	4.937275	-0.114153
57	C	-8.184998	6.203694	-0.413167
58	H	-9.147986	4.849822	0.969828
59	H	-7.189542	6.151810	0.042392
60	H	-8.047528	6.339794	-1.492056
61	H	-9.993990	5.025773	-0.558393
62	H	-10.107986	2.453768	-0.787430
63	H	-8.683403	7.098362	-0.025802
64	H	1.371628	5.982443	1.680480
65	C	3.034600	1.288958	-2.011063
66	C	3.048181	0.421781	-0.774770
67	O	2.217291	0.474002	0.117980
68	O	4.111956	-0.408023	-0.751003
69	C	4.333452	-1.234417	0.415442
70	C	5.751893	-0.962558	0.901642
71	O	5.784973	0.412959	1.315238
72	C	6.922759	1.008349	1.769237
73	O	6.833827	2.159719	2.144685
74	C	8.229277	0.241302	1.742884

75	C	8.978635	0.384562	0.394320
76	C	4.154103	-2.696366	0.030495
77	O	2.747798	-3.028450	-0.086665
78	P	1.982881	-3.248727	-1.482967
79	O	2.974151	-4.079181	-2.425821
80	O	1.560187	-1.999870	-2.193801
81	H	2.089376	1.097219	-2.527907
82	H	3.849225	0.992803	-2.676040
83	H	4.675001	-2.923291	-0.902403
84	H	4.543324	-3.341777	0.820127
85	H	3.612567	-0.958794	1.187454
86	H	5.977681	-1.619921	1.746259
87	H	6.470888	-1.144239	0.098076
88	H	8.354974	0.002996	-0.423799
89	H	9.854499	-0.272957	0.441783
90	H	8.843191	0.660497	2.544021
91	H	8.072412	-0.816936	1.965789
92	C	9.429945	1.813198	0.069271
93	C	10.201730	1.903806	-1.253135
94	H	10.061419	2.187384	0.886947
95	C	10.654914	3.328177	-1.586910
96	H	11.076726	1.241438	-1.208151
97	H	9.571140	1.520258	-2.066661
98	H	9.797773	4.005933	-1.672377
99	H	11.314712	3.726463	-0.807760
100	H	8.559489	2.479855	0.027408
101	C	3.126547	2.787470	-1.657454
102	C	4.477727	3.200480	-1.062493
103	H	5.275507	2.955273	-1.777870
104	H	4.685671	2.610146	-0.160265
105	H	2.317726	3.033595	-0.958767
106	C	4.550978	4.691659	-0.712141
107	C	5.911916	5.104401	-0.142989
108	H	3.762026	4.929617	0.014373
109	H	6.155715	4.522242	0.752224
110	H	6.711542	4.936219	-0.874068
111	H	4.329425	5.287104	-1.608266
112	H	2.936593	3.360627	-2.572337
113	H	5.927710	6.165327	0.127579
114	H	11.201331	3.361267	-2.535083
115	O	-1.090584	0.214489	-4.809857
116	H	-0.942097	1.168499	-4.861689
117	H	-0.849272	-0.132155	-5.679675
118	Ca	-0.579042	-1.037556	-2.748693
119	O	-0.526406	-0.073362	-0.545163
120	H	-0.716673	-0.869422	0.066764
121	H	0.341339	0.275604	-0.271831
122	H	3.185269	-4.971323	-2.106003
123	O	0.802876	-4.192085	-1.032104
124	H	-0.109606	-3.810364	-1.271795
125	O	-3.743489	-4.034987	-1.569568
126	H	-3.458410	-4.103806	-2.492794
127	H	-4.454673	-6.015005	-0.653484
128	O	-4.053931	-6.319260	0.176710
129	H	-3.051129	-5.130191	0.402054
130	H	-3.582491	-7.132618	-0.055846

E[B3LYP/6-31G(d,p)] = -4370.572338 h, E[APFD/6-311+G(2d,p)] = -4369.00201 h
Gcorr[B3LYP/6-31G(d,p)] = 0.957795 h

106. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 4th step, products

Center No.	Atom	X	Y	Z
1	C	-8.048092	-0.438435	1.856816
2	C	-6.608210	-0.310201	1.409164
3	O	-5.717411	0.209432	2.049164
4	O	-6.420679	-0.886790	0.191025
5	C	-5.097640	-0.828591	-0.379402
6	C	-5.076417	0.272591	-1.440722
7	O	-5.562271	1.511881	-0.900825
8	C	-4.771006	2.455430	-0.319455

9	O	-5.332932	3.391633	0.213389
10	C	-3.265139	2.345332	-0.423867
11	C	-2.717253	2.899977	-1.761300
12	C	-4.865836	-2.219727	-0.965458
13	O	-3.513262	-2.277458	-1.502461
14	P	-2.560607	-3.511672	-1.180779
15	O	-2.485764	-3.593546	0.377536
16	O	-1.245745	-3.291471	-1.903851
17	O	-1.783873	-0.575934	1.070160
18	C	-1.309645	-0.102769	2.331817
19	C	0.064303	-0.753244	2.627662
20	C	0.518847	-0.408472	4.041899
21	O	0.742902	0.910954	4.183572
22	O	0.638367	-1.211205	4.944632
23	N	-0.046274	-2.187125	2.385117
24	H	-8.107183	-1.365564	2.442195
25	H	-8.684264	-0.581985	0.978837
26	H	-0.313370	-2.662425	3.244969
27	H	-1.618242	-1.542348	1.099915
28	H	0.850001	-2.572566	2.102221
29	H	0.995658	1.073664	5.109753
30	H	0.791924	-0.330360	1.927263
31	H	-1.228473	0.983626	2.277045
32	H	-2.029007	-0.362876	3.119664
33	H	-5.002728	-2.963474	-0.178477
34	H	-5.555972	-2.430547	-1.785619
35	H	-4.367224	-0.629086	0.407893
36	H	-4.076914	0.368551	-1.867577
37	H	-5.774552	0.025638	-2.244517
38	H	-3.165034	2.356830	-2.603874
39	H	-1.645924	2.672095	-1.783184
40	H	-2.863207	2.935217	0.403862
41	H	-2.929971	1.316170	-0.281370
42	C	-2.935217	4.405499	-1.951777
43	C	-2.348377	4.930992	-3.267479
44	H	-2.479858	4.944443	-1.109271
45	C	-2.553623	6.436841	-3.457789
46	H	-1.274913	4.700152	-3.302130
47	H	-2.804033	4.390211	-4.108115
48	H	-3.619133	6.693293	-3.460761
49	H	-2.079116	7.005748	-2.650158
50	H	-4.007865	4.635771	-1.915552
51	C	-8.513393	0.752646	2.705542
52	C	-8.650729	2.056164	1.908260
53	H	-9.378493	1.908046	1.097560
54	H	-7.695529	2.297317	1.423604
55	H	-7.805005	0.894252	3.529766
56	C	-9.087916	3.247541	2.769192
57	C	-9.214553	4.548467	1.970489
58	H	-8.364505	3.387657	3.583873
59	H	-8.261526	4.815673	1.499839
60	H	-9.960693	4.452329	1.173358
61	H	-10.047768	3.016501	3.250982
62	H	-9.478056	0.495795	3.158918
63	H	-9.517005	5.383963	2.610322
64	H	-2.125325	6.781921	-4.404443
65	C	3.476978	0.937032	-2.057203
66	C	3.240392	0.241384	-0.737897
67	O	2.275503	0.443948	-0.014012
68	O	4.230208	-0.616219	-0.427078
69	C	4.215931	-1.282519	0.858590
70	C	5.538803	-0.970655	1.547748
71	O	5.547853	0.446082	1.784080
72	C	6.612618	1.080599	2.350290
73	O	6.497904	2.269719	2.566142
74	C	7.881531	0.302321	2.631880
75	C	8.848644	0.288201	1.421253
76	C	4.046372	-2.779254	0.640299
77	O	2.671533	-3.098507	0.301811
78	P	2.153828	-3.444769	-1.170789
79	O	3.282280	-4.320645	-1.882757
80	O	1.808701	-2.275392	-2.037877

81	H	2.647038	0.668867	-2.720003
82	H	4.399351	0.562025	-2.506567
83	H	4.720643	-3.140936	-0.138934
84	H	4.249762	-3.318277	1.566923
85	H	3.388370	-0.892040	1.452352
86	H	5.589012	-1.515221	2.495287
87	H	6.378695	-1.266031	0.913089
88	H	8.355732	-0.168481	0.553671
89	H	9.682002	-0.374302	1.682447
90	H	8.364387	0.802342	3.475259
91	H	7.660048	-0.722934	2.937989
92	C	9.394614	1.667379	1.033731
93	C	10.375066	1.608192	-0.144197
94	H	9.896095	2.113747	1.903634
95	C	10.928782	2.982398	-0.532387
96	H	11.206021	0.936123	0.109199
97	H	9.872437	1.157709	-1.010790
98	H	10.122639	3.666003	-0.822503
99	H	11.467228	3.442624	0.303878
100	H	8.565416	2.340441	0.782203
101	C	3.522652	2.469645	-1.890214
102	C	4.735061	2.967582	-1.094620
103	H	5.655473	2.646026	-1.602118
104	H	4.752460	2.494474	-0.103617
105	H	2.595477	2.798591	-1.405919
106	C	4.755618	4.491069	-0.920434
107	C	5.979335	4.986401	-0.143582
108	H	3.839892	4.805765	-0.401908
109	H	6.030385	4.521178	0.846711
110	H	6.907767	4.739998	-0.672072
111	H	4.726506	4.970386	-1.908372
112	H	3.529965	2.915837	-2.891274
113	H	5.953682	6.072470	-0.006652
114	H	11.623111	2.909362	-1.375737
115	O	-0.766869	-0.400899	-5.109568
116	H	-0.746312	0.546093	-5.302999
117	H	-0.481299	-0.838112	-5.923327
118	Ca	-0.189650	-1.287138	-2.905547
119	O	-0.302938	0.291008	-1.078742
120	H	-0.845447	0.016290	-0.301353
121	H	0.568549	0.546174	-0.715250
122	H	3.461788	-5.181581	-1.470111
123	O	0.911914	-4.384418	-0.847193
124	H	0.083375	-4.061868	-1.315569
125	O	-3.292989	-4.863005	-1.615707
126	H	-3.274679	-5.032573	-2.571738
127	H	-1.008020	-6.123950	1.222892
128	O	-0.777279	-5.189714	1.333066
129	H	-1.811522	-4.269858	0.787730
130	H	0.039650	-5.055268	0.818279

E[B3LYP/6-31G(d,p)] = -4370.605348 h, E[APFD/6-311+G(2d,p)] = -4369.028463 h
Gcorr[B3LYP/6-31G(d,p)] = 0.956999 h

107. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 5th step, reactants

Center No.	Atom	X	Y	Z
1	C	8.516549	-0.392170	1.649504
2	C	7.344238	-0.247065	0.703987
3	O	7.432127	-0.109662	-0.499026
4	O	6.159328	-0.305071	1.370021
5	C	4.951260	-0.115462	0.605195
6	C	4.424577	1.290279	0.880098
7	O	5.411398	2.276497	0.536212
8	C	5.505959	2.852534	-0.693628
9	O	6.478247	3.550206	-0.901803
10	C	4.386637	2.672382	-1.700984
11	C	3.187682	3.615695	-1.434948
12	C	3.989908	-1.207319	1.081666
13	O	2.708697	-1.104454	0.421220
14	P	2.426391	-1.827643	-1.038331

15	O	3.276219	-1.029941	-2.094349
16	O	0.933546	-1.494353	-1.179338
17	O	0.230578	-2.984544	1.636069
18	C	1.131672	-4.040012	1.968091
19	C	0.824246	-5.326401	1.170496
20	C	-0.558442	-5.863010	1.522720
21	O	-0.525154	-6.630365	2.599034
22	O	-1.567695	-5.564266	0.907898
23	N	0.878081	-5.058377	-0.298626
24	H	8.859839	-1.431220	1.565807
25	H	8.172702	-0.249177	2.677300
26	H	0.022101	-4.586453	-0.631298
27	H	-0.617188	-3.112044	2.087728
28	H	0.969751	-5.928441	-0.828429
29	H	-1.433298	-6.895835	2.836049
30	H	1.583683	-6.071056	1.412797
31	H	2.131706	-3.697579	1.702828
32	H	1.110302	-4.271659	3.035839
33	H	4.427021	-2.192167	0.897722
34	H	3.791426	-1.105459	2.150751
35	H	5.180081	-0.239725	-0.454306
36	H	3.481517	1.450307	0.357295
37	H	4.254424	1.420757	1.951793
38	H	2.753058	3.403529	-0.449765
39	H	2.412953	3.372775	-2.171872
40	H	4.822851	2.906079	-2.675042
41	H	4.044592	1.634359	-1.738058
42	C	3.529212	5.108020	-1.526578
43	C	2.312771	6.011664	-1.290656
44	H	3.956025	5.320748	-2.516404
45	C	2.647187	7.503750	-1.378177
46	H	1.532477	5.766846	-2.023833
47	H	1.884253	5.790109	-0.303717
48	H	3.399862	7.784651	-0.632736
49	H	3.046850	7.762444	-2.365267
50	H	4.311427	5.357459	-0.797925
51	C	9.664640	0.568046	1.300088
52	C	9.315303	2.044913	1.524300
53	H	9.036523	2.194611	2.577225
54	H	8.430091	2.310373	0.931131
55	H	9.948737	0.408366	0.253584
56	C	10.459667	2.999615	1.163020
57	C	10.093866	4.473169	1.366519
58	H	10.748209	2.835999	0.115846
59	H	9.228324	4.751050	0.754358
60	H	9.837426	4.676395	2.412648
61	H	11.344773	2.752728	1.764967
62	H	10.535462	0.297684	1.908855
63	H	10.923016	5.133827	1.092834
64	H	1.760366	8.122066	-1.205385
65	C	-3.966903	0.670703	1.882164
66	C	-3.923113	0.689073	0.373470
67	O	-3.200757	1.418826	-0.292609
68	O	-4.786887	-0.183616	-0.172416
69	C	-4.912068	-0.243808	-1.614607
70	C	-6.359948	0.080041	-1.960120
71	O	-6.582194	1.429959	-1.520588
72	C	-7.799324	2.034583	-1.604138
73	O	-7.869793	3.189400	-1.235418
74	C	-8.993355	1.244482	-2.099229
75	C	-9.730099	0.501805	-0.956200
76	C	-4.515179	-1.639389	-2.073109
77	O	-3.077856	-1.800104	-2.028406
78	P	-2.250864	-2.516386	-0.868059
79	O	-3.152666	-3.770996	-0.500602
80	O	-1.884945	-1.626136	0.289966
81	H	-2.999213	0.284293	2.220710
82	H	-4.735311	-0.032111	2.212544
83	H	-5.000303	-2.408849	-1.468894
84	H	-4.791837	-1.780909	-3.119668
85	H	-4.247508	0.499275	-2.058328
86	H	-6.501227	0.000914	-3.041956

87	H	-7.038729	-0.611025	-1.453254
88	H	-9.045121	-0.198891	-0.462082
89	H	-10.510600	-0.111556	-1.421213
90	H	-9.671199	1.971375	-2.553926
91	H	-8.703354	0.532167	-2.875554
92	C	-10.362482	1.424973	0.091833
93	C	-11.115840	0.655141	1.183682
94	H	-11.053105	2.118179	-0.408130
95	C	-11.752483	1.571939	2.232433
96	H	-11.893475	0.034389	0.718560
97	H	-10.424899	-0.041542	1.677430
98	H	-10.994153	2.181046	2.737649
99	H	-12.474273	2.256947	1.773249
100	H	-9.588313	2.048836	0.555823
101	C	-4.208673	2.074879	2.467685
102	C	-5.603781	2.632094	2.158620
103	H	-6.361869	1.944615	2.559705
104	H	-5.762413	2.660294	1.071943
105	H	-3.439094	2.756312	2.085939
106	C	-5.836813	4.034950	2.731927
107	C	-7.241440	4.571699	2.439296
108	H	-5.087098	4.722338	2.317414
109	H	-7.435533	4.598806	1.361421
110	H	-8.009085	3.936425	2.896488
111	H	-5.667452	4.017210	3.817095
112	H	-4.066425	2.017152	3.552946
113	H	-7.372589	5.585501	2.831526
114	H	-12.281175	0.995446	2.998473
115	O	5.206734	-4.377171	-1.812601
116	H	5.002278	-5.101089	-2.420659
117	H	4.339858	-4.120876	-1.428488
118	Ca	0.152150	-0.468349	0.913601
119	O	-0.602544	1.808580	0.464667
120	H	-0.133314	2.355526	-0.179057
121	H	-1.551676	1.835165	0.205344
122	H	-2.704613	-4.425047	0.077065
123	O	-0.971580	-3.095213	-1.611690
124	H	-0.166589	-2.457689	-1.543533
125	O	2.801774	-3.301619	-0.947095
126	H	1.694519	-4.419904	-0.556283
127	H	5.172196	-2.229191	-4.075866
128	O	5.314528	-2.070289	-3.132006
129	H	4.101710	-1.493145	-2.533043
130	H	5.405726	-2.972774	-2.714163

E[B3LYP/6-31G(d,p)] = -4370.632453 h, E[APFD/6-311+G(2d,p)] = -4369.060562 h
Gcorr[B3LYP/6-31G(d,p)] = 0.96461 h

108. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 5th step, TS

Center No.	Atom	X	Y	Z
1	C	8.375282	-0.355478	1.728731
2	C	7.280564	-0.189092	0.695537
3	O	7.468057	0.070675	-0.476788
4	O	6.053360	-0.387686	1.238066
5	C	4.899247	-0.205189	0.382882
6	C	4.261422	1.135150	0.732678
7	O	5.205375	2.211421	0.575317
8	C	5.428362	2.846628	-0.606404
9	O	6.365718	3.619288	-0.651315
10	C	4.474098	2.639757	-1.766327
11	C	3.225253	3.550277	-1.665436
12	C	3.979261	-1.397707	0.673898
13	O	2.717366	-1.307189	0.010447
14	P	2.447283	-1.995021	-1.582112
15	O	3.540900	-0.948031	-2.194165
16	O	0.934164	-1.615984	-1.499919
17	O	0.480952	-2.771299	2.059349
18	C	1.425101	-3.807157	2.321932
19	C	1.064182	-5.123436	1.604017
20	C	-0.313514	-5.623501	2.026290

21	O	-0.284220	-6.155158	3.236925
22	O	-1.310277	-5.501904	1.336762
23	N	1.064002	-4.959281	0.117451
24	H	8.745643	-1.384128	1.629661
25	H	7.942861	-0.268973	2.729355
26	H	0.195608	-4.512821	-0.218685
27	H	-0.241296	-2.803070	2.702843
28	H	1.120105	-5.869296	-0.348312
29	H	-1.187371	-6.411136	3.501855
30	H	1.820203	-5.867360	1.862485
31	H	2.393853	-3.462848	1.957915
32	H	1.508894	-4.009471	3.391914
33	H	4.490586	-2.323016	0.394187
34	H	3.778370	-1.431118	1.750934
35	H	5.224232	-0.215783	-0.655801
36	H	3.359890	1.293044	0.140168
37	H	3.990167	1.157159	1.791453
38	H	2.700784	3.358313	-0.720318
39	H	2.537904	3.254024	-2.466773
40	H	5.035954	2.892812	-2.668857
41	H	4.165828	1.595165	-1.853039
42	C	3.528234	5.048941	-1.782744
43	C	2.268157	5.919201	-1.701203
44	H	4.040736	5.237849	-2.736232
45	C	2.563087	7.416471	-1.831674
46	H	1.565981	5.613970	-2.488776
47	H	1.758072	5.728150	-0.747233
48	H	3.237259	7.757469	-1.037763
49	H	3.041334	7.643063	-2.791363
50	H	4.230304	5.350560	-0.994995
51	C	9.527136	0.639315	1.522510
52	C	9.133728	2.095947	1.800400
53	H	8.788290	2.185188	2.840382
54	H	8.280882	2.375941	1.168044
55	H	9.890909	0.544031	0.492998
56	C	10.277366	3.088826	1.559652
57	C	9.869858	4.542966	1.816479
58	H	10.631129	2.986032	0.524786
59	H	9.035720	4.837233	1.169337
60	H	9.548812	4.686692	2.854604
61	H	11.130195	2.826222	2.200352
62	H	10.355943	0.349255	2.179104
63	H	10.699528	5.231760	1.626406
64	H	1.645915	8.010945	-1.768082
65	C	-3.638253	0.935025	1.761106
66	C	-3.712870	0.724238	0.268222
67	O	-3.023275	1.319305	-0.549903
68	O	-4.640906	-0.183569	-0.075818
69	C	-4.884013	-0.447826	-1.479961
70	C	-6.353990	-0.149105	-1.746808
71	O	-6.527147	1.255743	-1.498319
72	C	-7.747410	1.858644	-1.531884
73	O	-7.775994	3.060072	-1.357450
74	C	-8.990942	1.016667	-1.731380
75	C	-9.575244	0.496357	-0.393726
76	C	-4.537347	-1.901626	-1.769287
77	O	-3.105039	-2.081897	-1.860232
78	P	-2.158421	-2.617492	-0.690801
79	O	-3.002670	-3.812037	-0.068333
80	O	-1.711486	-1.563387	0.285933
81	H	-2.650369	0.585163	2.080447
82	H	-4.386417	0.309805	2.253871
83	H	-4.955164	-2.566458	-1.010116
84	H	-4.929061	-2.188820	-2.747061
85	H	-4.254344	0.212730	-2.078230
86	H	-6.589780	-0.382974	-2.789389
87	H	-6.990937	-0.744226	-1.087075
88	H	-8.830879	-0.120838	0.125192
89	H	-10.406184	-0.173400	-0.644027
90	H	-9.723516	1.665843	-2.217696
91	H	-8.797701	0.175571	-2.401636
92	C	-10.073147	1.597912	0.549312

93	C	-10.675805	1.042097	1.845548
94	H	-10.825789	2.205794	0.028322
95	C	-11.176557	2.137790	2.791345
96	H	-11.503700	0.363775	1.598960
97	H	-9.923385	0.429643	2.360663
98	H	-10.362400	2.811654	3.081967
99	H	-11.954689	2.745691	2.315929
100	H	-9.249212	2.279234	0.795437
101	C	-3.815612	2.418748	2.137540
102	C	-5.219382	2.960745	1.841302
103	H	-5.957789	2.373348	2.405117
104	H	-5.459939	2.813843	0.779598
105	H	-3.063779	3.011197	1.602717
106	C	-5.380424	4.446046	2.186342
107	C	-6.793013	4.971677	1.912234
108	H	-4.652473	5.030345	1.607459
109	H	-7.071796	4.822470	0.863324
110	H	-7.534211	4.448458	2.527741
111	H	-5.126659	4.603934	3.243343
112	H	-3.596389	2.524653	3.206213
113	H	-6.872457	6.040895	2.134442
114	H	-11.599434	1.712193	3.707166
115	O	3.182669	-4.714380	-3.213465
116	H	2.569742	-5.464416	-3.260140
117	H	3.157857	-4.272475	-2.181353
118	Ca	0.471563	-0.590454	0.683193
119	O	-0.400118	1.621536	0.148657
120	H	0.068952	2.202021	-0.464552
121	H	-1.346641	1.647948	-0.121690
122	H	-2.491061	-4.392167	0.535142
123	O	-0.937651	-3.284026	-1.454058
124	H	-0.147332	-2.616484	-1.578900
125	O	2.937217	-3.441338	-1.181205
126	H	1.867911	-4.372299	-0.247142
127	H	1.315891	-2.366944	-3.662996
128	O	2.234226	-2.525809	-3.405092
129	H	3.555201	-1.083794	-3.157046
130	H	2.675838	-3.805629	-3.558777

E[B3LYP/6-31G(d,p)] = -4370.582074 h, E[APFD/6-311+G(2d,p)] = -4369.007056 h
Gcorr[B3LYP/6-31G(d,p)] = 0.967961 h

109. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 5th step, products

Center No.	Atom	X	Y	Z
1	C	8.394171	-0.236110	1.578171
2	C	7.286980	-0.075806	0.557177
3	O	7.458203	0.223218	-0.608373
4	O	6.071417	-0.329837	1.101355
5	C	4.904246	-0.176081	0.257174
6	C	4.215768	1.130241	0.637127
7	O	5.121247	2.243821	0.515690
8	C	5.323456	2.924848	-0.643673
9	O	6.234055	3.729936	-0.661411
10	C	4.377099	2.725934	-1.811453
11	C	3.098363	3.589698	-1.680384
12	C	4.039984	-1.412932	0.537427
13	O	2.751812	-1.364581	-0.075311
14	P	2.424370	-1.999364	-1.697752
15	O	3.490589	-0.896575	-2.270259
16	O	0.910411	-1.671445	-1.480027
17	O	0.517801	-2.805603	2.127971
18	C	1.461492	-3.833207	2.419937
19	C	1.112241	-5.155830	1.709100
20	C	-0.266353	-5.661205	2.123283
21	O	-0.244627	-6.177535	3.340056
22	O	-1.254594	-5.554784	1.419596
23	N	1.112810	-4.995272	0.219793
24	H	8.817339	-1.237406	1.425612
25	H	7.963921	-0.221837	2.583273
26	H	0.251783	-4.533988	-0.121363

27	H	-0.215007	-2.828270	2.759960
28	H	1.156468	-5.907116	-0.244834
29	H	-1.147857	-6.438699	3.599758
30	H	1.871228	-5.895992	1.969414
31	H	2.436352	-3.488274	2.071843
32	H	1.527146	-4.025076	3.493009
33	H	4.584644	-2.305948	0.219774
34	H	3.879600	-1.483138	1.619739
35	H	5.222158	-0.152809	-0.783353
36	H	3.313646	1.270737	0.041033
37	H	3.936112	1.114614	1.693919
38	H	2.572620	3.334792	-0.750796
39	H	2.428402	3.309654	-2.502033
40	H	4.930303	3.029008	-2.703818
41	H	4.103675	1.675157	-1.934237
42	C	3.350900	5.101640	-1.721807
43	C	2.060689	5.923775	-1.615223
44	H	3.867878	5.353839	-2.658034
45	C	2.306133	7.434777	-1.664758
46	H	1.379843	5.636037	-2.427686
47	H	1.544791	5.667123	-0.679929
48	H	2.957069	7.756812	-0.843986
49	H	2.789767	7.726262	-2.604006
50	H	4.032553	5.388634	-0.911052
51	C	9.492265	0.826206	1.419095
52	C	9.025649	2.244371	1.771941
53	H	8.675845	2.261036	2.814168
54	H	8.159904	2.513666	1.152607
55	H	9.855020	0.801843	0.385075
56	C	10.117625	3.305100	1.587555
57	C	9.636846	4.721035	1.919953
58	H	10.476696	3.275491	0.549846
59	H	8.789643	5.006931	1.286190
60	H	9.307796	4.792658	2.963046
61	H	10.982283	3.052214	2.216197
62	H	10.338375	0.546478	2.057902
63	H	10.430826	5.459972	1.770040
64	H	1.368402	7.994242	-1.585400
65	C	-3.578876	0.887532	1.841031
66	C	-3.646623	0.676804	0.348059
67	O	-2.945488	1.263369	-0.466272
68	O	-4.583726	-0.220021	-0.001028
69	C	-4.817355	-0.486479	-1.406126
70	C	-6.276644	-0.157873	-1.695775
71	O	-6.426792	1.249824	-1.449111
72	C	-7.625556	1.886367	-1.557415
73	O	-7.634800	3.085363	-1.365043
74	C	-8.873862	1.083121	-1.860618
75	C	-9.572146	0.562304	-0.579142
76	C	-4.498686	-1.949377	-1.682299
77	O	-3.070142	-2.158985	-1.767036
78	P	-2.133019	-2.692955	-0.589520
79	O	-2.987920	-3.876125	0.040329
80	O	-1.677012	-1.635655	0.379504
81	H	-2.592540	0.537267	2.164391
82	H	-4.329695	0.262834	2.330401
83	H	-4.932205	-2.599441	-0.919104
84	H	-4.892061	-2.237372	-2.659141
85	H	-4.166255	0.156315	-2.000826
86	H	-6.497907	-0.389075	-2.741947
87	H	-6.937991	-0.738647	-1.046883
88	H	-8.889596	-0.088957	-0.018567
89	H	-10.403915	-0.074381	-0.902429
90	H	-9.549217	1.759991	-2.390131
91	H	-8.655357	0.245489	-2.527223
92	C	-10.102229	1.665319	0.344357
93	C	-10.823193	1.110333	1.579067
94	H	-10.790200	2.309199	-0.220947
95	C	-11.357056	2.207641	2.504647
96	H	-11.652882	0.467273	1.255892
97	H	-10.135431	0.461908	2.138611
98	H	-10.544747	2.846045	2.870603

99	H	-12.073702	2.851712	1.982466
100	H	-9.276300	2.311713	0.666373
101	C	-3.758003	2.371402	2.216522
102	C	-5.159778	2.913842	1.911741
103	H	-5.902158	2.325671	2.469484
104	H	-5.392934	2.768548	0.848219
105	H	-3.003135	2.963962	1.686070
106	C	-5.322917	4.398619	2.258065
107	C	-6.731283	4.926948	1.967796
108	H	-4.587264	4.983218	1.689288
109	H	-6.995598	4.783764	0.914303
110	H	-7.481237	4.401194	2.570367
111	H	-5.081658	4.553795	3.318392
112	H	-3.544968	2.477137	3.286459
113	H	-6.812717	5.995048	2.194625
114	H	-11.865003	1.782512	3.376386
115	O	3.377473	-5.020351	-3.300987
116	H	2.750599	-5.757290	-3.271665
117	H	3.190547	-4.085935	-1.971954
118	Ca	0.534569	-0.670760	0.716734
119	O	-0.305080	1.556197	0.174298
120	H	0.146441	2.082443	-0.498439
121	H	-1.261536	1.587039	-0.058612
122	H	-2.480523	-4.455511	0.647214
123	O	-0.916353	-3.376452	-1.346654
124	H	-0.145013	-2.695977	-1.520485
125	O	3.017982	-3.445906	-1.211801
126	H	1.920086	-4.433491	-0.133839
127	H	1.328981	-2.335152	-3.629298
128	O	2.207590	-2.595570	-3.321911
129	H	3.540060	-1.019301	-3.232802
130	H	2.900026	-4.301467	-3.763182

E[B3LYP/6-31G(d,p)] = -4370.593579 h, E[APFD/6-311+G(2d,p)] = -4369.018958 h
Gcorr[B3LYP/6-31G(d,p)] = 0.969965 h

110. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 6th step, reactants

Center No.	Atom	X	Y	Z
1	C	-8.266210	-0.943870	1.991238
2	C	-7.237314	-0.639083	0.922498
3	O	-7.425946	-0.752545	-0.272730
4	O	-6.074807	-0.200683	1.465898
5	C	-4.974323	0.089617	0.570259
6	C	-3.975415	-1.058576	0.660429
7	O	-4.605093	-2.315286	0.350077
8	C	-4.676873	-2.829510	-0.906174
9	O	-5.365419	-3.819384	-1.060149
10	C	-3.855585	-2.214803	-2.023433
11	C	-2.386649	-2.705234	-2.021816
12	C	-4.399094	1.424799	1.063760
13	O	-3.198352	1.816696	0.394074
14	P	-3.161282	2.764313	-1.090634
15	O	-3.900261	1.511318	-1.838998
16	O	-1.599236	2.879187	-0.948782
17	O	0.708396	3.459297	1.493482
18	C	0.809744	4.826709	1.868598
19	C	0.580473	5.776731	0.672683
20	C	1.680308	5.606251	-0.366924
21	O	2.798442	6.207164	0.003390
22	O	1.533299	4.940599	-1.379556
23	N	-0.741170	5.504949	0.039255
24	H	-8.931578	-0.072415	2.042790
25	H	-7.767675	-1.022913	2.961101
26	H	-0.780456	4.582192	-0.435937
27	H	1.431765	3.174957	0.906170
28	H	-0.970498	6.216745	-0.658351
29	H	3.499768	6.030340	-0.650869
30	H	0.581470	6.804225	1.042087
31	H	0.035000	5.003698	2.615718
32	H	1.784238	5.050667	2.310713

33	H	-5.165900	2.196776	0.965275
34	H	-4.150703	1.329233	2.126674
35	H	-5.359234	0.182381	-0.443777
36	H	-3.119910	-0.862403	0.014827
37	H	-3.620890	-1.169009	1.688713
38	H	-1.895764	-2.418418	-1.082826
39	H	-1.862905	-2.164445	-2.819171
40	H	-4.339128	-2.523211	-2.953522
41	H	-3.881460	-1.122709	-1.984819
42	C	-2.225464	-4.214663	-2.239243
43	C	-0.757794	-4.658706	-2.266107
44	H	-2.709591	-4.496674	-3.184465
45	C	-0.590262	-6.165603	-2.482940
46	H	-0.228961	-4.112911	-3.059123
47	H	-0.275460	-4.368910	-1.322560
48	H	-1.079960	-6.736597	-1.685914
49	H	-1.033287	-6.479881	-3.434785
50	H	-2.755400	-4.764123	-1.450573
51	C	-9.081133	-2.206359	1.671614
52	C	-8.253367	-3.496734	1.725845
53	H	-7.818311	-3.605382	2.729725
54	H	-7.406907	-3.422087	1.030446
55	H	-9.526166	-2.092916	0.676402
56	C	-9.065039	-4.752953	1.387432
57	C	-8.224183	-6.032973	1.419797
58	H	-9.512695	-4.634966	0.391273
59	H	-7.393359	-5.974932	0.707381
60	H	-7.795018	-6.199462	2.414554
61	H	-9.904747	-4.845333	2.089642
62	H	-9.911942	-2.270264	2.384274
63	H	-8.823065	-6.913259	1.164208
64	H	0.466395	-6.451854	-2.496685
65	C	3.671188	0.681343	1.858310
66	C	3.223801	-0.307015	0.809000
67	O	2.349068	-1.146646	0.978675
68	O	3.905568	-0.176020	-0.341652
69	C	3.632015	-1.085629	-1.436848
70	C	4.912507	-1.860782	-1.723493
71	O	5.208191	-2.611640	-0.535121
72	C	6.329158	-3.376626	-0.416678
73	O	6.468051	-3.997729	0.617404
74	C	7.350112	-3.384417	-1.536190
75	C	8.415677	-2.270191	-1.381403
76	C	3.196972	-0.264977	-2.643928
77	O	1.836612	0.201710	-2.498525
78	P	1.395617	1.609249	-1.893622
79	O	2.535770	2.594259	-2.412453
80	O	1.210746	1.631779	-0.393549
81	H	2.802940	1.307984	2.087910
82	H	4.450629	1.324688	1.444011
83	H	3.868090	0.580761	-2.806798
84	H	3.190852	-0.894103	-3.535832
85	H	2.837627	-1.771098	-1.137340
86	H	4.744791	-2.533418	-2.569836
87	H	5.729265	-1.173932	-1.961673
88	H	7.930992	-1.285702	-1.376103
89	H	9.041214	-2.296983	-2.281235
90	H	7.839696	-4.360673	-1.493646
91	H	6.868155	-3.298683	-2.512995
92	C	9.302862	-2.410443	-0.138996
93	C	10.374064	-1.316390	-0.049466
94	H	9.788354	-3.396123	-0.151561
95	C	11.264874	-1.449276	1.189322
96	H	10.996808	-1.344205	-0.953773
97	H	9.886404	-0.332140	-0.045812
98	H	10.673193	-1.389917	2.110081
99	H	11.791768	-2.410214	1.196652
100	H	8.684089	-2.387272	0.766633
101	C	4.153925	-0.018821	3.144249
102	C	5.435032	-0.840210	2.958494
103	H	6.233591	-0.184665	2.583433
104	H	5.279071	-1.605453	2.186325

105	H	3.350856	-0.663022	3.521546
106	C	5.901761	-1.522994	4.249996
107	C	7.182581	-2.342092	4.063439
108	H	5.100320	-2.176055	4.621115
109	H	7.046097	-3.113945	3.298230
110	H	8.015654	-1.704293	3.745173
111	H	6.059272	-0.762299	5.026608
112	H	4.317398	0.754227	3.903934
113	H	7.480263	-2.836897	4.993776
114	H	12.018467	-0.655906	1.226089
115	O	-2.719673	5.088090	1.827958
116	H	-3.163174	5.863225	2.200816
117	H	-4.336054	4.559848	-0.980727
118	Ca	-0.841699	1.539987	0.993767
119	O	0.154529	-0.230763	2.319040
120	H	0.282875	-0.150890	3.272956
121	H	0.962208	-0.665591	1.961749
122	H	2.392472	3.521565	-2.120179
123	O	0.054006	1.896778	-2.670563
124	H	-0.653053	2.307670	-2.066624
125	O	-4.106974	3.882484	-0.322470
126	H	-1.520787	5.484360	0.765620
127	H	-2.438311	4.096432	-2.741087
128	O	-3.280046	3.662448	-2.550315
129	H	-4.028728	1.762172	-2.769102
130	H	-3.378906	4.658588	1.245792

E[B3LYP/6-31G(d,p)] = -4370.601292 h, E[APFD/6-311+G(2d,p)] = -4369.021566 h
Gcorr[B3LYP/6-31G(d,p)] = 0.969953 h

111. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 6th step, TS

Center No.	Atom	X	Y	Z
1	C	-9.267078	-0.300382	0.306410
2	C	-7.910915	-0.300626	-0.367050
3	O	-7.662846	-0.838788	-1.428132
4	O	-7.000647	0.400312	0.354781
5	C	-5.642481	0.454983	-0.142883
6	C	-4.794688	-0.536218	0.648353
7	O	-5.350325	-1.862950	0.595587
8	C	-5.088716	-2.744277	-0.406021
9	O	-5.698538	-3.795501	-0.389650
10	C	-4.032280	-2.426195	-1.448004
11	C	-2.595367	-2.781476	-0.995263
12	C	-5.197841	1.907794	0.065820
13	O	-3.769288	2.070715	-0.009964
14	P	-2.917426	2.514325	-1.603075
15	O	-3.682248	1.202504	-2.206137
16	O	-1.556060	2.335685	-0.870007
17	O	0.475378	2.446129	2.290911
18	C	0.191411	3.542327	3.161150
19	C	0.039009	4.880459	2.404223
20	C	1.379218	5.257882	1.779084
21	O	2.189191	5.876988	2.626532
22	O	1.675250	4.956560	0.632147
23	N	-1.014618	4.796521	1.378716
24	H	-9.852377	0.495843	-0.171651
25	H	-9.148141	-0.020255	1.356634
26	H	-0.646514	4.344709	0.540741
27	H	1.321053	2.566731	1.828158
28	H	-1.294276	5.734152	1.092409
29	H	3.049646	6.032232	2.194568
30	H	-0.235548	5.639137	3.140264
31	H	-0.754920	3.307361	3.649904
32	H	0.968391	3.641830	3.925169
33	H	-5.697624	2.560097	-0.653948
34	H	-5.502319	2.215644	1.071910
35	H	-5.648522	0.195259	-1.199022
36	H	-3.766826	-0.513384	0.290576
37	H	-4.800433	-0.276052	1.709771
38	H	-2.295346	-2.143624	-0.154285

39	H	-1.927925	-2.523576	-1.826823
40	H	-4.292696	-3.029019	-2.321456
41	H	-4.068035	-1.376375	-1.748259
42	C	-2.387497	-4.252259	-0.614969
43	C	-0.921792	-4.579764	-0.302131
44	H	-2.738313	-4.894119	-1.434766
45	C	-0.711686	-6.029994	0.143136
46	H	-0.311819	-4.378863	-1.193520
47	H	-0.555606	-3.896235	0.475359
48	H	-1.279353	-6.250211	1.054453
49	H	-1.042051	-6.733398	-0.629711
50	H	-3.009325	-4.502984	0.254382
51	C	-9.993892	-1.645451	0.159193
52	C	-9.330142	-2.788606	0.937905
53	H	-9.292780	-2.525305	2.004730
54	H	-8.287590	-2.902496	0.612416
55	H	-10.043575	-1.901729	-0.905324
56	C	-10.052137	-4.131529	0.773332
57	C	-9.373269	-5.272866	1.536833
58	H	-10.101996	-4.385118	-0.294308
59	H	-8.340803	-5.413432	1.197195
60	H	-9.341646	-5.065576	2.612690
61	H	-11.092546	-4.029988	1.110962
62	H	-11.027439	-1.517670	0.502176
63	H	-9.903260	-6.220600	1.396064
64	H	0.343637	-6.235045	0.350475
65	C	3.806668	-0.094248	1.874238
66	C	3.583652	-0.552064	0.453184
67	O	2.801523	-1.434994	0.125084
68	O	4.354247	0.112335	-0.425058
69	C	4.294393	-0.237747	-1.830613
70	C	5.665449	-0.764706	-2.238331
71	O	5.903437	-1.939607	-1.447476
72	C	7.055493	-2.660411	-1.541383
73	O	7.145537	-3.651405	-0.845587
74	C	8.164687	-2.183126	-2.456769
75	C	9.141392	-1.205973	-1.755654
76	C	3.926335	1.013113	-2.618159
77	O	2.515657	1.310202	-2.512088
78	P	1.844648	2.259119	-1.419649
79	O	2.914738	3.423443	-1.251364
80	O	1.472060	1.578184	-0.123388
81	H	2.854823	0.319994	2.223636
82	H	4.546699	0.709087	1.885017
83	H	4.514850	1.871334	-2.287147
84	H	4.103363	0.846672	-3.682181
85	H	3.538713	-1.012367	-1.970610
86	H	5.650189	-1.014204	-3.303241
87	H	6.436543	-0.011637	-2.052782
88	H	8.599230	-0.316554	-1.410668
89	H	9.846811	-0.855579	-2.518133
90	H	8.709576	-3.079303	-2.764304
91	H	7.761719	-1.715587	-3.358482
92	C	9.918295	-1.819038	-0.584834
93	C	10.907494	-0.834089	0.050566
94	H	10.462347	-2.706100	-0.937742
95	C	11.688465	-1.439754	1.220595
96	H	11.610344	-0.481101	-0.716079
97	H	10.361667	0.054509	0.395552
98	H	11.012942	-1.770880	2.017721
99	H	12.271424	-2.310222	0.898851
100	H	9.219171	-2.175847	0.181758
101	C	4.232532	-1.253783	2.796507
102	C	5.607285	-1.841321	2.456503
103	H	6.362533	-1.044121	2.503823
104	H	5.611185	-2.205563	1.420478
105	H	3.470043	-2.040534	2.754082
106	C	6.018535	-2.987110	3.389306
107	C	7.394167	-3.569370	3.049945
108	H	5.261845	-3.781680	3.338200
109	H	7.418833	-3.943556	2.020698
110	H	8.178435	-2.809072	3.144541

111	H	6.014994	-2.629218	4.427808
112	H	4.235740	-0.877235	3.825907
113	H	7.653403	-4.398104	3.717010
114	H	12.384606	-0.714359	1.654031
115	O	-3.098989	3.416674	1.890762
116	H	-3.821221	4.000521	2.168095
117	H	-3.538888	4.446605	-2.270678
118	Ca	-0.625958	0.775498	0.760473
119	O	0.383636	-1.332901	1.377731
120	H	0.347854	-1.735971	2.254170
121	H	1.272590	-1.534039	1.005902
122	H	2.664129	4.066809	-0.551068
123	O	0.579797	2.821545	-2.176756
124	H	-0.289028	2.678553	-1.647638
125	O	-3.756431	3.904584	-1.494499
126	H	-2.217300	4.032532	1.703420
127	H	-1.476132	2.607734	-3.341063
128	O	-2.340276	2.986551	-3.127146
129	H	-3.548221	1.197872	-3.167553
130	H	-3.402366	2.810225	0.965553

E[B3LYP/6-31G(d,p)] = -4370.584438 h, E[APFD/6-311+G(2d,p)] = -4369.005671 h
Gcorr[B3LYP/6-31G(d,p)] = 0.969286 h

112. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 6th step, products

Center No.	Atom	X	Y	Z
1	C	6.869017	-2.436258	-3.523009
2	C	6.361735	-1.389087	-2.554552
3	O	7.053115	-0.548968	-2.014303
4	O	5.019097	-1.488324	-2.376008
5	C	4.397366	-0.589729	-1.431603
6	C	4.100534	-1.373449	-0.156925
7	O	5.301424	-1.950783	0.384235
8	C	6.082287	-1.340193	1.314346
9	O	7.150445	-1.860269	1.568930
10	C	5.569246	-0.111772	2.040452
11	C	4.606455	-0.464936	3.200608
12	C	3.121317	-0.060691	-2.094674
13	O	2.506986	0.940125	-1.286953
14	P	2.033854	3.940249	1.664975
15	O	3.106480	2.822813	2.006453
16	O	0.798575	3.276802	1.116456
17	O	-0.544611	1.705998	-2.219977
18	C	-0.155268	2.324510	-3.450770
19	C	-0.282098	3.851363	-3.406119
20	C	-1.729819	4.279290	-3.164652
21	O	-2.028281	5.455481	-3.695339
22	O	-2.519868	3.622343	-2.488231
23	N	0.584637	4.430250	-2.361177
24	H	6.936517	-1.948508	-4.504113
25	H	6.125672	-3.232884	-3.614695
26	H	0.199934	4.246290	-1.436247
27	H	-1.455052	1.994449	-2.023537
28	H	0.628354	5.442260	-2.463329
29	H	-2.939129	5.699741	-3.445670
30	H	0.042800	4.248181	-4.371090
31	H	0.889389	2.060000	-3.618774
32	H	-0.753392	1.927590	-4.278123
33	H	3.376827	0.340596	-3.080738
34	H	2.403503	-0.875479	-2.235845
35	H	5.083179	0.235883	-1.226218
36	H	3.587727	-0.736059	0.563793
37	H	3.456582	-2.225848	-0.388505
38	H	3.729720	-0.997974	2.810969
39	H	4.231844	0.479398	3.612503
40	H	6.452523	0.392431	2.439303
41	H	5.080146	0.581648	1.350983
42	C	5.249593	-1.291412	4.320736
43	C	4.278326	-1.594322	5.468335
44	H	6.121228	-0.749922	4.713586

45	C	4.915475	-2.416259	6.592722
46	H	3.894749	-0.649520	5.876602
47	H	3.406158	-2.131345	5.071355
48	H	5.277991	-3.381187	6.220496
49	H	5.769882	-1.889449	7.032605
50	H	5.635561	-2.235171	3.914303
51	C	8.242999	-2.989268	-3.116052
52	C	8.209429	-3.819163	-1.826235
53	H	7.522073	-4.666839	-1.959532
54	H	7.796205	-3.214227	-1.008314
55	H	8.937639	-2.149664	-2.998460
56	C	9.587648	-4.345711	-1.408248
57	C	9.548058	-5.157521	-0.109821
58	H	10.275765	-3.497907	-1.288373
59	H	9.159926	-4.554541	0.719001
60	H	8.899313	-6.035115	-0.211538
61	H	10.003005	-4.963019	-2.216418
62	H	8.625479	-3.603094	-3.940085
63	H	10.544952	-5.511588	0.172540
64	H	4.198672	-2.617018	7.395533
65	C	-3.264870	-0.958140	-1.360464
66	C	-3.419050	-0.775931	0.130818
67	O	-2.690970	-1.279884	0.975037
68	O	-4.459452	0.019831	0.435904
69	C	-4.783735	0.264730	1.826733
70	C	-6.119171	-0.415238	2.112165
71	O	-5.914561	-1.817395	1.877568
72	C	-6.936672	-2.716863	1.884331
73	O	-6.648952	-3.881747	1.697346
74	C	-8.358920	-2.231255	2.076361
75	C	-9.052068	-1.872375	0.737609
76	C	-4.868684	1.771239	2.035547
77	O	-3.558360	2.375355	2.137318
78	P	-2.674589	2.868773	0.904861
79	O	-3.734638	3.568540	-0.047852
80	O	-1.841595	1.809987	0.235192
81	H	-2.393017	-0.363267	-1.656623
82	H	-4.135032	-0.531052	-1.864763
83	H	-5.434556	2.245842	1.230887
84	H	-5.352178	1.986998	2.989761
85	H	-4.001782	-0.164954	2.455107
86	H	-6.403734	-0.240420	3.154117
87	H	-6.894621	-0.018142	1.451866
88	H	-8.496503	-1.073973	0.229409
89	H	-10.032789	-1.450480	0.986406
90	H	-8.898576	-3.053899	2.552509
91	H	-8.397772	-1.374642	2.753695
92	C	-9.233354	-3.057336	-0.218268
93	C	-9.955231	-2.669130	-1.514628
94	H	-9.799631	-3.848974	0.291726
95	C	-10.139972	-3.848801	-2.473819
96	H	-10.935544	-2.238939	-1.269124
97	H	-9.390719	-1.872762	-2.018299
98	H	-9.173859	-4.278576	-2.762591
99	H	-10.731215	-4.646809	-2.010494
100	H	-8.256369	-3.492111	-0.463441
101	C	-3.058630	-2.430251	-1.756876
102	C	-4.287936	-3.310411	-1.499966
103	H	-5.142053	-2.906963	-2.062081
104	H	-4.567854	-3.258685	-0.439104
105	H	-2.193891	-2.830095	-1.214552
106	C	-4.073421	-4.778431	-1.887251
107	C	-5.312716	-5.645735	-1.645563
108	H	-3.226389	-5.181391	-1.315729
109	H	-5.620603	-5.607736	-0.594799
110	H	-6.159635	-5.300227	-2.249953
111	H	-3.783076	-4.837006	-2.945011
112	H	-2.799677	-2.459643	-2.821578
113	H	-5.125446	-6.693034	-1.904289
114	H	-10.654910	-3.541692	-3.389907
115	O	3.158768	3.377080	-1.950202
116	H	3.470414	3.893194	-1.191945

117	H	2.382505	5.755410	0.483892
118	Ca	0.431322	1.070017	-0.037931
119	O	0.012658	-1.264644	0.535351
120	H	0.345517	-1.976264	-0.027026
121	H	-0.939555	-1.455330	0.692653
122	H	-3.416290	3.680768	-0.973936
123	O	-1.783452	3.996931	1.575296
124	H	-0.817667	3.813980	1.452103
125	O	2.820787	4.908475	0.672721
126	H	2.280204	3.783842	-2.179848
127	H	1.178014	4.500394	3.595577
128	O	1.773408	4.873794	2.924634
129	H	3.945711	3.154839	2.367004
130	H	2.855718	1.851160	-1.532466

E[B3LYP/6-31G(d,p)] = -4370.617326 h, E[APFD/6-311+G(2d,p)] = -4369.028324 h
Gcorr[B3LYP/6-31G(d,p)] = 0.968707 h

113. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 7th step, reactants (extra approaching water added)

Center No.	Atom	X	Y	Z
1	C	4.728987	-4.806569	2.443092
2	C	3.958337	-4.324657	1.233105
3	O	4.152372	-4.689275	0.091027
4	O	2.989595	-3.438136	1.584774
5	C	2.201776	-2.849649	0.528926
6	C	2.707477	-1.428657	0.288758
7	O	4.111695	-1.430695	-0.020657
8	C	4.608874	-1.593193	-1.277013
9	O	5.810545	-1.740279	-1.380351
10	C	3.685810	-1.501450	-2.475562
11	C	3.515627	-0.043528	-2.972634
12	C	0.748970	-2.890523	1.010253
13	O	-0.142092	-2.348883	0.026994
14	P	-2.527306	-4.005273	-2.124396
15	O	-0.922293	-3.999164	-2.150045
16	O	-2.980958	-2.883662	-1.234387
17	O	-4.384035	-1.323516	1.878439
18	C	-5.749946	-1.374690	1.432772
19	C	-6.657271	-0.548441	2.343748
20	C	-6.592190	-1.073275	3.781471
21	O	-7.607455	-0.624360	4.523899
22	O	-5.699722	-1.781912	4.221199
23	N	-6.290000	0.880630	2.282503
24	H	4.263969	-5.751925	2.751896
25	H	4.585736	-4.100072	3.265294
26	H	-5.305161	0.986848	2.523254
27	H	-4.390788	-1.689849	2.783848
28	H	-6.823564	1.410666	2.969693
29	H	-7.483662	-0.934345	5.439542
30	H	-7.689309	-0.647347	1.993231
31	H	-5.766216	-0.963717	0.423121
32	H	-6.100311	-2.411459	1.401485
33	H	0.481403	-3.923782	1.255135
34	H	0.630316	-2.281128	1.909728
35	H	2.319154	-3.455977	-0.373516
36	H	2.114522	-0.935944	-0.483108
37	H	2.626159	-0.847616	1.210501
38	H	3.135056	0.590508	-2.161859
39	H	2.739949	-0.054303	-3.747670
40	H	4.149547	-2.101900	-3.262236
41	H	2.707109	-1.938570	-2.266622
42	C	4.798565	0.571281	-3.546584
43	C	4.591125	1.991223	-4.088363
44	H	5.177244	-0.074706	-4.351256
45	C	5.869934	2.600615	-4.671392
46	H	3.810347	1.972241	-4.861230
47	H	4.211051	2.631261	-3.282430
48	H	6.659463	2.662915	-3.913638
49	H	6.255672	1.996533	-5.500721
50	H	5.580277	0.586310	-2.776663

51	C	6.218270	-5.027460	2.140102
52	C	6.984919	-3.728382	1.860059
53	H	6.901089	-3.064270	2.732239
54	H	6.517494	-3.195445	1.021535
55	H	6.305078	-5.702153	1.280698
56	C	8.466860	-3.957600	1.539173
57	C	9.221021	-2.658203	1.240370
58	H	8.548275	-4.633778	0.677299
59	H	8.777013	-2.133639	0.386655
60	H	9.190815	-1.976795	2.098374
61	H	8.946329	-4.477084	2.380012
62	H	6.669785	-5.544871	2.994801
63	H	10.272941	-2.849961	1.004589
64	H	5.693314	3.612413	-5.051004
65	C	-0.726969	1.919000	3.573408
66	C	-1.153783	1.720916	2.144557
67	O	-1.468124	0.634977	1.667742
68	O	-1.122940	2.849873	1.426707
69	C	-1.431910	2.780890	0.010233
70	C	-0.512090	3.754803	-0.698577
71	O	0.811066	3.195755	-0.625433
72	C	1.905150	3.842386	-1.109462
73	O	2.970212	3.260829	-1.033145
74	C	1.758361	5.243056	-1.666200
75	C	1.898141	6.336684	-0.577424
76	C	-2.917131	3.112301	-0.170100
77	O	-3.335274	2.770359	-1.508565
78	P	-3.958714	1.316458	-1.813815
79	O	-5.505350	1.504491	-2.057543
80	O	-3.631841	0.313196	-0.738591
81	H	-1.415014	1.341804	4.197576
82	H	-0.817497	2.975850	3.834636
83	H	-3.500787	2.566304	0.572682
84	H	-3.108024	4.180501	-0.052237
85	H	-1.239911	1.768063	-0.343360
86	H	-0.834760	3.847703	-1.739725
87	H	-0.551771	4.734422	-0.215046
88	H	1.129320	6.199492	0.193427
89	H	1.680078	7.297541	-1.057782
90	H	2.555312	5.363293	-2.404270
91	H	0.804790	5.361468	-2.186740
92	C	3.280039	6.397796	0.083548
93	C	3.390334	7.520433	1.122814
94	H	4.045012	6.541900	-0.691939
95	C	4.768093	7.588093	1.788298
96	H	3.167362	8.482418	0.641997
97	H	2.619012	7.378352	1.891857
98	H	5.002910	6.651632	2.307198
99	H	5.557112	7.762465	1.047965
100	H	3.508577	5.437196	0.561989
101	C	0.721494	1.426963	3.808977
102	C	1.788621	2.253808	3.082175
103	H	1.696067	3.306368	3.383931
104	H	1.609990	2.232172	1.999096
105	H	0.791106	0.373412	3.511584
106	C	3.216310	1.769598	3.363991
107	C	4.279718	2.585904	2.623032
108	H	3.303215	0.712121	3.079088
109	H	4.117836	2.552731	1.539942
110	H	4.253057	3.638156	2.929487
111	H	3.406229	1.808327	4.445000
112	H	0.902333	1.458749	4.889264
113	H	5.286731	2.206751	2.825100
114	H	4.816619	8.397546	2.523888
115	O	-6.904649	2.062580	-0.094453
116	H	-6.897261	3.015351	0.073517
117	H	-3.749231	-5.779513	-1.804802
118	Ca	-2.363423	-1.277207	0.481043
119	O	-4.172621	-1.525165	-3.429809
120	H	-6.643426	1.619851	0.776786
121	H	-4.083458	-1.697641	-2.471981
122	H	-5.147965	-1.343823	-3.582779

123	O	-3.333339	1.001455	-3.234785
124	H	-3.534617	0.055704	-3.490902
125	O	-2.839647	-5.487123	-1.631993
126	H	-6.086755	1.740316	-1.195252
127	H	-3.521891	-3.018340	-3.766585
128	O	-3.085526	-3.908900	-3.596724
129	H	-0.500602	-4.737849	-2.618929
130	H	-0.189307	-2.953411	-0.736759
131	O	-6.660535	-0.658241	-3.604567
132	H	-6.481170	0.177501	-3.132684
133	H	-6.892330	-0.392461	-4.505600

E[B3LYP/6-31G(d,p)] = -4447.06889 h, E[APFD/6-311+G(2d,p)] = -4445.44849 h
Gcorr[B3LYP/6-31G(d,p)] = 0.984351 h

114. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 7th step, TS

Center No.	Atom	X	Y	Z
1	C	5.548775	-4.607883	2.179239
2	C	4.724044	-4.197521	0.978440
3	O	5.025421	-4.404904	-0.179677
4	O	3.574515	-3.578941	1.356636
5	C	2.701315	-3.089885	0.317718
6	C	2.896038	-1.580536	0.189375
7	O	4.271321	-1.244869	-0.061279
8	C	4.818227	-1.193378	-1.306759
9	O	6.019431	-1.027255	-1.376053
10	C	3.924663	-1.269492	-2.529459
11	C	3.317841	0.102065	-2.914646
12	C	1.278976	-3.446913	0.757964
13	O	0.313275	-2.984211	-0.195276
14	P	-2.282575	-4.481477	-2.199150
15	O	-0.704955	-4.758890	-2.174731
16	O	-2.541009	-3.143137	-1.583099
17	O	-3.657842	-1.647983	1.888079
18	C	-5.049304	-1.871474	1.602690
19	C	-5.946679	-1.262647	2.682026
20	C	-5.637022	-1.887146	4.045701
21	O	-6.644701	-1.741697	4.908610
22	O	-4.573515	-2.414639	4.336433
23	N	-5.794586	0.206161	2.734302
24	H	5.303337	-5.658530	2.381839
25	H	5.224913	-4.033073	3.051228
26	H	-4.825329	0.439907	2.945988
27	H	-3.514357	-2.032165	2.776237
28	H	-6.360713	0.588221	3.490432
29	H	-6.366841	-2.095600	5.773283
30	H	-6.988304	-1.483955	2.431734
31	H	-5.256293	-1.399481	0.642241
32	H	-5.254367	-2.944445	1.519908
33	H	1.199744	-4.528772	0.900291
34	H	1.049365	-2.957733	1.708559
35	H	2.951585	-3.594659	-0.618803
36	H	2.228014	-1.176541	-0.572057
37	H	2.663922	-1.099670	1.142586
38	H	2.702515	0.485013	-2.090556
39	H	2.633461	-0.071764	-3.753472
40	H	4.560144	-1.626830	-3.343309
41	H	3.124772	-2.001482	-2.394410
42	C	4.354320	1.159220	-3.313714
43	C	3.714797	2.483628	-3.748653
44	H	4.972864	0.765554	-4.132321
45	C	4.746597	3.540091	-4.155837
46	H	3.033506	2.295344	-4.589823
47	H	3.094401	2.876840	-2.933153
48	H	5.424510	3.770801	-3.326045
49	H	5.359272	3.194526	-4.996440
50	H	5.039891	1.344297	-2.476830
51	C	7.057044	-4.458557	1.931937
52	C	7.511531	-2.999813	1.794815
53	H	7.251843	-2.452515	2.712290

54	H	6.957081	-2.515184	0.980274
55	H	7.320769	-5.015935	1.025825
56	C	9.014705	-2.856233	1.527901
57	C	9.456413	-1.397974	1.370638
58	H	9.274328	-3.416771	0.619598
59	H	8.927093	-0.914461	0.541662
60	H	9.245780	-0.820638	2.278217
61	H	9.577061	-3.325611	2.346540
62	H	7.590724	-4.934931	2.762786
63	H	10.530304	-1.323385	1.170478
64	H	4.262224	4.474245	-4.458411
65	C	-0.169949	1.534746	3.360222
66	C	-0.833791	1.324127	2.024218
67	O	-0.915124	0.227900	1.475259
68	O	-1.280512	2.454925	1.478070
69	C	-1.831871	2.417388	0.127559
70	C	-1.477130	3.737026	-0.523319
71	O	-0.052089	3.732801	-0.747338
72	C	0.606692	4.803690	-1.258240
73	O	1.803676	4.689549	-1.443658
74	C	-0.148877	6.089166	-1.528490
75	C	-0.174076	7.033524	-0.300557
76	C	-3.348160	2.188713	0.218933
77	O	-3.928341	2.043769	-1.064160
78	P	-3.942655	0.518395	-1.854690
79	O	-5.558451	0.339964	-1.421582
80	O	-2.855546	-0.169467	-1.031024
81	H	-0.527937	0.747015	4.029501
82	H	-0.468369	2.503713	3.767147
83	H	-3.520994	1.316066	0.854736
84	H	-3.820283	3.056523	0.694389
85	H	-1.377275	1.589845	-0.414541
86	H	-2.014163	3.806745	-1.472996
87	H	-1.764153	4.571010	0.123053
88	H	-0.657960	6.531956	0.547036
89	H	-0.817054	7.882635	-0.560146
90	H	0.373574	6.581855	-2.352511
91	H	-1.170600	5.885710	-1.857784
92	C	1.204585	7.549452	0.128067
93	C	1.134494	8.509083	1.322403
94	H	1.678961	8.059243	-0.721994
95	C	2.508312	9.031995	1.752493
96	H	0.482498	9.355981	1.069243
97	H	0.655591	7.998548	2.168914
98	H	3.171073	8.209188	2.043997
99	H	2.997258	9.576950	0.936980
100	H	1.858070	6.704546	0.378807
101	C	1.370017	1.449279	3.236413
102	C	1.993592	2.593964	2.428758
103	H	1.769255	3.546768	2.928345
104	H	1.526088	2.656333	1.437439
105	H	1.631739	0.482529	2.789034
106	C	3.511163	2.455797	2.254383
107	C	4.127159	3.630716	1.487974
108	H	3.731079	1.518200	1.725726
109	H	3.660375	3.747578	0.503595
110	H	3.987183	4.571921	2.032364
111	H	3.986195	2.368444	3.240851
112	H	1.783884	1.444188	4.250972
113	H	5.202695	3.490661	1.338244
114	H	2.427108	9.712667	2.606181
115	O	-6.626431	1.516625	0.467733
116	H	-6.429138	2.458457	0.562293
117	H	-3.839899	-5.827882	-1.475925
118	Ca	-1.768660	-1.709815	0.288749
119	O	-4.185099	-0.961268	-2.900707
120	H	-6.321067	1.066352	1.316487
121	H	-3.592275	-1.641290	-2.534497
122	H	-5.632466	-1.507569	-2.958485
123	O	-3.707093	1.333257	-3.246962
124	H	-3.727307	0.669400	-3.955789
125	O	-2.871210	-5.758873	-1.460570

126	H	-5.957994	0.938871	-0.642513
127	H	-2.709672	-3.860034	-4.245656
128	O	-2.820934	-4.647808	-3.688526
129	H	-0.412142	-5.608162	-2.544539
130	H	0.248720	-3.616071	-0.932986
131	O	-6.587995	-1.473147	-2.576543
132	H	-6.238276	-0.526579	-1.931801
133	H	-7.196774	-1.212442	-3.285290

E[B3LYP/6-31G(d,p)] = -4446.999412 h, E[APFD/6-311+G(2d,p)] = -4445.384456 h
Gcorr[B3LYP/6-31G(d,p)] = 0.984449 h

115. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 7th step, products

Center No.	Atom	X	Y	Z
1	C	4.458206	-5.227332	2.095311
2	C	3.835568	-4.594940	0.869319
3	O	4.183793	-4.801525	-0.275723
4	O	2.807910	-3.772331	1.205974
5	C	2.126274	-3.071932	0.144091
6	C	2.618327	-1.625708	0.124469
7	O	4.049317	-1.567026	0.001490
8	C	4.708756	-1.578644	-1.188737
9	O	5.919612	-1.670811	-1.146921
10	C	3.944055	-1.400105	-2.485344
11	C	3.813186	0.089897	-2.890883
12	C	0.635781	-3.177345	0.477080
13	O	-0.174445	-2.509452	-0.499915
14	P	-2.774988	-3.955591	-2.557318
15	O	-1.187676	-4.176147	-2.573381
16	O	-3.074792	-2.689870	-1.822257
17	O	-4.123765	-1.502740	1.694806
18	C	-5.530580	-1.354066	1.456859
19	C	-6.201412	-0.669800	2.645122
20	C	-6.050629	-1.508572	3.920157
21	O	-6.582508	-0.884722	4.971639
22	O	-5.507306	-2.592851	3.947653
23	N	-5.610573	0.690545	2.875061
24	H	4.024175	-6.231830	2.181516
25	H	4.151075	-4.669945	2.984313
26	H	-4.588373	0.623809	2.905585
27	H	-4.024305	-2.180092	2.385623
28	H	-5.925092	1.077061	3.769663
29	H	-6.444916	-1.423584	5.772096
30	H	-7.266864	-0.528594	2.443798
31	H	-5.652248	-0.760279	0.550988
32	H	-6.004954	-2.325182	1.297444
33	H	0.357066	-4.232546	0.558353
34	H	0.439397	-2.694845	1.438144
35	H	2.347290	-3.569291	-0.803894
36	H	2.112512	-1.059959	-0.659415
37	H	2.402687	-1.151471	1.085015
38	H	3.301108	0.653169	-2.100265
39	H	3.158105	0.127420	-3.769480
40	H	4.516344	-1.933450	-3.248758
41	H	2.954188	-1.859014	-2.441027
42	C	5.148656	0.767301	-3.223473
43	C	4.980799	2.209968	-3.716892
44	H	5.669133	0.177742	-3.991357
45	C	6.315764	2.887740	-4.041513
46	H	4.342821	2.212677	-4.611471
47	H	4.446164	2.792980	-2.956671
48	H	6.962521	2.930832	-3.157580
49	H	6.859344	2.342070	-4.821469
50	H	5.800267	0.757451	-2.340839
51	C	5.987699	-5.324252	1.991094
52	C	6.688668	-3.960302	2.027399
53	H	6.427935	-3.444967	2.962944
54	H	6.310857	-3.328618	1.212548
55	H	6.243623	-5.849359	1.063620
56	C	8.214563	-4.059921	1.913186

57	C	8.904391	-2.692341	1.928962
58	H	8.472750	-4.588944	0.985783
59	H	8.553222	-2.065850	1.101095
60	H	8.695958	-2.154850	2.861203
61	H	8.602209	-4.678021	2.734429
62	H	6.349616	-5.947443	2.817389
63	H	9.991066	-2.789936	1.836901
64	H	6.167734	3.913508	-4.394960
65	C	-0.734207	1.660217	3.480725
66	C	-1.168723	1.526853	2.043858
67	O	-1.436256	0.447692	1.518810
68	O	-1.194731	2.690166	1.396302
69	C	-1.497602	2.698967	-0.032353
70	C	-0.647967	3.785754	-0.652481
71	O	0.718635	3.323091	-0.610683
72	C	1.757858	4.057380	-1.079158
73	O	2.864977	3.554597	-1.022758
74	C	1.510940	5.459294	-1.597567
75	C	1.582357	6.529566	-0.479706
76	C	-3.005040	2.931817	-0.220426
77	O	-3.378278	2.800512	-1.573650
78	P	-3.910048	1.260158	-2.144049
79	O	-5.373455	1.524014	-1.419627
80	O	-2.843230	0.406437	-1.433576
81	H	-1.389016	1.019661	4.078458
82	H	-0.864802	2.695410	3.804941
83	H	-3.537221	2.231203	0.432156
84	H	-3.262587	3.947111	0.109359
85	H	-1.237081	1.732752	-0.457678
86	H	-0.975835	3.927403	-1.685652
87	H	-0.753494	4.724233	-0.100976
88	H	0.823142	6.323082	0.285162
89	H	1.304596	7.488018	-0.933595
90	H	2.293089	5.654220	-2.335663
91	H	0.547542	5.525787	-2.109019
92	C	2.957888	6.658993	0.185001
93	C	2.998691	7.756251	1.255869
94	H	3.712277	6.872486	-0.584931
95	C	4.369573	7.889527	1.925723
96	H	2.717086	8.716104	0.802277
97	H	2.237430	7.545153	2.019071
98	H	4.661679	6.954713	2.417774
99	H	5.146446	8.133477	1.192210
100	H	3.246475	5.701289	0.636053
101	C	0.736081	1.217212	3.671065
102	C	1.757023	2.135687	2.988905
103	H	1.641654	3.155022	3.383190
104	H	1.546220	2.201893	1.913719
105	H	0.845894	0.189392	3.303607
106	C	3.207127	1.677050	3.186096
107	C	4.221228	2.606911	2.512526
108	H	3.323031	0.660342	2.786342
109	H	4.028756	2.686192	1.436852
110	H	4.168398	3.617897	2.933292
111	H	3.424807	1.607964	4.260439
112	H	0.931810	1.184856	4.748894
113	H	5.245810	2.244824	2.646454
114	H	4.368195	8.678864	2.684437
115	O	-6.299077	2.426829	0.984447
116	H	-6.059671	3.337299	1.204703
117	H	-4.270443	-5.427447	-1.960771
118	Ca	-2.281816	-1.276285	0.016640
119	O	-4.627112	-0.190867	-2.975764
120	H	-5.878027	1.391938	2.096370
121	H	-4.034314	-0.925791	-2.751496
122	H	-6.176577	-0.750432	-2.403685
123	O	-3.717822	1.895726	-3.643547
124	H	-4.019180	1.198216	-4.248095
125	O	-3.306051	-5.316221	-1.931599
126	H	-5.905611	2.241782	0.099675
127	H	-3.267477	-3.165756	-4.527758
128	O	-3.324594	-4.009920	-4.051105

129	H	-0.870911	-4.977810	-3.021471
130	H	-0.256027	-3.075289	-1.288555
131	O	-6.914177	-0.680610	-1.747610
132	H	-6.006224	0.768114	-1.538532
133	H	-7.707927	-0.489936	-2.266293

E[B3LYP/6-31G(d,p)] = -4447.012683 h, E[APFD/6-311+G(2d,p)] = -4445.406582 h
Gcorr[B3LYP/6-31G(d,p)] = 0.988120 h

116. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 8th step, reactants

Center No.	Atom	X	Y	Z
1	C	-4.409501	-4.135739	-2.533180
2	C	-3.493450	-3.964838	-1.340747
3	O	-3.611853	-4.548795	-0.282625
4	O	-2.490286	-3.085971	-1.605942
5	C	-1.559398	-2.789025	-0.543024
6	C	-1.918420	-1.430542	0.053570
7	O	-3.290981	-1.408504	0.478563
8	C	-3.697772	-1.724853	1.735340
9	O	-4.895478	-1.777987	1.932542
10	C	-2.675060	-1.939090	2.835569
11	C	-2.169740	-0.622264	3.472782
12	C	-0.170746	-2.796024	-1.187129
13	O	0.850658	-2.464767	-0.237531
14	P	3.527242	-4.093836	1.467831
15	O	1.988377	-4.538675	1.428143
16	O	3.599061	-2.630935	1.167753
17	O	5.192786	-0.208918	-1.308968
18	C	6.137676	0.341063	-0.385821
19	C	6.838911	1.554869	-0.988554
20	C	7.612575	1.182480	-2.256974
21	O	8.032722	2.272984	-2.905004
22	O	7.814428	0.040044	-2.606565
23	N	5.841216	2.631807	-1.292075
24	H	-4.066241	-5.034262	-3.062349
25	H	-4.274795	-3.293862	-3.217708
26	H	5.054683	2.235112	-1.815523
27	H	5.672625	-0.709613	-1.988393
28	H	6.261207	3.364157	-1.871039
29	H	8.507725	2.004862	-3.712430
30	H	7.547350	1.970929	-0.265629
31	H	5.565978	0.632112	0.495559
32	H	6.890927	-0.397526	-0.101879
33	H	0.015386	-3.776210	-1.638127
34	H	-0.118812	-2.037850	-1.971094
35	H	-1.636775	-3.572209	0.215703
36	H	-1.230908	-1.181795	0.861599
37	H	-1.846662	-0.652855	-0.709143
38	H	-1.601222	-0.037526	2.738968
39	H	-1.460240	-0.903343	4.260684
40	H	-3.184867	-2.534280	3.596750
41	H	-1.825049	-2.527003	2.478336
42	C	-3.275422	0.255738	4.071684
43	C	-2.720286	1.463191	4.837347
44	H	-3.896342	-0.348923	4.746878
45	C	-3.816572	2.364374	5.413006
46	H	-2.072313	1.108535	5.650240
47	H	-2.074645	2.050570	4.170207
48	H	-4.457935	2.763429	4.618866
49	H	-4.458157	1.811327	6.108512
50	H	-3.939286	0.609309	3.272874
51	C	-5.880104	-4.299122	-2.121156
52	C	-6.491824	-3.027563	-1.519111
53	H	-6.422714	-2.211531	-2.252862
54	H	-5.903732	-2.708320	-0.648414
55	H	-5.952616	-5.122590	-1.401472
56	C	-7.954844	-3.202128	-1.094090
57	C	-8.553722	-1.932253	-0.481654
58	H	-8.023585	-4.025044	-0.369675
59	H	-7.986878	-1.617146	0.401771

60	H	-8.537177	-1.102242	-1.197332
61	H	-8.553001	-3.510196	-1.962481
62	H	-6.453463	-4.600842	-3.005650
63	H	-9.593413	-2.086464	-0.174783
64	H	-3.390870	3.214048	5.956575
65	C	0.343793	1.436750	-3.752657
66	C	0.763129	1.273975	-2.314177
67	O	1.314192	0.264759	-1.876459
68	O	0.429791	2.317635	-1.556095
69	C	0.683587	2.261750	-0.118307
70	C	-0.393499	3.084194	0.552630
71	O	-1.634612	2.356353	0.437216
72	C	-2.808578	2.852326	0.907194
73	O	-3.791812	2.141579	0.822003
74	C	-2.855935	4.262099	1.462519
75	C	-3.138794	5.322852	0.369383
76	C	2.094647	2.818532	0.126302
77	O	2.534241	2.718966	1.467315
78	P	2.752655	1.100035	2.205388
79	O	3.811305	1.882142	3.187815
80	O	3.191230	0.423989	0.895054
81	H	1.149476	1.036304	-4.374153
82	H	0.222481	2.499595	-3.975425
83	H	2.769974	2.286987	-0.551656
84	H	2.106870	3.882198	-0.140645
85	H	0.619822	1.224510	0.204175
86	H	-0.118434	3.203195	1.602359
87	H	-0.474723	4.063532	0.073218
88	H	-2.354026	5.288738	-0.396859
89	H	-3.057185	6.306680	0.846116
90	H	-3.666832	4.273917	2.195305
91	H	-1.931061	4.512616	1.987235
92	C	-4.512888	5.191878	-0.297878
93	C	-4.772246	6.285362	-1.341646
94	H	-5.294025	5.232061	0.473922
95	C	-6.144085	6.161700	-2.011335
96	H	-4.684856	7.270457	-0.863732
97	H	-3.986056	6.247913	-2.107866
98	H	-6.246999	5.200125	-2.527127
99	H	-6.951927	6.229039	-1.273803
100	H	-4.605257	4.207141	-0.772817
101	C	-0.968873	0.672165	-4.049952
102	C	-2.201192	1.239013	-3.334071
103	H	-2.376205	2.267479	-3.679232
104	H	-2.011257	1.315372	-2.255466
105	H	-0.830864	-0.383554	-3.785945
106	C	-3.465621	0.400387	-3.558175
107	C	-4.689571	0.966331	-2.831143
108	H	-3.279337	-0.625864	-3.213970
109	H	-4.514333	1.023220	-1.751021
110	H	-4.925812	1.977536	-3.182687
111	H	-3.672006	0.330943	-4.634673
112	H	-1.126607	0.700126	-5.133966
113	H	-5.574775	0.342922	-2.995254
114	H	-6.300682	6.954393	-2.750136
115	O	3.924939	-2.466943	-2.620014
116	H	3.517632	-2.485977	-3.496918
117	H	5.172492	-5.106530	0.455854
118	Ca	2.941928	-1.173747	-0.742328
119	O	2.916168	-0.327603	3.197470
120	H	4.257519	-3.362922	-2.470809
121	H	3.221146	-1.038576	2.612024
122	H	4.140863	3.373788	1.299236
123	O	1.166640	1.191103	2.657406
124	H	1.004892	0.386951	3.177423
125	O	4.201609	-5.096666	0.433440
126	H	5.464807	3.087744	-0.380788
127	H	4.082198	-3.864222	3.561623
128	O	4.174187	-4.526480	2.857453
129	H	1.808494	-5.482798	1.570492
130	H	0.988407	-3.216765	0.365326
131	O	5.015099	3.719562	0.974639

132	H	4.112911	1.210198	3.819598
133	H	4.907225	4.677572	0.896141

E[B3LYP/6-31G(d,p)] = -4447.016163 h, E[APFD/6-311+G(2d,p)] = -4445.421387 h
Gcorr[B3LYP/6-31G(d,p)] = 0.990760 h

117. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 8th step, TS

Center No.	Atom	X	Y	Z
1	C	-4.483013	-4.129012	-2.470965
2	C	-3.539833	-3.960403	-1.299602
3	O	-3.640364	-4.537820	-0.236097
4	O	-2.534855	-3.091689	-1.590851
5	C	-1.580694	-2.796140	-0.548559
6	C	-1.914276	-1.429204	0.042903
7	O	-3.275146	-1.391021	0.503164
8	C	-3.651379	-1.693264	1.773069
9	O	-4.843688	-1.736358	2.002037
10	C	-2.600695	-1.903007	2.847453
11	C	-2.068590	-0.581869	3.452884
12	C	-0.203289	-2.823068	-1.216134
13	O	0.837223	-2.507825	-0.282098
14	P	3.514938	-4.130587	1.414474
15	O	1.984939	-4.603182	1.362386
16	O	3.558937	-2.660321	1.144815
17	O	5.154574	-0.202913	-1.309695
18	C	6.103326	0.320004	-0.370503
19	C	6.808875	1.559405	-0.917374
20	C	7.561607	1.228468	-2.209860
21	O	8.237674	2.286799	-2.669002
22	O	7.537289	0.143771	-2.760598
23	N	5.843690	2.668683	-1.132603
24	H	-4.156828	-5.030784	-3.005424
25	H	-4.358586	-3.289636	-3.160503
26	H	5.087402	2.339933	-1.735248
27	H	5.661014	-0.566682	-2.055628
28	H	6.299727	3.435809	-1.628095
29	H	8.667479	2.044049	-3.508988
30	H	7.543556	1.900944	-0.180618
31	H	5.536209	0.575508	0.523811
32	H	6.851654	-0.436792	-0.116708
33	H	-0.038956	-3.805728	-1.670051
34	H	-0.151765	-2.065550	-2.000741
35	H	-1.651887	-3.571973	0.218243
36	H	-1.203810	-1.177797	0.829990
37	H	-1.856906	-0.660728	-0.730158
38	H	-1.530331	-0.004712	2.690576
39	H	-1.329437	-0.857171	4.215358
40	H	-3.093104	-2.484764	3.630115
41	H	-1.765322	-2.501639	2.473845
42	C	-3.148341	0.304373	4.085880
43	C	-2.561519	1.520557	4.813139
44	H	-3.740913	-0.291731	4.793314
45	C	-3.632643	2.429670	5.422662
46	H	-1.880460	1.175320	5.602719
47	H	-1.943914	2.099165	4.112585
48	H	-4.306271	2.819375	4.650960
49	H	-4.244849	1.885763	6.151049
50	H	-3.844134	0.648728	3.310649
51	C	-5.944896	-4.282638	-2.025597
52	C	-6.535272	-3.006143	-1.412697
53	H	-6.479726	-2.192486	-2.150221
54	H	-5.924479	-2.687588	-0.557506
55	H	-6.006027	-5.104045	-1.302504
56	C	-7.988394	-3.172025	-0.951758
57	C	-8.565775	-1.897835	-0.327752
58	H	-8.043722	-3.993050	-0.224058
59	H	-7.976649	-1.584200	0.541517
60	H	-8.561761	-1.069190	-1.045185
61	H	-8.609071	-3.478809	-1.804653
62	H	-6.539894	-4.582811	-2.896203

63	H	-9.598729	-2.045963	0.003869
64	H	-3.184362	3.285590	5.937491
65	C	0.301872	1.389915	-3.781869
66	C	0.743829	1.240753	-2.348878
67	O	1.296995	0.235302	-1.906809
68	O	0.428778	2.297101	-1.598253
69	C	0.707965	2.261681	-0.164856
70	C	-0.347176	3.112362	0.507776
71	O	-1.593089	2.388787	0.431612
72	C	-2.757174	2.898875	0.912371
73	O	-3.742637	2.188223	0.862070
74	C	-2.789964	4.321220	1.435203
75	C	-3.084834	5.358142	0.322594
76	C	2.130960	2.800209	0.025973
77	O	2.618080	2.725532	1.363562
78	P	2.748433	1.038628	2.183401
79	O	3.839732	1.818944	3.116965
80	O	3.134439	0.370186	0.863706
81	H	1.092670	0.972416	-4.411114
82	H	0.189248	2.451293	-4.015836
83	H	2.779352	2.237698	-0.652463
84	H	2.153687	3.855971	-0.268611
85	H	0.634746	1.231423	0.176699
86	H	-0.053606	3.256786	1.549048
87	H	-0.429649	4.079087	0.003780
88	H	-2.311011	5.304454	-0.453562
89	H	-2.993523	6.352002	0.776155
90	H	-3.589159	4.353742	2.180071
91	H	-1.855787	4.579161	1.939591
92	C	-4.468548	5.216847	-0.322352
93	C	-4.739230	6.287636	-1.386572
94	H	-5.238707	5.276690	0.459132
95	C	-6.120414	6.153129	-2.034629
96	H	-4.642724	7.282843	-0.931947
97	H	-3.963703	6.230828	-2.162396
98	H	-6.232831	5.180672	-2.527536
99	H	-6.917943	6.239098	-1.287872
100	H	-4.570490	4.222120	-0.774007
101	C	-1.024290	0.637458	-4.048753
102	C	-2.237892	1.224264	-3.317126
103	H	-2.406731	2.252026	-3.667291
104	H	-2.029318	1.306956	-2.242380
105	H	-0.893489	-0.417443	-3.778008
106	C	-3.515403	0.398644	-3.513951
107	C	-4.719618	0.981866	-2.767912
108	H	-3.334556	-0.627951	-3.167896
109	H	-4.524057	1.042276	-1.691457
110	H	-4.951155	1.993817	-3.120421
111	H	-3.741889	0.326113	-4.586171
112	H	-1.200206	0.657653	-5.130109
113	H	-5.614402	0.367385	-2.912512
114	H	-6.285007	6.929712	-2.788635
115	O	3.866225	-2.522995	-2.667197
116	H	3.400445	-2.630924	-3.507588
117	H	5.179845	-5.097341	0.389519
118	Ca	2.929252	-1.217020	-0.790077
119	O	2.826190	-0.357825	3.176192
120	H	4.299402	-3.371602	-2.501493
121	H	3.114882	-1.094940	2.613196
122	H	3.888824	3.252425	1.239835
123	O	1.184746	1.290129	2.617588
124	H	0.931782	0.520507	3.153094
125	O	4.209158	-5.098527	0.360335
126	H	5.304046	3.202052	0.046578
127	H	4.063223	-3.932683	3.512923
128	O	4.168630	-4.579044	2.795872
129	H	1.824317	-5.554583	1.477183
130	H	0.975774	-3.264115	0.314932
131	O	4.882155	3.637909	1.002598
132	H	4.134878	1.172619	3.777722
133	H	4.846643	4.603879	0.934265

E[B3LYP/6-31G(d,p)] = -4447.010604 h, E[APFD/6-311+G(2d,p)] = -4445.411797 h
Gcorr[B3LYP/6-31G(d,p)] = 0.988233 h

118. 2PS6Ca+4H_2O, ser1:ser2:gly1:gly2, 8th step, products

Center No.	Atom	X	Y	Z
1	C	-5.621865	-0.528381	-3.079344
2	C	-4.490162	-1.422347	-2.620714
3	O	-4.520864	-2.636519	-2.616071
4	O	-3.410970	-0.695917	-2.226021
5	C	-2.275014	-1.412934	-1.696633
6	C	-2.280168	-1.274098	-0.176696
7	O	-3.502501	-1.796679	0.378470
8	C	-3.683885	-3.102489	0.706211
9	O	-4.807765	-3.445327	1.017603
10	C	-2.497321	-4.046929	0.752534
11	C	-1.718033	-3.958634	2.087565
12	C	-1.036485	-0.783607	-2.339420
13	O	0.166294	-1.401298	-1.865399
14	P	2.674517	-4.007642	-1.635557
15	O	1.218443	-4.088830	-2.283025
16	O	2.705837	-2.809758	-0.731056
17	O	4.809378	-0.306550	-1.051079
18	C	5.848933	-0.664020	-0.131624
19	C	6.798640	0.508655	0.105795
20	C	7.500492	0.892037	-1.200753
21	O	8.580075	1.650487	-0.985844
22	O	7.104861	0.583447	-2.313151
23	N	6.060945	1.660172	0.664829
24	H	-5.570165	-0.495420	-4.175275
25	H	-5.446679	0.489239	-2.720515
26	H	5.332054	1.938750	0.008380
27	H	5.243827	-0.135434	-1.906673
28	H	6.684434	2.458694	0.772328
29	H	8.950102	1.913499	-1.848155
30	H	7.561197	0.208743	0.830747
31	H	5.367408	-0.950876	0.802420
32	H	6.409062	-1.525647	-0.509141
33	H	-1.113739	-0.860219	-3.428857
34	H	-0.966123	0.272451	-2.070339
35	H	-2.361882	-2.463071	-1.989124
36	H	-1.398899	-1.756236	0.248530
37	H	-2.274843	-0.218297	0.105513
38	H	-1.307474	-2.949992	2.217446
39	H	-0.855280	-4.630281	2.003065
40	H	-2.910662	-5.051872	0.637938
41	H	-1.814658	-3.877356	-0.084174
42	C	-2.541394	-4.342280	3.323130
43	C	-1.730360	-4.273537	4.623027
44	H	-2.935880	-5.359550	3.192660
45	C	-2.542576	-4.670843	5.859334
46	H	-0.851163	-4.926444	4.536859
47	H	-1.342947	-3.253827	4.753245
48	H	-3.410260	-4.014271	5.990013
49	H	-2.915022	-5.698020	5.774234
50	H	-3.416645	-3.685715	3.408168
51	C	-6.995618	-1.054172	-2.635241
52	C	-7.211338	-0.994886	-1.117519
53	H	-7.106075	0.045286	-0.777551
54	H	-6.423022	-1.565601	-0.609172
55	H	-7.105754	-2.086859	-2.985564
56	C	-8.577538	-1.535441	-0.678423
57	C	-8.773397	-1.499139	0.840401
58	H	-8.688344	-2.568045	-1.036380
59	H	-8.005958	-2.093329	1.349491
60	H	-8.705879	-0.474545	1.223853
61	H	-9.373298	-0.956783	-1.166946
62	H	-7.769052	-0.464461	-3.141342
63	H	-9.751320	-1.898590	1.128513
64	H	-1.938520	-4.609842	6.770394
65	C	1.338035	3.960621	-2.447094

66	C	1.564322	3.171524	-1.181652
67	O	1.753057	1.957898	-1.167306
68	O	1.534973	3.925516	-0.086278
69	C	1.716794	3.321444	1.228933
70	C	0.416320	3.471333	1.994521
71	O	-0.577035	2.660715	1.334254
72	C	-1.869674	2.623219	1.746161
73	O	-2.633238	1.903441	1.129467
74	C	-2.310750	3.484701	2.912335
75	C	-2.794224	4.890971	2.477732
76	C	2.865120	4.084091	1.910178
77	O	3.091411	3.610776	3.220958
78	P	2.535481	-1.204496	2.330124
79	O	3.290878	-0.581245	3.554303
80	O	2.252975	-0.278751	1.181098
81	H	2.245514	3.850360	-3.051832
82	H	1.224829	5.017712	-2.197070
83	H	3.757219	4.006832	1.274804
84	H	2.600794	5.145948	1.974208
85	H	1.965073	2.265469	1.109389
86	H	0.583010	3.126428	3.017647
87	H	0.105821	4.519923	2.006566
88	H	-1.992889	5.414854	1.941640
89	H	-2.973846	5.465473	3.393918
90	H	-3.137363	2.950538	3.387809
91	H	-1.511490	3.582686	3.650554
92	C	-4.066168	4.886279	1.622237
93	C	-4.536693	6.298867	1.253562
94	H	-4.865683	4.366578	2.168256
95	C	-5.814369	6.304821	0.409046
96	H	-4.702391	6.876698	2.172847
97	H	-3.735297	6.816411	0.709083
98	H	-5.668565	5.763875	-0.532954
99	H	-6.642719	5.823674	0.941430
100	H	-3.897844	4.308324	0.705126
101	C	0.122260	3.445836	-3.243311
102	C	-1.216072	3.651811	-2.523386
103	H	-1.342472	4.719137	-2.294595
104	H	-1.202681	3.132895	-1.554668
105	H	0.269739	2.382685	-3.467562
106	C	-2.420635	3.162117	-3.336645
107	C	-3.751371	3.348383	-2.601832
108	H	-2.287829	2.099470	-3.579855
109	H	-3.758888	2.790142	-1.658940
110	H	-3.928978	4.403829	-2.365018
111	H	-2.449556	3.694331	-4.296807
112	H	0.108514	3.969843	-4.205635
113	H	-4.594264	2.998021	-3.206595
114	H	-6.124909	7.325314	0.162349
115	O	3.360641	-0.935525	-3.395566
116	H	2.942421	-0.675305	-4.227952
117	H	4.550842	-4.242093	-2.738001
118	Ca	2.345348	-0.366967	-1.188725
119	O	3.417037	-2.470610	1.905581
120	H	3.687454	-1.837528	-3.539813
121	H	3.203960	-2.758043	0.985758
122	H	3.669014	2.821445	3.168312
123	O	1.145900	-1.754844	2.910983
124	H	1.240922	-2.428502	3.602586
125	O	3.640303	-3.943909	-2.903911
126	H	5.314173	1.440742	2.162341
127	H	2.724673	-5.525630	-0.062856
128	O	3.068134	-5.387268	-0.961397
129	H	1.077617	-4.795600	-2.935603
130	H	0.211420	-2.324388	-2.166148
131	O	4.828098	1.404114	3.055864
132	H	3.934676	0.182206	3.330229
133	H	5.505665	1.504644	3.740354

E[B3LYP/6-31G(d,p)] = -4447.063353 h, E[APFD/6-311+G(2d,p)] = -4445.449973 h
Gcorr[B3LYP/6-31G(d,p)] = 0.985600 h

X. Structures of molecules and transition states (TS) related to 2PS6Ca + 4 H_2O, where the hydrolysis proceeds in the sequence gly1:gly2:ser1:ser2, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

119. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	-9.580922	-1.073698	-0.427161
2	C	-8.409668	-0.577881	0.393502
3	O	-8.452764	0.339834	1.187452
4	O	-7.291290	-1.310924	0.149626
5	C	-6.074289	-0.927368	0.825687
6	C	-5.198127	-0.174254	-0.174135
7	O	-5.909586	0.944172	-0.732034
8	C	-5.866201	2.202489	-0.218353
9	O	-6.622102	3.022798	-0.699982
10	C	-4.851193	2.550444	0.853220
11	C	-3.455779	2.884797	0.271122
12	C	-5.447655	-2.235288	1.317679
13	O	-4.363779	-1.977658	2.229817
14	P	-2.803816	-2.106834	1.812510
15	O	-2.067730	-2.834122	2.913182
16	O	-2.677391	-2.516047	0.363253
17	O	-2.281533	-0.523291	1.836763
18	C	-1.825989	0.075872	3.058689
19	C	-0.293901	-0.021921	3.168101
20	C	0.234002	0.759340	4.372972
21	O	-0.071570	2.050891	4.284829
22	O	0.848481	0.238252	5.280144
23	N	0.173167	-1.439247	3.313368
24	H	-10.149167	-1.753384	0.221113
25	H	-9.207492	-1.671492	-1.263105
26	H	0.580949	-1.545149	4.252438
27	H	-0.642135	-2.119530	3.195470
28	H	0.903405	-1.664402	2.618071
29	H	0.270707	2.510934	5.072714
30	H	0.152430	0.393993	2.260591
31	H	-2.100431	1.130106	3.025685
32	H	-2.306208	-0.389785	3.922722
33	H	-6.201267	-2.793264	1.876928
34	H	-5.101808	-2.843299	0.478421
35	H	-6.326079	-0.290558	1.676794
36	H	-4.262072	0.130589	0.292832
37	H	-4.968476	-0.819050	-1.025449
38	H	-3.047233	2.015789	-0.259383
39	H	-2.787066	3.067344	1.120971
40	H	-5.249357	3.428300	1.367482
41	H	-4.762431	1.751305	1.593644
42	C	-3.436228	4.104697	-0.658049
43	C	-2.029331	4.435058	-1.171992
44	H	-3.842148	4.973883	-0.122303
45	C	-1.997758	5.655080	-2.097290
46	H	-1.363022	4.607201	-0.315932
47	H	-1.624783	3.562329	-1.702880
48	H	-2.627769	5.498709	-2.980293
49	H	-2.364915	6.550711	-1.583433
50	H	-4.103768	3.934950	-1.512537
51	C	-10.485128	0.070105	-0.909563
52	C	-9.821940	0.974000	-1.956855
53	H	-9.533555	0.366876	-2.826963
54	H	-8.890846	1.390751	-1.550726
55	H	-10.787797	0.667298	-0.041807
56	C	-10.722446	2.125833	-2.419583
57	C	-10.047925	3.033696	-3.452689
58	H	-11.019970	2.723221	-1.547087
59	H	-9.130696	3.476265	-3.047805
60	H	-9.773920	2.472636	-4.353551
61	H	-11.651457	1.716669	-2.839446
62	H	-11.399934	-0.367174	-1.326754
63	H	-10.707371	3.852576	-3.758420
64	H	-0.981141	5.864327	-2.445936
65	C	2.472889	0.991589	-2.093093

66	C	2.392849	0.724719	-0.610715
67	O	1.376416	0.877115	0.051337
68	O	3.571059	0.345770	-0.069867
69	C	3.647806	0.222005	1.378610
70	C	4.935392	0.898218	1.822287
71	O	4.767305	2.300347	1.555365
72	C	5.725729	3.221854	1.853457
73	O	5.459033	4.386795	1.639380
74	C	7.069305	2.759194	2.377554
75	C	8.077409	2.462814	1.238715
76	C	3.599646	-1.248997	1.780177
77	O	2.359092	-1.821175	1.314819
78	P	2.380109	-3.195113	0.409597
79	O	3.050007	-4.326064	1.133494
80	O	0.958784	-3.344041	-0.099942
81	O	3.340330	-2.677116	-0.828716
82	C	4.219521	-3.619648	-1.461402
83	C	4.976676	-2.832360	-2.532052
84	H	1.724822	0.357256	-2.580225
85	H	3.455840	0.715114	-2.477840
86	H	4.277695	-2.469505	-3.288289
87	H	4.904792	-4.048936	-0.723876
88	H	3.647081	-4.420967	-1.938936
89	H	4.451059	-1.799253	1.374971
90	H	3.630414	-1.328238	2.869852
91	H	2.796288	0.754421	1.802118
92	H	5.079437	0.725356	2.892842
93	H	5.792513	0.497092	1.274185
94	H	7.677521	1.682213	0.579074
95	H	8.974215	2.038405	1.704700
96	H	7.451984	3.574204	2.997096
97	H	6.966290	1.878980	3.016376
98	C	8.466436	3.689713	0.405741
99	C	9.491442	3.364560	-0.687845
100	H	8.876627	4.461376	1.071822
101	C	9.892776	4.588850	-1.515981
102	H	10.385972	2.924566	-0.226795
103	H	9.079800	2.592266	-1.351727
104	H	9.023276	5.030717	-2.015859
105	H	10.339972	5.364438	-0.883919
106	H	7.571767	4.128694	-0.053305
107	C	2.176856	2.476861	-2.398821
108	C	3.256580	3.431618	-1.875394
109	H	4.215642	3.184543	-2.352013
110	H	3.404994	3.275678	-0.798439
111	H	1.201912	2.736481	-1.969690
112	C	2.931113	4.909553	-2.122000
113	C	4.032523	5.850104	-1.622412
114	H	1.983250	5.156101	-1.624597
115	H	4.230523	5.694151	-0.556191
116	H	4.971845	5.675904	-2.160055
117	H	2.764247	5.072631	-3.195289
118	H	2.081747	2.582626	-3.485192
119	H	3.757398	6.899993	-1.766650
120	H	10.623243	4.326413	-2.288112
121	O	-1.971123	-2.483086	-3.458534
122	H	-2.431091	-3.262865	-3.797919
123	H	-1.551931	-2.073692	-4.227424
124	Ca	-0.923682	-2.477266	-1.234328
125	O	-1.116275	-0.092186	-0.719994
126	H	-1.575948	-0.064391	0.139978
127	H	-0.286383	0.406557	-0.577742
128	O	1.678418	-5.645557	-1.928024
129	H	2.024363	-6.241969	-1.227733
130	H	1.234937	-4.954541	-1.410865
131	O	2.778687	-6.936112	0.293312
132	H	2.908860	-6.045426	0.691082
133	H	3.666557	-7.206556	0.023019
134	C	6.078404	-3.659654	-3.187211
135	O	7.255656	-3.405160	-3.056607
136	O	5.563814	-4.673410	-3.877359
137	H	6.291581	-5.195923	-4.261015

138	N	5.626527	-1.625169	-1.919078
139	H	5.950842	-0.968882	-2.635125
140	H	4.957555	-1.136240	-1.307349
141	H	6.453929	-1.895218	-1.375287

E[B3LYP/6-31G(d,p)] = -4693.169506 h, E[APFD/6-311+G(2d,p)] = -4691.46849 h
Gcorr[B3LYP/6-31G(d,p)] = 1.046952 h

120. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 1st step, TS

Center No.	Atom	X	Y	Z
1	C	-9.592093	-0.986716	-0.510851
2	C	-8.410828	-0.574989	0.341527
3	O	-8.443809	0.259528	1.223042
4	O	-7.296545	-1.280413	0.013535
5	C	-6.072955	-0.970244	0.714636
6	C	-5.198958	-0.124413	-0.209482
7	O	-5.909184	1.044884	-0.652930
8	C	-5.860143	2.247299	-0.020425
9	O	-6.612704	3.113563	-0.420077
10	C	-4.844124	2.484420	1.079971
11	C	-3.444159	2.858612	0.534828
12	C	-5.445660	-2.321343	1.067824
13	O	-4.345843	-2.150421	1.979306
14	P	-2.792455	-2.286592	1.531373
15	O	-2.067037	-3.131562	2.548937
16	O	-2.696933	-2.562103	0.046925
17	O	-2.227798	-0.724384	1.693697
18	C	-1.737678	-0.262853	2.961239
19	C	-0.204007	-0.379908	3.017686
20	C	0.356858	0.245430	4.295757
21	O	0.053238	1.538995	4.378363
22	O	0.993477	-0.381801	5.116665
23	N	0.263254	-1.799910	2.965638
24	H	-10.148256	-1.734874	0.068899
25	H	-9.228340	-1.490361	-1.410695
26	H	0.689390	-2.025480	3.873897
27	H	-0.546596	-2.457397	2.790988
28	H	0.991243	-1.922534	2.217692
29	H	0.417760	1.894797	5.208961
30	H	0.222715	0.147854	2.159701
31	H	-2.007199	0.789436	3.051643
32	H	-2.196135	-0.820562	3.781541
33	H	-6.192709	-2.928675	1.583271
34	H	-5.116924	-2.846181	0.167674
35	H	-6.315517	-0.421344	1.627386
36	H	-4.260899	0.129831	0.283372
37	H	-4.973104	-0.682961	-1.120704
38	H	-3.038851	2.036211	-0.067613
39	H	-2.778482	2.961722	1.400096
40	H	-5.235678	3.313846	1.673550
41	H	-4.764397	1.618165	1.741848
42	C	-3.411589	4.153925	-0.285427
43	C	-1.999369	4.517670	-0.760763
44	H	-3.815700	4.976387	0.320765
45	C	-1.954801	5.810120	-1.581230
46	H	-1.338338	4.614091	0.111091
47	H	-1.595603	3.689595	-1.359450
48	H	-2.578713	5.731026	-2.478765
49	H	-2.321619	6.661978	-0.997463
50	H	-4.074566	4.062682	-1.155393
51	C	-10.506993	0.197289	-0.855959
52	C	-9.859186	1.212995	-1.805689
53	H	-9.581835	0.706834	-2.741489
54	H	-8.923121	1.583860	-1.367788
55	H	-10.801613	0.695212	0.074905
56	C	-10.766263	2.407261	-2.125853
57	C	-10.105416	3.425572	-3.060067
58	H	-11.052630	2.903294	-1.188529
59	H	-9.182507	3.820847	-2.620591
60	H	-9.843936	2.969063	-4.021660

61	H	-11.700471	2.045562	-2.576614
62	H	-11.424908	-0.196875	-1.307817
63	H	-10.768426	4.272913	-3.263364
64	H	-0.934530	6.042062	-1.903892
65	C	2.611891	1.265069	-2.089594
66	C	2.475976	0.833869	-0.649023
67	O	1.453915	0.972021	0.005325
68	O	3.615827	0.320980	-0.133130
69	C	3.657304	0.045670	1.302822
70	C	4.955690	0.632760	1.829963
71	O	4.845081	2.059896	1.682665
72	C	5.843037	2.913197	2.041394
73	O	5.621253	4.102482	1.934088
74	C	7.174911	2.354348	2.498164
75	C	8.149726	2.111888	1.318466
76	C	3.528849	-1.455695	1.551498
77	O	2.280062	-1.903894	1.042541
78	P	2.157500	-3.406129	0.169916
79	O	2.902417	-4.248931	1.250519
80	O	0.638315	-3.270115	0.016498
81	O	3.122314	-2.765282	-1.021134
82	C	3.958851	-3.517859	-1.897416
83	C	4.700817	-2.487015	-2.746193
84	H	1.899519	0.674221	-2.675508
85	H	3.616626	1.050315	-2.459043
86	H	3.972708	-1.907945	-3.321261
87	H	4.659900	-4.139332	-1.328156
88	H	3.378935	-4.162477	-2.554313
89	H	4.359729	-1.998736	1.093622
90	H	3.584866	-1.632118	2.633126
91	H	2.817374	0.573344	1.754352
92	H	5.064273	0.364756	2.885205
93	H	5.814698	0.249775	1.272528
94	H	7.706559	1.403986	0.606477
95	H	9.036795	1.616088	1.729438
96	H	7.602739	3.098928	3.174256
97	H	7.044714	1.429277	3.064849
98	C	8.573794	3.385790	0.578100
99	C	9.564442	3.109237	-0.559646
100	H	9.027399	4.084511	1.294663
101	C	9.998011	4.378611	-1.298881
102	H	10.449456	2.600764	-0.153991
103	H	9.110165	2.407578	-1.272333
104	H	9.137212	4.890947	-1.743495
105	H	10.487570	5.084750	-0.618641
106	H	7.689895	3.895542	0.174674
107	C	2.300090	2.768848	-2.247035
108	C	3.357286	3.675120	-1.604553
109	H	4.327490	3.490199	-2.086851
110	H	3.489340	3.407483	-0.547314
111	H	1.313134	2.970761	-1.814937
112	C	3.017924	5.167209	-1.701238
113	C	4.106922	6.062908	-1.102213
114	H	2.064590	5.352763	-1.188136
115	H	4.303742	5.799318	-0.057262
116	H	5.049802	5.955712	-1.650901
117	H	2.855906	5.437009	-2.753572
118	H	2.226806	2.986727	-3.318289
119	H	3.820373	7.119006	-1.137189
120	H	10.702585	4.150026	-2.105096
121	O	-1.932580	-2.346730	-3.714320
122	H	-2.189532	-3.162548	-4.164871
123	H	-1.649600	-1.742056	-4.413365
124	Ca	-0.902074	-2.347497	-1.478444
125	O	-1.043728	0.007423	-0.810833
126	H	-1.504131	-0.025121	0.048553
127	H	-0.211944	0.492214	-0.638049
128	O	2.024707	-5.057286	-0.978054
129	H	2.494055	-5.995985	-0.302948
130	H	1.066489	-5.158932	-1.058162
131	O	2.997622	-6.549715	0.601188
132	H	3.033747	-5.431161	1.053308

133	H	3.893078	-6.808183	0.339883
134	C	5.714449	-3.080845	-3.721019
135	O	6.840765	-2.648911	-3.835412
136	O	5.186306	-4.084151	-4.417095
137	H	5.855139	-4.418268	-5.042475
138	N	5.438812	-1.504855	-1.881542
139	H	6.014738	-0.885123	-2.461136
140	H	4.781429	-0.938640	-1.321613
141	H	6.084712	-1.977301	-1.240994

E[B3LYP/6-31G(d,p)] = -4693.11973 h, E[APFD/6-311+G(2d,p)] = -4691.415952 h
Gcorr[B3LYP/6-31G(d,p)] = 1.043999 h

121. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 1st step, products

Center No.	Atom	X	Y	Z
1	C	-9.589169	-1.008221	-0.578517
2	C	-8.418650	-0.628002	0.302782
3	O	-8.468207	0.157753	1.227286
4	O	-7.293036	-1.299924	-0.055318
5	C	-6.077011	-1.010998	0.667846
6	C	-5.206440	-0.113937	-0.209677
7	O	-5.925200	1.070258	-0.596047
8	C	-5.884273	2.240369	0.094839
9	O	-6.643453	3.119767	-0.261287
10	C	-4.869074	2.430253	1.205424
11	C	-3.469887	2.833516	0.679381
12	C	-5.438752	-2.371102	0.961402
13	O	-4.336337	-2.231110	1.874702
14	P	-2.784288	-2.331088	1.411403
15	O	-2.046919	-3.233421	2.368880
16	O	-2.696490	-2.514098	-0.087724
17	O	-2.229824	-0.777900	1.665900
18	C	-1.720897	-0.393943	2.951776
19	C	-0.185810	-0.505014	2.974469
20	C	0.395261	0.055822	4.273083
21	O	0.085043	1.341144	4.430399
22	O	1.051912	-0.608856	5.047463
23	N	0.290622	-1.915078	2.834833
24	H	-10.148415	-1.782010	-0.036715
25	H	-9.214309	-1.471317	-1.495376
26	H	0.724666	-2.192481	3.724267
27	H	-0.515480	-2.565306	2.630347
28	H	1.019427	-1.987921	2.068984
29	H	0.463992	1.654784	5.271449
30	H	0.219294	0.072763	2.138169
31	H	-1.994548	0.648986	3.111728
32	H	-2.163242	-1.004385	3.742815
33	H	-6.179232	-3.005478	1.453262
34	H	-5.110529	-2.854266	0.038069
35	H	-6.330932	-0.507130	1.603221
36	H	-4.272229	0.123461	0.298366
37	H	-4.972658	-0.624450	-1.146587
38	H	-3.057258	2.037282	0.047690
39	H	-2.807775	2.907563	1.550366
40	H	-5.263936	3.230410	1.835820
41	H	-4.786486	1.534924	1.827442
42	C	-3.442293	4.159195	-0.090989
43	C	-2.029683	4.551471	-0.541909
44	H	-3.857350	4.955168	0.542529
45	C	-1.990109	5.872702	-1.315416
46	H	-1.376244	4.622195	0.338052
47	H	-1.613959	3.748699	-1.166358
48	H	-2.606901	5.820600	-2.219829
49	H	-2.368264	6.700174	-0.704434
50	H	-4.098185	4.095676	-0.968838
51	C	-10.505337	0.186302	-0.882357
52	C	-9.850589	1.245734	-1.778043
53	H	-9.556482	0.781899	-2.730522
54	H	-8.923396	1.603157	-1.310917
55	H	-10.813751	0.641301	0.065853

56	C	-10.761009	2.447027	-2.060068
57	C	-10.093800	3.508212	-2.940500
58	H	-11.063981	2.900847	-1.106721
59	H	-9.179816	3.889900	-2.471387
60	H	-9.815811	3.094619	-3.916772
61	H	-11.686255	2.099173	-2.539307
62	H	-11.415692	-0.191369	-1.362704
63	H	-10.759467	4.359440	-3.117095
64	H	-0.969564	6.124407	-1.622115
65	C	2.606519	1.293600	-2.145213
66	C	2.454451	0.866431	-0.704896
67	O	1.428099	1.017622	-0.059411
68	O	3.583930	0.345097	-0.178119
69	C	3.598342	0.056599	1.255369
70	C	4.882819	0.645318	1.813087
71	O	4.765946	2.074159	1.681144
72	C	5.749482	2.930381	2.069068
73	O	5.522082	4.119392	1.967727
74	C	7.075102	2.377078	2.550345
75	C	8.082752	2.167909	1.391978
76	C	3.470318	-1.448595	1.488085
77	O	2.254790	-1.906657	0.917258
78	P	2.172567	-3.466774	0.043389
79	O	2.749387	-4.150254	1.397609
80	O	0.679445	-3.234982	-0.241581
81	O	3.316503	-2.802061	-0.977462
82	C	4.085664	-3.524146	-1.934457
83	C	4.786429	-2.455863	-2.775561
84	H	1.898694	0.703493	-2.737549
85	H	3.614338	1.073846	-2.503179
86	H	4.036312	-1.882164	-3.327501
87	H	4.814516	-4.173621	-1.436853
88	H	3.469901	-4.136030	-2.591112
89	H	4.329684	-1.976194	1.065766
90	H	3.484020	-1.625935	2.572196
91	H	2.747849	0.577527	1.694032
92	H	4.974859	0.365338	2.866840
93	H	5.754330	0.275305	1.266161
94	H	7.665182	1.470360	0.654659
95	H	8.963733	1.672271	1.816086
96	H	7.477160	3.113200	3.251168
97	H	6.941041	1.439972	3.095777
98	C	8.513316	3.460568	0.688791
99	C	9.535676	3.217016	-0.428196
100	H	8.941316	4.148608	1.431014
101	C	9.975528	4.505682	-1.129396
102	H	10.414945	2.708446	-0.010337
103	H	9.106826	2.526242	-1.166807
104	H	9.121391	5.019121	-1.585445
105	H	10.440279	5.201952	-0.422097
106	H	7.635060	3.970142	0.273158
107	C	2.300425	2.797705	-2.308265
108	C	3.346258	3.701798	-1.644234
109	H	4.325301	3.517591	-2.108633
110	H	3.458072	3.431108	-0.585396
111	H	1.305950	3.001004	-1.894325
112	C	3.009879	5.194468	-1.742142
113	C	4.085240	6.086858	-1.114233
114	H	2.045268	5.378263	-1.249827
115	H	4.256962	5.819033	-0.065891
116	H	5.040773	5.980964	-1.640842
117	H	2.871735	5.469180	-2.796596
118	H	2.247612	3.017085	-3.380467
119	H	3.800517	7.143373	-1.151746
120	H	10.702907	4.300838	-1.921622
121	O	-1.919132	-2.249214	-3.854846
122	H	-2.080190	-1.425049	-4.333989
123	H	-2.687850	-2.806664	-4.037143
124	Ca	-0.904053	-2.234846	-1.604170
125	O	-1.090059	0.077852	-0.814562
126	H	-1.520175	-0.006199	0.056979
127	H	-0.258173	0.565215	-0.648361

128	O	2.241269	-4.999256	-0.790706
129	H	2.770904	-6.500503	0.130224
130	H	1.390445	-5.095404	-1.239055
131	O	3.061970	-6.831290	1.006644
132	H	2.871594	-5.132269	1.327286
133	H	4.008209	-7.002810	0.901044
134	C	5.803272	-2.998520	-3.775675
135	O	6.912301	-2.526605	-3.902193
136	O	5.297847	-4.008718	-4.478760
137	H	5.966766	-4.310092	-5.120458
138	N	5.506549	-1.474685	-1.894178
139	H	6.090553	-0.851322	-2.462204
140	H	4.835231	-0.917157	-1.343534
141	H	6.138986	-1.947795	-1.241113

E[B3LYP/6-31G(d,p)] = -4693.13643 h, E[APFD/6-311+G(2d,p)] = -4691.429752 h
Gcorr[B3LYP/6-31G(d,p)] = 1.049307 h

122. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	C	-9.589180	-1.008366	-0.578399
2	C	-8.418608	-0.628029	0.302779
3	O	-8.468109	0.157817	1.227207
4	O	-7.293014	-1.299983	-0.055325
5	C	-6.076955	-1.011006	0.667762
6	C	-5.206423	-0.114003	-0.209860
7	O	-5.925195	1.070167	-0.596285
8	C	-5.884283	2.240307	0.094551
9	O	-6.643465	3.119685	-0.261621
10	C	-4.869099	2.430245	1.205141
11	C	-3.469913	2.833519	0.679103
12	C	-5.438682	-2.371090	0.961381
13	O	-4.336267	-2.231040	1.874671
14	P	-2.784217	-2.331030	1.411377
15	O	-2.046852	-3.233341	2.368878
16	O	-2.696415	-2.514075	-0.087746
17	O	-2.229756	-0.777837	1.665839
18	C	-1.720865	-0.393843	2.951717
19	C	-0.185778	-0.504908	2.974455
20	C	0.395250	0.055948	4.273080
21	O	0.085023	1.341271	4.430368
22	O	1.051876	-0.608718	5.047492
23	N	0.290663	-1.914972	2.834851
24	H	-10.148185	-1.782344	-0.036616
25	H	-9.214351	-1.471285	-1.495362
26	H	0.724696	-2.192356	3.724297
27	H	-0.515433	-2.565209	2.630367
28	H	1.019478	-1.987832	2.069013
29	H	0.463941	1.654924	5.271427
30	H	0.219350	0.072861	2.138161
31	H	-1.994525	0.649090	3.111633
32	H	-2.163229	-1.004265	3.742761
33	H	-6.179154	-3.005448	1.453275
34	H	-5.110456	-2.854298	0.038071
35	H	-6.330833	-0.507079	1.603116
36	H	-4.272189	0.123429	0.298124
37	H	-4.972683	-0.624582	-1.146745
38	H	-3.057258	2.037271	0.047446
39	H	-2.807816	2.907611	1.550095
40	H	-5.263982	3.230413	1.835509
41	H	-4.786497	1.534935	1.827185
42	C	-3.442334	4.159172	-0.091313
43	C	-2.029724	4.551464	-0.542220
44	H	-3.857421	4.955158	0.542169
45	C	-1.990164	5.872671	-1.315769
46	H	-1.376304	4.622231	0.337752
47	H	-1.613970	3.748680	-1.166634
48	H	-2.606935	5.820525	-2.220195
49	H	-2.368353	6.700154	-0.704822
50	H	-4.098209	4.095608	-0.969173

51	C	-10.505635	0.185999	-0.881973
52	C	-9.851246	1.245645	-1.777665
53	H	-9.557209	0.781961	-2.730240
54	H	-8.924043	1.603198	-1.310659
55	H	-10.813984	0.640847	0.066330
56	C	-10.761945	2.446789	-2.059419
57	C	-10.095108	3.508169	-2.939897
58	H	-11.064821	2.900476	-1.105977
59	H	-9.181098	3.889986	-2.470939
60	H	-9.817241	3.094708	-3.916259
61	H	-11.687217	2.098797	-2.538509
62	H	-11.415993	-0.191807	-1.362207
63	H	-10.760965	4.359291	-3.116287
64	H	-0.969619	6.124389	-1.622454
65	C	2.606669	1.293635	-2.145189
66	C	2.454568	0.866451	-0.704880
67	O	1.428205	1.017640	-0.059412
68	O	3.584036	0.345103	-0.178089
69	C	3.598430	0.056604	1.255399
70	C	4.882904	0.645318	1.813129
71	O	4.766038	2.074159	1.681185
72	C	5.749583	2.930376	2.069095
73	O	5.522191	4.119388	1.967751
74	C	7.075205	2.377065	2.550362
75	C	8.082840	2.167878	1.391985
76	C	3.470399	-1.448589	1.488112
77	O	2.254862	-1.906641	0.917295
78	P	2.172615	-3.466759	0.043432
79	O	2.749420	-4.150245	1.397655
80	O	0.679499	-3.234941	-0.241547
81	O	3.316563	-2.802067	-0.977419
82	C	4.085705	-3.524157	-1.934426
83	C	4.786466	-2.455872	-2.775530
84	H	1.898870	0.703523	-2.737551
85	H	3.614502	1.073898	-2.503126
86	H	4.036343	-1.882163	-3.327455
87	H	4.814559	-4.173641	-1.436838
88	H	3.469925	-4.136032	-2.591076
89	H	4.329756	-1.976189	1.065776
90	H	3.484115	-1.625937	2.572222
91	H	2.747934	0.577535	1.694054
92	H	4.974934	0.365338	2.866883
93	H	5.754417	0.275300	1.266211
94	H	7.665253	1.470329	0.654674
95	H	8.963819	1.672231	1.816086
96	H	7.477276	3.113189	3.251173
97	H	6.941140	1.439965	3.095803
98	C	8.513411	3.460527	0.688786
99	C	9.535755	3.216957	-0.428211
100	H	8.941427	4.148566	1.431000
101	C	9.975615	4.505614	-1.129423
102	H	10.415023	2.708379	-0.010360
103	H	9.106888	2.526185	-1.166814
104	H	9.121479	5.019061	-1.585465
105	H	10.440381	5.201883	-0.422133
106	H	7.635156	3.970110	0.273161
107	C	2.300559	2.797737	-2.308239
108	C	3.346370	3.701839	-1.644184
109	H	4.325423	3.517641	-2.108564
110	H	3.458164	3.431148	-0.585344
111	H	1.306074	3.001022	-1.894316
112	C	3.009977	5.194506	-1.742098
113	C	4.085318	6.086907	-1.114170
114	H	2.045355	5.378291	-1.249803
115	H	4.257021	5.819086	-0.065823
116	H	5.040862	5.981021	-1.640759
117	H	2.871852	5.469217	-2.796555
118	H	2.247763	3.017122	-3.380440
119	H	3.800586	7.143419	-1.151690
120	H	10.702982	4.300758	-1.921656
121	O	-1.919044	-2.249214	-3.854867
122	H	-2.080085	-1.425052	-4.334022

123	H	-2.687773	-2.806651	-4.037158
124	Ca	-0.903971	-2.234839	-1.604188
125	O	-1.089957	0.077873	-0.814614
126	H	-1.520088	-0.006159	0.056922
127	H	-0.258069	0.565231	-0.648407
128	O	2.241296	-4.999245	-0.790659
129	H	2.770904	-6.500497	0.130275
130	H	1.390472	-5.095380	-1.239012
131	O	3.061964	-6.831288	1.006696
132	H	2.871612	-5.132262	1.327335
133	H	4.008201	-7.002821	0.901098
134	C	5.803296	-2.998515	-3.775665
135	O	6.912309	-2.526571	-3.902216
136	O	5.297878	-4.008730	-4.478729
137	H	5.966787	-4.310090	-5.120445
138	N	5.506600	-1.474708	-1.894143
139	H	6.090625	-0.851365	-2.462170
140	H	4.835294	-0.917162	-1.343504
141	H	6.139020	-1.947832	-1.241069

E[B3LYP/6-31G(d,p)] = -4693.13643 h, E[APFD/6-311+G(2d,p)] = -4691.429751 h
Gcorr[B3LYP/6-31G(d,p)] = 1.049318 h

123. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 2nd step, TS

Center No.	Atom	X	Y	Z
1	C	-9.567255	-0.919561	-0.615308
2	C	-8.403118	-0.579650	0.290661
3	O	-8.455505	0.184586	1.233145
4	O	-7.281911	-1.256638	-0.069586
5	C	-6.069240	-0.997849	0.671623
6	C	-5.176508	-0.100464	-0.182138
7	O	-5.871139	1.104682	-0.549615
8	C	-5.818243	2.257259	0.168688
9	O	-6.561523	3.156416	-0.171919
10	C	-4.807479	2.406452	1.289517
11	C	-3.401731	2.807514	0.779167
12	C	-5.452231	-2.370627	0.951895
13	O	-4.350226	-2.256028	1.865436
14	P	-2.794396	-2.391844	1.400463
15	O	-2.078741	-3.329557	2.330434
16	O	-2.726694	-2.548183	-0.106442
17	O	-2.215831	-0.850698	1.669475
18	C	-1.695325	-0.487577	2.960094
19	C	-0.155540	-0.518434	2.937614
20	C	0.408704	0.047207	4.239772
21	O	0.033838	1.316369	4.429638
22	O	1.112618	-0.583857	5.001401
23	N	0.407002	-1.871467	2.719147
24	H	-10.171229	-1.664753	-0.081811
25	H	-9.191394	-1.402298	-1.521405
26	H	0.842733	-2.174119	3.594366
27	H	-0.349256	-2.543205	2.508809
28	H	1.308921	-1.891126	1.752195
29	H	0.410701	1.624909	5.273061
30	H	0.178241	0.139360	2.125976
31	H	-2.030583	0.528541	3.170534
32	H	-2.078261	-1.161599	3.730198
33	H	-6.205144	-2.998552	1.434059
34	H	-5.132031	-2.847574	0.022379
35	H	-6.326397	-0.503941	1.611401
36	H	-4.241554	0.108920	0.336537
37	H	-4.945990	-0.596380	-1.127542
38	H	-2.997537	2.025044	0.125162
39	H	-2.740991	2.847502	1.653444
40	H	-5.196263	3.194489	1.938719
41	H	-4.737354	1.494472	1.888309
42	C	-3.356921	4.155140	0.048663
43	C	-1.939664	4.543883	-0.390317
44	H	-3.762661	4.936905	0.705528
45	C	-1.884574	5.887871	-1.122591

46	H	-1.285191	4.579383	0.490968
47	H	-1.533884	3.755894	-1.039614
48	H	-2.502809	5.871293	-2.027379
49	H	-2.252060	6.700573	-0.485813
50	H	-4.013070	4.126004	-0.830786
51	C	-10.425722	0.310960	-0.945975
52	C	-9.702858	1.342139	-1.822036
53	H	-9.399170	0.865635	-2.765233
54	H	-8.776530	1.663359	-1.327627
55	H	-10.742666	0.778990	-0.006919
56	C	-10.555729	2.578510	-2.131336
57	C	-9.818449	3.613511	-2.986802
58	H	-10.871711	3.043186	-1.187474
59	H	-8.907051	3.959320	-2.485959
60	H	-9.523496	3.189883	-3.953769
61	H	-11.477759	2.267859	-2.641357
62	H	-11.336389	-0.030438	-1.452207
63	H	-10.444462	4.489817	-3.184570
64	H	-0.861375	6.136709	-1.422793
65	C	2.585762	1.317833	-2.182424
66	C	2.407956	0.901177	-0.742646
67	O	1.376377	1.066845	-0.111382
68	O	3.524596	0.366343	-0.195150
69	C	3.517524	0.107473	1.243822
70	C	4.803624	0.687177	1.808141
71	O	4.713275	2.113762	1.642454
72	C	5.700928	2.962523	2.038262
73	O	5.495684	4.152302	1.906007
74	C	7.004369	2.398598	2.565497
75	C	8.037941	2.148299	1.438504
76	C	3.364839	-1.390515	1.506845
77	O	2.159301	-1.867574	0.920901
78	P	2.102515	-3.626291	-0.042475
79	O	2.636634	-4.177836	1.365065
80	O	0.642087	-3.310703	-0.326063
81	O	3.252703	-2.876266	-0.957351
82	C	4.086747	-3.556941	-1.901254
83	C	4.746277	-2.456805	-2.729054
84	H	1.879365	0.731832	-2.780543
85	H	3.596122	1.085045	-2.524611
86	H	3.973496	-1.901479	-3.268801
87	H	4.833843	-4.166447	-1.382266
88	H	3.515149	-4.199154	-2.568521
89	H	4.213193	-1.947331	1.104087
90	H	3.357168	-1.548394	2.593216
91	H	2.668964	0.649463	1.660838
92	H	4.874242	0.428743	2.869015
93	H	5.676786	0.290089	1.283441
94	H	7.628986	1.440153	0.706483
95	H	8.900202	1.649769	1.896314
96	H	7.400274	3.143464	3.260539
97	H	6.841147	1.475971	3.127292
98	C	8.505288	3.418430	0.717992
99	C	9.548849	3.134933	-0.369570
100	H	8.927074	4.115707	1.455120
101	C	10.025674	4.401245	-1.087150
102	H	10.409893	2.621473	0.079112
103	H	9.125729	2.435524	-1.103349
104	H	9.190711	4.918508	-1.573388
105	H	10.485656	5.104830	-0.383992
106	H	7.644944	3.932397	0.271449
107	C	2.298381	2.824118	-2.359734
108	C	3.349638	3.721931	-1.695942
109	H	4.330112	3.521016	-2.150282
110	H	3.449356	3.461069	-0.633492
111	H	1.303229	3.041808	-1.955006
112	C	3.032171	5.217400	-1.812986
113	C	4.114757	6.104223	-1.189665
114	H	2.067187	5.418615	-1.328268
115	H	4.277491	5.846965	-0.137318
116	H	5.071761	5.980532	-1.709693
117	H	2.903083	5.481302	-2.871348

118	H	2.256081	3.034717	-3.434135
119	H	3.842941	7.163529	-1.241571
120	H	10.767398	4.168015	-1.857937
121	O	-1.991351	-2.262731	-3.888286
122	H	-2.156184	-1.436765	-4.363109
123	H	-2.763467	-2.817825	-4.063489
124	Ca	-0.970089	-2.247899	-1.640722
125	O	-1.138058	0.046248	-0.810764
126	H	-1.532742	-0.063427	0.076002
127	H	-0.315656	0.555541	-0.669892
128	O	2.221183	-5.125571	-0.819998
129	H	2.780874	-6.694416	0.269934
130	H	1.419797	-5.254326	-1.346588
131	O	3.002893	-6.807225	1.212527
132	H	2.780582	-5.170428	1.368718
133	H	3.949904	-7.006766	1.223039
134	C	5.767998	-2.954317	-3.751188
135	O	6.841650	-2.416050	-3.911200
136	O	5.304121	-3.997739	-4.431869
137	H	5.969258	-4.264592	-5.092676
138	N	5.450591	-1.463526	-1.848783
139	H	6.054063	-0.862192	-2.422092
140	H	4.778190	-0.881658	-1.325077
141	H	6.065451	-1.925552	-1.171201

E[B3LYP/6-31G(d,p)] = -4693.130015 h, E[APFD/6-311+G(2d,p)] = -4691.422539 h
Gcorr[B3LYP/6-31G(d,p)] = 1.04708 h

124. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 2nd step, products

Center No.	Atom	X	Y	Z
1	C	9.155885	1.516481	-1.016061
2	C	8.194314	0.842995	-0.060197
3	O	8.460043	-0.115696	0.636541
4	O	6.987889	1.467072	-0.054801
5	C	5.947790	0.917319	0.783690
6	C	4.971904	0.154907	-0.109547
7	O	5.658542	-0.852107	-0.874513
8	C	5.849908	-2.128062	-0.444886
9	O	6.582049	-2.832234	-1.111780
10	C	5.100364	-2.640059	0.769942
11	C	3.662604	-3.105576	0.431766
12	C	5.304928	2.112386	1.492140
13	O	4.387355	1.664740	2.499364
14	P	2.765582	1.811389	2.354512
15	O	2.214417	2.423283	3.607148
16	O	2.439486	2.365697	0.979946
17	O	2.292691	0.218829	2.268858
18	C	2.000826	-0.544840	3.456226
19	C	0.476628	-0.642847	3.655721
20	C	0.154627	-1.669473	4.739445
21	O	0.598603	-2.893505	4.414177
22	O	-0.440854	-1.418167	5.767344
23	N	-0.159818	0.643047	3.971837
24	H	9.728190	2.240643	-0.421436
25	H	8.586909	2.092930	-1.750919
26	H	-0.542571	0.583001	4.915068
27	H	0.543034	1.388904	3.972724
28	H	-1.404090	1.152488	2.845834
29	H	0.367268	-3.500213	5.139610
30	H	0.058464	-1.046326	2.722763
31	H	2.423161	-1.539192	3.304712
32	H	2.468417	-0.080447	4.328128
33	H	6.090279	2.682418	1.995058
34	H	4.799562	2.761125	0.772381
35	H	6.401765	0.248076	1.517923
36	H	4.162271	-0.266293	0.485914
37	H	4.542376	0.829837	-0.853557
38	H	3.071512	-2.263315	0.052486
39	H	3.192331	-3.410705	1.374448
40	H	5.679489	-3.488260	1.142622

41	H	5.068192	-1.891246	1.565521
42	C	3.594662	-4.267580	-0.566850
43	C	2.157940	-4.729304	-0.840879
44	H	4.182422	-5.112211	-0.181430
45	C	2.078763	-5.887532	-1.839816
46	H	1.687127	-5.028205	0.105329
47	H	1.571515	-3.880095	-1.217675
48	H	2.512662	-5.606800	-2.806290
49	H	2.625979	-6.763722	-1.473885
50	H	4.067271	-3.975286	-1.513444
51	C	10.108491	0.520812	-1.692627
52	C	9.409792	-0.417790	-2.685053
53	H	8.924379	0.181761	-3.468488
54	H	8.606189	-0.965556	-2.175258
55	H	10.610408	-0.067536	-0.916039
56	C	10.363498	-1.426025	-3.337314
57	C	9.658011	-2.369609	-4.316220
58	H	10.856050	-2.015445	-2.552100
59	H	8.870238	-2.941537	-3.812657
60	H	9.188966	-1.811867	-5.134971
61	H	11.164438	-0.885151	-3.859541
62	H	10.888954	1.089494	-2.211881
63	H	10.358678	-3.084829	-4.759394
64	H	1.041949	-6.192190	-2.016064
65	C	-2.420259	-0.525507	-1.757200
66	C	-2.326771	-0.683827	-0.257919
67	O	-1.359008	-1.171234	0.306598
68	O	-3.429032	-0.268346	0.399622
69	C	-3.487035	-0.497957	1.847455
70	C	-4.799790	-1.203128	2.138950
71	O	-4.747885	-2.471453	1.458409
72	C	-5.802733	-3.329243	1.423441
73	O	-5.634840	-4.394148	0.863335
74	C	-7.128147	-2.909561	2.026181
75	C	-8.020983	-2.138678	1.021854
76	C	-3.323562	0.839325	2.579371
77	O	-2.124204	1.488189	2.236237
78	P	-2.099004	4.357997	-1.031004
79	O	-2.716089	5.025109	0.241419
80	O	-0.800171	3.634749	-0.894755
81	O	-3.229451	3.309522	-1.498364
82	C	-4.539386	3.757716	-1.891596
83	C	-5.391727	2.504892	-2.041448
84	H	-1.653561	0.198585	-2.054624
85	H	-3.392304	-0.115558	-2.038497
86	H	-4.913646	1.825966	-2.753424
87	H	-4.954692	4.435931	-1.139520
88	H	-4.492612	4.271654	-2.852900
89	H	-4.162146	1.502679	2.334699
90	H	-3.386205	0.631303	3.657880
91	H	-2.657320	-1.158785	2.098524
92	H	-4.887053	-1.355726	3.219295
93	H	-5.652424	-0.612255	1.796201
94	H	-7.511912	-1.223121	0.695383
95	H	-8.913543	-1.811906	1.567879
96	H	-7.632233	-3.832358	2.324059
97	H	-6.980588	-2.307233	2.926176
98	C	-8.442497	-2.951096	-0.207977
99	C	-9.340281	-2.154468	-1.163192
100	H	-8.971258	-3.856496	0.120529
101	C	-9.764217	-2.956403	-2.397217
102	H	-10.233644	-1.815003	-0.621903
103	H	-8.813491	-1.244037	-1.480763
104	H	-8.892564	-3.280636	-2.977109
105	H	-10.323899	-3.854445	-2.112118
106	H	-7.553384	-3.298196	-0.749357
107	C	-2.186457	-1.870031	-2.475523
108	C	-3.317707	-2.879816	-2.245948
109	H	-4.255895	-2.461096	-2.636620
110	H	-3.476331	-3.026165	-1.168775
111	H	-1.231640	-2.288531	-2.137013
112	C	-3.058253	-4.242200	-2.899611

113	C	-4.216873	-5.224664	-2.701736
114	H	-2.136649	-4.670678	-2.483210
115	H	-4.434722	-5.367511	-1.637644
116	H	-5.132240	-4.854312	-3.177681
117	H	-2.872054	-4.102350	-3.973018
118	H	-2.081264	-1.667657	-3.547219
119	H	-3.989640	-6.203876	-3.135541
120	H	-10.402601	-2.362411	-3.059257
121	O	2.141086	2.086804	-2.991589
122	H	2.304957	1.274179	-3.488956
123	H	2.906729	2.652910	-3.159102
124	Ca	0.981656	2.092188	-0.827422
125	O	1.200726	-0.271371	-0.260272
126	H	1.580306	-0.256170	0.642129
127	H	0.353619	-0.754440	-0.175294
128	O	-2.070220	5.535726	-2.117737
129	H	-0.596775	6.485935	1.886113
130	H	-1.483893	5.350687	-2.868707
131	O	-1.356509	6.845164	1.404923
132	H	-2.158360	5.757016	0.690700
133	H	-0.986261	7.497650	0.792613
134	C	-6.820041	2.760145	-2.536563
135	O	-7.772739	2.168716	-2.076659
136	O	-6.845174	3.649696	-3.519891
137	H	-7.763034	3.757161	-3.830727
138	N	-5.522012	1.761158	-0.742706
139	H	-6.371457	1.180321	-0.792771
140	H	-4.712465	1.159228	-0.524850
141	H	-5.653633	2.401015	0.047563

E[B3LYP/6-31G(d,p)] = -4693.15118 h, E[APFD/6-311+G(2d,p)] = -4691.438927 h
Gcorr[B3LYP/6-31G(d,p)] = 1.038201 h

125. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 3rd step, reactants (hydrolised glycerol + carbon chains neglected)

Center No.	Atom	X	Y	Z
1	C	-3.451809	4.779161	0.503902
2	C	-3.229205	3.352014	0.053995
3	O	-3.475154	2.919400	-1.053174
4	O	-2.687664	2.599275	1.050677
5	C	-2.454418	1.202954	0.781210
6	C	-3.572312	0.388981	1.432793
7	O	-4.863439	0.826558	0.977801
8	C	-5.461023	0.365458	-0.155859
9	O	-6.504053	0.894962	-0.482655
10	C	-4.858329	-0.803008	-0.910148
11	C	-5.289583	-2.176335	-0.338970
12	C	-1.078549	0.905360	1.373845
13	O	-0.790980	-0.506216	1.194244
14	P	0.593811	-0.987415	0.555274
15	O	0.634957	-0.366714	-0.891555
16	O	1.819035	-0.713438	1.375320
17	O	0.384763	-2.575091	0.469234
18	C	-0.848483	-3.280081	0.140670
19	C	-0.767170	-3.842799	-1.294142
20	C	-1.950536	-4.789131	-1.486567
21	O	-1.798409	-5.922457	-0.780686
22	O	-2.927102	-4.541913	-2.163085
23	N	-0.760847	-2.865945	-2.369610
24	H	-2.576828	5.350686	0.167828
25	H	-3.453212	4.815409	1.596699
26	H	-1.675193	-2.423261	-2.430021
27	H	-0.081349	-2.134853	-2.175238
28	H	-2.599363	-6.462171	-0.905062
29	H	0.146328	-4.447245	-1.346734
30	H	-0.923982	-4.083204	0.875065
31	H	-1.696968	-2.603753	0.254115
32	H	-0.331280	1.526665	0.875446
33	H	-1.056840	1.109950	2.446564
34	H	-2.437740	1.047154	-0.299426
35	H	-3.418956	-0.677900	1.265524

36	H	-3.581369	0.570551	2.510136
37	H	-4.982742	-2.258715	0.711625
38	H	-4.727642	-2.942885	-0.884661
39	H	-5.213870	-0.710557	-1.939297
40	H	-3.768099	-0.738586	-0.936627
41	C	-6.792014	-2.459739	-0.455605
42	C	-7.178197	-3.843641	0.080955
43	H	-7.092299	-2.381089	-1.509742
44	C	-8.675689	-4.139442	-0.044480
45	H	-6.606030	-4.612134	-0.456122
46	H	-6.876729	-3.920116	1.134433
47	H	-9.271604	-3.406011	0.510584
48	H	-8.999481	-4.104370	-1.090923
49	H	-7.361349	-1.690014	0.080995
50	C	-4.734441	5.385710	-0.084100
51	C	-6.017927	4.748657	0.463940
52	H	-6.044766	4.872028	1.556059
53	H	-6.003030	3.666819	0.276952
54	H	-4.704118	5.281027	-1.174681
55	C	-7.295420	5.340130	-0.144063
56	C	-8.571045	4.682386	0.391334
57	H	-7.258560	5.230347	-1.236399
58	H	-8.575392	3.606393	0.183019
59	H	-8.655992	4.808795	1.476777
60	H	-7.327071	6.420416	0.052591
61	H	-4.735463	6.460887	0.130251
62	H	-9.467362	5.114845	-0.065239
63	H	-8.920655	-5.132225	0.346780
64	P	6.984515	0.209018	0.416931
65	O	7.226681	1.692924	0.945853
66	O	6.222341	-0.718579	1.301506
67	O	6.188881	0.463837	-0.942389
68	C	6.724534	1.301772	-2.004106
69	C	5.659817	2.296929	-2.482667
70	H	6.186062	2.986492	-3.155088
71	H	7.597503	1.853307	-1.652537
72	H	7.021593	0.643701	-2.823508
73	O	3.303920	0.072550	3.582692
74	H	3.331145	-0.070605	4.538197
75	H	2.369220	0.189486	3.352628
76	Ca	4.052028	-1.572380	1.910369
77	O	2.606443	-3.536745	2.163618
78	H	1.796965	-3.439599	1.632173
79	H	2.929357	-4.431855	1.993750
80	O	8.464229	-0.283295	0.066246
81	H	1.565186	-0.004765	-1.161749
82	H	8.549756	-1.249037	0.016374
83	O	2.992529	0.429946	-1.325225
84	H	7.866108	1.767899	1.672522
85	H	3.196571	1.134116	-0.682420
86	C	5.165584	3.118635	-1.289163
87	O	4.149170	2.909512	-0.654190
88	O	6.028665	4.096813	-1.001347
89	H	5.719067	4.552946	-0.198222
90	N	4.534155	1.626164	-3.150719
91	H	3.489856	0.785654	-2.139308
92	H	3.953877	2.324126	-3.613882
93	H	4.894147	1.027616	-3.892300
94	O	4.038423	-1.923424	-0.510303
95	H	4.899081	-2.100834	-0.912076
96	H	3.736333	-1.066582	-0.901278

E[B3LYP/6-31G(d,p)] = -3804.921386 h, E[APFD/6-311+G(2d,p)] = -3803.661101 h
Gcorr[B3LYP/6-31G(d,p)] = 0.671706 h

126. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 3rd step, TS

Center No.	Atom	X	Y	Z
1	C	-4.424545	4.612964	-0.226047
2	C	-4.079904	3.197306	-0.636866
3	O	-4.528404	2.626480	-1.610946

4	O	-3.179109	2.641791	0.213744
5	C	-2.775251	1.276692	-0.028084
6	C	-3.524127	0.374307	0.950608
7	O	-4.946249	0.565648	0.851502
8	C	-5.741698	-0.109301	-0.021098
9	O	-6.902540	0.243121	-0.095061
10	C	-5.192971	-1.293828	-0.791506
11	C	-5.247016	-2.612378	0.018342
12	C	-1.263603	1.249113	0.185720
13	O	-0.804812	-0.079159	-0.078596
14	P	0.827135	-0.357777	-0.040886
15	O	1.116200	0.455665	-1.399171
16	O	1.253895	0.181769	1.312833
17	O	0.708479	-1.981388	-0.230679
18	C	-0.494348	-2.733948	-0.536270
19	C	-0.590906	-3.006460	-2.055979
20	C	-1.815182	-3.893186	-2.261973
21	O	-1.570616	-5.170843	-1.920933
22	O	-2.898566	-3.493300	-2.636975
23	N	-0.698846	-1.839835	-2.918333
24	H	-3.819437	5.276583	-0.857130
25	H	-4.106083	4.776961	0.806920
26	H	-1.534356	-1.313793	-2.672247
27	H	0.092273	-1.220326	-2.761025
28	H	-2.402174	-5.668716	-2.016574
29	H	0.296317	-3.580017	-2.345263
30	H	-0.387929	-3.674279	0.009077
31	H	-1.373837	-2.202878	-0.177987
32	H	-0.797352	1.962802	-0.501021
33	H	-1.017211	1.537301	1.213426
34	H	-3.016587	1.013896	-1.060183
35	H	-3.238892	-0.667684	0.803079
36	H	-3.276322	0.657615	1.976488
37	H	-4.639323	-2.518636	0.927633
38	H	-4.765493	-3.380768	-0.596719
39	H	-5.820886	-1.389271	-1.680711
40	H	-4.170788	-1.117079	-1.133407
41	C	-6.663207	-3.063560	0.394883
42	C	-6.679817	-4.393602	1.158365
43	H	-7.265916	-3.160351	-0.518898
44	C	-8.091960	-4.852724	1.533676
45	H	-6.192447	-5.166734	0.549140
46	H	-6.072725	-4.295608	2.068560
47	H	-8.591373	-4.114432	2.171388
48	H	-8.712815	-4.992352	0.641390
49	H	-7.153547	-2.291469	1.001521
50	C	-5.916228	4.928848	-0.413233
51	C	-6.829104	4.152818	0.544718
52	H	-6.548617	4.388314	1.581412
53	H	-6.665568	3.074340	0.418962
54	H	-6.193625	4.708709	-1.450533
55	C	-8.318322	4.457080	0.341737
56	C	-9.224282	3.662262	1.287236
57	H	-8.592471	4.235894	-0.698731
58	H	-9.086500	2.583907	1.148643
59	H	-9.000735	3.891648	2.335497
60	H	-8.493458	5.532640	0.480607
61	H	-6.060530	6.006196	-0.269500
62	H	-10.281538	3.889183	1.115119
63	H	-8.071742	-5.802909	2.077262
64	P	6.986666	-0.747237	1.091525
65	O	8.144658	-0.027971	1.911233
66	O	5.715975	-1.038423	1.810330
67	O	6.726642	0.298939	-0.091615
68	C	7.785760	0.719061	-0.980223
69	C	7.231726	1.827039	-1.868322
70	H	8.053005	2.194576	-2.489240
71	H	8.624521	1.117579	-0.407026
72	H	8.124958	-0.128887	-1.580529
73	O	2.497956	1.186470	3.520635
74	H	2.259429	1.088496	4.452179
75	H	1.659246	1.260673	3.034704

76	Ca	3.372287	-0.698682	2.162066
77	O	2.169476	-2.850829	2.132465
78	H	1.697155	-2.829799	1.280158
79	H	2.643879	-3.692580	2.154896
80	O	7.715132	-2.027413	0.475122
81	H	2.068331	0.647166	-1.575611
82	H	7.102903	-2.735383	0.216695
83	O	3.826351	0.979354	-1.523513
84	H	8.547843	-0.568447	2.609930
85	H	3.900324	1.756892	-0.947378
86	C	6.673946	2.991350	-1.045030
87	O	5.510962	3.333894	-1.057293
88	O	7.640247	3.557287	-0.327276
89	H	7.257804	4.280004	0.202834
90	N	6.149379	1.329966	-2.773546
91	H	5.235023	1.087164	-2.250362
92	H	5.904482	2.046317	-3.462431
93	H	6.463842	0.509232	-3.297917
94	O	2.932024	-0.931704	-0.178596
95	H	3.026276	-1.745406	-0.691436
96	H	3.650806	0.157459	-0.914993

E[B3LYP/6-31G(d,p)] = -3804.883252 h, E[APFD/6-311+G(2d,p)] = -3803.627298 h
Gcorr[B3LYP/6-31G(d,p)] = 0.676633 h

127. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 3rd step, products

Center No.	Atom	X	Y	Z
1	C	4.302140	4.614132	0.227838
2	C	3.995527	3.189355	0.639226
3	O	4.471225	2.627622	1.606263
4	O	3.094683	2.617730	-0.197823
5	C	2.714579	1.244894	0.049482
6	C	3.469699	0.355916	-0.936223
7	O	4.889077	0.584367	-0.865966
8	C	5.718596	-0.060814	-0.003802
9	O	6.869720	0.326644	0.049673
10	C	5.219974	-1.258692	0.779496
11	C	5.306161	-2.577515	-0.027126
12	C	1.200784	1.191878	-0.150331
13	O	0.759883	-0.134393	0.113188
14	P	-0.900814	-0.428427	0.082409
15	O	-1.096665	0.414386	1.462745
16	O	-1.243883	0.154625	-1.291995
17	O	-0.680591	-2.064240	0.262762
18	C	0.548274	-2.770839	0.544781
19	C	0.680029	-3.040286	2.063608
20	C	1.927840	-3.895652	2.252285
21	O	1.713019	-5.178575	1.908923
22	O	3.005661	-3.471307	2.617386
23	N	0.771732	-1.869767	2.924155
24	H	3.676232	5.260684	0.856535
25	H	3.980610	4.768272	-0.805799
26	H	1.593280	-1.329029	2.662810
27	H	-0.029124	-1.263586	2.761727
28	H	2.558729	-5.653948	1.993856
29	H	-0.187824	-3.636104	2.367390
30	H	0.467582	-3.717730	0.005018
31	H	1.403361	-2.210875	0.172767
32	H	0.735474	1.905083	0.539147
33	H	0.946807	1.486040	-1.175389
34	H	2.972845	0.987747	1.078834
35	H	3.214239	-0.691969	-0.776351
36	H	3.196420	0.625114	-1.959488
37	H	4.687738	-2.503929	-0.931066
38	H	4.853324	-3.358104	0.594159
39	H	5.863176	-1.330125	1.660040
40	H	4.197474	-1.114733	1.135043
41	C	6.731725	-2.987241	-0.415353
42	C	6.781652	-4.318440	-1.175332
43	H	7.345099	-3.063390	0.493311

44	C	8.203788	-4.736656	-1.560632
45	H	6.322236	-5.103902	-0.560160
46	H	6.164727	-4.241202	-2.080913
47	H	8.676185	-3.985609	-2.204019
48	H	8.835415	-4.855434	-0.672888
49	H	7.193423	-2.202585	-1.028255
50	C	5.783104	4.973943	0.417543
51	C	6.719656	4.233145	-0.545445
52	H	6.432120	4.467331	-1.580523
53	H	6.589569	3.149248	-0.427539
54	H	6.066954	4.755100	1.453376
55	C	8.198592	4.582484	-0.339837
56	C	9.129370	3.825149	-1.291933
57	H	8.479829	4.361366	0.698761
58	H	9.026612	2.741770	-1.162394
59	H	8.898210	4.055918	-2.338237
60	H	8.339468	5.664220	-0.469548
61	H	5.895047	6.056141	0.281252
62	H	10.178825	4.084592	-1.117992
63	H	8.207553	-5.688486	-2.101709
64	P	-6.952592	-0.772223	-1.099423
65	O	-8.056217	-0.054671	-1.991283
66	O	-5.644796	-1.083027	-1.739195
67	O	-6.747844	0.288966	0.081616
68	C	-7.851468	0.741433	0.897244
69	C	-7.324450	1.845192	1.806778
70	H	-8.166105	2.228685	2.389106
71	H	-8.643125	1.153515	0.269295
72	H	-8.247714	-0.092157	1.482841
73	O	-2.433649	1.138904	-3.510900
74	H	-2.146225	1.027254	-4.426975
75	H	-1.620810	1.189499	-2.976902
76	Ca	-3.318169	-0.748235	-2.161453
77	O	-2.122464	-2.901740	-2.101719
78	H	-1.625494	-2.890423	-1.262235
79	H	-2.590176	-3.747047	-2.126470
80	O	-7.724892	-2.037444	-0.507696
81	H	-2.034880	0.583141	1.686135
82	H	-7.135760	-2.746447	-0.202258
83	O	-3.890204	0.972600	1.598492
84	H	-8.439791	-0.605868	-2.692571
85	H	-3.935916	1.777551	1.057182
86	C	-6.706361	2.996179	1.007677
87	O	-5.537509	3.313301	1.071008
88	O	-7.627238	3.580758	0.248005
89	H	-7.207308	4.294201	-0.266189
90	N	-6.292661	1.331964	2.762205
91	H	-5.375538	1.067679	2.278666
92	H	-6.056840	2.048133	3.454975
93	H	-6.644029	0.521559	3.279394
94	O	-2.752970	-0.949343	0.212852
95	H	-2.844098	-1.750160	0.749003
96	H	-3.706872	0.215346	0.974624

E[B3LYP/6-31G(d,p)] = -3804.884192 h, E[APFD/6-311+G(2d,p)] = -3803.629709 h
Gcorr[B3LYP/6-31G(d,p)] = 0.679344 h

128. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 4th step, reactants

Center No.	Atom	X	Y	Z
1	C	2.363907	-4.582809	-1.360214
2	C	2.372090	-3.068178	-1.359018
3	O	2.961775	-2.376370	-2.165605
4	O	1.610519	-2.571691	-0.353107
5	C	1.542556	-1.133548	-0.200110
6	C	2.461882	-0.744274	0.954179
7	O	3.800764	-1.228261	0.742056
8	C	4.763906	-0.531243	0.083973
9	O	5.803167	-1.113579	-0.157289
10	C	4.546564	0.933177	-0.238102
11	C	4.863172	1.854520	0.965878

12	C	0.074395	-0.812937	0.086942
13	O	-0.138896	0.600178	0.143749
14	P	-1.160461	1.301467	-1.082918
15	O	-0.135195	0.795116	-2.224857
16	O	-2.443369	0.553340	-0.692557
17	O	-0.871843	2.813735	-0.456803
18	C	0.299459	3.308934	0.231970
19	C	1.005759	4.331584	-0.686089
20	C	2.056007	5.081339	0.124990
21	O	1.492923	5.869350	1.057790
22	O	3.256038	4.973582	-0.024945
23	N	1.630542	3.781892	-1.881556
24	H	1.604064	-4.889061	-2.091033
25	H	2.027748	-4.942293	-0.383748
26	H	2.497032	3.316361	-1.620872
27	H	1.026949	3.077570	-2.298359
28	H	2.210296	6.290327	1.563834
29	H	0.245443	5.066893	-0.979381
30	H	-0.057034	3.791492	1.145075
31	H	0.966844	2.488134	0.488097
32	H	-0.539512	-1.282032	-0.684831
33	H	-0.214473	-1.245348	1.052568
34	H	1.851505	-0.660394	-1.133082
35	H	2.433835	0.333694	1.117613
36	H	2.131268	-1.239294	1.870805
37	H	4.230316	1.581738	1.820230
38	H	4.574278	2.872296	0.682237
39	H	5.222387	1.166054	-1.064490
40	H	3.527169	1.114067	-0.588986
41	C	6.335060	1.836073	1.395777
42	C	6.622025	2.778311	2.571421
43	H	6.963716	2.119679	0.540156
44	C	8.092558	2.773732	2.999521
45	H	6.322387	3.799093	2.298288
46	H	5.991462	2.494046	3.424756
47	H	8.410898	1.772056	3.310125
48	H	8.745094	3.087464	2.176788
49	H	6.634106	0.815467	1.667242
50	C	3.727468	-5.177473	-1.741763
51	C	4.813786	-4.943671	-0.684130
52	H	4.491270	-5.386483	0.269180
53	H	4.925908	-3.867022	-0.500887
54	H	4.042303	-4.745522	-2.698694
55	C	6.177004	-5.525940	-1.076734
56	C	7.261628	-5.266939	-0.026515
57	H	6.489148	-5.095578	-2.037990
58	H	7.399251	-4.192313	0.138994
59	H	6.995833	-5.717870	0.936531
60	H	6.077407	-6.606916	-1.245132
61	H	3.600054	-6.253883	-1.907276
62	H	8.226130	-5.683980	-0.334277
63	H	8.265961	3.453747	3.839915
64	P	-6.071389	-1.285851	-0.235448
65	O	-7.503177	-1.545952	0.388373
66	O	-5.489444	0.094858	-0.091541
67	O	-5.238967	-2.368336	0.589809
68	C	-3.821645	-2.212477	0.867063
69	C	-3.606487	-1.637961	2.266580
70	H	-2.555460	-1.789169	2.530989
71	H	-3.401763	-3.215851	0.822695
72	H	-3.332447	-1.573759	0.126736
73	O	-1.400114	0.789056	2.557246
74	H	-1.269681	1.638753	2.998426
75	H	-0.923519	0.840871	1.693633
76	Ca	-4.371578	1.754685	-1.502684
77	O	-3.613441	3.478437	0.077039
78	H	-2.640129	3.514426	0.012652
79	H	-3.919929	4.391769	-0.002229
80	O	-6.236410	-1.770677	-1.744713
81	H	-0.492844	0.866643	-3.154312
82	H	-5.556747	-1.448131	-2.358721
83	O	-1.272705	1.043812	-4.638232

84	H	-8.236788	-1.149169	-0.108865
85	H	-1.723251	0.214171	-4.850592
86	C	-4.461512	-2.321838	3.336365
87	O	-5.172111	-1.706130	4.102374
88	O	-4.295911	-3.640603	3.318267
89	H	-4.844951	-4.037155	4.018562
90	N	-3.874243	-0.167405	2.333255
91	H	-4.433902	0.150889	1.525547
92	H	-4.415036	0.020853	3.187643
93	H	-2.945395	0.357371	2.370288
94	O	-2.143856	2.240072	-2.356075
95	H	-1.797112	3.136801	-2.466221
96	H	-1.910360	1.549365	-4.092087

E[B3LYP/6-31G(d,p)] = -3804.87922 h, E[APFD/6-311+G(2d,p)] = -3803.637263 h
Gcorr[B3LYP/6-31G(d,p)] = 0.680224 h

129. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 4th step, TS

Center No.	Atom	X	Y	Z
1	C	2.917901	-4.298231	-1.841780
2	C	2.788897	-2.802931	-1.641741
3	O	3.394668	-1.960423	-2.273444
4	O	1.880168	-2.511461	-0.676348
5	C	1.668179	-1.119356	-0.348490
6	C	2.433711	-0.817924	0.939145
7	O	3.819518	-1.184414	0.821630
8	C	4.793540	-0.351386	0.367906
9	O	5.894840	-0.833213	0.190069
10	C	4.501545	1.123638	0.183044
11	C	4.607533	1.924655	1.503783
12	C	0.156253	-0.959216	-0.184361
13	O	-0.189777	0.425293	-0.002773
14	P	-1.277216	1.231215	-1.327537
15	O	-0.170594	0.738509	-2.378677
16	O	-2.492281	0.421453	-0.883788
17	O	-0.960733	2.679744	-0.610870
18	C	0.246877	3.180611	0.014355
19	C	0.969325	4.145650	-0.953083
20	C	2.003180	4.934134	-0.154523
21	O	1.422975	5.813198	0.679763
22	O	3.204014	4.773752	-0.234401
23	N	1.628646	3.534376	-2.098318
24	H	2.255614	-4.557468	-2.678150
25	H	2.529394	-4.814075	-0.959321
26	H	2.494623	3.098486	-1.789075
27	H	1.048074	2.799009	-2.492951
28	H	2.127550	6.252376	1.188560
29	H	0.216348	4.863722	-1.301706
30	H	-0.085198	3.710513	0.909614
31	H	0.896955	2.354590	0.295708
32	H	-0.338335	-1.364295	-1.067377
33	H	-0.190105	-1.519328	0.690822
34	H	2.020712	-0.500693	-1.175358
35	H	2.306040	0.227082	1.225601
36	H	2.050559	-1.443986	1.748801
37	H	3.885021	1.539434	2.234626
38	H	4.303440	2.952735	1.279257
39	H	5.246099	1.491768	-0.526863
40	H	3.518048	1.276929	-0.267942
41	C	6.009923	1.925494	2.124311
42	C	6.089731	2.757910	3.410021
43	H	6.728233	2.318035	1.391142
44	C	7.489832	2.771165	4.030724
45	H	5.774363	3.787710	3.194553
46	H	5.369162	2.365247	4.140212
47	H	7.818337	1.757577	4.287352
48	H	8.226369	3.191356	3.336420
49	H	6.326465	0.896586	2.338676
50	C	4.357431	-4.728198	-2.159332
51	C	5.319640	-4.565744	-0.975597

52	H	4.955239	-5.165453	-0.129171
53	H	5.316982	-3.521459	-0.636681
54	H	4.717749	-4.143361	-3.013435
55	C	6.759292	-4.978608	-1.305338
56	C	7.718005	-4.799648	-0.124100
57	H	7.116960	-4.387077	-2.159069
58	H	7.744080	-3.755021	0.206209
59	H	7.408360	-5.409077	0.732719
60	H	6.772042	-6.026599	-1.634551
61	H	4.340843	-5.776877	-2.479054
62	H	8.739509	-5.092069	-0.388576
63	H	7.515028	3.371198	4.946173
64	P	-6.378203	-1.240854	0.063012
65	O	-7.679104	-1.123970	0.964554
66	O	-5.594555	0.012132	-0.188643
67	O	-5.576946	-2.311688	0.926058
68	C	-4.123983	-2.385302	0.939549
69	C	-3.580264	-1.822025	2.252337
70	H	-2.538337	-2.161368	2.322077
71	H	-3.878280	-3.442494	0.852355
72	H	-3.694944	-1.834740	0.099283
73	O	-1.211178	0.514473	2.175603
74	H	-1.112758	1.364911	2.626230
75	H	-0.733911	0.526186	1.091897
76	Ca	-4.485937	1.571390	-1.640469
77	O	-3.728912	3.319192	-0.083513
78	H	-2.757753	3.390768	-0.114371
79	H	-4.064412	4.222780	-0.159062
80	O	-6.917411	-1.941231	-1.267981
81	H	-0.494102	0.764994	-3.333312
82	H	-6.366771	-1.775010	-2.049738
83	O	-1.152486	0.859720	-4.811157
84	H	-8.425219	-0.684716	0.525508
85	H	-1.485631	-0.002781	-5.097991
86	C	-4.305149	-2.411292	3.464831
87	O	-4.827997	-1.740483	4.329582
88	O	-4.262725	-3.747718	3.461027
89	H	-4.727885	-4.071847	4.252651
90	N	-3.615562	-0.347221	2.306680
91	H	-4.198025	0.028922	1.557285
92	H	-4.048970	-0.070386	3.190141
93	H	-2.249002	0.208560	2.211023
94	O	-2.230390	2.108798	-2.536343
95	H	-1.888612	3.000875	-2.694544
96	H	-1.928674	1.330841	-4.460610

E[B3LYP/6-31G(d,p)] = -3804.866928 h, E[APFD/6-311+G(2d,p)] = -3803.622428 h
Gcorr[B3LYP/6-31G(d,p)] = 0.671089 h

130. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 4th step, products

Center No.	Atom	X	Y	Z
1	C	6.251938	-2.543888	3.058522
2	C	5.070278	-2.515905	2.114040
3	O	4.761078	-3.428870	1.373807
4	O	4.408849	-1.333046	2.171965
5	C	3.307255	-1.117888	1.258516
6	C	3.590053	0.162323	0.488888
7	O	4.775723	-0.056658	-0.298976
8	C	4.978095	0.447561	-1.543976
9	O	6.041055	0.189878	-2.076651
10	C	3.913600	1.305630	-2.197171
11	C	3.864735	2.749170	-1.645419
12	C	2.030519	-1.042294	2.100671
13	O	0.885251	-0.941947	1.255288
14	P	-2.562678	-2.599949	-1.948194
15	O	-1.165036	-3.027258	-1.435319
16	O	-3.702877	-2.674926	-0.973341
17	O	-2.436128	-1.102117	-2.584747
18	C	-1.905725	0.008822	-1.808348
19	C	-0.509987	0.421366	-2.331405

20	C	-0.232003	1.828688	-1.807633
21	O	-0.868592	2.762276	-2.523831
22	O	0.451600	2.083444	-0.831987
23	N	0.596754	-0.452580	-1.981705
24	H	6.124214	-3.416061	3.708523
25	H	6.248238	-1.648319	3.684729
26	H	0.678590	-0.534404	-0.968285
27	H	0.415554	-1.388753	-2.334775
28	H	-0.701311	3.629373	-2.111881
29	H	-0.587322	0.489000	-3.421634
30	H	-2.618350	0.826483	-1.934261
31	H	-1.850615	-0.251060	-0.748185
32	H	1.968200	-1.949936	2.711533
33	H	2.073805	-0.181866	2.777639
34	H	3.249073	-1.962885	0.569133
35	H	2.726923	0.409585	-0.129170
36	H	3.784619	0.986304	1.183461
37	H	3.608316	2.739435	-0.579611
38	H	3.036400	3.261697	-2.147974
39	H	4.174232	1.332666	-3.258295
40	H	2.929178	0.832872	-2.113122
41	C	5.161540	3.540037	-1.856481
42	C	5.072536	4.983507	-1.346309
43	H	5.410866	3.546959	-2.926791
44	C	6.364600	5.777539	-1.560554
45	H	4.240625	5.493966	-1.850174
46	H	4.821144	4.974386	-0.277080
47	H	7.207556	5.309436	-1.039515
48	H	6.623234	5.832688	-2.624159
49	H	5.995473	3.030970	-1.354539
50	C	7.578759	-2.668447	2.281590
51	C	7.904882	-1.436911	1.427879
52	H	7.989748	-0.557252	2.081797
53	H	7.072036	-1.226277	0.744374
54	H	7.526468	-3.560724	1.646065
55	C	9.192332	-1.587269	0.608656
56	C	9.490524	-0.358927	-0.257270
57	H	9.108119	-2.475030	-0.032896
58	H	8.662295	-0.155856	-0.945275
59	H	9.633571	0.534587	0.361558
60	H	10.036756	-1.779020	1.284632
61	H	8.384404	-2.843418	3.004296
62	H	10.398786	-0.499096	-0.852739
63	H	6.270209	6.802478	-1.187274
64	P	-6.499048	0.823575	0.553480
65	O	-5.482964	1.417987	-0.509867
66	O	-6.587440	-0.675304	0.556803
67	O	-6.064017	1.449606	1.953697
68	C	-5.322113	0.716904	2.965775
69	C	-3.839878	1.122254	2.949837
70	H	-3.378001	0.614493	3.804809
71	H	-5.781947	0.978094	3.919287
72	H	-5.425777	-0.356702	2.794925
73	O	-0.361001	1.244651	1.831047
74	H	-0.146762	1.774636	1.045101
75	H	0.363358	-0.110047	1.501297
76	Ca	-6.060769	-2.445538	-0.959228
77	O	-5.277191	-0.464340	-2.443004
78	H	-4.359642	-0.600811	-2.752728
79	H	-5.801872	-0.254206	-3.231243
80	O	-7.851679	1.595875	0.207260
81	H	-0.941922	-3.070737	-0.362017
82	H	-8.589788	1.377450	0.798895
83	O	-0.533739	-3.095646	0.912145
84	H	-5.377020	0.821932	-1.299881
85	H	-0.009303	-2.256205	1.106023
86	C	-3.693422	2.625733	3.176824
87	O	-3.237687	3.403831	2.367682
88	O	-4.155476	2.980574	4.387026
89	H	-4.068404	3.946581	4.470378
90	N	-3.113108	0.758079	1.734154
91	H	-3.230063	-0.235001	1.544253

92	H	-3.492900	1.273104	0.941337
93	H	-1.349250	1.113836	1.805926
94	O	-2.908118	-3.455795	-3.251049
95	H	-2.165695	-3.565657	-3.865912
96	H	-1.274296	-3.121557	1.534204

E[B3LYP/6-31G(d,p)] = -3804.922726 h, E[APFD/6-311+G(2d,p)] = -3803.672794 h
Gcorr[B3LYP/6-31G(d,p)] = 0.672875 h

131. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 5th step, reactants (hydrolysed glycerol + carbon chains neglected)

Center No.	Atom	X	Y	Z
1	P	3.432086	0.351511	-0.751402
2	O	3.632800	1.313740	0.413859
3	O	3.031995	-1.077299	-0.431256
4	O	2.330429	1.035999	-1.756136
5	C	1.067049	1.394752	-1.187245
6	C	0.958174	2.914334	-0.982474
7	C	-0.360166	3.246148	-0.268207
8	O	-1.388186	2.729823	-0.906387
9	O	-0.382517	3.876898	0.773267
10	N	2.069601	3.448794	-0.126223
11	H	2.601196	4.177035	-0.604965
12	H	1.629326	3.871462	0.706490
13	H	-2.227063	2.748694	-0.356367
14	H	0.992825	3.417431	-1.950851
15	H	0.283901	1.091453	-1.881595
16	H	0.897712	0.877359	-0.237178
17	P	-2.523092	-2.063488	-0.880328
18	O	-2.791004	-2.005366	-2.448993
19	O	-1.100663	-1.809048	-0.479434
20	O	-3.580387	-1.027223	-0.300034
21	C	-3.854127	-0.882456	1.125207
22	C	-3.413278	0.519642	1.574857
23	H	-3.709378	0.606741	2.627424
24	H	-4.927196	-1.031210	1.246695
25	H	-3.316544	-1.638760	1.700794
26	O	1.821977	-3.374387	1.721475
27	H	2.717189	-2.986145	1.956174
28	Ca	1.175904	-2.564520	-0.451649
29	O	4.185434	-2.228421	1.929734
30	H	4.097177	-1.913159	1.010921
31	H	4.109846	-1.385152	2.441731
32	O	-3.120026	-3.467841	-0.424945
33	H	2.746917	2.681947	0.168611
34	H	-2.488044	-4.202725	-0.475657
35	O	3.931580	0.287469	2.974608
36	H	-2.234099	-1.361819	-2.915666
37	H	3.840468	0.728055	2.099783
38	C	-4.222243	1.596280	0.844896
39	O	-3.771768	2.522564	0.188292
40	O	-5.533208	1.428530	1.023148
41	H	-6.003883	2.134657	0.544775
42	N	-1.988519	0.780327	1.464055
43	H	-1.505593	0.348421	2.246637
44	H	-1.618446	0.346926	0.621273
45	H	1.253206	-3.241511	2.490404
46	O	4.714421	0.274795	-1.718953
47	H	5.173493	1.125321	-1.796053
48	H	3.066987	0.397134	3.392557

E[B3LYP/6-31G(d,p)] = -2840.259173 h, E[APFD/6-311+G(2d,p)] = -2839.506245 h
Gcorr[B3LYP/6-31G(d,p)] = 0.286434 h

132. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 5th step, TS

Center No.	Atom	X	Y	Z
1	P	3.710162	-0.454353	-0.173266
2	O	3.892006	1.067433	0.265577
3	O	2.765097	-1.386901	0.605265

4	O	2.594501	-0.024399	-1.466138
5	C	1.334172	0.484299	-1.121661
6	C	1.199364	1.945852	-1.603604
7	C	-0.092808	2.561411	-1.078279
8	O	-1.143215	1.848364	-1.433848
9	O	-0.099670	3.560385	-0.374751
10	N	2.347771	2.762601	-1.092368
11	H	2.847118	3.234139	-1.847180
12	H	1.969509	3.486355	-0.465978
13	H	-1.990543	2.159984	-1.005790
14	H	1.209017	1.973773	-2.694652
15	H	0.536672	-0.093470	-1.598430
16	H	1.166315	0.447329	-0.038517
17	P	-2.468982	-2.351306	-0.515344
18	O	-2.382202	-2.521220	-2.095617
19	O	-1.151734	-2.145488	0.165959
20	O	-3.510797	-1.158894	-0.344740
21	C	-4.121395	-0.822703	0.932677
22	C	-3.723404	0.611677	1.317723
23	H	-4.259014	0.836697	2.246684
24	H	-5.199810	-0.914916	0.797227
25	H	-3.797368	-1.514322	1.713175
26	O	-1.866358	3.678048	2.012058
27	H	-1.372149	3.912005	1.212711
28	Ca	0.997307	-2.787655	1.009163
29	O	5.142496	-0.951207	0.969726
30	H	4.738934	-1.608367	1.554573
31	H	5.513760	0.069183	1.642566
32	O	-3.302798	-3.615233	-0.021902
33	H	3.039174	2.139348	-0.556381
34	H	-2.758285	-4.390624	0.188757
35	O	5.577913	1.175738	1.955282
36	H	-1.660344	-2.018134	-2.504690
37	H	4.721377	1.302586	1.177964
38	C	-4.246890	1.603052	0.278298
39	O	-3.571402	2.281844	-0.479162
40	O	-5.578141	1.645398	0.278864
41	H	-5.871149	2.262690	-0.415832
42	N	-2.298048	0.814050	1.542926
43	H	-2.019260	0.330653	2.393346
44	H	-1.757002	0.402086	0.785466
45	H	-1.980291	2.711194	1.903470
46	O	4.694557	-1.029366	-1.349460
47	H	4.227210	-0.893331	-2.189750
48	H	5.207982	1.269010	2.845417

E[B3LYP/6-31G(d,p)] = -2840.19593 h, E[APFD/6-311+G(2d,p)] = -2839.451997 h
Gcorr[B3LYP/6-31G(d,p)] = 0.287162 h

133. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 5th step, products

Center No.	Atom	X	Y	Z
1	P	3.785085	-0.376068	-0.153741
2	O	3.823691	1.236731	0.202398
3	O	2.858449	-1.325068	0.631868
4	O	2.578524	0.045416	-1.402637
5	C	1.294304	0.447005	-1.017007
6	C	0.999078	1.842372	-1.613559
7	C	-0.320943	2.403092	-1.098288
8	O	-1.326824	1.599358	-1.377751
9	O	-0.381489	3.449920	-0.470271
10	N	2.087718	2.802272	-1.229619
11	H	2.499836	3.263085	-2.042270
12	H	1.672244	3.530503	-0.631111
13	H	-2.194774	1.914894	-0.992785
14	H	0.970511	1.770211	-2.702132
15	H	0.528105	-0.235832	-1.400461
16	H	1.186802	0.485315	0.073800
17	P	-2.215593	-2.386349	-0.475025
18	O	-1.897942	-2.182393	-2.022452
19	O	-1.016039	-2.462679	0.415365

20	O	-3.173545	-1.133966	-0.275184
21	C	-4.004487	-0.976235	0.907970
22	C	-3.896160	0.492325	1.350156
23	H	-4.563046	0.609308	2.209733
24	H	-5.027067	-1.244881	0.637113
25	H	-3.659181	-1.623041	1.717518
26	O	-2.246835	3.834086	1.845159
27	H	-1.722790	3.936259	1.036973
28	Ca	1.248029	-2.887921	1.040143
29	O	5.164954	-0.646700	0.869506
30	H	4.903911	-1.369246	1.455872
31	H	5.799817	0.739483	1.847182
32	O	-3.195829	-3.638744	-0.314128
33	H	2.849070	2.297041	-0.706082
34	H	-2.769402	-4.411062	0.089980
35	O	5.692250	1.691175	2.072871
36	H	-1.097995	-2.646629	-2.316272
37	H	4.463293	1.488335	0.924839
38	C	-4.441032	1.401024	0.248770
39	O	-3.774840	2.082352	-0.515746
40	O	-5.769655	1.353456	0.191473
41	H	-6.071319	1.907593	-0.551390
42	N	-2.553901	0.911503	1.735118
43	H	-2.314991	0.501789	2.634806
44	H	-1.870949	0.566381	1.063692
45	H	-2.369812	2.863352	1.886292
46	O	4.703642	-0.869524	-1.418762
47	H	4.165768	-0.759312	-2.219705
48	H	5.289631	1.689876	2.952619

E[B3LYP/6-31G(d,p)] = -2840.208734 h, E[APFD/6-311+G(2d,p)] = -2839.465292 h
Gcorr[B3LYP/6-31G(d,p)] = 0.287141 h

134. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 6th step, TS

Center No.	Atom	X	Y	Z
1	P	3.529473	-1.288544	0.267591
2	O	4.423312	-0.100391	0.866244
3	O	2.034549	-1.066146	0.104927
4	O	3.886609	-0.113471	-1.578175
5	C	2.905121	0.652596	-2.186785
6	C	3.085350	2.167329	-1.717685
7	C	2.085411	2.604961	-0.654578
8	O	0.857518	2.654618	-1.122113
9	O	2.431585	2.871134	0.489759
10	N	4.441411	2.212990	-1.113656
11	H	5.112747	2.777448	-1.630005
12	H	4.359205	2.543720	-0.144326
13	H	0.190017	2.981190	-0.405682
14	H	3.018376	2.849424	-2.565509
15	H	3.000897	0.631274	-3.282138
16	H	1.891025	0.331030	-1.923928
17	P	-3.835428	-1.931567	-0.623711
18	O	-4.249927	-1.915732	-2.160275
19	O	-2.391532	-2.226523	-0.366535
20	O	-4.347670	-0.516219	-0.104415
21	C	-4.370174	-0.166176	1.309805
22	C	-3.631570	1.166403	1.488197
23	H	-3.750037	1.449513	2.540912
24	H	-5.416920	-0.084173	1.602867
25	H	-3.885064	-0.940383	1.908377
26	O	-0.887091	3.458232	0.573973
27	H	-1.611156	3.855755	0.066117
28	Ca	-0.031143	-1.991970	-0.382076
29	O	3.606396	-2.319335	1.583618
30	H	2.706023	-2.479609	1.898602
31	H	4.692659	-1.637726	3.124509
32	O	-4.854148	-2.947246	0.057611
33	H	4.674001	1.146619	-1.129474
34	H	-4.550119	-3.869214	0.058625
35	O	5.154816	-0.802507	3.324176

36	H	-3.540353	-1.621314	-2.753189
37	H	4.707943	-0.280570	1.810552
38	C	-4.290854	2.275153	0.661229
39	O	-3.717113	2.998582	-0.126318
40	O	-5.603271	2.356372	0.923274
41	H	-5.975596	3.073212	0.379741
42	N	-2.203975	1.107395	1.180415
43	H	-1.732908	0.498363	1.845530
44	H	-2.073210	0.699887	0.256493
45	H	-1.329718	2.638814	0.936005
46	O	4.324402	-2.297246	-0.707738
47	H	4.410967	-1.768958	-1.536045
48	H	4.604184	-0.370517	3.992778

E[B3LYP/6-31G(d,p)] = -2840.210332 h, E[APFD/6-311+G(2d,p)] = -2839.453296 h
Gcorr[B3LYP/6-31G(d,p)] = 0.28594 h

135. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 6th step, products

Center No.	Atom	X	Y	Z
1	P	3.735159	-2.196698	0.105033
2	O	4.204683	-2.094961	1.606828
3	O	2.250218	-2.052045	-0.097938
4	O	3.818977	1.253288	-0.424233
5	C	3.341339	1.964074	-1.575598
6	C	3.284985	3.455763	-1.192801
7	C	2.112532	3.756611	-0.250392
8	O	0.961485	3.299312	-0.713125
9	O	2.253644	4.373782	0.794520
10	N	4.539788	3.772796	-0.505524
11	H	5.227167	4.152458	-1.148679
12	H	4.353860	4.461953	0.219231
13	H	0.196118	3.489949	-0.059308
14	H	3.115295	4.046002	-2.104255
15	H	4.026154	1.824569	-2.421422
16	H	2.357748	1.576829	-1.840323
17	P	-3.800393	-1.783719	-1.051795
18	O	-4.380888	-1.496271	-2.504624
19	O	-2.323579	-2.008771	-0.997776
20	O	-4.322406	-0.543380	-0.202159
21	C	-4.085863	-0.437684	1.231479
22	C	-3.396576	0.902968	1.513288
23	H	-3.349355	1.003272	2.604290
24	H	-5.058531	-0.495122	1.720254
25	H	-3.453190	-1.256458	1.581996
26	O	-1.030926	3.599589	0.894763
27	H	-1.784282	4.006552	0.441776
28	Ca	0.016299	-1.989217	-0.703785
29	O	4.280766	-3.634137	-0.362859
30	H	3.888060	-3.927528	-1.199130
31	H	2.900313	-4.470170	3.109622
32	O	-4.685861	-2.988723	-0.506445
33	H	4.477961	1.889717	-0.049299
34	H	-4.345206	-3.866617	-0.742433
35	O	2.865926	-3.526385	3.321783
36	H	-3.783002	-0.983358	-3.071617
37	H	3.664364	-2.646772	2.256233
38	C	-4.245858	2.071104	1.002362
39	O	-3.857394	2.944665	0.255420
40	O	-5.492317	2.011981	1.493588
41	H	-5.991059	2.770866	1.142544
42	N	-2.039990	1.015496	0.980725
43	H	-1.432501	0.337744	1.435866
44	H	-2.037505	0.800570	-0.014848
45	H	-1.354509	2.664706	1.030091
46	O	4.612590	-1.160887	-0.690428
47	H	4.310239	-0.189572	-0.601970
48	H	1.923104	-3.310506	3.353563

E[B3LYP/6-31G(d,p)] = -2840.244841 h, E[APFD/6-311+G(2d,p)] = -2839.483739 h
Gcorr[B3LYP/6-31G(d,p)] = 0.278752 h

136. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 7th step, reactants (hydrolysed serine neglected)

Center No.	Atom	X	Y	Z
1	P	-4.845763	0.089293	0.030126
2	O	-5.172564	1.647325	0.006871
3	O	-3.412625	-0.260363	-0.210742
4	P	2.402328	-0.899573	0.505772
5	O	2.705846	-1.029186	2.068831
6	O	1.093959	-1.608354	0.235297
7	O	2.329472	0.681478	0.285958
8	C	2.415422	1.269004	-1.041956
9	C	1.760319	2.658353	-0.976349
10	H	1.939890	3.119819	-1.954961
11	H	3.467792	1.333203	-1.325416
12	H	1.878842	0.649736	-1.766330
13	O	3.739686	-3.801846	-0.934093
14	H	2.838229	-4.168552	-0.710516
15	Ca	-1.161109	-0.931746	-0.188016
16	O	-5.869370	-0.520288	-1.025772
17	H	-5.667829	-1.435040	-1.279822
18	H	1.221969	-4.870093	0.610062
19	O	3.616988	-1.381707	-0.345710
20	H	3.679716	-2.408812	-0.587217
21	O	1.238255	-4.377336	-0.222393
22	H	3.561900	-0.658959	2.337363
23	H	-4.738305	2.127109	-0.716470
24	C	2.481714	3.514069	0.064850
25	O	1.994927	3.912415	1.100351
26	O	3.755139	3.754437	-0.301338
27	H	4.175640	4.268604	0.410183
28	N	0.331217	2.673178	-0.703515
29	H	-0.154972	2.122168	-1.406551
30	H	0.151117	2.242536	0.200669
31	H	4.365750	-4.261772	-0.356764
32	O	-5.435904	-0.386308	1.430339
33	H	-4.841292	-0.225780	2.180507
34	H	1.061518	-3.447978	0.031668

E[B3LYP/6-31G(d,p)] = -2441.234542 h, E[APFD/6-311+G(2d,p)] = -2440.654193 h
Gcorr[B3LYP/6-31G(d,p)] = 0.175997 h

137. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 7th step, TS

Center No.	Atom	X	Y	Z
1	P	4.914014	-0.443446	0.043479
2	O	5.532066	-1.516798	-0.956403
3	O	3.422399	-0.346436	0.015968
4	P	-2.255543	1.460910	0.122205
5	O	-2.576180	1.368357	1.720005
6	O	-0.776532	1.690256	-0.361773
7	O	-2.230227	-0.227590	0.061714
8	C	-2.384821	-0.986585	-1.139827
9	C	-2.309449	-2.479391	-0.761176
10	H	-2.507357	-3.044245	-1.679891
11	H	-3.344845	-0.764685	-1.612150
12	H	-1.582107	-0.757027	-1.853361
13	O	-2.524792	3.280072	0.358494
14	H	-1.402528	4.003709	-0.012495
15	Ca	1.160545	0.290862	-0.031894
16	O	5.691080	0.894784	-0.331730
17	H	5.335101	1.688690	0.098308
18	H	0.207626	4.420947	0.220446
19	O	-3.454100	1.539301	-0.970997
20	H	-3.737970	2.464698	-1.045181
21	O	-0.413284	4.089276	-0.447788
22	H	-2.664541	0.430491	1.957613
23	H	5.101867	-1.532531	-1.826269
24	C	-3.434348	-2.794826	0.220571
25	O	-3.287727	-3.061251	1.394851

26	O	-4.642273	-2.709861	-0.371586
27	H	-5.315355	-2.878255	0.311005
28	N	-1.046668	-2.933647	-0.191174
29	H	-0.289994	-2.718579	-0.835990
30	H	-0.867435	-2.414430	0.665591
31	H	-2.831843	3.447867	1.261201
32	O	5.537199	-0.845438	1.452338
33	H	5.059893	-1.561901	1.900623
34	H	-0.371110	2.999037	-0.480744

E[B3LYP/6-31G(d,p)] = -2441.186183 h, E[APFD/6-311+G(2d,p)] = -2440.603784 h
Gcorr[B3LYP/6-31G(d,p)] = 0.181117 h

138. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 7th step, products

Center No.	Atom	X	Y	Z
1	P	4.852869	-0.350085	0.066389
2	O	5.446196	-1.447959	-0.921448
3	O	3.366063	-0.200493	0.018488
4	P	-2.410205	1.394119	0.231259
5	O	-2.467603	1.142163	1.841065
6	O	-0.977448	1.743460	-0.479173
7	O	-2.105368	-0.266081	0.041171
8	C	-2.303554	-0.986737	-1.180707
9	C	-2.109951	-2.487875	-0.889033
10	H	-2.379427	-3.014297	-1.812911
11	H	-3.308290	-0.810491	-1.569189
12	H	-1.572921	-0.671332	-1.936766
13	O	-2.716191	3.057369	0.525963
14	H	-1.487834	4.412042	-0.245840
15	Ca	1.117920	0.470667	-0.028369
16	O	5.678668	0.960472	-0.301494
17	H	5.335414	1.767773	0.113885
18	H	0.031810	4.660631	-0.159013
19	O	-3.720626	1.305331	-0.722333
20	H	-4.139110	2.180853	-0.745765
21	O	-0.656370	4.319787	-0.748592
22	H	-2.405808	0.188237	2.013889
23	H	5.028660	-1.451444	-1.797629
24	C	-3.103963	-2.913296	0.187070
25	O	-2.813284	-3.227464	1.322446
26	O	-4.371807	-2.867346	-0.265362
27	H	-4.956775	-3.104465	0.475563
28	N	-0.774292	-2.903987	-0.481214
29	H	-0.089797	-2.552053	-1.146065
30	H	-0.561944	-2.495489	0.425696
31	H	-2.946738	3.194908	1.455133
32	O	5.443486	-0.768088	1.484422
33	H	4.940167	-1.470117	1.927007
34	H	-0.806631	2.737542	-0.592027

E[B3LYP/6-31G(d,p)] = -2441.197207 h, E[APFD/6-311+G(2d,p)] = -2440.61695 h
Gcorr[B3LYP/6-31G(d,p)] = 0.182915 h

139. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 8th step, reactants

Center No.	Atom	X	Y	Z
1	P	-4.963157	0.451169	-0.147325
2	O	-5.865282	0.953904	1.063333
3	O	-3.841945	-0.457576	0.248069
4	P	2.107960	-1.536483	-0.250090
5	O	2.473811	-1.978609	1.248299
6	O	0.546421	-1.757260	-0.813724
7	O	1.669627	0.008988	0.284604
8	C	1.417021	1.116149	-0.588771
9	C	2.308476	2.322088	-0.205296
10	H	2.011363	3.137986	-0.875411
11	H	1.576937	0.847641	-1.635310
12	H	0.370870	1.419606	-0.460754
13	O	2.487337	-3.102724	-0.816881

14	H	1.355325	0.330387	2.434398
15	Ca	-1.642028	-1.274955	0.345953
16	O	-4.529883	1.805440	-0.864141
17	H	-3.885979	1.682262	-1.579997
18	H	1.507431	-0.324460	3.828737
19	O	3.184842	-0.901829	-1.287995
20	H	3.622497	-1.632400	-1.754333
21	O	2.000809	-0.074873	3.034502
22	H	2.343990	-1.270657	1.944288
23	H	-5.362427	1.137039	1.872917
24	C	3.771218	2.009708	-0.492740
25	O	4.596196	1.711170	0.346015
26	O	4.046283	2.088176	-1.808069
27	H	4.972052	1.814020	-1.929688
28	N	2.196680	2.779423	1.175164
29	H	1.218122	2.925568	1.412002
30	H	2.560717	2.062637	1.798666
31	H	2.684858	-3.683128	-0.069303
32	O	-6.011722	-0.179917	-1.165560
33	H	-6.253759	-1.096801	-0.958327
34	H	0.537531	-2.633630	-1.238645

E[B3LYP/6-31G(d,p)] = -2441.192708 h, E[APFD/6-311+G(2d,p)] = -2440.617352 h
Gcorr[B3LYP/6-31G(d,p)] = 0.181756 h

140. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 8th step, TS

Center No.	Atom	X	Y	Z
1	P	-4.898565	0.444086	-0.156609
2	O	-5.800063	0.910091	1.068987
3	O	-3.771677	-0.468670	0.213292
4	P	2.155012	-1.683982	-0.111620
5	O	2.213528	-1.973957	1.398320
6	O	0.672353	-1.744231	-0.887793
7	O	1.703570	0.085741	0.227503
8	C	1.535912	1.107083	-0.762307
9	C	2.304244	2.386307	-0.359034
10	H	2.130493	3.108992	-1.165739
11	H	1.896159	0.736366	-1.723073
12	H	0.470931	1.352188	-0.856299
13	O	2.517692	-3.246632	-0.666174
14	H	1.402053	0.257210	1.450817
15	Ca	-1.564677	-1.273885	0.256877
16	O	-4.474554	1.819477	-0.837975
17	H	-3.841959	1.718488	-1.567277
18	H	0.442634	-0.122378	2.855582
19	O	3.374450	-1.053734	-0.981237
20	H	3.855488	-1.794590	-1.385082
21	O	1.362475	-0.025817	2.563369
22	H	1.746243	-0.994920	2.262653
23	H	-5.296046	1.070816	1.882533
24	C	3.799135	2.094852	-0.317558
25	O	4.445490	1.936204	0.697473
26	O	4.323029	2.007123	-1.553108
27	H	5.258284	1.755340	-1.458146
28	N	1.915179	2.986417	0.912119
29	H	0.902224	3.053680	0.972558
30	H	2.233810	2.399266	1.679014
31	H	2.570661	-3.835566	0.099315
32	O	-5.945455	-0.165732	-1.189361
33	H	-6.178925	-1.090474	-1.008877
34	H	0.646085	-2.611547	-1.329910

E[B3LYP/6-31G(d,p)] = -2441.174058 h, E[APFD/6-311+G(2d,p)] = -2440.600614 h
Gcorr[B3LYP/6-31G(d,p)] = 0.179388 h

141. 2PS6Ca+4H_2O, gly1:gly2:ser1:ser2, 8th step, products

Center No.	Atom	X	Y	Z
1	P	4.600600	0.175367	-0.028027

2	O	4.870618	-0.910370	1.105008
3	O	3.163926	0.379061	-0.388541
4	P	-2.612026	2.138308	0.136275
5	O	-2.195273	1.696299	1.493995
6	O	-1.330956	1.943057	-0.869836
7	O	-0.177903	-1.413766	0.440158
8	C	-0.413586	-2.701903	-0.132583
9	C	-1.922802	-3.042607	-0.251349
10	H	-1.986716	-3.919330	-0.907406
11	H	0.050828	-2.696994	-1.121380
12	H	0.064340	-3.483094	0.470685
13	O	-3.058866	3.662055	-0.012931
14	H	-0.657403	-1.302058	1.307606
15	Ca	0.825129	0.631532	-0.384489
16	O	5.527997	-0.308463	-1.228179
17	H	5.363926	0.161155	-2.061719
18	H	-1.221818	-0.682970	3.405334
19	O	-3.835888	1.438239	-0.567312
20	H	-3.757464	0.441496	-0.595856
21	O	-1.643307	-0.785959	2.541771
22	H	-1.909716	0.115710	2.253019
23	H	4.353127	-1.724610	0.998396
24	C	-2.620940	-1.894805	-0.962535
25	O	-3.425452	-1.149794	-0.417672
26	O	-2.229891	-1.759698	-2.229360
27	H	-2.690279	-1.001217	-2.630404
28	N	-2.621111	-3.334657	0.992842
29	H	-2.164064	-4.120276	1.449086
30	H	-2.556224	-2.539659	1.628201
31	H	-2.555601	4.263235	0.558468
32	O	5.348547	1.469841	0.519271
33	H	4.812658	2.001792	1.128928
34	H	-1.493469	2.245529	-1.778950

E[B3LYP/6-31G(d,p)] = -2441.236699 h, E[APFD/6-311+G(2d,p)] = -2440.65196 h
Gcorr[B3LYP/6-31G(d,p)] = 0.180181 h

XI. Structures of molecules and transition states (TS) related to 2PC6Ca + 4 H_2O, where the hydrolysis proceeds in the sequence cho1:cho2:gly1:gly2, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

142. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 1st step, reactants

Center No.	Atom	X	Y	Z
1	P	2.738926	-0.631430	-1.649348
2	C	4.139500	-2.694574	-2.537431
3	H	3.346239	-2.708571	-3.290703
4	H	5.099282	-2.794721	-3.047654
5	C	3.951133	-3.775208	-1.464610
6	H	4.805745	-3.765407	-0.785968
7	H	3.045967	-3.563207	-0.894884
8	C	3.749657	0.792680	0.368671
9	H	3.405198	-0.089017	0.916169
10	H	3.294296	1.680974	0.815555
11	C	5.268858	0.897618	0.430242
12	H	5.725520	0.092990	-0.148661
13	C	6.486421	2.166633	-1.220359
14	C	5.769824	0.870770	1.864900
15	H	5.404627	1.733773	2.429067
16	H	5.437809	-0.040346	2.371275
17	C	7.844705	0.906010	3.009792
18	C	6.751568	3.584939	-1.675563
19	H	5.781654	4.043743	-1.905797
20	H	7.141164	4.140902	-0.813507
21	C	5.021791	-5.605189	-2.791657
22	H	5.056335	-5.012431	-3.703600
23	H	5.919302	-5.440713	-2.196613
24	H	4.928553	-6.660403	-3.045059
25	C	2.567896	-5.362671	-2.803616
26	H	2.474645	-6.409979	-3.087509
27	H	1.714301	-5.058360	-2.199539
28	H	2.641212	-4.746795	-3.697189

29	C	3.716492	-6.107496	-0.772349
30	H	2.845922	-5.805620	-0.191445
31	H	3.605173	-7.134531	-1.117524
32	H	4.625154	-6.006088	-0.180414
33	N	3.819556	-5.202446	-1.976766
34	C	7.703087	3.678737	-2.868863
35	H	8.655650	3.201066	-2.609498
36	H	7.290358	3.102554	-3.705688
37	C	7.952520	5.125667	-3.309067
38	H	6.994287	5.600075	-3.564296
39	H	8.360399	5.699210	-2.464589
40	C	8.906658	5.238557	-4.504241
41	H	8.498430	4.664964	-5.347334
42	H	9.863487	4.763832	-4.248112
43	C	9.344877	0.960821	2.825970
44	H	9.632208	0.122527	2.179063
45	H	9.573781	1.867032	2.250752
46	C	10.120938	0.934480	4.143555
47	H	9.794734	1.772975	4.770512
48	H	9.863532	0.022426	4.695649
49	C	11.637899	1.002802	3.934994
50	H	11.889143	1.916544	3.377898
51	H	11.958205	0.162938	3.302195
52	C	12.429923	0.977417	5.247930
53	H	12.108178	1.816480	5.879528
54	H	12.177946	0.064134	5.803727
55	O	7.255125	0.871366	4.071892
56	O	6.948684	1.163527	-1.724987
57	O	7.208811	0.901269	1.815202
58	O	5.647960	2.164627	-0.154852
59	O	2.117424	-0.303274	-2.979359
60	O	1.925555	-1.399385	-0.614935
61	O	3.307788	0.741499	-0.998380
62	O	4.166902	-1.427569	-1.871190
63	C	13.945567	1.046857	5.038898
64	H	14.231070	1.966539	4.515493
65	H	14.482042	1.026900	5.993156
66	H	14.301468	0.201463	4.438950
67	C	9.154783	6.685009	-4.942415
68	H	9.594692	7.274636	-4.129924
69	H	9.838776	6.732555	-5.796064
70	H	8.219745	7.175071	-5.237101
71	O	-0.564543	0.200653	-2.959730
72	H	0.405633	0.020499	-3.015635
73	H	-0.967494	-0.662868	-2.737348
74	Ca	-0.190704	-2.199776	-0.093521
75	O	0.667917	-4.487640	0.423890
76	H	0.100068	-5.245571	0.222826
77	H	0.988398	-4.642414	1.324418
78	O	-0.896910	1.575659	-0.704895
79	H	-0.771599	1.131416	-1.591787
80	H	-1.468936	2.337845	-0.861602
81	O	-1.748643	-0.485989	0.736209
82	H	-2.606131	-0.703514	0.327706
83	H	-1.484617	0.366421	0.288095
84	P	-3.202339	-2.340782	-2.070992
85	C	-4.910652	-4.084865	-1.021368
86	H	-5.528509	-3.616625	-1.791440
87	H	-4.897692	-5.162628	-1.195889
88	C	-5.370590	-3.737530	0.397444
89	H	-4.729181	-4.246605	1.119248
90	H	-5.298152	-2.661095	0.551663
91	C	-4.281604	0.086843	-1.751952
92	H	-4.614265	-0.103107	-2.775666
93	H	-3.422093	0.765949	-1.768722
94	C	-5.419586	0.681960	-0.937288
95	H	-6.238351	-0.035114	-0.861662
96	C	-5.422465	0.277853	1.446107
97	C	-5.917906	1.987826	-1.530656
98	H	-5.151054	2.765807	-1.480428
99	H	-6.203280	1.848148	-2.577234
100	C	-7.662614	3.542477	-1.137050

101	C	-4.749201	0.713257	2.726537
102	H	-3.673262	0.542176	2.591265
103	H	-4.866974	1.801061	2.806279
104	C	-7.035088	-5.597807	0.556724
105	H	-6.967097	-5.845653	-0.500718
106	H	-6.285214	-6.147099	1.125297
107	H	-8.032176	-5.836404	0.924345
108	C	-7.783145	-3.336025	-0.089876
109	H	-8.790288	-3.592207	0.236395
110	H	-7.590018	-2.275765	0.067926
111	H	-7.661265	-3.600523	-1.138283
112	C	-7.025552	-3.770414	2.197440
113	H	-6.846255	-2.703144	2.322643
114	H	-8.053803	-4.020298	2.456585
115	H	-6.334401	-4.352181	2.805932
116	N	-6.801485	-4.121665	0.744713
117	C	-5.272803	0.005427	3.976506
118	H	-6.353870	0.169437	4.059920
119	H	-5.133277	-1.076747	3.865040
120	C	-4.576318	0.485233	5.255213
121	H	-3.492627	0.325851	5.162405
122	H	-4.716503	1.570166	5.361871
123	C	-5.085012	-0.217504	6.519673
124	H	-4.944756	-1.301510	6.411320
125	H	-6.167987	-0.058196	6.609907
126	C	-8.848451	3.853945	-0.251923
127	H	-9.525624	2.991334	-0.289789
128	H	-8.486447	3.897373	0.783135
129	C	-9.575037	5.143528	-0.636889
130	H	-8.868229	5.981131	-0.598701
131	H	-9.908435	5.072415	-1.679242
132	C	-10.774290	5.435814	0.271866
133	H	-10.434470	5.501515	1.315235
134	H	-11.476431	4.590873	0.233188
135	C	-11.514944	6.725844	-0.100760
136	H	-10.812462	7.569313	-0.061864
137	H	-11.853144	6.659330	-1.143662
138	O	-7.268194	4.213390	-2.069843
139	O	-6.287066	-0.576620	1.351968
140	O	-7.066508	2.386349	-0.760132
141	O	-4.921761	0.962096	0.394633
142	O	-1.684499	-2.209125	-1.952644
143	O	-3.861475	-2.388749	-3.408845
144	O	-3.886286	-1.151148	-1.130953
145	O	-3.553639	-3.627106	-1.120641
146	C	-12.713324	7.016191	0.807710
147	H	-12.401069	7.121595	1.853027
148	H	-13.220406	7.942001	0.516954
149	H	-13.449286	6.205212	0.763140
150	C	-4.389443	0.262888	7.796794
151	H	-4.541498	1.337422	7.949868
152	H	-4.773607	-0.256800	8.680577
153	H	-3.308873	0.085690	7.749542

E[B3LYP/6-31G(d,p)] = -4551.898100 h, E[APFD/6-311+G(2d,p)] = -4550.157324 h
Gcorr[B3LYP/6-31G(d,p)] = 1.170068 h

143. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 1st step, TS

Center No.	Atom	X	Y	Z
1	P	2.589035	-1.095300	-0.156142
2	C	4.034870	-2.958463	-1.392582
3	H	3.159634	-2.956210	-2.047807
4	H	4.927998	-2.892327	-2.017878
5	C	4.068781	-4.191282	-0.481605
6	H	4.961372	-4.154407	0.145355
7	H	3.182679	-4.186035	0.152450
8	C	4.442958	-0.246121	1.623266
9	H	4.642808	-1.311814	1.740870
10	H	4.258317	0.195355	2.605897
11	C	5.626469	0.438094	0.949642

12	H	5.732412	0.075005	-0.072798
13	C	5.221977	2.464160	-0.288009
14	C	6.913604	0.216749	1.725983
15	H	6.871024	0.687604	2.712281
16	H	7.103764	-0.852248	1.859644
17	C	9.215898	0.733672	1.496537
18	C	4.955310	3.942044	-0.106593
19	H	4.066774	4.040433	0.529728
20	H	5.783841	4.357023	0.481161
21	C	5.311972	-5.676708	-2.063393
22	H	5.264123	-4.947704	-2.869781
23	H	6.200286	-5.510715	-1.454874
24	H	5.325415	-6.682625	-2.480521
25	C	2.846068	-5.732629	-2.018954
26	H	2.855463	-6.745177	-2.420514
27	H	1.980158	-5.588227	-1.373930
28	H	2.839361	-5.015887	-2.837199
29	C	4.125325	-6.611832	-0.127419
30	H	3.223571	-6.524239	0.476713
31	H	4.159045	-7.584624	-0.616539
32	H	5.012082	-6.469657	0.488476
33	N	4.091821	-5.539465	-1.189642
34	C	4.778010	4.699489	-1.423087
35	H	5.677124	4.570462	-2.037627
36	H	3.953732	4.249906	-1.989792
37	C	4.506129	6.192863	-1.209691
38	H	3.606850	6.315326	-0.589395
39	H	5.333071	6.636731	-0.637317
40	C	4.325382	6.968259	-2.520313
41	H	3.499456	6.523519	-3.091719
42	H	5.224432	6.845357	-3.139241
43	C	10.238294	1.397831	0.601463
44	H	10.174844	0.921764	-0.385130
45	H	9.917561	2.435894	0.447106
46	C	11.663300	1.337670	1.153399
47	H	11.685815	1.805251	2.145118
48	H	11.948485	0.289344	1.303442
49	C	12.679737	2.024143	0.234115
50	H	12.385848	3.072595	0.083177
51	H	12.650238	1.553910	-0.759069
52	C	14.113846	1.974065	0.774940
53	H	14.141597	2.443565	1.767544
54	H	14.406247	0.926098	0.925761
55	O	9.439535	0.197669	2.564025
56	O	5.300594	1.885115	-1.352847
57	O	7.977874	0.806284	0.954993
58	O	5.366037	1.860022	0.917431
59	O	2.291732	-0.499293	-1.591000
60	O	1.745790	-2.235896	0.374391
61	O	3.230918	-0.020668	0.870852
62	O	4.041511	-1.808060	-0.548718
63	C	15.128672	2.660831	-0.143867
64	H	14.881070	3.719041	-0.285888
65	H	16.141333	2.608610	0.269172
66	H	15.147984	2.190546	-1.133690
67	C	4.053002	8.459976	-2.305006
68	H	4.878142	8.939076	-1.765639
69	H	3.928677	8.985341	-3.257560
70	H	3.140662	8.614855	-1.717667
71	O	-0.015073	0.588105	-1.887347
72	H	1.360668	-0.109731	-1.765543
73	H	-0.713701	-0.085990	-1.936109
74	Ca	-0.411183	-3.135089	0.490290
75	O	0.785807	-5.302632	0.942968
76	H	0.304018	-6.125976	0.777032
77	H	1.140890	-5.394882	1.839198
78	O	0.762509	0.259467	0.452104
79	H	0.166148	0.661762	-0.875423
80	H	1.116818	0.974708	0.994866
81	O	-1.284187	-0.992379	1.174205
82	H	-1.928275	-0.704755	0.506478
83	H	-0.439225	-0.406885	0.979695

84	P	-2.877192	-2.340131	-1.987146
85	C	-5.359568	-3.132163	-1.371803
86	H	-5.779421	-2.286433	-1.923406
87	H	-5.347932	-3.999883	-2.036864
88	C	-6.123559	-3.404583	-0.075715
89	H	-5.763787	-4.327840	0.381369
90	H	-5.954958	-2.572781	0.608733
91	C	-3.372896	0.327821	-2.091098
92	H	-3.680284	0.073270	-3.109089
93	H	-2.674922	1.168437	-2.127607
94	C	-4.600351	0.692577	-1.259682
95	H	-5.318303	-0.127826	-1.237203
96	C	-4.845899	0.393177	1.120756
97	C	-5.264478	1.945195	-1.809128
98	H	-4.606408	2.812539	-1.705294
99	H	-5.504870	1.817663	-2.868916
100	C	-7.187390	3.264428	-1.386455
101	C	-4.210457	0.757516	2.442035
102	H	-3.189126	0.354196	2.423560
103	H	-4.099147	1.848342	2.468785
104	C	-7.995167	-4.688442	-1.126129
105	H	-7.630742	-4.480286	-2.130217
106	H	-7.543212	-5.601836	-0.741212
107	H	-9.080111	-4.784541	-1.142351
108	C	-8.248587	-2.265139	-0.726284
109	H	-9.331052	-2.350507	-0.642145
110	H	-7.879086	-1.436411	-0.123141
111	H	-7.975458	-2.124034	-1.770009
112	C	-8.182390	-3.823855	1.163837
113	H	-7.940938	-2.981990	1.811272
114	H	-9.261944	-3.944609	1.088644
115	H	-7.727172	-4.736518	1.546088
116	N	-7.631161	-3.545246	-0.213902
117	C	-4.985411	0.246485	3.657588
118	H	-6.005918	0.647789	3.632458
119	H	-5.083542	-0.843763	3.590763
120	C	-4.313568	0.624440	4.982547
121	H	-3.289716	0.224448	4.999666
122	H	-4.214303	1.717438	5.043291
123	C	-5.075609	0.116768	6.212660
124	H	-5.174825	-0.975392	6.150282
125	H	-6.098374	0.516818	6.193840
126	C	-8.424201	3.383181	-0.524391
127	H	-9.008577	2.463780	-0.656922
128	H	-8.099907	3.376037	0.523777
129	C	-9.266986	4.621233	-0.833804
130	H	-8.650414	5.518873	-0.703871
131	H	-9.560626	4.602794	-1.890263
132	C	-10.515975	4.718734	0.049442
133	H	-10.215760	4.731643	1.106860
134	H	-11.127966	3.815071	-0.082098
135	C	-11.371198	5.956256	-0.248430
136	H	-10.758558	6.858334	-0.116726
137	H	-11.669536	5.942711	-1.305428
138	O	-6.849136	4.032621	-2.264753
139	O	-5.825166	-0.315503	0.977418
140	O	-6.473051	2.161432	-1.058650
141	O	-4.159452	0.949809	0.093696
142	O	-1.600197	-3.020607	-1.531233
143	O	-3.377689	-2.411631	-3.392319
144	O	-2.636230	-0.762216	-1.515876
145	O	-4.034683	-2.837316	-0.920987
146	C	-12.619443	6.052716	0.633806
147	H	-12.350946	6.102126	1.695299
148	H	-13.207885	6.945292	0.397539
149	H	-13.268598	5.180144	0.497703
150	C	-4.403425	0.494230	7.536052
151	H	-4.321274	1.582000	7.641951
152	H	-4.970499	0.118269	8.393875
153	H	-3.390979	0.079033	7.598209

E[B3LYP/6-31G(d,p)] = -4551.843999 h, E[APFD/6-311+G(2d,p)] = -4550.103574 h

Gcorr[B3LYP/6-31G(d,p)] = 1.176736 h

144. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 1st step, products

Center No.	Atom	X	Y	Z
1	P	2.407099	-0.977911	0.126956
2	C	3.996975	-2.843914	-1.029441
3	H	3.146899	-2.855013	-1.717077
4	H	4.909392	-2.737655	-1.626485
5	C	4.038579	-4.117196	-0.175387
6	H	4.882397	-4.068109	0.515662
7	H	3.111339	-4.187442	0.392404
8	C	4.405992	-0.188594	1.884323
9	H	4.631727	-1.248372	1.999231
10	H	4.302333	0.267258	2.873989
11	C	5.527636	0.501161	1.116415
12	H	5.529362	0.160124	0.081891
13	C	5.114213	2.579078	-0.034569
14	C	6.880069	0.249392	1.760129
15	H	6.936575	0.692886	2.758630
16	H	7.069809	-0.824305	1.846514
17	C	9.162424	0.707408	1.305731
18	C	4.883362	4.055292	0.206501
19	H	4.019120	4.150108	0.875914
20	H	5.739904	4.433819	0.778584
21	C	5.495850	-5.479879	-1.684889
22	H	5.502360	-4.713762	-2.457318
23	H	6.308404	-5.311096	-0.979208
24	H	5.595048	-6.463532	-2.142246
25	C	3.046620	-5.624738	-1.904306
26	H	3.141714	-6.611998	-2.354947
27	H	2.112491	-5.551089	-1.349177
28	H	3.092565	-4.862288	-2.678925
29	C	4.156991	-6.553022	0.067925
30	H	3.193011	-6.531240	0.573769
31	H	4.287428	-7.498266	-0.458099
32	H	4.965819	-6.406183	0.782457
33	N	4.188187	-5.430336	-0.938901
34	C	4.678570	4.859888	-1.077708
35	H	5.552430	4.730038	-1.727478
36	H	3.824849	4.447791	-1.629131
37	C	4.450337	6.351668	-0.809605
38	H	3.575227	6.476104	-0.156023
39	H	5.306360	6.758104	-0.252365
40	C	4.245820	7.170837	-2.089836
41	H	3.390766	6.763439	-2.646080
42	H	5.120660	7.045106	-2.742015
43	C	10.106520	1.380812	0.334322
44	H	9.909619	0.964526	-0.661616
45	H	9.818685	2.437976	0.272143
46	C	11.580850	1.232260	0.712904
47	H	11.740832	1.652003	1.713368
48	H	11.828798	0.166400	0.785745
49	C	12.517620	1.913931	-0.290736
50	H	12.262611	2.980803	-0.362402
51	H	12.348675	1.492913	-1.292057
52	C	14.000434	1.771812	0.073626
53	H	14.168222	2.193094	1.074039
54	H	14.253430	0.705406	0.146223
55	O	9.481443	0.109092	2.314548
56	O	5.148600	2.040691	-1.123333
57	O	7.877071	0.849710	0.909644
58	O	5.280683	1.928743	1.141394
59	O	2.395441	-0.519438	-1.436346
60	O	1.609936	-2.223536	0.543843
61	O	3.134666	0.004068	1.250302
62	O	3.931130	-1.743988	-0.144965
63	C	14.935626	2.451688	-0.930828
64	H	14.728933	3.525848	-0.999634
65	H	15.985451	2.332584	-0.643607
66	H	14.814588	2.027266	-1.934083

67	C	4.018015	8.661508	-1.822105
68	H	4.872145	9.104282	-1.297019
69	H	3.875700	9.217972	-2.754279
70	H	3.129579	8.820643	-1.200280
71	O	-0.043850	0.645844	-2.004725
72	H	1.547182	-0.095108	-1.710738
73	H	-0.693932	-0.076866	-2.034350
74	Ca	-0.418147	-3.322770	0.391405
75	O	0.724938	-5.504127	0.876933
76	H	0.290167	-6.321930	0.594555
77	H	0.967735	-5.653169	1.802423
78	O	0.985365	0.154695	0.432907
79	H	0.114010	0.758629	-1.041595
80	H	1.289255	0.858060	1.022808
81	O	-1.286233	-1.113916	1.017861
82	H	-1.873404	-0.796170	0.309614
83	H	-0.450273	-0.578998	0.916195
84	P	-2.853519	-2.403177	-2.082475
85	C	-5.332500	-3.180852	-1.430876
86	H	-5.763764	-2.351135	-1.997761
87	H	-5.318039	-4.063151	-2.076301
88	C	-6.083895	-3.432456	-0.123048
89	H	-5.720970	-4.349226	0.344468
90	H	-5.907277	-2.590719	0.547204
91	C	-3.331971	0.267084	-2.192367
92	H	-3.649234	0.006721	-3.205571
93	H	-2.636876	1.109085	-2.239372
94	C	-4.550509	0.632707	-1.349152
95	H	-5.264931	-0.189838	-1.308273
96	C	-4.773346	0.373811	1.038552
97	C	-5.224022	1.876897	-1.907174
98	H	-4.565402	2.746057	-1.824020
99	H	-5.477122	1.734183	-2.962062
100	C	-7.140473	3.202789	-1.482506
101	C	-4.124933	0.761881	2.346656
102	H	-3.114137	0.332616	2.336802
103	H	-3.986294	1.849706	2.340726
104	C	-7.967597	-4.720734	-1.146414
105	H	-7.615426	-4.517804	-2.156005
106	H	-7.510982	-5.632091	-0.762151
107	H	-9.052641	-4.817027	-1.149316
108	C	-8.214224	-2.294783	-0.757940
109	H	-9.295864	-2.378118	-0.662222
110	H	-7.837750	-1.463076	-0.163261
111	H	-7.951623	-2.159829	-1.805123
112	C	-8.130358	-3.842416	1.140445
113	H	-7.880213	-2.997479	1.780533
114	H	-9.210912	-3.961059	1.077322
115	H	-7.673346	-4.754002	1.523052
116	N	-7.592981	-3.572666	-0.244594
117	C	-4.906915	0.306443	3.579642
118	H	-5.918733	0.728441	3.543459
119	H	-5.028164	-0.783014	3.548567
120	C	-4.223571	0.714447	4.889745
121	H	-3.208900	0.292400	4.919067
122	H	-4.099652	1.806398	4.912149
123	C	-4.993843	0.267629	6.138161
124	H	-5.116512	-0.823676	6.115362
125	H	-6.007823	0.688652	6.106168
126	C	-8.368509	3.336200	-0.610231
127	H	-8.955461	2.415835	-0.723190
128	H	-8.034116	3.344554	0.434751
129	C	-9.212054	4.570914	-0.930949
130	H	-8.592710	5.469228	-0.820395
131	H	-9.514971	4.536751	-1.984382
132	C	-10.453119	4.684943	-0.038655
133	H	-10.143890	4.714066	1.015833
134	H	-11.068124	3.780699	-0.150630
135	C	-11.308051	5.919591	-0.349234
136	H	-10.692258	6.822177	-0.237150
137	H	-11.615123	5.889785	-1.403398
138	O	-6.810336	3.957367	-2.375561

139	O	-5.756467	-0.333351	0.917496
140	O	-6.423558	2.103884	-1.145856
141	O	-4.092891	0.907460	-0.004988
142	O	-1.582461	-3.100052	-1.636793
143	O	-3.372542	-2.474407	-3.480315
144	O	-2.581962	-0.821093	-1.624768
145	O	-4.006967	-2.863362	-0.996626
146	C	-12.548746	6.033377	0.541504
147	H	-12.271430	6.099315	1.599821
148	H	-13.136972	6.923488	0.295583
149	H	-13.201058	5.160353	0.424832
150	C	-4.311061	0.678338	7.446156
151	H	-4.205822	1.767262	7.512463
152	H	-4.884137	0.345760	8.317783
153	H	-3.307451	0.244402	7.521973

E[B3LYP/6-31G(d,p)] = -4551.851041 h, E[APFD/6-311+G(2d,p)] = -4550.109115 h
Gcorr[B3LYP/6-31G(d,p)] = 1.178938 h

145. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 2nd step, reactants

Center No.	Atom	X	Y	Z
1	P	-4.353498	-0.619886	-2.567764
2	C	-7.051222	-0.544064	-1.729121
3	H	-6.930827	0.463374	-2.140312
4	H	-7.988696	-0.960288	-2.120702
5	C	-7.075983	-0.501273	-0.195734
6	H	-7.161719	-1.517331	0.193994
7	H	-6.143390	-0.055020	0.146172
8	C	-2.641430	-2.739378	-2.627931
9	H	-2.377693	-2.319873	-3.599299
10	H	-2.899577	-3.796768	-2.750134
11	C	-1.438302	-2.623809	-1.694729
12	H	-1.197523	-1.579234	-1.503414
13	C	-1.875349	-2.553346	0.688831
14	C	-0.230379	-3.343928	-2.266248
15	H	-0.412657	-4.418996	-2.347229
16	H	0.004328	-2.956504	-3.261847
17	C	2.039558	-3.721983	-1.713925
18	C	-2.204980	-3.439106	1.867905
19	H	-2.893259	-4.218844	1.526196
20	H	-1.274694	-3.958087	2.137998
21	C	-9.547151	-0.308168	0.135383
22	H	-9.724571	-0.257473	-0.936729
23	H	-9.547413	-1.345560	0.468168
24	H	-10.316117	0.254837	0.663343
25	C	-8.176725	1.733771	-0.012970
26	H	-8.930232	2.290884	0.543022
27	H	-7.184748	2.137466	0.187110
28	H	-8.399528	1.774970	-1.076914
29	C	-7.995377	0.276706	1.941426
30	H	-7.046943	0.764680	2.161924
31	H	-8.814763	0.813246	2.418829
32	H	-7.977333	-0.758854	2.278686
33	N	-8.205989	0.299631	0.448875
34	C	-2.766107	-2.682526	3.074341
35	H	-2.057098	-1.902009	3.372879
36	H	-3.688647	-2.166123	2.780027
37	C	-3.051976	-3.607770	4.262611
38	H	-3.754438	-4.394314	3.953075
39	H	-2.125724	-4.123501	4.553431
40	C	-3.623341	-2.869032	5.478858
41	H	-4.547038	-2.351964	5.185819
42	H	-2.919552	-2.084314	5.787677
43	C	3.133105	-3.404197	-0.719025
44	H	3.336985	-2.327280	-0.790961
45	H	2.727501	-3.564745	0.287044
46	C	4.408286	-4.220386	-0.937935
47	H	4.160626	-5.288441	-0.906625
48	H	4.793214	-4.025314	-1.945725
49	C	5.490991	-3.912920	0.102176

50	H	5.094689	-4.104264	1.109485
51	H	5.734868	-2.841226	0.070573
52	C	6.772706	-4.729999	-0.100432
53	H	6.525599	-5.799824	-0.072581
54	H	7.169881	-4.535398	-1.105724
55	O	2.153065	-4.426044	-2.697497
56	O	-1.697751	-1.344446	0.767619
57	O	0.879743	-3.107928	-1.379351
58	O	-1.777707	-3.268794	-0.438210
59	O	-4.881120	-0.537878	-4.109866
60	O	-4.551153	0.492836	-1.519527
61	O	-3.800480	-2.110371	-2.080794
62	O	-5.992106	-1.397063	-2.107365
63	C	7.851756	-4.427911	0.943517
64	H	7.494635	-4.645639	1.956616
65	H	8.752350	-5.026427	0.772127
66	H	8.143909	-3.371627	0.916790
67	C	-3.909893	-3.794574	6.665011
68	H	-2.997520	-4.299618	7.002139
69	H	-4.316573	-3.238851	7.516183
70	H	-4.636236	-4.569766	6.395431
71	O	-6.799732	-2.526713	-4.383500
72	H	-5.669293	-1.106177	-4.266666
73	H	-7.712011	-2.238860	-4.521948
74	Ca	-3.584997	2.469280	-0.837440
75	O	-4.786359	2.323125	1.330069
76	H	-5.031282	3.132511	1.800893
77	H	-4.423897	1.733771	2.006835
78	O	-2.840080	-0.086575	-3.143206
79	H	-6.634043	-2.390790	-3.419490
80	H	-2.325775	0.254390	-2.389707
81	O	-1.645634	0.988556	-0.701410
82	H	-0.809645	1.490877	-0.624727
83	H	-1.587962	0.184144	-0.145432
84	P	-0.405969	4.306710	-1.216835
85	C	0.937840	5.546042	0.719778
86	H	1.701981	5.458361	-0.056074
87	H	0.769138	6.607600	0.918021
88	C	1.301719	4.771088	1.987581
89	H	0.492157	4.863556	2.713941
90	H	1.444357	3.719355	1.740102
91	C	1.318478	2.349628	-1.909330
92	H	1.607220	3.145587	-2.599142
93	H	0.820754	1.550570	-2.470021
94	C	2.550352	1.813115	-1.195222
95	H	3.004123	2.601935	-0.594020
96	C	2.340275	0.866394	1.016927
97	C	3.568809	1.255916	-2.174220
98	H	3.186567	0.365432	-2.681833
99	H	3.822682	2.004635	-2.929223
100	C	5.847879	0.599671	-2.133239
101	C	1.894359	-0.374217	1.754846
102	H	0.891288	-0.639623	1.400635
103	H	2.548627	-1.191370	1.424582
104	C	2.453944	6.639996	3.180585
105	H	2.384359	7.307845	2.324314
106	H	1.564503	6.728450	3.803399
107	H	3.343785	6.880220	3.761164
108	C	3.773739	5.078139	1.801509
109	H	4.662165	5.323606	2.382035
110	H	3.818365	4.047951	1.451515
111	H	3.683061	5.769305	0.965974
112	C	2.757868	4.308734	3.893214
113	H	2.849835	3.285754	3.530621
114	H	3.661400	4.612844	4.420255
115	H	1.891729	4.408125	4.546381
116	N	2.569921	5.217250	2.700745
117	C	1.935241	-0.233536	3.277508
118	H	2.941636	0.074659	3.583733
119	H	1.258812	0.573285	3.585923
120	C	1.552081	-1.532163	3.996238
121	H	0.547051	-1.843832	3.678412

122	H	2.233213	-2.336066	3.682972
123	C	1.584404	-1.408913	5.524381
124	H	0.900986	-0.607723	5.836622
125	H	2.588118	-1.092890	5.839098
126	C	7.016796	0.292568	-1.224364
127	H	7.146501	1.148382	-0.550268
128	H	6.724010	-0.546233	-0.579738
129	C	8.310008	-0.018253	-1.979374
130	H	8.141852	-0.871666	-2.647108
131	H	8.561889	0.830751	-2.626339
132	C	9.483016	-0.318157	-1.039455
133	H	9.224635	-1.168595	-0.392247
134	H	9.641658	0.537684	-0.368072
135	C	10.788712	-0.627281	-1.781880
136	H	10.628642	-1.481971	-2.452888
137	H	11.046038	0.222901	-2.427953
138	O	5.861556	0.582319	-3.347756
139	O	2.829533	1.855105	1.536909
140	O	4.743169	0.913062	-1.414266
141	O	2.139469	0.737157	-0.312089
142	O	-1.878710	3.978609	-1.362072
143	O	0.328705	5.092162	-2.254289
144	O	0.398992	2.866971	-0.929619
145	O	-0.302595	4.983169	0.275474
146	C	11.959808	-0.927658	-0.841665
147	H	11.745078	-1.794734	-0.206580
148	H	12.876026	-1.143557	-1.400861
149	H	12.165215	-0.077380	-0.181255
150	C	1.209968	-2.709144	6.241860
151	H	1.897078	-3.520291	5.975258
152	H	1.242806	-2.589042	7.329605
153	H	0.197575	-3.032330	5.973056

E[B3LYP/6-31G(d,p)] = -4551.848241 h, E[APFD/6-311+G(2d,p)] = -4550.118655 h
Gcorr[B3LYP/6-31G(d,p)] = 1.181379 h

146. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 2nd step, TS

Center No.	Atom	X	Y	Z
1	P	-4.070511	-1.048028	-2.602281
2	C	-7.130939	-0.932537	-1.854343
3	H	-6.936075	0.032303	-2.346559
4	H	-8.096463	-1.305993	-2.238079
5	C	-7.216804	-0.724949	-0.332625
6	H	-7.385802	-1.688857	0.151627
7	H	-6.270783	-0.309334	0.014989
8	C	-2.653843	-3.249368	-2.080435
9	H	-2.389542	-3.116968	-3.131342
10	H	-3.036795	-4.263987	-1.937625
11	C	-1.413225	-3.041654	-1.217719
12	H	-1.095522	-2.000470	-1.254616
13	C	-1.726188	-2.457091	1.115263
14	C	-0.277848	-3.953564	-1.648748
15	H	-0.526353	-5.004361	-1.476489
16	H	-0.064372	-3.817276	-2.712693
17	C	1.999575	-4.320174	-1.116821
18	C	-2.060482	-3.060768	2.459111
19	H	-2.867719	-3.786127	2.312279
20	H	-1.184349	-3.649265	2.764891
21	C	-9.677414	-0.324899	-0.138663
22	H	-9.804171	-0.341537	-1.218910
23	H	-9.766524	-1.333015	0.264806
24	H	-10.425613	0.326190	0.312502
25	C	-8.153802	1.593498	-0.374993
26	H	-8.915090	2.237776	0.064320
27	H	-7.160158	1.958491	-0.117152
28	H	-8.278750	1.555158	-1.454837
29	C	-8.171114	0.292602	1.692986
30	H	-7.194968	0.717941	1.922842
31	H	-8.962140	0.931489	2.085492
32	H	-8.256880	-0.710052	2.110004

33	N	-8.310886	0.208894	0.195245
34	C	-2.419247	-2.029901	3.531584
35	H	-1.595384	-1.314785	3.636745
36	H	-3.290517	-1.451120	3.199205
37	C	-2.720559	-2.678575	4.887439
38	H	-3.537449	-3.404736	4.772052
39	H	-1.844752	-3.255071	5.217889
40	C	-3.096453	-1.662100	5.972227
41	H	-3.970777	-1.086428	5.639505
42	H	-2.279378	-0.936946	6.085985
43	C	3.159940	-3.827907	-0.281776
44	H	3.349817	-2.787151	-0.576019
45	H	2.829619	-3.785454	0.763170
46	C	4.425177	-4.674053	-0.431609
47	H	4.208771	-5.705309	-0.126994
48	H	4.703946	-4.719965	-1.490937
49	C	5.597476	-4.126065	0.390035
50	H	5.309574	-4.074346	1.449702
51	H	5.806861	-3.091831	0.080788
52	C	6.875458	-4.962484	0.253498
53	H	6.666809	-5.994017	0.567785
54	H	7.158454	-5.018438	-0.806280
55	O	2.031610	-5.232154	-1.918493
56	O	-1.444679	-1.279141	0.939627
57	O	0.881433	-3.594500	-0.873551
58	O	-1.755089	-3.386259	0.150881
59	O	-4.515488	-1.396957	-4.091627
60	O	-4.526442	0.184992	-1.840434
61	O	-3.711834	-2.360441	-1.689504
62	O	-6.113871	-1.856499	-2.076422
63	C	8.048313	-4.407451	1.067102
64	H	7.806397	-4.369297	2.135427
65	H	8.944008	-5.026201	0.950504
66	H	8.303290	-3.389574	0.749768
67	C	-3.396900	-2.310826	7.326678
68	H	-2.529036	-2.865795	7.700755
69	H	-3.661729	-1.560612	8.078829
70	H	-4.232399	-3.016070	7.250884
71	O	-6.474250	-3.118203	-4.181486
72	H	-5.306567	-2.018797	-4.193803
73	H	-7.250073	-2.739868	-4.617034
74	Ca	-3.752744	2.148028	-0.878968
75	O	-4.907396	2.087075	1.320833
76	H	-5.148890	2.910671	1.767994
77	H	-4.558152	1.509803	2.014564
78	O	-2.538768	-0.635870	-3.075461
79	H	-6.479917	-2.724276	-3.219040
80	H	-2.118720	-0.096039	-2.373774
81	O	-1.665736	0.822545	-0.817669
82	H	-0.890653	1.422857	-0.814344
83	H	-1.505876	0.101828	-0.172880
84	P	-0.773160	4.231824	-1.413847
85	C	0.426064	5.593436	0.539059
86	H	1.179851	5.636036	-0.250633
87	H	0.119061	6.614883	0.777878
88	C	0.914899	4.832244	1.773358
89	H	0.108668	4.777843	2.507299
90	H	1.205758	3.822360	1.485005
91	C	1.137389	2.474783	-2.155405
92	H	1.320425	3.301209	-2.845638
93	H	0.725970	1.625322	-2.711564
94	C	2.433697	2.081908	-1.463231
95	H	2.810200	2.919840	-0.875352
96	C	2.415744	1.118034	0.749593
97	C	3.486969	1.623270	-2.457661
98	H	3.176606	0.708818	-2.971045
99	H	3.670539	2.397855	-3.207752
100	C	5.762252	0.955973	-2.421361
101	C	2.150590	-0.169427	1.493912
102	H	1.139212	-0.507480	1.237293
103	H	2.827810	-0.923664	1.073325
104	C	1.802774	6.806600	3.023385

105	H	1.624943	7.485572	2.192146
106	H	0.920339	6.745460	3.659307
107	H	2.658039	7.152477	3.602160
108	C	3.312519	5.496260	1.578177
109	H	4.164087	5.852939	2.156289
110	H	3.502780	4.494020	1.197045
111	H	3.109208	6.189094	0.764024
112	C	2.447988	4.522751	3.652600
113	H	2.675857	3.533973	3.256462
114	H	3.309143	4.935409	4.177056
115	H	1.588268	4.481398	4.320309
116	N	2.114295	5.431918	2.492891
117	C	2.336288	-0.057059	3.008016
118	H	3.345319	0.314830	3.221315
119	H	1.641563	0.693646	3.404448
120	C	2.116444	-1.393730	3.725614
121	H	1.106139	-1.765752	3.504064
122	H	2.812354	-2.142796	3.321710
123	C	2.299849	-1.301439	5.245255
124	H	1.602458	-0.554675	5.648336
125	H	3.308417	-0.925743	5.464292
126	C	6.945867	0.695517	-1.516929
127	H	7.079973	1.575687	-0.876685
128	H	6.664170	-0.121129	-0.838906
129	C	8.230591	0.357560	-2.274844
130	H	8.052419	-0.514248	-2.915414
131	H	8.480605	1.186195	-2.948737
132	C	9.410524	0.080236	-1.336596
133	H	9.154153	-0.750680	-0.663652
134	H	9.577508	0.953999	-0.690801
135	C	10.709219	-0.254009	-2.080340
136	H	10.541299	-1.126934	-2.725460
137	H	10.963873	0.576632	-2.752375
138	O	5.736703	0.814433	-3.627636
139	O	2.816909	2.153066	1.255177
140	O	4.690052	1.373640	-1.707437
141	O	2.159248	0.974518	-0.567648
142	O	-2.201511	3.744947	-1.560094
143	O	-0.134102	5.110813	-2.438811
144	O	0.179955	2.879395	-1.158537
145	O	-0.736524	4.885706	0.091063
146	C	11.886944	-0.531064	-1.141241
147	H	11.674811	-1.378978	-0.479935
148	H	12.798077	-0.765648	-1.701218
149	H	12.100007	0.337097	-0.507033
150	C	2.086285	-2.638932	5.960121
151	H	2.792708	-3.396409	5.601846
152	H	2.224042	-2.540315	7.041771
153	H	1.074337	-3.023192	5.787050

E[B3LYP/6-31G(d,p)] = -4551.844511 h, E[APFD/6-311+G(2d,p)] = -4550.113811 h
Gcorr[B3LYP/6-31G(d,p)] = 1.179772 h

147. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 2nd step, products

Center No.	Atom	X	Y	Z
1	P	3.538353	0.257619	-2.569463
2	C	7.765603	2.347532	-1.983884
3	H	7.804267	1.761481	-2.909924
4	H	8.793204	2.610666	-1.710025
5	C	7.082029	1.557417	-0.857850
6	H	7.095957	2.154748	0.056236
7	H	6.043330	1.361997	-1.127398
8	C	3.231679	2.745660	-1.635722
9	H	3.020838	2.920541	-2.695271
10	H	4.013819	3.443806	-1.323710
11	C	1.966171	2.952039	-0.809074
12	H	1.232868	2.182800	-1.054079
13	C	1.906687	1.755758	1.287216
14	C	1.374160	4.335231	-1.003240
15	H	2.044839	5.111855	-0.625054

16	H	1.188177	4.524223	-2.064440
17	C	-0.551937	5.538524	-0.324739
18	C	2.436454	1.782691	2.701489
19	H	3.528797	1.863364	2.639678
20	H	2.099200	2.722450	3.156813
21	C	9.103700	0.362901	-0.005634
22	H	9.726507	0.733661	-0.817401
23	H	9.111691	1.065670	0.826994
24	H	9.467490	-0.610303	0.322558
25	C	7.650838	-0.736783	-1.669005
26	H	8.040610	-1.701549	-1.344541
27	H	6.613871	-0.836334	-1.993609
28	H	8.275048	-0.342457	-2.468028
29	C	6.847170	-0.384846	0.610605
30	H	5.831504	-0.501346	0.236330
31	H	7.261798	-1.353726	0.886225
32	H	6.867366	0.289293	1.466331
33	N	7.688818	0.206401	-0.492245
34	C	2.016606	0.578803	3.545760
35	H	0.921943	0.523318	3.578757
36	H	2.356957	-0.342741	3.057196
37	C	2.574850	0.641760	4.972020
38	H	3.671585	0.702801	4.932381
39	H	2.235224	1.568251	5.455940
40	C	2.165560	-0.558572	5.833960
41	H	2.503530	-1.483994	5.347919
42	H	1.069451	-0.617557	5.873097
43	C	-1.834670	5.448555	0.471038
44	H	-2.426109	4.625310	0.050179
45	H	-1.573660	5.131049	1.488231
46	C	-2.637014	6.750487	0.486673
47	H	-2.014678	7.553132	0.900568
48	H	-2.868549	7.044030	-0.544222
49	C	-3.933653	6.631582	1.295333
50	H	-3.695187	6.331642	2.325858
51	H	-4.551360	5.823504	0.878375
52	C	-4.750398	7.929245	1.323192
53	H	-4.131952	8.735955	1.739319
54	H	-4.987768	8.228116	0.293255
55	O	-0.156612	6.508998	-0.939607
56	O	1.180049	0.887540	0.823250
57	O	0.131242	4.370437	-0.276596
58	O	2.324337	2.824246	0.594001
59	O	3.974550	0.763960	-3.920142
60	O	4.231518	-0.950335	-1.946350
61	O	3.746205	1.424598	-1.424839
62	O	7.026115	3.537335	-2.166669
63	C	-6.045353	7.808680	2.132000
64	H	-5.837160	7.543654	3.174932
65	H	-6.604999	8.749729	2.133152
66	H	-6.699482	7.032617	1.718322
67	C	2.725388	-0.495454	7.258095
68	H	2.376735	0.402589	7.780635
69	H	2.416399	-1.364678	7.847694
70	H	3.821046	-0.469482	7.251661
71	O	5.470802	2.953163	-4.287963
72	H	4.947740	2.119230	-4.159666
73	H	6.057607	2.772972	-5.033909
74	Ca	3.481096	-2.887580	-0.848154
75	O	4.546638	-2.899603	1.379945
76	H	5.205148	-3.573614	1.597394
77	H	4.022827	-2.782979	2.184127
78	O	1.938589	0.017246	-2.631297
79	H	6.405616	3.371571	-2.919884
80	H	1.629306	-0.517493	-1.860896
81	O	1.424665	-1.535950	-0.423217
82	H	0.612669	-2.084893	-0.486666
83	H	1.276035	-0.818533	0.225347
84	P	0.394198	-4.862708	-1.069500
85	C	-0.848875	-5.807659	1.085914
86	H	-1.583252	-6.012417	0.303167
87	H	-0.586535	-6.751296	1.569817

88	C	-1.336480	-4.762257	2.092617
89	H	-0.550905	-4.577608	2.827637
90	H	-1.565727	-3.831591	1.573534
91	C	-1.327176	-3.076176	-2.107702
92	H	-1.548299	-3.965007	-2.703054
93	H	-0.789694	-2.350485	-2.727660
94	C	-2.621521	-2.476054	-1.582902
95	H	-3.100463	-3.172621	-0.893493
96	C	-2.655376	-1.145020	0.433060
97	C	-3.573990	-2.117014	-2.711654
98	H	-3.157490	-1.332131	-3.349049
99	H	-3.783265	-2.994070	-3.330783
100	C	-5.767591	-1.246677	-2.944237
101	C	-2.368810	0.246213	0.945755
102	H	-1.335120	0.497152	0.680800
103	H	-2.998443	0.933125	0.364693
104	C	-2.382620	-6.397754	3.669323
105	H	-2.273780	-7.237405	2.985663
106	H	-1.489515	-6.290429	4.283909
107	H	-3.255362	-6.553075	4.302206
108	C	-3.774593	-5.279783	1.964705
109	H	-4.656394	-5.470684	2.575259
110	H	-3.891732	-4.351870	1.406698
111	H	-3.608830	-6.119179	1.292289
112	C	-2.861690	-3.994885	3.840897
113	H	-3.004375	-3.084130	3.260544
114	H	-3.760870	-4.233601	4.407623
115	H	-2.011063	-3.894040	4.514070
116	N	-2.585308	-5.129544	2.881848
117	C	-2.613916	0.416923	2.445630
118	H	-3.644725	0.127045	2.680873
119	H	-1.965821	-0.273974	2.999286
120	C	-2.357937	1.852745	2.918186
121	H	-1.328019	2.141153	2.664926
122	H	-3.011799	2.540564	2.363521
123	C	-2.582903	2.043975	4.422784
124	H	-1.927934	1.357021	4.975761
125	H	-3.611577	1.752168	4.673889
126	C	-6.979027	-0.763766	-2.178760
127	H	-7.288224	-1.570397	-1.502355
128	H	-6.651397	0.056199	-1.526954
129	C	-8.134460	-0.323187	-3.078650
130	H	-7.785280	0.468992	-3.751765
131	H	-8.431846	-1.161032	-3.720858
132	C	-9.345267	0.171663	-2.279525
133	H	-9.039996	1.008041	-1.634767
134	H	-9.686960	-0.624788	-1.603278
135	C	-10.513986	0.617558	-3.166560
136	H	-10.171128	1.412669	-3.842330
137	H	-10.817945	-0.218888	-3.810298
138	O	-5.649608	-1.281336	-4.152792
139	O	-3.139036	-2.054498	1.086020
140	O	-4.789967	-1.650542	-2.098507
141	O	-2.308786	-1.254752	-0.867623
142	O	1.839757	-4.477188	-1.318056
143	O	-0.311092	-5.848854	-1.941794
144	O	-0.495982	-3.445049	-0.989731
145	O	0.354159	-5.273110	0.517942
146	C	-11.722668	1.112389	-2.366564
147	H	-11.457189	1.970735	-1.738813
148	H	-12.539079	1.422874	-3.026760
149	H	-12.108492	0.327225	-1.706291
150	C	-2.329467	3.479718	4.891802
151	H	-2.993676	4.186079	4.380430
152	H	-2.498244	3.584743	5.968507
153	H	-1.297876	3.787105	4.685030

E[B3LYP/6-31G(d,p)] = -4551.900526 h, E[APFD/6-311+G(2d,p)] = -4550.170383 h
Gcorr[B3LYP/6-31G(d,p)] = 1.176775 h

148. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 3rd step, reactants (hydrolised choline neglected)

Center No.	Atom	X	Y	Z
1	P	3.268112	2.094372	-3.641210
2	H	3.257255	-3.605509	-3.841180
3	C	1.884870	4.259170	-2.958790
4	H	1.530384	4.104407	-3.983233
5	H	2.241226	5.291107	-2.874151
6	C	0.740452	4.028067	-1.975398
7	H	0.466819	2.972578	-1.964349
8	C	1.372058	3.462182	0.288101
9	C	-0.464821	4.892621	-2.291974
10	H	-0.233869	5.955329	-2.174968
11	H	-0.793177	4.721576	-3.320932
12	C	-2.695939	5.168055	-1.546496
13	C	1.895334	4.053127	1.576525
14	H	2.635791	4.819165	1.323007
15	H	1.056407	4.591014	2.039709
16	C	2.469187	3.012570	2.541475
17	H	1.701046	2.261169	2.758616
18	H	3.294662	2.481821	2.051391
19	C	2.967771	3.636542	3.849847
20	H	3.721755	4.404103	3.625092
21	H	2.138374	4.159726	4.346426
22	C	3.568436	2.606569	4.814392
23	H	4.395713	2.084747	4.313966
24	H	2.814905	1.839215	5.038010
25	C	-3.716743	4.708221	-0.530295
26	H	-3.788385	3.615786	-0.600924
27	H	-3.304044	4.910541	0.466195
28	C	-5.087186	5.365333	-0.701393
29	H	-4.975065	6.454492	-0.640646
30	H	-5.466237	5.152915	-1.708394
31	C	-6.101998	4.890050	0.344425
32	H	-5.715068	5.102354	1.351368
33	H	-6.206508	3.797519	0.282427
34	C	-7.482181	5.539722	0.186962
35	H	-7.376091	6.631268	0.247731
36	H	-7.868275	5.326970	-0.819067
37	O	-2.873839	6.002426	-2.411762
38	O	1.095062	2.280654	0.125143
39	O	-1.516436	4.524022	-1.378498
40	O	1.215255	4.402207	-0.651845
41	O	3.339553	2.514259	-5.075301
42	O	4.459419	1.420924	-2.964398
43	O	2.981475	3.396010	-2.657099
44	O	3.140016	-2.632309	-3.809386
45	C	-8.494259	5.065343	1.234036
46	H	-8.150537	5.295209	2.249089
47	H	-9.468007	5.546412	1.095564
48	H	-8.646665	3.981588	1.174541
49	C	4.070971	3.225887	6.121832
50	H	3.258016	3.725655	6.660789
51	H	4.493977	2.466303	6.787301
52	H	4.849708	3.973274	5.931723
53	O	3.561082	-5.391277	-3.428902
54	H	4.488962	-5.544348	-3.652353
55	H	3.567698	-5.242123	-2.455759
56	Ca	4.826458	0.052681	-1.129040
57	O	5.410512	1.303206	0.921525
58	H	5.772862	2.199060	0.899362
59	H	5.754353	0.900426	1.730031
60	O	1.942491	1.165857	-3.440357
61	H	3.664637	-2.388911	-3.029489
62	H	1.978118	0.695491	-2.577139
63	O	2.352833	0.084578	-0.914079
64	H	1.982469	-0.789986	-0.679930
65	H	1.889354	0.771637	-0.391504
66	P	3.465015	-3.249437	-0.394170
67	C	3.173902	-3.840237	2.182841
68	H	2.661779	-4.684042	1.714847

69	H	3.977416	-4.227393	2.812319
70	C	2.219970	-2.927449	2.957842
71	H	2.785549	-2.099595	3.389288
72	H	1.462902	-2.529941	2.281771
73	C	0.963040	-3.273899	-1.376160
74	H	1.233463	-4.317491	-1.553149
75	H	1.019164	-2.732291	-2.324330
76	C	-0.420273	-3.217326	-0.749911
77	H	-0.417771	-3.755335	0.198911
78	C	-1.026360	-1.454112	0.779581
79	C	-1.478268	-3.794933	-1.675139
80	H	-1.598334	-3.181144	-2.572052
81	H	-1.210422	-4.810348	-1.980999
82	C	-3.794405	-4.299833	-1.585528
83	C	-1.529648	-0.031043	0.827005
84	H	-0.858267	0.589161	0.222767
85	H	-2.495624	-0.020260	0.304458
86	C	2.414033	-4.145681	5.132214
87	H	2.974273	-4.969603	4.694753
88	H	3.091440	-3.356430	5.456499
89	H	1.830431	-4.509041	5.977006
90	C	0.548031	-4.665210	3.600710
91	H	-0.024557	-5.048439	4.444417
92	H	-0.116531	-4.227924	2.856960
93	H	1.140295	-5.468689	3.167400
94	C	0.620910	-2.508066	4.757488
95	H	-0.058299	-2.106606	4.006398
96	H	0.063131	-2.960105	5.576685
97	H	1.278959	-1.728243	5.139057
98	N	1.466026	-3.579407	4.107325
99	C	-1.668407	0.523628	2.245658
100	H	-2.316470	-0.137966	2.832220
101	H	-0.686998	0.507345	2.736184
102	C	-2.227824	1.950485	2.267322
103	H	-1.584381	2.602521	1.660764
104	H	-3.215798	1.962251	1.785610
105	C	-2.347696	2.526588	3.683550
106	H	-1.360649	2.507020	4.165188
107	H	-2.992767	1.872444	4.285524
108	C	-5.020998	-4.256732	-0.702134
109	H	-4.783521	-4.797965	0.222233
110	H	-5.172709	-3.212624	-0.399913
111	C	-6.274925	-4.824505	-1.368628
112	H	-6.474242	-4.270505	-2.293751
113	H	-6.086031	-5.862408	-1.668520
114	C	-7.503577	-4.765289	-0.453921
115	H	-7.684820	-3.723672	-0.152866
116	H	-7.295666	-5.318118	0.473222
117	C	-8.771154	-5.330669	-1.105986
118	H	-8.978020	-4.777505	-2.032065
119	H	-8.588778	-6.371073	-1.407203
120	O	-3.748073	-4.704173	-2.730087
121	O	-0.872204	-2.180106	1.747412
122	O	-2.710918	-3.817523	-0.931793
123	O	-0.772394	-1.834606	-0.492178
124	O	4.354810	-2.256165	-1.124543
125	O	3.492833	-4.705522	-0.763259
126	O	1.906379	-2.684585	-0.451785
127	O	3.788505	-3.007630	1.185882
128	C	-9.997318	-5.271103	-0.190127
129	H	-10.224332	-4.238979	0.100551
130	H	-10.884913	-5.680785	-0.683209
131	H	-9.832623	-5.844445	0.729367
132	C	-2.899857	3.954702	3.711380
133	H	-3.900832	4.001155	3.267195
134	H	-2.972814	4.335614	4.735332
135	H	-2.255127	4.639073	3.147679

E[B3LYP/6-31G(d,p)] = -4299.539446 h, E[APFD/6-311+G(2d,p)] = -4297.963253 h
Gcorr[B3LYP/6-31G(d,p)] = 1.012021 h

149. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 3rd step, TS

Center No.	Atom	X	Y	Z
1	P	3.782869	2.264501	-3.103927
2	H	3.024063	-4.673191	-3.469281
3	C	2.403807	4.427991	-2.407290
4	H	2.179196	4.382785	-3.478068
5	H	2.779329	5.431146	-2.179976
6	C	1.135816	4.157645	-1.599766
7	H	0.818152	3.124303	-1.742110
8	C	1.516287	3.306164	0.629593
9	C	0.018386	5.117628	-1.958437
10	H	0.268315	6.143238	-1.671337
11	H	-0.167191	5.096129	-3.035748
12	C	-2.299203	5.377798	-1.548423
13	C	1.949108	3.717596	2.017771
14	H	2.705807	4.502741	1.919418
15	H	1.079950	4.196453	2.490050
16	C	2.453993	2.554643	2.876089
17	H	1.670289	1.791294	2.945025
18	H	3.308669	2.079141	2.378865
19	C	2.866222	3.002277	4.283125
20	H	3.636172	3.782983	4.207121
21	H	2.007171	3.468796	4.785684
22	C	3.397850	1.852836	5.147846
23	H	4.252925	1.386450	4.639750
24	H	2.627103	1.073729	5.225981
25	C	-3.475500	4.849458	-0.759095
26	H	-3.523384	3.764947	-0.915876
27	H	-3.243191	4.981483	0.305350
28	C	-4.801954	5.521326	-1.117829
29	H	-4.712657	6.602693	-0.959676
30	H	-4.998465	5.384385	-2.188195
31	C	-5.978123	4.972940	-0.302017
32	H	-5.774302	5.108946	0.769750
33	H	-6.059044	3.888246	-0.461118
34	C	-7.316587	5.635820	-0.649641
35	H	-7.234624	6.719517	-0.490586
36	H	-7.518939	5.499828	-1.720626
37	O	-2.328562	6.292907	-2.347340
38	O	1.219887	2.165480	0.299523
39	O	-1.166712	4.694827	-1.255313
40	O	1.461655	4.359102	-0.196201
41	O	4.064335	2.796894	-4.473698
42	O	4.841429	1.473065	-2.340383
43	O	3.424481	3.494505	-2.054227
44	O	2.869774	-3.482139	-3.180272
45	C	-8.490715	5.086621	0.166171
46	H	-8.332224	5.239186	1.239908
47	H	-9.430548	5.578703	-0.104681
48	H	-8.618426	4.010669	0.000863
49	C	3.817283	2.298295	6.551782
50	H	2.973488	2.738027	7.095608
51	H	4.192077	1.456456	7.142981
52	H	4.610580	3.053118	6.506450
53	O	3.152539	-5.841665	-3.324069
54	H	4.016564	-6.093646	-3.679247
55	H	3.311218	-5.468515	-2.125627
56	Ca	4.921299	-0.234214	-0.778247
57	O	5.490872	0.687575	1.425136
58	H	5.955598	1.525737	1.550289
59	H	5.689686	0.156841	2.207846
60	O	2.404088	1.395806	-3.161138
61	H	3.608266	-2.958659	-3.519703
62	H	2.310175	0.841609	-2.353195
63	O	2.435585	-0.032956	-0.777434
64	H	1.951492	-0.883519	-0.770898
65	H	1.955785	0.613014	-0.220322
66	P	3.260004	-3.331143	-1.171824
67	C	2.780964	-3.862750	1.446567
68	H	2.015591	-4.476151	0.965519

69	H	3.483724	-4.537391	1.949672
70	C	2.148586	-2.866468	2.421787
71	H	2.914461	-2.190461	2.806569
72	H	1.388083	-2.286954	1.899260
73	C	0.606443	-3.179820	-1.874386
74	H	0.752334	-4.216387	-2.185565
75	H	0.554960	-2.554740	-2.767748
76	C	-0.676248	-3.086196	-1.061514
77	H	-0.565971	-3.622850	-0.118344
78	C	-1.173920	-1.315543	0.505512
79	C	-1.862616	-3.634328	-1.839625
80	H	-2.063027	-3.034378	-2.731775
81	H	-1.675713	-4.666504	-2.148904
82	C	-4.169868	-4.040206	-1.471810
83	C	-1.627132	0.123746	0.573144
84	H	-0.902714	0.733795	0.021397
85	H	-2.565454	0.188151	0.006700
86	C	2.465469	-4.102274	4.568781
87	H	2.960635	-4.925712	4.058746
88	H	3.193756	-3.347511	4.862909
89	H	1.938076	-4.476500	5.445491
90	C	0.432889	-4.494701	3.233693
91	H	-0.095864	-4.820362	4.128772
92	H	-0.256364	-4.025535	2.533108
93	H	0.934847	-5.345424	2.776722
94	C	0.758700	-2.350638	4.371439
95	H	0.006829	-1.928788	3.705550
96	H	0.290811	-2.759571	5.266421
97	H	1.496233	-1.596837	4.645788
98	N	1.461444	-3.469929	3.642207
99	C	-1.809370	0.641859	2.000427
100	H	-2.493922	-0.021056	2.542510
101	H	-0.848571	0.589310	2.527411
102	C	-2.339753	2.079203	2.042134
103	H	-1.663346	2.734622	1.476419
104	H	-3.309550	2.124160	1.526638
105	C	-2.499432	2.619487	3.468548
106	H	-1.530265	2.570339	3.983270
107	H	-3.175565	1.960581	4.029876
108	C	-5.285015	-3.927478	-0.456604
109	H	-4.960213	-4.447065	0.453440
110	H	-5.369554	-2.869688	-0.176293
111	C	-6.623236	-4.472631	-0.957434
112	H	-6.908531	-3.941754	-1.873535
113	H	-6.501021	-5.525378	-1.239844
114	C	-7.738684	-4.342915	0.085793
115	H	-7.854627	-3.286589	0.367146
116	H	-7.444056	-4.871669	1.003409
117	C	-9.087129	-4.887692	-0.400583
118	H	-9.380485	-4.358757	-1.317426
119	H	-8.969413	-5.942763	-0.682399
120	O	-4.270923	-4.471553	-2.602998
121	O	-1.028158	-2.053677	1.465105
122	O	-3.000674	-3.588534	-0.959074
123	O	-0.947281	-1.690304	-0.772767
124	O	4.360358	-2.347907	-1.582948
125	O	3.377914	-4.892754	-1.126936
126	O	1.696670	-2.753099	-1.040826
127	O	3.486286	-3.076586	0.499167
128	C	-10.200852	-4.758524	0.642796
129	H	-10.364844	-3.710591	0.918905
130	H	-11.149201	-5.155784	0.266481
131	H	-9.950412	-5.306005	1.558687
132	C	-3.029466	4.055488	3.516259
133	H	-4.012846	4.131005	3.037928
134	H	-3.133771	4.409487	4.547135
135	H	-2.353813	4.744208	2.995762

E[B3LYP/6-31G(d,p)] = -4299.485822 h, E[APFD/6-311+G(2d,p)] = -4297.906697 h
Gcorr[B3LYP/6-31G(d,p)] = 1.011059 h

150. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 3rd step, products

Center No.	Atom	X	Y	Z
1	P	4.081193	2.201973	-2.852642
2	H	3.279666	-5.662804	-3.379659
3	C	2.557020	4.302083	-2.292001
4	H	2.424259	4.228531	-3.376319
5	H	2.894374	5.317574	-2.059273
6	C	1.227644	4.030201	-1.591591
7	H	0.947138	2.983773	-1.716579
8	C	1.371836	3.305279	0.716704
9	C	0.125238	4.942524	-2.094866
10	H	0.326250	5.986310	-1.836435
11	H	0.038349	4.866597	-3.182041
12	C	-2.224408	5.160595	-1.909701
13	C	1.640399	3.818268	2.112959
14	H	2.461303	4.541005	2.051201
15	H	0.757272	4.398244	2.413891
16	C	1.938687	2.719184	3.134984
17	H	1.094929	2.020251	3.170142
18	H	2.808287	2.138474	2.802151
19	C	2.201156	3.284111	4.535923
20	H	3.048160	3.983279	4.494955
21	H	1.332941	3.875428	4.859457
22	C	2.490947	2.199458	5.580363
23	H	3.352581	1.602384	5.251524
24	H	1.638210	1.508435	5.627461
25	C	-3.457627	4.639327	-1.207491
26	H	-3.462755	3.547101	-1.306716
27	H	-3.333381	4.835584	-0.134810
28	C	-4.759142	5.250427	-1.729290
29	H	-4.714706	6.340540	-1.619961
30	H	-4.843703	5.054457	-2.805127
31	C	-5.996370	4.706586	-1.006144
32	H	-5.905133	4.901941	0.071905
33	H	-6.032443	3.613349	-1.115393
34	C	-7.309708	5.309315	-1.519633
35	H	-7.272844	6.401518	-1.409410
36	H	-7.398566	5.115024	-2.597043
37	O	-2.198979	6.036071	-2.751938
38	O	1.121316	2.140100	0.439561
39	O	-1.109005	4.521978	-1.481038
40	O	1.416406	4.302445	-0.176223
41	O	4.616740	2.786551	-4.121804
42	O	4.971340	1.350610	-1.951877
43	O	3.552182	3.391038	-1.825854
44	O	2.848718	-3.909347	-3.025629
45	C	-8.545829	4.764003	-0.798317
46	H	-8.501240	4.973268	0.276631
47	H	-9.465785	5.212945	-1.186815
48	H	-8.628024	3.677865	-0.920174
49	C	2.764721	2.764887	6.977274
50	H	1.907418	3.339434	7.346029
51	H	2.965795	1.966580	7.699002
52	H	3.632612	3.434019	6.969736
53	O	3.649226	-6.477551	-2.977356
54	H	4.527507	-6.566508	-3.373216
55	H	3.796189	-5.368320	-1.655982
56	Ca	4.702642	-0.444405	-0.500338
57	O	5.036774	0.701507	1.687866
58	H	5.204465	1.653332	1.718387
59	H	5.580937	0.320782	2.390561
60	O	2.716375	1.379633	-3.199930
61	H	3.106240	-3.254871	-3.688879
62	H	2.447410	0.821563	-2.434322
63	O	2.254624	0.004835	-0.859061
64	H	1.771330	-0.842238	-0.868914
65	H	1.751309	0.662777	-0.337178
66	P	3.292345	-3.220633	-1.493972
67	C	3.257808	-3.261178	1.331981
68	H	2.649149	-4.128812	1.071198

69	H	4.143263	-3.622819	1.868269
70	C	2.453436	-2.273440	2.183995
71	H	3.056400	-1.392772	2.412840
72	H	1.563905	-1.964395	1.636734
73	C	0.568168	-3.359202	-1.839296
74	H	0.708359	-4.405853	-2.112748
75	H	0.444008	-2.777707	-2.757375
76	C	-0.667177	-3.243315	-0.959974
77	H	-0.481543	-3.702072	0.012313
78	C	-1.206161	-1.391134	0.494903
79	C	-1.869729	-3.891689	-1.629798
80	H	-2.121192	-3.385948	-2.566152
81	H	-1.665449	-4.944066	-1.846579
82	C	-4.163634	-4.258720	-1.165587
83	C	-1.749814	0.018477	0.471750
84	H	-1.052040	0.639877	-0.102198
85	H	-2.677307	-0.006529	-0.114554
86	C	3.109659	-3.155433	4.429889
87	H	3.673047	-3.978463	3.995532
88	H	3.747647	-2.279330	4.541957
89	H	2.710452	-3.454729	5.398351
90	C	1.073057	-4.011975	3.335810
91	H	0.671452	-4.296773	4.307810
92	H	0.266718	-3.739373	2.656161
93	H	1.662423	-4.831664	2.930508
94	C	1.137488	-1.714800	4.174283
95	H	0.288850	-1.495793	3.527193
96	H	0.793558	-2.070097	5.145112
97	H	1.763567	-0.832147	4.300302
98	N	1.957271	-2.804375	3.526339
99	C	-1.991010	0.607329	1.862007
100	H	-2.653930	-0.057720	2.428035
101	H	-1.041309	0.636097	2.409443
102	C	-2.592391	2.015937	1.807079
103	H	-1.926493	2.673234	1.231097
104	H	-3.543078	1.985627	1.256146
105	C	-2.831696	2.621980	3.195370
106	H	-1.882360	2.644860	3.747544
107	H	-3.499619	1.962740	3.766035
108	C	-5.248634	-4.080662	-0.127515
109	H	-4.915019	-4.579391	0.791152
110	H	-5.297910	-3.012590	0.119551
111	C	-6.612429	-4.605982	-0.578480
112	H	-6.902769	-4.102001	-1.508147
113	H	-6.525663	-5.671542	-0.823076
114	C	-7.701795	-4.405528	0.480859
115	H	-7.781236	-3.336819	0.725696
116	H	-7.404512	-4.909783	1.411299
117	C	-9.074886	-4.926645	0.039404
118	H	-9.369647	-4.422780	-0.891025
119	H	-8.993814	-5.994333	-0.205390
120	O	-4.301208	-4.751398	-2.267489
121	O	-0.987060	-2.046630	1.499147
122	O	-2.975650	-3.789970	-0.714058
123	O	-0.980463	-1.840426	-0.760423
124	O	4.156679	-2.102698	-2.099217
125	O	3.827598	-4.656256	-0.964900
126	O	1.697367	-2.875828	-1.091567
127	O	3.666154	-2.573717	0.162364
128	C	-10.164559	-4.725880	1.096694
129	H	-10.292041	-3.664105	1.336849
130	H	-11.131152	-5.107419	0.751830
131	H	-9.913599	-5.247208	2.027563
132	C	-3.426329	4.032409	3.145329
133	H	-4.390701	4.037518	2.624294
134	H	-3.589980	4.433643	4.150872
135	H	-2.760251	4.724095	2.616483

E[B3LYP/6-31G(d,p)] = -4299.508012 h, E[APFD/6-311+G(2d,p)] = -4297.923940 h
Gcorr[B3LYP/6-31G(d,p)] = 1.018967 h

151. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 4th step, products (choline hydrolysed by proton transfer from neighboring OH, with no TS)

Center No.	Atom	X	Y	Z
1	P	2.327157	-2.273911	-2.776269
2	H	-1.908954	-4.890311	-1.297480
3	C	4.628244	-0.947123	-2.539966
4	H	4.169767	-0.405836	-3.373024
5	H	5.555631	-1.407938	-2.894797
6	C	4.924584	0.027456	-1.404369
7	H	3.993375	0.439520	-1.012217
8	C	4.947175	-0.957747	0.803869
9	C	5.854393	1.146902	-1.834186
10	H	6.847152	0.763454	-2.085691
11	H	5.450089	1.664229	-2.708908
12	C	6.739890	3.147028	-0.921823
13	C	5.828880	-1.708964	1.773062
14	H	6.424776	-2.427699	1.200642
15	H	6.546258	-0.982008	2.178512
16	C	5.052868	-2.392828	2.901641
17	H	4.475133	-1.638581	3.448221
18	H	4.323191	-3.085508	2.464360
19	C	5.971346	-3.145506	3.870720
20	H	6.552914	-3.895451	3.316163
21	H	6.704172	-2.445995	4.297343
22	C	5.209737	-3.836515	5.008312
23	H	4.477407	-4.534380	4.580157
24	H	4.628471	-3.086229	5.561149
25	C	6.764040	4.025987	0.308465
26	H	5.726433	4.294942	0.543363
27	H	7.104737	3.409152	1.149640
28	C	7.634917	5.273195	0.150079
29	H	8.660171	4.969005	-0.092898
30	H	7.277718	5.855865	-0.707587
31	C	7.639238	6.150896	1.406683
32	H	7.994224	5.560763	2.263497
33	H	6.608846	6.448329	1.648021
34	C	8.507497	7.406817	1.263369
35	H	9.536647	7.108370	1.022074
36	H	8.152379	7.994996	0.406414
37	O	7.332231	3.353590	-1.962236
38	O	3.803597	-0.599742	1.047811
39	O	5.952429	2.062557	-0.727488
40	O	5.591577	-0.706848	-0.344795
41	O	2.459303	-2.562439	-4.233734
42	O	1.666319	-3.274534	-1.827863
43	O	3.769950	-1.981066	-2.046192
44	O	-0.996354	-0.867967	-3.679877
45	C	8.510569	8.283635	2.519097
46	H	8.893174	7.732386	3.385720
47	H	9.138108	9.170864	2.385590
48	H	7.498742	8.625343	2.765538
49	C	6.126711	-4.588750	5.977318
50	H	6.847942	-3.910075	6.446820
51	H	5.554280	-5.070726	6.776565
52	H	6.696186	-5.368377	5.458564
53	O	-2.683696	-4.844877	-2.659124
54	H	-2.110184	-5.158086	-3.371595
55	H	-2.848341	-3.875597	-2.862129
56	Ca	0.047858	-2.994414	-0.088136
57	O	2.203971	-3.954503	0.724051
58	H	2.512943	-3.940765	-0.204567
59	H	2.314909	-4.862412	1.035651
60	O	1.554069	-0.823511	-2.610331
61	H	-0.086182	-0.817566	-3.304367
62	H	1.406979	-0.634906	-1.651225
63	O	1.257376	-0.777684	0.118504
64	H	0.752169	-0.033600	0.475546
65	H	2.172188	-0.691277	0.475376
66	P	-2.098271	-1.287707	-2.569306
67	C	-2.258490	-5.607110	0.530562

68	H	-1.944677	-5.322354	1.537289
69	H	-3.311189	-5.331473	0.407133
70	C	-2.030601	-7.103966	0.275545
71	H	-2.302942	-7.343456	-0.754325
72	H	-0.973959	-7.336515	0.419182
73	C	-2.326993	1.273759	-1.948171
74	H	-1.785118	1.727064	-2.786366
75	H	-1.613640	1.051094	-1.146660
76	C	-3.391709	2.235451	-1.441543
77	H	-4.179242	2.349048	-2.189262
78	C	-5.299863	1.394462	-0.232184
79	C	-2.803911	3.590434	-1.086413
80	H	-2.107792	3.513559	-0.246404
81	H	-2.270186	4.014621	-1.941831
82	C	-3.576850	5.701043	-0.330965
83	C	-5.701576	0.799857	1.099967
84	H	-5.114590	-0.117074	1.240371
85	H	-5.364447	1.487031	1.885848
86	C	-4.297714	-7.911506	0.949166
87	H	-4.610407	-6.925407	1.285382
88	H	-4.516525	-8.037680	-0.110381
89	H	-4.809698	-8.676078	1.531927
90	C	-2.482755	-7.853425	2.615066
91	H	-2.987583	-8.622565	3.197566
92	H	-1.404202	-7.931710	2.746201
93	H	-2.832931	-6.871106	2.925133
94	C	-2.414029	-9.472102	0.772833
95	H	-1.342717	-9.588230	0.930564
96	H	-2.964397	-10.174351	1.397629
97	H	-2.659941	-9.628917	-0.276560
98	N	-2.811917	-8.067603	1.159235
99	C	-7.199532	0.515681	1.217833
100	H	-7.757214	1.446950	1.060649
101	H	-7.502597	-0.161649	0.410501
102	C	-7.577980	-0.091474	2.573474
103	H	-7.013197	-1.022056	2.727295
104	H	-7.267079	0.589493	3.378508
105	C	-9.077576	-0.382313	2.708639
106	H	-9.387161	-1.062612	1.903785
107	H	-9.640841	0.547904	2.554223
108	C	-4.813903	6.497190	0.020622
109	H	-5.461544	6.508859	-0.865283
110	H	-5.367629	5.932241	0.780914
111	C	-4.510416	7.917523	0.499671
112	H	-3.853193	7.870006	1.376406
113	H	-3.945702	8.447254	-0.276933
114	C	-5.778987	8.705092	0.846008
115	H	-6.343024	8.166898	1.621017
116	H	-6.435421	8.745981	-0.034800
117	C	-5.491627	10.131892	1.329055
118	H	-4.835141	10.089681	2.208679
119	H	-4.927798	10.668492	0.554066
120	O	-2.430120	6.100203	-0.279619
121	O	-6.046086	1.600323	-1.167672
122	O	-3.903058	4.448859	-0.726375
123	O	-3.972338	1.670614	-0.243475
124	O	-1.384112	-1.598990	-1.259781
125	O	-3.062602	-2.294347	-3.147534
126	O	-2.981696	0.078352	-2.380704
127	O	-1.449437	-4.895062	-0.393465
128	C	-6.759873	10.917765	1.675021
129	H	-7.327192	10.422739	2.471518
130	H	-6.522044	11.930659	2.016051
131	H	-7.420492	11.005797	0.804897
132	C	-9.453947	-0.988743	4.063764
133	H	-9.187297	-0.315311	4.886381
134	H	-10.529175	-1.184652	4.129394
135	H	-8.931680	-1.937681	4.231426

E[B3LYP/6-31G(d,p)] = -4299.553400 h, E[APFD/6-311+G(2d,p)] = -4297.952654 h
Gcorr[B3LYP/6-31G(d,p)] = 1.007101 h

152. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 5th step, reactants (hydrolised choline neglected)

Center No.	Atom	X	Y	Z
1	P	-0.767653	-1.428204	-0.030708
2	C	-2.934868	-1.818727	-1.576243
3	H	-2.688671	-2.868045	-1.386697
4	H	-3.139026	-1.691207	-2.642475
5	C	-4.163885	-1.419159	-0.760169
6	H	-3.953622	-1.484118	0.307606
7	C	-4.153670	0.966629	-0.305935
8	C	-5.366508	-2.277818	-1.104849
9	H	-5.693333	-2.107309	-2.134434
10	H	-5.121238	-3.337197	-0.989335
11	C	-7.587567	-2.588209	-0.340896
12	C	-4.659292	2.285995	-0.827131
13	H	-5.575744	2.113368	-1.397335
14	H	-4.895398	2.917877	0.033900
15	C	-3.600658	2.980427	-1.713694
16	H	-2.728172	3.233749	-1.102304
17	H	-3.261667	2.283712	-2.490049
18	C	-4.144253	4.257528	-2.364491
19	H	-5.005995	4.009315	-2.999936
20	H	-4.522875	4.930192	-1.582015
21	C	-3.085693	4.995402	-3.193796
22	H	-2.696632	4.318698	-3.967140
23	H	-2.239491	5.240373	-2.540201
24	C	-8.613736	-2.114978	0.663875
25	H	-8.179270	-2.237030	1.664056
26	H	-8.735412	-1.032984	0.527148
27	C	-9.956035	-2.839353	0.552384
28	H	-10.350355	-2.713433	-0.463154
29	H	-9.797449	-3.916122	0.687243
30	C	-10.982877	-2.335750	1.572853
31	H	-11.134738	-1.255695	1.435701
32	H	-10.580355	-2.459936	2.588185
33	C	-12.334687	-3.053001	1.473555
34	H	-12.735134	-2.928972	0.458302
35	H	-12.181531	-4.132002	1.610502
36	O	-7.750936	-3.449382	-1.182176
37	O	-3.457271	0.846451	0.700935
38	O	-6.420044	-1.917835	-0.193076
39	O	-4.528502	-0.049264	-1.087377
40	O	-0.390330	-2.870575	-0.139302
41	O	0.292995	-0.339432	-0.099632
42	O	-1.807644	-0.987885	-1.269190
43	O	1.764062	4.779764	2.430723
44	C	-13.360629	-2.548879	2.492863
45	H	-13.559834	-1.479560	2.358076
46	H	-14.313522	-3.079550	2.396873
47	H	-13.002006	-2.691186	3.518736
48	C	-3.619872	6.270257	-3.853678
49	H	-3.987370	6.979805	-3.103395
50	H	-2.841482	6.775255	-4.435146
51	H	-4.451105	6.047895	-4.532724
52	Ca	1.158533	1.534417	-1.136143
53	O	-0.590737	1.007735	-2.772482
54	H	-1.107354	0.269914	-2.381755
55	H	-0.367371	0.734447	-3.671776
56	O	-1.694124	-1.219290	1.287768
57	H	1.702794	4.909819	3.388988
58	H	-2.252543	-0.415433	1.206144
59	O	2.264363	3.594714	-2.016598
60	H	2.224766	4.022101	-1.141758
61	H	3.193410	3.613211	-2.282869
62	P	1.413903	3.242644	2.019984
63	C	4.015221	2.792762	1.797263
64	H	4.461429	3.610143	2.374320
65	H	3.858176	3.134370	0.768796
66	C	4.944992	1.590631	1.804415
67	H	4.994678	1.155510	2.804450
68	C	4.195003	-0.660293	1.375408

69	C	6.341661	1.970454	1.322427
70	H	6.319753	2.339905	0.295915
71	H	6.769194	2.731622	1.979643
72	C	7.659653	0.281346	0.240949
73	C	3.628842	-1.551796	0.295564
74	H	2.564377	-1.294649	0.198009
75	H	4.096710	-1.281213	-0.657559
76	C	3.794422	-3.044926	0.595052
77	H	4.862399	-3.279238	0.693931
78	H	3.340891	-3.266478	1.568025
79	C	3.165761	-3.933353	-0.484662
80	H	2.094897	-3.702952	-0.561100
81	H	3.608855	-3.689336	-1.461332
82	C	3.346480	-5.431875	-0.212007
83	H	2.908189	-5.675878	0.765321
84	H	4.417963	-5.660330	-0.130133
85	C	8.508657	-0.936849	0.528011
86	H	9.305870	-0.629640	1.216461
87	H	7.888582	-1.642860	1.095008
88	C	9.084747	-1.592011	-0.727921
89	H	8.262874	-1.878952	-1.394956
90	H	9.681502	-0.854465	-1.278039
91	C	9.945129	-2.819749	-0.408541
92	H	9.343519	-3.553015	0.147134
93	H	10.764433	-2.526825	0.263250
94	C	10.530704	-3.489023	-1.657856
95	H	9.711250	-3.781143	-2.328404
96	H	11.130879	-2.755131	-2.212535
97	O	7.414779	0.732475	-0.859502
98	O	4.420189	-0.994044	2.520931
99	O	7.201847	0.819864	1.400620
100	O	4.408547	0.597726	0.900371
101	O	1.279074	3.287538	0.493074
102	O	0.306876	2.658911	2.850041
103	O	2.768419	2.407250	2.392498
104	C	11.390773	-4.715122	-1.337353
105	H	10.808199	-5.480854	-0.812430
106	H	11.793850	-5.169868	-2.248152
107	H	12.238010	-4.447284	-0.695689
108	C	2.715951	-6.319536	-1.289369
109	H	3.158232	-6.122655	-2.272830
110	H	2.858684	-7.382274	-1.067396
111	H	1.638148	-6.137755	-1.370064
112	O	-2.314936	3.200309	2.063998
113	H	-2.677434	2.404255	1.638442
114	H	-1.425457	2.939725	2.390783
115	O	-1.154409	4.816409	0.087863
116	H	-0.308607	4.335644	0.079428
117	H	-1.677090	4.309062	0.746377

E[B3LYP/6-31G(d,p)] = -4047.184188 h, E[APFD/6-311+G(2d,p)] = -4045.746855 h
Gcorr[B3LYP/6-31G(d,p)] = 0.849494 h

153. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 5th step, TS

Center No.	Atom	X	Y	Z
1	P	-0.728482	-1.601359	-0.530192
2	C	-3.006272	-1.855243	-1.942012
3	H	-2.774062	-2.917348	-1.818003
4	H	-3.267013	-1.671031	-2.987591
5	C	-4.178627	-1.472750	-1.038739
6	H	-3.915806	-1.606698	0.010891
7	C	-4.086031	0.875778	-0.433698
8	C	-5.420748	-2.276871	-1.374859
9	H	-5.784706	-2.040878	-2.378623
10	H	-5.201921	-3.347434	-1.328047
11	C	-7.631251	-2.534793	-0.567067
12	C	-4.627103	2.236412	-0.798975
13	H	-5.258664	2.145626	-1.685339
14	H	-5.265207	2.555279	0.034695
15	C	-3.506926	3.269243	-1.015594

16	H	-2.886709	3.304190	-0.115294
17	H	-2.855728	2.930605	-1.830524
18	C	-4.044991	4.672001	-1.315990
19	H	-4.651282	4.646425	-2.231940
20	H	-4.721867	4.982351	-0.507667
21	C	-2.929463	5.714180	-1.469671
22	H	-2.255724	5.404798	-2.280532
23	H	-2.321925	5.726728	-0.554480
24	C	-8.604297	-2.095413	0.503631
25	H	-8.165967	-2.355150	1.475667
26	H	-8.646259	-0.999222	0.484220
27	C	-9.998183	-2.705024	0.346362
28	H	-10.396575	-2.442974	-0.641298
29	H	-9.917883	-3.798592	0.362981
30	C	-10.971001	-2.240594	1.435899
31	H	-11.042503	-1.143797	1.418513
32	H	-10.566626	-2.503690	2.423617
33	C	-12.374224	-2.841128	1.287170
34	H	-12.775808	-2.578728	0.299053
35	H	-12.301384	-3.936960	1.304720
36	O	-7.862655	-3.313849	-1.470177
37	O	-3.340654	0.672341	0.522684
38	O	-6.425364	-1.940449	-0.401302
39	O	-4.517496	-0.075295	-1.265750
40	O	-0.401916	-3.043619	-0.749973
41	O	0.355060	-0.537427	-0.615961
42	O	-1.843851	-1.066441	-1.661169
43	O	1.477019	4.581521	2.289822
44	C	-13.347458	-2.375926	2.374367
45	H	-13.466910	-1.286533	2.358643
46	H	-14.338701	-2.821329	2.240653
47	H	-12.988930	-2.654421	3.371942
48	C	-3.456594	7.123731	-1.753907
49	H	-4.106560	7.473421	-0.943796
50	H	-2.637401	7.842591	-1.857523
51	H	-4.040833	7.147939	-2.680822
52	Ca	1.231137	1.358666	-1.616175
53	O	-0.939123	1.305331	-2.744736
54	H	-1.382730	0.467892	-2.487923
55	H	-1.067027	1.407338	-3.696417
56	O	-1.556176	-1.447884	0.860302
57	H	2.297526	4.433944	2.784663
58	H	-2.106529	-0.635125	0.859797
59	O	2.219156	3.499011	-2.454335
60	H	2.085998	3.870324	-1.559693
61	H	3.161593	3.590133	-2.647935
62	P	1.128619	3.158833	1.536313
63	C	3.823953	2.867514	1.237285
64	H	4.255962	3.797100	1.640960
65	H	3.605375	3.034896	0.176950
66	C	4.862796	1.761195	1.373113
67	H	5.004347	1.505357	2.424849
68	C	4.200016	-0.558440	1.394882
69	C	6.193123	2.151979	0.742400
70	H	6.093346	2.309346	-0.332712
71	H	6.577043	3.060176	1.213561
72	C	7.612340	0.390205	-0.065682
73	C	3.662611	-1.660574	0.510395
74	H	2.644025	-1.374153	0.214678
75	H	4.251437	-1.668082	-0.414884
76	C	3.666483	-3.035979	1.181803
77	H	4.690999	-3.291288	1.480960
78	H	3.082459	-2.983960	2.108438
79	C	3.100698	-4.134636	0.274543
80	H	2.076060	-3.871558	-0.020393
81	H	3.687882	-4.177938	-0.654446
82	C	3.099436	-5.519865	0.932996
83	H	2.519069	-5.475573	1.864686
84	H	4.124621	-5.784723	1.225920
85	C	8.580691	-0.672836	0.404475
86	H	9.376394	-0.169892	0.968189
87	H	8.052686	-1.296276	1.137223

88	C	9.158323	-1.522408	-0.728101
89	H	8.337136	-1.998816	-1.277141
90	H	9.667406	-0.868643	-1.446617
91	C	10.132134	-2.592209	-0.221154
92	H	9.617420	-3.241438	0.501336
93	H	10.949469	-2.108972	0.332814
94	C	10.722888	-3.453812	-1.343676
95	H	9.905519	-3.935722	-1.896981
96	H	11.236925	-2.804032	-2.064813
97	O	7.277665	0.584408	-1.217194
98	O	4.445028	-0.662441	2.580263
99	O	7.163431	1.115749	0.988650
100	O	4.372135	0.585681	0.683768
101	O	1.234741	3.094862	-0.005203
102	O	0.368842	2.074894	2.371629
103	O	2.659052	2.487035	1.946417
104	C	11.695134	-4.522192	-0.834620
105	H	11.199938	-5.207783	-0.137454
106	H	12.099642	-5.119751	-1.658101
107	H	12.540952	-4.067847	-0.305962
108	C	2.527045	-6.614961	0.027791
109	H	3.107735	-6.707294	-0.897322
110	H	2.535421	-7.590879	0.524375
111	H	1.491338	-6.392875	-0.253694
112	O	-1.981824	2.551420	2.411776
113	H	-2.479646	1.968653	1.811656
114	H	-0.806203	2.183063	2.450024
115	O	-0.631774	4.135705	1.244740
116	H	-0.709579	4.064059	0.284166
117	H	-1.493252	3.425811	1.780596

E[B3LYP/6-31G(d,p)] = -4047.129460 h, E[APFD/6-311+G(2d,p)] = -4045.689363 h
Gcorr[B3LYP/6-31G(d,p)] = 0.848003 h

154. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 5th step, products

Center No.	Atom	X	Y	Z
1	P	-0.749190	-1.579506	-0.496315
2	C	-3.021908	-1.796179	-1.925941
3	H	-2.795526	-2.861422	-1.819495
4	H	-3.270475	-1.591321	-2.970669
5	C	-4.201126	-1.424286	-1.027456
6	H	-3.952046	-1.587176	0.021382
7	C	-4.089716	0.902300	-0.355370
8	C	-5.449056	-2.203746	-1.397051
9	H	-5.801217	-1.936015	-2.397100
10	H	-5.242675	-3.277648	-1.378031
11	C	-7.664716	-2.470824	-0.606506
12	C	-4.569928	2.288491	-0.704188
13	H	-5.247838	2.232178	-1.558494
14	H	-5.140431	2.653635	0.158115
15	C	-3.398465	3.248163	-0.990549
16	H	-2.727913	3.253817	-0.125069
17	H	-2.811190	2.863891	-1.833171
18	C	-3.872142	4.675862	-1.283628
19	H	-4.510884	4.673122	-2.177508
20	H	-4.503442	5.027163	-0.455590
21	C	-2.713429	5.660342	-1.487517
22	H	-2.069128	5.298822	-2.300527
23	H	-2.090221	5.673729	-0.582710
24	C	-8.642368	-2.049664	0.467257
25	H	-8.207164	-2.323476	1.436797
26	H	-8.686114	-0.953338	0.464411
27	C	-10.034653	-2.658990	0.295375
28	H	-10.430409	-2.381198	-0.689028
29	H	-9.952388	-3.752555	0.293934
30	C	-11.011652	-2.214529	1.389498
31	H	-11.085281	-1.117734	1.390020
32	H	-10.609669	-2.493119	2.373937
33	C	-12.413230	-2.815266	1.226754
34	H	-12.812527	-2.537326	0.241968

35	H	-12.338233	-3.911093	1.226380
36	O	-7.892908	-3.232033	-1.525460
37	O	-3.381528	0.654890	0.619906
38	O	-6.458343	-1.882477	-0.423203
39	O	-4.516680	-0.016121	-1.223384
40	O	-0.417119	-3.014004	-0.755825
41	O	0.329452	-0.508455	-0.546150
42	O	-1.861337	-1.015802	-1.616401
43	O	1.533756	4.610749	2.264402
44	C	-13.390467	-2.370051	2.318723
45	H	-13.511980	-1.280774	2.320779
46	H	-14.380461	-2.815038	2.174772
47	H	-13.034238	-2.664424	3.312558
48	C	-3.181774	7.084378	-1.801529
49	H	-3.802584	7.483803	-0.991615
50	H	-2.333006	7.762487	-1.936366
51	H	-3.778831	7.110034	-2.720111
52	Ca	1.299567	1.305970	-1.616954
53	O	-0.860076	1.279990	-2.767936
54	H	-1.336157	0.471503	-2.478174
55	H	-0.972977	1.340216	-3.725069
56	O	-1.583759	-1.470423	0.894130
57	H	2.368849	4.407936	2.711609
58	H	-2.129123	-0.655444	0.921682
59	O	2.275843	3.446460	-2.496162
60	H	2.112723	3.810497	-1.601583
61	H	3.221881	3.549099	-2.664008
62	P	1.075481	3.240349	1.459815
63	C	3.797121	2.867690	1.192930
64	H	4.240414	3.797350	1.590468
65	H	3.602750	3.030225	0.126584
66	C	4.830290	1.756835	1.348020
67	H	4.956990	1.504948	2.402531
68	C	4.165120	-0.562831	1.370132
69	C	6.170246	2.136592	0.731608
70	H	6.083405	2.291992	-0.344885
71	H	6.554865	3.043509	1.204617
72	C	7.587425	0.363441	-0.056206
73	C	3.634022	-1.667910	0.484949
74	H	2.611707	-1.389316	0.194497
75	H	4.219201	-1.669847	-0.442567
76	C	3.649519	-3.044298	1.154263
77	H	4.677416	-3.295742	1.445195
78	H	3.072387	-2.996113	2.085378
79	C	3.081178	-4.143847	0.249736
80	H	2.053449	-3.883393	-0.036827
81	H	3.661284	-4.183586	-0.683862
82	C	3.090182	-5.530036	0.906072
83	H	2.516194	-5.489506	1.841876
84	H	4.118511	-5.790904	1.191474
85	C	8.544358	-0.704052	0.427580
86	H	9.335594	-0.204612	1.000576
87	H	8.003751	-1.323496	1.154542
88	C	9.131612	-1.558840	-0.696068
89	H	8.314852	-2.031379	-1.254965
90	H	9.653848	-0.909345	-1.409027
91	C	10.092430	-2.633498	-0.174768
92	H	9.564535	-3.278297	0.542161
93	H	10.905416	-2.154139	0.388891
94	C	10.692508	-3.500731	-1.287955
95	H	9.879506	-3.978718	-1.851014
96	H	11.219851	-2.855439	-2.003493
97	O	7.265665	0.554818	-1.212049
98	O	4.398693	-0.664623	2.558379
99	O	7.132917	1.095557	0.990513
100	O	4.344329	0.578299	0.657951
101	O	1.258356	3.093916	-0.079874
102	O	0.427438	2.056283	2.365544
103	O	2.625117	2.504602	1.885402
104	C	11.651514	-4.574045	-0.764343
105	H	11.143114	-5.255238	-0.072387
106	H	12.063012	-5.175660	-1.581382

107	H	12.493169	-4.123848	-0.225585
108	C	2.516334	-6.626473	0.003427
109	H	3.090851	-6.714893	-0.925913
110	H	2.532718	-7.603014	0.498591
111	H	1.477626	-6.408865	-0.270401
112	O	-2.266551	2.471392	2.613380
113	H	-2.710210	1.914810	1.947427
114	H	-0.553941	2.146590	2.463329
115	O	-0.495825	4.025046	1.271261
116	H	-0.608251	4.085074	0.314032
117	H	-1.933909	3.247480	2.113812

E[B3LYP/6-31G(d,p)] = -4047.144990 h, E[APFD/6-311+G(2d,p)] = -4045.703467 h
Gcorr[B3LYP/6-31G(d,p)] = 0.855290 h

155. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 6th step, reactants

Center No.	Atom	X	Y	Z
1	P	-0.802280	-1.630705	-0.684214
2	C	-3.118219	-1.860565	-2.042934
3	H	-2.901589	-2.925814	-1.917714
4	H	-3.399694	-1.677958	-3.083549
5	C	-4.260370	-1.448870	-1.113593
6	H	-3.974467	-1.592028	-0.071087
7	C	-4.088893	0.883625	-0.486385
8	C	-5.531352	-2.221912	-1.413025
9	H	-5.924825	-1.970249	-2.401777
10	H	-5.339016	-3.298086	-1.379338
11	C	-7.711373	-2.444455	-0.510375
12	C	-4.593961	2.265378	-0.826378
13	H	-5.164530	2.222322	-1.757086
14	H	-5.290360	2.550403	-0.027011
15	C	-3.456592	3.296633	-0.915366
16	H	-2.890024	3.280239	0.022201
17	H	-2.763194	2.990758	-1.709422
18	C	-3.971262	4.714599	-1.187809
19	H	-4.569837	4.717102	-2.109524
20	H	-4.652878	5.014851	-0.379481
21	C	-2.845652	5.749575	-1.313512
22	H	-2.178211	5.456088	-2.135791
23	H	-2.233922	5.732187	-0.401960
24	C	-8.629765	-1.982289	0.598593
25	H	-8.143043	-2.220999	1.552707
26	H	-8.672586	-0.886605	0.557444
27	C	-10.030391	-2.592130	0.525773
28	H	-10.478672	-2.351180	-0.445695
29	H	-9.950834	-3.685272	0.563039
30	C	-10.944549	-2.100661	1.653756
31	H	-11.015616	-1.004380	1.614605
32	H	-10.488811	-2.341493	2.624669
33	C	-12.354399	-2.700942	1.594076
34	H	-12.807969	-2.460666	0.622979
35	H	-12.282261	-3.796242	1.633552
36	O	-7.993605	-3.226935	-1.395996
37	O	-3.343530	0.649202	0.456381
38	O	-6.492090	-1.865780	-0.401906
39	O	-4.565261	-0.044606	-1.329863
40	O	-0.498533	-3.079014	-0.900636
41	O	0.295424	-0.583910	-0.808092
42	O	-1.935044	-1.090553	-1.795432
43	O	1.569270	4.810583	1.868838
44	C	-13.267323	-2.207759	2.720619
45	H	-13.385766	-1.118693	2.685748
46	H	-14.264997	-2.653388	2.650762
47	H	-12.856244	-2.463817	3.703845
48	C	-3.359921	7.171307	-1.558740
49	H	-4.002251	7.506498	-0.736450
50	H	-2.534209	7.884668	-1.648189
51	H	-3.948775	7.225420	-2.481533
52	Ca	1.173208	1.302965	-1.824382
53	O	-1.027880	1.274823	-2.895482

54	H	-1.476907	0.444272	-2.626022
55	H	-1.186559	1.383198	-3.841689
56	O	-1.590941	-1.453369	0.723650
57	H	2.284854	4.666643	2.530351
58	H	-2.146593	-0.640568	0.727209
59	O	2.213288	3.408412	-2.731520
60	H	2.076796	3.777775	-1.834749
61	H	3.163096	3.459186	-2.902721
62	P	1.054438	3.400980	1.224022
63	C	3.773142	2.857762	1.001235
64	H	4.251444	3.790803	1.340647
65	H	3.559872	2.963726	-0.066958
66	C	4.763558	1.715960	1.206460
67	H	4.919347	1.531734	2.271456
68	C	3.991017	-0.559613	1.421070
69	C	6.095732	1.999302	0.522374
70	H	5.972837	2.106077	-0.556513
71	H	6.540724	2.908239	0.934257
72	C	7.364162	0.101617	-0.222371
73	C	3.437055	-1.717769	0.622415
74	H	2.457880	-1.410644	0.230742
75	H	4.079990	-1.854212	-0.256158
76	C	3.321312	-3.013383	1.428767
77	H	4.304248	-3.273851	1.840974
78	H	2.665748	-2.841675	2.291150
79	C	2.782422	-4.180453	0.593153
80	H	1.805503	-3.908574	0.171572
81	H	3.450550	-4.352493	-0.263478
82	C	2.645768	-5.482133	1.392825
83	H	1.984721	-5.308892	2.253011
84	H	3.623515	-5.757024	1.811730
85	C	8.297632	-0.981353	0.272867
86	H	9.159470	-0.487413	0.739044
87	H	7.786368	-1.508321	1.088369
88	C	8.743123	-1.954723	-0.819142
89	H	7.858509	-2.418934	-1.271686
90	H	9.238756	-1.395186	-1.621631
91	C	9.683923	-3.042643	-0.288939
92	H	9.184565	-3.594760	0.519903
93	H	10.567848	-2.572133	0.164617
94	C	10.136255	-4.030818	-1.370857
95	H	9.252072	-4.499408	-1.823777
96	H	10.635203	-3.478344	-2.178507
97	O	6.974965	0.231865	-1.365862
98	O	4.211719	-0.568889	2.615984
99	O	7.019384	0.927755	0.796447
100	O	4.215881	0.511267	0.617643
101	O	1.254638	3.082500	-0.283052
102	O	0.380785	2.324896	2.275765
103	O	2.589697	2.590096	1.727567
104	C	11.075022	-5.118027	-0.839342
105	H	10.591014	-5.708964	-0.053329
106	H	11.379316	-5.807071	-1.633983
107	H	11.984366	-4.680963	-0.411139
108	C	2.101208	-6.645575	0.558468
109	H	2.759389	-6.866361	-0.289834
110	H	2.010040	-7.559222	1.155169
111	H	1.109863	-6.410813	0.154260
112	O	3.267394	3.985823	3.915066
113	H	3.051113	3.196389	3.367792
114	H	-0.564688	2.543438	2.272539
115	O	-0.507224	4.123831	0.993848
116	H	-0.712492	3.991465	0.060157
117	H	2.655743	3.943685	4.662913

E[B3LYP/6-31G(d,p)] = -4047.138863 h, E[APFD/6-311+G(2d,p)] = -4045.697999 h
Gcorr[B3LYP/6-31G(d,p)] = 0.851005 h

156. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 6th step, TS

Center No.	Atom	X	Y	Z

1	P	-0.826921	-1.804689	-0.071614
2	C	-2.965064	-2.279649	-1.643215
3	H	-2.805569	-3.300623	-1.283294
4	H	-3.110348	-2.306615	-2.726546
5	C	-4.194685	-1.674591	-0.965808
6	H	-4.044176	-1.613550	0.112285
7	C	-4.010425	0.732427	-0.781959
8	C	-5.453358	-2.467435	-1.264754
9	H	-5.720179	-2.405091	-2.323446
10	H	-5.312389	-3.520005	-1.003145
11	C	-7.721205	-2.487167	-0.570048
12	C	-4.437097	2.023386	-1.440079
13	H	-4.649389	1.830316	-2.494895
14	H	-5.390319	2.309175	-0.974007
15	C	-3.407904	3.147381	-1.269302
16	H	-3.199020	3.266802	-0.199650
17	H	-2.471298	2.835346	-1.749080
18	C	-3.878582	4.480294	-1.860955
19	H	-4.121825	4.343716	-2.923735
20	H	-4.811925	4.788235	-1.369455
21	C	-2.837286	5.598135	-1.721635
22	H	-1.909720	5.290463	-2.224094
23	H	-2.583419	5.728263	-0.660383
24	C	-8.733986	-1.793570	0.313230
25	H	-8.338519	-1.796670	1.336687
26	H	-8.764167	-0.738134	0.013980
27	C	-10.127308	-2.421507	0.257886
28	H	-10.485461	-2.415125	-0.778614
29	H	-10.060138	-3.476003	0.551718
30	C	-11.133239	-1.695526	1.158364
31	H	-11.192774	-0.638863	0.861078
32	H	-10.765402	-1.699700	2.194255
33	C	-12.536902	-2.311630	1.118122
34	H	-12.902848	-2.308700	0.082492
35	H	-12.476538	-3.366934	1.416653
36	O	-7.931972	-3.441523	-1.291737
37	O	-3.401227	0.675981	0.278224
38	O	-6.505644	-1.900765	-0.462257
39	O	-4.409437	-0.335577	-1.488737
40	O	-0.520968	-3.264636	0.027624
41	O	0.292113	-0.787702	-0.242520
42	O	-1.793185	-1.489362	-1.404405
43	O	1.256320	4.753443	2.119870
44	C	-13.540215	-1.582642	2.016904
45	H	-13.647555	-0.533047	1.720009
46	H	-14.531255	-2.045464	1.967450
47	H	-13.217288	-1.598063	3.064179
48	C	-3.307824	6.936934	-2.297755
49	H	-4.214092	7.287999	-1.791577
50	H	-2.541856	7.710902	-2.185392
51	H	-3.538068	6.847558	-3.365426
52	Ca	1.167625	1.097171	-1.259928
53	O	-0.840676	0.811428	-2.608447
54	H	-1.279502	-0.023755	-2.337331
55	H	-0.903658	0.865312	-3.570180
56	O	-1.788947	-1.376291	1.165008
57	H	1.912643	4.509878	2.896660
58	H	-2.305778	-0.565755	0.954522
59	O	2.267973	3.036386	-2.398685
60	H	2.076661	3.628369	-1.648881
61	H	3.217462	3.106206	-2.564224
62	P	0.608608	3.511308	1.393921
63	C	3.721825	2.859889	1.175730
64	H	4.186847	3.803778	1.523961
65	H	3.428211	3.033855	0.128878
66	C	4.831206	1.799059	1.193556
67	H	5.176189	1.632421	2.215832
68	C	4.223495	-0.509664	1.541940
69	C	6.000888	2.177547	0.297027
70	H	5.695438	2.231701	-0.749201
71	H	6.414428	3.139380	0.609963
72	C	7.311053	0.372613	-0.598802

73	C	3.633200	-1.717486	0.847008
74	H	2.602235	-1.467409	0.563330
75	H	4.175694	-1.859131	-0.096247
76	C	3.668850	-2.986887	1.701066
77	H	4.705527	-3.202422	1.988710
78	H	3.125719	-2.804352	2.636306
79	C	3.065786	-4.199366	0.982411
80	H	2.030384	-3.974633	0.693451
81	H	3.615316	-4.378772	0.046721
82	C	3.088794	-5.476352	1.831786
83	H	2.546379	-5.294831	2.769729
84	H	4.124510	-5.703856	2.119054
85	C	8.419293	-0.593892	-0.239446
86	H	9.308018	0.001348	0.006716
87	H	8.133375	-1.092325	0.695061
88	C	8.727191	-1.613014	-1.337215
89	H	7.817334	-2.180206	-1.568749
90	H	8.998360	-1.082029	-2.257607
91	C	9.851514	-2.577916	-0.944152
92	H	9.576583	-3.100277	-0.016781
93	H	10.760358	-2.004657	-0.712110
94	C	10.169789	-3.612232	-2.030720
95	H	9.260684	-4.183552	-2.262339
96	H	10.445174	-3.089904	-2.956908
97	O	6.724668	0.409396	-1.662939
98	O	4.590486	-0.480213	2.701048
99	O	7.064655	1.211146	0.435589
100	O	4.298771	0.544201	0.695258
101	O	0.965682	3.135347	-0.038485
102	O	0.178801	2.322948	2.420386
103	O	2.627041	2.486588	1.951490
104	C	11.291927	-4.576301	-1.634281
105	H	11.030125	-5.137516	-0.729954
106	H	11.495360	-5.301675	-2.428819
107	H	12.223550	-4.036422	-1.429591
108	C	2.478828	-6.685840	1.116762
109	H	3.021440	-6.914046	0.192081
110	H	2.506009	-7.580471	1.747645
111	H	1.432846	-6.499078	0.847861
112	O	2.817805	3.917659	3.901777
113	H	2.810709	3.127569	3.154607
114	H	-0.778840	2.410098	2.557180
115	O	-0.908609	4.167234	1.207142
116	H	-1.186173	4.012157	0.293764
117	H	2.267569	3.600634	4.631185

E[B3LYP/6-31G(d,p)] = -4047.128716 h, E[APFD/6-311+G(2d,p)] = -4045.692044 h
Gcorr[B3LYP/6-31G(d,p)] = 0.848350 h

157. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 6th step, products

Center No.	Atom	X	Y	Z
1	P	0.892951	2.519596	0.880167
2	C	2.958554	2.887356	-0.818321
3	H	3.121831	3.756526	-0.174357
4	H	2.995613	3.210521	-1.861889
5	C	4.035823	1.834378	-0.557280
6	H	4.015469	1.509272	0.483289
7	C	3.194515	-0.410404	-0.931068
8	C	5.417356	2.348996	-0.914945
9	H	5.505696	2.529348	-1.989665
10	H	5.619199	3.286250	-0.388103
11	C	7.662392	1.605385	-0.795567
12	C	3.075690	-1.477612	-1.989356
13	H	2.397705	-1.066318	-2.747844
14	H	4.053569	-1.573132	-2.474679
15	C	2.562451	-2.826430	-1.483893
16	H	3.236620	-3.209395	-0.708440
17	H	1.586306	-2.688089	-1.005720
18	C	2.438302	-3.857690	-2.611707
19	H	1.768367	-3.466645	-3.390661

20	H	3.417045	-3.996440	-3.091923
21	C	1.913739	-5.215115	-2.127787
22	H	0.936108	-5.072868	-1.646852
23	H	2.583326	-5.603822	-1.348821
24	C	8.557051	0.479447	-0.328991
25	H	8.421490	0.378880	0.755561
26	H	8.172073	-0.452775	-0.760499
27	C	10.030563	0.686682	-0.682689
28	H	10.128338	0.797099	-1.769512
29	H	10.376666	1.631609	-0.247084
30	C	10.919743	-0.463946	-0.198190
31	H	10.563716	-1.408834	-0.632710
32	H	10.816729	-0.571813	0.890892
33	C	12.399991	-0.271842	-0.549917
34	H	12.500867	-0.163112	-1.638259
35	H	12.754365	0.672757	-0.115644
36	O	8.021684	2.622954	-1.353345
37	O	2.795471	-0.514307	0.229450
38	O	6.363958	1.344867	-0.508973
39	O	3.782920	0.684775	-1.414048
40	O	0.970992	3.922153	1.379891
41	O	-0.442863	1.836372	0.636129
42	O	1.647960	2.350426	-0.599814
43	O	0.059741	-2.126724	3.568302
44	C	13.288541	-1.421886	-0.066666
45	H	12.979073	-2.374728	-0.511211
46	H	14.337481	-1.255619	-0.332935
47	H	13.234878	-1.532731	1.022413
48	C	1.784399	-6.246795	-3.252255
49	H	2.752858	-6.434857	-3.729618
50	H	1.407945	-7.203168	-2.875076
51	H	1.094191	-5.900249	-4.029889
52	Ca	-1.139236	-0.252327	-0.164015
53	O	0.242503	0.463955	-2.068227
54	H	0.746426	1.248337	-1.766292
55	H	-0.084539	0.662965	-2.954825
56	O	1.822468	1.564258	1.840301
57	H	0.180189	-0.443617	3.908329
58	H	2.113401	0.754789	1.365856
59	O	-2.591784	-2.159126	-0.705481
60	H	-2.173810	-2.758551	-0.065490
61	H	-3.553806	-2.163884	-0.524059
62	P	0.377538	-2.687154	2.205901
63	C	-2.999196	-0.251922	3.568226
64	H	-3.259262	-0.799339	4.490933
65	H	-2.272721	-0.871628	3.026211
66	C	-4.280299	-0.123733	2.745902
67	H	-5.036064	0.431533	3.304559
68	C	-4.523718	1.856979	1.389640
69	C	-4.810711	-1.490311	2.342833
70	H	-4.119314	-1.989927	1.664479
71	H	-4.964157	-2.110724	3.228466
72	C	-6.237506	-1.606713	0.403483
73	C	-4.039831	2.501849	0.110305
74	H	-2.961542	2.675064	0.228475
75	H	-4.135861	1.766138	-0.697865
76	C	-4.766483	3.802751	-0.234913
77	H	-5.841560	3.604820	-0.327755
78	H	-4.655478	4.508296	0.596741
79	C	-4.245458	4.439546	-1.528341
80	H	-3.167656	4.633479	-1.430772
81	H	-4.353147	3.724657	-2.356736
82	C	-4.962990	5.745092	-1.892070
83	H	-4.854162	6.458885	-1.064442
84	H	-6.039850	5.550360	-1.986555
85	C	-7.662525	-1.380227	-0.044346
86	H	-8.312303	-1.957107	0.624985
87	H	-7.899956	-0.327064	0.153890
88	C	-7.918296	-1.736940	-1.509232
89	H	-7.255713	-1.141329	-2.148426
90	H	-7.647090	-2.785956	-1.678352
91	C	-9.377592	-1.507697	-1.919064

92	H	-9.645361	-0.455989	-1.744582
93	H	-10.036431	-2.101438	-1.269727
94	C	-9.656755	-1.864730	-3.384024
95	H	-8.998881	-1.270306	-4.032307
96	H	-9.386565	-2.915188	-3.557092
97	O	-5.332617	-1.977879	-0.327867
98	O	-5.276096	2.366506	2.194468
99	O	-6.103788	-1.353463	1.716341
100	O	-3.999914	0.609390	1.528020
101	O	-0.368969	-2.134804	0.989111
102	O	1.970062	-2.620034	1.889698
103	O	-2.478843	1.028502	3.850505
104	C	-11.115905	-1.638574	-3.790748
105	H	-11.405082	-0.589498	-3.660162
106	H	-11.283658	-1.901961	-4.840144
107	H	-11.794972	-2.246521	-3.182043
108	C	-4.442831	6.378794	-3.185745
109	H	-4.570097	5.700820	-4.037530
110	H	-4.974147	7.307629	-3.417625
111	H	-3.375511	6.615924	-3.108958
112	O	0.175554	0.529137	4.090791
113	H	-1.499078	0.924715	3.947225
114	H	2.180808	-1.942212	1.214058
115	O	0.124078	-4.294580	2.311096
116	H	0.305664	-4.735306	1.467932
117	H	0.726915	0.914215	3.387685

E[B3LYP/6-31G(d,p)] = -4047.195717 h, E[APFD/6-311+G(2d,p)] = -4045.756445 h
Gcorr[B3LYP/6-31G(d,p)] = 0.855072 h

158. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 7th step, reactants (hydrolysed glycerol + carbon chains neglected)

Center No.	Atom	X	Y	Z
1	P	2.039247	-2.760259	-0.307376
2	C	-0.177250	-2.530121	-1.825078
3	H	-0.321070	-3.568645	-1.513176
4	H	-0.326411	-2.463539	-2.905545
5	C	-1.171827	-1.623621	-1.099216
6	H	-1.039128	-1.689368	-0.019592
7	C	-0.248492	0.590165	-0.748046
8	C	-2.605770	-1.956549	-1.464518
9	H	-2.810048	-1.727997	-2.514331
10	H	-2.802092	-3.019135	-1.295602
11	C	-4.785664	-1.368768	-0.747549
12	C	-0.130293	1.963993	-1.354683
13	H	0.921789	2.075342	-1.645484
14	H	-0.729861	1.999849	-2.266964
15	C	-0.532031	3.088827	-0.383644
16	H	-1.575402	2.945099	-0.075852
17	H	0.078007	3.022029	0.523039
18	C	-0.369075	4.476341	-1.014608
19	H	0.676079	4.612084	-1.326679
20	H	-0.972687	4.534910	-1.930948
21	C	-0.769432	5.616039	-0.069837
22	H	-0.166277	5.554807	0.845898
23	H	-1.813053	5.476304	0.242423
24	C	-5.566291	-0.480632	0.194549
25	H	-5.199273	-0.672799	1.210602
26	H	-5.290397	0.558515	-0.025271
27	C	-7.080104	-0.680268	0.107086
28	H	-7.410841	-0.487547	-0.920624
29	H	-7.317703	-1.730950	0.312803
30	C	-7.849059	0.223705	1.077174
31	H	-7.603430	1.274927	0.869884
32	H	-7.509864	0.028838	2.104477
33	C	-9.369120	0.035301	1.002512
34	H	-9.706978	0.230750	-0.024178
35	H	-9.612892	-1.015757	1.208198
36	O	-5.252638	-2.172738	-1.529227
37	O	0.239098	0.274834	0.339680
38	O	-3.453010	-1.161358	-0.616512

39	O	-0.937947	-0.248626	-1.520133
40	O	1.984093	-4.260701	-0.343681
41	O	3.364208	-2.033978	-0.398558
42	O	1.174512	-2.119587	-1.574440
43	O	4.172314	0.774068	2.588756
44	C	-10.136352	0.937414	1.973739
45	H	-9.938620	1.996158	1.770626
46	H	-11.217124	0.779980	1.896576
47	H	-9.844290	0.740196	3.011569
48	C	-0.605199	7.002776	-0.698928
49	H	-1.223196	7.105051	-1.598249
50	H	-0.898449	7.794242	-0.001636
51	H	0.435550	7.184310	-0.990551
52	Ca	4.484734	-0.095086	-1.005781
53	O	2.646532	0.013213	-2.613108
54	H	2.059992	-0.753111	-2.446911
55	H	2.750348	0.080369	-3.570890
56	O	1.188349	-2.258811	0.990128
57	H	0.930853	-1.314044	0.910564
58	O	5.754596	2.029535	-1.292727
59	H	5.132725	2.378309	-0.618169
60	H	6.637376	2.110847	-0.906836
61	P	3.424074	1.776992	1.765833
62	O	3.575965	1.718264	0.234100
63	O	1.825406	1.799664	2.085900
64	H	1.318914	1.300287	1.410270
65	O	3.860678	3.265604	2.280165
66	H	3.403052	3.957925	1.781153
67	O	3.121768	-3.198760	3.078125
68	H	2.379800	-2.758729	2.636467
69	H	3.049171	-4.117875	2.744930
70	O	2.727701	-5.707151	1.845244
71	H	1.886498	-5.996558	2.223330
72	H	2.467194	-5.249719	1.010019

E[B3LYP/6-31G(d,p)] = -3158.937670 h, E[APFD/6-311+G(2d,p)] = -3157.982455 h
Gcorr[B3LYP/6-31G(d,p)] = 0.484468 h

159. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 7th step, TS

Center No.	Atom	X	Y	Z
1	P	2.068782	-2.793007	0.031861
2	C	-0.235183	-2.379615	-1.515293
3	H	-0.418843	-3.407855	-1.190963
4	H	-0.369454	-2.335448	-2.603147
5	C	-1.262693	-1.455000	-0.857182
6	H	-1.166174	-1.469644	0.229503
7	C	-0.306938	0.754503	-0.607151
8	C	-2.679651	-1.820906	-1.252284
9	H	-2.851439	-1.643849	-2.317701
10	H	-2.866066	-2.877887	-1.042628
11	C	-4.896114	-1.231043	-0.661116
12	C	-0.170503	2.100104	-1.271779
13	H	0.801320	2.073040	-1.783359
14	H	-0.936077	2.185406	-2.047134
15	C	-0.229931	3.284619	-0.296277
16	H	-1.198619	3.279900	0.219505
17	H	0.536605	3.162931	0.475854
18	C	-0.035383	4.627678	-1.009503
19	H	0.934798	4.626683	-1.526359
20	H	-0.798629	4.740599	-1.792081
21	C	-0.103131	5.829242	-0.059126
22	H	0.660284	5.715345	0.722187
23	H	-1.071826	5.825809	0.458457
24	C	-5.731898	-0.316766	0.206429
25	H	-5.410860	-0.460367	1.245756
26	H	-5.460383	0.716556	-0.044433
27	C	-7.236886	-0.543633	0.056280
28	H	-7.519500	-0.403534	-0.994024
29	H	-7.469927	-1.587541	0.298577
30	C	-8.065789	0.390700	0.944630

31	H	-7.825896	1.435382	0.700737
32	H	-7.775287	0.249035	1.995310
33	C	-9.577247	0.172661	0.804106
34	H	-9.866036	0.314495	-0.246115
35	H	-9.814976	-0.871941	1.046539
36	O	-5.318679	-2.068030	-1.434164
37	O	0.211262	0.457097	0.471233
38	O	-3.574604	-1.004782	-0.473338
39	O	-1.042181	-0.089964	-1.325230
40	O	1.550313	-4.227050	-0.331466
41	O	3.387587	-2.236467	-0.493614
42	O	1.099902	-1.999843	-1.226132
43	O	4.166972	0.310297	2.605562
44	C	-10.406159	1.104907	1.692606
45	H	-10.214975	2.156472	1.449821
46	H	-11.479115	0.924764	1.569552
47	H	-10.163605	0.961172	2.751752
48	C	0.090607	7.170834	-0.772137
49	H	-0.679324	7.327552	-1.536242
50	H	0.036771	8.008083	-0.068716
51	H	1.065422	7.216820	-1.270959
52	Ca	4.435843	-0.278311	-1.122922
53	O	2.415346	-0.040080	-2.462596
54	H	1.863776	-0.794479	-2.120563
55	H	2.415032	-0.109163	-3.425705
56	O	1.284883	-1.990855	1.228294
57	H	0.862636	-1.174520	0.883271
58	O	5.705470	1.847410	-1.493700
59	H	5.214427	2.157055	-0.702071
60	H	6.641692	1.881737	-1.255134
61	P	3.617468	1.477818	1.845416
62	O	3.782494	1.493034	0.314805
63	O	2.043597	1.765979	2.162606
64	H	1.454501	1.342067	1.502955
65	O	4.292949	2.833964	2.459615
66	H	3.974705	3.623663	1.998245
67	O	3.019724	-3.594623	1.601837
68	H	2.716164	-3.092417	2.370576
69	H	2.654832	-4.743509	1.686504
70	O	2.154598	-5.801124	1.378623
71	H	1.396859	-5.947242	1.962257
72	H	1.760913	-5.080543	0.427360

E[B3LYP/6-31G(d,p)] = -3158.890021 h, E[APFD/6-311+G(2d,p)] = -3157.926509 h
Gcorr[B3LYP/6-31G(d,p)] = 0.484796 h

160. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 7th step, products

Center No.	Atom	X	Y	Z
1	P	2.090009	-2.841974	0.115750
2	C	-0.226798	-2.330478	-1.512751
3	H	-0.455829	-3.352108	-1.193982
4	H	-0.347149	-2.288501	-2.604311
5	C	-1.254138	-1.384681	-0.880733
6	H	-1.180390	-1.396259	0.207756
7	C	-0.268694	0.806964	-0.613721
8	C	-2.669215	-1.728604	-1.300466
9	H	-2.821030	-1.548265	-2.368531
10	H	-2.875526	-2.782491	-1.094880
11	C	-4.887595	-1.142154	-0.707932
12	C	-0.092028	2.148624	-1.277544
13	H	0.888103	2.100138	-1.770900
14	H	-0.840949	2.247458	-2.067582
15	C	-0.146629	3.337162	-0.307160
16	H	-1.124013	3.352600	0.191855
17	H	0.604007	3.204441	0.478731
18	C	0.084739	4.673384	-1.022323
19	H	1.063531	4.652293	-1.522299
20	H	-0.662528	4.796096	-1.818785
21	C	0.022246	5.881189	-0.079641
22	H	0.770364	5.758493	0.715027

23	H	-0.954907	5.897681	0.421555
24	C	-5.725129	-0.210471	0.139491
25	H	-5.353651	-0.270002	1.169744
26	H	-5.511913	0.814510	-0.190920
27	C	-7.223780	-0.508269	0.071620
28	H	-7.555122	-0.453949	-0.972201
29	H	-7.400893	-1.541389	0.394802
30	C	-8.055230	0.451195	0.930295
31	H	-7.873608	1.484913	0.603394
32	H	-7.713621	0.397541	1.973753
33	C	-9.559909	0.160128	0.875436
34	H	-9.899757	0.212797	-0.167734
35	H	-9.739433	-0.873115	1.202039
36	O	-5.309905	-2.002063	-1.455849
37	O	0.215907	0.499902	0.477045
38	O	-3.567251	-0.900181	-0.536447
39	O	-1.003316	-0.024309	-1.347679
40	O	1.529963	-4.230964	-0.515135
41	O	3.378910	-2.216004	-0.424899
42	O	1.106776	-1.990323	-1.196495
43	O	4.110917	0.239963	2.613308
44	C	-10.391162	1.118898	1.733003
45	H	-10.258779	2.157049	1.407422
46	H	-11.459126	0.885008	1.673178
47	H	-10.096582	1.063380	2.787249
48	C	0.251359	7.215032	-0.796753
49	H	-0.502941	7.380623	-1.574474
50	H	0.200654	8.057337	-0.099157
51	H	1.234918	7.240961	-1.279621
52	Ca	4.413661	-0.268807	-1.081670
53	O	2.395478	-0.059401	-2.414818
54	H	1.854549	-0.820820	-2.045672
55	H	2.387458	-0.149998	-3.375858
56	O	1.214547	-2.021571	1.241380
57	H	0.833221	-1.205401	0.858022
58	O	5.687073	1.855318	-1.453997
59	H	5.200435	2.162796	-0.658723
60	H	6.624521	1.887583	-1.220103
61	P	3.593397	1.445070	1.889227
62	O	3.771745	1.504560	0.361000
63	O	2.025138	1.759118	2.204174
64	H	1.431555	1.351602	1.536617
65	O	4.295460	2.763620	2.553373
66	H	4.000546	3.575499	2.115659
67	O	2.790908	-3.741272	1.435827
68	H	2.874543	-3.147776	2.193354
69	H	2.368057	-5.457052	1.679108
70	O	1.960507	-6.263306	1.288900
71	H	1.122268	-6.362229	1.761233
72	H	1.673628	-5.013925	0.071540

E[B3LYP/6-31G(d,p)] = -3158.905133 h, E[APFD/6-311+G(2d,p)] = -3157.939555 h
Gcorr[B3LYP/6-31G(d,p)] = 0.488526 h

161. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 8th step, reactants

Center No.	Atom	X	Y	Z
1	P	-2.399858	0.012885	2.499154
2	C	0.121135	-1.272830	2.139480
3	H	0.157002	-2.364093	2.279134
4	H	0.289298	-0.798561	3.111092
5	C	1.251171	-0.879731	1.185040
6	H	0.989111	-1.176686	0.167575
7	C	0.842783	1.325243	0.287387
8	C	2.583733	-1.480169	1.589472
9	H	2.920099	-1.089843	2.554317
10	H	2.502890	-2.567973	1.665978
11	C	4.805444	-1.577338	0.766566
12	C	0.943916	2.788913	0.648037
13	H	0.195869	2.950984	1.436018
14	H	1.917354	2.954678	1.121915

15	C	0.720299	3.749366	-0.522366
16	H	1.458470	3.544009	-1.308031
17	H	-0.264231	3.561570	-0.964799
18	C	0.820209	5.218085	-0.093731
19	H	0.085044	5.415920	0.699336
20	H	1.807265	5.402305	0.353470
21	C	0.596128	6.202707	-1.247648
22	H	-0.390272	6.017223	-1.693906
23	H	1.330876	6.004286	-2.039615
24	C	5.715732	-1.137993	-0.359107
25	H	5.287907	-1.512563	-1.297634
26	H	5.655468	-0.044317	-0.425358
27	C	7.163436	-1.600735	-0.188836
28	H	7.550824	-1.227874	0.767019
29	H	7.187220	-2.695136	-0.121815
30	C	8.070212	-1.132263	-1.332389
31	H	8.038613	-0.035350	-1.397503
32	H	7.675824	-1.505248	-2.288290
33	C	9.526067	-1.587343	-1.173773
34	H	9.917642	-1.216259	-0.216977
35	H	9.556598	-2.683478	-1.110340
36	O	5.132652	-2.237327	1.733547
37	O	0.309668	0.877532	-0.720761
38	O	3.542567	-1.136059	0.569241
39	O	1.413132	0.562965	1.226579
40	O	-1.198220	1.055891	2.929861
41	O	-3.206833	0.247387	1.219527
42	O	-1.124920	-0.888706	1.582052
43	O	-5.411029	-1.506873	-0.771012
44	C	10.432852	-1.115785	-2.314415
45	H	10.449397	-0.021844	-2.380261
46	H	11.463775	-1.456142	-2.172326
47	H	10.085582	-1.499493	-3.280571
48	C	0.694110	7.668672	-0.814962
49	H	1.681587	7.892028	-0.395092
50	H	0.530312	8.346592	-1.658984
51	H	-0.052023	7.905441	-0.047811
52	Ca	-4.075357	0.546173	-0.871771
53	O	-2.116576	1.770921	-1.661399
54	H	-1.205532	1.500716	-1.411380
55	H	-2.157145	1.764089	-2.628359
56	O	-2.679876	-1.373750	3.364443
57	H	-2.275819	-2.112190	2.886169
58	O	-4.120274	0.706145	-3.392295
59	H	-3.880828	-0.249761	-3.387495
60	H	-4.933040	0.782946	-3.909194
61	P	-4.527747	-2.404936	-1.621273
62	O	-3.394636	-1.616911	-2.309149
63	O	-3.886644	-3.635177	-0.809258
64	H	-2.948761	-3.384907	-0.543760
65	O	-5.495022	-3.143486	-2.695162
66	H	-5.012089	-3.790474	-3.231095
67	O	-3.396871	0.840297	3.624947
68	H	-4.168390	0.295705	3.828163
69	H	-1.456912	-1.943477	0.264152
70	O	-1.485421	-2.595674	-0.482219
71	H	-1.776897	-2.072757	-1.253404
72	H	-1.567793	1.637041	3.612804

E[B3LYP/6-31G(d,p)] = -3158.909251 h, E[APFD/6-311+G(2d,p)] = -3157.934540 h
Gcorr[B3LYP/6-31G(d,p)] = 0.491331 h

162. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 8th step, TS

Center No.	Atom	X	Y	Z
1	P	-2.747458	-0.477141	2.404845
2	C	0.133964	-1.751057	1.428465
3	H	0.120184	-2.837315	1.218688
4	H	0.287361	-1.632090	2.510437
5	C	1.358403	-1.172495	0.702933
6	H	1.215275	-1.222399	-0.378070

7	C	1.062160	1.180573	0.248406
8	C	2.652920	-1.852019	1.098609
9	H	2.894589	-1.666442	2.149044
10	H	2.574233	-2.932478	0.948437
11	C	4.942185	-1.827265	0.471221
12	C	1.091576	2.540074	0.911840
13	H	0.188222	2.600653	1.535048
14	H	1.936055	2.560853	1.608247
15	C	1.144233	3.716137	-0.067722
16	H	2.034848	3.620072	-0.701617
17	H	0.279201	3.670281	-0.738291
18	C	1.167632	5.070625	0.650064
19	H	0.276938	5.159504	1.288383
20	H	2.032678	5.111321	1.326938
21	C	1.221452	6.263699	-0.311758
22	H	0.356620	6.221640	-0.987642
23	H	2.111066	6.173322	-0.949601
24	C	5.951293	-1.189459	-0.458828
25	H	5.600189	-1.345664	-1.486669
26	H	5.911169	-0.104801	-0.297165
27	C	7.373140	-1.721680	-0.274737
28	H	7.685572	-1.563252	0.764522
29	H	7.375363	-2.807130	-0.431747
30	C	8.378015	-1.059193	-1.223836
31	H	8.368052	0.028559	-1.065149
32	H	8.058247	-1.217819	-2.263567
33	C	9.809056	-1.582197	-1.049675
34	H	10.126788	-1.424252	-0.010161
35	H	9.817837	-2.668994	-1.208655
36	O	5.180263	-2.680246	1.304499
37	O	0.700205	0.970637	-0.904385
38	O	3.705632	-1.324182	0.262942
39	O	1.485741	0.228769	1.082083
40	O	-1.462214	-0.302808	3.372176
41	O	-2.999213	0.587660	1.362454
42	O	-1.039701	-1.121344	1.010678
43	O	-5.581101	-0.488755	-0.640539
44	C	10.812879	-0.918809	-1.997295
45	H	10.851105	0.164873	-1.837634
46	H	11.823580	-1.312835	-1.848739
47	H	10.539819	-1.088701	-3.045092
48	C	1.243335	7.615839	0.407299
49	H	2.116064	7.700057	1.064959
50	H	1.281819	8.446681	-0.304739
51	H	0.349021	7.749120	1.026753
52	Ca	-3.637432	0.987162	-0.855586
53	O	-1.649555	2.090077	-1.769069
54	H	-0.753274	1.745980	-1.558785
55	H	-1.785747	1.971325	-2.721395
56	O	-3.253543	-1.968450	2.096766
57	H	-2.972508	-2.284614	1.197574
58	O	-3.721652	1.128300	-3.391478
59	H	-3.827551	0.148592	-3.381831
60	H	-4.478716	1.482939	-3.876023
61	P	-5.159387	-1.615051	-1.567879
62	O	-3.853122	-1.293438	-2.315499
63	O	-4.999749	-3.040939	-0.825905
64	H	-4.064146	-3.138772	-0.517278
65	O	-6.394240	-1.896430	-2.577793
66	H	-6.209136	-2.628234	-3.185838
67	O	-3.817755	-0.204463	3.637899
68	H	-4.685019	-0.577389	3.427024
69	H	-1.665114	-1.966258	0.171447
70	O	-2.316324	-2.681773	-0.354645
71	H	-2.553197	-2.209810	-1.174997
72	H	-1.789022	-0.184465	4.279049

E[B3LYP/6-31G(d,p)] = -3158.896919 h, E[APFD/6-311+G(2d,p)] = -3157.922815 h
Gcorr[B3LYP/6-31G(d,p)] = 0.488519 h

163. 2PC6Ca+4H_2O, cho1:cho2:gly1:gly2, 8th step, products

Center No.	Atom	X	Y	Z
1	P	-3.379685	1.480239	1.467287
2	C	0.105974	-1.279060	3.405160
3	H	0.108147	-2.351543	3.634757
4	H	0.493633	-0.745970	4.278488
5	C	1.025584	-1.025863	2.209817
6	H	0.593488	-1.435256	1.294459
7	C	0.878962	0.985351	0.875814
8	C	2.414665	-1.596774	2.439276
9	H	2.901030	-1.118720	3.294075
10	H	2.357765	-2.672606	2.629476
11	C	4.490852	-1.708918	1.301134
12	C	1.056531	2.482955	0.936289
13	H	0.098490	2.876894	1.301071
14	H	1.798834	2.710895	1.706898
15	C	1.430351	3.124031	-0.405039
16	H	2.375809	2.695396	-0.761564
17	H	0.673673	2.874204	-1.156490
18	C	1.565179	4.647714	-0.300668
19	H	0.618807	5.071641	0.063994
20	H	2.322767	4.897192	0.455489
21	C	1.939110	5.312936	-1.630726
22	H	1.181055	5.062346	-2.385085
23	H	2.883713	4.886741	-1.994743
24	C	5.193514	-1.389647	0.000577
25	H	4.679105	-1.941622	-0.796551
26	H	5.021195	-0.328664	-0.218909
27	C	6.687698	-1.715284	0.020085
28	H	7.166104	-1.163137	0.838139
29	H	6.822182	-2.779043	0.249980
30	C	7.381371	-1.379596	-1.304855
31	H	7.237143	-0.313967	-1.532965
32	H	6.897628	-1.933891	-2.121657
33	C	8.881814	-1.696343	-1.297531
34	H	9.363061	-1.143238	-0.479634
35	H	9.024663	-2.761353	-1.069928
36	O	4.996862	-2.216964	2.282073
37	O	0.507303	0.351689	-0.103320
38	O	3.185299	-1.354186	1.247370
39	O	1.157349	0.412904	2.057529
40	O	-2.001339	1.633198	2.307488
41	O	-3.114374	1.705070	-0.013171
42	O	-1.220005	-0.818882	3.189986
43	O	-5.165595	-1.122314	-1.765967
44	C	9.575734	-1.358602	-2.620429
45	H	9.478738	-0.292849	-2.857199
46	H	10.644105	-1.595297	-2.583208
47	H	9.138371	-1.922781	-3.452116
48	C	2.072051	6.835132	-1.525671
49	H	2.846851	7.115722	-0.803035
50	H	2.339147	7.280270	-2.489658
51	H	1.132065	7.292581	-1.196450
52	Ca	-3.264967	0.426353	-1.945626
53	O	-0.923604	1.068446	-2.355374
54	H	-0.338069	0.887260	-1.587506
55	H	-0.684982	0.414784	-3.031615
56	O	-4.098810	0.207972	1.880672
57	H	-3.413679	-1.211020	1.597979
58	O	-2.101851	-1.078609	-3.688353
59	H	-2.206073	-1.807643	-3.037888
60	H	-2.508340	-1.384031	-4.510146
61	P	-4.406088	-2.394619	-1.433626
62	O	-2.886245	-2.149747	-1.346860
63	O	-4.905228	-3.128345	-0.088134
64	H	-4.292662	-2.902252	0.659213
65	O	-4.779586	-3.482353	-2.577030
66	H	-4.395472	-4.352577	-2.390979
67	O	-4.220102	2.794429	1.941179
68	H	-4.474719	2.727052	2.873140

69	H	-1.710321	-1.448243	2.610374
70	O	-2.936356	-2.091377	1.472867
71	H	-2.553448	-2.036425	0.572474
72	H	-1.679960	0.762142	2.657900

E[B3LYP/6-31G(d,p)] = -3158.961072 h, E[APFD/6-311+G(2d,p)] = -3157.984479 h
Gcorr[B3LYP/6-31G(d,p)] = 0.489270 h

XII. Structures of molecules and transition states (TS) related to 2PC6Ca + 4 H_2O, where the hydrolysis proceeds in the sequence cho1:gly2:cho2:gly1, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

164. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 1st and 2nd steps, same as in XI (choline hydrolysis)

165. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 3rd step, reactants (hydrolised choline neglected)

Center No.	Atom	X	Y	Z
1	P	-1.401279	-2.514203	-4.173617
2	H	-6.517288	3.370460	-0.936867
3	C	0.540955	-4.172569	-3.428956
4	H	0.986540	-3.732384	-4.327259
5	H	0.588630	-5.262381	-3.523181
6	C	1.322941	-3.728271	-2.195238
7	H	1.179052	-2.660632	-2.026897
8	C	0.164814	-3.793906	-0.074961
9	C	2.798295	-4.061984	-2.308285
10	H	2.959366	-5.143187	-2.343767
11	H	3.218313	-3.619806	-3.216215
12	C	4.794831	-3.707659	-1.084596
13	C	-0.315009	-4.727839	1.011381
14	H	-0.564619	-5.690935	0.555786
15	H	0.550017	-4.915555	1.663214
16	C	-1.484056	-4.167808	1.827932
17	H	-1.199405	-3.191992	2.237811
18	H	-2.339395	-3.990628	1.163565
19	C	-1.906493	-5.104773	2.965343
20	H	-2.168406	-6.088630	2.551295
21	H	-1.052274	-5.273448	3.636205
22	C	-3.091028	-4.567090	3.777313
23	H	-3.943490	-4.402599	3.104178
24	H	-2.830649	-3.581385	4.186091
25	C	5.373628	-3.093631	0.170175
26	H	5.085605	-2.034987	0.185250
27	H	4.862051	-3.548538	1.027847
28	C	6.890237	-3.256009	0.283025
29	H	7.141822	-4.322937	0.252098
30	H	7.367568	-2.804261	-0.594996
31	C	7.456968	-2.627356	1.560869
32	H	6.972349	-3.081088	2.437213
33	H	7.198397	-1.559258	1.588627
34	C	8.977382	-2.782773	1.687655
35	H	9.234478	-3.850242	1.658829
36	H	9.460378	-2.329653	0.811393
37	O	5.417173	-4.303431	-1.941476
38	O	0.028223	-2.576530	-0.056442
39	O	3.456585	-3.512548	-1.150509
40	O	0.794508	-4.457372	-1.051613
41	O	-1.002610	-2.611584	-5.612062
42	O	-2.873573	-2.464927	-3.772130
43	O	-0.834940	-3.810128	-3.310265
44	O	-7.464097	3.485256	-0.689096
45	C	9.543057	-2.154990	2.964951
46	H	9.103474	-2.612218	3.858822
47	H	10.628822	-2.282246	3.025831
48	H	9.330843	-1.080452	3.005298
49	C	-3.513006	-5.498452	4.917527
50	H	-2.691070	-5.654219	5.625564
51	H	-4.360266	-5.087658	5.476195
52	H	-3.810855	-6.481601	4.535619
53	O	-7.547046	1.751691	1.520240
54	H	-6.766455	1.223171	1.303403
55	H	-7.590600	2.385650	0.771325

56	Ca	-4.087151	-1.822880	-1.910285
57	O	-4.662494	-3.513813	-0.237759
58	H	-4.707445	-4.466516	-0.392777
59	H	-5.169921	-3.350132	0.567990
60	O	-0.624739	-1.244243	-3.506564
61	H	-7.947835	3.031945	-1.392450
62	H	-1.002688	-1.042472	-2.620998
63	O	-1.922052	-0.959991	-1.060704
64	H	-1.989603	-0.044731	-0.721651
65	H	-1.300885	-1.468182	-0.499105
66	P	-4.314407	1.660337	-0.732338
67	C	-4.412431	2.566776	1.773687
68	H	-4.172387	3.475815	1.217916
69	H	-5.359473	2.713845	2.296135
70	C	-3.277289	2.127747	2.699540
71	H	-3.552084	1.193753	3.193017
72	H	-2.368186	1.971382	2.118611
73	C	-1.923228	2.507514	-1.626084
74	H	-2.551489	3.332578	-1.968615
75	H	-1.649564	1.880996	-2.481626
76	C	-0.682014	3.054776	-0.938264
77	H	-0.967939	3.627317	-0.054883
78	C	0.415826	1.778322	0.794029
79	C	0.145990	3.914575	-1.878985
80	H	0.548731	3.323514	-2.705945
81	H	-0.461485	4.724373	-2.293596
82	C	2.125149	5.215301	-1.780605
83	C	1.377609	0.632989	1.004223
84	H	1.047146	-0.208595	0.385773
85	H	2.341926	0.949342	0.583746
86	C	-4.088106	3.367443	4.712999
87	H	-4.867044	3.889416	4.161001
88	H	-4.461715	2.413911	5.084743
89	H	-3.750610	3.986827	5.542779
90	C	-2.417356	4.411207	3.225881
91	H	-2.099040	5.050681	4.048414
92	H	-1.578561	4.191670	2.566793
93	H	-3.223721	4.896147	2.679115
94	C	-1.794291	2.488334	4.608004
95	H	-0.954457	2.306510	3.938355
96	H	-1.510715	3.182709	5.397968
97	H	-2.151210	1.554542	5.040938
98	N	-2.914044	3.108718	3.804662
99	C	1.532013	0.217257	2.468211
100	H	1.872241	1.077096	3.056932
101	H	0.549655	-0.062077	2.869263
102	C	2.506582	-0.953190	2.642178
103	H	2.160434	-1.803960	2.039023
104	H	3.490145	-0.672453	2.239402
105	C	2.664511	-1.394363	4.102250
106	H	1.679484	-1.666212	4.505218
107	H	3.013657	-0.542419	4.701134
108	C	3.215485	5.717087	-0.860852
109	H	2.733365	6.287096	-0.056481
110	H	3.665515	4.843615	-0.372525
111	C	4.274708	6.558036	-1.574931
112	H	4.722410	5.964638	-2.381245
113	H	3.789344	7.414082	-2.058854
114	C	5.372387	7.052953	-0.626438
115	H	5.851125	6.191106	-0.140195
116	H	4.918521	7.644713	0.181152
117	C	6.443300	7.895247	-1.330325
118	H	6.894361	7.303245	-2.138106
119	H	5.963935	8.756296	-1.815349
120	O	2.033111	5.437190	-2.971356
121	O	-0.054859	2.477947	1.674755
122	O	1.226416	4.462418	-1.101972
123	O	0.142595	1.938662	-0.520278
124	O	-4.751965	0.358590	-1.364904
125	O	-4.822517	2.977753	-1.249340
126	O	-2.655247	1.705118	-0.675197
127	O	-4.624118	1.467845	0.865811

128	C	7.541527	8.387992	-0.383314
129	H	8.062062	7.547716	0.090278
130	H	8.289292	8.985455	-0.914999
131	H	7.124523	9.011032	0.416194
132	C	3.629193	-2.571105	4.275989
133	H	4.632079	-2.317817	3.913503
134	H	3.719477	-2.862685	5.327505
135	H	3.286992	-3.448861	3.715524

E[B3LYP/6-31G(d,p)] = -4299.537450 h, E[APFD/6-311+G(2d,p)] = -4297.958937 h
Gcorr[B3LYP/6-31G(d,p)] = 1.010865 h

166. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 3rd step, TS

Center No.	Atom	X	Y	Z
1	P	-1.357582	-1.446274	-4.164982
2	H	-5.842174	3.703856	-0.708319
3	C	0.589016	-3.236514	-3.844069
4	H	1.035977	-2.598851	-4.613997
5	H	0.641506	-4.275380	-4.186086
6	C	1.363402	-3.088653	-2.535125
7	H	1.238192	-2.081039	-2.137713
8	C	0.108221	-3.593744	-0.532750
9	C	2.832081	-3.421887	-2.713959
10	H	2.969769	-4.475379	-2.974035
11	H	3.265125	-2.810549	-3.510686
12	C	4.841282	-3.344739	-1.465223
13	C	-0.434571	-4.736175	0.294784
14	H	-0.679390	-5.563258	-0.378987
15	H	0.394619	-5.092209	0.922151
16	C	-1.633606	-4.343334	1.162792
17	H	-1.346799	-3.512579	1.817846
18	H	-2.440234	-3.969450	0.520110
19	C	-2.161758	-5.510290	2.004640
20	H	-2.408778	-6.354137	1.345026
21	H	-1.368716	-5.869037	2.675810
22	C	-3.399782	-5.136992	2.829426
23	H	-4.183946	-4.774494	2.150902
24	H	-3.153504	-4.293694	3.488880
25	C	5.438893	-3.019446	-0.115040
26	H	5.145571	-1.993500	0.139749
27	H	4.944831	-3.658004	0.628145
28	C	6.958122	-3.189571	-0.064312
29	H	7.214537	-4.221100	-0.334053
30	H	7.418282	-2.550972	-0.828028
31	C	7.542608	-2.853171	1.312192
32	H	7.075078	-3.493228	2.073916
33	H	7.278413	-1.819856	1.578680
34	C	9.065787	-3.018300	1.379864
35	H	9.328956	-4.050787	1.113168
36	H	9.532110	-2.378868	0.618228
37	O	5.451212	-3.738651	-2.439654
38	O	-0.042931	-2.408248	-0.269595
39	O	3.502412	-3.140843	-1.469638
40	O	0.808901	-4.040081	-1.584320
41	O	-0.874505	-1.130939	-5.545205
42	O	-2.851259	-1.544639	-3.863190
43	O	-0.789966	-2.917973	-3.658608
44	O	-7.087644	3.858841	-0.869153
45	C	9.647521	-2.681576	2.756070
46	H	9.224391	-3.328034	3.533476
47	H	10.734827	-2.809186	2.772624
48	H	9.429682	-1.644168	3.034712
49	C	-3.940995	-6.299535	3.666515
50	H	-3.187896	-6.659817	4.376597
51	H	-4.824154	-6.001378	4.240881
52	H	-4.226896	-7.145331	3.030828
53	O	-6.655622	1.628126	-0.141485
54	H	-6.874324	1.529956	0.795507
55	H	-7.084005	2.736049	-0.527716
56	Ca	-4.150614	-1.431170	-1.951774

57	O	-4.928387	-3.276359	-0.497018
58	H	-4.994526	-4.189566	-0.806872
59	H	-5.634194	-3.168667	0.154660
60	O	-0.672587	-0.391807	-3.124993
61	H	-7.272688	3.878065	-1.818813
62	H	-1.096681	-0.451969	-2.238918
63	O	-2.133565	-0.701238	-0.758372
64	H	-2.292044	0.169576	-0.316038
65	H	-1.492546	-1.237093	-0.254891
66	P	-4.629606	1.771669	-0.256804
67	C	-4.299294	2.055582	2.374977
68	H	-3.970188	3.023077	1.993618
69	H	-5.168205	2.209397	3.020898
70	C	-3.167106	1.322115	3.094056
71	H	-3.482870	0.304993	3.333583
72	H	-2.292522	1.289706	2.445839
73	C	-2.122227	2.577746	-1.039704
74	H	-2.672817	3.471920	-1.344623
75	H	-1.932368	1.962917	-1.929807
76	C	-0.801339	3.014045	-0.419605
77	H	-0.987719	3.509302	0.534587
78	C	0.416567	1.558016	1.081215
79	C	-0.018437	3.929257	-1.345575
80	H	0.280447	3.409200	-2.260025
81	H	-0.620528	4.799601	-1.621082
82	C	1.994229	5.182752	-1.296408
83	C	1.415112	0.423768	1.095654
84	H	1.115794	-0.312584	0.343795
85	H	2.368343	0.845121	0.746553
86	C	-3.802148	1.900445	5.443511
87	H	-4.642652	2.512462	5.123647
88	H	-4.115079	0.864819	5.570656
89	H	-3.402900	2.288370	6.379670
90	C	-2.275123	3.381365	4.190103
91	H	-1.864466	3.756311	5.127149
92	H	-1.515532	3.390919	3.409587
93	H	-3.135348	3.983271	3.903395
94	C	-1.526411	1.160195	4.900992
95	H	-0.731061	1.239043	4.161264
96	H	-1.206401	1.580529	5.853607
97	H	-1.830934	0.122492	5.033086
98	N	-2.712567	1.952488	4.404236
99	C	1.582910	-0.223854	2.471998
100	H	1.847606	0.546284	3.205623
101	H	0.618537	-0.638946	2.792162
102	C	2.639144	-1.334318	2.481234
103	H	2.380245	-2.089231	1.726154
104	H	3.609681	-0.916950	2.177408
105	C	2.783695	-2.009827	3.850646
106	H	1.810522	-2.418769	4.154480
107	H	3.042031	-1.250674	4.601254
108	C	3.188615	5.548997	-0.443749
109	H	2.809415	5.984565	0.489247
110	H	3.684939	4.614997	-0.151108
111	C	4.165306	6.498053	-1.139611
112	H	4.513058	6.037431	-2.072113
113	H	3.633916	7.412292	-1.430413
114	C	5.367590	6.856448	-0.259009
115	H	5.893904	5.936631	0.033140
116	H	5.012666	7.313823	0.675477
117	C	6.355515	7.808261	-0.944388
118	H	6.709559	7.349920	-1.877671
119	H	5.828001	8.726101	-1.237254
120	O	1.783725	5.560103	-2.432208
121	O	0.018680	2.153598	2.069510
122	O	1.155321	4.357861	-0.627883
123	O	0.025688	1.842682	-0.176953
124	O	-4.681838	0.751814	-1.384834
125	O	-4.782961	3.317553	-0.459576
126	O	-2.876515	1.844502	-0.076309
127	O	-4.714919	1.204188	1.296498
128	C	7.556005	8.167614	-0.063805

129	H	8.122859	7.272565	0.217028
130	H	8.241626	8.847111	-0.580548
131	H	7.234804	8.658933	0.861800
132	C	3.833102	-3.124935	3.870004
133	H	4.824533	-2.740998	3.604202
134	H	3.909237	-3.584779	4.860806
135	H	3.582087	-3.916716	3.154678

E[B3LYP/6-31G(d,p)] = -4299.483395 h, E[APFD/6-311+G(2d,p)] = -4297.902194 h
Gcorr[B3LYP/6-31G(d,p)] = 1.012173 h

167. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 3rd step, products

Center No.	Atom	X	Y	Z
1	P	-1.435124	-1.400187	-4.116692
2	H	-5.568086	3.773746	-0.661445
3	C	0.487748	-3.221723	-3.837440
4	H	0.931069	-2.589064	-4.613606
5	H	0.522200	-4.261084	-4.180355
6	C	1.284185	-3.085023	-2.540185
7	H	1.181122	-2.075334	-2.141578
8	C	0.039950	-3.571931	-0.525475
9	C	2.743739	-3.441593	-2.746328
10	H	2.859253	-4.498703	-3.002642
11	H	3.169118	-2.842478	-3.556275
12	C	4.784089	-3.377332	-1.550278
13	C	-0.509571	-4.709068	0.305454
14	H	-0.768077	-5.532855	-0.367285
15	H	0.319343	-5.075088	0.927351
16	C	-1.698989	-4.303781	1.180801
17	H	-1.398267	-3.479334	1.837631
18	H	-2.503494	-3.916669	0.543311
19	C	-2.238588	-5.466979	2.020562
20	H	-2.499992	-6.304663	1.358617
21	H	-1.447186	-5.839160	2.686337
22	C	-3.467593	-5.080919	2.852898
23	H	-4.249597	-4.703979	2.179786
24	H	-3.206721	-4.244629	3.515655
25	C	5.421308	-3.050903	-0.218676
26	H	5.142197	-2.021976	0.039902
27	H	4.943958	-3.682968	0.540728
28	C	6.940216	-3.231229	-0.209582
29	H	7.182135	-4.265641	-0.481662
30	H	7.383268	-2.599057	-0.988628
31	C	7.565146	-2.892866	1.148570
32	H	7.115454	-3.526984	1.925863
33	H	7.314750	-1.856906	1.418025
34	C	9.088600	-3.067050	1.174045
35	H	9.337981	-4.102206	0.904467
36	H	9.537068	-2.433611	0.396836
37	O	5.364353	-3.779642	-2.539349
38	O	-0.098884	-2.385371	-0.263299
39	O	3.447007	-3.163552	-1.519503
40	O	0.731110	-4.027759	-1.580522
41	O	-0.948710	-1.070865	-5.492772
42	O	-2.929997	-1.486469	-3.817152
43	O	-0.884319	-2.886350	-3.633684
44	O	-7.162940	4.055965	-1.279581
45	C	9.710921	-2.728194	2.531849
46	H	9.306266	-3.369035	3.323613
47	H	10.797513	-2.862079	2.518206
48	H	9.506958	-1.688418	2.812159
49	C	-4.021196	-6.240314	3.686242
50	H	-3.269974	-6.614964	4.390856
51	H	-4.897485	-5.933037	4.266297
52	H	-4.321770	-7.078550	3.047312
53	O	-6.439658	1.706687	-0.193820
54	H	-6.738157	1.797184	0.722085
55	H	-7.224925	3.107661	-1.020032
56	Ca	-4.220187	-1.346618	-1.900886
57	O	-4.998414	-3.196933	-0.451809

58	H	-5.064392	-4.108530	-0.766429
59	H	-5.703210	-3.093496	0.201637
60	O	-0.738179	-0.369461	-3.062276
61	H	-7.100552	4.044287	-2.244909
62	H	-1.165334	-0.428166	-2.176705
63	O	-2.196497	-0.643502	-0.691252
64	H	-2.355357	0.241281	-0.265679
65	H	-1.557648	-1.171673	-0.179809
66	P	-4.678997	1.812879	-0.219468
67	C	-4.186403	2.052313	2.422653
68	H	-3.793699	2.993742	2.038604
69	H	-5.022220	2.265087	3.096259
70	C	-3.091444	1.240660	3.114567
71	H	-3.454887	0.232678	3.323753
72	H	-2.218193	1.188548	2.466325
73	C	-2.103158	2.592676	-0.967290
74	H	-2.621235	3.500240	-1.291269
75	H	-1.929041	1.963694	-1.851340
76	C	-0.766460	3.004588	-0.360718
77	H	-0.932220	3.487456	0.603557
78	C	0.469008	1.516565	1.096250
79	C	0.016591	3.924171	-1.282046
80	H	0.295825	3.415898	-2.209380
81	H	-0.576430	4.807540	-1.534231
82	C	2.034017	5.172067	-1.229280
83	C	1.458606	0.373957	1.074197
84	H	1.147223	-0.341027	0.307131
85	H	2.412909	0.796915	0.729806
86	C	-3.690703	1.732223	5.493762
87	H	-4.532586	2.357047	5.203641
88	H	-4.006567	0.694304	5.591533
89	H	-3.279594	2.088341	6.437444
90	C	-2.160495	3.243603	4.281575
91	H	-1.726628	3.573260	5.224979
92	H	-1.415857	3.276427	3.487420
93	H	-3.018102	3.867868	4.038095
94	C	-1.430616	0.989569	4.898181
95	H	-0.638881	1.095419	4.158062
96	H	-1.101387	1.364020	5.866970
97	H	-1.742510	-0.050592	4.985381
98	N	-2.612431	1.812548	4.444532
99	C	1.630645	-0.309604	2.432588
100	H	1.898793	0.440825	3.185104
101	H	0.666690	-0.731930	2.744518
102	C	2.684577	-1.421971	2.410829
103	H	2.424023	-2.155392	1.635482
104	H	3.655948	-0.998516	2.118353
105	C	2.827707	-2.134851	3.761369
106	H	1.853327	-2.548702	4.054517
107	H	3.088717	-1.397087	4.532116
108	C	3.243456	5.509605	-0.385650
109	H	2.880961	5.898420	0.574153
110	H	3.753207	4.567468	-0.146809
111	C	4.198311	6.497753	-1.056934
112	H	4.531311	6.082888	-2.015896
113	H	3.653834	7.419407	-1.295618
114	C	5.414666	6.826991	-0.184242
115	H	5.954903	5.899879	0.054574
116	H	5.074224	7.237009	0.777232
117	C	6.380256	7.819377	-0.843356
118	H	6.719956	7.408567	-1.803707
119	H	5.838828	8.744606	-1.082690
120	O	1.804372	5.587961	-2.347952
121	O	0.099261	2.101361	2.102282
122	O	1.206903	4.325532	-0.574379
123	O	0.052899	1.820475	-0.147533
124	O	-4.573666	0.886668	-1.434355
125	O	-4.689095	3.428848	-0.353211
126	O	-2.875385	1.902086	0.005826
127	O	-4.703339	1.249249	1.355361
128	C	7.594571	8.149180	0.029834
129	H	8.174972	7.247690	0.257333

130	H	8.263669	8.858953	-0.467500
131	H	7.287201	8.593391	0.983523
132	C	3.873333	-3.253627	3.750488
133	H	4.866006	-2.866211	3.494503
134	H	3.948357	-3.739947	4.728660
135	H	3.619149	-4.025331	3.014607

E[B3LYP/6-31G(d,p)] = -4299.495966 h, E[APFD/6-311+G(2d,p)] = -4297.913402 h
Gcorr[B3LYP/6-31G(d,p)] = 1.018514 h

168. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 4th step, reactants

Center No.	Atom	X	Y	Z
1	P	2.021412	-3.006106	-2.617466
2	H	-4.081951	-5.102805	-1.327796
3	C	2.577277	-0.360630	-2.369702
4	H	1.883865	0.420255	-2.697113
5	H	3.207809	-0.653380	-3.213659
6	C	3.453198	0.177241	-1.239433
7	H	2.852329	0.342738	-0.342750
8	C	4.340922	-1.580544	0.149164
9	C	4.172736	1.454059	-1.633834
10	H	4.887798	1.274171	-2.441611
11	H	3.456526	2.209527	-1.967769
12	C	5.568399	3.075777	-0.610860
13	C	5.365963	-2.686946	0.157462
14	H	5.144359	-3.304462	-0.722788
15	H	6.346524	-2.235234	-0.035113
16	C	5.376406	-3.520639	1.439615
17	H	5.571917	-2.866580	2.298310
18	H	4.380819	-3.951726	1.600585
19	C	6.419761	-4.643151	1.397358
20	H	6.224204	-5.289324	0.530005
21	H	7.416599	-4.209191	1.235744
22	C	6.439648	-5.497335	2.670618
23	H	5.442503	-5.929293	2.830537
24	H	6.633763	-4.850180	3.536634
25	C	6.298607	3.430870	0.665034
26	H	5.570162	3.413972	1.484873
27	H	6.998500	2.612300	0.877924
28	C	7.029532	4.772753	0.599567
29	H	7.730325	4.761005	-0.243667
30	H	6.305852	5.568546	0.385157
31	C	7.782102	5.094600	1.895638
32	H	8.503221	4.292485	2.107769
33	H	7.075135	5.098552	2.737426
34	C	8.519677	6.438255	1.849046
35	H	9.225658	6.433356	1.007633
36	H	7.798290	7.238775	1.636377
37	O	5.586568	3.709490	-1.648072
38	O	3.491074	-1.389552	1.010335
39	O	4.871246	1.924667	-0.465522
40	O	4.466871	-0.815160	-0.943928
41	O	3.467203	-3.243478	-2.916717
42	O	1.247750	-3.841467	-1.603189
43	O	1.818750	-1.484311	-1.911403
44	C	9.270822	6.758104	3.144912
45	H	10.023008	5.992093	3.365657
46	H	9.786320	7.721922	3.080764
47	H	8.585177	6.803283	3.998830
48	C	7.481567	-6.619038	2.626689
49	H	8.492801	-6.215225	2.501794
50	H	7.470872	-7.210647	3.547909
51	H	7.292872	-7.301575	1.790175
52	O	-3.652328	-5.152001	0.677577
53	H	-2.996220	-5.548937	1.266148
54	Ca	0.075371	-2.372484	-0.130493
55	O	1.518024	-3.123935	1.726907
56	H	2.336737	-2.585871	1.676602
57	H	1.157391	-2.970983	2.610842
58	O	1.184052	-2.893052	-3.993181

59	H	0.221723	-3.110255	-3.850384
60	O	-1.189706	-1.332985	1.776140
61	H	-2.050367	-1.781439	1.723833
62	H	-1.388904	-0.397260	1.567126
63	P	-2.903299	-3.825385	-0.085100
64	C	-4.784722	-3.034867	1.735581
65	H	-5.524266	-3.674177	1.253681
66	H	-4.358594	-3.573208	2.583983
67	C	-5.378888	-1.686827	2.148886
68	H	-4.599744	-1.046472	2.565399
69	H	-5.811332	-1.190397	1.279269
70	C	-3.152848	-1.489691	-1.717463
71	H	-4.157032	-1.918626	-1.771343
72	H	-2.797757	-1.349056	-2.745972
73	C	-3.241984	-0.122744	-1.048401
74	H	-3.291819	-0.232757	0.033189
75	C	-1.453064	1.389014	-0.439118
76	C	-4.442513	0.661606	-1.557964
77	H	-4.377632	0.828594	-2.637121
78	H	-5.369570	0.121954	-1.345775
79	C	-5.444168	2.784195	-1.207510
80	C	-0.576389	2.457735	-1.045414
81	H	0.005618	2.006020	-1.856856
82	H	-1.256608	3.167363	-1.536092
83	C	-5.976728	-2.352337	4.485638
84	H	-5.733146	-3.400737	4.328746
85	H	-5.094140	-1.800849	4.807053
86	H	-6.765224	-2.266536	5.232043
87	C	-7.661570	-2.549648	2.697760
88	H	-8.450210	-2.495478	3.446758
89	H	-8.005753	-2.118747	1.758434
90	H	-7.365736	-3.586511	2.553582
91	C	-6.931844	-0.336862	3.467335
92	H	-7.295641	0.099870	2.538374
93	H	-7.729244	-0.364231	4.208278
94	H	-6.085135	0.233991	3.846262
95	N	-6.480729	-1.752854	3.195762
96	C	0.318607	3.174136	-0.033529
97	H	-0.302216	3.561123	0.782465
98	H	1.005107	2.448854	0.421135
99	C	1.119949	4.319413	-0.662149
100	H	1.731189	3.930672	-1.488884
101	H	0.427986	5.044202	-1.113713
102	C	2.025949	5.041566	0.342298
103	H	2.690527	4.308258	0.819084
104	H	1.407753	5.460469	1.147626
105	C	-5.330826	4.077042	-0.431678
106	H	-5.285573	3.822283	0.634446
107	H	-4.354920	4.519670	-0.669186
108	C	-6.465525	5.061922	-0.717757
109	H	-6.485680	5.287245	-1.790737
110	H	-7.425256	4.583342	-0.487871
111	C	-6.330642	6.361942	0.083018
112	H	-5.365880	6.835235	-0.148478
113	H	-6.304986	6.128325	1.156888
114	C	-7.462096	7.360431	-0.189899
115	H	-7.486490	7.593786	-1.262908
116	H	-8.425503	6.885734	0.040269
117	O	-6.297883	2.512373	-2.027665
118	O	-1.611536	1.220806	0.761434
119	O	-4.449091	1.927948	-0.872439
120	O	-2.056173	0.651387	-1.389838
121	O	-1.464616	-4.132477	0.341044
122	O	-3.625347	-4.262211	-1.493291
123	O	-2.269570	-2.389045	-1.052129
124	O	-3.749117	-2.679828	0.802504
125	C	-7.326840	8.657889	0.612620
126	H	-6.387935	9.172311	0.377883
127	H	-8.147996	9.349093	0.396473
128	H	-7.333837	8.459034	1.690453
129	C	2.866132	6.152690	-0.294509
130	H	2.230535	6.902119	-0.780075

131	H	3.475827	6.669376	0.454162
132	H	3.544057	5.746160	-1.053007
133	O	-1.361708	-3.611460	-3.570568
134	H	-2.036087	-3.371499	-4.219052
135	H	-1.722631	-3.337944	-2.704962

E[B3LYP/6-31G(d,p)] = -4299.505775 h, E[APFD/6-311+G(2d,p)] = -4297.919283 h
Gcorr[B3LYP/6-31G(d,p)] = 1.021327 h

169. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 4th step, TS

Center No.	Atom	X	Y	Z
1	P	1.672050	-2.787856	-3.043518
2	H	-4.472305	-5.064787	-1.495808
3	C	2.537933	-0.329896	-2.293842
4	H	1.843218	0.476192	-2.561132
5	H	3.158557	-0.563550	-3.164950
6	C	3.427206	0.152302	-1.150417
7	H	2.833464	0.331336	-0.251831
8	C	4.319109	-1.570439	0.285821
9	C	4.203090	1.398215	-1.536705
10	H	4.928226	1.180498	-2.324883
11	H	3.524399	2.176222	-1.896479
12	C	5.784731	2.863078	-0.547266
13	C	5.399140	-2.623630	0.367895
14	H	5.253338	-3.304607	-0.480400
15	H	6.356811	-2.122972	0.180091
16	C	5.423206	-3.387191	1.692873
17	H	5.516485	-2.672917	2.519833
18	H	4.464289	-3.900319	1.833467
19	C	6.566991	-4.404957	1.760227
20	H	6.472611	-5.117845	0.929045
21	H	7.524564	-3.886549	1.610514
22	C	6.610558	-5.174176	3.085722
23	H	5.656667	-5.699138	3.230331
24	H	6.693649	-4.458968	3.915207
25	C	6.475091	3.225587	0.748433
26	H	5.698004	3.481962	1.479452
27	H	6.951953	2.315600	1.134084
28	C	7.490161	4.359900	0.599924
29	H	8.236975	4.078627	-0.152208
30	H	6.982165	5.249433	0.208184
31	C	8.189197	4.702125	1.920321
32	H	8.692138	3.805821	2.310309
33	H	7.436379	4.979949	2.671629
34	C	9.211722	5.836969	1.784943
35	H	9.962184	5.558274	1.032890
36	H	8.708059	6.731817	1.395039
37	O	5.980681	3.377951	-1.630548
38	O	3.473555	-1.356789	1.146340
39	O	4.892036	1.861831	-0.359273
40	O	4.406336	-0.879066	-0.857684
41	O	3.023275	-2.991696	-3.677034
42	O	1.148133	-3.842213	-2.050456
43	O	1.821822	-1.493696	-1.903328
44	C	9.911890	6.178033	3.103676
45	H	10.452972	5.311199	3.500061
46	H	10.634360	6.990480	2.974156
47	H	9.189482	6.492964	3.865411
48	C	7.764213	-6.178085	3.159125
49	H	8.732645	-5.676046	3.052766
50	H	7.769425	-6.712002	4.115008
51	H	7.690141	-6.925294	2.360735
52	O	-3.658329	-5.261496	0.464620
53	H	-2.916971	-5.664411	0.938734
54	Ca	0.274125	-2.620280	-0.235881
55	O	1.666259	-3.347177	1.654241
56	H	2.390806	-2.693526	1.746410
57	H	1.302837	-3.480754	2.539318
58	O	0.558749	-2.298731	-4.018822
59	H	-0.651782	-2.648016	-3.728458

60	O	-1.185376	-1.438263	1.373483
61	H	-2.055699	-1.865934	1.308440
62	H	-1.352540	-0.505011	1.126744
63	P	-3.127798	-3.899069	-0.327987
64	C	-4.702470	-3.163095	1.737080
65	H	-5.495939	-3.783635	1.321414
66	H	-4.168767	-3.733903	2.497938
67	C	-5.240090	-1.836253	2.273930
68	H	-4.413472	-1.193889	2.581069
69	H	-5.812463	-1.326354	1.498088
70	C	-3.777034	-1.291685	-1.820993
71	H	-4.748898	-1.741208	-1.595313
72	H	-3.732866	-1.119003	-2.903341
73	C	-3.681098	0.047265	-1.100714
74	H	-3.515208	-0.107715	-0.035404
75	C	-1.688800	1.377433	-0.794402
76	C	-4.930578	0.886636	-1.323021
77	H	-5.072035	1.112862	-2.383511
78	H	-5.816784	0.358392	-0.959634
79	C	-5.726801	3.045498	-0.743522
80	C	-0.819825	2.393038	-1.497283
81	H	-0.346049	1.895108	-2.352608
82	H	-1.492047	3.143176	-1.932878
83	C	-5.422445	-2.527612	4.669389
84	H	-5.146928	-3.559956	4.466286
85	H	-4.533183	-1.925937	4.853435
86	H	-6.086184	-2.489881	5.531813
87	C	-7.360070	-2.814692	3.168619
88	H	-8.032488	-2.783123	4.024522
89	H	-7.857198	-2.413364	2.286330
90	H	-7.039806	-3.839772	2.993423
91	C	-6.633743	-0.566186	3.829043
92	H	-7.180203	-0.160440	2.979006
93	H	-7.286368	-0.632855	4.698097
94	H	-5.768050	0.054897	4.054377
95	N	-6.157501	-1.957402	3.480304
96	C	0.215270	3.043449	-0.578207
97	H	-0.301650	3.511802	0.267546
98	H	0.855264	2.263560	-0.147651
99	C	1.081807	4.085994	-1.292808
100	H	1.589587	3.618518	-2.148683
101	H	0.439802	4.870826	-1.716482
102	C	2.123272	4.726864	-0.366408
103	H	2.733236	3.936186	0.091475
104	H	1.604796	5.227500	0.462202
105	C	-5.411431	4.291944	0.052431
106	H	-5.292510	3.994204	1.101934
107	H	-4.422722	4.645902	-0.265636
108	C	-6.463974	5.391884	-0.093788
109	H	-6.571653	5.648747	-1.154519
110	H	-7.438420	5.004304	0.227084
111	C	-6.115705	6.649500	0.710348
112	H	-5.135830	7.029215	0.387775
113	H	-6.005498	6.386088	1.771899
114	C	-7.159889	7.764018	0.571603
115	H	-7.270778	8.024182	-0.489739
116	H	-8.138308	7.384418	0.895706
117	O	-6.705789	2.868659	-1.440562
118	O	-1.613651	1.114170	0.397625
119	O	-4.757968	2.111740	-0.586540
120	O	-2.562583	0.805101	-1.639337
121	O	-1.624892	-4.059666	-0.270366
122	O	-4.062100	-4.192264	-1.619741
123	O	-2.727497	-2.182199	-1.446687
124	O	-3.784936	-2.772809	0.689946
125	C	-6.808591	9.021659	1.372013
126	H	-5.851036	9.443530	1.045831
127	H	-7.571856	9.797537	1.252743
128	H	-6.724108	8.799211	2.441908
129	C	3.038245	5.726630	-1.079731
130	H	2.457813	6.524996	-1.556173
131	H	3.736025	6.196498	-0.378745

132	H	3.632510	5.234519	-1.857272
133	O	-1.714225	-2.968240	-3.500559
134	H	-2.270813	-2.765818	-4.263159
135	H	-2.229922	-2.557676	-2.433215

E[B3LYP/6-31G(d,p)] = -4299.483496 h, E[APFD/6-311+G(2d,p)] = -4297.907294 h
Gcorr[B3LYP/6-31G(d,p)] = 1.015873 h

170. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 4th step, products

Center No.	Atom	X	Y	Z
1	P	1.115478	-4.056253	-1.029987
2	H	-2.620391	-3.586584	-2.030296
3	C	2.175170	-1.685231	-1.882837
4	H	1.599324	-0.922102	-2.416053
5	H	2.605515	-2.374311	-2.614986
6	C	3.285501	-1.015729	-1.076685
7	H	2.854040	-0.478113	-0.229877
8	C	4.076372	-2.417823	0.714309
9	C	4.120225	-0.068329	-1.919775
10	H	4.658221	-0.602402	-2.708917
11	H	3.485891	0.690522	-2.384313
12	C	5.783505	1.587103	-1.539686
13	C	4.961176	-3.603986	0.999781
14	H	4.491974	-4.441837	0.467925
15	H	5.928032	-3.433873	0.512568
16	C	5.128181	-3.915631	2.487823
17	H	5.559248	-3.045787	2.999210
18	H	4.140618	-4.077926	2.936032
19	C	6.012042	-5.145138	2.727757
20	H	5.579795	-6.010884	2.206277
21	H	6.999414	-4.978843	2.274057
22	C	6.189042	-5.485521	4.212268
23	H	5.202057	-5.652317	4.664458
24	H	6.619985	-4.619485	4.732644
25	C	6.755183	2.120647	-0.510256
26	H	6.164410	2.483987	0.340730
27	H	7.330112	1.269554	-0.125393
28	C	7.679654	3.216217	-1.042967
29	H	8.237505	2.830919	-1.905167
30	H	7.074849	4.050529	-1.417156
31	C	8.658587	3.724562	0.021649
32	H	9.261444	2.884414	0.394555
33	H	8.093972	4.101253	0.886401
34	C	9.591850	4.827752	-0.491762
35	H	10.154918	4.450901	-1.356267
36	H	8.988377	5.666691	-0.863881
37	O	5.637218	2.002426	-2.673041
38	O	3.352237	-1.858429	1.524636
39	O	5.067270	0.557178	-1.033144
40	O	4.174277	-2.040757	-0.572079
41	O	2.443159	-4.733269	-0.914386
42	O	0.044728	-4.186368	0.048846
43	O	1.279204	-2.378589	-1.007402
44	C	10.568902	5.333894	0.573592
45	H	11.209496	4.523525	0.939966
46	H	11.220298	6.119830	0.177621
47	H	10.034160	5.747686	1.436230
48	C	7.072890	-6.714369	4.446117
49	H	8.077361	-6.563336	4.034343
50	H	7.180190	-6.932769	5.513634
51	H	6.649292	-7.603464	3.965104
52	O	-4.472797	-4.618546	1.375534
53	H	-4.501916	-4.323436	2.298044
54	Ca	-0.579329	-1.967878	0.745242
55	O	0.887951	-2.114809	2.753994
56	H	1.826088	-2.137017	2.478351
57	H	0.731647	-1.200092	3.041870
58	O	0.503584	-4.340023	-2.497361
59	H	-0.413780	-3.973310	-2.592410
60	O	-0.633175	0.142296	2.191379

61	H	-1.382673	0.377164	2.754681
62	H	-0.447087	0.926942	1.630870
63	P	-3.888658	-3.454517	0.398673
64	C	-6.340192	-2.794175	-0.358976
65	H	-6.105876	-3.285694	-1.307115
66	H	-6.874949	-3.499302	0.285161
67	C	-7.118709	-1.494971	-0.564251
68	H	-7.228052	-0.981492	0.392240
69	H	-6.571431	-0.844513	-1.248244
70	C	-2.709298	-0.086521	-1.468362
71	H	-3.561827	-0.594222	-1.001301
72	H	-2.946734	0.099151	-2.522490
73	C	-2.486952	1.237835	-0.754407
74	H	-2.150348	1.059514	0.266277
75	C	-0.312104	2.305087	-0.857649
76	C	-3.742523	2.091729	-0.725161
77	H	-4.007252	2.442931	-1.726809
78	H	-4.583806	1.523416	-0.320274
79	C	-4.518229	4.000912	0.452614
80	C	0.604602	3.054033	-1.796151
81	H	1.046564	2.300573	-2.463443
82	H	-0.009404	3.695014	-2.436782
83	C	-9.417145	-2.401401	-0.187462
84	H	-9.056242	-3.421276	-0.075359
85	H	-9.415004	-1.889992	0.774245
86	H	-10.423307	-2.411206	-0.603877
87	C	-8.483415	-2.358749	-2.469514
88	H	-9.489459	-2.356789	-2.886703
89	H	-7.801755	-1.826668	-3.131848
90	H	-8.149364	-3.384137	-2.325351
91	C	-9.083463	-0.263620	-1.340290
92	H	-8.446266	0.275967	-2.039554
93	H	-10.091024	-0.356034	-1.742742
94	H	-9.107681	0.248122	-0.379078
95	N	-8.518076	-1.649641	-1.138174
96	C	1.701878	3.852130	-1.087135
97	H	1.237270	4.614835	-0.449545
98	H	2.258270	3.186678	-0.417523
99	C	2.665687	4.519582	-2.074930
100	H	3.167000	3.745076	-2.671814
101	H	2.095927	5.135895	-2.784624
102	C	3.725986	5.390082	-1.390198
103	H	4.283081	4.779174	-0.667002
104	H	3.227787	6.175027	-0.805419
105	C	-4.092693	5.135079	1.357706
106	H	-3.467934	4.713574	2.153960
107	H	-3.427690	5.786232	0.774880
108	C	-5.266938	5.928576	1.933698
109	H	-5.866054	6.335775	1.110778
110	H	-5.926751	5.246778	2.484349
111	C	-4.811826	7.063438	2.858091
112	H	-4.152023	7.745161	2.302885
113	H	-4.203008	6.647577	3.673436
114	C	-5.977597	7.861093	3.455126
115	H	-6.583253	8.280290	2.640360
116	H	-6.638353	7.177044	4.004667
117	O	-5.644754	3.789359	0.049874
118	O	-0.027798	2.018472	0.296701
119	O	-3.461927	3.218087	0.127043
120	O	-1.463518	1.981242	-1.465011
121	O	-2.797133	-2.675090	1.099696
122	O	-3.653578	-4.112698	-0.939372
123	O	-1.527773	-0.884743	-1.366426
124	O	-5.131379	-2.378473	0.284220
125	C	-5.521631	8.988538	4.386103
126	H	-4.885938	9.706998	3.856056
127	H	-6.375173	9.538389	4.795890
128	H	-4.942879	8.595117	5.229655
129	C	4.704800	6.029098	-2.379813
130	H	4.180126	6.668484	-3.099071
131	H	5.447776	6.647456	-1.865427
132	H	5.243177	5.262771	-2.948793

133	O	-1.944862	-3.191531	-2.667588
134	H	-2.354034	-3.179768	-3.543599
135	H	-1.644249	-1.664378	-1.968923

E[B3LYP/6-31G(d,p)] = -4299.558415 h, E[APFD/6-311+G(2d,p)] = -4297.960346 h
Gcorr[B3LYP/6-31G(d,p)] = 1.018650 h

171. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 5th step, reactants (hydrolysed glycerol + carbon chains neglected)

Center No.	Atom	X	Y	Z
1	P	-0.812546	-2.188031	-1.492534
2	C	0.364071	0.249183	-1.314391
3	H	-0.273890	1.130113	-1.193935
4	H	0.469544	0.026314	-2.379792
5	C	1.736409	0.516337	-0.703457
6	H	1.653537	0.619344	0.380121
7	C	2.848111	-1.513574	-0.033404
8	C	2.399328	1.745863	-1.295654
9	H	2.639885	1.598133	-2.352304
10	H	1.741380	2.614935	-1.207644
11	C	4.331328	3.061936	-0.899621
12	C	3.519473	-2.741518	-0.596510
13	H	2.798925	-3.183105	-1.297641
14	H	4.364492	-2.407979	-1.210879
15	C	3.961242	-3.753382	0.461878
16	H	4.657560	-3.270815	1.158628
17	H	3.091605	-4.058855	1.056175
18	C	4.621875	-4.992112	-0.154031
19	H	3.923240	-5.465165	-0.858433
20	H	5.492935	-4.683577	-0.749093
21	C	5.062244	-6.023590	0.891685
22	H	4.190414	-6.329580	1.485619
23	H	5.759158	-5.549123	1.595689
24	C	5.576880	3.181232	-0.050293
25	H	5.264743	3.167156	1.001385
26	H	6.162931	2.264549	-0.194652
27	C	6.412486	4.423426	-0.362639
28	H	6.696466	4.410205	-1.421763
29	H	5.794162	5.318533	-0.223310
30	C	7.668860	4.521445	0.510041
31	H	8.282919	3.620670	0.368905
32	H	7.377742	4.528138	1.570067
33	C	8.517041	5.763532	0.211065
34	H	8.807368	5.755815	-0.848210
35	H	7.902043	6.662712	0.351502
36	O	3.992076	3.820658	-1.785860
37	O	2.565317	-1.331020	1.143873
38	O	3.608950	1.971939	-0.548270
39	O	2.580297	-0.624175	-1.001244
40	O	0.197596	-2.699793	-2.464784
41	O	-1.271016	-3.036981	-0.301318
42	O	-0.248279	-0.858413	-0.638885
43	C	9.771562	5.860778	1.084285
44	H	10.422809	4.991176	0.939543
45	H	10.354980	6.756520	0.847517
46	H	9.510865	5.904582	2.147974
47	C	5.721157	-7.261391	0.275774
48	H	6.615731	-6.990062	-0.296362
49	H	6.023517	-7.978122	1.046246
50	H	5.035641	-7.775886	-0.407283
51	O	-5.785254	-1.123393	0.912485
52	H	-5.968995	-1.176755	1.862664
53	Ca	-1.096113	-1.752322	1.705254
54	O	0.879902	-2.899709	2.577162
55	H	1.672183	-2.451209	2.211015
56	H	1.042890	-3.019294	3.521786
57	O	-2.080377	-1.585432	-2.291023
58	H	-2.761592	-1.173739	-1.686559
59	P	-4.343484	-0.443038	0.611935
60	C	-5.397446	1.914882	0.044395
61	H	-4.862479	2.098856	-0.891018

62	H	-6.320370	1.370648	-0.175562
63	C	-5.677736	3.198337	0.826240
64	H	-6.262036	2.961580	1.716667
65	H	-4.733396	3.648182	1.137538
66	C	-7.766726	3.747466	-0.430042
67	H	-7.590517	2.991264	-1.192132
68	H	-8.316803	3.321684	0.408145
69	H	-8.323176	4.578225	-0.861444
70	C	-5.638429	4.807520	-1.084049
71	H	-6.202038	5.614415	-1.549925
72	H	-4.689034	5.182963	-0.704531
73	H	-5.468176	4.013587	-1.807694
74	C	-6.710577	5.405116	1.038288
75	H	-5.757997	5.777507	1.412303
76	H	-7.241309	6.194186	0.507704
77	H	-7.318098	5.029795	1.860517
78	N	-6.445207	4.273095	0.073685
79	O	-3.318593	-0.875670	1.642836
80	O	-4.094703	-0.632525	-0.869584
81	O	-4.568974	1.149354	0.928217
82	O	-3.824329	-4.229235	-0.032419
83	H	-4.296268	-3.874411	-0.810741
84	H	-2.923060	-3.876001	-0.155748
85	O	-4.865694	-2.886833	-2.336117
86	H	-4.004259	-2.868280	-2.780272
87	H	-4.841594	-2.053953	-1.821879
88	O	-1.244448	0.456068	2.827604
89	H	-1.114359	0.558987	3.780059
90	H	-2.207742	0.488301	2.680398

E[B3LYP/6-31G(d,p)] = -3411.300403 h, E[APFD/6-311+G(2d,p)] = -3410.189650 h
Gcorr[B3LYP/6-31G(d,p)] = 0.649096 h

172. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 5th step, TS

Center No.	Atom	X	Y	Z
1	P	0.831503	1.803349	-1.574239
2	C	-0.559250	-0.494070	-1.249444
3	H	0.022943	-1.407661	-1.095633
4	H	-0.660402	-0.310888	-2.322627
5	C	-1.939632	-0.645799	-0.619339
6	H	-1.854974	-0.724517	0.466101
7	C	-2.929044	1.453199	0.018525
8	C	-2.693068	-1.840743	-1.173477
9	H	-2.925918	-1.707472	-2.233481
10	H	-2.100023	-2.752932	-1.060367
11	C	-4.751953	-2.950994	-0.788429
12	C	-3.516531	2.718640	-0.555355
13	H	-2.766725	3.113135	-1.253909
14	H	-4.377083	2.436426	-1.173933
15	C	-3.900797	3.758561	0.498476
16	H	-4.629865	3.320738	1.191169
17	H	-3.017462	4.009276	1.098230
18	C	-4.479774	5.035273	-0.121694
19	H	-3.748473	5.465409	-0.820430
20	H	-5.363594	4.780601	-0.723362
21	C	-4.864414	6.090702	0.922191
22	H	-3.980025	6.342719	1.522880
23	H	-5.593823	5.658518	1.620474
24	C	-5.991440	-2.964282	0.077766
25	H	-5.665807	-3.124611	1.113777
26	H	-6.423087	-1.956082	0.058613
27	C	-7.019087	-4.015630	-0.343656
28	H	-7.316609	-3.832855	-1.383428
29	H	-6.548290	-5.005831	-0.330103
30	C	-8.259909	-4.018859	0.556278
31	H	-8.723231	-3.022098	0.543491
32	H	-7.955712	-4.199659	1.597061
33	C	-9.302028	-5.065952	0.144920
34	H	-9.605129	-4.884087	-0.895028
35	H	-8.837669	-6.061283	0.156899

36	O	-4.504911	-3.716723	-1.698766
37	O	-2.675990	1.257465	1.200203
38	O	-3.912901	-1.954893	-0.417664
39	O	-2.701116	0.544809	-0.942088
40	O	-0.153316	2.387187	-2.530696
41	O	1.455564	2.641910	-0.451914
42	O	0.129977	0.602908	-0.629342
43	C	-10.540946	-5.068908	1.045369
44	H	-11.045547	-4.096107	1.027242
45	H	-11.265263	-5.825468	0.726328
46	H	-10.272965	-5.282466	2.086466
47	C	-5.442824	7.366787	0.303638
48	H	-6.347994	7.150740	-0.275322
49	H	-5.706931	8.099409	1.073232
50	H	-4.722569	7.839891	-0.373563
51	O	5.982757	1.414770	0.862391
52	H	6.436976	0.683821	1.307870
53	Ca	1.036238	1.476363	1.625770
54	O	-0.847104	2.695341	2.592963
55	H	-1.677078	2.297034	2.254408
56	H	-0.964732	2.812865	3.544521
57	O	1.968639	1.002156	-2.394127
58	H	2.729446	0.701037	-1.835786
59	P	4.499421	0.856621	0.422258
60	C	5.684407	-1.598436	0.053270
61	H	5.093290	-1.895561	-0.818993
62	H	6.585844	-1.090811	-0.315830
63	C	6.057552	-2.799941	0.924768
64	H	6.680319	-2.473140	1.759325
65	H	5.148794	-3.252146	1.326079
66	C	8.123582	-3.412809	-0.340843
67	H	7.917384	-2.700070	-1.136378
68	H	8.693005	-2.936075	0.456164
69	H	8.676545	-4.261612	-0.740964
70	C	5.997823	-4.542376	-0.866865
71	H	6.548876	-5.390040	-1.272057
72	H	5.051643	-4.877068	-0.443365
73	H	5.821323	-3.808967	-1.650112
74	C	7.128607	-4.976435	1.262201
75	H	6.190010	-5.345862	1.672971
76	H	7.673001	-5.787010	0.779567
77	H	7.735180	-4.531859	2.049919
78	N	6.823414	-3.918998	0.230200
79	O	3.320855	0.923255	1.407149
80	O	4.320505	0.453017	-1.116771
81	O	4.928608	-0.768012	0.914645
82	O	4.241841	2.682785	-0.062974
83	H	4.690580	2.767912	-1.244011
84	H	3.268461	2.781359	-0.163729
85	O	5.053150	2.409137	-2.297402
86	H	4.386218	2.676324	-2.946752
87	H	4.718546	1.317617	-1.842601
88	O	1.693981	-0.664776	2.747285
89	H	1.769292	-0.695541	3.710407
90	H	2.594837	-0.459117	2.408578

E[B3LYP/6-31G(d,p)] = -3411.247908 h, E[APFD/6-311+G(2d,p)] = -3410.131153 h
Gcorr[B3LYP/6-31G(d,p)] = 0.651830h

173. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 5th step, products

Center No.	Atom	X	Y	Z
1	P	0.773342	1.764804	-1.603697
2	C	-0.685986	-0.505366	-1.428861
3	H	-0.133055	-1.447056	-1.363522
4	H	-0.814138	-0.235612	-2.480617
5	C	-2.048503	-0.652751	-0.761640
6	H	-1.928665	-0.789649	0.314599
7	C	-2.967961	1.429068	0.022918
8	C	-2.858984	-1.795710	-1.344502
9	H	-3.129377	-1.602900	-2.386366

10	H	-2.291268	-2.729564	-1.299801
11	C	-4.923693	-2.878594	-0.906907
12	C	-3.545558	2.736204	-0.460693
13	H	-2.809937	3.155703	-1.159657
14	H	-4.429914	2.505224	-1.066800
15	C	-3.876896	3.723784	0.659320
16	H	-4.596647	3.263999	1.347524
17	H	-2.972058	3.922665	1.246229
18	C	-4.443324	5.044416	0.125374
19	H	-3.721765	5.495599	-0.570214
20	H	-5.349042	4.841774	-0.463363
21	C	-4.774256	6.050250	1.234537
22	H	-3.868101	6.249600	1.822417
23	H	-5.494615	5.597554	1.929198
24	C	-6.127355	-2.888573	0.008409
25	H	-5.760749	-3.022059	1.034135
26	H	-6.570238	-1.884970	-0.016190
27	C	-7.161093	-3.956893	-0.350441
28	H	-7.498179	-3.801124	-1.382342
29	H	-6.682650	-4.943483	-0.330565
30	C	-8.367065	-3.946393	0.595699
31	H	-8.838342	-2.953473	0.575409
32	H	-8.022130	-4.098265	1.628362
33	C	-9.416068	-5.010714	0.251643
34	H	-9.760389	-4.857771	-0.780090
35	H	-8.944067	-6.002321	0.271157
36	O	-4.730231	-3.622883	-1.847366
37	O	-2.686798	1.159161	1.183356
38	O	-4.050182	-1.909512	-0.544257
39	O	-2.783524	0.575029	-0.995191
40	O	-0.181832	2.418308	-2.542941
41	O	1.413015	2.522558	-0.436882
42	O	0.062882	0.516232	-0.749199
43	C	-10.619209	-4.998403	1.199321
44	H	-11.131425	-4.029702	1.175858
45	H	-11.349648	-5.767681	0.928272
46	H	-10.309531	-5.183080	2.234362
47	C	-5.338383	7.370461	0.701253
48	H	-6.263768	7.206376	0.137379
49	H	-5.563948	8.066408	1.515825
50	H	-4.625473	7.862927	0.030106
51	O	6.027753	1.486810	0.825067
52	H	6.468579	0.763097	1.294141
53	Ca	1.032526	1.288927	1.602941
54	O	-0.830510	2.511818	2.619754
55	H	-1.667492	2.136873	2.271548
56	H	-0.940428	2.591815	3.576165
57	O	1.921063	0.999247	-2.468355
58	H	2.599142	0.575087	-1.899694
59	P	4.529774	0.945038	0.411720
60	C	5.831427	-1.517054	0.123399
61	H	5.261306	-1.929438	-0.716669
62	H	6.681068	-0.963260	-0.300111
63	C	6.325113	-2.621492	1.062749
64	H	6.961530	-2.194459	1.839849
65	H	5.466767	-3.097413	1.540135
66	C	8.356669	-3.198517	-0.273248
67	H	8.052561	-2.576083	-1.112052
68	H	8.930770	-2.613221	0.444175
69	H	8.950310	-4.037767	-0.633162
70	C	6.293512	-4.507746	-0.577805
71	H	6.882769	-5.344032	-0.951819
72	H	5.400666	-4.873583	-0.071987
73	H	6.019674	-3.852548	-1.401369
74	C	7.566621	-4.689614	1.505603
75	H	6.680180	-5.080621	2.003103
76	H	8.134104	-5.502958	1.055020
77	H	8.188297	-4.145909	2.215555
78	N	7.131185	-3.742511	0.415217
79	O	3.356995	0.910028	1.414418
80	O	4.341319	0.329983	-1.119003
81	O	5.018024	-0.699531	0.937719

82	O	4.233278	2.555609	-0.159208
83	H	4.595631	2.818430	-1.947921
84	H	3.259354	2.654422	-0.220064
85	O	4.675987	2.398034	-2.834715
86	H	3.765672	2.384688	-3.169474
87	H	4.567184	1.014490	-1.805086
88	O	1.795025	-1.021634	2.271676
89	H	1.822318	-1.251250	3.210076
90	H	2.691439	-0.676297	2.046920

E[B3LYP/6-31G(d,p)] = -3411.260274 h, E[APFD/6-311+G(2d,p)] = -3410.142798 h
Gcorr[B3LYP/6-31G(d,p)] = 0.657524 h

174. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 6th step, reactants

Center No.	Atom	X	Y	Z
1	P	-0.919996	-2.042542	-1.780467
2	C	0.496474	0.231355	-1.464762
3	H	-0.157265	1.102655	-1.357175
4	H	0.652683	0.029334	-2.528304
5	C	1.834280	0.501073	-0.788817
6	H	1.708732	0.543458	0.294869
7	C	3.084012	-1.458330	-0.146267
8	C	2.480440	1.780351	-1.288836
9	H	2.760842	1.699452	-2.342896
10	H	1.794225	2.624170	-1.175661
11	C	4.347282	3.134799	-0.743788
12	C	3.903945	-2.595197	-0.706869
13	H	3.291628	-3.082007	-1.476578
14	H	4.752613	-2.153164	-1.243513
15	C	4.374329	-3.599982	0.346037
16	H	4.961328	-3.075868	1.109807
17	H	3.501644	-4.020030	0.860973
18	C	5.209491	-4.733470	-0.260488
19	H	4.619176	-5.250464	-1.030063
20	H	6.080124	-4.307434	-0.778705
21	C	5.688550	-5.752715	0.780157
22	H	4.817289	-6.177786	1.296498
23	H	6.275695	-5.233818	1.549825
24	C	5.555549	3.249225	0.158161
25	H	5.205742	3.163230	1.194499
26	H	6.181808	2.364693	-0.014694
27	C	6.351643	4.538053	-0.051759
28	H	6.677740	4.594080	-1.097239
29	H	5.691821	5.399259	0.108905
30	C	7.567451	4.637746	0.876363
31	H	8.224010	3.771329	0.713237
32	H	7.234950	4.575021	1.922277
33	C	8.373153	5.927448	0.678596
34	H	8.704769	5.988919	-0.366710
35	H	7.715307	6.792042	0.840416
36	O	4.008902	3.934216	-1.593727
37	O	2.777496	-1.316221	1.030123
38	O	3.656590	1.998113	-0.487851
39	O	2.723386	-0.599219	-1.111503
40	O	-0.010135	-2.602277	-2.821649
41	O	-1.496940	-2.913787	-0.659253
42	O	-0.124382	-0.902730	-0.841175
43	C	9.587179	6.028158	1.606905
44	H	10.280036	5.194664	1.444090
45	H	10.140746	6.958221	1.441517
46	H	9.283350	6.004133	2.659727
47	C	6.525616	-6.882994	0.173975
48	H	7.422050	-6.490522	-0.319589
49	H	6.851788	-7.593595	0.940369
50	H	5.953232	-7.441009	-0.575819
51	O	-5.581584	-1.465571	1.568570
52	H	-5.800222	-0.697080	2.145297
53	Ca	-0.874762	-1.881212	1.452125
54	O	1.099601	-3.034730	2.299563
55	H	1.894431	-2.535931	2.016455

56	H	1.222247	-3.242155	3.235053
57	O	-2.085699	-1.183047	-2.501228
58	H	-2.852317	-0.982659	-1.920206
59	P	-4.277712	-1.142893	0.642699
60	C	-5.881165	1.085261	0.002226
61	H	-5.797111	0.935366	-1.078543
62	H	-6.766748	0.534969	0.348388
63	C	-5.997838	2.572422	0.350705
64	H	-6.148729	2.694056	1.424875
65	H	-5.077026	3.084382	0.065712
66	C	-8.469556	2.706862	0.002972
67	H	-8.520331	1.710646	-0.430927
68	H	-8.573656	2.653290	1.086085
69	H	-9.254439	3.333068	-0.419309
70	C	-6.951551	3.362379	-1.821856
71	H	-7.746087	3.970194	-2.252899
72	H	-5.980030	3.802449	-2.043945
73	H	-7.005971	2.350299	-2.216155
74	C	-7.120119	4.744686	0.193851
75	H	-6.154235	5.191451	-0.037934
76	H	-7.919496	5.303848	-0.290576
77	H	-7.275889	4.723819	1.271516
78	N	-7.136083	3.328511	-0.325955
79	O	-2.914431	-0.806696	1.263321
80	O	-4.481924	-1.010561	-1.029822
81	O	-4.706647	0.639983	0.657423
82	O	-4.094138	-2.832509	0.443649
83	H	-5.043859	0.979190	2.410361
84	H	-3.248246	-2.984959	-0.026655
85	O	-5.663444	0.808852	3.155839
86	H	-5.103658	0.643087	3.926672
87	H	-4.669442	-1.913399	-1.334898

E[B3LYP/6-31G(d,p)] = -3334.809136 h, E[APFD/6-311+G(2d,p)] = -3333.723561 h
Gcorr[B3LYP/6-31G(d,p)] = 0.633606 h

175. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 6th step, TS

Center No.	Atom	X	Y	Z
1	P	0.900413	1.968487	-1.782285
2	C	-0.539780	-0.291644	-1.465265
3	H	0.096963	-1.173610	-1.346540
4	H	-0.683759	-0.092944	-2.530944
5	C	-1.886853	-0.528389	-0.795500
6	H	-1.767072	-0.571168	0.288804
7	C	-3.086926	1.464498	-0.163870
8	C	-2.561519	-1.793394	-1.293958
9	H	-2.842593	-1.706419	-2.347367
10	H	-1.894074	-2.652219	-1.182038
11	C	-4.446162	-3.115050	-0.728372
12	C	-3.866225	2.626164	-0.730974
13	H	-3.234231	3.089694	-1.499158
14	H	-4.727044	2.211728	-1.270306
15	C	-4.306258	3.649177	0.317538
16	H	-4.920223	3.149022	1.076142
17	H	-3.422330	4.034697	0.840222
18	C	-5.090247	4.814569	-0.296718
19	H	-4.472950	5.306725	-1.061392
20	H	-5.972802	4.423464	-0.822223
21	C	-5.536618	5.853191	0.739303
22	H	-4.653341	6.242545	1.263360
23	H	-6.151430	5.359281	1.503778
24	C	-5.653868	-3.200757	0.177436
25	H	-5.303404	-3.087059	1.210773
26	H	-6.277336	-2.319245	-0.019840
27	C	-6.454935	-4.491899	0.003477
28	H	-6.782442	-4.575356	-1.039685
29	H	-5.798234	-5.350950	0.187154
30	C	-7.669769	-4.561193	0.935638
31	H	-8.323568	-3.697436	0.748995
32	H	-7.335418	-4.469972	1.978855

33	C	-8.480288	-5.853143	0.775942
34	H	-8.814384	-5.942991	-0.266515
35	H	-7.825067	-6.715108	0.960814
36	O	-4.120227	-3.930377	-1.567914
37	O	-2.792229	1.314290	1.014458
38	O	-3.740019	-1.984038	-0.489588
39	O	-2.746833	0.592570	-1.125235
40	O	0.002602	2.542926	-2.823637
41	O	1.487419	2.828727	-0.654814
42	O	0.100296	0.835019	-0.843408
43	C	-9.692582	-5.923264	1.709325
44	H	-10.382914	-5.092265	1.524509
45	H	-10.249768	-6.855664	1.571557
46	H	-9.386262	-5.870526	2.760377
47	C	-6.321122	7.016439	0.125251
48	H	-7.228309	6.660705	-0.376432
49	H	-6.624925	7.740232	0.888487
50	H	-5.719500	7.550106	-0.619357
51	O	5.687898	1.719020	1.368578
52	H	5.919065	1.004588	2.060671
53	Ca	0.876250	1.774737	1.457040
54	O	-1.075650	2.948788	2.316783
55	H	-1.883198	2.481178	2.016298
56	H	-1.199608	3.142261	3.255034
57	O	2.063498	1.101071	-2.500672
58	H	2.798545	0.862104	-1.899223
59	P	4.321833	1.447027	0.609780
60	C	5.922967	-1.269144	0.102471
61	H	5.722381	-1.136327	-0.970010
62	H	6.894923	-0.782579	0.306146
63	C	6.008222	-2.763958	0.452848
64	H	6.253738	-2.877990	1.510705
65	H	5.038421	-3.229658	0.267368
66	C	8.427834	-3.071021	-0.099243
67	H	8.502187	-2.079365	-0.539606
68	H	8.625996	-3.023487	0.971110
69	H	9.134808	-3.745591	-0.581276
70	C	6.719313	-3.632850	-1.779384
71	H	7.430028	-4.292904	-2.275575
72	H	5.704959	-4.008099	-1.910446
73	H	6.801940	-2.626454	-2.183432
74	C	6.974651	-5.013606	0.226874
75	H	5.966289	-5.399604	0.083692
76	H	7.692545	-5.627401	-0.316310
77	H	7.222481	-4.995563	1.287451
78	N	7.035680	-3.606165	-0.307556
79	O	3.078021	1.003386	1.355108
80	O	4.465968	0.937262	-0.961050
81	O	4.889816	-0.744417	0.878809
82	O	4.073959	3.028863	0.218876
83	H	5.471897	-0.618290	2.214410
84	H	3.177773	3.108759	-0.187951
85	O	6.047793	-0.233576	3.003950
86	H	5.441386	-0.115475	3.747858
87	H	4.733932	1.715876	-1.478141

E[B3LYP/6-31G(d,p)] = -3334.803149 h, E[APFD/6-311+G(2d,p)] = -3333.718134 h
Gcorr[B3LYP/6-31G(d,p)] = 0.628660 h

176. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 6th step, products

Center No.	Atom	X	Y	Z
1	P	0.564828	1.849557	-1.682301
2	C	-0.769918	-0.483431	-1.362396
3	H	-0.164262	-1.381845	-1.211326
4	H	-0.882202	-0.302572	-2.434808
5	C	-2.140934	-0.665445	-0.720406
6	H	-2.044432	-0.725069	0.365380
7	C	-3.191249	1.413275	-0.107149
8	C	-2.863978	-1.891572	-1.245942
9	H	-3.129410	-1.775179	-2.300494

10	H	-2.235888	-2.780760	-1.142067
11	C	-4.821134	-3.127687	-0.734331
12	C	-3.818897	2.650978	-0.698405
13	H	-3.084576	3.055987	-1.407247
14	H	-4.673594	2.333178	-1.307781
15	C	-4.228649	3.697071	0.339472
16	H	-4.942211	3.250721	1.042757
17	H	-3.350468	3.983381	0.930925
18	C	-4.846383	4.945273	-0.301153
19	H	-4.130323	5.383156	-1.010779
20	H	-5.724638	4.654199	-0.894414
21	C	-5.257664	6.008615	0.724287
22	H	-4.378777	6.297783	1.316227
23	H	-5.971581	5.568845	1.433740
24	C	-6.037592	-3.176989	0.162565
25	H	-5.685902	-3.132035	1.200873
26	H	-6.603101	-2.249879	0.003983
27	C	-6.917598	-4.406026	-0.069909
28	H	-7.247791	-4.421034	-1.115523
29	H	-6.316690	-5.312192	0.073850
30	C	-8.136213	-4.440612	0.859247
31	H	-8.732999	-3.529018	0.713595
32	H	-7.798512	-4.419294	1.905168
33	C	-9.027801	-5.669074	0.641169
34	H	-9.365329	-5.689117	-0.403861
35	H	-8.429659	-6.578992	0.785256
36	O	-4.532555	-3.933405	-1.596570
37	O	-2.928183	1.243295	1.076161
38	O	-4.058226	-2.043747	-0.456479
39	O	-2.938668	0.497878	-1.055253
40	O	-0.427277	2.406583	-2.644810
41	O	1.150068	2.703681	-0.543796
42	O	-0.102916	0.630109	-0.745012
43	C	-10.243594	-5.703914	1.571977
44	H	-10.878889	-4.822731	1.426358
45	H	-10.859279	-6.591328	1.392430
46	H	-9.936220	-5.719105	2.623935
47	C	-5.875430	7.255077	0.083708
48	H	-6.776096	7.001474	-0.486995
49	H	-6.157887	7.994607	0.840046
50	H	-5.171900	7.735598	-0.605750
51	O	5.582184	1.611467	0.899935
52	H	6.066239	0.520341	2.079785
53	Ca	0.768937	1.508930	1.539336
54	O	-1.137914	2.714124	2.479335
55	H	-1.959371	2.310485	2.126655
56	H	-1.266660	2.813439	3.431617
57	O	1.750509	1.107420	-2.485585
58	H	2.521730	0.880606	-1.914408
59	P	4.141822	1.595379	0.459354
60	C	5.853364	-2.284500	0.312684
61	H	5.368609	-2.943946	-0.412665
62	H	5.941726	-1.289556	-0.140914
63	C	7.229086	-2.832007	0.724783
64	H	7.645084	-2.193726	1.507086
65	H	7.113803	-3.842781	1.120404
66	C	8.633701	-1.536746	-0.882889
67	H	7.762718	-1.103021	-1.368976
68	H	8.943302	-0.917219	-0.042058
69	H	9.447757	-1.630255	-1.600500
70	C	7.820670	-3.772560	-1.514891
71	H	8.636190	-3.868175	-2.230813
72	H	7.544031	-4.752853	-1.128257
73	H	6.965644	-3.300841	-1.994494
74	C	9.529650	-3.528174	0.227276
75	H	9.287286	-4.527468	0.586019
76	H	10.299461	-3.581573	-0.541679
77	H	9.866337	-2.903642	1.053679
78	N	8.289199	-2.912022	-0.369983
79	O	3.060330	1.075546	1.392954
80	O	3.995650	0.634010	-0.898171
81	O	5.041077	-2.252197	1.467948

82	O	3.759769	3.063745	-0.089563
83	H	5.406495	-1.527338	2.034169
84	H	2.798917	3.077654	-0.349368
85	O	6.314491	-0.211675	2.705667
86	H	5.949729	0.051234	3.560873
87	H	4.767381	0.747371	-1.474550

E[B3LYP/6-31G(d,p)] = -3334.857503 h, E[APFD/6-311+G(2d,p)] = -3333.772473 h
Gcorr[B3LYP/6-31G(d,p)] = 0.630383 h

177. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 7th step, reactants (hydrolysed choline neglected)

Center No.	Atom	X	Y	Z
1	P	2.039247	-2.760259	-0.307376
2	C	-0.177250	-2.530121	-1.825078
3	H	-0.321070	-3.568645	-1.513176
4	H	-0.326411	-2.463539	-2.905545
5	C	-1.171827	-1.623621	-1.099216
6	H	-1.039128	-1.689368	-0.019592
7	C	-0.248492	0.590165	-0.748046
8	C	-2.605770	-1.956549	-1.464518
9	H	-2.810048	-1.727997	-2.514331
10	H	-2.802092	-3.019135	-1.295602
11	C	-4.785664	-1.368768	-0.747549
12	C	-0.130293	1.963993	-1.354683
13	H	0.921789	2.075342	-1.645484
14	H	-0.729861	1.999849	-2.266964
15	C	-0.532031	3.088827	-0.383644
16	H	-1.575402	2.945099	-0.075852
17	H	0.078007	3.022029	0.523039
18	C	-0.369075	4.476341	-1.014608
19	H	0.676079	4.612084	-1.326679
20	H	-0.972687	4.534910	-1.930948
21	C	-0.769432	5.616039	-0.069837
22	H	-0.166277	5.554807	0.845898
23	H	-1.813053	5.476304	0.242423
24	C	-5.566291	-0.480632	0.194549
25	H	-5.199273	-0.672799	1.210602
26	H	-5.290397	0.558515	-0.025271
27	C	-7.080104	-0.680268	0.107086
28	H	-7.410841	-0.487547	-0.920624
29	H	-7.317703	-1.730950	0.312803
30	C	-7.849059	0.223705	1.077174
31	H	-7.603430	1.274927	0.869884
32	H	-7.509864	0.028838	2.104477
33	C	-9.369120	0.035301	1.002512
34	H	-9.706978	0.230750	-0.024178
35	H	-9.612892	-1.015757	1.208198
36	O	-5.252638	-2.172738	-1.529227
37	O	0.239098	0.274834	0.339680
38	O	-3.453010	-1.161358	-0.616512
39	O	-0.937947	-0.248626	-1.520133
40	O	1.984093	-4.260701	-0.343681
41	O	3.364208	-2.033978	-0.398558
42	O	1.174512	-2.119587	-1.574440
43	O	4.172314	0.774068	2.588756
44	C	-10.136352	0.937414	1.973739
45	H	-9.938620	1.996158	1.770626
46	H	-11.217124	0.779980	1.896576
47	H	-9.844290	0.740196	3.011569
48	C	-0.605199	7.002776	-0.698928
49	H	-1.223196	7.105051	-1.598249
50	H	-0.898449	7.794242	-0.001636
51	H	0.435550	7.184310	-0.990551
52	Ca	4.484734	-0.095086	-1.005781
53	O	2.646532	0.013213	-2.613108
54	H	2.059992	-0.753111	-2.446911
55	H	2.750348	0.080369	-3.570890
56	O	1.188349	-2.258811	0.990128
57	H	0.930853	-1.314044	0.910564
58	O	5.754596	2.029535	-1.292727

59	H	5.132725	2.378309	-0.618169
60	H	6.637376	2.110847	-0.906836
61	P	3.424074	1.776992	1.765833
62	O	3.575965	1.718264	0.234100
63	O	1.825406	1.799664	2.085900
64	H	1.318914	1.300287	1.410270
65	O	3.860678	3.265604	2.280165
66	H	3.403052	3.957925	1.781153
67	O	3.121768	-3.198760	3.078125
68	H	2.379800	-2.758729	2.636467
69	H	3.049171	-4.117875	2.744930
70	O	2.727701	-5.707151	1.845244
71	H	1.886498	-5.996558	2.223330
72	H	2.467194	-5.249719	1.010019

E[B3LYP/6-31G(d,p)] = -2441.236699 h, E[APFD/6-311+G(2d,p)] = -3157.982455 h
Gcorr[B3LYP/6-31G(d,p)] = 0.180181 h

178. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 7th step, TS

Center No.	Atom	X	Y	Z
1	P	2.068782	-2.793007	0.031861
2	C	-0.235183	-2.379615	-1.515293
3	H	-0.418843	-3.407855	-1.190963
4	H	-0.369454	-2.335448	-2.603147
5	C	-1.262693	-1.455000	-0.857182
6	H	-1.166174	-1.469644	0.229503
7	C	-0.306938	0.754503	-0.607151
8	C	-2.679651	-1.820906	-1.252284
9	H	-2.851439	-1.643849	-2.317701
10	H	-2.866066	-2.877887	-1.042628
11	C	-4.896114	-1.231043	-0.661116
12	C	-0.170503	2.100104	-1.271779
13	H	0.801320	2.073040	-1.783359
14	H	-0.936077	2.185406	-2.047134
15	C	-0.229931	3.284619	-0.296277
16	H	-1.198619	3.279900	0.219505
17	H	0.536605	3.162931	0.475854
18	C	-0.035383	4.627678	-1.009503
19	H	0.934798	4.626683	-1.526359
20	H	-0.798629	4.740599	-1.792081
21	C	-0.103131	5.829242	-0.059126
22	H	0.660284	5.715345	0.722187
23	H	-1.071826	5.825809	0.458457
24	C	-5.731898	-0.316766	0.206429
25	H	-5.410860	-0.460367	1.245756
26	H	-5.460383	0.716556	-0.044433
27	C	-7.236886	-0.543633	0.056280
28	H	-7.519500	-0.403534	-0.994024
29	H	-7.469927	-1.587541	0.298577
30	C	-8.065789	0.390700	0.944630
31	H	-7.825896	1.435382	0.700737
32	H	-7.775287	0.249035	1.995310
33	C	-9.577247	0.172661	0.804106
34	H	-9.866036	0.314495	-0.246115
35	H	-9.814976	-0.871941	1.046539
36	O	-5.318679	-2.068030	-1.434164
37	O	0.211262	0.457097	0.471233
38	O	-3.574604	-1.004782	-0.473338
39	O	-1.042181	-0.089964	-1.325230
40	O	1.550313	-4.227050	-0.331466
41	O	3.387587	-2.236467	-0.493614
42	O	1.099902	-1.999843	-1.226132
43	O	4.166972	0.310297	2.605562
44	C	-10.406159	1.104907	1.692606
45	H	-10.214975	2.156472	1.449821
46	H	-11.479115	0.924764	1.569552
47	H	-10.163605	0.961172	2.751752
48	C	0.090607	7.170834	-0.772137
49	H	-0.679324	7.327552	-1.536242
50	H	0.036771	8.008083	-0.068716

51	H	1.065422	7.216820	-1.270959
52	Ca	4.435843	-0.278311	-1.122922
53	O	2.415346	-0.040080	-2.462596
54	H	1.863776	-0.794479	-2.120563
55	H	2.415032	-0.109163	-3.425705
56	O	1.284883	-1.990855	1.228294
57	H	0.862636	-1.174520	0.883271
58	O	5.705470	1.847410	-1.493700
59	H	5.214427	2.157055	-0.702071
60	H	6.641692	1.881737	-1.255134
61	P	3.617468	1.477818	1.845416
62	O	3.782494	1.493034	0.314805
63	O	2.043597	1.765979	2.162606
64	H	1.454501	1.342067	1.502955
65	O	4.292949	2.833964	2.459615
66	H	3.974705	3.623663	1.998245
67	O	3.019724	-3.594623	1.601837
68	H	2.716164	-3.092417	2.370576
69	H	2.654832	-4.743509	1.686504
70	O	2.154598	-5.801124	1.378623
71	H	1.396859	-5.947242	1.962257
72	H	1.760913	-5.080543	0.427360

E[B3LYP/6-31G(d,p)] = -3158.890021 h, E[APFD/6-311+G(2d,p)] = -3157.926509 h
Gcorr[B3LYP/6-31G(d,p)] = 0.484796 h

179. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 7th step, products

Center No.	Atom	X	Y	Z
1	P	2.090009	-2.841974	0.115750
2	C	-0.226798	-2.330478	-1.512751
3	H	-0.455829	-3.352108	-1.193982
4	H	-0.347149	-2.288501	-2.604311
5	C	-1.254138	-1.384681	-0.880733
6	H	-1.180390	-1.396259	0.207756
7	C	-0.268694	0.806964	-0.613721
8	C	-2.669215	-1.728604	-1.300466
9	H	-2.821030	-1.548265	-2.368531
10	H	-2.875526	-2.782491	-1.094880
11	C	-4.887595	-1.142154	-0.707932
12	C	-0.092028	2.148624	-1.277544
13	H	0.888103	2.100138	-1.770900
14	H	-0.840949	2.247458	-2.067582
15	C	-0.146629	3.337162	-0.307160
16	H	-1.124013	3.352600	0.191855
17	H	0.604007	3.204441	0.478731
18	C	0.084739	4.673384	-1.022323
19	H	1.063531	4.652293	-1.522299
20	H	-0.662528	4.796096	-1.818785
21	C	0.022246	5.881189	-0.079641
22	H	0.770364	5.758493	0.715027
23	H	-0.954907	5.897681	0.421555
24	C	-5.725129	-0.210471	0.139491
25	H	-5.353651	-0.270002	1.169744
26	H	-5.511913	0.814510	-0.190920
27	C	-7.223780	-0.508269	0.071620
28	H	-7.555122	-0.453949	-0.972201
29	H	-7.400893	-1.541389	0.394802
30	C	-8.055230	0.451195	0.930295
31	H	-7.873608	1.484913	0.603394
32	H	-7.713621	0.397541	1.973753
33	C	-9.559909	0.160128	0.875436
34	H	-9.899757	0.212797	-0.167734
35	H	-9.739433	-0.873115	1.202039
36	O	-5.309905	-2.002063	-1.455849
37	O	0.215907	0.499902	0.477045
38	O	-3.567251	-0.900181	-0.536447
39	O	-1.003316	-0.024309	-1.347679
40	O	1.529963	-4.230964	-0.515135
41	O	3.378910	-2.216004	-0.424899
42	O	1.106776	-1.990323	-1.196495

43	O	4.110917	0.239963	2.613308
44	C	-10.391162	1.118898	1.733003
45	H	-10.258779	2.157049	1.407422
46	H	-11.459126	0.885008	1.673178
47	H	-10.096582	1.063380	2.787249
48	C	0.251359	7.215032	-0.796753
49	H	-0.502941	7.380623	-1.574474
50	H	0.200654	8.057337	-0.099157
51	H	1.234918	7.240961	-1.279621
52	Ca	4.413661	-0.268807	-1.081670
53	O	2.395478	-0.059401	-2.414818
54	H	1.854549	-0.820820	-2.045672
55	H	2.387458	-0.149998	-3.375858
56	O	1.214547	-2.021571	1.241380
57	H	0.833221	-1.205401	0.858022
58	O	5.687073	1.855318	-1.453997
59	H	5.200435	2.162796	-0.658723
60	H	6.624521	1.887583	-1.220103
61	P	3.593397	1.445070	1.889227
62	O	3.771745	1.504560	0.361000
63	O	2.025138	1.759118	2.204174
64	H	1.431555	1.351602	1.536617
65	O	4.295460	2.763620	2.553373
66	H	4.000546	3.575499	2.115659
67	O	2.790908	-3.741272	1.435827
68	H	2.874543	-3.147776	2.193354
69	H	2.368057	-5.457052	1.679108
70	O	1.960507	-6.263306	1.288900
71	H	1.122268	-6.362229	1.761233
72	H	1.673628	-5.013925	0.071540

E[B3LYP/6-31G(d,p)] = -3158.905133 h, E[APFD/6-311+G(2d,p)] = -3157.939555 h
Gcorr[B3LYP/6-31G(d,p)] = 0.488526 h

180. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 8th step, reactants

Center No.	Atom	X	Y	Z
1	P	-2.399858	0.012885	2.499154
2	C	0.121135	-1.272830	2.139480
3	H	0.157002	-2.364093	2.279134
4	H	0.289298	-0.798561	3.111092
5	C	1.251171	-0.879731	1.185040
6	H	0.989111	-1.176686	0.167575
7	C	0.842783	1.325243	0.287387
8	C	2.583733	-1.480169	1.589472
9	H	2.920099	-1.089843	2.554317
10	H	2.502890	-2.567973	1.665978
11	C	4.805444	-1.577338	0.766566
12	C	0.943916	2.788913	0.648037
13	H	0.195869	2.950984	1.436018
14	H	1.917354	2.954678	1.121915
15	C	0.720299	3.749366	-0.522366
16	H	1.458470	3.544009	-1.308031
17	H	-0.264231	3.561570	-0.964799
18	C	0.820209	5.218085	-0.093731
19	H	0.085044	5.415920	0.699336
20	H	1.807265	5.402305	0.353470
21	C	0.596128	6.202707	-1.247648
22	H	-0.390272	6.017223	-1.693906
23	H	1.330876	6.004286	-2.039615
24	C	5.715732	-1.137993	-0.359107
25	H	5.287907	-1.512563	-1.297634
26	H	5.655468	-0.044317	-0.425358
27	C	7.163436	-1.600735	-0.188836
28	H	7.550824	-1.227874	0.767019
29	H	7.187220	-2.695136	-0.121815
30	C	8.070212	-1.132263	-1.332389
31	H	8.038613	-0.035350	-1.397503
32	H	7.675824	-1.505248	-2.288290
33	C	9.526067	-1.587343	-1.173773
34	H	9.917642	-1.216259	-0.216977

35	H	9.556598	-2.683478	-1.110340
36	O	5.132652	-2.237327	1.733547
37	O	0.309668	0.877532	-0.720761
38	O	3.542567	-1.136059	0.569241
39	O	1.413132	0.562965	1.226579
40	O	-1.198220	1.055891	2.929861
41	O	-3.206833	0.247387	1.219527
42	O	-1.124920	-0.888706	1.582052
43	O	-5.411029	-1.506873	-0.771012
44	C	10.432852	-1.115785	-2.314415
45	H	10.449397	-0.021844	-2.380261
46	H	11.463775	-1.456142	-2.172326
47	H	10.085582	-1.499493	-3.280571
48	C	0.694110	7.668672	-0.814962
49	H	1.681587	7.892028	-0.395092
50	H	0.530312	8.346592	-1.658984
51	H	-0.052023	7.905441	-0.047811
52	Ca	-4.075357	0.546173	-0.871771
53	O	-2.116576	1.770921	-1.661399
54	H	-1.205532	1.500716	-1.411380
55	H	-2.157145	1.764089	-2.628359
56	O	-2.679876	-1.373750	3.364443
57	H	-2.275819	-2.112190	2.886169
58	O	-4.120274	0.706145	-3.392295
59	H	-3.880828	-0.249761	-3.387495
60	H	-4.933040	0.782946	-3.909194
61	P	-4.527747	-2.404936	-1.621273
62	O	-3.394636	-1.616911	-2.309149
63	O	-3.886644	-3.635177	-0.809258
64	H	-2.948761	-3.384907	-0.543760
65	O	-5.495022	-3.143486	-2.695162
66	H	-5.012089	-3.790474	-3.231095
67	O	-3.396871	0.840297	3.624947
68	H	-4.168390	0.295705	3.828163
69	H	-1.456912	-1.943477	0.264152
70	O	-1.485421	-2.595674	-0.482219
71	H	-1.776897	-2.072757	-1.253404
72	H	-1.567793	1.637041	3.612804

E[B3LYP/6-31G(d,p)] = -3158.909251 h, E[APFD/6-311+G(2d,p)] = -3157.934540 h
Gcorr[B3LYP/6-31G(d,p)] = 0.491331 h

181. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 8th step, TS

Center No.	Atom	X	Y	Z
1	P	-2.747458	-0.477141	2.404845
2	C	0.133964	-1.751057	1.428465
3	H	0.120184	-2.837315	1.218688
4	H	0.287361	-1.632090	2.510437
5	C	1.358403	-1.172495	0.702933
6	H	1.215275	-1.222399	-0.378070
7	C	1.062160	1.180573	0.248406
8	C	2.652920	-1.852019	1.098609
9	H	2.894589	-1.666442	2.149044
10	H	2.574233	-2.932478	0.948437
11	C	4.942185	-1.827265	0.471221
12	C	1.091576	2.540074	0.911840
13	H	0.188222	2.600653	1.535048
14	H	1.936055	2.560853	1.608247
15	C	1.144233	3.716137	-0.067722
16	H	2.034848	3.620072	-0.701617
17	H	0.279201	3.670281	-0.738291
18	C	1.167632	5.070625	0.650064
19	H	0.276938	5.159504	1.288383
20	H	2.032678	5.111321	1.326938
21	C	1.221452	6.263699	-0.311758
22	H	0.356620	6.221640	-0.987642
23	H	2.111066	6.173322	-0.949601
24	C	5.951293	-1.189459	-0.458828
25	H	5.600189	-1.345664	-1.486669
26	H	5.911169	-0.104801	-0.297165

27	C	7.373140	-1.721680	-0.274737
28	H	7.685572	-1.563252	0.764522
29	H	7.375363	-2.807130	-0.431747
30	C	8.378015	-1.059193	-1.223836
31	H	8.368052	0.028559	-1.065149
32	H	8.058247	-1.217819	-2.263567
33	C	9.809056	-1.582197	-1.049675
34	H	10.126788	-1.424252	-0.010161
35	H	9.817837	-2.668994	-1.208655
36	O	5.180263	-2.680246	1.304499
37	O	0.700205	0.970637	-0.904385
38	O	3.705632	-1.324182	0.262942
39	O	1.485741	0.228769	1.082083
40	O	-1.462214	-0.302808	3.372176
41	O	-2.999213	0.587660	1.362454
42	O	-1.039701	-1.121344	1.010678
43	O	-5.581101	-0.488755	-0.640539
44	C	10.812879	-0.918809	-1.997295
45	H	10.851105	0.164873	-1.837634
46	H	11.823580	-1.312835	-1.848739
47	H	10.539819	-1.088701	-3.045092
48	C	1.243335	7.615839	0.407299
49	H	2.116064	7.700057	1.064959
50	H	1.281819	8.446681	-0.304739
51	H	0.349021	7.749120	1.026753
52	Ca	-3.637432	0.987162	-0.855586
53	O	-1.649555	2.090077	-1.769069
54	H	-0.753274	1.745980	-1.558785
55	H	-1.785747	1.971325	-2.721395
56	O	-3.253543	-1.968450	2.096766
57	H	-2.972508	-2.284614	1.197574
58	O	-3.721652	1.128300	-3.391478
59	H	-3.827551	0.148592	-3.381831
60	H	-4.478716	1.482939	-3.876023
61	P	-5.159387	-1.615051	-1.567879
62	O	-3.853122	-1.293438	-2.315499
63	O	-4.999749	-3.040939	-0.825905
64	H	-4.064146	-3.138772	-0.517278
65	O	-6.394240	-1.896430	-2.577793
66	H	-6.209136	-2.628234	-3.185838
67	O	-3.817755	-0.204463	3.637899
68	H	-4.685019	-0.577389	3.427024
69	H	-1.665114	-1.966258	0.171447
70	O	-2.316324	-2.681773	-0.354645
71	H	-2.553197	-2.209810	-1.174997
72	H	-1.789022	-0.184465	4.279049

E[B3LYP/6-31G(d,p)] = -3158.896919 h, E[APFD/6-311+G(2d,p)] = -3157.922815 h
Gcorr[B3LYP/6-31G(d,p)] = 0.488519 h

182. 2PC6Ca+4H_2O, cho1:gly2:cho2:gly1, 8th step, products

Center No.	Atom	X	Y	Z
1	P	-3.379685	1.480239	1.467287
2	C	0.105974	-1.279060	3.405160
3	H	0.108147	-2.351543	3.634757
4	H	0.493633	-0.745970	4.278488
5	C	1.025584	-1.025863	2.209817
6	H	0.593488	-1.435256	1.294459
7	C	0.878962	0.985351	0.875814
8	C	2.414665	-1.596774	2.439276
9	H	2.901030	-1.118720	3.294075
10	H	2.357765	-2.672606	2.629476
11	C	4.490852	-1.708918	1.301134
12	C	1.056531	2.482955	0.936289
13	H	0.098490	2.876894	1.301071
14	H	1.798834	2.710895	1.706898
15	C	1.430351	3.124031	-0.405039
16	H	2.375809	2.695396	-0.761564
17	H	0.673673	2.874204	-1.156490
18	C	1.565179	4.647714	-0.300668

19	H	0.618807	5.071641	0.063994
20	H	2.322767	4.897192	0.455489
21	C	1.939110	5.312936	-1.630726
22	H	1.181055	5.062346	-2.385085
23	H	2.883713	4.886741	-1.994743
24	C	5.193514	-1.389647	0.000577
25	H	4.679105	-1.941622	-0.796551
26	H	5.021195	-0.328664	-0.218909
27	C	6.687698	-1.715284	0.020085
28	H	7.166104	-1.163137	0.838139
29	H	6.822182	-2.779043	0.249980
30	C	7.381371	-1.379596	-1.304855
31	H	7.237143	-0.313967	-1.532965
32	H	6.897628	-1.933891	-2.121657
33	C	8.881814	-1.696343	-1.297531
34	H	9.363061	-1.143238	-0.479634
35	H	9.024663	-2.761353	-1.069928
36	O	4.996862	-2.216964	2.282073
37	O	0.507303	0.351689	-0.103320
38	O	3.185299	-1.354186	1.247370
39	O	1.157349	0.412904	2.057529
40	O	-2.001339	1.633198	2.307488
41	O	-3.114374	1.705070	-0.013171
42	O	-1.220005	-0.818882	3.189986
43	O	-5.165595	-1.122314	-1.765967
44	C	9.575734	-1.358602	-2.620429
45	H	9.478738	-0.292849	-2.857199
46	H	10.644105	-1.595297	-2.583208
47	H	9.138371	-1.922781	-3.452116
48	C	2.072051	6.835132	-1.525671
49	H	2.846851	7.115722	-0.803035
50	H	2.339147	7.280270	-2.489658
51	H	1.132065	7.292581	-1.196450
52	Ca	-3.264967	0.426353	-1.945626
53	O	-0.923604	1.068446	-2.355374
54	H	-0.338069	0.887260	-1.587506
55	H	-0.684982	0.414784	-3.031615
56	O	-4.098810	0.207972	1.880672
57	H	-3.413679	-1.211020	1.597979
58	O	-2.101851	-1.078609	-3.688353
59	H	-2.206073	-1.807643	-3.037888
60	H	-2.508340	-1.384031	-4.510146
61	P	-4.406088	-2.394619	-1.433626
62	O	-2.886245	-2.149747	-1.346860
63	O	-4.905228	-3.128345	-0.088134
64	H	-4.292662	-2.902252	0.659213
65	O	-4.779586	-3.482353	-2.577030
66	H	-4.395472	-4.352577	-2.390979
67	O	-4.220102	2.794429	1.941179
68	H	-4.474719	2.727052	2.873140
69	H	-1.710321	-1.448243	2.610374
70	O	-2.936356	-2.091377	1.472867
71	H	-2.553448	-2.036425	0.572474
72	H	-1.679960	0.762142	2.657900

E[B3LYP/6-31G(d,p)] = -3158.961072 h, E[APFD/6-311+G(2d,p)] = -3157.984480 h
Gcorr[B3LYP/6-31G(d,p)] = 0.489270 h

XIII. Structures of molecules and transition states (TS) related to the hydrolysis at the glycerol backbone of PS6, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

183. PS6+2H_2O, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	-2.823954	-2.162052	-2.214228
2	C	-1.932424	-2.013894	-1.001102
3	O	-1.831927	-2.833070	-0.105992
4	O	-1.229245	-0.860350	-1.053035
5	C	-0.296755	-0.550407	0.010012
6	C	-0.527931	0.900099	0.393820
7	O	-1.785588	0.927355	1.101038

8	C	-2.374078	2.065862	1.512247
9	O	-3.368455	1.953616	2.215703
10	C	-1.840249	3.404687	1.058545
11	C	-2.411694	3.832521	-0.316916
12	C	1.104590	-0.804936	-0.540833
13	O	2.039171	-0.526713	0.520818
14	P	3.586467	-0.943107	0.336852
15	O	4.168865	-0.677921	1.777956
16	O	3.809878	-2.281805	-0.269850
17	O	4.124442	0.300740	-0.564364
18	C	5.442975	0.314399	-1.136928
19	C	6.555260	0.096870	-0.083979
20	C	7.917505	0.505325	-0.644359
21	O	8.145542	-0.061929	-1.839344
22	O	8.698774	1.234128	-0.072878
23	N	6.240182	0.779819	1.176780
24	H	-2.187334	-2.562146	-3.014669
25	H	-3.136034	-1.165870	-2.542626
26	H	6.067003	1.771295	1.015742
27	H	4.983724	-0.024963	1.704138
28	H	7.045078	0.728017	1.799029
29	H	9.025311	0.220972	-2.146883
30	H	6.620797	-0.976953	0.132287
31	H	5.529543	-0.445147	-1.916527
32	H	5.535843	1.301699	-1.594474
33	H	1.190489	-1.848462	-0.854150
34	H	1.311509	-0.154917	-1.397484
35	H	-0.490602	-1.186769	0.876104
36	H	0.277076	1.237546	1.051245
37	H	-0.567894	1.529952	-0.498299
38	H	-2.154100	3.085032	-1.077666
39	H	-1.895051	4.754753	-0.606334
40	H	-2.137640	4.130344	1.819299
41	H	-0.748145	3.392322	1.018270
42	C	-3.926344	4.070384	-0.322129
43	C	-4.449455	4.530838	-1.688394
44	H	-4.175484	4.824639	0.437038
45	C	-5.961151	4.776535	-1.699478
46	H	-3.926253	5.449723	-1.985370
47	H	-4.195169	3.777059	-2.445716
48	H	-6.511869	3.865554	-1.438856
49	H	-6.241473	5.550650	-0.976130
50	H	-4.450332	3.153461	-0.023546
51	C	-4.025041	-3.084139	-1.976233
52	C	-5.065514	-2.503465	-1.009927
53	H	-5.420657	-1.537865	-1.396814
54	H	-4.587481	-2.292054	-0.043672
55	H	-3.664217	-4.046876	-1.596832
56	C	-6.264830	-3.431875	-0.784998
57	C	-7.304586	-2.849769	0.177095
58	H	-5.907345	-4.396013	-0.399047
59	H	-6.865651	-2.653664	1.162311
60	H	-7.706314	-1.902359	-0.200039
61	H	-6.740205	-3.648086	-1.751372
62	H	-4.497931	-3.284045	-2.944901
63	H	-8.146363	-3.535364	0.319054
64	H	-6.304922	5.102722	-2.686411
65	O	-1.554507	-2.324585	2.761731
66	H	-2.322725	-1.724724	2.870580
67	H	-1.662861	-2.663007	1.859769
68	O	-3.856314	-0.705238	3.096279
69	H	-4.515085	-1.071797	2.492026
70	H	-3.688548	0.197489	2.752887

E[B3LYP/6-31G(d,p)] = -2007.834518 h, E[APFD/6-311+G(2d,p)] = -2007.000395 h
Gcorr[B3LYP/6-31G(d,p)] = 0.505112 h

184. PS6+2H_2O, 1st step, TS

Center No.	Atom	X	Y	Z
1	C	3.259970	-3.453247	-0.112059

2	C	2.635380	-2.094713	-0.336734
3	O	3.011299	-1.288486	-1.180251
4	O	1.574937	-1.907232	0.460066
5	C	0.673788	-0.794652	0.199387
6	C	0.864070	0.307358	1.250558
7	O	2.109651	0.932695	1.251694
8	C	2.843874	2.258703	0.025922
9	O	3.414607	3.044787	0.737808
10	C	1.732897	2.533676	-0.958379
11	C	0.704886	3.552820	-0.437902
12	C	-0.719939	-1.420018	0.231874
13	O	-1.655156	-0.406758	-0.197307
14	P	-3.129476	-0.842764	-0.674337
15	O	-3.692765	0.510645	-1.259996
16	O	-3.186746	-2.050816	-1.539929
17	O	-3.879220	-1.014974	0.760550
18	C	-5.196950	-1.580126	0.865157
19	C	-6.227763	-0.866817	-0.040253
20	C	-7.654146	-1.238648	0.364458
21	O	-7.805862	-2.568919	0.461269
22	O	-8.540070	-0.434070	0.554492
23	N	-6.009537	0.584737	-0.057821
24	H	2.575023	-4.169524	-0.585640
25	H	3.224524	-3.674953	0.959876
26	H	-6.016423	0.960210	0.889841
27	H	-4.609088	0.721352	-0.807185
28	H	-6.779614	1.035997	-0.548746
29	H	-8.729912	-2.751707	0.709013
30	H	-6.094912	-1.232322	-1.066373
31	H	-5.176929	-2.644015	0.620537
32	H	-5.465976	-1.464496	1.917569
33	H	-0.761414	-2.278010	-0.443560
34	H	-0.979275	-1.746821	1.244635
35	H	0.875841	-0.421580	-0.806105
36	H	0.047411	1.028377	1.087020
37	H	0.678602	-0.150971	2.237795
38	H	0.424129	3.288331	0.588384
39	H	-0.203930	3.450493	-1.043209
40	H	2.220354	2.919538	-1.864080
41	H	1.245941	1.601059	-1.244654
42	C	1.178367	5.011585	-0.485222
43	C	0.124491	5.999662	0.028786
44	H	1.441534	5.269242	-1.521289
45	C	0.587953	7.458327	-0.031866
46	H	-0.798293	5.883964	-0.556175
47	H	-0.137897	5.742015	1.063958
48	H	1.490628	7.611554	0.570599
49	H	0.823154	7.756178	-1.060136
50	H	2.097028	5.113231	0.103247
51	C	4.673981	-3.606433	-0.681102
52	C	5.758239	-2.915187	0.154959
53	H	5.763924	-3.351149	1.164357
54	H	5.508410	-1.854903	0.284409
55	H	4.686877	-3.216835	-1.705451
56	C	7.158702	-3.039341	-0.457115
57	C	8.246676	-2.369888	0.387992
58	H	7.153049	-2.597962	-1.463025
59	H	8.046275	-1.299848	0.514853
60	H	8.301523	-2.815997	1.387650
61	H	7.402475	-4.101928	-0.593137
62	H	4.898240	-4.677374	-0.750944
63	H	9.233233	-2.471155	-0.076100
64	H	-0.182715	8.139453	0.343752
65	O	3.830624	1.205333	-0.595631
66	H	4.313716	0.795901	0.313398
67	H	3.346583	0.415179	-0.953018
68	O	4.441607	0.231930	1.546843
69	H	3.410037	0.391866	1.659782
70	H	4.886669	0.854470	2.140313

E[B3LYP/6-31G(d,p)] = -2007.769463 h, E[APFD/6-311+G(2d,p)] = -2006.937064 h
Gcorr[B3LYP/6-31G(d,p)] = 0.505234 h

185. PS6+2H_2O, 1st step, products

Center No.	Atom	X	Y	Z
1	C	2.312080	-3.648314	-0.374994
2	C	1.796220	-2.230038	-0.292811
3	O	2.338824	-1.241841	-0.770010
4	O	0.626355	-2.189372	0.364952
5	C	-0.089700	-0.931286	0.501467
6	C	-0.044885	-0.483926	1.961899
7	O	1.207274	0.040027	2.352723
8	C	4.250661	1.425460	0.802512
9	O	5.117727	1.943463	1.473234
10	C	3.026748	2.127821	0.249575
11	C	3.089187	3.654737	0.341366
12	C	-1.502037	-1.232941	0.004681
13	O	-2.226832	0.014945	0.002190
14	P	-3.674916	0.087131	-0.699153
15	O	-3.980388	1.634457	-0.656410
16	O	-3.779548	-0.604467	-2.011368
17	O	-4.608298	-0.553077	0.471137
18	C	-5.997590	-0.854029	0.259068
19	C	-6.805259	0.368878	-0.236734
20	C	-8.305800	0.132544	-0.066564
21	O	-8.677151	-1.050647	-0.580403
22	O	-9.065629	0.922580	0.449931
23	N	-6.355608	1.606304	0.412775
24	H	1.483511	-4.261544	-0.746766
25	H	2.487961	-3.977160	0.656540
26	H	-6.392460	1.514910	1.427230
27	H	-4.892583	1.791319	-0.170046
28	H	-6.991256	2.364773	0.171372
29	H	-9.638375	-1.147615	-0.456464
30	H	-6.632511	0.482935	-1.314499
31	H	-6.107592	-1.673400	-0.454101
32	H	-6.361856	-1.184567	1.234297
33	H	-1.463019	-1.646268	-1.006240
34	H	-2.004267	-1.948187	0.665013
35	H	0.381386	-0.181640	-0.136794
36	H	-0.784265	0.313340	2.085697
37	H	-0.355269	-1.328096	2.596374
38	H	3.346414	3.937214	1.368858
39	H	2.084530	4.050445	0.148970
40	H	2.866675	1.801152	-0.785739
41	H	2.181838	1.728861	0.827974
42	C	4.083545	4.296514	-0.634385
43	C	4.126856	5.825917	-0.533369
44	H	3.818998	4.008404	-1.661964
45	C	5.115039	6.467245	-1.512243
46	H	3.120617	6.229099	-0.711840
47	H	4.391028	6.112238	0.493721
48	H	6.135505	6.108265	-1.335871
49	H	4.855792	6.227754	-2.549937
50	H	5.086405	3.892077	-0.447482
51	C	3.565195	-3.837419	-1.238066
52	C	4.876522	-3.391190	-0.578653
53	H	4.991463	-3.910740	0.383097
54	H	4.832717	-2.321478	-0.346411
55	H	3.430518	-3.310603	-2.190396
56	C	6.106691	-3.664703	-1.452639
57	C	7.419575	-3.226289	-0.796788
58	H	5.988113	-3.148174	-2.414870
59	H	7.413910	-2.151840	-0.580610
60	H	7.583523	-3.752640	0.150536
61	H	6.153823	-4.736939	-1.687089
62	H	3.638162	-4.903808	-1.483540
63	H	8.278511	-3.431177	-1.444205
64	H	5.124420	7.557846	-1.414939
65	O	4.322865	0.091783	0.546587
66	H	3.932407	-1.220945	2.002012
67	H	3.577947	-0.224982	-0.013729

68	O	3.279886	-1.804042	2.428273
69	H	1.860282	-0.689918	2.427277
70	H	3.611027	-1.944350	3.325821

E[B3LYP/6-31G(d,p)] = -2007.842137 h, E[APFD/6-311+G(2d,p)] = -2007.004212 h
Gcorr[B3LYP/6-31G(d,p)] = 0.504273 h

186. PS6+2H_2O, 2nd step, reactants (hydrolysed carbon chain neglected)

Center No.	Atom	X	Y	Z
1	C	4.141535	-0.445947	1.609360
2	C	3.168750	-0.764268	0.494402
3	O	3.255672	-1.689487	-0.282816
4	O	2.131273	0.124546	0.488754
5	C	1.112222	0.004475	-0.542459
6	C	1.137274	1.283436	-1.381430
7	O	2.347788	1.426593	-2.091595
8	C	-0.202791	-0.242306	0.190805
9	O	-1.220215	-0.439449	-0.814894
10	P	-2.679693	-0.954542	-0.370040
11	O	-3.379085	-1.197630	-1.763542
12	O	-2.687462	-2.070722	0.612464
13	O	-3.330993	0.430438	0.185528
14	C	-4.602633	0.459444	0.854209
15	C	-5.737007	-0.166310	0.007678
16	C	-7.105617	0.242753	0.551509
17	O	-7.193633	0.022419	1.872829
18	O	-8.002855	0.691791	-0.127884
19	N	-5.580912	0.153620	-1.416474
20	H	3.670624	-0.795289	2.537874
21	H	4.220720	0.641898	1.699865
22	H	-5.519165	1.161620	-1.554537
23	H	-4.261808	-0.639864	-1.806583
24	H	-6.408874	-0.153679	-1.924075
25	H	-8.083374	0.288545	2.166441
26	H	-5.680339	-1.257646	0.106709
27	H	-4.542234	-0.055577	1.815159
28	H	-4.797483	1.519085	1.033922
29	H	-0.121672	-1.132097	0.820719
30	H	-0.470608	0.615612	0.817344
31	H	1.360497	-0.854379	-1.167971
32	H	0.315466	1.222558	-2.103134
33	H	0.939176	2.147110	-0.728405
34	C	5.518539	-1.093615	1.429184
35	C	6.337782	-0.497953	0.277018
36	H	6.444390	0.585122	0.429461
37	H	5.787044	-0.622817	-0.664190
38	H	5.388656	-2.170723	1.273526
39	C	7.726823	-1.131945	0.136465
40	C	8.546016	-0.538590	-1.013614
41	H	7.615924	-2.214472	-0.013290
42	H	8.036050	-0.675557	-1.974040
43	H	8.702937	0.537096	-0.873725
44	H	8.277213	-1.010244	1.079361
45	H	6.072318	-0.976322	2.368288
46	H	9.530649	-1.011547	-1.089090
47	H	4.166343	3.657721	-0.782845
48	O	4.074059	2.768348	-0.415623
49	H	2.997488	1.870275	-1.498915
50	H	3.536922	2.884972	0.401622
51	O	2.375057	2.737000	1.734170
52	H	2.737893	2.794789	2.628509
53	H	2.144804	1.800777	1.610029

E[B3LYP/6-31G(d,p)] = -1697.910064 h, E[APFD/6-311+G(2d,p)] = -1697.251930 h
Gcorr[B3LYP/6-31G(d,p)] = 0.364273 h

187. PS6+2H_2O, 2nd step, TS

Center No.	Atom	X	Y	Z

1	C	4.121088	-1.344919	0.483305
2	C	3.470899	-0.142242	-0.190654
3	O	3.449310	0.047126	-1.389702
4	O	2.019599	-0.044680	0.545791
5	C	0.994214	0.637696	-0.205197
6	C	0.947026	2.137305	0.107748
7	O	2.047686	2.858724	-0.412111
8	C	-0.306666	-0.091475	0.122196
9	O	-1.335737	0.426581	-0.753507
10	P	-2.751681	-0.331278	-0.836232
11	O	-3.471856	0.448545	-2.005577
12	O	-2.679574	-1.813521	-0.936397
13	O	-3.468774	0.209246	0.522637
14	C	-4.713028	-0.334992	0.991891
15	C	-5.829948	-0.282900	-0.077440
16	C	-7.200957	-0.499916	0.562575
17	O	-7.212888	-1.598787	1.333794
18	O	-8.159925	0.218381	0.381702
19	N	-5.764103	0.957753	-0.858885
20	H	3.418256	-2.174278	0.347010
21	H	4.211571	-1.181172	1.560037
22	H	-5.792839	1.770867	-0.244970
23	H	-4.396026	0.791740	-1.666251
24	H	-6.585288	1.023682	-1.457991
25	H	-8.106637	-1.696753	1.708304
26	H	-5.679646	-1.118044	-0.773170
27	H	-4.578853	-1.366445	1.324052
28	H	-4.977994	0.281657	1.853747
29	H	-0.178186	-1.163483	-0.044509
30	H	-0.605593	0.076286	1.163146
31	H	1.236070	0.503301	-1.263820
32	H	0.044812	2.549225	-0.355470
33	H	0.843031	2.271789	1.197533
34	C	5.474786	-1.734682	-0.129702
35	C	6.604214	-0.707400	0.024394
36	H	6.678449	-0.390080	1.074491
37	H	6.370561	0.188771	-0.567680
38	H	5.326603	-1.951709	-1.193975
39	C	7.966555	-1.244156	-0.434426
40	C	9.093576	-0.214767	-0.310941
41	H	7.888099	-1.579707	-1.477169
42	H	8.887036	0.673357	-0.918999
43	H	9.215527	0.116036	0.726808
44	H	8.216767	-2.136153	0.155278
45	H	5.785203	-2.676190	0.340142
46	H	10.050787	-0.629918	-0.642637
47	H	5.023054	1.322354	0.511523
48	O	4.070012	1.256949	0.666440
49	H	2.864947	2.438718	-0.072683
50	H	3.555007	1.165990	1.960197
51	O	2.734360	0.917729	2.620805
52	H	3.016812	0.306617	3.317912
53	H	2.224133	0.372781	1.741324

E[B3LYP/6-31G(d,p)] = -1697.840520 h, E[APFD/6-311+G(2d,p)] = -1697.187617 h
Gcorr[B3LYP/6-31G(d,p)] = 0.367700 h

188. PS6+2H_2O, 2nd step, products

Center No.	Atom	X	Y	Z
1	C	5.559803	0.034304	-0.552414
2	C	4.264098	-0.335847	0.139698
3	O	3.227806	0.303594	0.085131
4	O	0.975775	-3.592879	-0.811276
5	C	0.711398	-2.339767	-0.192502
6	C	0.827209	-2.426433	1.331616
7	O	2.165756	-2.693396	1.772429
8	C	-0.702839	-1.973320	-0.632547
9	O	-1.016745	-0.660120	-0.112831
10	P	-2.339373	0.095781	-0.623355
11	O	-2.160067	1.530633	0.013158

12	O	-2.600240	0.016708	-2.085715
13	O	-3.479864	-0.619768	0.293807
14	C	-4.881995	-0.404595	0.065316
15	C	-5.266957	1.093756	0.066132
16	C	-6.780087	1.261804	0.203090
17	O	-7.439574	0.511786	-0.694233
18	O	-7.315263	1.993133	1.007516
19	N	-4.523811	1.837252	1.090388
20	H	5.672624	-0.669046	-1.388311
21	H	6.388188	-0.183331	0.131160
22	H	-4.661909	1.418622	2.009348
23	H	-3.017256	1.770865	0.553586
24	H	-4.890119	2.785771	1.151226
25	H	-8.394215	0.661583	-0.572339
26	H	-4.996957	1.518323	-0.909096
27	H	-5.189201	-0.854644	-0.880841
28	H	-5.380637	-0.929209	0.883496
29	H	-0.754171	-1.966366	-1.723859
30	H	-1.425700	-2.700094	-0.245351
31	H	1.400178	-1.560623	-0.550033
32	H	0.538724	-1.475552	1.784899
33	H	0.152215	-3.210137	1.701380
34	C	5.610096	1.479810	-1.055126
35	C	5.718720	2.521942	0.065266
36	H	6.617330	2.316408	0.664536
37	H	4.862802	2.415401	0.743927
38	H	4.715308	1.677673	-1.656756
39	C	5.776187	3.963568	-0.454054
40	C	5.891045	5.003299	0.664763
41	H	4.877927	4.167461	-1.052544
42	H	5.035555	4.945548	1.347497
43	H	6.798573	4.846435	1.259056
44	H	6.628234	4.067600	-1.139705
45	H	6.470056	1.579872	-1.728379
46	H	5.928200	6.021293	0.263191
47	H	3.480555	-1.726171	1.222497
48	O	4.365488	-1.493630	0.819469
49	H	2.478458	-3.517747	1.351256
50	H	4.277658	-3.431012	-0.073590
51	O	3.619797	-4.145209	-0.084057
52	H	4.108205	-4.971209	-0.195708
53	H	1.933635	-3.773129	-0.755544

E[B3LYP/6-31G(d,p)] = -1697.915009 h, E[APFD/6-311+G(2d,p)] = -1697.249466 h
Gcorr[B3LYP/6-31G(d,p)] = 0.365587 h

XIV. Structures of molecules and transition states (TS) related to the hydrolysis at the glycerol backbone of PS6Ca, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

189. PS6Ca+5H_2O, 1st step, reactants

Center No.	Atom	X	Y	Z
1	C	-3.941107	-2.328852	-2.094232
2	C	-3.214024	-1.646369	-0.958841
3	O	-3.481344	-1.766434	0.228933
4	O	-2.194555	-0.905797	-1.428155
5	C	-1.310025	-0.200918	-0.523991
6	C	-1.330576	1.273896	-0.904166
7	O	-2.542838	1.905675	-0.443291
8	C	-2.616241	2.612561	0.706549
9	O	-3.714881	3.048737	1.017282
10	C	-1.379596	2.888564	1.533727
11	C	-0.604907	4.142701	1.056525
12	C	0.075601	-0.826579	-0.696494
13	O	0.945281	-0.153442	0.235253
14	P	2.552726	-0.211765	0.048563
15	O	3.174933	0.539690	1.205567
16	O	3.029029	-1.614570	-0.275403
17	O	2.687603	0.724778	-1.302563
18	C	3.925014	0.826604	-2.005928
19	C	5.067820	1.332462	-1.095355

20	C	6.252527	1.908973	-1.860651
21	O	6.605457	1.111397	-2.868686
22	O	6.796337	2.947505	-1.554781
23	N	4.569985	2.360196	-0.133233
24	H	-3.211078	-3.017444	-2.539098
25	H	-4.139865	-1.576694	-2.866385
26	H	3.995705	3.072955	-0.590447
27	H	3.980498	1.835514	0.586309
28	H	5.361451	2.841351	0.304078
29	H	7.374706	1.501111	-3.322547
30	H	5.440941	0.506686	-0.481923
31	H	4.223723	-0.134705	-2.430903
32	H	3.745018	1.531269	-2.820522
33	H	0.034120	-1.892199	-0.456755
34	H	0.429904	-0.690522	-1.723122
35	H	-1.648084	-0.335514	0.504744
36	H	-0.444437	1.771410	-0.514822
37	H	-1.341776	1.377703	-1.990903
38	H	-0.274253	4.009218	0.018923
39	H	0.305747	4.204614	1.663316
40	H	-1.735373	3.049807	2.553932
41	H	-0.712818	2.023039	1.551072
42	C	-1.392484	5.452428	1.181168
43	C	-0.575034	6.678624	0.756412
44	H	-1.721906	5.576738	2.221928
45	C	-1.351851	7.991705	0.890895
46	H	0.340211	6.730396	1.361358
47	H	-0.246304	6.551856	-0.283879
48	H	-2.255547	7.982068	0.271008
49	H	-1.663826	8.162122	1.927562
50	H	-2.306936	5.399449	0.576642
51	C	-5.215803	-3.076998	-1.692683
52	C	-6.410316	-2.167257	-1.380104
53	H	-6.606906	-1.519590	-2.246780
54	H	-6.166581	-1.506105	-0.541058
55	H	-4.999006	-3.716608	-0.829031
56	C	-7.683731	-2.949963	-1.035373
57	C	-8.867867	-2.041541	-0.690473
58	H	-7.477331	-3.616828	-0.187021
59	H	-8.634525	-1.404184	0.169618
60	H	-9.120641	-1.384292	-1.530469
61	H	-7.951754	-3.602939	-1.877255
62	H	-5.478868	-3.748719	-2.518548
63	H	-9.761557	-2.623908	-0.443146
64	H	-0.744261	8.848007	0.580836
65	O	-5.770663	-0.244139	1.567632
66	H	-5.830088	0.483524	0.912554
67	H	-5.004007	-0.750561	1.262992
68	O	-5.815045	1.821026	-0.349364
69	H	-5.378046	1.407613	-1.106257
70	H	-5.102508	2.357174	0.059667
71	Ca	4.062953	-3.320136	0.958427
72	O	4.379742	-5.330279	-0.393308
73	H	4.797454	-5.290733	-1.264288
74	H	4.680875	-6.160127	0.001104
75	O	6.069263	-2.544030	2.104928
76	H	6.555283	-1.751343	1.841120
77	H	6.176135	-2.609019	3.063467
78	O	2.336331	-3.852554	2.543050
79	H	1.425418	-3.830927	2.130609
80	H	2.268681	-3.368264	3.375625
81	O	0.037106	-3.714017	1.257278
82	H	-0.394521	-4.568827	1.126498
83	H	-0.628071	-3.150999	1.731758
84	O	-1.745565	-2.064938	2.420567
85	H	-2.177195	-2.413559	3.212286
86	H	-2.451584	-1.990311	1.750379

E[B3LYP/6-31G(d,p)] = -3067.510231 h, E[APFD/6-311+G(2d,p)] = -3066.498604 h
Gcorr[B3LYP/6-31G(d,p)] = 0.610154 h

190. PS6Ca+5H_2O, TS

Center No.	Atom	X	Y	Z
1	C	-3.576372	-2.574254	-2.186234
2	C	-2.880434	-1.616523	-1.250426
3	O	-3.224370	-1.408002	-0.083363
4	O	-1.848981	-1.017605	-1.838813
5	C	-1.092194	0.002849	-1.123809
6	C	-1.559019	1.388058	-1.598017
7	O	-2.923652	1.622454	-1.439883
8	C	-3.968483	2.239474	0.086999
9	O	-4.624354	3.152183	-0.334327
10	C	-3.010025	2.224013	1.252120
11	C	-2.150825	3.497472	1.342349
12	C	0.368808	-0.298190	-1.447074
13	O	1.169126	0.628330	-0.687274
14	P	2.725849	0.316434	-0.388338
15	O	3.266985	1.444827	0.463179
16	O	2.924409	-1.119158	0.058521
17	O	3.330328	0.491373	-1.913895
18	C	4.684498	0.153698	-2.209090
19	C	5.684150	0.973330	-1.357902
20	C	7.081384	1.053106	-1.959965
21	O	7.493279	-0.145612	-2.373655
22	O	7.720419	2.080678	-2.019276
23	N	5.176857	2.358702	-1.127812
24	H	-2.797215	-3.108669	-2.739267
25	H	-4.095469	-1.950295	-2.926172
26	H	4.829033	2.792930	-1.986350
27	H	4.375423	2.265687	-0.427186
28	H	5.930384	2.952298	-0.768963
29	H	8.394705	-0.060687	-2.734043
30	H	5.777052	0.523556	-0.364717
31	H	4.877892	-0.908665	-2.040772
32	H	4.819763	0.371452	-3.270402
33	H	0.609683	-1.326921	-1.165456
34	H	0.570862	-0.161670	-2.514788
35	H	-1.254245	-0.124941	-0.053938
36	H	-0.945339	2.124868	-1.057822
37	H	-1.289530	1.479575	-2.664719
38	H	-1.739443	3.728569	0.352977
39	H	-1.293417	3.275904	1.989246
40	H	-3.635840	2.132830	2.150752
41	H	-2.388404	1.328440	1.218895
42	C	-2.892217	4.723347	1.891934
43	C	-2.003561	5.969860	1.979895
44	H	-3.284358	4.486397	2.891441
45	C	-2.736568	7.191912	2.541522
46	H	-1.127775	5.748621	2.605279
47	H	-1.611825	6.205524	0.981014
48	H	-3.598030	7.456990	1.917984
49	H	-3.109036	6.998999	3.554131
50	H	-3.761627	4.935201	1.259417
51	C	-4.551817	-3.548468	-1.512286
52	C	-5.889906	-2.931455	-1.084192
53	H	-6.367796	-2.465579	-1.957403
54	H	-5.710607	-2.126300	-0.362532
55	H	-4.061924	-4.010121	-0.646378
56	C	-6.849105	-3.957984	-0.469400
57	C	-8.189955	-3.350442	-0.046486
58	H	-6.368532	-4.425581	0.400731
59	H	-8.048340	-2.560540	0.699994
60	H	-8.710532	-2.906121	-0.902529
61	H	-7.024723	-4.767357	-1.191114
62	H	-4.746762	-4.359858	-2.223717
63	H	-8.851531	-4.105973	0.389754
64	H	-2.078842	8.065954	2.589837
65	O	-4.794057	0.875147	0.103288
66	H	-5.092982	0.765008	-0.958795
67	H	-4.185638	0.111880	0.244388
68	O	-4.998563	0.673296	-2.312024

69	H	-4.035610	1.082670	-2.214015
70	H	-5.555435	1.335450	-2.746489
71	Ca	3.677399	-2.276955	1.940632
72	O	4.225901	-4.492716	1.050578
73	H	4.201270	-4.678999	0.102327
74	H	4.962863	-5.012686	1.398541
75	O	5.650820	-1.392175	3.083049
76	H	6.492783	-1.867036	3.085071
77	H	5.881635	-0.454383	3.041742
78	O	2.122902	-2.756386	3.698554
79	H	1.172016	-3.008174	3.514784
80	H	2.116253	-2.259545	4.525973
81	O	-0.386530	-3.401229	3.185254
82	H	-0.849326	-2.604494	2.828092
83	H	-0.423286	-4.054715	2.474058
84	O	-1.610497	-1.143368	2.242424
85	H	-2.215784	-1.351836	1.505681
86	H	-2.181602	-0.801113	2.944279

E[B3LYP/6-31G(d,p)] = -3067.445414 h, E[APFD/6-311+G(2d,p)] = -3066.431871 h
Gcorr[B3LYP/6-31G(d,p)] = 0.609188 h

191. PS6Ca+5H_2O, products

Center No.	Atom	X	Y	Z
1	C	-2.243164	-3.339929	-0.148024
2	C	-1.843951	-1.952873	-0.588482
3	O	-2.054630	-0.923126	0.060074
4	O	-1.154916	-1.957046	-1.724945
5	C	-0.401913	-0.767454	-2.126863
6	C	-0.939672	-0.240326	-3.454631
7	O	-2.120986	0.523270	-3.335416
8	C	-4.227205	2.005026	-0.321831
9	O	-5.247184	2.654885	-0.315562
10	C	-2.830098	2.536867	-0.563908
11	C	-2.749572	4.064413	-0.640443
12	C	1.054138	-1.232459	-2.207143
13	O	1.892124	-0.071002	-2.352990
14	P	2.974021	0.310213	-1.211918
15	O	3.469207	1.712221	-1.490956
16	O	2.452995	-0.034657	0.168032
17	O	4.171533	-0.745254	-1.631232
18	C	5.325832	-0.932739	-0.810610
19	C	6.057557	0.396421	-0.520076
20	C	7.489776	0.211640	-0.035073
21	O	7.554086	-0.705648	0.931191
22	O	8.425507	0.845391	-0.471257
23	N	6.063194	1.274626	-1.727597
24	H	-1.383456	-3.690512	0.441104
25	H	-2.287961	-3.987490	-1.028169
26	H	6.324593	0.765427	-2.575343
27	H	5.063277	1.643172	-1.826215
28	H	6.739000	2.034785	-1.607605
29	H	8.479000	-0.783018	1.228087
30	H	5.515407	0.953993	0.249863
31	H	5.064098	-1.405942	0.138927
32	H	5.976663	-1.607802	-1.371337
33	H	1.307902	-1.787681	-1.301624
34	H	1.219115	-1.875702	-3.076353
35	H	-0.504063	-0.008506	-1.350559
36	H	-0.170265	0.418422	-3.870698
37	H	-1.060336	-1.087151	-4.146778
38	H	-3.507179	4.424292	-1.346308
39	H	-1.774293	4.332167	-1.064519
40	H	-2.170980	2.148942	0.224233
41	H	-2.483249	2.073392	-1.498717
42	C	-2.925643	4.769133	0.710491
43	C	-2.832636	6.296335	0.609022
44	H	-2.159380	4.405172	1.410215
45	C	-2.997447	7.001583	1.958565
46	H	-1.865027	6.571513	0.167511

47	H	-3.599217	6.658573	-0.089312
48	H	-3.970009	6.771811	2.408646
49	H	-2.223004	6.686140	2.667193
50	H	-3.896002	4.492152	1.140927
51	C	-3.525169	-3.422401	0.694294
52	C	-4.813986	-3.461836	-0.137159
53	H	-4.798096	-4.351185	-0.783498
54	H	-4.846896	-2.598552	-0.813295
55	H	-3.563840	-2.577313	1.389805
56	C	-6.076939	-3.481601	0.732909
57	C	-7.370687	-3.508934	-0.086412
58	H	-6.067509	-2.601718	1.388487
59	H	-7.446618	-2.628618	-0.735165
60	H	-7.415971	-4.396237	-0.728535
61	H	-6.045486	-4.357936	1.395390
62	H	-3.466719	-4.327126	1.310205
63	H	-8.254141	-3.521735	0.560518
64	H	-2.928344	8.089194	1.852769
65	O	-4.310854	0.649177	-0.139195
66	H	-4.733106	-0.377001	-1.892154
67	H	-3.424404	0.224088	-0.126560
68	O	-4.349042	-0.925769	-2.595924
69	H	-2.881989	-0.067922	-3.147036
70	H	-5.043106	-1.007707	-3.264222
71	Ca	2.368782	-0.703404	2.390089
72	O	3.494390	-2.719953	1.594587
73	H	3.961415	-3.369246	2.137502
74	H	3.185532	-3.199316	0.813872
75	O	3.903061	0.092678	4.151774
76	H	3.771630	0.956022	4.567007
77	H	4.176873	-0.498444	4.866327
78	O	0.409434	-1.502996	3.542714
79	H	-0.490844	-1.144284	3.347459
80	H	0.287517	-2.432496	3.773483
81	O	-1.985799	-0.439939	2.800229
82	H	-1.968922	-0.633704	1.838516
83	H	-1.876241	0.520465	2.864950
84	O	-4.940479	-0.497076	2.670077
85	H	-3.989379	-0.524533	2.873714
86	H	-4.967208	-0.114772	1.780116

E[B3LYP/6-31G(d,p)] = -3067.517181 h, E[APFD/6-311+G(2d,p)] = -3066.501041 h
Gcorr[B3LYP/6-31G(d,p)] = 0.616408 h

XV. Structures of molecules and transition states (TS) related to the hydrolysis at the glycerol backbone of 2PS6Ca, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

192. 2PS6Ca+2H_2O, reactants

Center No.	Atom	X	Y	Z
1	C	-6.587336	-0.424244	2.010147
2	C	-5.173166	-0.376783	1.482313
3	O	-4.439155	0.596952	1.524073
4	O	-4.803609	-1.573596	0.974303
5	C	-3.454852	-1.729657	0.473531
6	C	-3.543174	-2.209521	-0.962867
7	O	-3.941787	-1.082003	-1.777363
8	C	-4.748403	-1.164029	-2.848885
9	O	-4.876100	-0.146294	-3.521448
10	C	-5.501878	-2.433983	-3.163899
11	C	-6.789672	-2.586103	-2.315628
12	C	-2.684964	-2.693025	1.389045
13	O	-1.287369	-2.387557	1.315388
14	P	-0.254300	-3.267855	0.372547
15	O	-0.569351	-4.725923	0.467385
16	O	-0.118711	-2.595254	-0.982951
17	O	1.137007	-2.865768	1.166723
18	C	1.289083	-3.294365	2.519459
19	C	0.984771	-2.127384	3.464004
20	C	1.031653	-2.481702	4.949720
21	O	0.361900	-3.600476	5.207544

22	O	1.593426	-1.786090	5.770185
23	N	1.952661	-0.995280	3.266154
24	H	-6.590960	-1.164001	2.820447
25	H	-7.221904	-0.849282	1.223223
26	H	1.698927	-0.344194	2.499946
27	H	2.013441	-0.469171	4.149269
28	H	0.388723	-3.770181	6.166804
29	H	-0.014484	-1.747802	3.234514
30	H	0.620644	-4.124500	2.757362
31	H	2.320289	-3.637793	2.648141
32	H	-3.001361	-2.519083	2.419975
33	H	-2.865057	-3.743511	1.140607
34	H	-2.949562	-0.766784	0.519630
35	H	-2.557186	-2.530975	-1.307030
36	H	-4.252316	-3.033459	-1.038632
37	H	-6.536363	-2.604859	-1.248786
38	H	-7.213754	-3.568697	-2.551226
39	H	-5.765330	-2.374409	-4.222120
40	H	-4.858240	-3.307663	-3.033280
41	C	-7.838762	-1.498145	-2.576079
42	C	-9.132179	-1.717925	-1.781760
43	H	-8.071601	-1.469541	-3.649375
44	C	-10.178472	-0.626851	-2.027140
45	H	-9.554295	-2.697609	-2.042634
46	H	-8.896572	-1.764438	-0.709784
47	H	-9.796820	0.359151	-1.738091
48	H	-10.456720	-0.576390	-3.085943
49	H	-7.425468	-0.511781	-2.327592
50	C	-7.124520	0.924761	2.498296
51	C	-7.384563	1.945043	1.382375
52	H	-8.086566	1.515104	0.653306
53	H	-6.451673	2.140847	0.841223
54	H	-6.421169	1.346696	3.225900
55	C	-7.948177	3.272000	1.906048
56	C	-8.145232	4.316985	0.803500
57	H	-7.269001	3.674157	2.670238
58	H	-7.192473	4.554860	0.317925
59	H	-8.832080	3.953048	0.030540
60	H	-8.903269	3.086000	2.415909
61	H	-8.057643	0.734347	3.041824
62	H	-8.559832	5.247896	1.204378
63	H	-11.090764	-0.812789	-1.451308
64	P	0.705470	1.926934	0.452961
65	O	0.028685	0.812780	-0.349511
66	O	-0.369951	2.278728	1.648044
67	C	-1.290404	3.364668	1.513410
68	C	-2.069354	3.338124	0.178221
69	H	-1.390525	3.645747	-0.623079
70	H	-1.973858	3.272625	2.360206
71	H	-0.773931	4.325172	1.577059
72	O	-0.714090	0.751831	-3.640005
73	H	-0.777217	0.531991	-4.578161
74	H	-1.577820	1.164451	-3.399886
75	Ca	0.543145	-0.671957	-2.113592
76	O	1.214427	3.155475	-0.227453
77	H	2.895965	-1.345218	3.072028
78	C	-3.260458	4.287791	0.182682
79	O	-4.387396	3.953456	-0.111921
80	O	-2.888592	5.518597	0.542934
81	H	-3.674307	6.094751	0.534504
82	N	-2.547836	1.970777	-0.168047
83	H	-2.953180	1.961819	-1.135096
84	H	-1.720650	1.336488	-0.196216
85	H	-3.247343	1.599260	0.496366
86	C	4.124105	-2.144199	-0.516918
87	C	3.675326	-0.708180	-0.580684
88	O	2.827529	-0.289600	-1.365920
89	O	4.316905	0.083158	0.281565
90	C	4.050478	1.513534	0.271005
91	C	5.399895	2.211080	0.331295
92	O	6.065525	1.908905	-0.907257
93	C	7.327946	2.340047	-1.181223

94	O	7.777254	2.077617	-2.278450
95	C	8.116839	3.066499	-0.111400
96	C	8.917021	2.096226	0.793955
97	C	3.163131	1.863638	1.460851
98	O	1.882068	1.200224	1.355624
99	H	3.226261	-2.746768	-0.347350
100	H	4.795157	-2.278211	0.334745
101	H	3.613659	1.520553	2.394007
102	H	3.023719	2.945193	1.506415
103	H	3.541246	1.770763	-0.658152
104	H	5.244320	3.289618	0.427768
105	H	5.980673	1.850360	1.184487
106	H	8.232516	1.395042	1.288073
107	H	9.367079	2.697318	1.592532
108	H	8.811322	3.725070	-0.639125
109	H	7.468232	3.694850	0.503711
110	C	10.014095	1.312632	0.063947
111	C	10.807028	0.390525	0.998466
112	H	10.701626	2.020591	-0.419347
113	C	11.907184	-0.392542	0.275819
114	H	11.251873	0.988143	1.805525
115	H	10.116738	-0.312010	1.484795
116	H	11.487989	-1.024993	-0.515100
117	H	12.632342	0.283493	-0.191286
118	H	9.572437	0.717324	-0.744938
119	C	4.813624	-2.572056	-1.831087
120	C	6.154065	-1.867878	-2.074521
121	H	6.839918	-2.108227	-1.250070
122	H	6.016308	-0.778476	-2.045287
123	H	4.129461	-2.381522	-2.666970
124	C	6.807216	-2.249276	-3.408135
125	C	8.156631	-1.557643	-3.626851
126	H	6.124675	-1.990974	-4.229119
127	H	8.052735	-0.468055	-3.577739
128	H	8.880126	-1.854434	-2.858536
129	H	6.938679	-3.338868	-3.451818
130	H	4.966154	-3.656444	-1.791216
131	H	8.584197	-1.813440	-4.601836
132	H	12.454395	-1.042097	0.966694
133	O	-3.130391	1.805824	-2.867925
134	H	-3.823208	1.130454	-3.097510
135	H	-3.384467	2.623682	-3.318576

E[B3LYP/6-31G(d,p)] = -4540.302067 h, E[APFD/6-311+G(2d,p)] = -4538.637039 h
Gcorr[B3LYP/6-31G(d,p)] = 1.007983 h

193. 2PS6Ca+2H_2O, TS

Center No.	Atom	X	Y	Z
1	C	7.519794	-1.453545	1.096684
2	C	6.024993	-1.463911	0.901223
3	O	5.419503	-2.284898	0.234187
4	O	5.421673	-0.413007	1.515098
5	C	4.006496	-0.263354	1.290730
6	C	3.684146	1.207921	1.108631
7	O	4.188202	1.675178	-0.177153
8	C	3.561782	3.093952	-0.967872
9	O	4.155507	3.250504	-1.970597
10	C	2.939581	3.993389	0.045956
11	C	3.997572	4.811496	0.823867
12	C	3.214597	-0.911678	2.433217
13	O	1.871021	-1.125576	1.980444
14	P	0.620001	-0.233057	2.603161
15	O	0.865854	0.075463	4.044453
16	O	0.282390	0.875584	1.621416
17	O	-0.571220	-1.352815	2.390059
18	C	-0.535443	-2.535311	3.191504
19	C	-0.981983	-3.700843	2.310578
20	C	-1.039839	-5.044227	3.037357
21	O	0.061140	-5.265580	3.747847
22	O	-1.981098	-5.803181	2.933392

23	N	-2.344081	-3.464637	1.725017
24	H	7.827780	-2.483950	1.294964
25	H	7.773617	-0.838962	1.963891
26	H	-2.297360	-3.054489	0.766787
27	H	-2.829857	-4.372666	1.683104
28	H	-0.007578	-6.140171	4.172432
29	H	-0.292246	-3.792305	1.466784
30	H	0.470645	-2.753152	3.554924
31	H	-1.199902	-2.417696	4.054677
32	H	3.655620	-1.887680	2.650816
33	H	3.229074	-0.308522	3.344983
34	H	3.755105	-0.798437	0.379453
35	H	2.599792	1.330764	1.144297
36	H	4.159153	1.819004	1.877043
37	H	4.707489	4.131642	1.309721
38	H	3.455354	5.316663	1.631199
39	H	2.285524	4.658834	-0.526485
40	H	2.308392	3.419690	0.720860
41	C	4.755163	5.846985	-0.014522
42	C	5.744628	6.667988	0.822486
43	H	4.032971	6.522733	-0.492928
44	C	6.503671	7.711619	-0.002040
45	H	5.202461	7.166781	1.636857
46	H	6.460981	5.988731	1.303550
47	H	7.081811	7.238416	-0.803733
48	H	5.814916	8.425738	-0.467404
49	H	5.296627	5.347711	-0.827702
50	C	8.241424	-0.932700	-0.168876
51	C	7.985783	0.549436	-0.468575
52	H	8.321808	1.153285	0.385910
53	H	6.907743	0.734428	-0.562100
54	H	7.936000	-1.547864	-1.024103
55	C	8.684870	1.036987	-1.743284
56	C	8.408742	2.513141	-2.045827
57	H	8.357172	0.421601	-2.591996
58	H	7.334904	2.697326	-2.166895
59	H	8.764428	3.156433	-1.232911
60	H	9.767222	0.875940	-1.649662
61	H	9.315688	-1.100459	-0.030763
62	H	8.908277	2.832944	-2.966055
63	H	7.201514	8.279670	0.621419
64	P	-0.918331	-2.142661	-1.739371
65	O	-0.478292	-0.737348	-1.391250
66	O	0.045600	-3.162780	-0.851155
67	C	0.858577	-4.116885	-1.539527
68	C	2.067686	-3.398475	-2.175018
69	H	1.711205	-2.802974	-3.018282
70	H	1.186174	-4.837785	-0.787058
71	H	0.302888	-4.628225	-2.326232
72	O	1.803701	2.000402	-1.542479
73	H	1.649010	2.502515	-2.356893
74	H	2.527798	0.874599	-1.921288
75	Ca	-0.332066	1.432761	-0.555418
76	O	-1.015763	-2.591757	-3.160226
77	H	-2.910242	-2.845563	2.311038
78	C	3.126234	-4.378081	-2.665915
79	O	4.243560	-4.443025	-2.200742
80	O	2.643674	-5.145801	-3.642002
81	H	3.334387	-5.776067	-3.916032
82	N	2.701918	-2.476255	-1.183188
83	H	2.900719	-1.521356	-1.588737
84	H	2.068483	-2.329748	-0.386424
85	H	3.599611	-2.857898	-0.841007
86	C	-3.838077	0.628503	2.081519
87	C	-3.499939	0.465883	0.621865
88	O	-2.668138	1.151857	0.036999
89	O	-4.196722	-0.507514	0.028617
90	C	-4.006331	-0.758594	-1.390467
91	C	-5.319724	-0.440056	-2.089936
92	O	-5.530273	0.971006	-1.908588
93	C	-6.659166	1.607022	-2.327877
94	O	-6.714683	2.807066	-2.150596

95	C	-7.785441	0.800739	-2.940683
96	C	-8.798612	0.294643	-1.882998
97	C	-3.589135	-2.215703	-1.554394
98	O	-2.325318	-2.468880	-0.909366
99	H	-2.952742	0.290293	2.633770
100	H	-4.667206	-0.035353	2.337522
101	H	-4.314730	-2.879742	-1.079685
102	H	-3.512722	-2.468395	-2.615187
103	H	-3.224740	-0.093949	-1.759509
104	H	-5.234276	-0.681668	-3.153650
105	H	-6.138064	-1.016109	-1.650170
106	H	-8.288346	-0.344269	-1.151073
107	H	-9.513220	-0.351401	-2.406067
108	H	-8.295261	1.470873	-3.637621
109	H	-7.400176	-0.044372	-3.516223
110	C	-9.557166	1.407877	-1.151078
111	C	-10.582055	0.866961	-0.146427
112	H	-10.069016	2.040976	-1.889073
113	C	-11.342089	1.974837	0.588980
114	H	-11.296192	0.217906	-0.670900
115	H	-10.069305	0.227354	0.584687
116	H	-10.656031	2.619257	1.150670
117	H	-11.892109	2.611113	-0.113675
118	H	-8.847926	2.062007	-0.628976
119	C	-4.157877	2.090793	2.443323
120	C	-5.452138	2.605864	1.801779
121	H	-6.291789	1.976953	2.129448
122	H	-5.396178	2.495385	0.710005
123	H	-3.312750	2.721525	2.143945
124	C	-5.753552	4.071503	2.136382
125	C	-7.048515	4.574941	1.491268
126	H	-4.912493	4.696110	1.806160
127	H	-7.010129	4.472230	0.400961
128	H	-7.914219	4.003863	1.846595
129	H	-5.813050	4.191215	3.226555
130	H	-4.231749	2.159834	3.534451
131	H	-7.228224	5.629629	1.723876
132	H	-12.065117	1.559749	1.298625
133	O	3.289010	0.101729	-1.963043
134	H	3.996833	0.964459	-0.903735
135	H	3.740618	0.164129	-2.817768

E[B3LYP/6-31G(d,p)] = -4540.228180 h, E[APFD/6-311+G(2d,p)] = -4538.566525 h
Gcorr[B3LYP/6-31G(d,p)] = 1.007826 h

194. 2PS6Ca+2H_2O, products

Center No.	Atom	X	Y	Z
1	C	7.820863	-1.672871	1.482374
2	C	6.386406	-1.400024	1.106874
3	O	5.752473	-2.063319	0.298663
4	O	5.894780	-0.306427	1.723244
5	C	4.570587	0.127181	1.329428
6	C	4.536032	1.649571	1.345409
7	O	5.267678	2.212537	0.264273
8	C	1.961547	4.074632	-2.131915
9	O	1.793774	4.924196	-2.973173
10	C	2.434316	4.266407	-0.713472
11	C	2.437964	5.731319	-0.264081
12	C	3.530202	-0.557496	2.220795
13	O	2.267499	-0.573842	1.525983
14	P	0.983701	0.325120	2.068479
15	O	1.295296	0.917398	3.403933
16	O	0.517257	1.186511	0.913279
17	O	-0.164369	-0.861543	2.174927
18	C	0.049631	-1.916484	3.112961
19	C	0.013174	-3.248884	2.364051
20	C	0.367888	-4.465986	3.219725
21	O	1.470901	-4.261102	3.932516
22	O	-0.282366	-5.490325	3.199601
23	N	-1.338240	-3.519367	1.770069

24	H	7.941903	-2.757755	1.540611
25	H	8.031136	-1.241999	2.464771
26	H	-1.435698	-3.163928	0.793121
27	H	-1.486599	-4.538873	1.775560
28	H	1.676676	-5.070326	4.434990
29	H	0.719417	-3.200409	1.530684
30	H	1.013975	-1.830755	3.616686
31	H	-0.733323	-1.878876	3.877777
32	H	3.824341	-1.596495	2.388855
33	H	3.422790	-0.053627	3.183892
34	H	4.409380	-0.198031	0.304871
35	H	3.483473	1.964070	1.322752
36	H	4.977973	2.028601	2.271831
37	H	2.981363	6.330132	-1.004075
38	H	3.007265	5.794855	0.670440
39	H	1.815908	3.645972	-0.054146
40	H	3.445022	3.839716	-0.654135
41	C	1.037524	6.318533	-0.047638
42	C	1.062438	7.781415	0.411829
43	H	0.504094	5.713457	0.699576
44	C	-0.335632	8.365836	0.633870
45	H	1.644266	7.858845	1.340245
46	H	1.597416	8.384228	-0.334315
47	H	-0.929247	8.331441	-0.286861
48	H	-0.881884	7.804601	1.400647
49	H	0.461458	6.243254	-0.979012
50	C	8.793062	-1.098918	0.423844
51	C	8.824082	0.433435	0.360241
52	H	9.113502	0.826771	1.345020
53	H	7.818565	0.827148	0.162958
54	H	8.527069	-1.511724	-0.557274
55	C	9.793400	0.965887	-0.702387
56	C	9.836631	2.495898	-0.759768
57	H	9.504325	0.570463	-1.685591
58	H	8.847548	2.910928	-0.984926
59	H	10.161431	2.918460	0.197895
60	H	10.801216	0.577439	-0.502559
61	H	9.795337	-1.475939	0.658469
62	H	10.529542	2.847776	-1.531007
63	H	-0.285372	9.410210	0.958569
64	P	-0.595979	-2.200910	-1.888945
65	O	-0.488412	-0.692208	-1.800235
66	O	0.631801	-2.836668	-0.972799
67	C	1.630254	-3.622924	-1.631027
68	C	2.667733	-2.687737	-2.275129
69	H	2.164914	-2.089915	-3.039266
70	H	2.093266	-4.250652	-0.866319
71	H	1.192246	-4.249683	-2.408416
72	O	1.737894	2.741180	-2.429197
73	H	1.483923	2.699940	-3.370119
74	H	3.140853	1.445719	-2.143800
75	Ca	-0.693459	1.475522	-1.023133
76	O	-0.692860	-2.877224	-3.216327
77	H	-2.090366	-3.108940	2.330919
78	C	3.814581	-3.442338	-2.937668
79	O	4.973504	-3.334573	-2.604358
80	O	3.356366	-4.228587	-3.913880
81	H	4.108585	-4.706971	-4.306945
82	N	3.232474	-1.751988	-1.256129
83	H	3.472080	-0.817441	-1.664915
84	H	2.548742	-1.573978	-0.504592
85	H	4.103170	-2.118721	-0.827693
86	C	-3.661723	0.210914	2.136564
87	C	-3.410850	0.014193	0.664293
88	O	-2.764748	0.799605	-0.023163
89	O	-3.965275	-1.099676	0.181602
90	C	-3.855787	-1.402893	-1.236259
91	C	-5.263803	-1.404525	-1.812169
92	O	-5.746260	-0.055959	-1.685498
93	C	-7.011650	0.306811	-2.036115
94	O	-7.300644	1.480695	-1.922779
95	C	-7.990420	-0.752844	-2.498543

96	C	-8.786003	-1.382311	-1.327274
97	C	-3.163312	-2.753857	-1.373186
98	O	-1.815207	-2.695578	-0.868588
99	H	-2.686836	0.096452	2.625234
100	H	-4.318282	-0.582448	2.501226
101	H	-3.681205	-3.514497	-0.784626
102	H	-3.146918	-3.065036	-2.421249
103	H	-3.264291	-0.623193	-1.716145
104	H	-5.223777	-1.700476	-2.864886
105	H	-5.903038	-2.099866	-1.261988
106	H	-8.096354	-1.857415	-0.618124
107	H	-9.393310	-2.191045	-1.750114
108	H	-8.684089	-0.250102	-3.177318
109	H	-7.485346	-1.539204	-3.064576
110	C	-9.694014	-0.399157	-0.579526
111	C	-10.499227	-1.068770	0.541022
112	H	-10.384295	0.069505	-1.294582
113	C	-11.408497	-0.090943	1.291202
114	H	-11.104539	-1.881174	0.116857
115	H	-9.807275	-1.542835	1.250255
116	H	-10.826300	0.713907	1.754543
117	H	-12.133979	0.373906	0.613950
118	H	-9.093976	0.416371	-0.157010
119	C	-4.243414	1.604818	2.440667
120	C	-5.657283	1.809403	1.882717
121	H	-6.329231	1.057025	2.318953
122	H	-5.660264	1.628602	0.798928
123	H	-3.565706	2.365665	2.036140
124	C	-6.218809	3.210561	2.151991
125	C	-7.631554	3.402652	1.591763
126	H	-5.545235	3.958451	1.712021
127	H	-7.653123	3.222242	0.511217
128	H	-8.338667	2.706018	2.057106
129	H	-6.220943	3.400599	3.233743
130	H	-4.251258	1.736513	3.528458
131	H	-7.999073	4.418261	1.771320
132	H	-11.969265	-0.595582	2.084626
133	O	3.918131	0.876467	-1.979565
134	H	4.904415	1.828374	-0.556483
135	H	4.458476	0.942400	-2.781033

E[B3LYP/6-31G(d,p)] = -2441.236699 h, E[APFD/6-311+G(2d,p)] = -4538.632142 h
Gcorr[B3LYP/6-31G(d,p)] = 0.180181 h

XVI. Structures of molecules and transition states (TS) related to the hydrolysis at the glycerol backbone of PC6, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

195. PC6+2H_2O, 1st step, reactants

Center No.	Atom	X	Y	Z
1	O	-3.269045	0.375415	-1.930088
2	H	-3.337485	0.906894	-1.125083
3	H	-2.755529	-0.409055	-1.666541
4	O	-5.890064	-0.630347	-2.198047
5	H	-5.827619	-1.310271	-2.881606
6	H	-4.993521	-0.236508	-2.182321
7	P	4.294754	-1.597050	-1.077259
8	C	4.367369	-0.548951	1.369650
9	H	3.865087	-1.502834	1.552609
10	H	5.239815	-0.489374	2.026884
11	C	3.433875	0.650864	1.558706
12	H	3.997114	1.575216	1.417529
13	H	2.633728	0.601651	0.820649
14	C	1.733851	-2.022475	-1.595934
15	H	1.943170	-3.025799	-1.208526
16	H	1.761716	-2.059961	-2.693418
17	C	0.349701	-1.585068	-1.131856
18	H	0.325995	-1.506197	-0.043734
19	C	0.076224	0.806400	-0.902527
20	C	-0.723183	-2.545430	-1.614896
21	H	-0.816379	-2.514677	-2.703767

22	H	-0.497593	-3.564570	-1.299997
23	C	-2.775518	-3.134155	-0.497643
24	C	-0.206036	2.053548	-1.707677
25	H	0.519490	2.084666	-2.529862
26	H	-1.185254	1.903612	-2.179758
27	C	3.767381	0.806076	4.032344
28	H	4.280526	-0.151740	4.091023
29	H	4.479274	1.606018	3.830760
30	H	3.243604	0.999065	4.967887
31	C	1.801127	-0.382280	3.132546
32	H	1.293985	-0.235166	4.085367
33	H	1.083178	-0.381026	2.313613
34	H	2.358735	-1.316318	3.155872
35	C	1.964241	2.051592	2.925303
36	H	1.245994	2.013836	2.107107
37	H	1.452463	2.138261	3.883440
38	H	2.654085	2.884419	2.793646
39	N	2.755793	0.765686	2.918450
40	C	-0.173471	3.345018	-0.890002
41	H	-0.899843	3.273890	-0.071395
42	H	0.811225	3.452547	-0.419033
43	C	-0.474294	4.583293	-1.742535
44	H	0.252504	4.645223	-2.564844
45	H	-1.460007	4.469999	-2.215566
46	C	-0.444199	5.890855	-0.942063
47	H	0.540749	6.001486	-0.468657
48	H	-1.171314	5.828531	-0.121151
49	C	-4.060088	-2.572484	0.057637
50	H	-4.609903	-2.078141	-0.753130
51	H	-4.654547	-3.424020	0.397848
52	C	-3.848228	-1.569889	1.210263
53	H	-3.301957	-2.059427	2.026480
54	H	-3.214828	-0.744752	0.864937
55	C	-5.176973	-1.013040	1.734563
56	H	-5.805816	-1.843581	2.084514
57	H	-5.721332	-0.545282	0.902937
58	C	-5.000342	0.002537	2.869755
59	H	-4.452014	-0.469806	3.695961
60	H	-4.369160	0.830257	2.519017
61	O	-2.439002	-4.298318	-0.470231
62	O	0.273126	0.767524	0.300513
63	O	-1.998499	-2.153100	-1.055011
64	O	0.054980	-0.282883	-1.698436
65	O	4.976258	-1.251675	-2.368508
66	O	4.339298	-2.980907	-0.487323
67	O	2.699031	-1.094582	-1.109426
68	O	4.831848	-0.476350	0.023356
69	C	-6.329339	0.558607	3.389965
70	H	-6.967826	-0.242350	3.779762
71	H	-6.171321	1.281078	4.197314
72	H	-6.884932	1.065613	2.592843
73	C	-0.742210	7.126584	-1.796440
74	H	-1.735131	7.060034	-2.255719
75	H	-0.713056	8.042956	-1.197942
76	H	-0.010702	7.233737	-2.605561

E[B3LYP/6-31G(d,p)] = -1937.181989 h, E[APFD/6-311+G(2d,p)] = -1936.359217 h
Gcorr[B3LYP/6-31G(d,p)] = 0.577759 h

196. PC6+2H_2O, 1st step, TS

Center No.	Atom	X	Y	Z
1	O	-4.101727	-1.713285	-2.846740
2	H	-4.669372	-0.928691	-2.882300
3	H	-3.258972	-1.536107	-2.176888
4	O	-4.525621	-3.189298	-1.019497
5	H	-4.268037	-4.105938	-1.213413
6	H	-4.493076	-2.484280	-2.058811
7	P	3.861456	-2.050541	-0.969613
8	C	3.985551	-0.652274	1.293659
9	H	3.348128	-1.490534	1.588191

10	H	4.828407	-0.600685	1.989094
11	C	3.218806	0.672825	1.234939
12	H	3.902847	1.472659	0.945069
13	H	2.423993	0.593930	0.493405
14	C	1.283173	-2.192218	-1.567986
15	H	1.369816	-3.168680	-1.078724
16	H	1.308967	-2.344031	-2.655530
17	C	-0.034579	-1.549985	-1.166109
18	H	-0.030415	-1.324635	-0.099063
19	C	-0.172327	0.861920	-1.225186
20	C	-1.236672	-2.421736	-1.508392
21	H	-1.260011	-2.624570	-2.587681
22	H	-1.149666	-3.377084	-0.976042
23	C	-3.367609	-2.697157	-0.006603
24	C	-0.369076	2.027468	-2.170695
25	H	0.431645	1.980734	-2.919531
26	H	-1.298244	1.843625	-2.724566
27	C	3.560043	1.265814	3.641509
28	H	3.966506	0.287584	3.890224
29	H	4.356790	1.932897	3.313953
30	H	3.055040	1.684473	4.511333
31	C	1.472871	0.156191	2.938190
32	H	0.979019	0.549382	3.826261
33	H	0.765493	0.072456	2.114195
34	H	1.919074	-0.809993	3.165091
35	C	1.915616	2.467555	2.268318
36	H	1.182976	2.346042	1.471166
37	H	1.432369	2.803936	3.184958
38	H	2.692085	3.173025	1.974157
39	N	2.554922	1.124550	2.529698
40	C	-0.400504	3.391800	-1.481310
41	H	-1.187065	3.392652	-0.717157
42	H	0.545149	3.551154	-0.949168
43	C	-0.636031	4.542250	-2.466892
44	H	0.151774	4.534065	-3.233424
45	H	-1.582373	4.376997	-3.001213
46	C	-0.670455	5.918544	-1.791400
47	H	0.275762	6.082641	-1.258280
48	H	-1.456813	5.924347	-1.024512
49	C	-4.040061	-1.598159	0.800118
50	H	-4.470937	-0.851956	0.124850
51	H	-4.875458	-2.073132	1.328555
52	C	-3.087791	-0.938961	1.802344
53	H	-2.634234	-1.721365	2.423363
54	H	-2.269271	-0.457248	1.255136
55	C	-3.786966	0.090851	2.697614
56	H	-4.607218	-0.395956	3.244417
57	H	-4.255968	0.862612	2.070515
58	C	-2.840893	0.763144	3.700107
59	H	-2.368847	-0.008495	4.323470
60	H	-2.024740	1.253026	3.151899
61	O	-2.744559	-3.638324	0.468943
62	O	-0.031316	0.959659	-0.015005
63	O	-2.439697	-1.784779	-1.108897
64	O	-0.178401	-0.299776	-1.896487
65	O	4.636250	-2.003227	-2.254233
66	O	3.689414	-3.321714	-0.181720
67	O	2.360903	-1.345623	-1.166646
68	O	4.514330	-0.858118	-0.014235
69	C	-3.540648	1.787664	4.598295
70	H	-4.339349	1.319149	5.184748
71	H	-2.839354	2.249668	5.300968
72	H	-3.994275	2.589771	4.004792
73	C	-0.908270	7.067374	-2.775952
74	H	-1.863857	6.948456	-3.299395
75	H	-0.927496	8.035030	-2.263990
76	H	-0.118754	7.107782	-3.535086

E[B3LYP/6-31G(d,p)] = -1937.124093 h, E[APFD/6-311+G(2d,p)] = -1936.305345 h
Gcorr[B3LYP/6-31G(d,p)] = 0.576171 h

197. PC6+2H_2O, 1st step, products

Center No.	Atom	X	Y	Z
1	O	1.255538	5.093266	-2.591332
2	H	2.178795	5.374381	-2.648624
3	H	1.076685	3.312274	-2.485105
4	O	0.316828	4.920633	0.147823
5	H	-0.650858	4.984967	0.234434
6	H	0.985393	5.305189	-1.680808
7	P	-4.419455	-0.659838	-0.731797
8	C	-3.583163	-0.996233	1.774073
9	H	-3.560476	0.093148	1.679894
10	H	-4.193872	-1.253267	2.644600
11	C	-2.180269	-1.604260	1.870674
12	H	-2.263968	-2.686354	1.987894
13	H	-1.628261	-1.384262	0.957083
14	C	-2.438588	0.640005	-1.930695
15	H	-3.028604	1.520049	-1.652990
16	H	-2.629832	0.411675	-2.987944
17	C	-0.963024	0.940716	-1.723839
18	H	-0.755962	1.097592	-0.664763
19	C	0.493417	-0.939725	-1.291202
20	C	-0.490991	2.150195	-2.518042
21	H	-0.639854	1.962386	-3.593488
22	H	-1.126257	3.004320	-2.241854
23	C	0.704193	3.756085	0.741079
24	C	1.220686	-2.073738	-1.981605
25	H	0.466807	-2.670304	-2.510799
26	H	1.846985	-1.631269	-2.766299
27	C	-1.996781	-1.321718	4.348829
28	H	-2.870043	-0.675355	4.412965
29	H	-2.292177	-2.367284	4.432096
30	H	-1.295461	-1.067896	5.142789
31	C	-0.972295	0.345784	2.847035
32	H	-0.319172	0.646392	3.665766
33	H	-0.465199	0.471299	1.892971
34	H	-1.885373	0.936631	2.873545
35	C	-0.031160	-1.908684	2.999272
36	H	0.439938	-1.765508	2.027408
37	H	0.616885	-1.545628	3.796543
38	H	-0.269757	-2.959402	3.161238
39	N	-1.314093	-1.112919	3.024007
40	C	2.050926	-2.946742	-1.040380
41	H	2.781920	-2.319609	-0.515491
42	H	1.397539	-3.368861	-0.267328
43	C	2.775701	-4.078820	-1.777492
44	H	2.039022	-4.700428	-2.305983
45	H	3.426107	-3.651518	-2.553862
46	C	3.612887	-4.966679	-0.848866
47	H	2.962062	-5.391952	-0.072931
48	H	4.348746	-4.344608	-0.321582
49	C	2.199258	3.572128	0.680513
50	H	2.500252	3.707325	-0.363889
51	H	2.650202	4.406515	1.234012
52	C	2.676754	2.225313	1.223059
53	H	2.344860	2.116496	2.262600
54	H	2.193537	1.420819	0.657460
55	C	4.199924	2.070129	1.147554
56	H	4.680402	2.881520	1.712604
57	H	4.527723	2.189497	0.105102
58	C	4.694707	0.720174	1.680904
59	H	4.369016	0.602609	2.723316
60	H	4.209973	-0.089046	1.117816
61	O	-0.104264	3.012604	1.257338
62	O	0.527116	-0.717128	-0.089994
63	O	0.871183	2.391015	-2.215989
64	O	-0.194862	-0.207930	-2.179872
65	O	-5.091970	-1.564767	-1.722670
66	O	-4.980718	0.687727	-0.363488
67	O	-2.805744	-0.472978	-1.114910
68	O	-4.194049	-1.586509	0.629036

69	C	6.215676	0.560287	1.599407
70	H	6.726755	1.336231	2.180799
71	H	6.536910	-0.411901	1.987328
72	H	6.566786	0.638353	0.564088
73	C	4.334880	-6.098022	-1.586799
74	H	5.018847	-5.701946	-2.346140
75	H	4.922743	-6.713465	-0.897979
76	H	3.621813	-6.756450	-2.096005

E[B3LYP/6-31G(d,p)] = -1937.184221 h, E[APFD/6-311+G(2d,p)] = -1936.361920 h
Gcorr[B3LYP/6-31G(d,p)] = 0.577050 h

198. PC6+2H_2O, 2nd step, reactants (hydrolysed carbon chain neglected)

Center No.	Atom	X	Y	Z
1	P	3.421330	-0.854190	-1.450844
2	C	3.406813	1.526015	-0.253797
3	H	3.644081	0.860476	0.580762
4	H	4.188164	2.288929	-0.317828
5	C	2.014646	2.152492	-0.125231
6	H	1.831652	2.804067	-0.981846
7	H	1.264581	1.362196	-0.110534
8	C	1.590614	-2.283838	-0.164808
9	H	2.468081	-2.626694	0.393610
10	H	1.315455	-3.058054	-0.893677
11	C	0.443669	-2.048046	0.805623
12	H	0.692155	-1.232058	1.485146
13	C	-1.231632	-0.402341	0.189411
14	C	0.083247	-3.286940	1.609100
15	H	-0.347613	-4.053591	0.952170
16	H	1.000328	-3.692350	2.054623
17	C	-2.373268	-0.140533	-0.764120
18	H	-1.920024	0.228261	-1.695230
19	H	-2.854912	-1.090875	-1.003074
20	C	2.765072	4.126441	1.212643
21	H	3.761174	3.720052	1.375531
22	H	2.737036	4.697761	0.285318
23	H	2.486498	4.762326	2.052020
24	C	1.838093	2.150500	2.362649
25	H	1.601951	2.780053	3.219875
26	H	1.106269	1.349616	2.265721
27	H	2.842294	1.746070	2.471323
28	C	0.380665	3.578166	1.011506
29	H	-0.326703	2.753143	0.933794
30	H	0.183657	4.168707	1.905785
31	H	0.333890	4.211901	0.126697
32	N	1.771493	2.999502	1.117716
33	C	-3.391317	0.868605	-0.224640
34	H	-3.824991	0.456298	0.693557
35	H	-2.874475	1.794416	0.052231
36	C	-4.502373	1.176200	-1.234504
37	H	-4.057686	1.571956	-2.158791
38	H	-5.009672	0.242587	-1.516106
39	C	-5.539543	2.173891	-0.704530
40	H	-5.032307	3.106908	-0.423964
41	H	-5.981217	1.777903	0.219850
42	O	-0.781229	0.408347	0.979797
43	O	-0.841765	-2.901700	2.628926
44	O	-0.728955	-1.650163	0.035591
45	O	3.467642	-1.282622	-2.888061
46	O	4.409518	-1.349966	-0.429334
47	O	1.880783	-1.058348	-0.833735
48	O	3.402889	0.806093	-1.484295
49	C	-6.651388	2.479610	-1.712526
50	H	-7.198696	1.570167	-1.985743
51	H	-7.374785	3.193700	-1.305569
52	H	-6.242624	2.908483	-2.634643
53	H	-1.052310	-3.688542	3.150676
54	O	-2.688174	-3.721237	-0.647093
55	H	-1.926147	-3.128283	-0.745893
56	H	-3.111212	-3.731925	-1.516164

57	O	-3.493250	-2.196358	1.647394
58	H	-3.442288	-2.746113	0.844258
59	H	-2.619462	-2.344844	2.050590

E[B3LYP/6-31G(d,p)] = -1627.247979 h, E[APFD/6-311+G(2d,p)] = -1626.606610 h
Gcorr[B3LYP/6-31G(d,p)] = 0.439767 h

199. PC6+2H_2O, 2nd step, TS

Center No.	Atom	X	Y	Z
1	P	3.440459	-0.085280	-1.649874
2	C	2.835731	1.977064	-0.072001
3	H	3.235067	1.254521	0.645114
4	H	3.413356	2.902149	0.018207
5	C	1.337488	2.229228	0.128952
6	H	0.980456	2.894728	-0.659337
7	H	0.786459	1.289083	0.082312
8	C	2.008118	-2.058905	-0.549258
9	H	2.969702	-2.215477	-0.050170
10	H	1.865952	-2.854271	-1.293497
11	C	0.879095	-2.087038	0.475875
12	H	0.976804	-1.202380	1.115650
13	C	-1.485902	-0.959013	0.576529
14	C	0.947128	-3.322332	1.374520
15	H	0.713284	-4.230426	0.804379
16	H	1.962493	-3.423824	1.778212
17	C	-2.385285	-0.563985	-0.589138
18	H	-1.763137	0.020292	-1.274751
19	H	-2.715090	-1.452066	-1.137707
20	C	1.632579	4.209534	1.632303
21	H	2.701523	4.053690	1.762119
22	H	1.444698	4.826915	0.754045
23	H	1.222942	4.689612	2.520221
24	C	1.267752	1.972344	2.608578
25	H	0.948226	2.463576	3.527419
26	H	0.722791	1.039918	2.463613
27	H	2.341589	1.798334	2.642127
28	C	-0.548509	3.102139	1.424290
29	H	-1.024011	2.129777	1.291981
30	H	-0.844986	3.552503	2.371581
31	H	-0.787874	3.774432	0.600823
32	N	0.945761	2.883183	1.449697
33	C	-3.602450	0.256269	-0.141341
34	H	-4.199256	-0.336616	0.562873
35	H	-3.256888	1.138493	0.411132
36	C	-4.483288	0.699450	-1.315470
37	H	-3.880182	1.287558	-2.021878
38	H	-4.824298	-0.185921	-1.870844
39	C	-5.701835	1.523971	-0.882527
40	H	-5.360473	2.407854	-0.326773
41	H	-6.303656	0.935187	-0.177008
42	O	-0.925934	-0.116622	1.295430
43	O	0.011665	-3.148152	2.452943
44	O	-0.375940	-1.979878	-0.195177
45	O	3.633860	-0.210324	-3.133720
46	O	4.509428	-0.480201	-0.664776
47	O	2.001679	-0.785665	-1.199604
48	O	2.993863	1.500004	-1.405341
49	C	-6.579368	1.966787	-2.057200
50	H	-6.963296	1.102990	-2.612008
51	H	-7.439590	2.552007	-1.715885
52	H	-6.013492	2.586656	-2.762111
53	H	-0.076774	-3.990884	2.918093
54	O	-1.889880	-3.851490	-0.138187
55	H	-1.089713	-3.140638	-0.374176
56	H	-2.486195	-3.973500	-0.892138
57	O	-2.251075	-2.037761	1.379642
58	H	-2.286457	-3.078018	0.627386
59	H	-1.586029	-2.311689	2.056883

E[B3LYP/6-31G(d,p)] = -1627.189945 h, E[APFD/6-311+G(2d,p)] = -1626.548915 h

Gcorr[B3LYP/6-31G(d,p)] = 0.441760 h

200. PC6+2H_2O, 2nd step, products

Center No.	Atom	X	Y	Z
1	P	-4.318444	-0.875676	0.041680
2	C	-2.445817	-2.771978	0.041620
3	H	-2.451700	-2.481552	1.096045
4	H	-2.559273	-3.858086	-0.019750
5	C	-1.181571	-2.298798	-0.685951
6	H	-1.253336	-2.569097	-1.740970
7	H	-1.102949	-1.214316	-0.605002
8	C	-3.034449	1.375877	0.594323
9	H	-2.943964	1.032215	1.630357
10	H	-3.934688	2.001044	0.515959
11	C	-1.820482	2.201549	0.198895
12	H	-0.959257	1.524711	0.102472
13	C	2.266613	1.596662	0.136550
14	C	-1.488199	3.228710	1.286315
15	H	-2.317714	3.939828	1.394915
16	H	-1.332002	2.729613	2.246663
17	C	3.613331	1.251563	-0.461768
18	H	3.424788	0.835089	-1.459894
19	H	4.195377	2.166826	-0.595453
20	C	0.142210	-4.380769	-0.305993
21	H	-0.600620	-4.804770	0.366257
22	H	-0.084613	-4.650044	-1.337091
23	H	1.132130	-4.743866	-0.032968
24	C	0.393776	-2.478958	1.245693
25	H	1.357020	-2.890299	1.545943
26	H	0.421243	-1.391328	1.299773
27	H	-0.391121	-2.882206	1.882186
28	C	1.242543	-2.314218	-1.042677
29	H	1.276417	-1.235506	-0.891829
30	H	2.183892	-2.764958	-0.729476
31	H	1.039900	-2.559246	-2.084565
32	N	0.135211	-2.879261	-0.185722
33	C	4.385205	0.226154	0.385404
34	H	4.571970	0.648607	1.381302
35	H	3.755455	-0.657884	0.535778
36	C	5.716178	-0.183217	-0.254354
37	H	5.525496	-0.605106	-1.251347
38	H	6.334663	0.711020	-0.414479
39	C	6.502053	-1.198193	0.584749
40	H	5.882705	-2.091081	0.744695
41	H	6.689345	-0.775038	1.580845
42	O	1.439060	0.764952	0.486139
43	O	-0.274482	3.943697	1.012494
44	O	-2.106351	2.839499	-1.043712
45	O	-5.519020	-0.626399	-0.824696
46	O	-4.426687	-1.052832	1.533270
47	O	-3.133461	0.247057	-0.280702
48	O	-3.554462	-2.190857	-0.637426
49	C	7.832326	-1.606291	-0.055323
50	H	8.486247	-0.738080	-0.196063
51	H	8.369301	-2.330106	0.566360
52	H	7.674552	-2.063854	-1.038668
53	H	-0.350250	4.380864	0.140473
54	O	0.227721	4.328399	-1.666729
55	H	-1.277371	3.193019	-1.412721
56	H	0.275477	5.084048	-2.267308
57	O	2.065613	2.914534	0.249118
58	H	1.135853	4.005997	-1.561966
59	H	1.171472	3.110542	0.657423

E[B3LYP/6-31G(d,p)] = -1627.254809 h, E[APFD/6-311+G(2d,p)] = -1626.604208 h
Gcorr[B3LYP/6-31G(d,p)] = 0.439844 h

XVII. Structures of molecules and transition states (TS) related to the hydrolysis at the glycerol backbone of PC6Ca, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

201. PC6Ca+4H_2O, 1st step, reactants

Center No.	Atom	X	Y	Z
1	O	-3.965912	-0.735337	-4.445866
2	H	-4.552785	0.028556	-4.527952
3	H	-3.319383	-0.480828	-3.766457
4	Ca	5.917890	0.238014	-0.956441
5	O	8.358262	0.040339	-1.031269
6	H	8.861769	-0.032898	-0.208796
7	H	8.766199	-0.592786	-1.637954
8	O	-5.040657	-2.824734	-2.887223
9	H	-4.304202	-3.448413	-2.857117
10	H	-4.737346	-2.135305	-3.512609
11	O	3.674401	1.114389	-1.437661
12	H	3.045057	0.408287	-1.173427
13	H	3.454105	1.332876	-2.353282
14	P	3.401506	-2.129487	0.205661
15	C	2.032150	-1.896790	2.482825
16	H	1.396283	-2.585868	1.921862
17	H	2.347505	-2.393339	3.403520
18	C	1.346832	-0.555510	2.760624
19	H	2.042638	0.098165	3.289409
20	H	1.066635	-0.083879	1.818837
21	C	1.388461	-1.705434	-1.556317
22	H	1.284461	-2.780555	-1.395319
23	H	1.790439	-1.527916	-2.559753
24	C	0.050339	-1.009725	-1.372910
25	H	-0.285871	-1.144546	-0.346990
26	C	-0.120312	1.283768	-0.656400
27	C	-1.026133	-1.510491	-2.326498
28	H	-0.772965	-1.288590	-3.363811
29	H	-1.172053	-2.584893	-2.199529
30	C	-3.004468	-1.221774	-1.003869
31	C	0.251377	2.693747	-1.048249
32	H	1.346057	2.715585	-1.134796
33	H	-0.128019	2.868705	-2.062098
34	C	0.352012	-1.204198	4.961258
35	H	0.627361	-2.251198	4.851811
36	H	1.159842	-0.647094	5.434519
37	H	-0.556010	-1.125922	5.557639
38	C	-1.002154	-1.399060	2.909551
39	H	-1.899020	-1.360769	3.526869
40	H	-1.193136	-0.945532	1.938286
41	H	-0.681468	-2.432905	2.797138
42	C	-0.403844	0.811772	3.778461
43	H	-0.593935	1.233036	2.791937
44	H	-1.318558	0.793120	4.369429
45	H	0.366234	1.380855	4.297994
46	N	0.080640	-0.609190	3.603755
47	C	-0.247292	3.760534	-0.072573
48	H	-1.339078	3.694953	0.008511
49	H	0.148682	3.548618	0.927639
50	C	0.155613	5.177121	-0.498027
51	H	1.249989	5.234797	-0.584193
52	H	-0.240464	5.383891	-1.502252
53	C	-0.333466	6.259778	0.471676
54	H	0.062260	6.051115	1.474809
55	H	-1.426845	6.200165	0.557242
56	C	-4.209125	-0.338165	-0.799347
57	H	-3.828183	0.615101	-0.406628
58	H	-4.642860	-0.116085	-1.778532
59	C	-5.249160	-0.943957	0.144301
60	H	-5.605922	-1.882048	-0.295267
61	H	-4.767458	-1.202064	1.094544
62	C	-6.431113	-0.002223	0.399165
63	H	-6.905133	0.257694	-0.557977
64	H	-6.062164	0.942867	0.822698
65	C	-7.485432	-0.599733	1.339028

66	H	-7.852611	-1.544054	0.915020
67	H	-7.010546	-0.859803	2.294750
68	O	-2.661431	-2.149300	-0.301747
69	O	-0.667289	0.957061	0.384272
70	O	-2.271536	-0.815310	-2.086177
71	O	0.256359	0.405364	-1.611429
72	O	4.779289	-1.633477	-0.189908
73	O	3.005252	-3.561233	0.054945
74	O	2.297115	-1.154430	-0.583665
75	O	3.214839	-1.576087	1.739979
76	C	-8.667420	0.340045	1.594659
77	H	-9.182984	0.590577	0.660478
78	H	-9.401308	-0.114629	2.268094
79	H	-8.334577	1.279690	2.050317
80	C	0.069710	7.675034	0.047305
81	H	-0.340608	7.924807	-0.937806
82	H	-0.293391	8.423924	0.758664
83	H	1.159489	7.774501	-0.013847

E[B3LYP/6-31G(d,p)] = -2767.533131 h, E[APFD/6-311+G(2d,p)] = -2766.602568 h
Gcorr[B3LYP/6-31G(d,p)] = 0.617903 h

202. PC6Ca+4H_2O, 1st step, TS

Center No.	Atom	X	Y	Z
1	O	-3.336778	-1.080655	-4.592978
2	H	-3.971636	-0.379544	-4.805356
3	H	-2.640659	-0.742328	-3.828840
4	Ca	5.912218	0.661264	-0.537065
5	O	8.353188	0.605953	-0.334386
6	H	8.760489	0.531917	0.539591
7	H	8.871945	0.025638	-0.908270
8	O	-3.893195	-2.417268	-2.694097
9	H	-3.517676	-3.312822	-2.719642
10	H	-3.767437	-1.809860	-3.814549
11	O	3.656568	1.489816	-1.031400
12	H	3.054401	0.730522	-0.870144
13	H	3.467087	1.787826	-1.931368
14	P	3.438040	-1.906738	0.282368
15	C	1.766071	-2.146335	2.342993
16	H	1.296513	-2.806588	1.609444
17	H	2.003262	-2.735416	3.232161
18	C	0.901664	-0.927179	2.676295
19	H	1.428938	-0.300440	3.397757
20	H	0.717321	-0.347493	1.771630
21	C	1.608059	-1.416805	-1.649796
22	H	1.573093	-2.507536	-1.615109
23	H	2.117740	-1.104841	-2.568402
24	C	0.204954	-0.842417	-1.586940
25	H	-0.258506	-1.097393	-0.637160
26	C	-0.188959	1.354831	-0.676973
27	C	-0.690328	-1.336840	-2.718379
28	H	-0.280396	-1.038712	-3.689814
29	H	-0.723719	-2.431692	-2.670292
30	C	-3.000534	-1.676818	-1.585860
31	C	0.052599	2.824440	-0.936794
32	H	1.141123	2.971022	-0.912853
33	H	-0.252308	3.038426	-1.967795
34	C	-0.337560	-1.998268	4.564160
35	H	0.047928	-2.992973	4.349416
36	H	0.337816	-1.465793	5.233001
37	H	-1.325241	-2.079027	5.016268
38	C	-1.334417	-1.980944	2.308961
39	H	-2.317216	-2.107615	2.761670
40	H	-1.417554	-1.413252	1.384258
41	H	-0.893927	-2.957386	2.117505
42	C	-1.120646	0.108400	3.573075
43	H	-1.189742	0.669345	2.641957
44	H	-2.111829	-0.080817	3.983347
45	H	-0.511199	0.644762	4.299734
46	N	-0.464241	-1.220744	3.280236

47	C	-0.646098	3.752661	0.057637
48	H	-1.726688	3.566140	0.028819
49	H	-0.318888	3.504479	1.074113
50	C	-0.369855	5.232945	-0.229066
51	H	0.714276	5.413323	-0.203758
52	H	-0.694768	5.473945	-1.251109
53	C	-1.063699	6.179156	0.758250
54	H	-0.737431	5.938224	1.779009
55	H	-2.146338	5.995621	0.733433
56	C	-3.902718	-0.580348	-1.040390
57	H	-3.255043	0.101051	-0.479363
58	H	-4.334188	-0.008512	-1.868851
59	C	-5.009701	-1.136207	-0.136147
60	H	-5.632723	-1.829487	-0.714234
61	H	-4.548723	-1.726823	0.665225
62	C	-5.889243	-0.038194	0.472710
63	H	-6.344341	0.554518	-0.333689
64	H	-5.260018	0.659144	1.044147
65	C	-6.995614	-0.583466	1.384267
66	H	-7.623360	-1.280175	0.812321
67	H	-6.540155	-1.176029	2.189341
68	O	-2.380942	-2.483073	-0.892012
69	O	-0.741388	0.898501	0.311538
70	O	-1.996899	-0.786649	-2.608531
71	O	0.315781	0.603430	-1.674417
72	O	4.795836	-1.240190	0.166498
73	O	3.222958	-3.328911	-0.121131
74	O	2.352033	-0.922318	-0.515682
75	O	2.999117	-1.619042	1.838088
76	C	-7.873697	0.514452	1.992048
77	H	-8.369828	1.101955	1.210997
78	H	-8.652273	0.093506	2.636709
79	H	-7.278331	1.207215	2.597875
80	C	-0.789320	7.657950	0.469194
81	H	-1.136740	7.936329	-0.532330
82	H	-1.297327	8.306983	1.189910
83	H	0.283019	7.878827	0.520010

E[B3LYP/6-31G(d,p)] = -2767.477927 h, E[APFD/6-311+G(2d,p)] = -2766.547276 h
Gcorr[B3LYP/6-31G(d,p)] = 0.618804 h

203. PC6Ca+4H_2O, 1st step, products

Center No.	Atom	X	Y	Z
1	O	-3.447275	-2.624259	-4.279734
2	H	-4.196465	-2.109897	-4.610649
3	H	-2.257535	-1.534594	-3.519814
4	Ca	5.838008	0.387039	-0.878433
5	O	8.279369	0.320974	-0.681197
6	H	8.695191	0.433265	0.184657
7	H	8.775741	-0.387849	-1.113034
8	O	-3.778648	-3.431196	-1.508344
9	H	-3.260707	-4.238082	-1.336419
10	H	-3.771050	-3.031188	-3.457295
11	O	3.571295	1.209480	-1.327570
12	H	2.961563	0.539908	-0.948700
13	H	3.283898	1.333198	-2.242241
14	P	3.403555	-1.839642	0.677146
15	C	1.808407	-1.506147	2.779156
16	H	1.299732	-2.315490	2.249949
17	H	2.046070	-1.850063	3.788512
18	C	0.994251	-0.209105	2.789068
19	H	1.557208	0.564571	3.314455
20	H	0.814296	0.114437	1.763917
21	C	1.651587	-1.700913	-1.366875
22	H	1.549036	-2.764930	-1.143199
23	H	2.282219	-1.584120	-2.256180
24	C	0.282996	-1.078563	-1.587881
25	H	-0.343105	-1.218781	-0.706989
26	C	-0.121778	1.217192	-0.951205
27	C	-0.430762	-1.638251	-2.811350

28	H	0.184981	-1.461465	-3.707629
29	H	-0.521687	-2.726743	-2.680992
30	C	-3.324075	-2.468616	-0.657792
31	C	0.169011	2.644212	-1.358745
32	H	1.260093	2.764023	-1.347373
33	H	-0.129379	2.754836	-2.408455
34	C	-0.249844	-0.686060	4.904179
35	H	0.119607	-1.707558	4.967759
36	H	0.435920	-0.002909	5.404275
37	H	-1.237011	-0.625811	5.360418
38	C	-1.274670	-1.244479	2.728256
39	H	-2.258201	-1.207670	3.195524
40	H	-1.340632	-0.942406	1.685511
41	H	-0.872778	-2.252506	2.806832
42	C	-0.983810	1.096387	3.384339
43	H	-1.067910	1.377477	2.335156
44	H	-1.967052	1.060008	3.851992
45	H	-0.340683	1.793722	3.920067
46	N	-0.369984	-0.282089	3.458618
47	C	-0.508437	3.692344	-0.475289
48	H	-1.593030	3.530883	-0.488885
49	H	-0.189447	3.549734	0.564155
50	C	-0.192658	5.125362	-0.918935
51	H	0.895935	5.278236	-0.911151
52	H	-0.512234	5.264097	-1.961438
53	C	-0.859222	6.190054	-0.039299
54	H	-0.540207	6.048845	1.002227
55	H	-1.946686	6.036029	-0.048072
56	C	-4.112835	-1.190153	-0.758497
57	H	-3.442335	-0.370290	-0.491831
58	H	-4.438618	-1.046122	-1.791898
59	C	-5.334313	-1.218822	0.185250
60	H	-5.977845	-2.066523	-0.080725
61	H	-4.989265	-1.394541	1.211843
62	C	-6.143879	0.081558	0.128650
63	H	-6.480634	0.255188	-0.902838
64	H	-5.490469	0.927159	0.384664
65	C	-7.357899	0.074968	1.065656
66	H	-8.008239	-0.771737	0.808141
67	H	-7.018564	-0.103202	2.094891
68	O	-2.419531	-2.695433	0.121347
69	O	-0.787259	0.884525	0.016261
70	O	-1.692078	-1.008566	-2.912460
71	O	0.472916	0.349417	-1.794382
72	O	4.770249	-1.267957	0.345082
73	O	3.139279	-3.308804	0.619765
74	O	2.277867	-1.029437	-0.254009
75	O	3.048265	-1.181875	2.136921
76	C	-8.165508	1.375282	1.011387
77	H	-8.546764	1.562553	0.001095
78	H	-9.023947	1.340193	1.689991
79	H	-7.549747	2.235729	1.297114
80	C	-0.542014	7.621703	-0.481299
81	H	-0.880423	7.803130	-1.507836
82	H	-1.031565	8.357198	0.165340
83	H	0.536225	7.815851	-0.449800

E[B3LYP/6-31G(d,p)] = -2441.236699 h, E[APFD/6-311+G(2d,p)] = -2766.599787 h
Gcorr[B3LYP/6-31G(d,p)] = 0.180181 h

204. PC6Ca+4H_2O, 2nd step, reactants (hydrolysed carbon chain neglected)

Center No.	Atom	X	Y	Z
1	P	3.421330	-0.854190	-1.450844
2	C	3.406813	1.526015	-0.253797
3	H	3.644081	0.860476	0.580762
4	H	4.188164	2.288929	-0.317828
5	C	2.014646	2.152492	-0.125231
6	H	1.831652	2.804067	-0.981846
7	H	1.264581	1.362196	-0.110534
8	C	1.590614	-2.283838	-0.164808

9	H	2.468081	-2.626694	0.393610
10	H	1.315455	-3.058054	-0.893677
11	C	0.443669	-2.048046	0.805623
12	H	0.692155	-1.232058	1.485146
13	C	-1.231632	-0.402341	0.189411
14	C	0.083247	-3.286940	1.609100
15	H	-0.347613	-4.053591	0.952170
16	H	1.000328	-3.692350	2.054623
17	C	-2.373268	-0.140533	-0.764120
18	H	-1.920024	0.228261	-1.695230
19	H	-2.854912	-1.090875	-1.003074
20	C	2.765072	4.126441	1.212643
21	H	3.761174	3.720052	1.375531
22	H	2.737036	4.697761	0.285318
23	H	2.486498	4.762326	2.052020
24	C	1.838093	2.150500	2.362649
25	H	1.601951	2.780053	3.219875
26	H	1.106269	1.349616	2.265721
27	H	2.842294	1.746070	2.471323
28	C	0.380665	3.578166	1.011506
29	H	-0.326703	2.753143	0.933794
30	H	0.183657	4.168707	1.905785
31	H	0.333890	4.211901	0.126697
32	N	1.771493	2.999502	1.117716
33	C	-3.391317	0.868605	-0.224640
34	H	-3.824991	0.456298	0.693557
35	H	-2.874475	1.794416	0.052231
36	C	-4.502373	1.176200	-1.234504
37	H	-4.057686	1.571956	-2.158791
38	H	-5.009672	0.242587	-1.516106
39	C	-5.539543	2.173891	-0.704530
40	H	-5.032307	3.106908	-0.423964
41	H	-5.981217	1.777903	0.219850
42	O	-0.781229	0.408347	0.979797
43	O	-0.841765	-2.901700	2.628926
44	O	-0.728955	-1.650163	0.035591
45	O	3.467642	-1.282622	-2.888061
46	O	4.409518	-1.349966	-0.429334
47	O	1.880783	-1.058348	-0.833735
48	O	3.402889	0.806093	-1.484295
49	C	-6.651388	2.479610	-1.712526
50	H	-7.198696	1.570167	-1.985743
51	H	-7.374785	3.193700	-1.305569
52	H	-6.242624	2.908483	-2.634643
53	H	-1.052310	-3.688542	3.150676
54	O	-2.688174	-3.721237	-0.647093
55	H	-1.926147	-3.128283	-0.745893
56	H	-3.111212	-3.731925	-1.516164
57	O	-3.493250	-2.196358	1.647394
58	H	-3.442288	-2.746113	0.844258
59	H	-2.619462	-2.344844	2.050590

E[B3LYP/6-31G(d,p)] = -1627.247979 h, E[APFD/6-311+G(2d,p)] = -1626.606610 h
Gcorr[B3LYP/6-31G(d,p)] = 0.439767 h

205. PC6Ca+4H_2O, 2nd step, TS

Center No.	Atom	X	Y	Z
1	P	3.440459	-0.085280	-1.649874
2	C	2.835731	1.977064	-0.072001
3	H	3.235067	1.254521	0.645114
4	H	3.413356	2.902149	0.018207
5	C	1.337488	2.229228	0.128952
6	H	0.980456	2.894728	-0.659337
7	H	0.786459	1.289083	0.082312
8	C	2.008118	-2.058905	-0.549258
9	H	2.969702	-2.215477	-0.050170
10	H	1.865952	-2.854271	-1.293497
11	C	0.879095	-2.087038	0.475875
12	H	0.976804	-1.202380	1.115650
13	C	-1.485902	-0.959013	0.576529

14	C	0.947128	-3.322332	1.374520
15	H	0.713284	-4.230426	0.804379
16	H	1.962493	-3.423824	1.778212
17	C	-2.385285	-0.563985	-0.589138
18	H	-1.763137	0.020292	-1.274751
19	H	-2.715090	-1.452066	-1.137707
20	C	1.632579	4.209534	1.632303
21	H	2.701523	4.053690	1.762119
22	H	1.444698	4.826915	0.754045
23	H	1.222942	4.689612	2.520221
24	C	1.267752	1.972344	2.608578
25	H	0.948226	2.463576	3.527419
26	H	0.722791	1.039918	2.463613
27	H	2.341589	1.798334	2.642127
28	C	-0.548509	3.102139	1.424290
29	H	-1.024011	2.129777	1.291981
30	H	-0.844986	3.552503	2.371581
31	H	-0.787874	3.774432	0.600823
32	N	0.945761	2.883183	1.449697
33	C	-3.602450	0.256269	-0.141341
34	H	-4.199256	-0.336616	0.562873
35	H	-3.256888	1.138493	0.411132
36	C	-4.483288	0.699450	-1.315470
37	H	-3.880182	1.287558	-2.021878
38	H	-4.824298	-0.185921	-1.870844
39	C	-5.701835	1.523971	-0.882527
40	H	-5.360473	2.407854	-0.326773
41	H	-6.303656	0.935187	-0.177008
42	O	-0.925934	-0.116622	1.295430
43	O	0.011665	-3.148152	2.452943
44	O	-0.375940	-1.979878	-0.195177
45	O	3.633860	-0.210324	-3.133720
46	O	4.509428	-0.480201	-0.664776
47	O	2.001679	-0.785665	-1.199604
48	O	2.993863	1.500004	-1.405341
49	C	-6.579368	1.966787	-2.057200
50	H	-6.963296	1.102990	-2.612008
51	H	-7.439590	2.552007	-1.715885
52	H	-6.013492	2.586656	-2.762111
53	H	-0.076774	-3.990884	2.918093
54	O	-1.889880	-3.851490	-0.138187
55	H	-1.089713	-3.140638	-0.374176
56	H	-2.486195	-3.973500	-0.892138
57	O	-2.251075	-2.037761	1.379642
58	H	-2.286457	-3.078018	0.627386
59	H	-1.586029	-2.311689	2.056883

E[B3LYP/6-31G(d,p)] = -1627.189945 h, E[APFD/6-311+G(2d,p)] = -1626.548914 h
Gcorr[B3LYP/6-31G(d,p)] = 0.441760 h

206. PC6Ca+4H_2O, 2nd step, products

Center No.	Atom	X	Y	Z
1	P	-4.318444	-0.875676	0.041680
2	C	-2.445817	-2.771978	0.041620
3	H	-2.451700	-2.481552	1.096045
4	H	-2.559273	-3.858086	-0.019750
5	C	-1.181571	-2.298798	-0.685951
6	H	-1.253336	-2.569097	-1.740970
7	H	-1.102949	-1.214316	-0.605002
8	C	-3.034449	1.375877	0.594323
9	H	-2.943964	1.032215	1.630357
10	H	-3.934688	2.001044	0.515959
11	C	-1.820482	2.201549	0.198895
12	H	-0.959257	1.524711	0.102472
13	C	2.266613	1.596662	0.136550
14	C	-1.488199	3.228710	1.286315
15	H	-2.317714	3.939828	1.394915
16	H	-1.332002	2.729613	2.246663
17	C	3.613331	1.251563	-0.461768
18	H	3.424788	0.835089	-1.459894

19	H	4.195377	2.166826	-0.595453
20	C	0.142210	-4.380769	-0.305993
21	H	-0.600620	-4.804770	0.366257
22	H	-0.084613	-4.650044	-1.337091
23	H	1.132130	-4.743866	-0.032968
24	C	0.393776	-2.478958	1.245693
25	H	1.357020	-2.890299	1.545943
26	H	0.421243	-1.391328	1.299773
27	H	-0.391121	-2.882206	1.882186
28	C	1.242543	-2.314218	-1.042677
29	H	1.276417	-1.235506	-0.891829
30	H	2.183892	-2.764958	-0.729476
31	H	1.039900	-2.559246	-2.084565
32	N	0.135211	-2.879261	-0.185722
33	C	4.385205	0.226154	0.385404
34	H	4.571970	0.648607	1.381302
35	H	3.755455	-0.657884	0.535778
36	C	5.716178	-0.183217	-0.254354
37	H	5.525496	-0.605106	-1.251347
38	H	6.334663	0.711020	-0.414479
39	C	6.502053	-1.198193	0.584749
40	H	5.882705	-2.091081	0.744695
41	H	6.689345	-0.775038	1.580845
42	O	1.439060	0.764952	0.486139
43	O	-0.274482	3.943697	1.012494
44	O	-2.106351	2.839499	-1.043712
45	O	-5.519020	-0.626399	-0.824696
46	O	-4.426687	-1.052832	1.533270
47	O	-3.133461	0.247057	-0.280702
48	O	-3.554462	-2.190857	-0.637426
49	C	7.832326	-1.606291	-0.055323
50	H	8.486247	-0.738080	-0.196063
51	H	8.369301	-2.330106	0.566360
52	H	7.674552	-2.063854	-1.038668
53	H	-0.350250	4.380864	0.140473
54	O	0.227721	4.328399	-1.666729
55	H	-1.277371	3.193019	-1.412721
56	H	0.275477	5.084048	-2.267308
57	O	2.065613	2.914534	0.249118
58	H	1.135853	4.005997	-1.561966
59	H	1.171472	3.110542	0.657423

E[B3LYP/6-31G(d,p)] = -1627.254809 h, E[APFD/6-311+G(2d,p)] = -2440.65196 h
Gcorr[B3LYP/6-31G(d,p)] = -1626.604208 h

XVIII. Structures of molecules and transition states (TS) related to the hydrolysis at the glycerol backbone of 2PC6Ca, as optimized through Gaussian16, at B3LYP/6-31G(d,p) level.

207. 2PC6Ca+4H_2O, 1st step, reactants

Center No.	Atom	X	Y	Z
1	P	1.944415	-0.937104	1.445798
2	C	1.863855	-1.692639	-1.089750
3	H	1.189903	-2.410965	-0.621732
4	H	1.286172	-1.053360	-1.760418
5	C	3.005215	-2.400063	-1.819169
6	H	3.628452	-1.670001	-2.338776
7	H	3.622402	-2.931428	-1.093038
8	C	4.467829	-0.807745	2.291703
9	H	4.419026	-1.866955	2.023334
10	H	4.783971	-0.728790	3.335484
11	C	5.452661	-0.078462	1.385627
12	H	5.068922	-0.048020	0.364630
13	C	5.242529	2.299333	1.050986
14	C	6.825966	-0.727817	1.419503
15	H	7.274029	-0.657132	2.414795
16	H	6.759148	-1.784290	1.143480
17	C	8.933561	-0.448395	0.371576
18	C	5.460023	3.625886	1.745153
19	H	4.896814	3.603244	2.686431
20	H	6.516837	3.674301	2.037190

21	C	1.691334	-2.800894	-3.908406
22	H	0.731120	-2.542811	-3.460816
23	H	2.196617	-1.922687	-4.309793
24	H	1.541433	-3.536259	-4.698462
25	C	1.832541	-4.570063	-2.202495
26	H	1.685104	-5.345246	-2.953779
27	H	2.429230	-4.953201	-1.375002
28	H	0.868469	-4.215702	-1.843500
29	C	3.823330	-3.961205	-3.507548
30	H	4.455325	-4.409861	-2.741993
31	H	3.536131	-4.710260	-4.243966
32	H	4.345270	-3.137886	-3.993567
33	N	2.574281	-3.426225	-2.853872
34	C	5.067387	4.834348	0.894353
35	H	5.636640	4.816064	-0.042774
36	H	4.011151	4.748691	0.611824
37	C	5.302920	6.165316	1.617268
38	H	4.732867	6.176740	2.557113
39	H	6.361619	6.243891	1.902628
40	C	4.914325	7.386854	0.775481
41	H	3.856528	7.306933	0.490586
42	H	5.484085	7.373897	-0.163504
43	C	9.696786	0.369827	-0.645977
44	H	9.158947	0.298273	-1.599792
45	H	9.623307	1.422875	-0.346292
46	C	11.156587	-0.058947	-0.801612
47	H	11.658452	0.010981	0.170990
48	H	11.193311	-1.116761	-1.088804
49	C	11.911100	0.784830	-1.835134
50	H	11.867484	1.843962	-1.544048
51	H	11.401211	0.715023	-2.806497
52	C	13.376967	0.366512	-2.002354
53	H	13.884898	0.435652	-1.030919
54	H	13.419229	-0.691859	-2.293128
55	O	9.379434	-1.366242	1.031532
56	O	4.824327	2.152827	-0.079657
57	O	7.650500	-0.028715	0.467897
58	O	5.586026	1.276495	1.872539
59	O	0.712810	-0.088689	1.641309
60	O	1.865255	-2.408806	1.847697
61	O	3.168944	-0.196286	2.204678
62	O	2.495791	-0.864113	-0.100684
63	C	14.130576	1.210664	-3.034427
64	H	14.134823	2.269742	-2.752263
65	H	15.172354	0.887880	-3.130952
66	H	13.665196	1.134450	-4.023826
67	C	5.149996	8.716553	1.498029
68	H	6.205757	8.839952	1.765314
69	H	4.863550	9.567970	0.872034
70	H	4.566272	8.772639	2.423997
71	O	-3.551294	5.562882	-0.844613
72	H	-4.118789	6.136806	-0.312341
73	H	-3.744862	4.662950	-0.533037
74	Ca	-0.027588	-3.824456	2.231260
75	O	1.975220	-5.088111	1.455007
76	H	2.431640	-5.746102	1.996462
77	H	2.521013	-4.280991	1.489094
78	O	-4.529941	5.081776	-3.444141
79	H	-3.880468	4.454185	-3.785681
80	H	-4.159155	5.354579	-2.580100
81	O	-1.283403	-1.712776	2.483875
82	H	-1.869264	-1.679512	1.705139
83	H	-0.601529	-1.018737	2.285586
84	P	-1.743075	-3.049658	-0.951223
85	C	-4.224317	-3.563675	-1.799249
86	H	-3.977652	-2.696353	-2.416445
87	H	-4.473196	-4.396242	-2.460993
88	C	-5.341656	-3.270748	-0.792695
89	H	-5.496289	-4.152531	-0.168689
90	H	-5.053031	-2.433182	-0.157441
91	C	-2.004094	-0.373167	-0.719182
92	H	-1.769562	-0.434949	-1.784104

93	H	-1.130956	-0.001190	-0.172806
94	C	-3.210647	0.522244	-0.497726
95	H	-4.087649	0.070968	-0.956438
96	C	-4.627198	0.238978	1.430986
97	C	-3.014940	1.926149	-1.054777
98	H	-2.217434	2.452937	-0.529624
99	H	-2.791369	1.879578	-2.122379
100	C	-5.251976	2.511081	-1.687055
101	C	-4.644330	0.383802	2.934124
102	H	-3.790675	-0.187552	3.320839
103	H	-4.421316	1.433708	3.162692
104	C	-7.234958	-4.033113	-2.235800
105	H	-6.604723	-4.151875	-3.114744
106	H	-7.244735	-4.951157	-1.649045
107	H	-8.247105	-3.774248	-2.544023
108	C	-6.624745	-1.643437	-2.188522
109	H	-7.628156	-1.403848	-2.538273
110	H	-6.249012	-0.848398	-1.546540
111	H	-5.967186	-1.795468	-3.042093
112	C	-7.645391	-2.688101	-0.222816
113	H	-7.248744	-1.880304	0.391125
114	H	-8.621383	-2.420026	-0.625594
115	H	-7.718352	-3.609704	0.353409
116	N	-6.699777	-2.915012	-1.379505
117	C	-5.955384	-0.057013	3.585820
118	H	-6.784753	0.513689	3.151255
119	H	-6.145221	-1.109331	3.342017
120	C	-5.941999	0.126387	5.107773
121	H	-5.105422	-0.443015	5.536995
122	H	-5.746331	1.181413	5.346168
123	C	-7.249236	-0.309979	5.780219
124	H	-7.443371	-1.364484	5.541950
125	H	-8.084091	0.258422	5.348553
126	C	-6.442480	3.354265	-1.304139
127	H	-6.847352	2.922744	-0.378117
128	H	-6.082863	4.354222	-1.044761
129	C	-7.512266	3.416588	-2.395149
130	H	-7.062840	3.860035	-3.290541
131	H	-7.815099	2.397735	-2.663397
132	C	-8.740216	4.228812	-1.969303
133	H	-8.428546	5.246762	-1.695461
134	H	-9.174356	3.788449	-1.060291
135	C	-9.817507	4.306140	-3.058007
136	H	-9.381463	4.744093	-3.965987
137	H	-10.128548	3.288478	-3.330367
138	O	-5.200183	1.702375	-2.589628
139	O	-5.548659	-0.173728	0.746010
140	O	-4.199329	2.728470	-0.839892
141	O	-3.434268	0.625445	0.929897
142	O	-0.860437	-3.772491	0.049022
143	O	-1.212156	-2.705321	-2.309944
144	O	-2.340766	-1.685901	-0.218713
145	O	-3.099034	-3.969022	-1.008779
146	C	-11.044365	5.120005	-2.635999
147	H	-10.769168	6.152216	-2.390898
148	H	-11.793936	5.155882	-3.433301
149	H	-11.521393	4.686171	-1.749674
150	C	-7.235673	-0.123341	7.300306
151	H	-7.077578	0.927522	7.568469
152	H	-8.181092	-0.443063	7.750514
153	H	-6.431885	-0.706922	7.763557

E[B3LYP/6-31G(d,p)] = -4551.884210 h, E[APFD/6-311+G(2d,p)] = -4550.160776 h
Gcorr[B3LYP/6-31G(d,p)] = 1.175136 h

208. 2PC6Ca+4H_2O, 1st step, TS

Center No.	Atom	X	Y	Z
1	P	1.987142	-0.537703	1.623638
2	C	1.918858	-1.698401	-0.756192
3	H	1.249616	-2.347077	-0.189634

4	H	1.327945	-1.138133	-1.483498
5	C	3.039157	-2.497939	-1.419482
6	H	3.672472	-1.834081	-2.010585
7	H	3.651364	-2.966887	-0.647385
8	C	4.493132	-0.331789	2.512919
9	H	4.406126	-1.421722	2.482520
10	H	4.803065	-0.036651	3.519174
11	C	5.512679	0.146456	1.485398
12	H	5.140026	-0.034742	0.476111
13	C	5.433960	2.394804	0.620196
14	C	6.861378	-0.525595	1.681729
15	H	7.305984	-0.250737	2.642592
16	H	6.759383	-1.614170	1.645478
17	C	8.976932	-0.572318	0.611295
18	C	5.673216	3.835700	1.014693
19	H	5.036370	4.050074	1.882260
20	H	6.704369	3.911075	1.382178
21	C	1.756203	-3.068082	-3.488217
22	H	0.802820	-2.713724	-3.096359
23	H	2.315417	-2.267950	-3.972847
24	H	1.583668	-3.880090	-4.194248
25	C	1.773927	-4.641693	-1.594296
26	H	1.622999	-5.496695	-2.252404
27	H	2.324288	-4.942435	-0.702946
28	H	0.812552	-4.209365	-1.324835
29	C	3.821159	-4.269642	-2.903530
30	H	4.411088	-4.663328	-2.076837
31	H	3.516644	-5.078912	-3.565455
32	H	4.394713	-3.527137	-3.457064
33	N	2.583816	-3.611867	-2.346886
34	C	5.415980	4.829979	-0.118438
35	H	6.058155	4.578769	-0.971245
36	H	4.383457	4.716313	-0.470025
37	C	5.662020	6.282792	0.303742
38	H	5.018770	6.528521	1.160639
39	H	6.696670	6.390092	0.659305
40	C	5.408091	7.290169	-0.824374
41	H	4.374240	7.181389	-1.179076
42	H	6.050839	7.042987	-1.680111
43	C	9.769798	-0.028704	-0.556367
44	H	9.226366	-0.287874	-1.473884
45	H	9.739065	1.066505	-0.497137
46	C	11.210696	-0.538895	-0.606521
47	H	11.721733	-0.268575	0.325458
48	H	11.204115	-1.634912	-0.644245
49	C	11.989713	0.016419	-1.804118
50	H	11.987600	1.114938	-1.763784
51	H	11.471131	-0.254771	-2.734708
52	C	13.437781	-0.484259	-1.868129
53	H	13.954896	-0.212580	-0.937958
54	H	13.438624	-1.581959	-1.907302
55	O	9.383676	-1.347444	1.454197
56	O	5.065674	2.013688	-0.472340
57	O	7.715437	-0.082391	0.609938
58	O	5.688865	1.570490	1.666490
59	O	0.786179	0.374156	1.611912
60	O	1.835053	-1.904967	2.290018
61	O	3.218110	0.289548	2.275670
62	O	2.589081	-0.771422	0.112906
63	C	14.214684	0.070615	-3.065740
64	H	14.259343	1.165321	-3.035598
65	H	15.243359	-0.303990	-3.083263
66	H	13.740243	-0.214538	-4.011733
67	C	5.653861	8.742051	-0.403280
68	H	6.689431	8.889238	-0.075829
69	H	5.464407	9.435347	-1.229293
70	H	5.000558	9.028816	0.428733
71	O	-4.068128	5.056918	-2.127095
72	H	-4.575886	5.734921	-1.655296
73	H	-4.057937	4.132997	-1.561533
74	Ca	-0.146984	-3.181481	2.800457
75	O	1.818998	-4.606706	2.150735

76	H	2.245592	-5.210613	2.773639
77	H	2.380648	-3.809358	2.118887
78	O	-5.356353	3.558615	-3.471386
79	H	-4.863135	3.182150	-4.218973
80	H	-4.712832	4.524800	-2.907736
81	O	-1.291155	-1.010866	2.639524
82	H	-1.857348	-1.089263	1.848938
83	H	-0.576807	-0.385123	2.348228
84	P	-1.720560	-2.866016	-0.528332
85	C	-4.107848	-3.531177	-1.517648
86	H	-3.753175	-2.843103	-2.288913
87	H	-4.341414	-4.487056	-1.992507
88	C	-5.298685	-2.968760	-0.735073
89	H	-5.541292	-3.651097	0.081858
90	H	-5.043391	-1.997062	-0.310608
91	C	-2.036002	-0.190457	-0.747345
92	H	-1.828369	-0.423884	-1.793653
93	H	-1.152055	0.275425	-0.298811
94	C	-3.246794	0.717274	-0.638131
95	H	-4.140437	0.190087	-0.965267
96	C	-4.549741	0.736251	1.390958
97	C	-3.111270	1.996489	-1.456912
98	H	-2.276984	2.603293	-1.089099
99	H	-2.917064	1.718784	-2.498923
100	C	-5.468731	2.329520	-2.458881
101	C	-4.514745	1.196925	2.830814
102	H	-3.629365	0.738268	3.290049
103	H	-4.318495	2.276357	2.827515
104	C	-7.133685	-4.095925	-1.999413
105	H	-6.446590	-4.544151	-2.714018
106	H	-7.262547	-4.749686	-1.137588
107	H	-8.094424	-3.915048	-2.479523
108	C	-6.367534	-1.868176	-2.716198
109	H	-7.330876	-1.721974	-3.204007
110	H	-5.969482	-0.906231	-2.390430
111	H	-5.680345	-2.346262	-3.411953
112	C	-7.590879	-2.130435	-0.605031
113	H	-7.173393	-1.196582	-0.231276
114	H	-8.505602	-1.949740	-1.168121
115	H	-7.789520	-2.811469	0.221823
116	N	-6.582964	-2.774180	-1.528255
117	C	-5.783726	0.867139	3.617311
118	H	-6.647478	1.320638	3.116206
119	H	-5.951569	-0.216432	3.595194
120	C	-5.715497	1.351361	5.070131
121	H	-4.845259	0.897960	5.565744
122	H	-5.542579	2.436820	5.085159
123	C	-6.980475	1.030098	5.875149
124	H	-7.151484	-0.054825	5.861183
125	H	-7.849205	1.481556	5.377210
126	C	-6.740103	2.598163	-1.666234
127	H	-6.714055	1.923561	-0.804154
128	H	-6.724391	3.621417	-1.276018
129	C	-8.006991	2.359560	-2.496577
130	H	-8.002233	3.032118	-3.363018
131	H	-7.981651	1.338096	-2.895793
132	C	-9.294810	2.566606	-1.690957
133	H	-9.313840	3.589723	-1.288997
134	H	-9.291369	1.897779	-0.818312
135	C	-10.568736	2.322370	-2.509295
136	H	-10.571087	2.990671	-3.381059
137	H	-10.549233	1.299940	-2.910561
138	O	-5.215308	1.259058	-3.021612
139	O	-5.469612	0.129067	0.869063
140	O	-4.295775	2.779567	-1.358828
141	O	-3.408141	1.075367	0.758748
142	O	-0.913387	-3.446453	0.617071
143	O	-1.108146	-2.724500	-1.889937
144	O	-2.329048	-1.410127	-0.026589
145	O	-3.082552	-3.781546	-0.547619
146	C	-11.854169	2.530073	-1.702758
147	H	-11.918365	3.554153	-1.317424

148	H	-12.744269	2.348348	-2.314048
149	H	-11.896179	1.851030	-0.843360
150	C	-6.911803	1.518360	7.325200
151	H	-6.775803	2.604961	7.370634
152	H	-7.827898	1.274507	7.873007
153	H	-6.072185	1.058005	7.858504

E[B3LYP/6-31G(d,p)] = -4551.828873 h, E[APFD/6-311+G(2d,p)] = -4550.104557 h
Gcorr[B3LYP/6-31G(d,p)] = 1.176680 h

209. 2PC6Ca+4H_2O, 1st step, products

Center No.	Atom	X	Y	Z
1	P	2.031324	-0.779984	1.561213
2	C	1.937476	-1.768514	-0.896596
3	H	1.207610	-2.391944	-0.379088
4	H	1.417287	-1.164077	-1.642436
5	C	3.047958	-2.612443	-1.521628
6	H	3.721446	-1.977321	-2.099773
7	H	3.621104	-3.096748	-0.729497
8	C	4.581432	-0.715549	2.332301
9	H	4.494809	-1.777082	2.082723
10	H	4.928795	-0.629499	3.365562
11	C	5.559607	-0.029638	1.385637
12	H	5.148652	-0.013586	0.375047
13	C	5.357964	2.343066	1.015406
14	C	6.919817	-0.705972	1.395335
15	H	7.400407	-0.618674	2.374067
16	H	6.824288	-1.767510	1.149100
17	C	8.989019	-0.510200	0.253270
18	C	5.619887	3.680365	1.672542
19	H	5.100573	3.681225	2.639040
20	H	6.689457	3.724131	1.914478
21	C	1.753940	-3.157593	-3.590485
22	H	0.801471	-2.799480	-3.197841
23	H	2.318688	-2.357130	-4.068187
24	H	1.576998	-3.962409	-4.303695
25	C	1.757165	-4.740630	-1.704764
26	H	1.567586	-5.575959	-2.378040
27	H	2.318658	-5.075957	-0.833051
28	H	0.814891	-4.292113	-1.397291
29	C	3.805145	-4.388097	-3.015369
30	H	4.397621	-4.781610	-2.190356
31	H	3.489184	-5.198805	-3.670115
32	H	4.381003	-3.653892	-3.577498
33	N	2.577407	-3.716719	-2.453732
34	C	5.198476	4.875842	0.817180
35	H	5.722901	4.833636	-0.145010
36	H	4.129452	4.794820	0.586114
37	C	5.479347	6.218233	1.501734
38	H	4.954982	6.252959	2.467270
39	H	6.551091	6.292514	1.734769
40	C	5.061069	7.426967	0.655715
41	H	3.990115	7.351609	0.423636
42	H	5.584729	7.390538	-0.309144
43	C	9.732338	0.272233	-0.806347
44	H	9.146897	0.214894	-1.732638
45	H	9.711952	1.329154	-0.511827
46	C	11.166402	-0.210493	-1.028648
47	H	11.717449	-0.152017	-0.082268
48	H	11.151167	-1.270904	-1.308144
49	C	11.898646	0.598424	-2.105263
50	H	11.906808	1.660473	-1.821734
51	H	11.339222	0.540066	-3.049762
52	C	13.338810	0.127195	-2.340924
53	H	13.896635	0.185500	-1.396533
54	H	13.329551	-0.934098	-2.623844
55	O	9.433346	-1.435524	0.903755
56	O	4.882019	2.179555	-0.089828
57	O	7.726206	-0.046653	0.400537
58	O	5.735286	1.332628	1.837411

59	O	0.865341	0.171084	1.664530
60	O	1.839064	-2.199202	2.092884
61	O	3.301348	-0.063443	2.267331
62	O	2.600135	-0.885400	0.023111
63	C	14.069037	0.936645	-3.416717
64	H	14.123907	1.997030	-3.144943
65	H	15.092948	0.576888	-3.561573
66	H	13.552775	0.869338	-4.381216
67	C	5.342684	8.768026	1.339802
68	H	6.411149	8.886610	1.553402
69	H	5.033485	9.609935	0.711773
70	H	4.804959	8.847377	2.291572
71	O	-3.609536	5.155360	-2.672806
72	H	-4.148819	5.903082	-2.380702
73	H	-3.605529	3.869450	-1.434183
74	Ca	-0.150134	-3.467168	2.563998
75	O	1.817549	-4.892680	1.921908
76	H	2.231308	-5.512249	2.537951
77	H	2.384327	-4.098565	1.912970
78	O	-5.142639	3.136591	-4.088102
79	H	-4.568106	2.644107	-4.701463
80	H	-4.164157	4.688079	-3.321520
81	O	-1.245477	-1.262308	2.543971
82	H	-1.823895	-1.264535	1.759522
83	H	-0.521520	-0.626305	2.303345
84	P	-1.740706	-2.886806	-0.732442
85	C	-4.246645	-3.396485	-1.501745
86	H	-3.999609	-2.561654	-2.161884
87	H	-4.520651	-4.255648	-2.118403
88	C	-5.337901	-3.030285	-0.492060
89	H	-5.476114	-3.861662	0.201281
90	H	-5.031305	-2.145194	0.065688
91	C	-1.893037	-0.195141	-0.736959
92	H	-1.676347	-0.335537	-1.798151
93	H	-0.983410	0.132503	-0.221842
94	C	-3.008083	0.821177	-0.559918
95	H	-3.920476	0.476909	-1.047180
96	C	-4.474010	0.623727	1.351985
97	C	-2.637396	2.199013	-1.093033
98	H	-1.738880	2.564086	-0.570784
99	H	-2.382410	2.093437	-2.157927
100	C	-5.675418	2.233810	-3.217652
101	C	-4.520861	0.849158	2.846825
102	H	-3.663885	0.318518	3.280349
103	H	-4.324230	1.915096	3.020013
104	C	-7.297919	-3.913439	-1.768683
105	H	-6.695799	-4.161020	-2.640491
106	H	-7.319088	-4.751936	-1.073283
107	H	-8.309882	-3.662221	-2.084040
108	C	-6.628290	-1.551781	-2.027277
109	H	-7.639474	-1.304949	-2.349088
110	H	-6.176513	-0.707522	-1.511796
111	H	-6.030104	-1.832955	-2.891392
112	C	-7.605153	-2.328670	0.081280
113	H	-7.174499	-1.455581	0.570228
114	H	-8.593588	-2.098357	-0.314411
115	H	-7.665669	-3.167402	0.774202
116	N	-6.708436	-2.716156	-1.071064
117	C	-5.834472	0.419726	3.500528
118	H	-6.666388	0.952236	3.024423
119	H	-6.002848	-0.647130	3.308586
120	C	-5.849572	0.680105	5.011237
121	H	-5.009369	0.149701	5.481569
122	H	-5.677521	1.749462	5.198751
123	C	-7.158733	0.252651	5.685672
124	H	-7.329549	-0.815987	5.497610
125	H	-7.997273	0.782553	5.213985
126	C	-6.661803	2.861304	-2.268874
127	H	-6.648166	2.275072	-1.347435
128	H	-6.339473	3.878867	-2.033278
129	C	-8.080903	2.880560	-2.876347
130	H	-8.065195	3.446886	-3.815762

131	H	-8.375461	1.854790	-3.131059
132	C	-9.112648	3.492282	-1.921991
133	H	-8.807508	4.516410	-1.665940
134	H	-9.114369	2.927848	-0.979169
135	C	-10.531426	3.514939	-2.503787
136	H	-10.525887	4.076836	-3.447400
137	H	-10.832819	2.490520	-2.760625
138	O	-5.397675	1.053118	-3.288831
139	O	-5.396847	0.198488	0.674400
140	O	-3.741557	3.059394	-0.895337
141	O	-3.263711	0.950631	0.864640
142	O	-0.882890	-3.523267	0.346768
143	O	-1.183223	-2.700371	-2.111433
144	O	-2.327439	-1.447642	-0.158975
145	O	-3.115147	-3.779815	-0.709841
146	C	-11.561566	4.127208	-1.549901
147	H	-11.304721	5.163467	-1.302304
148	H	-12.563065	4.129020	-1.992215
149	H	-11.613291	3.565895	-0.610008
150	C	-7.172432	0.514666	7.194619
151	H	-7.037990	1.580384	7.412307
152	H	-8.118613	0.199491	7.646486
153	H	-6.365212	-0.029566	7.698111

E[B3LYP/6-31G(d,p)] = -4551.887034 h, E[APFD/6-311+G(2d,p)] = -4550.104557 h
Gcorr[B3LYP/6-31G(d,p)] = 1.176818 h

210. 2PC6Ca+4H_2O, 2nd step, reactants (hydrolysed carbon chain neglected)

Center No.	Atom	X	Y	Z
1	P	-1.434264	-0.304080	-1.252132
2	C	-1.586483	-0.070081	1.411676
3	H	-1.483975	-1.073137	1.839716
4	H	-0.581769	0.352513	1.308054
5	C	-2.467456	0.733280	2.355979
6	H	-3.512009	0.489798	2.155037
7	H	-2.235883	0.484824	3.393184
8	C	-3.609115	-1.453875	-2.297193
9	H	-3.110680	-2.370268	-1.966002
10	H	-3.913488	-1.580570	-3.339700
11	C	-4.830902	-1.178920	-1.423028
12	H	-4.521519	-0.959879	-0.401274
13	C	-5.729336	1.045386	-1.154667
14	C	-5.802540	-2.347019	-1.448072
15	H	-6.214015	-2.500527	-2.449773
16	H	-5.305228	-3.268884	-1.132204
17	C	-7.866828	-2.940392	-0.441079
18	C	-6.442130	2.141925	-1.915344
19	H	-5.818643	2.399765	-2.780785
20	H	-7.358824	1.708154	-2.334178
21	C	-2.462112	2.736741	0.832404
22	H	-1.621645	2.361636	0.251069
23	H	-3.398663	2.367188	0.417489
24	H	-2.453215	3.826560	0.852240
25	C	-1.044582	2.718203	2.850078
26	H	-0.994947	3.802340	2.750985
27	H	-1.028000	2.443363	3.904817
28	H	-0.210003	2.249440	2.327376
29	C	-3.489751	2.845043	3.050021
30	H	-3.451994	2.459055	4.068232
31	H	-3.381566	3.928850	3.056937
32	H	-4.427353	2.563368	2.571791
33	N	-2.351854	2.253363	2.258236
34	C	-6.752980	3.378842	-1.071809
35	H	-7.357193	3.083390	-0.205614
36	H	-5.818255	3.786691	-0.668583
37	C	-7.486895	4.462789	-1.869593
38	H	-6.879645	4.749932	-2.739758
39	H	-8.421395	4.048757	-2.274105
40	C	-7.804950	5.712982	-1.040516
41	H	-6.870497	6.125500	-0.636633

42	H	-8.411279	5.424838	-0.171152
43	C	-8.927766	-2.481253	0.534286
44	H	-8.434739	-2.293380	1.496425
45	H	-9.287705	-1.502231	0.193421
46	C	-10.084493	-3.469442	0.690340
47	H	-10.540331	-3.649074	-0.290779
48	H	-9.690737	-4.436498	1.025884
49	C	-11.150846	-2.974633	1.673991
50	H	-11.538067	-2.003485	1.334342
51	H	-10.687371	-2.791449	2.653807
52	C	-12.319305	-3.953380	1.842519
53	H	-12.780441	-4.136841	0.862645
54	H	-11.931669	-4.923127	2.182778
55	O	-7.876716	-3.977188	-1.074809
56	O	-5.395027	1.099537	0.014712
57	O	-6.868273	-2.031555	-0.531887
58	O	-5.509713	-0.018216	-1.960262
59	O	-0.668150	0.968698	-1.540530
60	O	-0.672227	-1.619930	-1.270917
61	O	-2.694667	-0.346670	-2.278051
62	O	-2.263364	-0.168117	0.149457
63	C	-13.384862	-3.455886	2.823758
64	H	-13.815202	-2.504220	2.491434
65	H	-14.204412	-4.175178	2.922522
66	H	-12.960193	-3.295686	3.821399
67	C	-8.538083	6.794849	-1.839166
68	H	-9.492766	6.421629	-2.227178
69	H	-8.750671	7.673159	-1.220963
70	H	-7.940812	7.127260	-2.695944
71	O	6.763769	1.664231	-3.888510
72	H	6.201106	1.770784	-4.668800
73	H	6.792039	3.146156	-2.695611
74	Ca	1.652843	-2.015515	-1.484764
75	O	1.676775	0.221879	-2.474001
76	H	1.737111	0.358156	-3.428252
77	H	0.807592	0.626369	-2.184539
78	H	6.231522	1.163425	-3.246492
79	O	3.955292	-2.780570	-1.960244
80	H	4.243740	-2.991789	-2.858813
81	H	4.385382	-3.434287	-1.391890
82	P	2.546907	0.068445	1.408795
83	C	4.002299	0.238416	3.635075
84	H	3.873661	1.299188	3.405668
85	H	3.660646	0.060792	4.657263
86	C	5.443617	-0.233628	3.417315
87	H	5.527000	-1.281735	3.710003
88	H	5.694842	-0.132615	2.361872
89	C	3.810268	1.783428	-0.183635
90	H	3.307237	2.635484	0.285413
91	H	3.231404	1.466076	-1.058362
92	C	5.214908	2.188702	-0.599889
93	H	5.813183	2.459667	0.270616
94	C	6.749375	0.310840	-0.516102
95	C	5.210431	3.345768	-1.602003
96	H	4.603891	3.075456	-2.478204
97	H	4.722961	4.200126	-1.119519
98	C	7.191477	-0.911269	-1.283373
99	H	6.284529	-1.443620	-1.597636
100	H	7.684112	-0.575072	-2.206204
101	C	6.279677	0.458952	5.668732
102	H	5.370251	1.006779	5.908262
103	H	6.183788	-0.584085	5.969019
104	H	7.127491	0.918317	6.175282
105	C	6.605806	1.950534	3.728043
106	H	7.434705	2.427976	4.249358
107	H	6.778389	1.953519	2.652655
108	H	5.677433	2.463109	3.971488
109	C	7.841538	-0.155752	3.873644
110	H	7.995849	-0.120403	2.795782
111	H	8.633835	0.381992	4.393272
112	H	7.798136	-1.187081	4.221442
113	N	6.523801	0.514775	4.184184

114	C	8.127946	-1.830038	-0.495971
115	H	9.003537	-1.257507	-0.167629
116	H	7.624930	-2.174639	0.415937
117	C	8.581497	-3.036275	-1.326671
118	H	7.699522	-3.603891	-1.656859
119	H	9.074541	-2.678725	-2.241437
120	C	9.530047	-3.972482	-0.568601
121	H	9.035134	-4.324432	0.346705
122	H	10.410516	-3.404381	-0.239282
123	O	7.134548	0.628236	0.594300
124	O	6.515016	3.743458	-1.975814
125	O	5.851931	1.037507	-1.233201
126	O	2.101645	-1.146875	0.615625
127	O	1.566100	1.166308	1.706841
128	O	3.914441	0.698154	0.752776
129	O	3.203587	-0.576170	2.769962
130	C	9.980736	-5.176365	-1.401222
131	H	10.509012	-4.855672	-2.306375
132	H	10.656277	-5.824723	-0.833714
133	H	9.123773	-5.782716	-1.716378
134	O	8.946387	-0.136561	-4.215303
135	H	8.243492	0.541562	-4.202616
136	H	8.523981	-0.888485	-4.650694

E[B3LYP/6-31G(d,p)] = -4241.953048 h, E[APFD/6-311+G(2d,p)] = -4240.399083 h
Gcorr[B3LYP/6-31G(d,p)] = 1.035925 h

211. 2PC6Ca+4H_2O, 2nd step, TS

Center No.	Atom	X	Y	Z
1	P	-1.203640	-0.546685	-1.140385
2	C	-1.305141	-0.009893	1.486357
3	H	-1.273799	-0.974429	2.003202
4	H	-0.272198	0.321597	1.347609
5	C	-2.115074	0.943249	2.351044
6	H	-3.176715	0.764218	2.173279
7	H	-1.895336	0.776271	3.406677
8	C	-3.466238	-1.716008	-1.957581
9	H	-3.018308	-2.597957	-1.488919
10	H	-3.799637	-1.988456	-2.962622
11	C	-4.650260	-1.226887	-1.125116
12	H	-4.310173	-0.890880	-0.145899
13	C	-5.360440	1.078753	-1.171861
14	C	-5.708143	-2.308242	-0.982551
15	H	-6.143944	-2.567556	-1.951501
16	H	-5.277698	-3.212729	-0.542265
17	C	-7.812462	-2.581576	0.077010
18	C	-5.986077	2.114917	-2.079620
19	H	-5.346708	2.201117	-2.967434
20	H	-6.936497	1.703972	-2.442323
21	C	-1.955951	2.785797	0.644128
22	H	-1.150522	2.291921	0.103893
23	H	-2.919887	2.452872	0.261878
24	H	-1.860129	3.868223	0.560395
25	C	-0.538731	2.845057	2.664275
26	H	-0.391696	3.902339	2.445347
27	H	-0.550809	2.688842	3.743121
28	H	0.254540	2.249174	2.211554
29	C	-2.964791	3.187405	2.835640
30	H	-2.958594	2.895931	3.885425
31	H	-2.768237	4.254851	2.742557
32	H	-3.922514	2.940282	2.378949
33	N	-1.879823	2.433115	2.110001
34	C	-6.191102	3.476295	-1.414123
35	H	-6.813875	3.351621	-0.520033
36	H	-5.224410	3.857113	-1.063238
37	C	-6.836729	4.498820	-2.356263
38	H	-6.211937	4.614362	-3.253302
39	H	-7.804211	4.112492	-2.707062
40	C	-7.046199	5.871765	-1.706039
41	H	-6.078943	6.256086	-1.354999

42	H	-7.670694	5.755183	-0.810004
43	C	-8.822381	-1.912147	0.982286
44	H	-8.316199	-1.678794	1.927624
45	H	-9.073800	-0.941322	0.537020
46	C	-10.078368	-2.751278	1.221600
47	H	-10.546608	-2.982193	0.257133
48	H	-9.790883	-3.714553	1.659886
49	C	-11.090273	-2.047872	2.133047
50	H	-11.369092	-1.080804	1.690917
51	H	-10.614850	-1.815975	3.096699
52	C	-12.358038	-2.874378	2.380625
53	H	-12.831156	-3.106580	1.416935
54	H	-12.078648	-3.840142	2.822985
55	O	-7.921241	-3.682203	-0.426411
56	O	-5.005203	1.269051	-0.023188
57	O	-6.734115	-1.787075	-0.116198
58	O	-5.246134	-0.103907	-1.817738
59	O	-0.387112	0.630499	-1.630593
60	O	-0.490390	-1.880255	-0.977061
61	O	-2.486739	-0.679981	-2.128324
62	O	-1.994241	-0.166354	0.238048
63	C	-13.369034	-2.168959	3.289480
64	H	-13.692806	-1.215713	2.856117
65	H	-14.261695	-2.783099	3.446937
66	H	-12.934868	-1.954114	4.272662
67	C	-7.690097	6.892857	-2.648647
68	H	-8.674205	6.551266	-2.989385
69	H	-7.826155	7.861267	-2.156226
70	H	-7.070878	7.055580	-3.538242
71	O	6.686559	1.955482	-3.554610
72	H	6.691092	1.401992	-4.351104
73	H	6.345156	4.569713	-1.414433
74	Ca	1.876042	-2.171086	-1.035941
75	O	1.713223	-0.468694	-2.802179
76	H	1.506552	-0.732989	-3.708240
77	H	0.925325	0.057560	-2.481871
78	H	6.049078	1.509846	-2.780449
79	O	2.472078	-3.810507	-2.753941
80	H	3.205134	-3.698290	-3.373962
81	H	2.371508	-4.765001	-2.638090
82	P	2.712236	-0.288384	1.459425
83	C	4.725807	0.308502	3.132858
84	H	4.610512	1.284087	2.654945
85	H	4.369192	0.389728	4.163734
86	C	6.158320	-0.217501	3.039874
87	H	6.222664	-1.188159	3.535025
88	H	6.428402	-0.319034	1.987728
89	C	3.551106	1.224878	-0.641667
90	H	2.918328	1.929609	-0.096467
91	H	3.172302	1.114919	-1.660048
92	C	4.990744	1.732802	-0.669115
93	H	5.448054	1.632535	0.319830
94	C	7.178572	0.342006	-0.988925
95	C	4.997984	3.211251	-1.067889
96	H	4.579775	3.324007	-2.079379
97	H	4.340222	3.760183	-0.377715
98	C	7.290281	-1.016537	-1.686074
99	H	7.079486	-0.905550	-2.755015
100	H	8.340842	-1.326525	-1.600281
101	C	7.065014	0.761351	5.153687
102	H	6.129369	1.272285	5.373047
103	H	7.055758	-0.241573	5.579204
104	H	7.898990	1.332941	5.559437
105	C	7.252392	2.031523	3.044550
106	H	8.108469	2.573482	3.445520
107	H	7.338759	1.912554	1.964087
108	H	6.336159	2.555360	3.310760
109	C	8.561885	-0.008596	3.360615
110	H	8.669599	-0.058146	2.277489
111	H	9.357781	0.589149	3.803210
112	H	8.558854	-1.008384	3.793823
113	N	7.238706	0.654001	3.663175

114	C	6.398577	-2.100430	-1.073655
115	H	6.605561	-2.161718	0.001574
116	H	5.348682	-1.800627	-1.172743
117	C	6.620068	-3.475663	-1.715786
118	H	6.436600	-3.410553	-2.798092
119	H	7.676114	-3.760713	-1.604246
120	C	5.735969	-4.579355	-1.122189
121	H	4.681258	-4.319769	-1.282678
122	H	5.883534	-4.615605	-0.034138
123	O	7.295023	0.451280	0.242802
124	O	6.331203	3.695245	-1.003990
125	O	5.773936	0.939254	-1.569370
126	O	1.955937	-1.590128	1.265384
127	O	2.043242	0.977503	1.905900
128	O	3.427859	-0.078982	-0.026522
129	O	3.951037	-0.690160	2.456013
130	C	6.012830	-5.961727	-1.721685
131	H	7.051135	-6.267339	-1.549228
132	H	5.363689	-6.726148	-1.282010
133	H	5.843973	-5.964098	-2.804784
134	O	8.150736	1.313710	-1.773963
135	H	7.556242	1.724495	-2.912899
136	H	8.989260	0.841151	-1.888102

E[B3LYP/6-31G(d,p)] = -2441.236699 h, E[APFD/6-311+G(2d,p)] = -4240.337716 h
Gcorr[B3LYP/6-31G(d,p)] = 0.180181 h

212. 2PC6Ca+4H_2O, 2nd step, products

Center No.	Atom	X	Y	Z
1	P	-1.240017	-0.314234	-1.744137
2	C	-1.456935	-0.058427	0.923182
3	H	-1.498762	-1.145192	1.043325
4	H	-0.420803	0.255447	1.080759
5	C	-2.413697	0.543727	1.937466
6	H	-3.435478	0.448509	1.567967
7	H	-2.320774	0.023078	2.892272
8	C	-3.493778	-1.634881	-2.356382
9	H	-2.968359	-2.501455	-1.942383
10	H	-3.931444	-1.919627	-3.317160
11	C	-4.595408	-1.197082	-1.390114
12	H	-4.173109	-0.912840	-0.427332
13	C	-5.435018	1.058025	-1.197647
14	C	-5.624753	-2.301397	-1.210186
15	H	-6.153258	-2.502380	-2.146349
16	H	-5.144057	-3.226479	-0.877703
17	C	-7.610757	-2.675969	0.031345
18	C	-6.129730	2.141414	-1.992509
19	H	-5.499614	2.363088	-2.863320
20	H	-7.051810	1.709567	-2.400921
21	C	-2.160052	2.865471	1.005065
22	H	-1.273448	2.600683	0.434838
23	H	-3.054814	2.664537	0.418847
24	H	-2.118357	3.911962	1.305572
25	C	-0.953338	2.228838	3.058376
26	H	-0.853820	3.292971	3.272251
27	H	-1.046347	1.672238	3.990935
28	H	-0.090702	1.873812	2.493302
29	C	-3.399311	2.470094	3.075804
30	H	-3.467829	1.843555	3.964343
31	H	-3.254453	3.511012	3.362177
32	H	-4.296863	2.365808	2.467115
33	N	-2.214274	2.025507	2.256810
34	C	-6.422458	3.408228	-1.187668
35	H	-7.033325	3.148958	-0.314523
36	H	-5.482306	3.813255	-0.794538
37	C	-7.136747	4.479783	-2.019319
38	H	-6.522977	4.730832	-2.896021
39	H	-8.077289	4.069658	-2.413596
40	C	-7.435077	5.759001	-1.227950
41	H	-6.494560	6.166694	-0.833347

42	H	-8.048586	5.506920	-0.352436
43	C	-8.523407	-2.086928	1.083763
44	H	-7.925954	-1.940625	1.992815
45	H	-8.805062	-1.079520	0.753099
46	C	-9.759660	-2.940640	1.369930
47	H	-10.325514	-3.079295	0.440674
48	H	-9.442232	-3.941381	1.686659
49	C	-10.665575	-2.320658	2.439768
50	H	-10.974614	-1.315757	2.118673
51	H	-10.092402	-2.180680	3.367322
52	C	-11.912863	-3.161354	2.738288
53	H	-12.484145	-3.301280	1.810660
54	H	-11.603304	-4.165091	3.059414
55	O	-7.764051	-3.739034	-0.536800
56	O	-5.081310	1.153741	-0.036474
57	O	-6.562399	-1.855274	-0.212711
58	O	-5.256855	-0.043826	-1.960313
59	O	-0.458429	0.757146	-2.468187
60	O	-0.539390	-1.620101	-1.398267
61	O	-2.570775	-0.577778	-2.645769
62	O	-1.915783	0.304796	-0.388716
63	C	-12.817019	-2.538918	3.806386
64	H	-13.169720	-1.548140	3.497732
65	H	-13.697604	-3.161085	3.996851
66	H	-12.282797	-2.418206	4.755779
67	C	-8.147012	6.829934	-2.059806
68	H	-9.107083	6.462438	-2.439876
69	H	-8.345730	7.729285	-1.467786
70	H	-7.541695	7.126977	-2.923880
71	O	7.725474	1.883177	-2.721196
72	H	8.415734	1.631083	-2.088455
73	H	6.150682	4.670505	-1.869658
74	Ca	1.814997	-1.992316	-1.462664
75	O	1.722379	-0.430470	-3.361622
76	H	1.590135	-0.811803	-4.239471
77	H	0.900358	0.101548	-3.162808
78	H	6.113470	1.173621	-2.310162
79	O	3.256755	-3.155324	-3.084483
80	H	4.075363	-2.758427	-3.411639
81	H	3.410735	-4.109563	-3.089367
82	P	2.566778	-0.196993	1.084904
83	C	4.516624	0.714267	2.660337
84	H	4.622152	1.607110	2.037599
85	H	3.848437	0.949428	3.492566
86	C	5.875358	0.189072	3.120412
87	H	5.734832	-0.664371	3.785917
88	H	6.447575	-0.123101	2.246473
89	C	3.181528	1.509121	-0.952619
90	H	2.721524	2.196377	-0.238386
91	H	2.637730	1.555597	-1.899175
92	C	4.647178	1.864962	-1.186724
93	H	5.198592	1.766554	-0.237181
94	C	8.534777	-0.339809	-0.281400
95	C	4.736058	3.331550	-1.621502
96	H	4.356819	3.425125	-2.647365
97	H	4.117952	3.955174	-0.962588
98	C	8.416645	-1.793813	-0.680759
99	H	8.625465	-1.884462	-1.753665
100	H	9.225620	-2.333463	-0.168249
101	C	6.087813	1.654648	5.135510
102	H	5.186588	2.212275	4.887920
103	H	5.840181	0.786643	5.745500
104	H	6.784438	2.300796	5.668370
105	C	7.085762	2.372460	2.995568
106	H	7.807248	2.990048	3.528999
107	H	7.508703	2.004219	2.061199
108	H	6.183096	2.950511	2.808453
109	C	8.035010	0.473526	4.214690
110	H	8.508085	0.148922	3.288951
111	H	8.682611	1.167204	4.748871
112	H	7.801958	-0.384348	4.844206
113	N	6.749551	1.184826	3.866506

114	C	7.055813	-2.408984	-0.342499
115	H	6.866633	-2.296130	0.730625
116	H	6.272219	-1.839797	-0.858286
117	C	6.971828	-3.889779	-0.729073
118	H	7.194235	-4.003745	-1.799320
119	H	7.751324	-4.449738	-0.193601
120	C	5.602811	-4.512021	-0.429534
121	H	4.832497	-3.963961	-0.987996
122	H	5.367503	-4.375265	0.634634
123	O	7.820792	0.227353	0.521211
124	O	6.103369	3.762714	-1.539669
125	O	5.163238	0.971985	-2.158429
126	O	2.025458	-1.601650	0.897516
127	O	1.761462	0.923224	1.673005
128	O	3.032178	0.157370	-0.468052
129	O	3.982280	-0.374080	1.897276
130	C	5.526761	-6.000378	-0.783562
131	H	6.264705	-6.580324	-0.217781
132	H	4.537494	-6.413499	-0.560714
133	H	5.724715	-6.164230	-1.849102
134	O	9.528955	0.372706	-0.870246
135	H	7.336028	2.705099	-2.356390
136	H	10.044231	-0.183371	-1.476994

E[B3LYP/6-31G(d,p)] = -4241.946650 h, E[APFD/6-311+G(2d,p)] = -4240.395370 h
Gcorr[B3LYP/6-31G(d,p)] = 1.037485 h