Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Mechanisms and Stereoselectivities of DABCO-Catalyzed Rauhut-Currier Reaction of α,β-unsaturated ketones and aryl acrylates: A Computational Investigation

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Fig S1. Free energy profiles for the formation of P(*R*RS). The solvation-corrected relative free energies at SMD(CH_3CN)/M06-2X/6-311++G(d,p) level are given in kcal/mol. Red line: in the absence; bule lind: in the presence of PhOH.

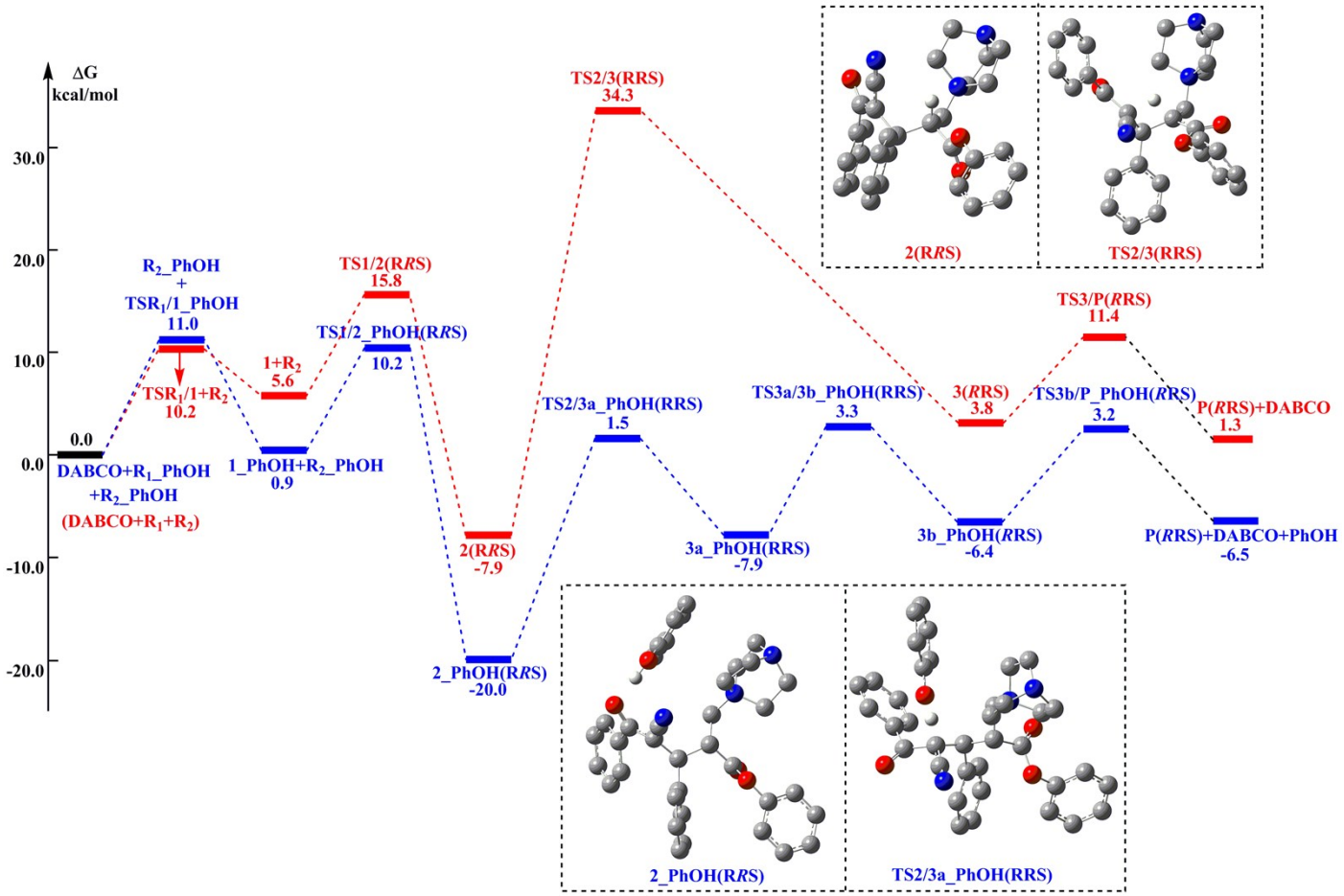


Fig S2. Free energy profiles for the formation of P(RSR). The solvation-corrected relative free energies at SMD(CH_3CN)/M06-2X/6-311++G(d,p) level are given in kcal/mol. Red line: in the absence; bule lind: in the presence of PhOH.

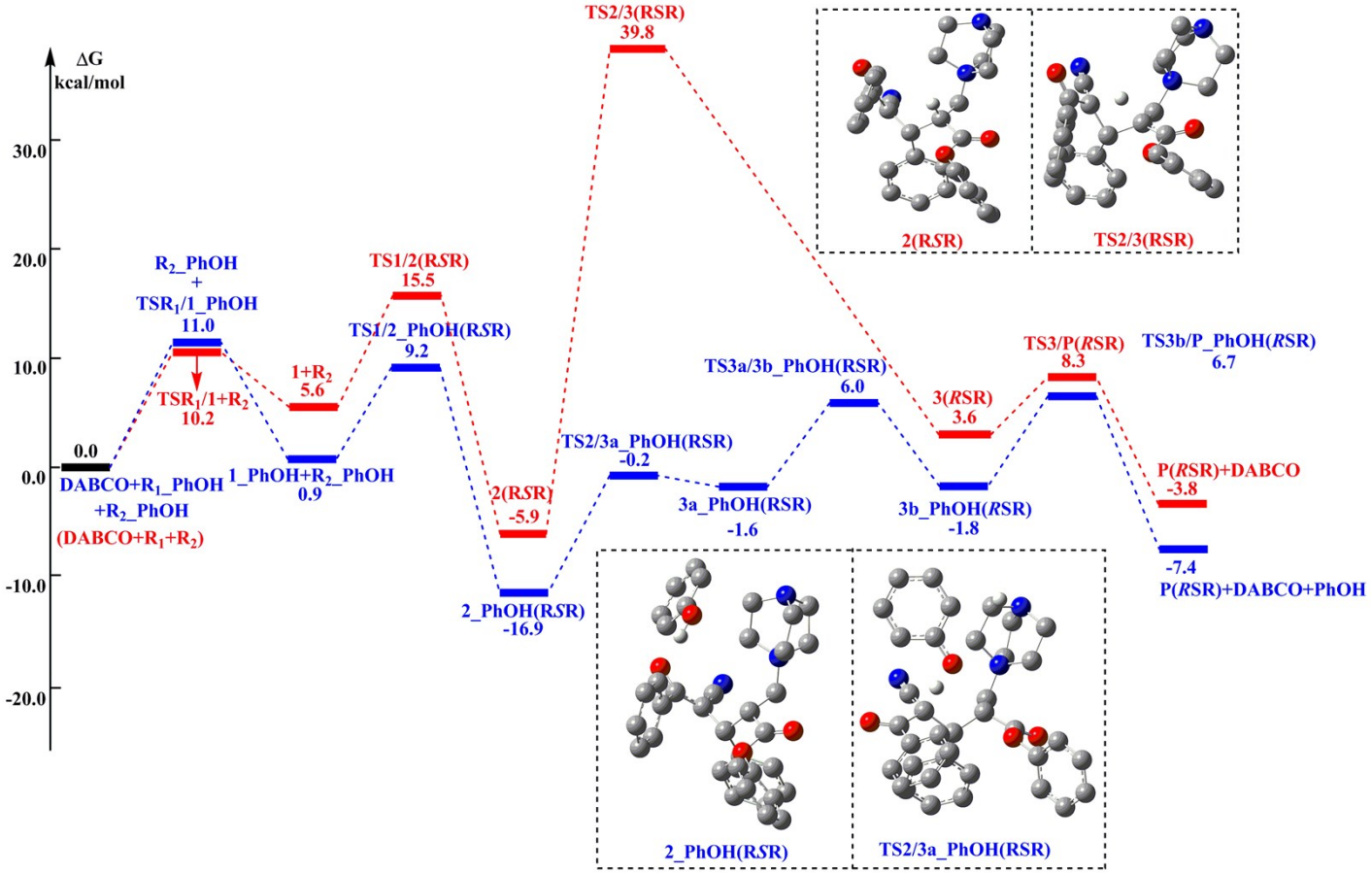


Fig S3. Free energy profiles for the formation of P(SRS). The solvation-corrected relative free energies at SMD(CH_3CN)/M06-2X/6-311++G(d,p) level are given in kcal/mol. Red line: in the absence; bule lind: in the presence of PhOH.

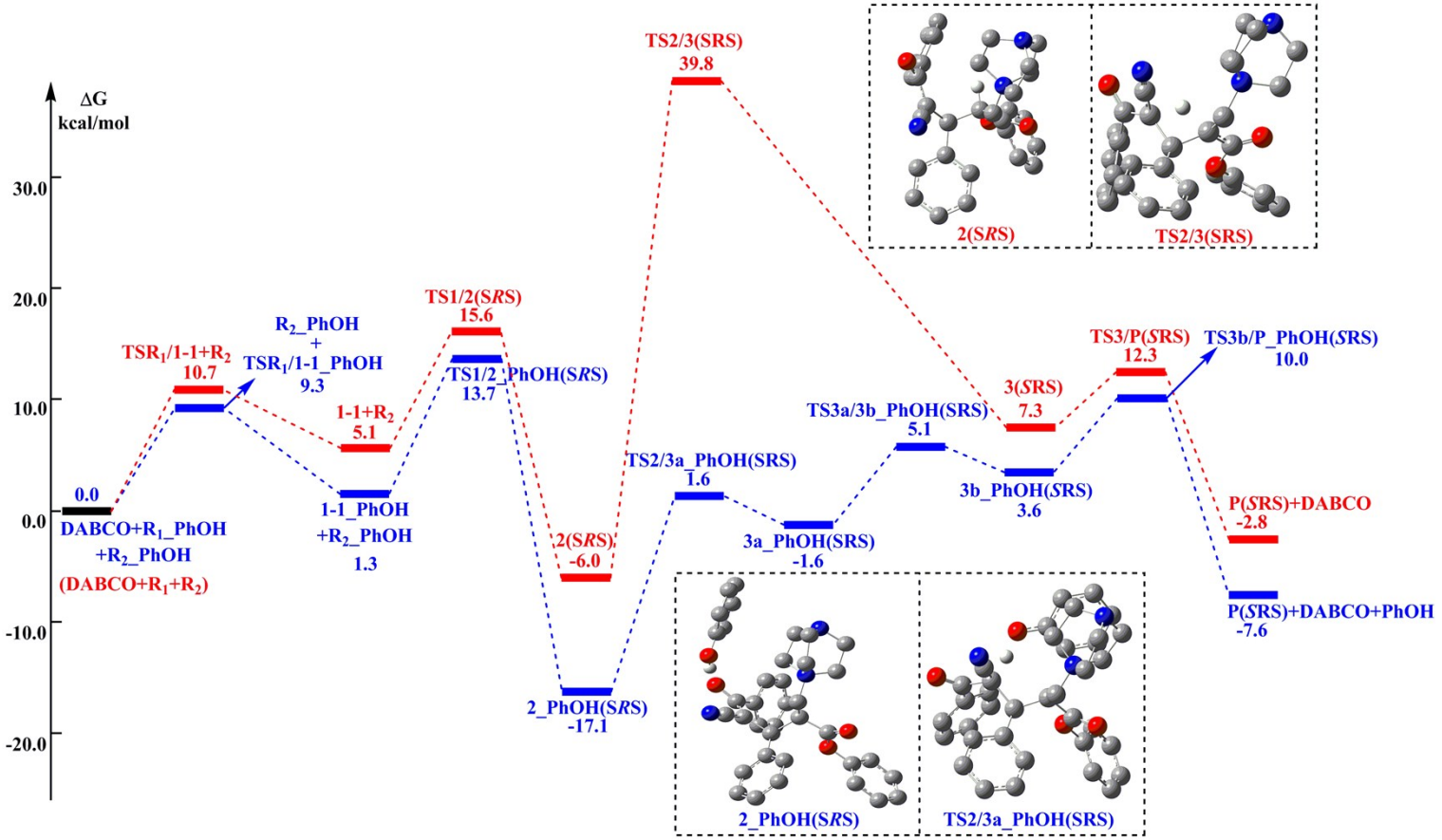
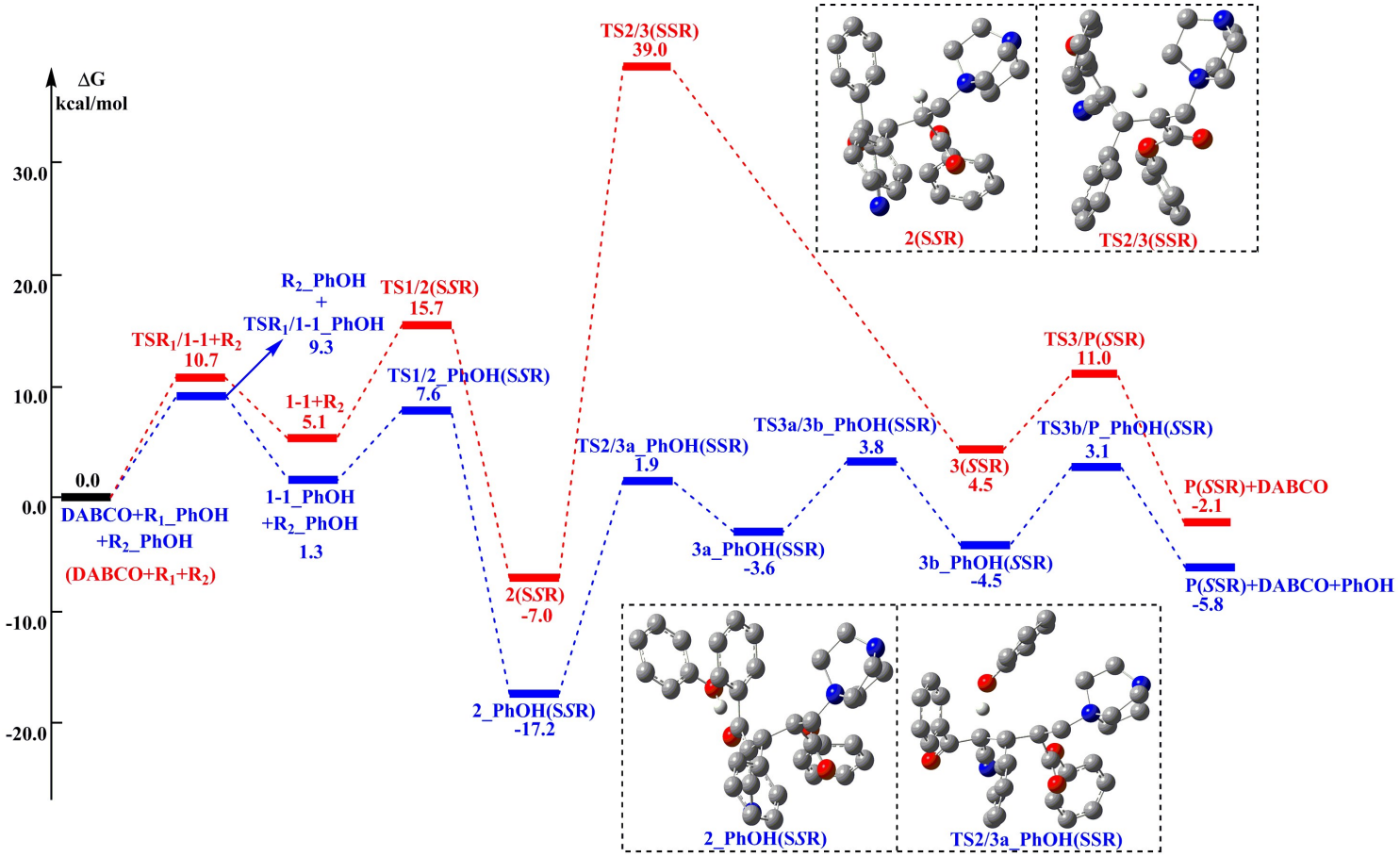


Fig S4. Free energy profiles for the formation of P(SSR). The solvation-corrected relative free energies at SMD(CH_3CN)/M06-2X/6-311++G(d,p) level are given in kcal/mol. Red line: in the absence; bule lind: in the presence of PhOH.



Cartesian coordinates for optimized structures

(Energies are given in Hartree, imaginary frequencies are given in i)

Part 1 In the absence of PhOH

R_1

SCF Done: E(RM062X) = -498.006170182

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.012664	-0.411718	-0.376650
2	6	0	-4.119506	0.099516	0.156984
3	1	0	-3.029019	-1.165406	-1.157434
4	1	0	-5.104296	-0.218857	-0.169872
5	1	0	-4.062757	0.853597	0.937892
6	6	0	-1.686064	0.048476	0.096791
7	8	0	-1.485169	0.875266	0.951460
8	8	0	-0.697072	-0.605210	-0.567385
9	6	0	0.624600	-0.279181	-0.280396
10	6	0	1.453255	-1.299987	0.166539
11	6	0	1.105455	1.005600	-0.510138
12	6	0	2.801466	-1.025608	0.390125
13	1	0	1.039918	-2.290713	0.327513
14	6	0	2.452864	1.267503	-0.277907

15	1	0	0.434408	1.780863	-0.865215
16	6	0	3.302087	0.256043	0.171515
17	1	0	3.458266	-1.817828	0.736293
18	1	0	2.840406	2.266778	-0.451629
19	1	0	4.352043	0.467261	0.348672

R_2

SCF Done: E(RM062X) = -745.985911527

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.054573	1.116080	-0.008099
2	6	0	-0.660744	-0.082678	-0.175366
3	1	0	-0.008952	-0.911660	-0.443342
4	6	0	-0.776603	2.340181	0.201718
5	7	0	-1.330313	3.343762	0.365546
6	6	0	-2.079040	-0.428716	-0.109417
7	6	0	-3.043067	0.328176	0.576804
8	6	0	-2.476184	-1.607616	-0.761674
9	6	0	-4.372097	-0.077214	0.582185
10	1	0	-2.756871	1.215433	1.130111
11	6	0	-3.808718	-2.001055	-0.766283
12	1	0	-1.728033	-2.206508	-1.274494
13	6	0	-4.759625	-1.233988	-0.095078

14	1	0	-5.109011	0.509086	1.122237
15	1	0	-4.103331	-2.907455	-1.285767
16	1	0	-5.800964	-1.541715	-0.089760
17	6	0	1.416539	1.322552	-0.217355
18	8	0	1.816482	2.418978	-0.566287
19	6	0	2.366046	0.188172	-0.014193
20	6	0	2.178627	-0.784673	0.974054
21	6	0	3.520298	0.164019	-0.805525
22	6	0	3.137555	-1.777770	1.159448
23	1	0	1.301746	-0.753270	1.613807
24	6	0	4.464676	-0.840037	-0.630708
25	1	0	3.660715	0.933552	-1.558301
26	6	0	4.273732	-1.811337	0.353330
27	1	0	2.996953	-2.524032	1.934973
28	1	0	5.351742	-0.864496	-1.255877
29	1	0	5.015421	-2.591673	0.494844

DABCO

SCF Done: E(RM062X) = -345.186667534

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.777913	-0.719727	-1.175483
2	6	0	-0.777698	-0.719924	-1.175504

3	1	0	1.175202	-0.231125	-2.071672
4	1	0	1.174286	-1.740424	-1.145068
5	1	0	-1.175086	-0.231598	-2.071800
6	1	0	-1.173805	-1.740718	-1.144902
7	6	0	0.777821	1.378412	-0.035090
8	1	0	1.175068	1.908820	0.837002
9	1	0	1.174948	1.863643	-0.933298
10	6	0	-0.777947	1.378335	-0.035329
11	1	0	-1.175514	1.908868	0.836542
12	1	0	-1.174849	1.863359	-0.933748
13	6	0	-0.778046	-0.658521	1.210772
14	1	0	-1.175390	-0.124174	2.080394
15	1	0	-1.174742	-1.679356	1.234340
16	6	0	0.777956	-0.658580	1.210797
17	1	0	1.175314	-0.124442	2.080542
18	1	0	1.174574	-1.679451	1.234166
19	7	0	1.286187	0.000534	-0.000169
20	7	0	-1.286188	0.000413	-0.000329

TSR_1/1

SCF Done: E(RM062X) = -843.190884153

Imaginary Frequencies = -166.7130

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.016151	-1.511592	0.960742
2	6	0	-1.101740	-1.981317	0.323087
3	1	0	0.108013	-1.505901	2.040443
4	1	0	-1.832892	-2.573857	0.867602
5	1	0	-1.065060	-2.141375	-0.752457
6	6	0	1.093351	-0.961481	0.178433
7	8	0	1.152574	-0.836148	-1.030801
8	8	0	2.138075	-0.564231	0.997340
9	6	0	3.294963	-0.077698	0.424696
10	6	0	3.773875	1.140769	0.896588
11	6	0	4.008516	-0.807761	-0.524542
12	6	0	4.982912	1.636705	0.412534
13	1	0	3.198346	1.682596	1.640771
14	6	0	5.211377	-0.298720	-1.006568
15	1	0	3.621264	-1.756693	-0.878195
16	6	0	5.702935	0.921584	-0.542025
17	1	0	5.359078	2.585320	0.783823
18	1	0	5.769159	-0.862893	-1.748331
19	1	0	6.643368	1.309837	-0.920655
20	6	0	-4.734589	0.129032	-0.895384
21	6	0	-3.673876	-1.004430	-0.771186
22	1	0	-5.666902	-0.153918	-0.396605
23	1	0	-4.959742	0.337120	-1.945741
24	1	0	-4.080746	-1.890507	-0.272724

25	1	0	-3.282983	-1.305737	-1.748550
26	6	0	-4.011461	1.117871	1.155653
27	1	0	-3.609140	2.034614	1.597670
28	1	0	-4.973771	0.904870	1.631192
29	6	0	-3.027738	-0.071460	1.344318
30	1	0	-2.152325	0.205991	1.941767
31	1	0	-3.514659	-0.928270	1.821322
32	6	0	-1.906836	0.617091	-0.662920
33	1	0	-1.075657	0.956380	-0.035244
34	1	0	-1.491344	0.241313	-1.602572
35	6	0	-2.964185	1.733939	-0.895083
36	1	0	-2.631868	2.683909	-0.465252
37	1	0	-3.137759	1.887697	-1.964696
38	7	0	-4.243018	1.365198	-0.273266
39	7	0	-2.547197	-0.508436	0.028132

TSR_1/1-1

SCF Done: E(RM062X) = -843.190944930

Imaginary Frequencies = -175.7559

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013375	-1.872301	0.298006
2	6	0	1.125670	-2.044399	-0.445872

3	1	0	-0.110758	-2.258198	1.305916
4	1	0	1.870157	-2.777226	-0.143747
5	1	0	1.099866	-1.804182	-1.506845
6	6	0	-1.094530	-1.091494	-0.243177
7	8	0	-1.160323	-0.550052	-1.331829
8	8	0	-2.152284	-1.031894	0.651644
9	6	0	-3.240162	-0.244758	0.334913
10	6	0	-4.494558	-0.845198	0.331763
11	6	0	-3.100073	1.123049	0.106458
12	6	0	-5.626258	-0.066275	0.096363
13	1	0	-4.571236	-1.912095	0.517176
14	6	0	-4.235890	1.890280	-0.134520
15	1	0	-2.111689	1.571048	0.118660
16	6	0	-5.500571	1.300663	-0.140937
17	1	0	-6.606901	-0.533011	0.096629
18	1	0	-4.131369	2.956169	-0.315061
19	1	0	-6.382625	1.905060	-0.329235
20	6	0	3.594590	-0.574545	-1.128295
21	6	0	4.612165	0.558534	-0.799552
22	1	0	4.054915	-1.566472	-1.072297
23	1	0	3.155618	-0.450361	-2.123288
24	1	0	5.575122	0.139790	-0.490991
25	1	0	4.781778	1.193523	-1.674398
26	6	0	3.047571	-0.650153	1.208057
27	1	0	2.201655	-0.707068	1.902004
28	1	0	3.600314	-1.593867	1.257719

29	6	0	3.965740	0.570399	1.499829
30	1	0	3.545705	1.196680	2.293100
31	1	0	4.959857	0.240533	1.816587
32	6	0	2.786382	1.917784	-0.072618
33	1	0	2.448410	2.593539	0.719076
34	1	0	2.893434	2.499414	-0.993620
35	6	0	1.781215	0.748873	-0.274123
36	1	0	0.987478	0.750286	0.481532
37	1	0	1.310386	0.772353	-1.261310
38	7	0	2.502157	-0.524204	-0.148816
39	7	0	4.109734	1.398048	0.295401

1

SCF Done: E(RM062X) = -843.201122008

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.105439	-0.872790	1.232817
2	6	0	-1.322398	-1.483899	0.697484
3	1	0	-0.002305	-0.672188	2.291362
4	1	0	-1.866620	-2.095734	1.424243
5	1	0	-1.123771	-2.072688	-0.204164
6	6	0	0.954341	-0.631129	0.368839
7	8	0	1.031964	-0.795446	-0.855215

8	8	0	2.076629	-0.099194	1.068308
9	6	0	3.267733	0.055175	0.422928
10	6	0	3.985463	1.221613	0.695865
11	6	0	3.821333	-0.923336	-0.409679
12	6	0	5.248669	1.412779	0.140918
13	1	0	3.540679	1.965879	1.349822
14	6	0	5.080506	-0.716830	-0.967017
15	1	0	3.261390	-1.825966	-0.620002
16	6	0	5.801124	0.447097	-0.698330
17	1	0	5.798929	2.322438	0.364499
18	1	0	5.503935	-1.478343	-1.616308
19	1	0	6.783108	0.596648	-1.136786
20	6	0	-4.717236	-0.274959	-0.699954
21	6	0	-3.558762	-1.257175	-0.404384
22	1	0	-5.529371	-0.412494	0.019092
23	1	0	-5.111364	-0.456020	-1.703219
24	1	0	-3.843148	-2.037805	0.304750
25	1	0	-3.163059	-1.722730	-1.310301
26	6	0	-3.909410	1.398141	0.789096
27	1	0	-3.436253	2.383090	0.827865
28	1	0	-4.824506	1.432798	1.385800
29	6	0	-2.958238	0.316006	1.351246
30	1	0	-2.093945	0.738798	1.867277
31	1	0	-3.468133	-0.386942	2.015478
32	6	0	-1.872782	0.446816	-0.825216
33	1	0	-1.144496	1.072441	-0.306837

34	1	0	-1.344013	-0.161846	-1.560134
35	6	0	-3.044960	1.257573	-1.424468
36	1	0	-2.775451	2.315692	-1.477833
37	1	0	-3.275286	0.910980	-2.435932
38	7	0	-4.254435	1.112782	-0.607126
39	7	0	-2.427670	-0.488406	0.206514

1-1

SCF Done: E(RM062X) = -843.201244461

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.113084	-1.648254	0.289464
2	6	0	1.383269	-1.710501	-0.435420
3	1	0	-0.007483	-2.141850	1.245114
4	1	0	1.981896	-2.599673	-0.212083
5	1	0	1.241231	-1.625515	-1.517798
6	6	0	-0.966340	-1.016414	-0.311164
7	8	0	-1.035432	-0.408778	-1.387271
8	8	0	-2.151841	-1.168310	0.467641
9	6	0	-3.211658	-0.342418	0.241256
10	6	0	-4.486015	-0.904122	0.342355
11	6	0	-3.073622	1.030245	0.007819
12	6	0	-5.616715	-0.100649	0.216227

13	1	0	-4.572364	-1.970955	0.526059
14	6	0	-4.210642	1.822003	-0.124522
15	1	0	-2.083162	1.461866	-0.077000
16	6	0	-5.486422	1.266152	-0.021776
17	1	0	-6.602594	-0.548806	0.302567
18	1	0	-4.096302	2.887259	-0.305922
19	1	0	-6.367467	1.892487	-0.123177
20	6	0	3.579450	-0.664329	-1.030612
21	6	0	4.638474	0.368900	-0.576253
22	1	0	3.940466	-1.692747	-0.958379
23	1	0	3.223864	-0.479685	-2.047260
24	1	0	5.462715	-0.127987	-0.057513
25	1	0	5.044532	0.889927	-1.447121
26	6	0	2.847398	-0.605877	1.287426
27	1	0	1.953254	-0.679388	1.909412
28	1	0	3.433359	-1.523433	1.386632
29	6	0	3.679291	0.664165	1.582556
30	1	0	3.108142	1.362992	2.200076
31	1	0	4.589059	0.392778	2.124243
32	6	0	2.823137	1.877197	-0.278986
33	1	0	2.455368	2.715843	0.318082
34	1	0	3.080466	2.251642	-1.273711
35	6	0	1.735572	0.783781	-0.372848
36	1	0	0.965244	0.886991	0.392927
37	1	0	1.247872	0.734875	-1.347632
38	7	0	2.385397	-0.546991	-0.134474

39	7	0	4.044675	1.348534	0.338245

TS1/2(R*R*S)

SCF Done: E(RM062X) = -1589.19485197

Imaginary Frequencies = -181.7942

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.040293	0.667704	-0.808582
2	6	0	1.456844	0.467926	-0.476327
3	1	0	-0.272229	0.783103	-1.839223
4	1	0	1.954639	-0.232190	-1.158812
5	1	0	1.570722	0.113455	0.553612
6	6	0	-0.856514	1.002246	0.222937
7	8	0	-0.647575	0.989377	1.437028
8	8	0	-2.113625	1.335690	-0.289162
9	6	0	-3.175021	1.636291	0.523478
10	6	0	-4.071684	2.576506	0.011000
11	6	0	-3.437175	1.016487	1.749499
12	6	0	-5.226858	2.899440	0.717532
13	1	0	-3.850847	3.040253	-0.945750
14	6	0	-4.594380	1.353999	2.448455
15	1	0	-2.742720	0.288679	2.144830
16	6	0	-5.493736	2.291755	1.942966

17	1	0	-5.918078	3.629645	0.306651
18	1	0	-4.793364	0.869457	3.400373
19	1	0	-6.392656	2.543641	2.497097
20	6	0	4.643788	2.583767	-0.130862
21	6	0	3.775923	1.308816	-0.241048
22	1	0	5.564632	2.455643	-0.705255
23	1	0	4.911812	2.775006	0.911542
24	1	0	4.088405	0.656109	-1.060051
25	1	0	3.754300	0.735561	0.688558
26	6	0	3.402337	3.437792	-1.973976
27	1	0	2.982413	4.344609	-2.416283
28	1	0	4.239990	3.107740	-2.594096
29	6	0	2.314518	2.340117	-1.903473
30	1	0	1.306048	2.739271	-2.025211
31	1	0	2.475292	1.540449	-2.630223
32	6	0	1.938061	2.742784	0.472377
33	1	0	0.871715	2.915812	0.326912
34	1	0	2.096206	2.291820	1.454548
35	6	0	2.783530	4.019469	0.249741
36	1	0	2.175517	4.805660	-0.205798
37	1	0	3.157944	4.386039	1.208607
38	7	0	3.917001	3.749578	-0.638342
39	7	0	2.360398	1.716615	-0.538613
40	6	0	0.557114	-2.524879	-1.095021
41	6	0	-0.447087	-1.783427	-0.506724
42	1	0	-0.306439	-1.520048	0.538347

43	6	0	0.443834	-3.019234	-2.432243
44	7	0	0.361333	-3.439821	-3.510827
45	6	0	-1.840982	-1.686055	-0.977811
46	6	0	-2.203669	-1.514383	-2.320881
47	6	0	-2.848550	-1.771509	-0.009770
48	6	0	-3.544612	-1.445697	-2.680521
49	1	0	-1.437744	-1.398966	-3.081035
50	6	0	-4.191525	-1.713669	-0.372891
51	1	0	-2.573076	-1.894016	1.035086
52	6	0	-4.543177	-1.550864	-1.710119
53	1	0	-3.812842	-1.301025	-3.722932
54	1	0	-4.959656	-1.784636	0.391917
55	1	0	-5.589113	-1.497254	-1.997372
56	6	0	1.866472	-2.802730	-0.469172
57	8	0	2.821394	-3.160958	-1.148605
58	6	0	2.036407	-2.662522	1.015884
59	6	0	3.253981	-2.152403	1.479882
60	6	0	1.073754	-3.093656	1.933503
61	6	0	3.490848	-2.035156	2.845088
62	1	0	4.004986	-1.844693	0.757378
63	6	0	1.321692	-2.995452	3.301303
64	1	0	0.140859	-3.525668	1.581562
65	6	0	2.522902	-2.456973	3.757748
66	1	0	4.431310	-1.624092	3.199693
67	1	0	0.575996	-3.343412	4.009568
68	1	0	2.709331	-2.372354	4.824306

TS1/2(R*S*R)

SCF Done: E(RM062X) = -1589.19503746

Imaginary Frequencies = -176.0713

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.134226	2.534843	1.323113
2	6	0	0.515971	1.321616	1.426387
3	1	0	1.328626	1.158320	0.729056
4	6	0	-1.133894	2.974056	2.244158
5	7	0	-1.935187	3.366329	2.987293
6	6	0	0.494167	0.362663	2.536331
7	6	0	-0.558778	0.224535	3.455934
8	6	0	1.611173	-0.479239	2.662408
9	6	0	-0.476162	-0.713343	4.480284
10	1	0	-1.452064	0.832256	3.368218
11	6	0	1.697211	-1.405203	3.695929
12	1	0	2.422255	-0.391276	1.943027
13	6	0	0.651844	-1.523797	4.610162
14	1	0	-1.299128	-0.811861	5.181695
15	1	0	2.576033	-2.037342	3.782278
16	1	0	0.710996	-2.249184	5.416021
17	6	0	0.028762	3.424035	0.156696

18	8	0	-0.760064	4.336097	-0.057391
19	6	0	1.153767	3.180305	-0.808350
20	6	0	2.477356	3.005027	-0.392043
21	6	0	0.853192	3.194089	-2.173881
22	6	0	3.486870	2.830311	-1.335784
23	1	0	2.719117	3.020543	0.667387
24	6	0	1.860239	2.997949	-3.114199
25	1	0	-0.175000	3.349505	-2.488453
26	6	0	3.178366	2.816777	-2.695400
27	1	0	4.514542	2.704855	-1.008863
28	1	0	1.618898	2.992724	-4.172767
29	1	0	3.965760	2.670156	-3.428730
30	6	0	-0.567210	-0.153158	-0.298221
31	6	0	-1.863610	-0.325677	0.365548
32	1	0	-0.379141	0.698114	-0.939369
33	1	0	-2.268912	0.619887	0.749740
34	1	0	-1.791130	-1.049556	1.183652
35	6	0	0.377343	-1.189285	-0.241639
36	8	0	0.283345	-2.294638	0.289113
37	8	0	1.581622	-0.778679	-0.845669
38	6	0	2.652507	-1.625123	-0.976389
39	6	0	3.377493	-1.497921	-2.163639
40	6	0	3.082205	-2.510709	0.016518
41	6	0	4.528249	-2.254112	-2.363425
42	1	0	3.027294	-0.796038	-2.914504
43	6	0	4.232675	-3.267616	-0.201074

44	1	0	2.516722	-2.606733	0.933798
45	6	0	4.960390	-3.147202	-1.383603
46	1	0	5.085920	-2.144770	-3.289017
47	1	0	4.563499	-3.956357	0.571175
48	1	0	5.856539	-3.739938	-1.538714
49	6	0	-5.410134	-1.463655	-0.584765
50	6	0	-4.223143	-1.101638	0.338598
51	1	0	-6.108439	-0.625886	-0.658659
52	1	0	-5.945853	-2.324087	-0.176589
53	1	0	-4.395869	-0.183584	0.904129
54	1	0	-3.968538	-1.907839	1.030448
55	6	0	-4.387514	-0.570696	-2.540110
56	1	0	-3.916094	-0.845441	-3.487393
57	1	0	-5.203210	0.125471	-2.750163
58	6	0	-3.359334	0.099400	-1.597743
59	1	0	-2.431057	0.360173	-2.108835
60	1	0	-3.759385	0.985771	-1.099263
61	6	0	-2.615068	-2.179323	-1.145964
62	1	0	-1.819608	-1.946530	-1.855585
63	1	0	-2.203438	-2.809071	-0.355636
64	6	0	-3.865566	-2.782518	-1.826909
65	1	0	-3.605622	-3.135832	-2.827853
66	1	0	-4.245367	-3.630645	-1.250944
67	7	0	-4.936406	-1.786464	-1.933229
68	7	0	-3.008327	-0.875039	-0.513146

TS1/2(S*R*S)

SCF Done: E(RM062X) = -1589.19562912

Imaginary Frequencies = -152.7075

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.720620	2.071322	1.467497
2	6	0	-0.420458	1.653670	0.819069
3	1	0	-0.532632	1.954127	-0.216210
4	6	0	0.932931	1.827205	2.859986
5	7	0	1.115584	1.654867	3.993374
6	6	0	-1.667642	1.205320	1.460656
7	6	0	-1.711963	0.332570	2.556410
8	6	0	-2.869053	1.725490	0.956626
9	6	0	-2.928341	0.030637	3.162023
10	1	0	-0.797532	-0.120849	2.925732
11	6	0	-4.081281	1.436633	1.574909
12	1	0	-2.842077	2.379823	0.088662
13	6	0	-4.112612	0.592238	2.683835
14	1	0	-2.951233	-0.647122	4.010209
15	1	0	-5.001384	1.861423	1.184657
16	1	0	-5.057834	0.360801	3.166260
17	6	0	1.898235	2.615345	0.758241
18	8	0	3.015138	2.549644	1.257938

19	6	0	1.725647	3.240519	-0.593955
20	6	0	2.737028	3.044461	-1.540348
21	6	0	0.641097	4.069031	-0.902183
22	6	0	2.650755	3.645368	-2.791712
23	1	0	3.586919	2.418952	-1.283370
24	6	0	0.566678	4.685030	-2.148767
25	1	0	-0.131445	4.249878	-0.160020
26	6	0	1.565198	4.467176	-3.096485
27	1	0	3.431200	3.479603	-3.528039
28	1	0	-0.271067	5.336019	-2.379163
29	1	0	1.500039	4.941783	-4.071093
30	6	0	0.330102	-0.503415	-0.325276
31	6	0	1.340832	-0.885823	0.667499
32	1	0	0.584447	0.141933	-1.156921
33	1	0	1.976452	-0.046765	0.975750
34	1	0	0.869396	-1.325692	1.552208
35	6	0	-0.897775	-1.182496	-0.324308
36	8	0	-1.279297	-2.075408	0.432176
37	8	0	-1.743079	-0.690698	-1.334333
38	6	0	-3.029099	-1.148492	-1.450570
39	6	0	-3.871184	-1.356497	-0.355280
40	6	0	-3.510731	-1.320474	-2.749014
41	6	0	-5.192042	-1.739161	-0.574675
42	1	0	-3.485713	-1.218800	0.646778
43	6	0	-4.835189	-1.698685	-2.955013
44	1	0	-2.838115	-1.147117	-3.583788

45	6	0	-5.682109	-1.912808	-1.869050
46	1	0	-5.845001	-1.897024	0.279725
47	1	0	-5.203550	-1.826294	-3.968888
48	1	0	-6.714459	-2.208667	-2.029347
49	6	0	3.237254	-2.309392	1.396240
50	6	0	4.380262	-3.222187	0.894519
51	1	0	3.603787	-1.373550	1.823584
52	1	0	2.589535	-2.806377	2.122218
53	1	0	5.324450	-2.672046	0.860658
54	1	0	4.499713	-4.070303	1.573313
55	6	0	3.235411	-1.428389	-0.875197
56	1	0	2.573474	-1.034954	-1.648560
57	1	0	3.817988	-0.608567	-0.446282
58	6	0	4.121529	-2.589822	-1.386170
59	1	0	3.767398	-2.941719	-2.358806
60	1	0	5.152333	-2.244654	-1.498773
61	6	0	2.740096	-4.293954	-0.457918
62	1	0	2.570355	-4.799888	-1.411799
63	1	0	2.683613	-5.038754	0.340792
64	6	0	1.672425	-3.195259	-0.252924
65	1	0	1.164405	-2.921810	-1.179539
66	1	0	0.920360	-3.453116	0.494655
67	7	0	2.365554	-1.952484	0.227513
68	7	0	4.089484	-3.719461	-0.452725

TS1/2(S*S*R)

SCF Done: E(RM062X) = -1589.19818499

Imaginary Frequencies = -167.3595

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.587985	-0.197666	0.210060
2	6	0	-1.875785	0.217625	-0.368489
3	1	0	-0.444033	-0.207665	1.283680
4	1	0	-2.314384	1.080505	0.145168
5	1	0	-1.771288	0.446760	-1.433666
6	6	0	0.350200	-0.849451	-0.607263
7	8	0	0.309730	-1.039249	-1.823720
8	8	0	1.480738	-1.225001	0.131007
9	6	0	2.424477	-2.038355	-0.449210
10	6	0	3.762315	-1.724627	-0.216766
11	6	0	2.079259	-3.190694	-1.159068
12	6	0	4.760934	-2.567240	-0.702355
13	1	0	3.998728	-0.827501	0.348699
14	6	0	3.086902	-4.019885	-1.643897
15	1	0	1.035104	-3.425168	-1.330977
16	6	0	4.429878	-3.714102	-1.420978
17	1	0	5.802630	-2.321252	-0.517269
18	1	0	2.818050	-4.914914	-2.197633
19	1	0	5.209462	-4.366962	-1.801304

20	6	0	-4.202775	-0.296977	-1.056113
21	6	0	-5.389585	-1.261670	-0.829900
22	1	0	-4.396346	0.704428	-0.665613
23	1	0	-3.915348	-0.223414	-2.107506
24	1	0	-6.104168	-0.832486	-0.122557
25	1	0	-5.906018	-1.439354	-1.776404
26	6	0	-3.401930	-1.138335	1.086782
27	1	0	-2.488740	-1.380190	1.633067
28	1	0	-3.833823	-0.219630	1.490895
29	6	0	-4.410446	-2.311834	1.067472
30	1	0	-3.933137	-3.233090	1.411816
31	1	0	-5.247595	-2.088229	1.733211
32	6	0	-3.818968	-3.024993	-1.126456
33	1	0	-3.562224	-4.044227	-0.827471
34	1	0	-4.165417	-3.048274	-2.163132
35	6	0	-2.577068	-2.114281	-0.989232
36	1	0	-1.807639	-2.548173	-0.347897
37	1	0	-2.126038	-1.847590	-1.946123
38	7	0	-3.004694	-0.834767	-0.327222
39	7	0	-4.919547	-2.539379	-0.287888
40	6	0	1.986677	1.709726	0.352682
41	6	0	0.653127	1.965535	0.093417
42	1	0	0.021373	2.149061	0.954242
43	6	0	2.965759	1.633414	-0.684528
44	7	0	3.785581	1.590854	-1.506053
45	6	0	0.078513	2.419188	-1.181711

46	6	0	0.521657	1.975125	-2.437407
47	6	0	-0.995878	3.321201	-1.123202
48	6	0	-0.085585	2.445020	-3.598619
49	1	0	1.306499	1.232486	-2.508157
50	6	0	-1.592327	3.796498	-2.285992
51	1	0	-1.354648	3.654180	-0.152300
52	6	0	-1.136168	3.359360	-3.529133
53	1	0	0.260733	2.088750	-4.564173
54	1	0	-2.414183	4.503173	-2.222064
55	1	0	-1.601832	3.724079	-4.439793
56	6	0	2.497352	1.343196	1.679843
57	8	0	3.636478	0.912329	1.831450
58	6	0	1.606325	1.468280	2.882426
59	6	0	0.926631	2.649843	3.194287
60	6	0	1.533257	0.376369	3.753016
61	6	0	0.174369	2.732637	4.364096
62	1	0	1.003937	3.509975	2.534438
63	6	0	0.763585	0.454522	4.909863
64	1	0	2.079280	-0.531063	3.510762
65	6	0	0.084931	1.633967	5.217233
66	1	0	-0.340648	3.656490	4.609248
67	1	0	0.699111	-0.400692	5.575755
68	1	0	-0.508396	1.698323	6.124399

2(R*R*S)

SCF Done: E(RM062X) = -1589.24120685

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.098222	0.417163	0.039097
2	6	0	-1.093908	0.900648	-0.794434
3	1	0	0.196409	0.949186	0.989464
4	1	0	-1.912555	0.177442	-0.751984
5	1	0	-0.797255	1.029201	-1.838598
6	6	0	1.388713	0.585782	-0.730779
7	8	0	1.549553	0.279608	-1.884743
8	8	0	2.363449	1.090510	0.061781
9	6	0	3.674057	1.082113	-0.410821
10	6	0	4.341418	2.295717	-0.491320
11	6	0	4.299299	-0.124850	-0.705238
12	6	0	5.680201	2.300587	-0.880290
13	1	0	3.816028	3.213662	-0.247096
14	6	0	5.635082	-0.104378	-1.095752
15	1	0	3.742887	-1.055555	-0.629188
16	6	0	6.327127	1.104269	-1.183012
17	1	0	6.215022	3.243218	-0.944873
18	1	0	6.137941	-1.038587	-1.327029
19	1	0	7.370012	1.111659	-1.484351
20	6	0	-3.349773	3.946962	-1.003837
21	6	0	-2.844720	2.518198	-1.306219

22	1	0	-4.442088	3.950993	-0.980774
23	1	0	-3.016801	4.642361	-1.778665
24	1	0	-3.604458	1.753732	-1.128957
25	1	0	-2.458966	2.418155	-2.321951
26	6	0	-3.111897	3.386946	1.294279
27	1	0	-2.875687	3.782549	2.284933
28	1	0	-4.179344	3.154216	1.261360
29	6	0	-2.270894	2.115344	1.035803
30	1	0	-1.424113	2.045349	1.720095
31	1	0	-2.856970	1.193282	1.095346
32	6	0	-0.716117	3.336580	-0.427329
33	1	0	0.174555	3.038966	0.129107
34	1	0	-0.460913	3.456990	-1.483216
35	6	0	-1.386370	4.593554	0.176523
36	1	0	-0.990667	4.793435	1.175560
37	1	0	-1.175556	5.457694	-0.457868
38	7	0	-2.835379	4.411794	0.284950
39	7	0	-1.706116	2.202950	-0.363257
40	6	0	-1.244319	-1.227669	1.374084
41	6	0	-0.120010	-1.106305	0.362996
42	1	0	-0.458663	-1.558650	-0.573940
43	6	0	-1.060721	-0.572526	2.607552
44	7	0	-0.863151	-0.011366	3.614714
45	6	0	1.174266	-1.809681	0.739069
46	6	0	1.945755	-1.418843	1.841202
47	6	0	1.625232	-2.874062	-0.047640

48	6	0	3.124587	-2.091575	2.155088
49	1	0	1.625296	-0.581932	2.456358
50	6	0	2.802508	-3.552672	0.266735
51	1	0	1.043621	-3.174033	-0.916862
52	6	0	3.555265	-3.163290	1.372039
53	1	0	3.710675	-1.777088	3.013958
54	1	0	3.130271	-4.381310	-0.354454
55	1	0	4.473649	-3.687070	1.620512
56	6	0	-2.578156	-1.626083	1.092165
57	8	0	-3.556771	-1.354898	1.820583
58	6	0	-2.855289	-2.427517	-0.159068
59	6	0	-3.998715	-2.123171	-0.904092
60	6	0	-2.057247	-3.507337	-0.549085
61	6	0	-4.320889	-2.861515	-2.039646
62	1	0	-4.630978	-1.301344	-0.578288
63	6	0	-2.387769	-4.260198	-1.674784
64	1	0	-1.182096	-3.766558	0.042578
65	6	0	-3.515686	-3.933324	-2.426433
66	1	0	-5.203412	-2.607617	-2.619867
67	1	0	-1.767968	-5.105002	-1.961397
68	1	0	-3.770698	-4.515954	-3.306843

2(R*S*R)

SCF Done: E(RM062X) = -1589.23658931

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.990357	1.186964	1.770163
2	6	0	-0.246926	1.041737	0.896267
3	1	0	-0.975086	0.428879	1.431534
4	6	0	1.810115	2.314921	1.572867
5	7	0	2.477236	3.258906	1.390882
6	6	0	-0.943502	2.370070	0.627442
7	6	0	-1.276388	3.177493	1.725330
8	6	0	-1.312599	2.811278	-0.645118
9	6	0	-1.959350	4.375846	1.557395
10	1	0	-0.988203	2.854243	2.722734
11	6	0	-1.996079	4.017576	-0.819097
12	1	0	-1.077667	2.228161	-1.530210
13	6	0	-2.323439	4.803761	0.279158
14	1	0	-2.208383	4.979160	2.425677
15	1	0	-2.268134	4.336048	-1.821243
16	1	0	-2.852801	5.742265	0.144512
17	6	0	1.590712	0.124483	2.495911
18	8	0	2.772356	0.131901	2.900909
19	6	0	0.780315	-1.125221	2.767072
20	6	0	-0.516983	-1.093975	3.288969
21	6	0	1.389195	-2.365180	2.543901
22	6	0	-1.201832	-2.278570	3.554545
23	1	0	-0.985628	-0.137300	3.507600

24	6	0	0.700929	-3.550230	2.791192
25	1	0	2.413574	-2.386605	2.181086
26	6	0	-0.598905	-3.508766	3.294924
27	1	0	-2.205212	-2.240096	3.968808
28	1	0	1.180993	-4.506068	2.601284
29	1	0	-1.135656	-4.431402	3.495910
30	6	0	0.100750	0.213199	-0.379985
31	6	0	1.157561	0.873540	-1.271080
32	1	0	0.480291	-0.733721	0.025460
33	1	0	1.558103	1.773947	-0.801230
34	1	0	0.736340	1.141688	-2.242499
35	6	0	-1.110936	-0.217702	-1.190227
36	8	0	-1.182353	-0.252233	-2.393372
37	8	0	-2.102661	-0.624246	-0.366233
38	6	0	-3.296166	-1.085748	-0.919527
39	6	0	-3.692100	-2.373109	-0.584858
40	6	0	-4.085289	-0.251853	-1.703204
41	6	0	-4.916770	-2.842719	-1.055974
42	1	0	-3.049536	-2.984413	0.041240
43	6	0	-5.303428	-0.736794	-2.172369
44	1	0	-3.751831	0.755442	-1.932466
45	6	0	-5.720716	-2.028611	-1.851644
46	1	0	-5.239228	-3.846698	-0.797835
47	1	0	-5.930320	-0.098478	-2.787303
48	1	0	-6.673222	-2.397740	-2.218653
49	6	0	4.437892	-0.045094	-2.946621

50	6	0	3.317760	0.867134	-2.402121
51	1	0	5.404491	0.448029	-2.819196
52	1	0	4.287114	-0.244040	-4.010750
53	1	0	3.690734	1.634675	-1.719897
54	1	0	2.739115	1.339070	-3.198213
55	6	0	4.441165	-1.058727	-0.796639
56	1	0	4.605369	-1.993394	-0.254426
57	1	0	5.267319	-0.379368	-0.571235
58	6	0	3.095247	-0.438175	-0.353301
59	1	0	2.459490	-1.173401	0.142818
60	1	0	3.219557	0.427040	0.301122
61	6	0	1.978635	-1.181194	-2.412096
62	1	0	1.178271	-1.706769	-1.889542
63	1	0	1.595631	-0.794499	-3.358726
64	6	0	3.234784	-2.066127	-2.586056
65	1	0	3.174612	-2.946411	-1.940956
66	1	0	3.301328	-2.402049	-3.623682
67	7	0	4.448426	-1.325537	-2.236486
68	7	0	2.360880	0.022231	-1.590607

2(S*R*S)

SCF Done: E(RM062X) = -1589.23658977

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

1	6	0	-0.990114	1.185966	1.770974
2	6	0	0.247191	1.040713	0.897112
3	1	0	0.975066	0.427246	1.432068
4	6	0	-1.809239	2.314499	1.574381
5	7	0	-2.475774	3.259027	1.393068
6	6	0	0.944292	2.368923	0.629059
7	6	0	1.277535	3.175562	1.727422
8	6	0	1.313440	2.810778	-0.643253
9	6	0	1.960897	4.373780	1.560169
10	1	0	0.989282	2.851816	2.724646
11	6	0	1.997330	4.016946	-0.816546
12	1	0	1.078245	2.228276	-1.528678
13	6	0	2.325041	4.802352	0.282161
14	1	0	2.210184	4.976481	2.428802
15	1	0	2.269401	4.335932	-1.818523
16	1	0	2.854699	5.740764	0.148041
17	6	0	-1.591082	0.123228	2.495839
18	8	0	-2.772809	0.130835	2.900598
19	6	0	-0.781241	-1.126992	2.766268
20	6	0	-1.390573	-2.366549	2.542106
21	6	0	0.515983	-1.096633	3.288399
22	6	0	-0.702821	-3.552050	2.788676
23	1	0	-2.414902	-2.387307	2.179118
24	6	0	1.200311	-2.281687	3.553259
25	1	0	0.984974	-0.140297	3.507767

26	6	0	0.596939	-3.511461	3.292659
27	1	0	-1.183237	-4.507562	2.598020
28	1	0	2.203636	-2.243901	3.967712
29	1	0	1.133283	-4.434454	3.493090
30	6	0	-0.100755	0.213105	-0.379688
31	6	0	-1.157239	0.874513	-1.270364
32	1	0	-0.480622	-0.733952	0.025124
33	1	0	-1.557502	1.774707	-0.799871
34	1	0	-0.735795	1.143251	-2.241519
35	6	0	1.110852	-0.217526	-1.190177
36	8	0	1.182449	-0.250874	-2.393344
37	8	0	2.102331	-0.625181	-0.366426
38	6	0	3.296029	-1.085887	-0.919967
39	6	0	4.085241	-0.250916	-1.702416
40	6	0	3.692087	-2.373577	-0.586718
41	6	0	5.303578	-0.735084	-2.171839
42	1	0	3.751687	0.756610	-1.930517
43	6	0	4.916962	-2.842416	-1.058081
44	1	0	3.049465	-2.985725	0.038499
45	6	0	5.720985	-2.027223	-1.852561
46	1	0	5.930547	-0.095912	-2.785807
47	1	0	5.239529	-3.846647	-0.801067
48	1	0	6.673655	-2.395752	-2.219750
49	6	0	-3.317262	0.869666	-2.401743
50	6	0	-4.437583	-0.041811	-2.947086
51	1	0	-3.690113	1.636810	-1.719009

52	1	0	-2.738339	1.342014	-3.197383
53	1	0	-5.404035	0.451575	-2.819581
54	1	0	-4.286616	-0.240125	-4.011304
55	6	0	-3.095490	-0.437175	-0.353803
56	1	0	-2.460062	-1.173028	0.141796
57	1	0	-3.219511	0.427589	0.301271
58	6	0	-4.441584	-1.056861	-0.797761
59	1	0	-4.606296	-1.991792	-0.256159
60	1	0	-5.267481	-0.377288	-0.572070
61	6	0	-3.235260	-2.063515	-2.587650
62	1	0	-3.175463	-2.944196	-1.943059
63	1	0	-3.301761	-2.398811	-3.625478
64	6	0	-1.978847	-1.179101	-2.412981
65	1	0	-1.178691	-1.705300	-1.890738
66	1	0	-1.595652	-0.791844	-3.359304
67	7	0	-2.360794	0.023871	-1.590684
68	7	0	-4.448712	-1.322729	-2.237794

2(S*S*R)

SCF Done: E(RM062X) = -1589.23576710

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.465811	0.218742	-0.175790

2	6	0	-1.856232	0.269417	-0.798732
3	1	0	-0.514939	-0.113292	0.864983
4	1	0	-2.360418	1.202389	-0.531310
5	1	0	-1.791740	0.204670	-1.888298
6	6	0	0.457368	-0.748365	-0.889319
7	8	0	0.531091	-0.911109	-2.082696
8	8	0	1.216173	-1.417311	0.006019
9	6	0	2.254295	-2.219091	-0.473094
10	6	0	3.551376	-1.812448	-0.189656
11	6	0	1.974630	-3.402369	-1.144738
12	6	0	4.604763	-2.629147	-0.599726
13	1	0	3.711277	-0.877410	0.346428
14	6	0	3.038827	-4.204372	-1.550249
15	1	0	0.945304	-3.686392	-1.341526
16	6	0	4.351902	-3.819627	-1.279439
17	1	0	5.626968	-2.331914	-0.385138
18	1	0	2.839213	-5.132634	-2.076921
19	1	0	5.177578	-4.449842	-1.595477
20	6	0	-4.031291	-0.759256	-1.236009
21	6	0	-5.091026	-1.722245	-0.656270
22	1	0	-4.362800	0.280477	-1.237200
23	1	0	-3.710933	-1.040276	-2.241655
24	1	0	-5.872041	-1.165191	-0.132575
25	1	0	-5.554395	-2.285429	-1.469896
26	6	0	-3.232639	-0.655975	1.066572
27	1	0	-2.343612	-0.528194	1.685272

28	1	0	-3.824170	0.261694	1.091016
29	6	0	-4.049340	-1.903187	1.475308
30	1	0	-3.447829	-2.565404	2.103146
31	1	0	-4.927879	-1.590537	2.044548
32	6	0	-3.298772	-3.252869	-0.336236
33	1	0	-2.922531	-4.061990	0.294069
34	1	0	-3.600353	-3.674248	-1.298531
35	6	0	-2.185032	-2.198011	-0.534794
36	1	0	-1.399107	-2.291092	0.219072
37	1	0	-1.748701	-2.235764	-1.535117
38	7	0	-2.795570	-0.829524	-0.367676
39	7	0	-4.476485	-2.653792	0.292364
40	6	0	1.663524	1.603950	0.200526
41	6	0	0.173673	1.660964	-0.099370
42	1	0	-0.331592	2.101387	0.763237
43	6	0	2.563012	1.550027	-0.883585
44	7	0	3.304415	1.518891	-1.787194
45	6	0	-0.150444	2.580599	-1.268943
46	6	0	0.026629	2.217404	-2.609297
47	6	0	-0.614278	3.870195	-0.986159
48	6	0	-0.256977	3.121002	-3.632895
49	1	0	0.380237	1.221554	-2.858328
50	6	0	-0.892100	4.776676	-2.006473
51	1	0	-0.757936	4.166388	0.050954
52	6	0	-0.714745	4.403056	-3.337156
53	1	0	-0.116566	2.818883	-4.666978

54	1	0	-1.250389	5.772335	-1.760828
55	1	0	-0.932568	5.104620	-4.137139
56	6	0	2.211710	1.266314	1.461371
57	8	0	3.405865	0.947896	1.658123
58	6	0	1.300095	1.264124	2.668821
59	6	0	0.550141	2.382242	3.046950
60	6	0	1.261716	0.117927	3.469365
61	6	0	-0.237714	2.349537	4.196539
62	1	0	0.595677	3.286212	2.443621
63	6	0	0.461084	0.076733	4.608374
64	1	0	1.864555	-0.741040	3.186391
65	6	0	-0.290625	1.193843	4.974463
66	1	0	-0.808232	3.227527	4.485626
67	1	0	0.429132	-0.823431	5.215568
68	1	0	-0.909090	1.166361	5.866806

TS2/3(RRS)

SCF Done: E(RM062X) = -1589.16689676

Imaginary Frequencies = -1703.7458

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.079392	-1.056014	0.535137
2	6	0	-0.670432	-2.231034	1.087785

3	1	0	-0.508893	0.124162	-0.206474
4	1	0	-0.930026	-2.083886	2.140419
5	1	0	-0.105138	-3.162521	0.983177
6	6	0	1.152112	-1.444738	-0.354130
7	8	0	1.297423	-2.525746	-0.903697
8	8	0	2.011335	-0.398405	-0.603450
9	6	0	3.059208	-0.596630	-1.482121
10	6	0	3.052130	0.107470	-2.680772
11	6	0	4.123443	-1.425020	-1.136647
12	6	0	4.134217	-0.019942	-3.549940
13	1	0	2.210016	0.751779	-2.912128
14	6	0	5.196485	-1.549458	-2.015188
15	1	0	4.101639	-1.957708	-0.190839
16	6	0	5.205430	-0.848723	-3.221612
17	1	0	4.137193	0.531281	-4.485504
18	1	0	6.030864	-2.193453	-1.753565
19	1	0	6.046031	-0.946548	-3.901672
20	6	0	-3.970015	-4.049803	0.430300
21	6	0	-2.532317	-3.840193	0.959033
22	1	0	-4.700812	-3.861911	1.221251
23	1	0	-4.088815	-5.081068	0.088843
24	1	0	-2.490953	-3.769435	2.047644
25	1	0	-1.843794	-4.618204	0.621487
26	6	0	-4.280229	-1.766693	-0.163974
27	1	0	-4.342740	-1.082695	-1.014990
28	1	0	-5.172869	-1.631807	0.452322

29	6	0	-3.017799	-1.469042	0.677565
30	1	0	-2.560554	-0.513070	0.423122
31	1	0	-3.211363	-1.490927	1.753015
32	6	0	-1.840799	-2.695893	-1.078863
33	1	0	-1.592571	-1.704862	-1.462828
34	1	0	-0.990614	-3.359901	-1.239246
35	6	0	-3.164919	-3.244556	-1.659029
36	1	0	-3.434235	-2.681461	-2.556008
37	1	0	-3.055958	-4.297375	-1.933231
38	7	0	-4.250957	-3.137342	-0.680606
39	7	0	-2.006049	-2.543155	0.408452
40	6	0	-0.224662	1.322090	0.432141
41	6	0	0.231576	0.205648	1.411360
42	1	0	-0.588671	0.161774	2.138011
43	6	0	0.764210	2.055701	-0.294728
44	7	0	1.561374	2.653232	-0.894729
45	6	0	1.520286	0.422015	2.175639
46	6	0	1.887361	1.701579	2.605092
47	6	0	2.337203	-0.657751	2.525995
48	6	0	3.042129	1.898482	3.359748
49	1	0	1.262052	2.553714	2.347811
50	6	0	3.491417	-0.464971	3.281801
51	1	0	2.067375	-1.661131	2.202369
52	6	0	3.850302	0.815446	3.700245
53	1	0	3.311053	2.901236	3.679548
54	1	0	4.112392	-1.317686	3.541794

55	1	0	4.753448	0.968327	4.283794
56	6	0	-1.506871	1.975274	0.731920
57	8	0	-2.272438	1.513152	1.578470
58	6	0	-1.996521	3.123495	-0.110114
59	6	0	-3.298607	3.030176	-0.614913
60	6	0	-1.253086	4.284580	-0.339479
61	6	0	-3.835732	4.063189	-1.374974
62	1	0	-3.881431	2.136478	-0.409183
63	6	0	-1.802549	5.329452	-1.080959
64	1	0	-0.255430	4.386421	0.074528
65	6	0	-3.086877	5.216520	-1.608913
66	1	0	-4.839653	3.973180	-1.779175
67	1	0	-1.224533	6.234048	-1.245411
68	1	0	-3.507057	6.028170	-2.195717

TS2/3(RSR)

SCF Done: E(RM062X) = -1589.15842523

Imaginary Frequencies = -1719.8831

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.019194	-1.564146	-1.145040
2	6	0	-0.205968	-1.190748	0.346251
3	1	0	-1.244165	-0.872096	0.438720

4	6	0	1.200774	-2.234190	-1.486763
5	7	0	2.224681	-2.727031	-1.735734
6	6	0	0.052478	-2.253429	1.392890
7	6	0	0.040711	-3.615918	1.081187
8	6	0	0.262542	-1.872518	2.724318
9	6	0	0.232393	-4.575967	2.075733
10	1	0	-0.125435	-3.934098	0.054670
11	6	0	0.451924	-2.828306	3.718102
12	1	0	0.273153	-0.814177	2.978063
13	6	0	0.439557	-4.185927	3.395755
14	1	0	0.220405	-5.630055	1.813733
15	1	0	0.611713	-2.513872	4.745597
16	1	0	0.590962	-4.932791	4.169326
17	6	0	-1.091145	-1.750908	-2.136850
18	8	0	-0.830872	-2.017724	-3.307074
19	6	0	-2.522220	-1.495200	-1.752361
20	6	0	-3.102061	-2.046853	-0.605702
21	6	0	-3.311807	-0.745667	-2.630299
22	6	0	-4.450346	-1.830190	-0.329619
23	1	0	-2.506033	-2.664650	0.062320
24	6	0	-4.653820	-0.512730	-2.343340
25	1	0	-2.861828	-0.344590	-3.533899
26	6	0	-5.223763	-1.053375	-1.190408
27	1	0	-4.896078	-2.268965	0.557956
28	1	0	-5.257031	0.085666	-3.019783
29	1	0	-6.271575	-0.874909	-0.967505

30	6	0	0.629435	0.108660	0.417823
31	6	0	2.082976	-0.068410	0.773652
32	1	0	0.387060	-0.257177	-1.022310
33	1	0	2.345608	-1.120657	0.642890
34	1	0	2.313649	0.197342	1.811433
35	6	0	0.003711	1.349297	0.770307
36	8	0	0.561323	2.424388	0.957311
37	8	0	-1.378253	1.261961	0.772321
38	6	0	-2.144677	2.404574	0.876360
39	6	0	-3.128788	2.580670	-0.092434
40	6	0	-2.015493	3.295805	1.939377
41	6	0	-3.993573	3.668429	-0.001915
42	1	0	-3.207694	1.859191	-0.900670
43	6	0	-2.881660	4.384222	2.014488
44	1	0	-1.249398	3.135486	2.688943
45	6	0	-3.869832	4.575713	1.048684
46	1	0	-4.763309	3.804661	-0.755592
47	1	0	-2.784706	5.085341	2.838185
48	1	0	-4.542021	5.425370	1.117818
49	6	0	5.515626	0.641357	-0.779324
50	6	0	4.349657	-0.195477	-0.204682
51	1	0	6.008660	0.080494	-1.577263
52	1	0	6.253668	0.854946	-0.001602
53	1	0	4.037597	-1.004560	-0.870420
54	1	0	4.579531	-0.607609	0.780165
55	6	0	3.896862	1.644592	-2.200425

56	1	0	3.615083	2.565683	-2.716772
57	1	0	4.215685	0.914413	-2.949190
58	6	0	2.680393	1.106056	-1.409283
59	1	0	1.902239	1.856557	-1.261340
60	1	0	2.253311	0.224496	-1.888422
61	6	0	3.598968	1.930846	0.707863
62	1	0	2.700431	2.478738	0.986356
63	1	0	4.101161	1.563110	1.605777
64	6	0	4.550129	2.738492	-0.200087
65	1	0	4.037709	3.609878	-0.617552
66	1	0	5.403638	3.089058	0.386074
67	7	0	5.029219	1.915540	-1.313354
68	7	0	3.145771	0.698386	-0.039730

TS2/3(SRS)

SCF Done: E(RM062X) = -1589.15842532

Imaginary Frequencies = -1719.8481

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.019154	-1.564040	-1.145140
2	6	0	0.205927	-1.190702	0.346167
3	1	0	1.244117	-0.872030	0.438648
4	6	0	-1.200819	-2.234047	-1.486917

5	7	0	-2.224743	-2.726837	-1.735922
6	6	0	-0.052495	-2.253416	1.392778
7	6	0	-0.041038	-3.615891	1.081009
8	6	0	-0.262207	-1.872532	2.724270
9	6	0	-0.232670	-4.575951	2.075556
10	1	0	0.124838	-3.934069	0.054450
11	6	0	-0.451522	-2.828330	3.718055
12	1	0	-0.272602	-0.814199	2.978063
13	6	0	-0.439463	-4.185940	3.395643
14	1	0	-0.220919	-5.630029	1.813503
15	1	0	-0.611022	-2.513914	4.745600
16	1	0	-0.590806	-4.932813	4.169217
17	6	0	1.091131	-1.750718	-2.136944
18	8	0	0.830888	-2.017354	-3.307213
19	6	0	2.522200	-1.495138	-1.752356
20	6	0	3.311794	-0.745370	-2.630089
21	6	0	3.102019	-2.047077	-0.605826
22	6	0	4.653793	-0.512478	-2.343043
23	1	0	2.861821	-0.344072	-3.533594
24	6	0	4.450300	-1.830472	-0.329670
25	1	0	2.505985	-2.665054	0.062024
26	6	0	5.223723	-1.053416	-1.190242
27	1	0	5.257004	0.086103	-3.019321
28	1	0	4.896031	-2.269462	0.557800
29	1	0	6.271526	-0.874984	-0.967270
30	6	0	-0.629488	0.108697	0.417802

31	6	0	-2.083020	-0.068457	0.773624
32	1	0	-0.387134	-0.257105	-1.022371
33	1	0	-2.345576	-1.120699	0.642644
34	1	0	-2.313738	0.197070	1.811457
35	6	0	-0.003744	1.349335	0.770222
36	8	0	-0.561327	2.424454	0.957160
37	8	0	1.378218	1.261955	0.772252
38	6	0	2.144759	2.404486	0.876281
39	6	0	2.015507	3.295893	1.939146
40	6	0	3.129082	2.580298	-0.092347
41	6	0	2.881843	4.384175	2.014279
42	1	0	1.249219	3.135819	2.688569
43	6	0	3.994037	3.667919	-0.001799
44	1	0	3.208021	1.858694	-0.900472
45	6	0	3.870249	4.575361	1.048660
46	1	0	2.784851	5.085411	2.837873
47	1	0	4.763964	3.803905	-0.755329
48	1	0	4.542582	5.424901	1.117826
49	6	0	-4.349850	-0.195379	-0.204305
50	6	0	-5.515857	0.641539	-0.778742
51	1	0	-4.037988	-1.004510	-0.870083
52	1	0	-4.579558	-0.607457	0.780604
53	1	0	-6.009195	0.080626	-1.576458
54	1	0	-6.253650	0.855356	-0.000846
55	6	0	-2.680654	1.105933	-1.409284
56	1	0	-1.902574	1.856546	-1.261487

57	1	0	-2.253507	0.224380	-1.888374
58	6	0	-3.897254	1.644257	-2.200351
59	1	0	-3.615527	2.565135	-2.717108
60	1	0	-4.216297	0.913820	-2.948770
61	6	0	-4.549927	2.738651	-0.200084
62	1	0	-4.037302	3.609778	-0.617843
63	1	0	-5.403240	3.089632	0.386117
64	6	0	-3.598873	1.930950	0.707919
65	1	0	-2.700281	2.478753	0.986408
66	1	0	-4.101137	1.563304	1.605832
67	7	0	-3.145852	0.698393	-0.039625
68	7	0	-5.029398	1.915569	-1.313103

TS2/3(SSR)

SCF Done: E(RM062X) = -1589.16019036

Imaginary Frequencies = -1709.4006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.230067	0.568711	-0.448466
2	6	0	0.665992	1.193863	-1.477054
3	1	0	0.145560	0.332001	0.991097
4	1	0	1.164381	0.435768	-2.089644
5	1	0	0.122668	1.884487	-2.128289

6	6	0	-1.516079	1.221414	-0.366806
7	8	0	-1.788719	2.349674	-0.744899
8	8	0	-2.444638	0.440923	0.283106
9	6	0	-3.745307	0.892490	0.402739
10	6	0	-4.281675	0.998412	1.681286
11	6	0	-4.517577	1.146998	-0.728293
12	6	0	-5.617613	1.369109	1.828491
13	1	0	-3.653707	0.776480	2.538068
14	6	0	-5.847684	1.524172	-0.567757
15	1	0	-4.075531	1.048171	-1.714331
16	6	0	-6.401530	1.636066	0.708146
17	1	0	-6.043576	1.450074	2.824158
18	1	0	-6.454594	1.728601	-1.444877
19	1	0	-7.440851	1.926882	0.826565
20	6	0	2.580577	2.621844	-2.074483
21	6	0	3.812212	3.377368	-1.519958
22	1	0	2.856542	1.788591	-2.723528
23	1	0	1.888421	3.278591	-2.606081
24	1	0	4.732720	2.850571	-1.784338
25	1	0	3.854068	4.381606	-1.948514
26	6	0	2.741586	1.213722	-0.085653
27	1	0	2.139923	0.743242	0.691671
28	1	0	3.150348	0.442944	-0.745257
29	6	0	3.828045	2.140488	0.512792
30	1	0	3.699386	2.222495	1.595301
31	1	0	4.819439	1.726043	0.313088

32	6	0	2.463609	4.084641	0.312419
33	1	0	2.454813	4.253822	1.391914
34	1	0	2.381000	5.052739	-0.188294
35	6	0	1.277178	3.172409	-0.085275
36	1	0	0.785414	2.715257	0.775151
37	1	0	0.526300	3.684415	-0.689405
38	7	0	1.808984	2.041123	-0.920920
39	7	0	3.745834	3.483550	-0.061889
40	6	0	0.043946	-1.020876	1.338512
41	6	0	-0.071409	-0.955310	-0.206384
42	1	0	0.951841	-1.137163	-0.541073
43	6	0	-1.114375	-1.137385	2.174897
44	7	0	-2.016450	-1.246738	2.900519
45	6	0	-0.945347	-1.920929	-0.984181
46	6	0	-2.199421	-2.369124	-0.551933
47	6	0	-0.471392	-2.377173	-2.222137
48	6	0	-2.954391	-3.236707	-1.339146
49	1	0	-2.594989	-2.039040	0.401777
50	6	0	-1.227797	-3.238108	-3.014148
51	1	0	0.510696	-2.054964	-2.564239
52	6	0	-2.476925	-3.671096	-2.574204
53	1	0	-3.923213	-3.574746	-0.982256
54	1	0	-0.837077	-3.576974	-3.969449
55	1	0	-3.070119	-4.345584	-3.184693
56	6	0	1.247695	-1.517565	2.042247
57	8	0	1.326262	-1.479595	3.267002

58	6	0	2.452706	-1.988904	1.269934
59	6	0	2.365284	-2.920740	0.232003
60	6	0	3.708912	-1.524095	1.673126
61	6	0	3.520177	-3.365334	-0.408852
62	1	0	1.395281	-3.309985	-0.069010
63	6	0	4.860080	-1.949931	1.017267
64	1	0	3.770022	-0.819897	2.498678
65	6	0	4.766278	-2.871757	-0.026106
66	1	0	3.444410	-4.097311	-1.207468
67	1	0	5.830342	-1.571012	1.324706
68	1	0	5.664145	-3.209700	-0.535216

3(*R*RS)

SCF Done: E(RM062X) = -1589.22349698

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.266485	0.004188	-0.826240
2	6	0	0.625705	-0.025818	-2.009416
3	1	0	-2.113352	0.932574	1.214949
4	1	0	0.761943	0.963469	-2.463388
5	1	0	0.252154	-0.723859	-2.763933
6	6	0	-1.081059	-1.129801	-0.721279
7	8	0	-0.942662	-2.217313	-1.293443

8	8	0	-2.207590	-0.956393	0.118191
9	6	0	-2.811037	-2.059008	0.661232
10	6	0	-2.086712	-3.129457	1.191278
11	6	0	-4.201849	-2.042398	0.743154
12	6	0	-2.768288	-4.181340	1.794718
13	1	0	-1.004577	-3.128822	1.126034
14	6	0	-4.873693	-3.097549	1.358527
15	1	0	-4.742571	-1.197890	0.325498
16	6	0	-4.161629	-4.173294	1.882887
17	1	0	-2.204145	-5.013486	2.206814
18	1	0	-5.957857	-3.075609	1.422630
19	1	0	-4.683716	-4.997209	2.359510
20	6	0	4.336753	0.019903	-0.933333
21	6	0	2.843110	0.423020	-0.902757
22	1	0	4.739796	0.031614	0.082746
23	1	0	4.913532	0.722612	-1.541127
24	1	0	2.402673	0.319585	0.089632
25	1	0	2.675233	1.437687	-1.272285
26	6	0	3.569008	-2.228227	-0.825397
27	1	0	3.783954	-3.256387	-1.128316
28	1	0	3.739593	-2.144687	0.252455
29	6	0	2.103714	-1.877301	-1.168569
30	1	0	1.654350	-2.557295	-1.893992
31	1	0	1.460857	-1.827032	-0.288164
32	6	0	2.778904	-0.578652	-3.120973
33	1	0	2.129757	-1.132116	-3.802334

34	1	0	2.872929	0.451752	-3.472636
35	6	0	4.148027	-1.266932	-2.924654
36	1	0	4.120684	-2.290416	-3.308112
37	1	0	4.920465	-0.716087	-3.467249
38	7	0	4.500489	-1.320201	-1.502824
39	7	0	2.081492	-0.512971	-1.793204
40	6	0	-1.091265	1.316271	1.242671
41	6	0	-0.511118	1.370184	-0.205915
42	1	0	0.466015	1.863237	-0.112118
43	6	0	-1.158344	2.660663	1.825495
44	7	0	-1.217813	3.726026	2.272779
45	6	0	-1.375430	2.296817	-1.056978
46	6	0	-2.636281	1.886657	-1.506871
47	6	0	-0.923771	3.573871	-1.396489
48	6	0	-3.426850	2.738527	-2.271910
49	1	0	-2.993015	0.891094	-1.252770
50	6	0	-1.710162	4.426838	-2.173147
51	1	0	0.054378	3.902891	-1.050446
52	6	0	-2.964722	4.011516	-2.610827
53	1	0	-4.404553	2.407748	-2.610928
54	1	0	-1.340046	5.414000	-2.435502
55	1	0	-3.579760	4.672300	-3.214696
56	6	0	-0.312654	0.341462	2.148796
57	8	0	-0.906137	-0.563470	2.694746
58	6	0	1.164834	0.496917	2.318394
59	6	0	1.897859	-0.657689	2.623212

60	6	0	1.826959	1.723416	2.196872
61	6	0	3.276140	-0.589688	2.791221
62	1	0	1.372688	-1.603824	2.717370
63	6	0	3.206266	1.791793	2.385328
64	1	0	1.281461	2.633978	1.970671
65	6	0	3.931191	0.638537	2.678102
66	1	0	3.839994	-1.489690	3.017649
67	1	0	3.712636	2.748416	2.301887
68	1	0	5.006986	0.694203	2.817147

3(*R*SR)

SCF Done: E(RM062X) = -1589.22369272

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.545461	-0.774322	-1.299437
2	6	0	-0.164751	-0.677125	0.229528
3	1	0	-1.144380	-0.533825	0.700053
4	6	0	0.607143	-0.773369	-2.201150
5	7	0	1.512395	-0.745191	-2.921337
6	6	0	0.375796	-1.967799	0.821086
7	6	0	1.052036	-2.949511	0.093365
8	6	0	0.202955	-2.164768	2.198196
9	6	0	1.551985	-4.089960	0.726035

10	1	0	1.189585	-2.846274	-0.978863
11	6	0	0.701458	-3.297130	2.832670
12	1	0	-0.324814	-1.407652	2.774957
13	6	0	1.382638	-4.266849	2.095189
14	1	0	2.073450	-4.841154	0.139827
15	1	0	0.554756	-3.426600	3.901207
16	1	0	1.772725	-5.154132	2.585035
17	6	0	-1.457593	-1.960784	-1.619879
18	8	0	-1.062178	-2.889638	-2.297035
19	6	0	-2.841748	-1.947302	-1.056666
20	6	0	-3.569782	-3.142719	-1.094369
21	6	0	-3.433865	-0.792603	-0.531455
22	6	0	-4.869569	-3.186282	-0.606250
23	1	0	-3.100746	-4.029745	-1.508504
24	6	0	-4.740178	-0.837362	-0.051633
25	1	0	-2.889021	0.147171	-0.496778
26	6	0	-5.456586	-2.031969	-0.085353
27	1	0	-5.427450	-4.117271	-0.631060
28	1	0	-5.195593	0.063433	0.348172
29	1	0	-6.473821	-2.065038	0.293506
30	6	0	0.681656	0.545668	0.552627
31	6	0	1.990053	0.504843	1.232944
32	1	0	-1.084559	0.155226	-1.514632
33	1	0	2.174538	-0.417516	1.791722
34	1	0	2.083542	1.361230	1.906975
35	6	0	0.094510	1.816547	0.514973

36	8	0	0.575939	2.914807	0.810962
37	8	0	-1.248547	1.765595	0.046816
38	6	0	-2.042291	2.880462	0.134914
39	6	0	-2.815872	3.199828	-0.980059
40	6	0	-2.158148	3.622130	1.311974
41	6	0	-3.709098	4.267850	-0.919541
42	1	0	-2.708876	2.606522	-1.884041
43	6	0	-3.047049	4.692187	1.357538
44	1	0	-1.552716	3.360300	2.171753
45	6	0	-3.825064	5.021019	0.246602
46	1	0	-4.311039	4.511702	-1.790100
47	1	0	-3.134839	5.270770	2.272768
48	1	0	-4.517346	5.856084	0.292250
49	6	0	4.793136	-0.418637	-1.276597
50	6	0	3.626427	-0.663271	-0.293711
51	1	0	4.423419	-0.394804	-2.306142
52	1	0	5.524324	-1.226855	-1.191298
53	1	0	2.730613	-1.020247	-0.798982
54	1	0	3.888462	-1.358348	0.508732
55	6	0	4.514398	1.942444	-1.329352
56	1	0	4.942372	2.884390	-0.975065
57	1	0	4.410359	2.000672	-2.416087
58	6	0	3.130395	1.695970	-0.686164
59	1	0	2.713961	2.576499	-0.193432
60	1	0	2.398286	1.314196	-1.399490
61	6	0	4.426430	1.015645	1.258264

62	1	0	4.221298	2.029333	1.610747
63	1	0	4.414985	0.330895	2.109541
64	6	0	5.737334	0.928638	0.441918
65	1	0	6.355289	1.806904	0.645425
66	1	0	6.306320	0.036780	0.718532
67	7	0	5.448000	0.861925	-0.993654
68	7	0	3.282979	0.636320	0.364977

3(*S*RS)

SCF Done: E(RM062X) = -1589.21813616

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022557	1.391486	-1.330754
2	6	0	-0.026562	1.184604	0.233743
3	1	0	-1.074715	0.942073	0.425503
4	6	0	1.151360	2.211562	-1.776600
5	7	0	2.067425	2.832249	-2.112223
6	6	0	0.234994	2.476857	1.022885
7	6	0	0.022482	3.754533	0.489234
8	6	0	0.620820	2.389494	2.367242
9	6	0	0.206710	4.899259	1.264181
10	1	0	-0.293443	3.879597	-0.541537
11	6	0	0.800887	3.530325	3.144902

12	1	0	0.779567	1.410518	2.810412
13	6	0	0.599368	4.794713	2.595321
14	1	0	0.040794	5.876131	0.818790
15	1	0	1.102067	3.428652	4.183805
16	1	0	0.745847	5.686904	3.197128
17	6	0	-1.287532	1.918209	-1.934965
18	8	0	-1.352798	3.020928	-2.440634
19	6	0	-2.473796	1.007831	-1.896705
20	6	0	-2.406364	-0.319806	-1.454410
21	6	0	-3.695149	1.525126	-2.347243
22	6	0	-3.550166	-1.114842	-1.464139
23	1	0	-1.473538	-0.746418	-1.091453
24	6	0	-4.833696	0.729621	-2.354858
25	1	0	-3.733955	2.554991	-2.687735
26	6	0	-4.761203	-0.592101	-1.913217
27	1	0	-3.492599	-2.143253	-1.117970
28	1	0	-5.777153	1.136649	-2.705143
29	1	0	-5.650699	-1.215085	-1.917727
30	6	0	0.760682	-0.013781	0.723628
31	6	0	2.234326	0.076426	0.903293
32	1	0	0.174277	0.399799	-1.767015
33	1	0	2.609745	1.089176	0.716714
34	1	0	2.540719	-0.240382	1.907431
35	6	0	0.134531	-0.993503	1.501712
36	8	0	0.644406	-1.915603	2.147591
37	8	0	-1.280837	-0.851996	1.570336

38	6	0	-2.059606	-1.964878	1.468315
39	6	0	-3.357013	-1.863992	1.975569
40	6	0	-1.654276	-3.129576	0.808900
41	6	0	-4.252003	-2.916637	1.811002
42	1	0	-3.649936	-0.947987	2.479853
43	6	0	-2.559308	-4.178172	0.656267
44	1	0	-0.642767	-3.212624	0.426681
45	6	0	-3.860097	-4.080583	1.149828
46	1	0	-5.261023	-2.824381	2.202715
47	1	0	-2.240916	-5.080133	0.140723
48	1	0	-4.558628	-4.901796	1.023806
49	6	0	4.560044	-0.655107	0.464745
50	6	0	5.490877	-1.382012	-0.534834
51	1	0	4.767003	0.415293	0.525645
52	1	0	4.605606	-1.087599	1.466658
53	1	0	6.036326	-0.658349	-1.146544
54	1	0	6.217903	-1.986848	0.012899
55	6	0	3.065781	-0.399566	-1.435379
56	1	0	2.011242	-0.400064	-1.710356
57	1	0	3.460241	0.616944	-1.494559
58	6	0	3.879641	-1.405851	-2.281960
59	1	0	3.210473	-2.055564	-2.852450
60	1	0	4.514494	-0.862718	-2.986558
61	6	0	3.845095	-3.097049	-0.611516
62	1	0	3.371129	-3.843858	-1.253854
63	1	0	4.467217	-3.620522	0.119913

64	6	0	2.761169	-2.258625	0.103409
65	1	0	1.778192	-2.348062	-0.364143
66	1	0	2.659539	-2.491347	1.162272
67	7	0	3.137852	-0.807620	0.001855
68	7	0	4.718197	-2.248658	-1.427832

3(*S*SR)

SCF Done: E(RM062X) = -1589.22346973

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.311961	-0.059166	0.819077
2	6	0	0.549331	-0.182481	2.019323
3	1	0	-2.083772	1.024657	-1.209320
4	1	0	0.682121	0.771248	2.544901
5	1	0	0.150717	-0.927820	2.713514
6	6	0	-1.127634	-1.177522	0.608030
7	8	0	-1.007930	-2.305031	1.101570
8	8	0	-2.230919	-0.937701	-0.245808
9	6	0	-2.803212	-1.995355	-0.901085
10	6	0	-4.191403	-1.993190	-1.018382
11	6	0	-2.046293	-3.001913	-1.505502
12	6	0	-4.827858	-2.998466	-1.745142
13	1	0	-4.757240	-1.198723	-0.540396

14	6	0	-2.692302	-4.004910	-2.220519
15	1	0	-0.966119	-2.987555	-1.412488
16	6	0	-4.083038	-4.010707	-2.345094
17	1	0	-5.910256	-2.988610	-1.836175
18	1	0	-2.102925	-4.787084	-2.690944
19	1	0	-4.578697	-4.797163	-2.905901
20	6	0	2.664680	-0.841385	3.145416
21	6	0	4.037576	-1.519139	2.936499
22	1	0	2.751685	0.157615	3.579519
23	1	0	1.994626	-1.443441	3.761900
24	1	0	4.797654	-1.008119	3.532912
25	1	0	3.999507	-2.565769	3.250257
26	6	0	2.803294	0.325409	1.013923
27	1	0	2.382711	0.312857	0.007533
28	1	0	2.641565	1.308308	1.463096
29	6	0	4.291001	-0.102138	1.043464
30	1	0	4.713540	-0.028298	0.038055
31	1	0	4.865355	0.549847	1.707622
32	6	0	3.505605	-2.328585	0.761319
33	1	0	3.710400	-2.177048	-0.303069
34	1	0	3.699965	-3.376778	1.002769
35	6	0	2.034168	-1.981243	1.082122
36	1	0	1.421965	-1.853534	0.187861
37	1	0	1.550247	-2.706714	1.738150
38	7	0	2.007573	-0.667695	1.807245
39	7	0	4.425937	-1.479295	1.524269

40	6	0	-1.063826	1.412366	-1.168546
41	6	0	-0.534206	1.351024	0.299257
42	1	0	0.447500	1.843255	0.274795
43	6	0	-1.117131	2.797656	-1.648048
44	7	0	-1.164051	3.894319	-2.013797
45	6	0	-1.419530	2.215754	1.192835
46	6	0	-2.679663	1.768668	1.606646
47	6	0	-0.982505	3.474714	1.610988
48	6	0	-3.483118	2.566843	2.415683
49	1	0	-3.025659	0.787500	1.289866
50	6	0	-1.781878	4.273637	2.430017
51	1	0	-0.004272	3.831083	1.293447
52	6	0	-3.035231	3.821625	2.833077
53	1	0	-4.459859	2.208313	2.728336
54	1	0	-1.422316	5.246226	2.753833
55	1	0	-3.660362	4.439915	3.470620
56	6	0	-0.245904	0.511353	-2.115337
57	8	0	-0.811778	-0.362771	-2.735620
58	6	0	1.234447	0.693283	-2.229436
59	6	0	1.882519	1.909100	-1.985419
60	6	0	1.986987	-0.428536	-2.602432
61	6	0	3.266780	1.999978	-2.120655
62	1	0	1.323728	2.795515	-1.702649
63	6	0	3.369325	-0.339719	-2.717253
64	1	0	1.472809	-1.366843	-2.789239
65	6	0	4.010467	0.878541	-2.481732

66	1	0	3.762379	2.949280	-1.942811
67	1	0	3.947969	-1.215488	-2.995279
68	1	0	5.089955	0.951140	-2.578148

TS3/P(*R*RS)

SCF Done: E(RM062X) = -1589.21059535

Imaginary Frequencies = -137.9798

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.485848	0.112565	-1.082443
2	6	0	0.407572	0.072130	-2.129407
3	1	0	-1.908064	0.660815	1.327951
4	1	0	0.870546	0.993845	-2.476759
5	1	0	0.301253	-0.715545	-2.869281
6	6	0	-1.264566	-1.098876	-0.897131
7	8	0	-1.058457	-2.178012	-1.419636
8	8	0	-2.358334	-0.914723	-0.073427
9	6	0	-3.089686	-2.022638	0.319800
10	6	0	-2.488060	-3.069212	1.014367
11	6	0	-4.456345	-2.012840	0.068700
12	6	0	-3.278708	-4.126962	1.453467
13	1	0	-1.421325	-3.038980	1.206633
14	6	0	-5.238716	-3.074430	0.520972

15	1	0	-4.894577	-1.177737	-0.469741
16	6	0	-4.652919	-4.134152	1.209601
17	1	0	-2.817298	-4.948633	1.993282
18	1	0	-6.307629	-3.070610	0.329712
19	1	0	-5.263341	-4.962221	1.556578
20	6	0	4.614744	-0.293697	-0.986400
21	6	0	3.192600	0.311320	-1.156162
22	1	0	4.999161	-0.099866	0.019996
23	1	0	5.313981	0.140070	-1.708202
24	1	0	2.773160	0.632211	-0.198074
25	1	0	3.193430	1.167339	-1.838957
26	6	0	3.546607	-2.320919	-0.330435
27	1	0	3.596768	-3.412094	-0.398534
28	1	0	3.784385	-2.033111	0.699363
29	6	0	2.138983	-1.811287	-0.742987
30	1	0	1.543465	-2.589868	-1.227539
31	1	0	1.562681	-1.432797	0.109558
32	6	0	2.878501	-1.248589	-2.951076
33	1	0	2.147011	-1.919833	-3.412589
34	1	0	3.049231	-0.404229	-3.627153
35	6	0	4.201116	-1.992327	-2.605299
36	1	0	4.084919	-3.072644	-2.737744
37	1	0	5.016359	-1.655424	-3.252838
38	7	0	4.576907	-1.744424	-1.207051
39	7	0	2.297725	-0.717012	-1.709308
40	6	0	-0.955678	1.185950	1.227762

41	6	0	-0.665246	1.407915	-0.300699
42	1	0	0.301379	1.921936	-0.352592
43	6	0	-1.105699	2.450182	1.953262
44	7	0	-1.247525	3.441545	2.531739
45	6	0	-1.693603	2.370577	-0.886719
46	6	0	-2.925586	1.934939	-1.384537
47	6	0	-1.404753	3.738786	-0.914131
48	6	0	-3.848009	2.848813	-1.889508
49	1	0	-3.163440	0.875582	-1.381741
50	6	0	-2.324911	4.654609	-1.421123
51	1	0	-0.446634	4.088423	-0.534656
52	6	0	-3.552050	4.211182	-1.909148
53	1	0	-4.800472	2.493374	-2.272214
54	1	0	-2.079646	5.712635	-1.437855
55	1	0	-4.271306	4.921185	-2.306508
56	6	0	0.101880	0.260123	1.852550
57	8	0	-0.206912	-0.895055	2.067770
58	6	0	1.493756	0.743024	2.104635
59	6	0	2.425192	-0.208404	2.544594
60	6	0	1.913701	2.059875	1.879425
61	6	0	3.752503	0.146340	2.747915
62	1	0	2.091695	-1.227451	2.715636
63	6	0	3.245679	2.412750	2.083547
64	1	0	1.225148	2.824307	1.536787
65	6	0	4.165246	1.459371	2.513892
66	1	0	4.466734	-0.598237	3.086678

67	1	0	3.562416	3.435130	1.902970
68	1	0	5.203709	1.737289	2.668809

TS3/P(*R*SR)

SCF Done: E(RM062X) = -1589.21152246

Imaginary Frequencies = -135.8430

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.736846	-0.701265	-1.077961
2	6	0	-0.359658	-0.727886	0.446016
3	1	0	-1.330502	-0.616484	0.941569
4	6	0	0.405728	-0.619694	-1.990929
5	7	0	1.285810	-0.531651	-2.736098
6	6	0	0.199578	-2.056906	0.921532
7	6	0	1.036586	-2.866918	0.149959
8	6	0	-0.109888	-2.465903	2.224081
9	6	0	1.555703	-4.052815	0.671765
10	1	0	1.282303	-2.594307	-0.871431
11	6	0	0.407348	-3.646542	2.747999
12	1	0	-0.762305	-1.843595	2.832860
13	6	0	1.246402	-4.445227	1.970847
14	1	0	2.201034	-4.670649	0.054145
15	1	0	0.151601	-3.944819	3.760562

16	1	0	1.649950	-5.369247	2.374011
17	6	0	-1.609901	-1.901797	-1.466657
18	8	0	-1.172640	-2.774352	-2.188675
19	6	0	-2.994308	-1.969899	-0.911271
20	6	0	-3.678420	-3.184819	-1.038448
21	6	0	-3.629199	-0.876832	-0.309074
22	6	0	-4.977744	-3.309829	-0.564003
23	1	0	-3.175423	-4.021890	-1.511950
24	6	0	-4.934252	-1.003728	0.159388
25	1	0	-3.122130	0.079109	-0.204823
26	6	0	-5.607134	-2.217523	0.034834
27	1	0	-5.501238	-4.255950	-0.660749
28	1	0	-5.424258	-0.152478	0.621368
29	1	0	-6.623589	-2.313219	0.404975
30	6	0	0.490631	0.458164	0.881776
31	6	0	1.704852	0.365458	1.519565
32	1	0	-1.306102	0.220572	-1.240392
33	1	0	2.078636	-0.596806	1.858660
34	1	0	2.051701	1.235357	2.069840
35	6	0	-0.064407	1.800138	0.792674
36	8	0	0.501997	2.849232	1.023034
37	8	0	-1.399268	1.773679	0.420862
38	6	0	-2.106646	2.962028	0.333011
39	6	0	-2.785481	3.210049	-0.854959
40	6	0	-2.205009	3.830308	1.417248
41	6	0	-3.575994	4.352945	-0.961853

42	1	0	-2.690334	2.509668	-1.679871
43	6	0	-2.992043	4.972000	1.295017
44	1	0	-1.670286	3.612188	2.334882
45	6	0	-3.678019	5.237500	0.109599
46	1	0	-4.109547	4.549828	-1.886858
47	1	0	-3.071321	5.656570	2.134303
48	1	0	-4.291141	6.129369	0.024464
49	6	0	5.109820	-0.458683	-1.123984
50	6	0	3.785048	-0.660054	-0.335364
51	1	0	5.007266	-0.821216	-2.151613
52	1	0	5.934513	-1.001339	-0.651032
53	1	0	2.959256	-0.931040	-0.996927
54	1	0	3.880728	-1.434378	0.433420
55	6	0	4.308257	1.716063	-1.673269
56	1	0	4.605860	2.756337	-1.838552
57	1	0	4.031478	1.283352	-2.640715
58	6	0	3.126385	1.634858	-0.671183
59	1	0	2.978507	2.574637	-0.131046
60	1	0	2.182481	1.375092	-1.160496
61	6	0	4.556527	1.047041	1.153662
62	1	0	4.233967	1.908638	1.747570
63	1	0	4.812714	0.231067	1.837564
64	6	0	5.743541	1.409783	0.213335
65	1	0	5.905262	2.492230	0.191521
66	1	0	6.668098	0.934513	0.555126
67	7	0	5.464229	0.965964	-1.159286

68	7	0	3.426156	0.601449	0.327916

TS3/P(*S*RS)

SCF Done: E(RM062X) = -1589.20675607

Imaginary Frequencies = -168.6421

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.053235	1.311243	-1.116440
2	6	0	-0.113665	1.224646	0.442364
3	1	0	-1.177580	1.006738	0.577780
4	6	0	1.326854	1.915512	-1.514495
5	7	0	2.346995	2.368521	-1.816436
6	6	0	0.141003	2.539056	1.184801
7	6	0	0.219018	3.784967	0.554993
8	6	0	0.223551	2.506527	2.584678
9	6	0	0.392676	4.954804	1.297688
10	1	0	0.142211	3.873392	-0.523268
11	6	0	0.388948	3.670750	3.326440
12	1	0	0.159039	1.550575	3.096480
13	6	0	0.480575	4.905475	2.684099
14	1	0	0.458644	5.907388	0.779740
15	1	0	0.448886	3.612545	4.409563
16	1	0	0.617549	5.816674	3.258927

17	6	0	-1.115601	2.000657	-1.838970
18	8	0	-0.965469	3.062890	-2.407984
19	6	0	-2.443044	1.315589	-1.808167
20	6	0	-2.595874	-0.038687	-1.486870
21	6	0	-3.570110	2.080861	-2.133772
22	6	0	-3.862822	-0.616312	-1.488710
23	1	0	-1.738082	-0.657415	-1.240748
24	6	0	-4.833322	1.503621	-2.127993
25	1	0	-3.438367	3.129062	-2.383619
26	6	0	-4.980313	0.153906	-1.805087
27	1	0	-3.974635	-1.669468	-1.245529
28	1	0	-5.704030	2.102864	-2.375193
29	1	0	-5.967792	-0.298120	-1.801876
30	6	0	0.638704	0.044379	1.031261
31	6	0	1.980868	0.069320	1.359494
32	1	0	0.087263	0.276629	-1.476507
33	1	0	2.523638	1.011683	1.296123
34	1	0	2.334006	-0.624823	2.115856
35	6	0	-0.053395	-1.187518	1.334110
36	8	0	0.450647	-2.247646	1.664343
37	8	0	-1.429014	-1.057914	1.242694
38	6	0	-2.227518	-2.178945	1.170305
39	6	0	-3.395482	-2.168769	1.925895
40	6	0	-1.948720	-3.224304	0.290654
41	6	0	-4.302731	-3.218204	1.796038
42	1	0	-3.586018	-1.335479	2.595113

43	6	0	-2.861566	-4.269444	0.173691
44	1	0	-1.034029	-3.213992	-0.292910
45	6	0	-4.039908	-4.270566	0.921287
46	1	0	-5.217512	-3.209140	2.380900
47	1	0	-2.651084	-5.085435	-0.511362
48	1	0	-4.748682	-5.086522	0.820800
49	6	0	4.402477	-0.076951	-0.335942
50	6	0	5.258088	-0.870399	-1.365812
51	1	0	4.016993	0.853814	-0.760324
52	1	0	4.971372	0.162449	0.568032
53	1	0	5.146226	-0.446945	-2.368888
54	1	0	6.317972	-0.833948	-1.096760
55	6	0	2.537845	-1.370304	-1.124892
56	1	0	1.608662	-1.849326	-0.797756
57	1	0	2.284620	-0.486406	-1.715907
58	6	0	3.456030	-2.331593	-1.929389
59	1	0	3.108152	-3.366154	-1.848624
60	1	0	3.462716	-2.056907	-2.988455
61	6	0	4.832228	-2.809046	-0.047729
62	1	0	4.630770	-3.883826	-0.087952
63	1	0	5.833131	-2.666191	0.371096
64	6	0	3.761857	-2.085051	0.812071
65	1	0	2.898344	-2.718685	1.032401
66	1	0	4.178347	-1.731502	1.760741
67	7	0	3.259802	-0.912712	0.069484
68	7	0	4.830437	-2.274877	-1.415035

TS3/P(*S*SR)

SCF Done: E(RM062X) = -1589.21095959

Imaginary Frequencies = -157.4215

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.432446	0.106786	1.008744
2	6	0	0.472705	0.039459	2.050590
3	1	0	-1.750997	0.690638	-1.492436
4	1	0	0.937722	0.954568	2.413561
5	1	0	0.332286	-0.742136	2.792175
6	6	0	-1.256076	-1.067902	0.823481
7	8	0	-1.088332	-2.168864	1.315850
8	8	0	-2.353028	-0.812450	0.022811
9	6	0	-3.135072	-1.879915	-0.381643
10	6	0	-4.470854	-1.895045	0.000528
11	6	0	-2.607646	-2.861252	-1.216554
12	6	0	-5.297983	-2.916640	-0.464982
13	1	0	-4.847179	-1.111084	0.650887
14	6	0	-3.441201	-3.879705	-1.668950
15	1	0	-1.562801	-2.808224	-1.504695
16	6	0	-4.785986	-3.910521	-1.296210
17	1	0	-6.344011	-2.933428	-0.173799

18	1	0	-3.039766	-4.649253	-2.321734
19	1	0	-5.432070	-4.705656	-1.655446
20	6	0	2.827060	-1.368911	2.895094
21	6	0	4.147058	-2.125917	2.569720
22	1	0	2.985303	-0.559241	3.615016
23	1	0	2.063245	-2.043808	3.294044
24	1	0	4.945055	-1.824285	3.254827
25	1	0	4.007186	-3.207262	2.664609
26	6	0	3.253494	0.256457	1.182596
27	1	0	2.874597	0.640023	0.231521
28	1	0	3.258926	1.074200	1.910496
29	6	0	4.660536	-0.386237	1.025226
30	1	0	5.073181	-0.170684	0.034641
31	1	0	5.354462	0.003779	1.776361
32	6	0	3.562833	-2.358308	0.263726
33	1	0	3.847543	-2.045988	-0.746755
34	1	0	3.577329	-3.451944	0.298475
35	6	0	2.155886	-1.818940	0.638502
36	1	0	1.628098	-1.388116	-0.219147
37	1	0	1.515279	-2.593903	1.068314
38	7	0	2.308722	-0.769210	1.655004
39	7	0	4.576364	-1.841316	1.194530
40	6	0	-0.834478	1.246178	-1.286015
41	6	0	-0.667919	1.413131	0.260290
42	1	0	0.237306	2.011414	0.415992
43	6	0	-0.978500	2.545238	-1.949421

44	7	0	-1.115603	3.569383	-2.468976
45	6	0	-1.823547	2.215116	0.858301
46	6	0	-3.140728	2.136618	0.395885
47	6	0	-1.550081	3.042788	1.953080
48	6	0	-4.156536	2.859967	1.021146
49	1	0	-3.391373	1.506939	-0.452408
50	6	0	-2.562203	3.763513	2.580309
51	1	0	-0.527700	3.119798	2.316885
52	6	0	-3.873720	3.672769	2.115874
53	1	0	-5.173378	2.785639	0.646247
54	1	0	-2.324675	4.399253	3.428457
55	1	0	-4.667157	4.233652	2.600812
56	6	0	0.277770	0.367951	-1.875869
57	8	0	0.002566	-0.789059	-2.127992
58	6	0	1.665685	0.884972	-2.055084
59	6	0	2.051241	2.193801	-1.741266
60	6	0	2.628582	-0.025190	-2.513935
61	6	0	3.382595	2.579898	-1.878607
62	1	0	1.334304	2.922324	-1.378882
63	6	0	3.954543	0.362703	-2.651298
64	1	0	2.319671	-1.038135	-2.753238
65	6	0	4.333964	1.667820	-2.329610
66	1	0	3.674264	3.595093	-1.628949
67	1	0	4.693886	-0.349383	-3.005632
68	1	0	5.371567	1.972101	-2.431339

P(*R*RS)

SCF Done: E(RM062X) = -1244.02133061

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.339314	0.115558	-0.990882
2	6	0	0.660555	0.004063	-1.868103
3	1	0	-1.615632	0.627769	1.509675
4	1	0	1.330698	0.835351	-2.068230
5	1	0	0.823847	-0.923304	-2.408214
6	6	0	-1.167205	-1.116643	-0.779419
7	8	0	-0.912721	-2.202232	-1.234453
8	8	0	-2.261438	-0.876247	-0.014944
9	6	0	-3.058275	-1.972653	0.325316
10	6	0	-2.760333	-2.671826	1.487027
11	6	0	-4.148474	-2.291308	-0.472109
12	6	0	-3.589125	-3.727090	1.860656
13	1	0	-1.893838	-2.382819	2.073214
14	6	0	-4.969528	-3.349195	-0.085612
15	1	0	-4.346264	-1.718353	-1.373134
16	6	0	-4.691768	-4.066529	1.077202
17	1	0	-3.371091	-4.284107	2.766739
18	1	0	-5.828176	-3.611064	-0.696158
19	1	0	-5.334456	-4.889979	1.372702

20	6	0	-0.675808	1.148185	1.310906
21	6	0	-0.561724	1.415823	-0.232694
22	1	0	0.358656	1.989037	-0.379800
23	6	0	-0.713716	2.381086	2.099846
24	7	0	-0.762719	3.343401	2.738713
25	6	0	-1.697557	2.291957	-0.748957
26	6	0	-2.812795	1.788127	-1.422968
27	6	0	-1.595780	3.676892	-0.566891
28	6	0	-3.811528	2.646046	-1.881362
29	1	0	-2.911160	0.724173	-1.606613
30	6	0	-2.595123	4.534014	-1.018698
31	1	0	-0.716687	4.088836	-0.076955
32	6	0	-3.711179	4.019371	-1.675433
33	1	0	-4.669032	2.233901	-2.405251
34	1	0	-2.494037	5.604689	-0.867299
35	1	0	-4.489860	4.685536	-2.034669
36	6	0	0.436559	0.180373	1.766642
37	8	0	0.135419	-0.989026	1.904465
38	6	0	1.840262	0.642481	1.962095
39	6	0	2.758368	-0.299317	2.448115
40	6	0	2.274542	1.942070	1.673301
41	6	0	4.085170	0.054161	2.650960
42	1	0	2.413006	-1.304761	2.666003
43	6	0	3.607637	2.290958	1.871647
44	1	0	1.593727	2.695469	1.291805
45	6	0	4.511392	1.351428	2.362350

46	1	0	4.788558	-0.678387	3.034139
47	1	0	3.937127	3.299489	1.643224
48	1	0	5.549291	1.628856	2.521096

P(*R*SR)

SCF Done: E(RM062X) = -1244.02583319

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.612233	-0.636393	-1.107271
2	6	0	-0.236014	-0.662845	0.417935
3	1	0	-1.185057	-0.504509	0.937990
4	6	0	0.569626	-0.561897	-1.971290
5	7	0	1.507406	-0.468228	-2.639807
6	6	0	0.287015	-2.015930	0.862634
7	6	0	1.404001	-2.627427	0.279725
8	6	0	-0.395505	-2.693411	1.877225
9	6	0	1.829695	-3.880834	0.712463
10	1	0	1.954256	-2.126879	-0.511603
11	6	0	0.031073	-3.946599	2.312791
12	1	0	-1.271313	-2.233265	2.328878
13	6	0	1.146330	-4.543566	1.730872
14	1	0	2.699024	-4.339712	0.251023
15	1	0	-0.510806	-4.455239	3.104543

16	1	0	1.481379	-5.520338	2.066730
17	6	0	-1.451905	-1.867512	-1.478765
18	8	0	-0.985540	-2.733099	-2.188553
19	6	0	-2.824580	-1.972076	-0.904189
20	6	0	-3.462442	-3.215906	-0.984089
21	6	0	-3.486357	-0.889802	-0.311634
22	6	0	-4.744100	-3.378295	-0.474113
23	1	0	-2.938447	-4.045646	-1.447733
24	6	0	-4.773163	-1.054799	0.193233
25	1	0	-3.016624	0.088120	-0.245306
26	6	0	-5.400298	-2.296687	0.115256
27	1	0	-5.232877	-4.345700	-0.534837
28	1	0	-5.284076	-0.212071	0.647989
29	1	0	-6.402232	-2.422372	0.514682
30	6	0	0.656179	0.518819	0.754694
31	6	0	1.929950	0.448132	1.143231
32	1	0	-1.193818	0.272276	-1.301201
33	1	0	2.442964	-0.498969	1.270647
34	1	0	2.483705	1.357042	1.357643
35	6	0	0.066782	1.892318	0.646106
36	8	0	0.682507	2.925384	0.690154
37	8	0	-1.284772	1.834581	0.496105
38	6	0	-1.989508	3.028120	0.328303
39	6	0	-2.639294	3.219581	-0.883344
40	6	0	-2.081778	3.945333	1.367924
41	6	0	-3.403841	4.371061	-1.060317

42	1	0	-2.541237	2.476401	-1.669467
43	6	0	-2.845806	5.093390	1.175613
44	1	0	-1.565717	3.760248	2.304370
45	6	0	-3.506138	5.308327	-0.034213
46	1	0	-3.916980	4.532927	-2.003194
47	1	0	-2.926675	5.821552	1.976849
48	1	0	-4.099858	6.206075	-0.176112

P(*S*RS)

SCF Done: E(RM062X) = -1244.02543707

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.099322	0.734547	-0.996895
2	6	0	-0.276488	0.998362	0.534737
3	1	0	-1.324951	0.764418	0.738016
4	6	0	1.306602	0.764008	-1.411602
5	7	0	2.421630	0.760779	-1.714615
6	6	0	-0.066193	2.437952	0.972699
7	6	0	0.843346	3.316171	0.377738
8	6	0	-0.821082	2.888649	2.062125
9	6	0	0.991992	4.615278	0.865771
10	1	0	1.439781	3.007234	-0.474691
11	6	0	-0.671867	4.181979	2.550916

12	1	0	-1.534808	2.212269	2.527101
13	6	0	0.238652	5.051655	1.951681
14	1	0	1.701505	5.285964	0.390182
15	1	0	-1.269736	4.511273	3.395566
16	1	0	0.356600	6.063504	2.327665
17	6	0	-0.923292	1.720288	-1.839468
18	8	0	-0.369282	2.557612	-2.519926
19	6	0	-2.409913	1.627662	-1.758777
20	6	0	-3.074268	0.508096	-1.243914
21	6	0	-3.151296	2.711483	-2.244463
22	6	0	-4.465460	0.476998	-1.217467
23	1	0	-2.522265	-0.350546	-0.871190
24	6	0	-4.539378	2.680573	-2.208634
25	1	0	-2.623822	3.572591	-2.642739
26	6	0	-5.197448	1.561934	-1.695577
27	1	0	-4.975199	-0.396360	-0.822845
28	1	0	-5.110013	3.526676	-2.578874
29	1	0	-6.282785	1.536500	-1.668973
30	6	0	0.565364	0.005063	1.318203
31	6	0	1.733324	0.292830	1.894478
32	1	0	-0.451911	-0.285229	-1.192900
33	1	0	2.152606	1.294235	1.863668
34	1	0	2.291530	-0.478130	2.416700
35	6	0	0.080652	-1.406034	1.428520
36	8	0	0.648002	-2.300453	2.000596
37	8	0	-1.109853	-1.566304	0.788154

38	6	0	-1.731018	-2.814917	0.832760
39	6	0	-2.202371	-3.318787	2.039378
40	6	0	-1.924446	-3.480928	-0.369322
41	6	0	-2.882774	-4.533229	2.033629
42	1	0	-2.039056	-2.767131	2.959698
43	6	0	-2.612077	-4.693545	-0.360563
44	1	0	-1.541312	-3.052162	-1.290537
45	6	0	-3.089613	-5.220734	0.837476
46	1	0	-3.257012	-4.939485	2.968197
47	1	0	-2.773219	-5.223112	-1.294444
48	1	0	-3.625318	-6.164796	0.840181

P(*S*SR)

SCF Done: E(RM062X) = -1244.02423924

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.237683	0.179567	0.894360
2	6	0	0.863136	0.067290	1.640030
3	1	0	-1.572720	0.683048	-1.611776
4	1	0	1.556353	0.896326	1.752027
5	1	0	1.090362	-0.860942	2.155508
6	6	0	-1.106432	-1.031621	0.773233
7	8	0	-0.867298	-2.111328	1.250198

8	8	0	-2.220941	-0.765370	0.049238
9	6	0	-3.058979	-1.828456	-0.285186
10	6	0	-4.336742	-1.853084	0.253985
11	6	0	-2.622092	-2.780647	-1.198401
12	6	0	-5.205106	-2.872898	-0.134399
13	1	0	-4.639033	-1.082813	0.956780
14	6	0	-3.497728	-3.795807	-1.572425
15	1	0	-1.618079	-2.710368	-1.605249
16	6	0	-4.787483	-3.843925	-1.042209
17	1	0	-6.209651	-2.905521	0.276149
18	1	0	-3.171101	-4.548223	-2.283814
19	1	0	-5.466762	-4.636565	-1.340274
20	6	0	-0.665062	1.241120	-1.370331
21	6	0	-0.589601	1.468163	0.169336
22	1	0	0.249890	2.145433	0.356915
23	6	0	-0.742921	2.512681	-2.093839
24	7	0	-0.823285	3.513568	-2.666757
25	6	0	-1.831518	2.135913	0.753952
26	6	0	-3.062896	2.206145	0.100544
27	6	0	-1.711718	2.699749	2.028993
28	6	0	-4.151502	2.829430	0.711738
29	1	0	-3.195820	1.772941	-0.886654
30	6	0	-2.796557	3.318867	2.640936
31	1	0	-0.754858	2.647468	2.544519
32	6	0	-4.023496	3.385498	1.981661
33	1	0	-5.102122	2.877057	0.188731

34	1	0	-2.682743	3.752151	3.630234
35	1	0	-4.872640	3.869570	2.454630
36	6	0	0.479985	0.316506	-1.833265
37	8	0	0.202386	-0.854607	-2.000831
38	6	0	1.875943	0.811418	-1.989553
39	6	0	2.275159	2.112966	-1.662655
40	6	0	2.825282	-0.102424	-2.468405
41	6	0	3.605885	2.491870	-1.817731
42	1	0	1.568185	2.843276	-1.284218
43	6	0	4.149534	0.280711	-2.627441
44	1	0	2.506004	-1.110057	-2.713892
45	6	0	4.541476	1.580317	-2.301586
46	1	0	3.908882	3.501638	-1.560038
47	1	0	4.877733	-0.430475	-3.004495
48	1	0	5.577651	1.881322	-2.424564

Part 2 In the presence of PhOH

PhOH

SCF Done: E(RM062X) = -307.343025435

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.805105	0.669198	-0.008904
2	6	0	-0.414454	0.646723	-0.011158
3	6	0	0.295361	1.849965	-0.015936
4	6	0	-0.387306	3.067824	-0.018572
5	6	0	-1.780533	3.075462	-0.016283
6	6	0	-2.497430	1.880724	-0.011485
7	1	0	-2.351721	-0.269535	-0.005016
8	1	0	0.136296	-0.288954	-0.009058
9	1	0	0.173169	3.999752	-0.022416
10	1	0	-2.305557	4.026435	-0.018464
11	1	0	-3.582717	1.892204	-0.009742
12	8	0	1.652849	1.775586	-0.017849
13	1	0	2.022135	2.675457	-0.019933

R_1_PhOH

SCF Done: E(RM062X) = -805.364840277

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.168116	-0.770938	-0.609704
2	6	0	-4.394306	-0.737807	-0.092253
3	1	0	-2.915211	-1.349023	-1.492096
4	1	0	-5.207700	-1.300399	-0.539349
5	1	0	-4.613756	-0.142773	0.790090
6	6	0	-2.082623	0.016903	0.010865
7	8	0	-2.195307	0.695022	1.011640
8	8	0	-0.942119	-0.105191	-0.693841
9	6	0	0.193399	0.597326	-0.287637
10	6	0	0.795122	0.332553	0.935919
11	6	0	0.728042	1.507225	-1.191382
12	6	0	1.960109	1.022472	1.265656
13	1	0	0.359389	-0.393691	1.614743
14	6	0	1.896990	2.183539	-0.851118
15	1	0	0.229162	1.674843	-2.140592
16	6	0	2.509814	1.947794	0.379232
17	1	0	2.434565	0.837954	2.224883
18	1	0	2.322903	2.899941	-1.546804
19	1	0	3.414274	2.485028	0.647466
20	6	0	-0.228089	3.173716	2.523091
21	6	0	-0.638089	3.693455	1.291205
22	6	0	-0.051663	4.858099	0.802106

23	6	0	0.930599	5.522557	1.534541
24	6	0	1.321861	5.007898	2.771240
25	6	0	0.751574	3.839442	3.267033
26	1	0	-1.403869	3.175516	0.719921
27	1	0	-0.371240	5.247402	-0.160858
28	1	0	1.382292	6.431257	1.149278
29	1	0	2.085037	5.516214	3.354091
30	1	0	1.059564	3.422937	4.221713
31	8	0	-0.752655	2.033743	3.033251
32	1	0	-1.248104	1.570453	2.328914

R_2_PhOH

SCF Done: E(RM062X) = -1053.34287005

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.666540	0.821841	0.151510
2	6	0	-1.848189	-0.384086	0.745574
3	1	0	-1.000169	-1.064256	0.697772
4	6	0	-2.710876	1.795591	-0.006104
5	7	0	-3.534504	2.595459	-0.153677
6	6	0	-3.026466	-0.937327	1.402270
7	6	0	-4.088158	-0.163813	1.901771
8	6	0	-3.068010	-2.333593	1.557203

9	6	0	-5.170124	-0.781245	2.515966
10	1	0	-4.061189	0.918088	1.839856
11	6	0	-4.159782	-2.947477	2.157832
12	1	0	-2.237202	-2.931977	1.192499
13	6	0	-5.213409	-2.170922	2.637304
14	1	0	-5.981084	-0.175327	2.907746
15	1	0	-4.184824	-4.027642	2.260964
16	1	0	-6.063966	-2.646554	3.116182
17	6	0	-0.391304	1.196940	-0.517115
18	8	0	-0.388869	2.126202	-1.318837
19	6	0	0.870052	0.470645	-0.204769
20	6	0	1.251291	0.214462	1.117088
21	6	0	1.749299	0.193698	-1.256818
22	6	0	2.518389	-0.296929	1.381985
23	1	0	0.578503	0.453106	1.935936
24	6	0	3.005600	-0.336737	-0.986957
25	1	0	1.449382	0.409273	-2.278125
26	6	0	3.394113	-0.571245	0.332345
27	1	0	2.823945	-0.474520	2.408390
28	1	0	3.686788	-0.554790	-1.803716
29	1	0	4.382440	-0.969734	0.541766
30	6	0	4.349823	3.194943	-1.757960
31	6	0	3.007646	3.178860	-1.367477
32	6	0	2.679533	3.238404	-0.008945
33	6	0	3.690955	3.285166	0.946833
34	6	0	5.031583	3.293496	0.564090

35	6	0	5.351221	3.255531	-0.793432
36	1	0	4.588440	3.150185	-2.816501
37	1	0	1.634728	3.243650	0.291377
38	1	0	3.423853	3.317565	1.999706
39	1	0	5.816592	3.332357	1.312830
40	1	0	6.391360	3.264682	-1.107261
41	8	0	2.064350	3.102006	-2.337374
42	1	0	1.202041	2.851510	-1.943478

TSR_1/1_PhOH

SCF Done: E(RM062X) = -1150.55147435

Imaginary Frequencies = -155.4593

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.697507	-2.071007	2.245081
2	6	0	-2.777918	-2.569353	1.580553
3	1	0	-1.587834	-2.146178	3.320645
4	1	0	-3.489319	-3.213982	2.087777
5	1	0	-2.768802	-2.612898	0.494848
6	6	0	-0.672990	-1.377551	1.506645
7	8	0	-0.657236	-1.159174	0.300835
8	8	0	0.346191	-0.960995	2.320870
9	6	0	1.496270	-0.429263	1.756293

10	6	0	1.962247	0.774527	2.274030
11	6	0	2.203811	-1.115429	0.772299
12	6	0	3.156020	1.306352	1.789477
13	1	0	1.391978	1.278302	3.048815
14	6	0	3.391505	-0.570469	0.293121
15	1	0	1.826333	-2.057308	0.389886
16	6	0	3.870595	0.638896	0.797152
17	1	0	3.524538	2.245531	2.190618
18	1	0	3.945930	-1.097956	-0.477172
19	1	0	4.798563	1.056191	0.418901
20	6	0	-6.421399	-0.232849	0.310099
21	6	0	-5.371583	-1.384278	0.359345
22	1	0	-7.396523	-0.578991	0.667417
23	1	0	-6.545554	0.138095	-0.711983
24	1	0	-5.831267	-2.341233	0.627841
25	1	0	-4.858942	-1.504414	-0.600866
26	6	0	-5.934444	0.419790	2.554866
27	1	0	-5.556116	1.242279	3.170313
28	1	0	-6.949906	0.184489	2.888720
29	6	0	-5.013281	-0.829544	2.663235
30	1	0	-4.230057	-0.695689	3.417903
31	1	0	-5.582716	-1.730490	2.913836
32	6	0	-3.637784	0.153564	0.968406
33	1	0	-2.920954	0.383007	1.764193
34	1	0	-3.072143	-0.073126	0.059250
35	6	0	-4.651149	1.310214	0.750469

36	1	0	-4.368947	2.196860	1.329198
37	1	0	-4.695302	1.595696	-0.305789
38	7	0	-5.997392	0.886347	1.163262
39	7	0	-4.360432	-1.056930	1.369891
40	6	0	-2.050739	3.236661	-1.084183
41	6	0	-1.411195	2.153025	-0.472817
42	6	0	-1.088429	2.217979	0.886855
43	6	0	-1.407133	3.356233	1.623801
44	6	0	-2.045073	4.438802	1.019596
45	6	0	-2.362412	4.369083	-0.337885
46	1	0	-2.296434	3.172843	-2.140148
47	1	0	-0.592222	1.375418	1.361124
48	1	0	-1.150683	3.392158	2.679224
49	1	0	-2.291319	5.324269	1.596855
50	1	0	-2.859726	5.204162	-0.823190
51	8	0	-1.127784	1.071393	-1.235694
52	1	0	-0.800566	0.339625	-0.670019

TSR_1/1-1_PhOH

SCF Done: E(RM062X) = -1150.55375460

Imaginary Frequencies = -150.1906

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

1	6	0	-0.619218	-2.567621	-1.168737
2	6	0	0.595371	-2.343182	-1.748040
3	1	0	-0.890426	-3.530395	-0.751462
4	1	0	1.243900	-3.174809	-2.006523
5	1	0	0.780779	-1.407763	-2.271595
6	6	0	-1.548516	-1.483325	-0.994618
7	8	0	-1.443184	-0.323333	-1.385209
8	8	0	-2.669531	-1.883899	-0.324945
9	6	0	-3.613700	-0.922445	0.006249
10	6	0	-4.878462	-1.026166	-0.557210
11	6	0	-3.310290	0.068421	0.935623
12	6	0	-5.863869	-0.114473	-0.181467
13	1	0	-5.078738	-1.814701	-1.275773
14	6	0	-4.299670	0.978441	1.296851
15	1	0	-2.313307	0.118413	1.364353
16	6	0	-5.576653	0.889523	0.740735
17	1	0	-6.856550	-0.191503	-0.614544
18	1	0	-4.072885	1.757392	2.018827
19	1	0	-6.345524	1.599437	1.029637
20	6	0	3.078069	-0.846778	-0.951914
21	6	0	4.093531	-0.349212	0.117482
22	1	0	3.565657	-1.447491	-1.727215
23	1	0	2.556529	-0.016496	-1.438362
24	1	0	5.085676	-0.780115	-0.050580
25	1	0	4.184584	0.741775	0.086844
26	6	0	2.733022	-2.793755	0.401756

27	1	0	1.960475	-3.466985	0.789036
28	1	0	3.331527	-3.342027	-0.332763
29	6	0	3.617586	-2.206385	1.542018
30	1	0	3.222053	-2.482348	2.524746
31	1	0	4.643081	-2.581758	1.470303
32	6	0	2.288373	-0.227958	1.672583
33	1	0	1.996368	-0.429571	2.708091
34	1	0	2.306926	0.858963	1.527975
35	6	0	1.305297	-0.895447	0.673845
36	1	0	0.601522	-1.570940	1.173227
37	1	0	0.719795	-0.157845	0.120445
38	7	0	2.067314	-1.687695	-0.296034
39	7	0	3.649948	-0.739594	1.462127
40	6	0	-0.132351	2.329328	-0.038043
41	6	0	0.135831	3.184463	1.028145
42	6	0	1.355431	3.855480	1.114692
43	6	0	2.311431	3.662372	0.116662
44	6	0	2.060265	2.803452	-0.950413
45	6	0	0.836546	2.131451	-1.028790
46	1	0	-1.081978	1.804220	-0.110351
47	1	0	-0.620432	3.327350	1.795173
48	1	0	1.558346	4.521556	1.947285
49	1	0	3.264950	4.180558	0.169359
50	1	0	2.800486	2.641743	-1.729069
51	8	0	0.638178	1.290880	-2.074680
52	1	0	-0.147638	0.722912	-1.901319

1_PhOH

SCF Done: E(RM062X) = -1150.56740005

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.204245	-0.640668	1.380276
2	6	0	-1.498465	-1.316616	1.196459
3	1	0	-0.005627	-0.070652	2.278925
4	1	0	-1.988449	-1.567671	2.141947
5	1	0	-1.410899	-2.217664	0.581589
6	6	0	0.771712	-0.755504	0.419507
7	8	0	0.733781	-1.384444	-0.673124
8	8	0	1.933747	-0.029736	0.734685
9	6	0	3.063591	-0.186865	-0.022931
10	6	0	3.761049	0.973278	-0.358491
11	6	0	3.569223	-1.439954	-0.377926
12	6	0	4.968842	0.883228	-1.046617
13	1	0	3.348483	1.934495	-0.067028
14	6	0	4.772164	-1.516956	-1.074611
15	1	0	3.018584	-2.334672	-0.112573
16	6	0	5.477898	-0.361427	-1.411422
17	1	0	5.509570	1.790572	-1.299846
18	1	0	5.163125	-2.491749	-1.352497

19	1	0	6.417093	-0.432391	-1.951457
20	6	0	-4.925984	-0.410550	-0.313812
21	6	0	-3.814676	-1.313455	0.272863
22	1	0	-5.668470	-0.170676	0.452287
23	1	0	-5.431087	-0.930027	-1.131851
24	1	0	-4.076713	-1.717187	1.253259
25	1	0	-3.547505	-2.135818	-0.395154
26	6	0	-3.853672	1.617950	0.322563
27	1	0	-3.309781	2.481766	-0.069516
28	1	0	-4.696717	1.981329	0.915609
29	6	0	-2.927557	0.751615	1.208772
30	1	0	-1.989950	1.253981	1.452907
31	1	0	-3.414059	0.421984	2.130424
32	6	0	-2.072488	-0.097149	-0.912192
33	1	0	-1.246091	0.596047	-0.750702
34	1	0	-1.683721	-1.004856	-1.374335
35	6	0	-3.238795	0.533325	-1.705042
36	1	0	-2.902446	1.452854	-2.191398
37	1	0	-3.591726	-0.154855	-2.479619
38	7	0	-4.362975	0.845685	-0.815495
39	7	0	-2.574625	-0.487898	0.446880
40	6	0	-0.747125	0.642502	-4.609916
41	6	0	-0.230989	-0.214740	-3.629319
42	6	0	-0.563637	-1.577140	-3.663569
43	6	0	-1.407929	-2.061629	-4.659505
44	6	0	-1.925217	-1.209618	-5.634955

45	6	0	-1.585763	0.143576	-5.601938
46	1	0	-0.482149	1.695323	-4.574504
47	1	0	-0.162531	-2.238744	-2.900124
48	1	0	-1.660703	-3.118468	-4.671286
49	1	0	-2.582797	-1.593530	-6.408432
50	1	0	-1.979785	0.821443	-6.354245
51	8	0	0.572270	0.308107	-2.681713
52	1	0	0.730851	-0.366350	-1.958877

1-1_PhOH

SCF Done: E(RM062X) = -1150.56880203

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.303152	-1.455988	0.035536
2	6	0	0.844370	-1.294436	-0.868185
3	1	0	-0.178668	-1.887142	1.020698
4	1	0	1.610752	-2.067777	-0.759121
5	1	0	0.530891	-1.253078	-1.914737
6	6	0	-1.554299	-1.063929	-0.379288
7	8	0	-1.925694	-0.540747	-1.464397
8	8	0	-2.557813	-1.352718	0.562070
9	6	0	-3.720624	-0.632417	0.525737
10	6	0	-4.909348	-1.325947	0.744012

11	6	0	-3.734655	0.756492	0.370230
12	6	0	-6.116178	-0.631631	0.803880
13	1	0	-4.872563	-2.404082	0.867365
14	6	0	-4.946547	1.438490	0.420524
15	1	0	-2.802231	1.288513	0.210442
16	6	0	-6.141859	0.751319	0.637117
17	1	0	-7.039001	-1.177706	0.977612
18	1	0	-4.954864	2.517617	0.294959
19	1	0	-7.083020	1.290933	0.677744
20	6	0	2.498878	0.244276	-1.906165
21	6	0	3.457960	1.423490	-1.631162
22	1	0	3.026605	-0.691846	-2.103337
23	1	0	1.805012	0.445102	-2.726569
24	1	0	4.471169	1.062568	-1.434135
25	1	0	3.488556	2.081403	-2.503805
26	6	0	2.543292	-0.049535	0.512038
27	1	0	1.928453	-0.373085	1.354925
28	1	0	3.294857	-0.813063	0.297981
29	6	0	3.166197	1.351409	0.730963
30	1	0	2.683029	1.860412	1.569220
31	1	0	4.230239	1.248011	0.958219
32	6	0	1.579551	2.487352	-0.637143
33	1	0	1.265917	3.209489	0.121285
34	1	0	1.439847	2.941754	-1.623794
35	6	0	0.737520	1.202135	-0.506872
36	1	0	0.289731	1.094870	0.481478

37	1	0	-0.050120	1.122668	-1.253526
38	7	0	1.649877	0.023596	-0.687314
39	7	0	3.006125	2.187587	-0.464535
40	6	0	-1.668511	2.321351	-2.907847
41	6	0	-1.753877	3.706953	-3.019148
42	6	0	-0.877253	4.412889	-3.842395
43	6	0	0.093626	3.713370	-4.560207
44	6	0	0.196260	2.329024	-4.453538
45	6	0	-0.684734	1.625153	-3.623789
46	1	0	-2.346777	1.763388	-2.266493
47	1	0	-2.518110	4.237161	-2.457230
48	1	0	-0.950291	5.492683	-3.925701
49	1	0	0.781895	4.249784	-5.207764
50	1	0	0.952787	1.776659	-5.004103
51	8	0	-0.539875	0.284305	-3.528142
52	1	0	-1.092910	-0.071753	-2.769735

TS1/2_PhOH(R*R*S)

SCF Done: E(RM062X) = -1896.55709539

Imaginary Frequencies = -119.7886

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.775208	-0.890555	0.575483

2	6	0	0.447572	-0.568397	-0.163949
3	1	0	-0.737579	-1.176141	1.619353
4	1	0	1.181380	-0.018474	0.438702
5	1	0	0.217723	0.000199	-1.071622
6	6	0	-1.985428	-0.978409	-0.125748
7	8	0	-2.199039	-0.731801	-1.316665
8	8	0	-3.023116	-1.381628	0.725046
9	6	0	-4.332440	-1.464803	0.341492
10	6	0	-5.112138	-2.311419	1.136825
11	6	0	-4.933281	-0.733227	-0.689790
12	6	0	-6.478131	-2.432830	0.907476
13	1	0	-4.626175	-2.859014	1.938787
14	6	0	-6.303308	-0.871349	-0.910770
15	1	0	-4.336563	-0.075817	-1.304875
16	6	0	-7.084083	-1.714170	-0.122333
17	1	0	-7.069675	-3.091151	1.537338
18	1	0	-6.764135	-0.301833	-1.713398
19	1	0	-8.149947	-1.807697	-0.306224
20	6	0	3.335667	-2.399034	-1.897662
21	6	0	2.368633	-1.239632	-1.570931
22	1	0	4.269029	-2.286255	-1.337685
23	1	0	3.569743	-2.396645	-2.965229
24	1	0	2.860710	-0.424096	-1.035626
25	1	0	1.874594	-0.839314	-2.460201
26	6	0	2.615844	-3.750407	-0.077471
27	1	0	2.063226	-4.657272	0.182446

28	1	0	3.616327	-3.818196	0.359147
29	6	0	1.894451	-2.496942	0.470296
30	1	0	1.083568	-2.743660	1.158441
31	1	0	2.576780	-1.792737	0.954190
32	6	0	0.442050	-2.723257	-1.472769
33	1	0	-0.256670	-3.175859	-0.767534
34	1	0	-0.123671	-2.136075	-2.199019
35	6	0	1.392043	-3.758084	-2.123705
36	1	0	0.992850	-4.765328	-1.980787
37	1	0	1.481491	-3.573030	-3.197693
38	7	0	2.734064	-3.685699	-1.536666
39	7	0	1.278392	-1.762182	-0.681737
40	6	0	0.091308	2.221317	1.259418
41	6	0	-1.156635	1.713117	0.986076
42	1	0	-1.437213	1.678304	-0.063664
43	6	0	0.617390	2.324561	2.586794
44	7	0	1.086357	2.423458	3.642883
45	6	0	-2.270033	1.474764	1.910611
46	6	0	-2.125235	1.125231	3.262420
47	6	0	-3.560962	1.598816	1.377960
48	6	0	-3.248715	0.916417	4.052538
49	1	0	-1.139829	0.979153	3.691310
50	6	0	-4.683977	1.401916	2.174830
51	1	0	-3.677204	1.849397	0.326008
52	6	0	-4.530124	1.058333	3.515369
53	1	0	-3.125138	0.632736	5.093383

54	1	0	-5.675890	1.499010	1.742779
55	1	0	-5.402778	0.889745	4.139444
56	6	0	1.070607	2.572095	0.215975
57	8	0	2.274662	2.625221	0.484657
58	6	0	0.630373	2.877822	-1.176318
59	6	0	1.471328	2.473571	-2.220249
60	6	0	-0.536119	3.595604	-1.459798
61	6	0	1.131270	2.754404	-3.538119
62	1	0	2.383753	1.931687	-1.984846
63	6	0	-0.862018	3.893810	-2.780624
64	1	0	-1.173911	3.941748	-0.651447
65	6	0	-0.036017	3.466418	-3.818358
66	1	0	1.776731	2.425395	-4.346750
67	1	0	-1.760784	4.462165	-2.998509
68	1	0	-0.297957	3.693094	-4.847540
69	6	0	6.261004	-1.415104	0.570060
70	6	0	6.680838	-0.644004	-0.514833
71	6	0	6.008623	0.542024	-0.805339
72	6	0	4.932521	0.962632	-0.026335
73	6	0	4.511943	0.179999	1.054953
74	6	0	5.180894	-1.012907	1.351670
75	1	0	6.776989	-2.340183	0.812100
76	1	0	7.521609	-0.962118	-1.122952
77	1	0	6.323599	1.154746	-1.645371
78	1	0	4.409736	1.887991	-0.252116
79	1	0	4.848950	-1.605706	2.199560

80	8	0	3.458605	0.525948	1.838058
81	1	0	3.061441	1.362701	1.511315

TS1/2_PhOH(R*S*R)

SCF Done: E(RM062X) = -1896.56103327

Imaginary Frequencies = -168.1450

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.741463	1.170516	-2.284742
2	6	0	-1.449222	0.080995	-1.814460
3	1	0	-2.125856	0.292891	-0.990801
4	6	0	0.338021	1.020273	-3.207324
5	7	0	1.231776	0.915342	-3.940794
6	6	0	-1.678019	-1.220428	-2.455302
7	6	0	-1.301082	-1.521289	-3.771617
8	6	0	-2.369308	-2.191785	-1.709919
9	6	0	-1.597392	-2.767823	-4.318527
10	1	0	-0.795931	-0.782784	-4.384328
11	6	0	-2.660436	-3.433436	-2.257105
12	1	0	-2.645600	-1.963781	-0.681926
13	6	0	-2.272915	-3.725934	-3.566503
14	1	0	-1.305372	-2.985671	-5.341379
15	1	0	-3.190784	-4.174389	-1.666512

16	1	0	-2.502110	-4.695153	-3.999422
17	6	0	-0.790368	2.481766	-1.626591
18	8	0	0.193463	3.231465	-1.632772
19	6	0	-2.050418	2.959328	-0.983682
20	6	0	-3.320132	2.550082	-1.408049
21	6	0	-1.938584	3.916926	0.031968
22	6	0	-4.460400	3.083210	-0.811512
23	1	0	-3.421230	1.838133	-2.221653
24	6	0	-3.077354	4.442178	0.630723
25	1	0	-0.949350	4.235721	0.347045
26	6	0	-4.340970	4.024551	0.209366
27	1	0	-5.442163	2.767754	-1.150930
28	1	0	-2.981428	5.173575	1.427727
29	1	0	-5.231927	4.436327	0.674661
30	6	0	0.206272	-0.814255	-0.115596
31	6	0	0.534865	-2.211108	-0.438865
32	1	0	0.815618	-0.014093	-0.507286
33	1	0	0.768993	-2.362770	-1.499331
34	1	0	-0.278736	-2.883294	-0.149681
35	6	0	-0.687303	-0.544192	0.930852
36	8	0	-1.375324	-1.326936	1.587601
37	8	0	-0.788432	0.845547	1.154336
38	6	0	-1.718479	1.315232	2.048847
39	6	0	-1.280057	2.241697	2.993400
40	6	0	-3.068423	0.969461	1.968858
41	6	0	-2.196799	2.832011	3.860726

42	1	0	-0.225503	2.501802	3.025038
43	6	0	-3.975217	1.561284	2.844940
44	1	0	-3.396783	0.246781	1.229260
45	6	0	-3.547178	2.494027	3.790629
46	1	0	-1.851265	3.558304	4.590719
47	1	0	-5.026940	1.296075	2.781552
48	1	0	-4.262041	2.952015	4.467426
49	6	0	3.250366	-4.749283	0.520248
50	6	0	1.903905	-4.238596	-0.041048
51	1	0	3.971645	-4.899762	-0.287204
52	1	0	3.098802	-5.704461	1.029217
53	1	0	1.838935	-4.332136	-1.127119
54	1	0	1.044214	-4.735013	0.414944
55	6	0	4.192429	-2.573210	0.725513
56	1	0	4.478749	-1.807071	1.450912
57	1	0	5.057335	-2.791594	0.093739
58	6	0	3.019391	-2.069410	-0.148493
59	1	0	2.842365	-0.997371	-0.027754
60	1	0	3.152251	-2.299002	-1.208715
61	6	0	1.638676	-2.630603	1.777527
62	1	0	1.703279	-1.559921	1.982323
63	1	0	0.643541	-2.984202	2.053951
64	6	0	2.783231	-3.427856	2.444365
65	1	0	3.234436	-2.826887	3.238494
66	1	0	2.402312	-4.352514	2.886431
67	7	0	3.814938	-3.781436	1.463744

68	7	0	1.770123	-2.779434	0.287885
69	6	0	4.802874	1.031367	1.110968
70	6	0	3.837502	0.876738	2.109656
71	6	0	2.534691	1.307085	1.863658
72	6	0	2.194067	1.892728	0.645917
73	6	0	3.160125	2.027988	-0.357186
74	6	0	4.471203	1.596190	-0.115882
75	1	0	5.823629	0.701740	1.286308
76	1	0	4.099314	0.426080	3.062540
77	1	0	1.764816	1.186628	2.622070
78	1	0	1.172440	2.215165	0.464810
79	1	0	5.212854	1.711706	-0.900775
80	8	0	2.886512	2.563399	-1.567748
81	1	0	1.924197	2.746926	-1.651371

TS1/2_PhOH(S*R*S)

SCF Done: E(RM062X) = -1896.55328704

Imaginary Frequencies = -211.8417

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.080334	4.368713	-1.289618
2	6	0	2.775631	4.095168	-2.453025
3	1	0	3.451083	3.248246	-2.469974

4	6	0	1.212514	5.505924	-1.211017
5	7	0	0.517731	6.430221	-1.111203
6	6	0	2.952255	5.122704	-3.511401
7	6	0	3.358951	6.409822	-3.126261
8	6	0	2.790701	4.846192	-4.874829
9	6	0	3.602219	7.393190	-4.080833
10	1	0	3.511080	6.633937	-2.074232
11	6	0	3.025510	5.837126	-5.824976
12	1	0	2.455471	3.867869	-5.201446
13	6	0	3.432988	7.111213	-5.434376
14	1	0	3.925603	8.379655	-3.762499
15	1	0	2.883596	5.609709	-6.877528
16	1	0	3.615531	7.879288	-6.179925
17	6	0	1.935343	3.413504	-0.187555
18	8	0	0.954227	3.454594	0.564132
19	6	0	2.964595	2.354927	0.022052
20	6	0	2.533591	1.097864	0.462447
21	6	0	4.330564	2.600273	-0.155581
22	6	0	3.458460	0.086149	0.693513
23	1	0	1.470985	0.922696	0.607769
24	6	0	5.254950	1.590165	0.096425
25	1	0	4.670483	3.584134	-0.465690
26	6	0	4.819900	0.332696	0.511371
27	1	0	3.120472	-0.892618	1.019505
28	1	0	6.315123	1.786284	-0.030146
29	1	0	5.543132	-0.455869	0.696510

30	6	0	1.406789	2.200259	-3.330793
31	6	0	0.123388	2.899080	-3.482468
32	1	0	1.688946	1.810769	-2.361321
33	1	0	-0.018055	3.669954	-2.713616
34	1	0	0.019332	3.348838	-4.474514
35	6	0	2.056732	1.648363	-4.452490
36	8	0	1.780539	1.769146	-5.645566
37	8	0	3.191527	0.922940	-4.059064
38	6	0	4.084175	0.520976	-5.023973
39	6	0	4.663891	1.430455	-5.909305
40	6	0	4.462010	-0.818965	-5.036188
41	6	0	5.623007	0.984184	-6.813654
42	1	0	4.365493	2.473558	-5.879326
43	6	0	5.429385	-1.253967	-5.940461
44	1	0	3.999116	-1.504266	-4.332618
45	6	0	6.009422	-0.356700	-6.834609
46	1	0	6.073562	1.691116	-7.504364
47	1	0	5.725817	-2.298841	-5.945259
48	1	0	6.759826	-0.698059	-7.541032
49	6	0	-2.352467	2.908427	-3.305340
50	6	0	-3.611879	2.012600	-3.327433
51	1	0	-2.278720	3.512808	-2.396445
52	1	0	-2.286248	3.561255	-4.178533
53	1	0	-4.324741	2.362733	-2.575866
54	1	0	-4.094928	2.051839	-4.307406
55	6	0	-1.088487	1.258908	-2.032445

56	1	0	-0.276497	0.536156	-2.128938
57	1	0	-0.837298	1.976400	-1.245220
58	6	0	-2.461243	0.579449	-1.815381
59	1	0	-2.311501	-0.461799	-1.518003
60	1	0	-3.020719	1.087263	-1.024810
61	6	0	-2.450022	0.103249	-4.150255
62	1	0	-2.082596	-0.887816	-3.870152
63	1	0	-3.079209	-0.000851	-5.037907
64	6	0	-1.267701	1.052518	-4.458705
65	1	0	-0.315968	0.527580	-4.547050
66	1	0	-1.430810	1.651412	-5.357777
67	7	0	-1.138146	2.024657	-3.323215
68	7	0	-3.260661	0.618523	-3.043270
69	6	0	-4.708850	2.593191	0.650504
70	6	0	-4.277668	1.566477	1.491561
71	6	0	-2.921931	1.463852	1.799577
72	6	0	-1.999392	2.367662	1.275243
73	6	0	-2.439072	3.389149	0.426088
74	6	0	-3.799000	3.502423	0.117726
75	1	0	-5.762818	2.689222	0.404411
76	1	0	-4.989624	0.857813	1.902469
77	1	0	-2.571638	0.671659	2.455485
78	1	0	-0.941809	2.287028	1.512977
79	1	0	-4.123288	4.306237	-0.537519
80	8	0	-1.592492	4.283755	-0.141420
81	1	0	-0.666003	4.107043	0.137942

TS1/2_PhOH(S*S*R)

SCF Done: E(RM062X) = -1896.55809415

Imaginary Frequencies = -122.0683

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.341716	-2.253529	1.015185
2	6	0	-4.810431	-2.235445	0.968508
3	1	0	-2.794885	-1.639786	1.720766
4	1	0	-5.241311	-1.244837	1.153269
5	1	0	-5.177390	-2.616196	0.009629
6	6	0	-2.657065	-3.181319	0.226037
7	8	0	-3.110878	-3.997387	-0.580909
8	8	0	-1.259372	-3.058926	0.377845
9	6	0	-0.469885	-4.095306	-0.057955
10	6	0	0.685910	-3.778442	-0.768313
11	6	0	-0.755515	-5.423289	0.269766
12	6	0	1.558172	-4.795498	-1.154489
13	1	0	0.889269	-2.738023	-1.003687
14	6	0	0.118833	-6.429810	-0.127305
15	1	0	-1.658317	-5.657713	0.823453
16	6	0	1.278452	-6.123550	-0.841088
17	1	0	2.458744	-4.543588	-1.707238

18	1	0	-0.107064	-7.461749	0.126259
19	1	0	1.956580	-6.914114	-1.147677
20	6	0	-6.998947	-3.128253	1.733727
21	6	0	-7.719465	-3.861001	2.889482
22	1	0	-7.307635	-2.084673	1.640930
23	1	0	-7.131786	-3.628295	0.771432
24	1	0	-8.249540	-3.146787	3.525487
25	1	0	-8.447840	-4.566771	2.482924
26	6	0	-5.296953	-2.607753	3.398348
27	1	0	-4.219425	-2.484528	3.521239
28	1	0	-5.780545	-1.628843	3.443630
29	6	0	-5.900308	-3.615792	4.405335
30	1	0	-5.107110	-4.162535	4.922340
31	1	0	-6.491569	-3.081321	5.153084
32	6	0	-5.920168	-5.419560	2.849459
33	1	0	-5.295802	-6.069000	3.468102
34	1	0	-6.578237	-6.050552	2.245819
35	6	0	-5.024567	-4.544253	1.942405
36	1	0	-3.986545	-4.518224	2.278011
37	1	0	-5.044311	-4.840820	0.892494
38	7	0	-5.524345	-3.129761	2.011803
39	7	0	-6.756361	-4.587970	3.720385
40	6	0	-1.546033	-0.551792	-1.199929
41	6	0	-2.870785	-0.419900	-0.856508
42	1	0	-3.086876	0.171184	0.025331
43	6	0	-1.114506	-1.192132	-2.405316

44	7	0	-0.732734	-1.688740	-3.381537
45	6	0	-4.047787	-0.763832	-1.655430
46	6	0	-4.083736	-1.825413	-2.573606
47	6	0	-5.214334	-0.011334	-1.439242
48	6	0	-5.256256	-2.104005	-3.269434
49	1	0	-3.219008	-2.462948	-2.709704
50	6	0	-6.379328	-0.286460	-2.145165
51	1	0	-5.194639	0.797832	-0.712953
52	6	0	-6.401468	-1.335484	-3.064137
53	1	0	-5.277424	-2.933220	-3.970244
54	1	0	-7.270212	0.309900	-1.972954
55	1	0	-7.311399	-1.559305	-3.613097
56	6	0	-0.452942	-0.178086	-0.300996
57	8	0	0.712575	-0.481993	-0.576788
58	6	0	-0.731243	0.537597	0.980905
59	6	0	-1.451525	1.735261	1.023691
60	6	0	-0.179332	0.009701	2.153068
61	6	0	-1.622441	2.396866	2.236897
62	1	0	-1.857578	2.156994	0.108222
63	6	0	-0.372482	0.663519	3.366209
64	1	0	0.385584	-0.917563	2.107461
65	6	0	-1.091368	1.857841	3.407679
66	1	0	-2.170076	3.333695	2.266854
67	1	0	0.043006	0.245083	4.277735
68	1	0	-1.234229	2.370937	4.353984
69	6	0	5.773655	2.262821	-0.180976

70	6	0	5.537016	2.397759	-1.549719
71	6	0	4.376017	1.851860	-2.094087
72	6	0	3.457932	1.180050	-1.290285
73	6	0	3.700842	1.049514	0.082306
74	6	0	4.865896	1.594934	0.633773
75	1	0	6.674616	2.681955	0.258578
76	1	0	6.247958	2.920367	-2.181895
77	1	0	4.177092	1.946813	-3.158122
78	1	0	2.554830	0.752667	-1.717668
79	1	0	5.040554	1.484673	1.699967
80	8	0	2.848755	0.409348	0.914125
81	1	0	2.066449	0.089647	0.409772

2_PhOH(R*R*S)

SCF Done: E(RM062X) = -1896.61253310

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037256	-0.697965	0.687222
2	6	0	-1.420287	-0.277650	0.856288
3	1	0	0.608635	-0.587604	1.613631
4	1	0	-1.998171	-1.089042	1.307037
5	1	0	-1.850060	-0.033439	-0.119849
6	6	0	0.707309	0.117688	-0.400653

7	8	0	0.226992	0.333057	-1.484781
8	8	0	1.929056	0.545094	-0.013739
9	6	0	2.690539	1.268394	-0.934302
10	6	0	2.288544	2.540373	-1.322959
11	6	0	3.873380	0.699054	-1.382915
12	6	0	3.099977	3.258295	-2.196882
13	1	0	1.359302	2.955480	-0.944670
14	6	0	4.678337	1.430913	-2.255043
15	1	0	4.151523	-0.295249	-1.045306
16	6	0	4.292535	2.705857	-2.664558
17	1	0	2.799081	4.253078	-2.510718
18	1	0	5.608223	1.000569	-2.613989
19	1	0	4.921804	3.271849	-3.344384
20	6	0	-3.408073	2.397693	2.670448
21	6	0	-3.100583	1.318550	1.610588
22	1	0	-3.991246	1.968968	3.490273
23	1	0	-3.988441	3.203954	2.215075
24	1	0	-3.690317	0.410585	1.750563
25	1	0	-3.224654	1.681929	0.587936
26	6	0	-1.507773	1.895768	4.007842
27	1	0	-0.521092	2.259793	4.305851
28	1	0	-2.090685	1.697463	4.910896
29	6	0	-1.376930	0.592306	3.186548
30	1	0	-0.378474	0.160167	3.254528
31	1	0	-2.109743	-0.169041	3.467285
32	6	0	-0.800240	2.097701	1.335947

33	1	0	0.234314	1.842609	1.579391
34	1	0	-0.910763	2.221450	0.255673
35	6	0	-1.289289	3.337154	2.123860
36	1	0	-0.426838	3.875688	2.523584
37	1	0	-1.844364	4.010723	1.466021
38	7	0	-2.167544	2.943566	3.226144
39	7	0	-1.648365	0.919593	1.738156
40	6	0	-0.524090	-3.081968	1.334453
41	6	0	0.095740	-2.206441	0.257060
42	1	0	-0.526597	-2.286194	-0.641552
43	6	0	-0.163920	-2.796150	2.673527
44	7	0	0.187927	-2.533795	3.755399
45	6	0	1.526043	-2.552621	-0.144220
46	6	0	2.522573	-2.772590	0.812921
47	6	0	1.871692	-2.611138	-1.498262
48	6	0	3.828731	-3.057401	0.422071
49	1	0	2.279270	-2.724015	1.871360
50	6	0	3.177354	-2.902147	-1.892365
51	1	0	1.104012	-2.439113	-2.250200
52	6	0	4.160383	-3.128323	-0.931484
53	1	0	4.590003	-3.228466	1.177744
54	1	0	3.423115	-2.952626	-2.949281
55	1	0	5.178175	-3.358677	-1.232601
56	6	0	-1.558420	-4.019712	1.169397
57	8	0	-2.256216	-4.458705	2.137124
58	6	0	-1.898415	-4.565175	-0.190973

59	6	0	-3.220595	-4.949213	-0.445856
60	6	0	-0.934586	-4.776966	-1.182997
61	6	0	-3.582508	-5.472724	-1.683165
62	1	0	-3.959817	-4.843197	0.341954
63	6	0	-1.291946	-5.311356	-2.418840
64	1	0	0.107527	-4.550775	-0.979915
65	6	0	-2.619321	-5.648446	-2.676855
66	1	0	-4.615343	-5.751688	-1.871065
67	1	0	-0.530009	-5.471252	-3.176217
68	1	0	-2.900815	-6.059811	-3.641930
69	6	0	-5.866420	-0.224869	3.370272
70	6	0	-6.293833	-0.481519	2.066157
71	6	0	-5.632356	-1.454823	1.318095
72	6	0	-4.558981	-2.162120	1.854840
73	6	0	-4.130921	-1.903308	3.165303
74	6	0	-4.794614	-0.922959	3.918690
75	1	0	-6.371051	0.529357	3.968446
76	1	0	-7.129401	0.066031	1.641727
77	1	0	-5.948816	-1.668436	0.300549
78	1	0	-4.041369	-2.913393	1.267507
79	1	0	-4.456516	-0.726913	4.932804
80	8	0	-3.088542	-2.537404	3.731972
81	1	0	-2.732612	-3.269257	3.139679

2_PhOH(R*S*R)

SCF Done: E(RM062X) = -1896.60359866

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.028368	3.033043	-0.621178
2	6	0	-1.732702	2.848077	-1.955929
3	1	0	-2.571401	2.172189	-1.780317
4	6	0	-0.201561	4.165765	-0.443078
5	7	0	0.470205	5.112727	-0.318097
6	6	0	-2.334917	4.133201	-2.512847
7	6	0	-2.991840	5.009555	-1.637691
8	6	0	-2.324856	4.452799	-3.874047
9	6	0	-3.619275	6.158889	-2.106132
10	1	0	-3.008961	4.782173	-0.574985
11	6	0	-2.950651	5.607282	-4.347428
12	1	0	-1.829393	3.811968	-4.597441
13	6	0	-3.600466	6.465170	-3.466929
14	1	0	-4.121693	6.819510	-1.405280
15	1	0	-2.923378	5.831330	-5.409802
16	1	0	-4.084489	7.365230	-3.834106
17	6	0	-0.948775	2.045011	0.369087
18	8	0	-0.161115	2.077883	1.364120
19	6	0	-1.819241	0.818735	0.266196
20	6	0	-3.212574	0.889399	0.171886
21	6	0	-1.201837	-0.434699	0.319951

22	6	0	-3.974525	-0.275703	0.113327
23	1	0	-3.701836	1.860921	0.154811
24	6	0	-1.961167	-1.599768	0.243604
25	1	0	-0.120810	-0.487614	0.421226
26	6	0	-3.349792	-1.521899	0.139468
27	1	0	-5.056742	-0.209963	0.048889
28	1	0	-1.470640	-2.568519	0.273086
29	1	0	-3.943595	-2.429825	0.087991
30	6	0	-0.806689	2.076853	-2.946568
31	6	0	0.396579	2.894201	-3.431989
32	1	0	-0.474446	1.207201	-2.365911
33	1	0	0.464577	3.848150	-2.903125
34	1	0	0.320919	3.095134	-4.502946
35	6	0	-1.545425	1.447889	-4.119199
36	8	0	-1.150865	1.395154	-5.257406
37	8	0	-2.704220	0.893420	-3.702839
38	6	0	-3.509022	0.246990	-4.642444
39	6	0	-3.703934	-1.118210	-4.491266
40	6	0	-4.142429	0.979016	-5.639157
41	6	0	-4.561317	-1.773024	-5.373611
42	1	0	-3.196684	-1.646291	-3.689929
43	6	0	-4.992859	0.311200	-6.516081
44	1	0	-3.972972	2.048805	-5.716868
45	6	0	-5.203151	-1.061748	-6.385684
46	1	0	-4.726933	-2.840543	-5.265974
47	1	0	-5.495904	0.867254	-7.301111

48	1	0	-5.870345	-1.575250	-7.071034
49	6	0	4.179941	2.575069	-3.552795
50	6	0	2.776834	3.106451	-3.921952
51	1	0	4.659897	3.236778	-2.827155
52	1	0	4.802548	2.534336	-4.449821
53	1	0	2.612516	4.129450	-3.578384
54	1	0	2.570117	3.043975	-4.992633
55	6	0	3.421622	1.348131	-1.662860
56	1	0	3.228077	0.338987	-1.289242
57	1	0	4.081917	1.854665	-0.955995
58	6	0	2.102791	2.142273	-1.782731
59	1	0	1.278164	1.652860	-1.262881
60	1	0	2.187040	3.168062	-1.419375
61	6	0	1.802041	0.869909	-3.868520
62	1	0	1.158902	0.215619	-3.277713
63	1	0	1.399732	0.960423	-4.878939
64	6	0	3.275224	0.394669	-3.843984
65	1	0	3.317414	-0.638641	-3.491743
66	1	0	3.704580	0.434866	-4.848513
67	7	0	4.085912	1.238052	-2.963817
68	7	0	1.740355	2.239851	-3.244008
69	6	0	4.691058	4.963098	2.491110
70	6	0	3.842686	5.726595	3.293410
71	6	0	2.484253	5.412428	3.334471
72	6	0	1.973369	4.354066	2.588891
73	6	0	2.829661	3.590014	1.783534

74	6	0	4.194105	3.902236	1.740184
75	1	0	5.752176	5.193841	2.448859
76	1	0	4.234218	6.553274	3.878036
77	1	0	1.810481	5.998496	3.953834
78	1	0	0.915059	4.109726	2.610307
79	1	0	4.849335	3.300363	1.116605
80	8	0	2.387689	2.549808	1.048872
81	1	0	1.394524	2.447372	1.156090

2_PhOH(S*R*S)

SCF Done: E(RM062X) = -1896.60633221

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.701876	4.187279	-1.473939
2	6	0	2.395551	3.677894	-2.729860
3	1	0	3.314722	3.175523	-2.424806
4	6	0	0.925538	5.365955	-1.574778
5	7	0	0.300731	6.345543	-1.680993
6	6	0	2.833397	4.812133	-3.647818
7	6	0	3.716416	5.769251	-3.125988
8	6	0	2.427081	4.947633	-4.976305
9	6	0	4.181158	6.819813	-3.906773
10	1	0	4.036922	5.681810	-2.090086

11	6	0	2.892226	6.003700	-5.765303
12	1	0	1.746262	4.234660	-5.429787
13	6	0	3.768416	6.942802	-5.235202
14	1	0	4.867922	7.545347	-3.480461
15	1	0	2.559025	6.085546	-6.795780
16	1	0	4.127533	7.764781	-5.847202
17	6	0	1.630259	3.501837	-0.254110
18	8	0	0.885107	3.839979	0.716109
19	6	0	2.447624	2.252360	-0.045674
20	6	0	1.790819	1.104078	0.411557
21	6	0	3.833368	2.212679	-0.230326
22	6	0	2.497320	-0.074256	0.636881
23	1	0	0.718771	1.143623	0.591284
24	6	0	4.544058	1.038676	0.011868
25	1	0	4.362554	3.110439	-0.540657
26	6	0	3.876651	-0.109689	0.434886
27	1	0	1.973225	-0.962304	0.978324
28	1	0	5.621294	1.023524	-0.125368
29	1	0	4.430436	-1.025866	0.617899
30	6	0	1.551912	2.554978	-3.412922
31	6	0	0.142572	2.993623	-3.818481
32	1	0	1.502491	1.772090	-2.645016
33	1	0	-0.104478	3.963031	-3.380172
34	1	0	0.049533	3.061710	-4.904134
35	6	0	2.283333	1.902262	-4.574797
36	8	0	1.811296	1.635272	-5.651496

37	8	0	3.560489	1.625511	-4.230255
38	6	0	4.404616	1.097369	-5.208441
39	6	0	4.771856	1.878518	-6.297679
40	6	0	4.907255	-0.180713	-5.014155
41	6	0	5.667731	1.351786	-7.223719
42	1	0	4.362697	2.878690	-6.408136
43	6	0	5.808943	-0.693317	-5.946204
44	1	0	4.599980	-0.753035	-4.144569
45	6	0	6.186899	0.068361	-7.050060
46	1	0	5.962641	1.948674	-8.081202
47	1	0	6.215074	-1.690264	-5.805854
48	1	0	6.888498	-0.335155	-7.773392
49	6	0	-2.254381	2.580317	-4.001427
50	6	0	-3.431873	1.785793	-3.397286
51	1	0	-2.311334	3.648067	-3.781680
52	1	0	-2.158016	2.435203	-5.079732
53	1	0	-3.960329	2.388430	-2.653016
54	1	0	-4.134749	1.517205	-4.189682
55	6	0	-1.143137	2.047574	-1.894071
56	1	0	-0.172280	1.831541	-1.445672
57	1	0	-1.450219	3.057598	-1.608314
58	6	0	-2.191156	0.962853	-1.548270
59	1	0	-1.699636	0.073717	-1.142562
60	1	0	-2.882262	1.350051	-0.795863
61	6	0	-2.054413	-0.137989	-3.658774
62	1	0	-1.812628	-1.118911	-3.242727

63	1	0	-2.581055	-0.284588	-4.605354
64	6	0	-0.749372	0.659295	-3.885043
65	1	0	0.083550	0.244331	-3.313024
66	1	0	-0.470944	0.727872	-4.937959
67	7	0	-0.968146	2.068125	-3.392390
68	7	0	-2.947496	0.570092	-2.739978
69	6	0	-4.548755	2.595075	1.026777
70	6	0	-4.015982	1.548189	1.781656
71	6	0	-2.647991	1.535399	2.049580
72	6	0	-1.814195	2.545186	1.571828
73	6	0	-2.352722	3.590331	0.806756
74	6	0	-3.728980	3.608745	0.540156
75	1	0	-5.613560	2.622418	0.811162
76	1	0	-4.659066	0.758176	2.156525
77	1	0	-2.217707	0.730962	2.640632
78	1	0	-0.748655	2.543718	1.782517
79	1	0	-4.134927	4.424556	-0.051534
80	8	0	-1.599356	4.585754	0.298839
81	1	0	-0.624861	4.399462	0.451053

2_PhOH(S*S*R)

SCF Done: E(RM062X) = -1896.60302173

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

1	6	0	-3.560971	-1.699996	0.112112
2	6	0	-4.867751	-2.381392	0.501165
3	1	0	-3.156787	-1.131569	0.953903
4	1	0	-5.701581	-1.678699	0.420686
5	1	0	-5.067058	-3.239379	-0.146466
6	6	0	-2.483656	-2.686557	-0.291099
7	8	0	-2.635472	-3.665333	-0.979085
8	8	0	-1.292302	-2.313065	0.226940
9	6	0	-0.155866	-3.026240	-0.162886
10	6	0	0.721395	-2.413639	-1.047498
11	6	0	0.090975	-4.278049	0.384683
12	6	0	1.891585	-3.090394	-1.391552
13	1	0	0.486212	-1.424416	-1.437352
14	6	0	1.262988	-4.940859	0.029873
15	1	0	-0.621232	-4.716115	1.077631
16	6	0	2.162309	-4.349114	-0.857294
17	1	0	2.593854	-2.629116	-2.079297
18	1	0	1.472973	-5.919819	0.449850
19	1	0	3.075649	-4.869393	-1.128775
20	6	0	-6.181724	-3.711140	2.078713
21	6	0	-6.355416	-4.052051	3.575133
22	1	0	-7.001881	-3.107322	1.686054
23	1	0	-6.052627	-4.599216	1.456129
24	1	0	-7.134594	-3.430209	4.023350
25	1	0	-6.647355	-5.099903	3.677767

26	6	0	-4.955578	-1.772463	2.918694
27	1	0	-4.134033	-1.089460	2.699340
28	1	0	-5.906224	-1.258953	2.757602
29	6	0	-4.838353	-2.382253	4.333928
30	1	0	-3.833229	-2.229261	4.735250
31	1	0	-5.554265	-1.893622	4.999113
32	6	0	-4.016662	-4.488571	3.588850
33	1	0	-3.110669	-4.459904	4.198298
34	1	0	-4.296340	-5.533582	3.432885
35	6	0	-3.744605	-3.795727	2.232177
36	1	0	-2.859848	-3.155818	2.273074
37	1	0	-3.651019	-4.509219	1.410347
38	7	0	-4.915894	-2.900175	1.916551
39	7	0	-5.106176	-3.821889	4.303948
40	6	0	-2.478926	-0.193050	-1.652776
41	6	0	-3.793069	-0.623773	-1.015081
42	1	0	-4.195011	0.227388	-0.459896
43	6	0	-2.069256	-0.797587	-2.864102
44	7	0	-1.736458	-1.295457	-3.865503
45	6	0	-4.858998	-0.972090	-2.043246
46	6	0	-4.869305	-2.169680	-2.768257
47	6	0	-5.864263	-0.031987	-2.293430
48	6	0	-5.863865	-2.415563	-3.714190
49	1	0	-4.101892	-2.916904	-2.590695
50	6	0	-6.855562	-0.273286	-3.241838
51	1	0	-5.866806	0.902534	-1.736704

52	6	0	-6.858861	-1.469988	-3.955166
53	1	0	-5.858370	-3.351297	-4.265755
54	1	0	-7.626077	0.471624	-3.417853
55	1	0	-7.631214	-1.664189	-4.693516
56	6	0	-1.513133	0.578153	-0.999793
57	8	0	-0.341710	0.772596	-1.455761
58	6	0	-1.841400	1.197177	0.333217
59	6	0	-2.862765	2.140447	0.479447
60	6	0	-1.049815	0.866004	1.437651
61	6	0	-3.091496	2.745121	1.714157
62	1	0	-3.462825	2.417893	-0.384476
63	6	0	-1.285649	1.461364	2.674351
64	1	0	-0.247233	0.143566	1.316912
65	6	0	-2.305379	2.403494	2.813760
66	1	0	-3.877413	3.487776	1.815772
67	1	0	-0.670363	1.195845	3.529196
68	1	0	-2.482088	2.874507	3.776376
69	6	0	0.537130	5.649295	1.284141
70	6	0	-0.432233	6.115193	0.394961
71	6	0	-0.846830	5.288481	-0.648714
72	6	0	-0.307158	4.014748	-0.807629
73	6	0	0.660093	3.544245	0.093203
74	6	0	1.078980	4.375913	1.140508
75	1	0	0.870621	6.280661	2.103473
76	1	0	-0.856709	7.107332	0.513064
77	1	0	-1.598409	5.637482	-1.352097

78	1	0	-0.627559	3.369990	-1.621523
79	1	0	1.825757	4.001148	1.834530
80	8	0	1.214919	2.323196	-0.016372
81	1	0	0.635225	1.736253	-0.592853

TS2/3a_PhOH(RRS)

SCF Done: E(RM062X) = -1896.57572623

Imaginary Frequencies = -1141.5594

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.793616	0.519567	0.218685
2	6	0	-0.257811	1.418792	-0.433326
3	1	0	1.057841	0.837472	1.231115
4	1	0	-1.261942	1.045948	-0.239352
5	1	0	-0.087826	1.447287	-1.512598
6	6	0	2.067254	0.530340	-0.608166
7	8	0	2.109393	0.549535	-1.811730
8	8	0	3.153545	0.489257	0.191965
9	6	0	4.410735	0.350675	-0.398321
10	6	0	4.920917	1.335708	-1.234671
11	6	0	5.139765	-0.779907	-0.058010
12	6	0	6.203362	1.168028	-1.751854
13	1	0	4.325275	2.210583	-1.474488

14	6	0	6.422774	-0.932747	-0.579873
15	1	0	4.698845	-1.515417	0.608655
16	6	0	6.953343	0.037044	-1.428701
17	1	0	6.616577	1.925861	-2.410332
18	1	0	7.004705	-1.812006	-0.321257
19	1	0	7.951787	-0.085346	-1.836800
20	6	0	0.938117	4.936969	0.522799
21	6	0	1.046266	3.528048	-0.112632
22	1	0	1.380964	5.674686	-0.150228
23	1	0	1.478194	4.965742	1.472565
24	1	0	1.257647	3.556791	-1.184790
25	1	0	1.797540	2.919595	0.395632
26	6	0	-1.227673	5.084376	-0.450630
27	1	0	-2.235901	5.484086	-0.318736
28	1	0	-0.739605	5.634177	-1.259352
29	6	0	-1.306989	3.581055	-0.792035
30	1	0	-2.275998	3.138954	-0.543910
31	1	0	-1.074491	3.375944	-1.838201
32	6	0	-0.713648	2.928063	1.490388
33	1	0	-1.593169	2.284523	1.593828
34	1	0	0.105603	2.529435	2.090613
35	6	0	-0.994676	4.412905	1.819462
36	1	0	-2.070601	4.591040	1.895353
37	1	0	-0.534004	4.666265	2.777233
38	7	0	-0.458624	5.292073	0.777472
39	7	0	-0.283644	2.843043	0.042722

40	6	0	-0.849178	-1.021469	1.396416
41	6	0	0.226358	-0.939531	0.292028
42	1	0	-0.274422	-1.111531	-0.669855
43	6	0	-0.433539	-0.444648	2.656597
44	7	0	-0.117893	0.093531	3.635819
45	6	0	1.331625	-1.985229	0.411936
46	6	0	1.799675	-2.452097	1.644002
47	6	0	1.897783	-2.509007	-0.758542
48	6	0	2.798459	-3.423798	1.702163
49	1	0	1.383754	-2.070966	2.572046
50	6	0	2.892985	-3.481669	-0.702690
51	1	0	1.536797	-2.162104	-1.724465
52	6	0	3.344962	-3.945814	0.531354
53	1	0	3.143000	-3.778987	2.668948
54	1	0	3.307260	-3.881372	-1.623621
55	1	0	4.115367	-4.709765	0.581482
56	6	0	-1.597183	-2.297372	1.629449
57	8	0	-1.868947	-2.679281	2.756982
58	6	0	-2.263866	-2.957417	0.452119
59	6	0	-1.607061	-3.397031	-0.699967
60	6	0	-3.654328	-3.093532	0.545157
61	6	0	-2.338422	-3.943213	-1.753848
62	1	0	-0.525997	-3.342839	-0.774616
63	6	0	-4.383117	-3.621769	-0.514874
64	1	0	-4.159207	-2.758265	1.446711
65	6	0	-3.725525	-4.042597	-1.670501

66	1	0	-1.819453	-4.290799	-2.642275
67	1	0	-5.463513	-3.703354	-0.440841
68	1	0	-4.291992	-4.455036	-2.500371
69	6	0	-5.269122	0.778122	-2.430206
70	6	0	-5.604261	1.495686	-1.279421
71	6	0	-4.835090	1.397657	-0.125258
72	6	0	-3.690392	0.565524	-0.070981
73	6	0	-3.359190	-0.143830	-1.251528
74	6	0	-4.138976	-0.040081	-2.399213
75	8	0	-2.977898	0.494777	1.033990
76	1	0	-1.890674	-0.287418	1.092177
77	1	0	-6.479376	2.141577	-1.280827
78	1	0	-5.100036	1.956733	0.768686
79	1	0	-2.486550	-0.794405	-1.243958
80	1	0	-3.857405	-0.610742	-3.281550
81	1	0	-5.874328	0.854004	-3.328211

TS2/3a_PhOH(RSR)

SCF Done: E(RM062X) = -1896.58019638

Imaginary Frequencies = -1102.1773

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.185941	1.619457	0.818791

2	6	0	0.709092	0.379166	1.044777
3	1	0	1.602473	0.564748	0.441479
4	6	0	-1.329243	1.685855	1.700993
5	7	0	-2.279141	1.688782	2.368600
6	6	0	1.194579	0.205093	2.485601
7	6	0	1.162729	1.267876	3.396423
8	6	0	1.757639	-1.005521	2.913419
9	6	0	1.671327	1.125277	4.686951
10	1	0	0.740728	2.226802	3.112180
11	6	0	2.263232	-1.150727	4.202814
12	1	0	1.810529	-1.857481	2.242601
13	6	0	2.222188	-0.084485	5.098125
14	1	0	1.631597	1.968099	5.370739
15	1	0	2.690070	-2.102562	4.505327
16	1	0	2.615707	-0.196269	6.103897
17	6	0	0.502640	2.940341	0.710551
18	8	0	0.090755	3.943232	1.279562
19	6	0	1.695898	3.032060	-0.194906
20	6	0	1.805356	2.257938	-1.356297
21	6	0	2.699242	3.952377	0.122699
22	6	0	2.919335	2.395360	-2.180204
23	1	0	1.007600	1.572799	-1.633423
24	6	0	3.817097	4.077346	-0.696005
25	1	0	2.596133	4.557475	1.018871
26	6	0	3.928851	3.297048	-1.847004
27	1	0	2.996452	1.798438	-3.084250

28	1	0	4.601590	4.782597	-0.438381
29	1	0	4.801312	3.395161	-2.486402
30	6	0	0.054852	-0.901297	0.425138
31	6	0	-0.910411	-1.615476	1.373833
32	1	0	-0.475371	-0.540483	-0.464105
33	1	0	-1.270581	-0.936069	2.150151
34	1	0	-0.429327	-2.470485	1.854589
35	6	0	1.107733	-1.846163	-0.130835
36	8	0	1.281479	-2.998318	0.178552
37	8	0	1.832493	-1.209373	-1.077787
38	6	0	2.912408	-1.882592	-1.652404
39	6	0	2.827369	-2.221817	-2.994796
40	6	0	4.053460	-2.126167	-0.898345
41	6	0	3.926983	-2.826513	-3.601829
42	1	0	1.917781	-2.007363	-3.546841
43	6	0	5.142326	-2.735392	-1.516193
44	1	0	4.083029	-1.836375	0.148049
45	6	0	5.081206	-3.085110	-2.865413
46	1	0	3.877899	-3.094387	-4.652755
47	1	0	6.041786	-2.934109	-0.941639
48	1	0	5.934674	-3.556809	-3.342224
49	6	0	-4.282352	-3.349135	1.162103
50	6	0	-2.899814	-2.978095	1.742654
51	1	0	-5.066843	-2.741334	1.620118
52	1	0	-4.493962	-4.400917	1.369633
53	1	0	-2.971724	-2.368824	2.645352

54	1	0	-2.279150	-3.853952	1.943794
55	6	0	-4.231045	-1.683284	-0.537751
56	1	0	-4.093219	-1.533491	-1.611966
57	1	0	-5.169710	-1.207812	-0.242249
58	6	0	-3.064480	-1.047920	0.252398
59	1	0	-2.475723	-0.360498	-0.359700
60	1	0	-3.397064	-0.533803	1.157277
61	6	0	-1.837262	-3.056840	-0.453899
62	1	0	-1.443088	-2.419947	-1.249627
63	1	0	-1.065946	-3.754313	-0.124847
64	6	0	-3.141644	-3.769965	-0.882157
65	1	0	-3.229845	-3.741302	-1.970743
66	1	0	-3.125783	-4.815410	-0.563754
67	7	0	-4.311446	-3.124026	-0.284322
68	7	0	-2.152450	-2.159359	0.716240
69	6	0	-4.841739	3.187191	-2.193481
70	6	0	-4.600082	1.948530	-2.791578
71	6	0	-3.407620	1.269896	-2.566123
72	6	0	-2.400973	1.810813	-1.734021
73	6	0	-2.657383	3.069306	-1.141621
74	6	0	-3.858598	3.735105	-1.369024
75	8	0	-1.280839	1.140839	-1.526498
76	1	0	-0.725385	1.464477	-0.360498
77	1	0	-5.350605	1.504551	-3.441543
78	1	0	-3.217887	0.306852	-3.034392
79	1	0	-1.900363	3.521357	-0.503756

80	1	0	-4.024857	4.700499	-0.896710
81	1	0	-5.774492	3.714123	-2.368814

TS2/3a_PhOH(SRS)

SCF Done: E(RM062X) = -1896.57673824

Imaginary Frequencies = -1216.9173

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.588453	-1.875168	-1.111958
2	6	0	0.834300	-1.134321	0.217540
3	1	0	1.631774	-0.421926	-0.010439
4	6	0	-0.330686	-2.983563	-1.008674
5	7	0	-1.106034	-3.844260	-0.925364
6	6	0	1.346280	-2.007014	1.364943
7	6	0	1.857572	-3.290990	1.145046
8	6	0	1.375136	-1.508514	2.675440
9	6	0	2.381169	-4.046059	2.194534
10	1	0	1.855187	-3.723782	0.149669
11	6	0	1.896053	-2.260113	3.724688
12	1	0	0.983326	-0.520562	2.903227
13	6	0	2.403971	-3.535785	3.488527
14	1	0	2.770407	-5.039842	1.992982
15	1	0	1.902788	-1.845200	4.728326

16	1	0	2.810474	-4.124718	4.305225
17	6	0	1.802510	-2.287291	-1.875856
18	8	0	1.914880	-3.390128	-2.395369
19	6	0	2.908481	-1.284288	-2.029776
20	6	0	2.644955	0.057139	-2.320487
21	6	0	4.229476	-1.725130	-1.915286
22	6	0	3.697140	0.954618	-2.482766
23	1	0	1.616425	0.380512	-2.454988
24	6	0	5.279278	-0.822756	-2.060388
25	1	0	4.423451	-2.772619	-1.702071
26	6	0	5.013936	0.517451	-2.342919
27	1	0	3.488354	1.993602	-2.720780
28	1	0	6.304801	-1.164330	-1.956205
29	1	0	5.833526	1.220401	-2.459509
30	6	0	-0.391477	-0.255682	0.614949
31	6	0	-1.485457	-0.997860	1.391504
32	1	0	-0.795872	0.107557	-0.333649
33	1	0	-1.373493	-2.079832	1.287694
34	1	0	-1.443131	-0.744952	2.452988
35	6	0	0.014614	1.024853	1.338995
36	8	0	-0.557156	1.510265	2.282703
37	8	0	1.098527	1.583265	0.757380
38	6	0	1.604180	2.783255	1.259899
39	6	0	2.049846	2.874012	2.573101
40	6	0	1.716746	3.841807	0.369052
41	6	0	2.608623	4.074461	3.003954

42	1	0	1.965401	2.021548	3.239353
43	6	0	2.282038	5.035650	0.813849
44	1	0	1.373627	3.722783	-0.654432
45	6	0	2.723357	5.155298	2.129894
46	1	0	2.959700	4.161254	4.027555
47	1	0	2.376451	5.870117	0.125988
48	1	0	3.160612	6.087227	2.474332
49	6	0	-3.824500	-1.283251	2.010320
50	6	0	-5.277491	-1.213298	1.491909
51	1	0	-3.494523	-2.307241	2.196139
52	1	0	-3.668516	-0.682211	2.908735
53	1	0	-5.627186	-2.205938	1.196919
54	1	0	-5.929316	-0.838359	2.284786
55	6	0	-3.226360	-1.371867	-0.358254
56	1	0	-2.465504	-1.074868	-1.087054
57	1	0	-3.145573	-2.445833	-0.181187
58	6	0	-4.648893	-0.944826	-0.785958
59	1	0	-4.598750	-0.218599	-1.600503
60	1	0	-5.199997	-1.822278	-1.133373
61	6	0	-4.727311	0.944663	0.654336
62	1	0	-4.910974	1.659252	-0.152718
63	1	0	-5.178267	1.332954	1.571326
64	6	0	-3.200654	0.769837	0.836176
65	1	0	-2.646377	1.137159	-0.032880
66	1	0	-2.827550	1.247722	1.741772
67	7	0	-2.904305	-0.706198	0.957665

68	7	0	-5.369370	-0.329775	0.329136
69	6	0	-2.756260	3.201694	-2.108282
70	6	0	-3.361505	2.144717	-2.793102
71	6	0	-2.670030	0.961929	-3.034089
72	6	0	-1.335959	0.785873	-2.599726
73	6	0	-0.727553	1.880798	-1.941628
74	6	0	-1.432989	3.055650	-1.690541
75	8	0	-0.723518	-0.367061	-2.813966
76	1	0	-0.046688	-1.003541	-1.942631
77	1	0	-4.388817	2.239655	-3.138332
78	1	0	-3.147674	0.135735	-3.555433
79	1	0	0.301947	1.785999	-1.605052
80	1	0	-0.938797	3.868454	-1.162922
81	1	0	-3.301102	4.120041	-1.912733

TS2/3a_PhOH(SSR)

SCF Done: E(RM062X) = -1896.57407125

Imaginary Frequencies = -1196.2234

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.347406	-0.092322	0.222383
2	6	0	0.569283	0.705694	1.517486
3	1	0	0.565472	0.514293	-0.662312

4	1	0	-0.275421	1.377969	1.690553
5	1	0	0.654680	0.019599	2.365003
6	6	0	1.276213	-1.299600	0.227808
7	8	0	1.351950	-2.093948	1.130138
8	8	0	2.066617	-1.322158	-0.867946
9	6	0	3.044342	-2.310780	-0.976444
10	6	0	2.724301	-3.662754	-0.910689
11	6	0	4.342141	-1.875188	-1.212815
12	6	0	3.743198	-4.596009	-1.083669
13	1	0	1.700090	-3.970999	-0.736486
14	6	0	5.350496	-2.821531	-1.386299
15	1	0	4.550336	-0.810437	-1.264825
16	6	0	5.053691	-4.181079	-1.319590
17	1	0	3.507451	-5.654808	-1.036010
18	1	0	6.367686	-2.491549	-1.573894
19	1	0	5.839976	-4.917237	-1.454273
20	6	0	1.963972	2.084070	2.975537
21	6	0	3.036257	3.197029	2.973842
22	1	0	0.990342	2.440901	3.316347
23	1	0	2.258837	1.212616	3.563866
24	1	0	2.569431	4.180175	3.072940
25	1	0	3.713736	3.049082	3.818184
26	6	0	1.595012	2.803404	0.672565
27	1	0	1.277104	2.460105	-0.313259
28	1	0	0.787591	3.377805	1.129778
29	6	0	2.925197	3.583163	0.626182

30	1	0	3.446499	3.398548	-0.317601
31	1	0	2.719499	4.654112	0.701570
32	6	0	4.251417	1.802242	1.484456
33	1	0	4.960142	1.790009	0.652655
34	1	0	4.762608	1.443255	2.381328
35	6	0	3.051937	0.887881	1.142212
36	1	0	2.973346	0.716179	0.067386
37	1	0	3.089549	-0.064796	1.675719
38	7	0	1.785885	1.593186	1.556582
39	7	0	3.803459	3.174190	1.726360
40	6	0	-1.581364	-1.000185	-1.246975
41	6	0	-1.168487	-0.473257	0.149509
42	1	0	-1.679288	0.491586	0.254065
43	6	0	-0.755481	-2.037130	-1.814796
44	7	0	-0.099887	-2.848760	-2.325403
45	6	0	-1.657244	-1.340976	1.302388
46	6	0	-1.613689	-2.738705	1.250486
47	6	0	-2.233816	-0.733022	2.422501
48	6	0	-2.118572	-3.504490	2.298137
49	1	0	-1.187131	-3.239081	0.385036
50	6	0	-2.737045	-1.495968	3.474688
51	1	0	-2.310585	0.352046	2.458844
52	6	0	-2.679655	-2.886277	3.415146
53	1	0	-2.076965	-4.588256	2.239173
54	1	0	-3.186935	-1.003593	4.331919
55	1	0	-3.077622	-3.486003	4.228504

56	6	0	-3.014982	-1.415403	-1.320265
57	8	0	-3.385218	-2.476236	-1.798498
58	6	0	-4.035358	-0.452717	-0.783957
59	6	0	-4.116062	0.846480	-1.286747
60	6	0	-4.941951	-0.888148	0.185582
61	6	0	-5.100945	1.712960	-0.813841
62	1	0	-3.415898	1.164889	-2.055798
63	6	0	-5.910430	-0.014133	0.670902
64	1	0	-4.870323	-1.903900	0.566812
65	6	0	-5.990900	1.286200	0.170357
66	1	0	-5.170382	2.720645	-1.213413
67	1	0	-6.604392	-0.347269	1.436934
68	1	0	-6.750066	1.965729	0.546385
69	6	0	0.235154	4.793917	-1.526364
70	6	0	-0.869499	4.185041	-0.929970
71	6	0	-1.288316	2.914363	-1.315139
72	6	0	-0.626879	2.204301	-2.348429
73	6	0	0.500012	2.835485	-2.932738
74	6	0	0.916747	4.099659	-2.530196
75	8	0	-1.019984	1.029518	-2.797265
76	1	0	-1.374355	0.076426	-2.017561
77	1	0	-1.412608	4.703991	-0.142951
78	1	0	-2.154712	2.466305	-0.836778
79	1	0	1.023989	2.303284	-3.722433
80	1	0	1.782477	4.552334	-3.008708
81	1	0	0.556092	5.785029	-1.220399

3a_PhOH(RRS)

SCF Done: E(RM062X) = -1896.59381605

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.736786	-0.539813	0.173114
2	6	0	0.533503	-1.138519	-0.436468
3	1	0	-0.939517	-0.926479	1.175733
4	1	0	1.422743	-0.544570	-0.195525
5	1	0	0.423174	-1.200076	-1.523267
6	6	0	-1.939029	-0.837481	-0.707514
7	8	0	-1.970008	-0.655619	-1.896991
8	8	0	-2.975980	-1.306954	0.018499
9	6	0	-4.226740	-1.402092	-0.593217
10	6	0	-4.855493	-2.638147	-0.582297
11	6	0	-4.837199	-0.265824	-1.113465
12	6	0	-6.140882	-2.740039	-1.112639
13	1	0	-4.344953	-3.497624	-0.159094
14	6	0	-6.118485	-0.384480	-1.644717
15	1	0	-4.312949	0.686280	-1.101543
16	6	0	-6.771327	-1.617531	-1.645023
17	1	0	-6.646819	-3.700571	-1.108121
18	1	0	-6.607920	0.492755	-2.056667

19	1	0	-7.771342	-1.701895	-2.058778
20	6	0	0.254124	-4.913712	0.146668
21	6	0	-0.280479	-3.483763	-0.115636
22	1	0	0.349996	-5.462353	-0.793823
23	1	0	-0.446309	-5.450391	0.790808
24	1	0	-0.670460	-3.362388	-1.129820
25	1	0	-1.042653	-3.193287	0.611302
26	6	0	2.544162	-4.335618	-0.161757
27	1	0	3.482950	-4.156247	0.369834
28	1	0	2.726508	-5.072955	-0.947201
29	6	0	2.023857	-3.027176	-0.791872
30	1	0	2.776743	-2.236187	-0.807017
31	1	0	1.628049	-3.172948	-1.799433
32	6	0	1.307322	-2.506605	1.487998
33	1	0	2.218235	-1.900944	1.509421
34	1	0	0.532442	-2.003418	2.067904
35	6	0	1.502328	-3.969933	1.944285
36	1	0	2.428153	-4.051712	2.519039
37	1	0	0.671424	-4.288992	2.579154
38	7	0	1.568763	-4.870606	0.790601
39	7	0	0.867148	-2.522700	0.041663
40	6	0	0.452481	1.408190	1.352489
41	6	0	-0.586437	1.005046	0.252045
42	1	0	-0.157478	1.338609	-0.700573
43	6	0	0.057038	0.918025	2.675319
44	7	0	-0.246353	0.478098	3.700578

45	6	0	-1.913236	1.720809	0.441946
46	6	0	-2.802968	1.358392	1.460488
47	6	0	-2.258334	2.770341	-0.414161
48	6	0	-4.009931	2.034303	1.617565
49	1	0	-2.564198	0.536989	2.130033
50	6	0	-3.466536	3.448904	-0.256517
51	1	0	-1.574370	3.056011	-1.210536
52	6	0	-4.345155	3.081367	0.760288
53	1	0	-4.690925	1.738032	2.409904
54	1	0	-3.719617	4.262402	-0.929984
55	1	0	-5.288445	3.605211	0.883236
56	6	0	0.571438	2.939166	1.378955
57	8	0	0.034247	3.585446	2.253627
58	6	0	1.297314	3.583595	0.248255
59	6	0	2.292200	2.912237	-0.472108
60	6	0	0.966514	4.905879	-0.072111
61	6	0	2.955893	3.572931	-1.503635
62	1	0	2.575003	1.892158	-0.210938
63	6	0	1.619598	5.551471	-1.115072
64	1	0	0.189495	5.408635	0.496167
65	6	0	2.617439	4.885205	-1.828990
66	1	0	3.741705	3.059029	-2.049708
67	1	0	1.355200	6.572633	-1.371908
68	1	0	3.132034	5.392274	-2.639820
69	6	0	6.597851	-0.747862	-1.513102
70	6	0	6.539773	-1.054822	-0.149655

71	6	0	5.391007	-0.818105	0.594050
72	6	0	4.217404	-0.248635	0.013085
73	6	0	4.304527	0.042511	-1.383369
74	6	0	5.462746	-0.199086	-2.114754
75	8	0	3.146496	-0.034816	0.703147
76	1	0	1.431538	0.955715	1.126718
77	1	0	7.408733	-1.490015	0.340868
78	1	0	5.359655	-1.059951	1.654574
79	1	0	3.424982	0.459069	-1.873109
80	1	0	5.478212	0.040876	-3.176503
81	1	0	7.499035	-0.936453	-2.088275

3a_PhOH(RSR)

SCF Done: E(RM062X) = -1896.59050049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.029998	-1.734212	-1.307344
2	6	0	-1.106175	-1.183212	0.148994
3	1	0	-1.819884	-0.357889	0.084187
4	6	0	-0.330386	-3.017251	-1.417172
5	7	0	0.253729	-4.012123	-1.496146
6	6	0	-1.650395	-2.155465	1.192290
7	6	0	-2.285802	-3.353950	0.850408

8	6	0	-1.566909	-1.822866	2.552275
9	6	0	-2.808848	-4.194497	1.833428
10	1	0	-2.390825	-3.654673	-0.186287
11	6	0	-2.087088	-2.660604	3.533595
12	1	0	-1.087133	-0.901270	2.869950
13	6	0	-2.710216	-3.855368	3.178287
14	1	0	-3.294979	-5.119270	1.536886
15	1	0	-2.003415	-2.375912	4.578201
16	1	0	-3.114791	-4.512821	3.941770
17	6	0	-2.400200	-1.817353	-2.000271
18	8	0	-2.842390	-2.877857	-2.393235
19	6	0	-3.151991	-0.539390	-2.170615
20	6	0	-2.525210	0.712912	-2.117910
21	6	0	-4.530280	-0.625387	-2.398535
22	6	0	-3.286281	1.867153	-2.285695
23	1	0	-1.445474	0.794650	-1.982437
24	6	0	-5.283429	0.531183	-2.557806
25	1	0	-4.998544	-1.604064	-2.442607
26	6	0	-4.661114	1.778853	-2.499109
27	1	0	-2.801248	2.838357	-2.251097
28	1	0	-6.353658	0.462664	-2.726804
29	1	0	-5.248835	2.683901	-2.622813
30	6	0	0.254878	-0.523649	0.536110
31	6	0	1.257178	-1.519410	1.125322
32	1	0	0.622111	-0.079383	-0.406395
33	1	0	0.983919	-2.543973	0.862006

34	1	0	1.285691	-1.441107	2.214484
35	6	0	0.068306	0.676400	1.449011
36	8	0	0.692931	0.906486	2.454627
37	8	0	-0.900344	1.486913	0.967516
38	6	0	-1.177212	2.693155	1.610497
39	6	0	-0.179754	3.637661	1.827882
40	6	0	-2.503917	2.934424	1.939822
41	6	0	-0.532647	4.856831	2.400660
42	1	0	0.846612	3.420261	1.551253
43	6	0	-2.841767	4.160162	2.509917
44	1	0	-3.251257	2.171423	1.744897
45	6	0	-1.858952	5.120426	2.742648
46	1	0	0.234977	5.604505	2.575010
47	1	0	-3.876239	4.362034	2.770075
48	1	0	-2.125678	6.074174	3.187306
49	6	0	4.961069	-2.335327	0.921899
50	6	0	3.520111	-2.329784	1.478050
51	1	0	5.166616	-3.276105	0.405226
52	1	0	5.672504	-2.229530	1.744611
53	1	0	3.038435	-3.306470	1.402769
54	1	0	3.469802	-1.978942	2.510968
55	6	0	4.315106	-1.479754	-1.199353
56	1	0	4.393465	-0.612047	-1.857562
57	1	0	4.688466	-2.357697	-1.732510
58	6	0	2.838016	-1.711784	-0.793927
59	1	0	2.146023	-1.083818	-1.366529

60	1	0	2.540267	-2.758927	-0.883847
61	6	0	3.222571	0.025986	0.899600
62	1	0	2.678500	0.695546	0.227169
63	1	0	2.996699	0.284866	1.934564
64	6	0	4.743043	0.015083	0.602984
65	1	0	4.986948	0.846583	-0.063403
66	1	0	5.308440	0.135788	1.530720
67	7	0	5.155005	-1.239873	-0.026485
68	7	0	2.685020	-1.364229	0.667470
69	6	0	3.542362	3.497594	-1.620359
70	6	0	2.265265	3.573505	-1.057303
71	6	0	1.310005	2.590152	-1.296179
72	6	0	1.584372	1.457450	-2.122068
73	6	0	2.889370	1.422241	-2.700821
74	6	0	3.834040	2.410915	-2.451918
75	8	0	0.724375	0.515198	-2.319030
76	1	0	-0.428182	-1.008575	-1.881737
77	1	0	2.005668	4.419001	-0.421692
78	1	0	0.315960	2.671234	-0.860730
79	1	0	3.123879	0.586412	-3.357140
80	1	0	4.816406	2.333914	-2.915045
81	1	0	4.283164	4.267888	-1.430101

3a_PhOH(SRS)

SCF Done: E(RM062X) = -1896.59050004

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.030710	-1.733610	-1.308013
2	6	0	1.106835	-1.183195	0.148571
3	1	0	1.820213	-0.357564	0.084027
4	6	0	0.331699	-3.016917	-1.418260
5	7	0	-0.251696	-4.012190	-1.497478
6	6	0	1.651563	-2.155674	1.191393
7	6	0	2.287909	-3.353508	0.848968
8	6	0	1.567593	-1.823881	2.551544
9	6	0	2.811397	-4.194207	1.831627
10	1	0	2.393386	-3.653610	-0.187859
11	6	0	2.088217	-2.661766	3.532499
12	1	0	1.087068	-0.902810	2.869609
13	6	0	2.712284	-3.855882	3.176651
14	1	0	3.298267	-5.118456	1.534670
15	1	0	2.004141	-2.377719	4.577247
16	1	0	3.117202	-4.513449	3.939851
17	6	0	2.400860	-1.815694	-2.001213
18	8	0	2.843701	-2.875738	-2.394631
19	6	0	3.151701	-0.537106	-2.171199
20	6	0	2.523957	0.714706	-2.118284
21	6	0	4.530072	-0.621998	-2.398985
22	6	0	3.284161	1.869565	-2.285768

23	1	0	1.444162	0.795635	-1.982838
24	6	0	5.282367	0.535185	-2.557891
25	1	0	4.999099	-1.600299	-2.443247
26	6	0	4.659094	1.782366	-2.499019
27	1	0	2.798357	2.840377	-2.251021
28	1	0	6.352669	0.467511	-2.726750
29	1	0	5.246138	2.687890	-2.622432
30	6	0	-0.254434	-0.524360	0.536082
31	6	0	-1.256262	-1.520701	1.125082
32	1	0	-0.621916	-0.080013	-0.406305
33	1	0	-0.982748	-2.545069	0.861274
34	1	0	-1.284637	-1.442854	2.214278
35	6	0	-0.068200	0.675486	1.449322
36	8	0	-0.692513	0.904853	2.455292
37	8	0	0.899730	1.486732	0.967653
38	6	0	1.176300	2.692770	1.611161
39	6	0	2.502904	2.934235	1.940726
40	6	0	0.178546	3.636867	1.828927
41	6	0	2.840346	4.159774	2.511496
42	1	0	3.250473	2.171540	1.745476
43	6	0	0.531026	4.855833	2.402387
44	1	0	-0.847711	3.419286	1.552027
45	6	0	1.857228	5.119620	2.744647
46	1	0	3.874732	4.361810	2.771863
47	1	0	-0.236817	5.603204	2.577075
48	1	0	2.123619	6.073204	3.189855

49	6	0	-3.519034	-2.331633	1.477855
50	6	0	-4.960003	-2.337286	0.921726
51	1	0	-3.037146	-3.308185	1.402296
52	1	0	-3.468742	-1.981038	2.510859
53	1	0	-5.165362	-3.277903	0.404689
54	1	0	-5.671449	-2.231947	1.744479
55	6	0	-2.837225	-1.712725	-0.794063
56	1	0	-2.145032	-1.084504	-1.366183
57	1	0	-2.539487	-2.759848	-0.884322
58	6	0	-4.314382	-1.480782	-1.199286
59	1	0	-4.393029	-0.612858	-1.857149
60	1	0	-4.687607	-2.358604	-1.732734
61	6	0	-4.742439	0.013279	0.603632
62	1	0	-4.986530	0.844975	-0.062437
63	1	0	-5.307784	0.133555	1.531453
64	6	0	-3.221940	0.024336	0.900131
65	1	0	-2.678036	0.694184	0.227862
66	1	0	-2.996029	0.282918	1.935156
67	7	0	-2.684200	-1.365706	0.667494
68	7	0	-5.154202	-1.241516	-0.026245
69	6	0	-3.543471	3.498281	-1.619806
70	6	0	-3.835495	2.411451	-2.451063
71	6	0	-2.891063	1.422534	-2.699841
72	6	0	-1.585978	1.457604	-2.121271
73	6	0	-1.311209	2.590518	-1.295814
74	6	0	-2.266258	3.574105	-1.057018

75	8	0	-0.726223	0.515121	-2.318185
76	1	0	0.428672	-1.007967	-1.882119
77	1	0	-4.817939	2.334550	-2.914036
78	1	0	-3.125743	0.586639	-3.356008
79	1	0	-0.317078	2.671567	-0.860553
80	1	0	-2.006377	4.419720	-0.421684
81	1	0	-4.284119	4.268735	-1.429612

3a_PhOH(SSR)

SCF Done: E(RM062X) = -1896.59140791

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.022268	0.409037	0.607328
2	6	0	-0.164973	-0.086927	2.047080
3	1	0	-0.375760	-0.309734	-0.120034
4	1	0	0.701878	-0.662386	2.382364
5	1	0	-0.318128	0.749262	2.734301
6	6	0	-0.741713	1.711783	0.427252
7	8	0	-0.810810	2.605964	1.232222
8	8	0	-1.420673	1.697970	-0.742272
9	6	0	-2.328783	2.723604	-1.012283
10	6	0	-1.920129	4.046855	-1.126760
11	6	0	-3.648728	2.340644	-1.214248

12	6	0	-2.871934	5.008397	-1.458358
13	1	0	-0.881329	4.312182	-0.966051
14	6	0	-4.588449	3.313387	-1.547901
15	1	0	-3.924500	1.294440	-1.111958
16	6	0	-4.202164	4.646720	-1.669248
17	1	0	-2.568440	6.046663	-1.551884
18	1	0	-5.622464	3.025894	-1.711778
19	1	0	-4.935876	5.403864	-1.928211
20	6	0	-1.617614	-1.232801	3.668309
21	6	0	-2.649305	-2.378547	3.788119
22	1	0	-0.663961	-1.473398	4.142199
23	1	0	-1.990687	-0.284513	4.060870
24	1	0	-2.157059	-3.308415	4.084701
25	1	0	-3.389089	-2.121618	4.550125
26	6	0	-1.049780	-2.353717	1.578567
27	1	0	-0.620491	-2.192053	0.586220
28	1	0	-0.297586	-2.813245	2.224768
29	6	0	-2.365561	-3.156773	1.546720
30	1	0	-2.816786	-3.115640	0.550127
31	1	0	-2.158174	-4.202243	1.789761
32	6	0	-3.793819	-1.314984	1.994653
33	1	0	-4.427941	-1.482919	1.119685
34	1	0	-4.389962	-0.827249	2.770115
35	6	0	-2.596177	-0.427150	1.586947
36	1	0	-2.449669	-0.431388	0.504617
37	1	0	-2.692046	0.597950	1.953760

38	7	0	-1.344646	-1.006415	2.201650
39	7	0	-3.326641	-2.603321	2.507854
40	6	0	1.794855	0.687518	-1.247241
41	6	0	1.537155	0.441631	0.271375
42	1	0	1.833936	-0.603152	0.414599
43	6	0	1.427744	2.035435	-1.688668
44	7	0	1.131162	3.097870	-2.034115
45	6	0	2.418554	1.275204	1.183274
46	6	0	2.324712	2.669747	1.274454
47	6	0	3.388855	0.617860	1.947835
48	6	0	3.177492	3.380041	2.116094
49	1	0	1.587590	3.213526	0.693896
50	6	0	4.240803	1.327662	2.791532
51	1	0	3.476525	-0.464251	1.877143
52	6	0	4.135630	2.713298	2.877826
53	1	0	3.090816	4.460950	2.175828
54	1	0	4.986244	0.796860	3.376218
55	1	0	4.797009	3.273054	3.532539
56	6	0	3.288928	0.471847	-1.551853
57	8	0	3.993972	1.418118	-1.836042
58	6	0	3.846587	-0.906792	-1.428308
59	6	0	5.237894	-1.026505	-1.316409
60	6	0	3.041340	-2.052528	-1.429840
61	6	0	5.823826	-2.280569	-1.203698
62	1	0	5.844959	-0.126680	-1.314655
63	6	0	3.639275	-3.307437	-1.326842

64	1	0	1.955669	-1.987948	-1.520685
65	6	0	5.022698	-3.424007	-1.210935
66	1	0	6.901816	-2.369989	-1.110030
67	1	0	3.018045	-4.198240	-1.336391
68	1	0	5.479482	-4.405594	-1.124141
69	6	0	-3.806502	-3.480836	-2.131482
70	6	0	-2.653778	-4.266689	-2.029673
71	6	0	-1.400204	-3.690798	-1.860459
72	6	0	-1.223756	-2.275921	-1.785039
73	6	0	-2.415208	-1.499862	-1.920876
74	6	0	-3.664664	-2.090521	-2.080292
75	8	0	-0.072279	-1.734998	-1.565922
76	1	0	1.163686	-0.035638	-1.789027
77	1	0	-2.737414	-5.351172	-2.076238
78	1	0	-0.512909	-4.315202	-1.773101
79	1	0	-2.312694	-0.416148	-1.892847
80	1	0	-4.544748	-1.455237	-2.171229
81	1	0	-4.782978	-3.937791	-2.258908

TS3a/3b_PhOH(RRS)

SCF Done: E(RM062X) = -1896.57540490

Imaginary Frequencies = -1174.0934

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

1	6	0	0.205502	0.001825	0.790981
2	6	0	-0.582070	-0.051094	2.085018
3	1	0	-0.324596	-0.699925	-0.341802
4	1	0	-0.928280	0.942909	2.386589
5	1	0	0.012234	-0.473645	2.899764
6	6	0	1.428693	-0.778588	0.890908
7	8	0	1.683180	-1.650364	1.701824
8	8	0	2.255823	-0.532736	-0.182215
9	6	0	3.503505	-1.119376	-0.266258
10	6	0	3.869951	-1.616690	-1.513152
11	6	0	4.392632	-1.133139	0.806288
12	6	0	5.146545	-2.146239	-1.688400
13	1	0	3.152806	-1.577250	-2.327915
14	6	0	5.663442	-1.671049	0.618454
15	1	0	4.087950	-0.739661	1.769708
16	6	0	6.044746	-2.178274	-0.623463
17	1	0	5.437114	-2.532648	-2.660713
18	1	0	6.360969	-1.688208	1.450655
19	1	0	7.038167	-2.594081	-0.760005
20	6	0	-2.828336	-3.116700	1.626576
21	6	0	-1.509846	-2.345730	1.844287
22	1	0	-2.795970	-4.060603	2.176510
23	1	0	-2.968106	-3.339907	0.564237
24	1	0	-0.970735	-2.670135	2.737287
25	1	0	-0.838444	-2.413834	0.988472

26	6	0	-3.685111	-1.821384	3.431586
27	1	0	-4.585686	-1.361435	3.845849
28	1	0	-3.409800	-2.670133	4.063116
29	6	0	-2.542369	-0.780763	3.392501
30	1	0	-2.906220	0.246976	3.459775
31	1	0	-1.793269	-0.950835	4.168007
32	6	0	-2.802132	-0.429440	0.997700
33	1	0	-2.904858	0.652421	1.117295
34	1	0	-2.338757	-0.646665	0.033972
35	6	0	-4.141653	-1.178686	1.187846
36	1	0	-4.897296	-0.515847	1.617744
37	1	0	-4.502679	-1.531661	0.218242
38	7	0	-3.973443	-2.324674	2.086050
39	7	0	-1.843535	-0.895957	2.062532
40	6	0	0.687202	1.642442	-1.250359
41	6	0	0.226113	1.444023	0.240877
42	1	0	-0.835545	1.716584	0.209284
43	6	0	2.134239	1.818502	-1.416514
44	7	0	3.267281	1.983701	-1.574545
45	6	0	0.887955	2.473974	1.146602
46	6	0	2.157149	2.273320	1.701441
47	6	0	0.214340	3.665831	1.431527
48	6	0	2.732112	3.239903	2.522915
49	1	0	2.711002	1.362798	1.486255
50	6	0	0.786419	4.634964	2.253802
51	1	0	-0.773098	3.831516	1.003892

52	6	0	2.048199	4.422496	2.803557
53	1	0	3.717500	3.068409	2.946466
54	1	0	0.243852	5.551312	2.467405
55	1	0	2.496835	5.171963	3.448883
56	6	0	0.004539	2.908172	-1.806970
57	8	0	0.647795	3.919670	-1.996887
58	6	0	-1.472696	2.878585	-2.043261
59	6	0	-2.213353	1.691466	-2.068503
60	6	0	-2.118053	4.105811	-2.237245
61	6	0	-3.589293	1.739845	-2.281278
62	1	0	-1.731779	0.725240	-1.933149
63	6	0	-3.491081	4.148663	-2.446957
64	1	0	-1.529678	5.017717	-2.215530
65	6	0	-4.228938	2.964125	-2.467470
66	1	0	-4.161342	0.816437	-2.302109
67	1	0	-3.987596	5.103171	-2.592141
68	1	0	-5.302329	2.996654	-2.629746
69	6	0	-0.939784	-5.189694	-2.009483
70	6	0	0.182901	-4.621351	-1.408784
71	6	0	0.267088	-3.245410	-1.208881
72	6	0	-0.790143	-2.399849	-1.595902
73	6	0	-1.919678	-2.982829	-2.202118
74	6	0	-1.987064	-4.357246	-2.408773
75	8	0	-0.752128	-1.078892	-1.405401
76	1	0	0.386771	0.759972	-1.827792
77	1	0	1.010244	-5.253498	-1.096573

78	1	0	1.153363	-2.812639	-0.750956
79	1	0	-2.736125	-2.331361	-2.504581
80	1	0	-2.868920	-4.783384	-2.880484
81	1	0	-0.997204	-6.262162	-2.167289

TS3a/3b_PhOH(RSR)

SCF Done: E(RM062X) = -1896.57387316

Imaginary Frequencies = -1101.6165

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.238103	-1.954151	-1.390226
2	6	0	-0.549476	-1.415029	0.050061
3	1	0	-1.449026	-0.808801	-0.089908
4	6	0	0.708907	-3.074150	-1.398256
5	7	0	1.480121	-3.935573	-1.388021
6	6	0	-0.926283	-2.515407	1.052740
7	6	0	-1.383746	-3.778311	0.655019
8	6	0	-0.874426	-2.253289	2.430252
9	6	0	-1.776175	-4.735324	1.590538
10	1	0	-1.440138	-4.044179	-0.394545
11	6	0	-1.268616	-3.205462	3.366216
12	1	0	-0.513225	-1.298684	2.799353
13	6	0	-1.723342	-4.455152	2.951768

14	1	0	-2.123181	-5.704605	1.244456
15	1	0	-1.214602	-2.966427	4.424414
16	1	0	-2.029326	-5.199981	3.680372
17	6	0	-1.482056	-2.331224	-2.219710
18	8	0	-1.642294	-3.464745	-2.625398
19	6	0	-2.470220	-1.254111	-2.521718
20	6	0	-2.152930	0.106318	-2.432664
21	6	0	-3.749720	-1.645314	-2.934008
22	6	0	-3.111743	1.063730	-2.751700
23	1	0	-1.154969	0.425404	-2.140387
24	6	0	-4.706598	-0.686098	-3.241448
25	1	0	-3.981119	-2.703799	-3.002625
26	6	0	-4.387946	0.669577	-3.150079
27	1	0	-2.857685	2.117903	-2.689369
28	1	0	-5.700588	-0.992721	-3.552029
29	1	0	-5.136115	1.419241	-3.390555
30	6	0	0.534896	-0.439525	0.557689
31	6	0	1.782252	-1.117094	1.103212
32	1	0	0.776878	0.375950	-0.616039
33	1	0	1.785760	-2.188660	0.881610
34	1	0	1.861569	-0.993955	2.188154
35	6	0	0.046529	0.563221	1.503078
36	8	0	0.691792	1.114565	2.376929
37	8	0	-1.285105	0.875316	1.310007
38	6	0	-1.876487	1.837410	2.111680
39	6	0	-1.371593	3.132860	2.197850

40	6	0	-3.047341	1.474303	2.767633
41	6	0	-2.061963	4.074578	2.956517
42	1	0	-0.454501	3.391711	1.681139
43	6	0	-3.730197	2.426906	3.521570
44	1	0	-3.409494	0.454564	2.677734
45	6	0	-3.239838	3.727654	3.618341
46	1	0	-1.674490	5.086513	3.029013
47	1	0	-4.645826	2.148418	4.034527
48	1	0	-3.772328	4.469045	4.206044
49	6	0	5.581167	-0.963447	0.776149
50	6	0	4.211814	-1.272802	1.422732
51	1	0	5.968120	-1.844850	0.257804
52	1	0	6.295579	-0.678238	1.552442
53	1	0	3.997505	-2.342876	1.458611
54	1	0	4.117327	-0.852405	2.426470
55	6	0	4.663144	-0.346265	-1.330220
56	1	0	4.428477	0.514811	-1.962795
57	1	0	5.249891	-1.056512	-1.918641
58	6	0	3.365483	-1.027064	-0.843007
59	1	0	2.499368	-0.707838	-1.422264
60	1	0	3.437787	-2.116838	-0.847143
61	6	0	3.278488	0.865188	0.724103
62	1	0	2.593857	1.308640	0.000994
63	1	0	2.957004	1.127445	1.731786
64	6	0	4.750522	1.238993	0.438120
65	1	0	4.782238	2.109393	-0.222749

66	1	0	5.271328	1.491919	1.365817
67	7	0	5.461371	0.125848	-0.195854
68	7	0	3.132246	-0.628857	0.590036
69	6	0	0.535598	5.013943	-1.847637
70	6	0	-0.409531	4.231131	-1.186809
71	6	0	-0.268308	2.845690	-1.119505
72	6	0	0.838184	2.210832	-1.712372
73	6	0	1.790465	3.009224	-2.372112
74	6	0	1.634874	4.389744	-2.440854
75	8	0	1.000081	0.882155	-1.673188
76	1	0	0.250343	-1.135431	-1.936561
77	1	0	-1.271482	4.698663	-0.716540
78	1	0	-1.016396	2.240493	-0.613042
79	1	0	2.644766	2.519355	-2.832126
80	1	0	2.381766	4.984640	-2.960378
81	1	0	0.418873	6.091926	-1.900660

TS3a/3b_PhOH(SRS)

SCF Done: E(RM062X) = -1896.57229641

Imaginary Frequencies = -1115.4263

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.256025	-2.047927	-0.640889

2	6	0	-0.325843	-0.492057	-0.801798
3	1	0	-1.080769	-0.225120	-0.057046
4	6	0	0.805464	-2.715751	-1.400237
5	7	0	1.640073	-3.254170	-1.992056
6	6	0	-0.910568	-0.087771	-2.150712
7	6	0	-0.289206	-0.369415	-3.374627
8	6	0	-2.133412	0.594442	-2.171965
9	6	0	-0.865327	0.036680	-4.576558
10	1	0	0.644654	-0.922742	-3.408946
11	6	0	-2.712130	1.001570	-3.373135
12	1	0	-2.634097	0.810311	-1.230370
13	6	0	-2.076592	0.726127	-4.581480
14	1	0	-0.365310	-0.192212	-5.513278
15	1	0	-3.660261	1.531808	-3.361418
16	1	0	-2.522759	1.041671	-5.520014
17	6	0	-1.596958	-2.654396	-1.105536
18	8	0	-1.643194	-3.329473	-2.112400
19	6	0	-2.836302	-2.316755	-0.346122
20	6	0	-2.832654	-1.994983	1.014708
21	6	0	-4.043619	-2.337919	-1.056133
22	6	0	-4.034274	-1.701951	1.656836
23	1	0	-1.904735	-1.986612	1.581786
24	6	0	-5.236350	-2.029071	-0.414973
25	1	0	-4.028058	-2.585512	-2.113187
26	6	0	-5.231500	-1.713102	0.944459
27	1	0	-4.030655	-1.462626	2.715491

28	1	0	-6.168461	-2.034111	-0.971423
29	1	0	-6.163102	-1.475227	1.449535
30	6	0	0.936527	0.297324	-0.376489
31	6	0	2.176581	0.171780	-1.248501
32	1	0	1.151027	-0.243134	0.940286
33	1	0	2.129608	-0.674871	-1.933807
34	1	0	2.343487	1.079330	-1.835953
35	6	0	0.637888	1.719616	-0.170377
36	8	0	1.399014	2.656542	-0.329860
37	8	0	-0.642889	1.946577	0.286055
38	6	0	-1.023123	3.268916	0.470275
39	6	0	-1.667105	3.930532	-0.569106
40	6	0	-0.809408	3.883062	1.698993
41	6	0	-2.115151	5.233955	-0.367490
42	1	0	-1.812068	3.420530	-1.517141
43	6	0	-1.261834	5.186924	1.890111
44	1	0	-0.294558	3.342574	2.487941
45	6	0	-1.914835	5.863708	0.860327
46	1	0	-2.621982	5.756815	-1.172931
47	1	0	-1.102223	5.674074	2.847356
48	1	0	-2.266746	6.879142	1.014381
49	6	0	4.619358	0.183890	-1.522647
50	6	0	5.951327	-0.277205	-0.888330
51	1	0	4.368105	-0.379708	-2.423632
52	1	0	4.612982	1.251895	-1.751624
53	1	0	6.259863	-1.243036	-1.297721

54	1	0	6.732192	0.455213	-1.108454
55	6	0	3.643800	-1.458890	-0.025932
56	1	0	2.743352	-1.703488	0.538562
57	1	0	3.707400	-2.088772	-0.915215
58	6	0	4.916683	-1.542776	0.841680
59	1	0	4.657751	-1.519344	1.904297
60	1	0	5.437204	-2.481691	0.634792
61	6	0	5.186199	0.805253	1.082363
62	1	0	5.224067	0.792947	2.174696
63	1	0	5.765588	1.662731	0.728899
64	6	0	3.715877	0.911153	0.619897
65	1	0	3.017118	0.613084	1.403052
66	1	0	3.453655	1.903842	0.256175
67	7	0	3.509803	-0.044972	-0.528403
68	7	0	5.811906	-0.414697	0.564012
69	6	0	-1.830317	-1.418654	4.525643
70	6	0	-0.897626	-2.435238	4.309709
71	6	0	0.170653	-2.245136	3.439229
72	6	0	0.338206	-1.022900	2.758838
73	6	0	-0.606556	-0.002483	2.983369
74	6	0	-1.673597	-0.205199	3.854326
75	8	0	1.373905	-0.868101	1.935639
76	1	0	-0.077879	-2.267104	0.420198
77	1	0	-1.004407	-3.387584	4.823078
78	1	0	0.899420	-3.032843	3.267365
79	1	0	-0.491193	0.943286	2.461827

80	1	0	-2.392322	0.596089	4.009154
81	1	0	-2.662554	-1.569216	5.206604

TS3a/3b_PhOH(SSR)

SCF Done: E(RM062X) = -1896.57663244

Imaginary Frequencies = -1237.6589

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.339693	0.384722	-0.048772
2	6	0	-2.837773	0.149110	-0.033322
3	1	0	-0.600073	-0.797930	-0.287739
4	1	0	-3.256615	0.309774	0.965604
5	1	0	-3.355290	0.807890	-0.736685
6	6	0	-0.961592	1.253267	-1.156769
7	8	0	-1.501829	1.317801	-2.245356
8	8	0	0.178196	1.984731	-0.883078
9	6	0	0.771512	2.729808	-1.888204
10	6	0	0.087902	3.752572	-2.539949
11	6	0	2.109092	2.464069	-2.162150
12	6	0	0.763586	4.510146	-3.493160
13	1	0	-0.952217	3.946418	-2.301680
14	6	0	2.775391	3.232505	-3.114508
15	1	0	2.609254	1.659243	-1.629881

16	6	0	2.103568	4.253439	-3.784356
17	1	0	0.238765	5.309065	-4.008345
18	1	0	3.819768	3.029569	-3.331660
19	1	0	2.622176	4.849693	-4.528739
20	6	0	-4.817857	-1.238996	-0.485947
21	6	0	-5.301366	-2.698432	-0.643456
22	1	0	-5.185573	-0.772901	0.430266
23	1	0	-5.082989	-0.614478	-1.341756
24	1	0	-5.703017	-3.075345	0.300816
25	1	0	-6.092871	-2.742500	-1.395809
26	6	0	-2.910933	-2.262587	0.619216
27	1	0	-1.846541	-2.147100	0.819133
28	1	0	-3.486047	-2.022321	1.516978
29	6	0	-3.241668	-3.662658	0.058641
30	1	0	-2.332925	-4.147133	-0.310824
31	1	0	-3.666619	-4.284218	0.851074
32	6	0	-3.518021	-2.946056	-2.195437
33	1	0	-2.794282	-3.651517	-2.610975
34	1	0	-4.269159	-2.732583	-2.960744
35	6	0	-2.788621	-1.652189	-1.766264
36	1	0	-1.715770	-1.805629	-1.652030
37	1	0	-2.965881	-0.813458	-2.441336
38	7	0	-3.313226	-1.243622	-0.414175
39	7	0	-4.194646	-3.567139	-1.052152
40	6	0	0.793358	0.514011	1.359487
41	6	0	-0.766029	0.671484	1.344591

42	1	0	-1.116968	-0.151178	1.978469
43	6	0	1.514394	1.739291	1.716915
44	7	0	2.117148	2.686669	1.994949
45	6	0	-1.243096	1.942468	2.040822
46	6	0	-1.899591	2.979768	1.377151
47	6	0	-1.019720	2.067555	3.418716
48	6	0	-2.316521	4.117538	2.070504
49	1	0	-2.103623	2.908695	0.312071
50	6	0	-1.429455	3.200938	4.112325
51	1	0	-0.515971	1.258733	3.945615
52	6	0	-2.080534	4.234231	3.436933
53	1	0	-2.827536	4.913470	1.536573
54	1	0	-1.245116	3.277198	5.180116
55	1	0	-2.403614	5.120511	3.975061
56	6	0	1.268549	-0.634075	2.280617
57	8	0	0.562128	-1.035406	3.180974
58	6	0	2.606366	-1.237366	2.008718
59	6	0	3.513133	-0.699871	1.086424
60	6	0	2.932787	-2.413723	2.693189
61	6	0	4.730350	-1.335058	0.856874
62	1	0	3.290878	0.214396	0.543952
63	6	0	4.141981	-3.053867	2.451127
64	1	0	2.220874	-2.821178	3.404024
65	6	0	5.041992	-2.514516	1.531223
66	1	0	5.429696	-0.914146	0.141208
67	1	0	4.384361	-3.971653	2.977920

68	1	0	5.987292	-3.014181	1.340421
69	6	0	3.454323	-2.469289	-2.434059
70	6	0	3.046191	-3.392243	-1.465698
71	6	0	1.890574	-3.181807	-0.726313
72	6	0	1.097465	-2.032790	-0.929655
73	6	0	1.497485	-1.124743	-1.930720
74	6	0	2.667297	-1.342470	-2.659769
75	8	0	0.021450	-1.851349	-0.171755
76	1	0	1.138840	0.267420	0.352127
77	1	0	3.642715	-4.281979	-1.277865
78	1	0	1.577217	-3.888090	0.038027
79	1	0	0.882354	-0.253868	-2.147529
80	1	0	2.957400	-0.618612	-3.418235
81	1	0	4.363676	-2.632756	-3.004032

3b_PhOH(*R*RS)

SCF Done: E(RM062X) = -1896.59059953

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.794125	-0.325738	0.211967
2	6	0	0.481323	-0.697938	-0.537686
3	1	0	-0.837760	-0.780783	1.205213
4	1	0	1.298692	-0.040448	-0.231410

5	1	0	0.323201	-0.595004	-1.615185
6	6	0	-2.025308	-0.731957	-0.570035
7	8	0	-2.197655	-0.509722	-1.741855
8	8	0	-2.935133	-1.339425	0.223476
9	6	0	-4.188870	-1.601707	-0.334180
10	6	0	-4.407487	-2.800934	-0.996649
11	6	0	-5.191723	-0.658795	-0.156180
12	6	0	-5.683148	-3.063544	-1.492456
13	1	0	-3.594649	-3.511496	-1.114301
14	6	0	-6.462191	-0.934220	-0.656422
15	1	0	-4.969582	0.264470	0.372665
16	6	0	-6.708661	-2.133519	-1.323764
17	1	0	-5.873959	-3.997928	-2.011375
18	1	0	-7.258657	-0.208566	-0.522994
19	1	0	-7.700671	-2.344376	-1.711201
20	6	0	0.610269	-4.530321	-0.562189
21	6	0	-0.056227	-3.132351	-0.626179
22	1	0	0.686607	-4.958300	-1.564585
23	1	0	0.002379	-5.195794	0.054815
24	1	0	-0.451173	-2.900050	-1.618496
25	1	0	-0.846006	-3.023562	0.121008
26	6	0	2.807862	-3.678604	-0.901879
27	1	0	3.783310	-3.542940	-0.427163
28	1	0	2.947429	-4.243009	-1.827143
29	6	0	2.174430	-2.306410	-1.219821
30	1	0	2.862155	-1.475909	-1.038955

31	1	0	1.787555	-2.244540	-2.239201
32	6	0	1.447506	-2.283452	1.118452
33	1	0	2.250581	-1.560083	1.282856
34	1	0	0.612949	-2.036720	1.775046
35	6	0	1.892840	-3.754798	1.293259
36	1	0	2.879980	-3.785557	1.762538
37	1	0	1.188691	-4.289661	1.935644
38	7	0	1.956036	-4.446722	0.005633
39	7	0	0.987514	-2.094664	-0.306886
40	6	0	0.350521	1.696285	1.211458
41	6	0	-0.835955	1.232470	0.386060
42	1	0	-0.722522	1.650192	-0.619489
43	6	0	0.538863	1.081431	2.472361
44	7	0	0.643993	0.555446	3.508743
45	6	0	-2.193827	1.680161	0.908968
46	6	0	-2.667619	1.272798	2.162599
47	6	0	-3.001894	2.508784	0.124998
48	6	0	-3.904791	1.709179	2.628835
49	1	0	-2.065288	0.612889	2.781932
50	6	0	-4.240903	2.950073	0.590981
51	1	0	-2.651015	2.818621	-0.857234
52	6	0	-4.693586	2.555048	1.847365
53	1	0	-4.255296	1.386385	3.604963
54	1	0	-4.850700	3.599637	-0.030305
55	1	0	-5.656506	2.897628	2.214605
56	6	0	1.398467	2.493964	0.733362

57	8	0	2.522025	2.626040	1.311745
58	6	0	1.209027	3.256373	-0.550209
59	6	0	2.174349	3.145681	-1.555183
60	6	0	0.116070	4.105862	-0.743548
61	6	0	2.038075	3.855423	-2.744985
62	1	0	3.024551	2.485840	-1.404465
63	6	0	-0.011657	4.831843	-1.926544
64	1	0	-0.631057	4.202066	0.040796
65	6	0	0.946711	4.703511	-2.931143
66	1	0	2.785466	3.750028	-3.526071
67	1	0	-0.858409	5.498529	-2.062869
68	1	0	0.844329	5.263319	-3.856269
69	6	0	6.364683	-0.673019	-0.978310
70	6	0	5.865227	0.626769	-0.902925
71	6	0	4.920973	0.976053	0.059912
72	6	0	4.453615	0.009914	0.962716
73	6	0	4.962220	-1.294979	0.896436
74	6	0	5.909931	-1.627347	-0.067309
75	8	0	3.530621	0.282047	1.906512
76	1	0	3.149305	1.204103	1.775710
77	1	0	6.217388	1.384735	-1.597724
78	1	0	4.536987	1.989362	0.132533
79	1	0	4.604067	-2.034584	1.608717
80	1	0	6.294829	-2.643111	-0.106203
81	1	0	7.101201	-0.937248	-1.730661

3b_PhOH(*R*SR)

SCF Done: E(RM062X) = -1896.58329907

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.993982	-1.582001	1.585394
2	6	0	1.505165	-1.135500	0.226858
3	1	0	2.079078	-0.223735	0.414553
4	6	0	0.404587	-2.881450	1.693008
5	7	0	-0.067767	-3.941134	1.739449
6	6	0	2.470602	-2.142467	-0.398050
7	6	0	3.274177	-2.948518	0.417826
8	6	0	2.638466	-2.232573	-1.784324
9	6	0	4.207301	-3.822969	-0.133128
10	1	0	3.176527	-2.887647	1.498373
11	6	0	3.572146	-3.107307	-2.338080
12	1	0	2.046546	-1.619675	-2.457989
13	6	0	4.358706	-3.908961	-1.515366
14	1	0	4.817069	-4.438347	0.521854
15	1	0	3.680123	-3.159355	-3.417455
16	1	0	5.082946	-4.593709	-1.946106
17	6	0	1.113531	-0.869007	2.736301
18	8	0	0.705602	-1.452895	3.880786
19	6	0	1.723509	0.475405	2.867362

20	6	0	2.693943	0.664519	3.862062
21	6	0	1.330343	1.547961	2.057887
22	6	0	3.289971	1.910397	4.024696
23	1	0	2.999982	-0.168769	4.489940
24	6	0	1.930778	2.793106	2.234310
25	1	0	0.533305	1.433939	1.321342
26	6	0	2.910688	2.975703	3.208437
27	1	0	4.051476	2.047772	4.785887
28	1	0	1.621461	3.626320	1.609737
29	1	0	3.375358	3.948811	3.336825
30	6	0	0.326950	-0.709149	-0.693565
31	6	0	-0.457591	-1.873886	-1.304547
32	1	0	-0.329396	-0.092101	-0.059555
33	1	0	-0.234490	-2.812908	-0.792762
34	1	0	-0.229994	-1.998615	-2.365890
35	6	0	0.718719	0.319422	-1.736558
36	8	0	0.342799	0.345386	-2.882743
37	8	0	1.510745	1.269964	-1.195250
38	6	0	1.644096	2.467378	-1.900770
39	6	0	0.605039	3.387720	-1.826897
40	6	0	2.818080	2.720445	-2.593785
41	6	0	0.758287	4.609173	-2.478133
42	1	0	-0.283939	3.119834	-1.256910
43	6	0	2.956083	3.949809	-3.238202
44	1	0	3.602160	1.970021	-2.623370
45	6	0	1.930096	4.891389	-3.181934

46	1	0	-0.038899	5.345420	-2.432071
47	1	0	3.868185	4.168691	-3.785008
48	1	0	2.044236	5.847025	-3.684480
49	6	0	-4.100527	-2.899818	-1.672115
50	6	0	-2.575895	-2.922073	-1.925902
51	1	0	-4.376729	-3.662789	-0.939360
52	1	0	-4.628199	-3.110660	-2.605559
53	1	0	-2.098564	-3.815646	-1.519180
54	1	0	-2.322727	-2.823109	-2.983826
55	6	0	-3.964649	-1.410311	0.181406
56	1	0	-4.137107	-0.373418	0.486391
57	1	0	-4.477167	-2.071182	0.885357
58	6	0	-2.453244	-1.725657	0.191958
59	1	0	-1.890537	-0.976623	0.751978
60	1	0	-2.232266	-2.718777	0.590275
61	6	0	-2.441996	-0.485252	-1.940503
62	1	0	-2.085655	0.370786	-1.357533
63	1	0	-1.964651	-0.482075	-2.920834
64	6	0	-3.985527	-0.550755	-2.033555
65	1	0	-4.407304	0.413331	-1.737776
66	1	0	-4.298768	-0.767638	-3.058617
67	7	0	-4.523963	-1.595170	-1.159573
68	7	0	-1.958852	-1.730825	-1.233049
69	6	0	-4.815583	1.870666	2.297404
70	6	0	-4.712197	2.420483	1.015919
71	6	0	-3.518454	2.368399	0.305270

72	6	0	-2.347321	1.749645	0.838146
73	6	0	-2.479749	1.215254	2.156292
74	6	0	-3.680659	1.273041	2.854145
75	8	0	-1.251143	1.658832	0.158484
76	1	0	0.718643	-0.800374	4.604288
77	1	0	-5.579391	2.897412	0.562498
78	1	0	-3.450337	2.799539	-0.692236
79	1	0	-1.605987	0.741150	2.603553
80	1	0	-3.735565	0.842106	3.852339
81	1	0	-5.750482	1.911048	2.847736

3b_PhOH(*S*RS)

SCF Done: E(RM062X) = -1896.57412314

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.993051	-1.581673	1.585989
2	6	0	-1.504600	-1.135974	0.227340
3	1	0	-2.078949	-0.224417	0.414715
4	6	0	-0.403036	-2.880805	1.694064
5	7	0	0.069832	-3.940240	1.740960
6	6	0	-2.469569	-2.143707	-0.397096
7	6	0	-3.272033	-2.950536	0.419092
8	6	0	-2.638029	-2.233840	-1.783303

9	6	0	-4.204648	-3.825782	-0.131488
10	1	0	-3.173949	-2.889679	1.499596
11	6	0	-3.571199	-3.109356	-2.336678
12	1	0	-2.046922	-1.620420	-2.457212
13	6	0	-4.356641	-3.911795	-1.513653
14	1	0	-4.813570	-4.441736	0.523740
15	1	0	-3.679655	-3.161409	-3.416005
16	1	0	-5.080485	-4.597139	-1.944104
17	6	0	-1.112789	-0.868318	2.736657
18	8	0	-0.704603	-1.451708	3.881297
19	6	0	-1.723128	0.475964	2.867314
20	6	0	-1.330390	1.548312	2.057350
21	6	0	-2.693336	0.665249	3.862201
22	6	0	-1.931020	2.793400	2.233488
23	1	0	-0.533543	1.434180	1.320619
24	6	0	-3.289577	1.911064	4.024540
25	1	0	-2.999076	-0.167870	4.490447
26	6	0	-2.910706	2.976154	3.207812
27	1	0	-1.622010	3.626464	1.608564
28	1	0	-4.050919	2.048561	4.785872
29	1	0	-3.375515	3.949225	3.335985
30	6	0	-0.326711	-0.709444	-0.693418
31	6	0	0.458101	-1.874086	-1.304227
32	1	0	0.329592	-0.091996	-0.059759
33	1	0	0.235335	-2.813056	-0.792205
34	1	0	0.230395	-1.999128	-2.365509

35	6	0	-0.719045	0.318678	-1.736660
36	8	0	-0.343211	0.344504	-2.882876
37	8	0	-1.511523	1.268967	-1.195581
38	6	0	-1.645564	2.466110	-1.901425
39	6	0	-2.820060	2.718726	-2.593720
40	6	0	-0.606643	3.386693	-1.828526
41	6	0	-2.958741	3.947879	-3.238414
42	1	0	-3.604040	1.968163	-2.622508
43	6	0	-0.760561	4.607901	-2.480043
44	1	0	0.282731	3.119196	-1.258973
45	6	0	-1.932898	4.889665	-3.183155
46	1	0	-3.871270	4.166399	-3.784658
47	1	0	0.036511	5.344322	-2.434744
48	1	0	-2.047561	5.845129	-3.685909
49	6	0	2.576661	-2.921748	-1.925612
50	6	0	4.101301	-2.899026	-1.671953
51	1	0	2.099611	-3.815381	-1.518694
52	1	0	2.323372	-2.823036	-2.983530
53	1	0	4.377793	-3.661818	-0.939122
54	1	0	4.628957	-3.109838	-2.605412
55	6	0	2.453833	-1.725073	0.192061
56	1	0	1.890934	-0.976192	0.752111
57	1	0	2.233234	-2.718225	0.590495
58	6	0	3.965134	-1.409276	0.181366
59	1	0	4.137290	-0.372273	0.486142
60	1	0	4.477895	-2.069862	0.885407

61	6	0	3.985637	-0.550031	-2.033701
62	1	0	4.407131	0.414209	-1.738025
63	1	0	4.298908	-0.766929	-3.058750
64	6	0	2.442085	-0.484978	-1.940600
65	1	0	2.085502	0.371088	-1.357817
66	1	0	1.964718	-0.482141	-2.920920
67	7	0	1.959333	-1.730560	-1.232906
68	7	0	4.524417	-1.594184	-1.159618
69	6	0	4.814082	1.873258	2.297358
70	6	0	4.711135	2.422441	1.015573
71	6	0	3.517730	2.369713	0.304384
72	6	0	2.346510	1.750948	0.837046
73	6	0	2.478515	1.217111	2.155461
74	6	0	3.679079	1.275547	2.853852
75	8	0	1.250587	1.659641	0.157038
76	1	0	-0.717830	-0.798985	4.604615
77	1	0	5.578414	2.899380	0.562323
78	1	0	3.449951	2.800409	-0.693336
79	1	0	1.604620	0.743035	2.602491
80	1	0	3.733647	0.845080	3.852266
81	1	0	5.748721	1.914154	2.848092

3b_PhOH(*S*SR)

SCF Done: E(RM062X) = -1896.58887152

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.671548	-0.029183	0.695914
2	6	0	0.326534	-0.625224	2.061547
3	1	0	-0.107417	-0.261666	-0.038194
4	1	0	0.784130	-1.613266	2.161669
5	1	0	0.686440	0.009381	2.875341
6	6	0	0.645719	1.487303	0.714391
7	8	0	0.483525	2.185396	1.686657
8	8	0	0.772694	1.972876	-0.533088
9	6	0	0.484630	3.322741	-0.731507
10	6	0	1.478805	4.277618	-0.573648
11	6	0	-0.803637	3.643445	-1.138489
12	6	0	1.163525	5.609519	-0.838576
13	1	0	2.472264	3.974384	-0.257522
14	6	0	-1.102601	4.978788	-1.399503
15	1	0	-1.524784	2.835094	-1.240647
16	6	0	-0.121973	5.960282	-1.250276
17	1	0	1.926197	6.373588	-0.722805
18	1	0	-2.103105	5.253333	-1.720433
19	1	0	-0.359249	6.999477	-1.456774
20	6	0	-1.262804	-1.404323	3.728465
21	6	0	-2.726547	-1.831934	3.970945
22	1	0	-0.566219	-2.241011	3.804041
23	1	0	-0.941054	-0.604712	4.399350

24	1	0	-2.811897	-2.921627	3.971581
25	1	0	-3.061036	-1.458818	4.942165
26	6	0	-1.740093	-1.844837	1.365241
27	1	0	-1.561040	-1.475827	0.353660
28	1	0	-1.208520	-2.785855	1.528147
29	6	0	-3.257809	-1.947567	1.656017
30	1	0	-3.824895	-1.457449	0.859409
31	1	0	-3.552038	-2.999453	1.695434
32	6	0	-3.364281	0.137046	2.797540
33	1	0	-4.104777	0.559472	2.113888
34	1	0	-3.498773	0.592528	3.782347
35	6	0	-1.943354	0.430242	2.255894
36	1	0	-1.945674	0.729490	1.201846
37	1	0	-1.411976	1.170694	2.854592
38	7	0	-1.141057	-0.848567	2.328551
39	7	0	-3.599407	-1.302710	2.923803
40	6	0	2.442687	-0.229555	-1.202882
41	6	0	1.974177	-0.699273	0.166622
42	1	0	1.687937	-1.748515	0.038877
43	6	0	3.267459	0.938440	-1.263066
44	7	0	3.943816	1.880958	-1.271791
45	6	0	3.143445	-0.688672	1.144256
46	6	0	3.449182	0.408009	1.954819
47	6	0	3.977705	-1.810633	1.186740
48	6	0	4.561758	0.377072	2.795889
49	1	0	2.822682	1.295811	1.944797

50	6	0	5.088940	-1.843055	2.023744
51	1	0	3.748160	-2.664394	0.552409
52	6	0	5.384420	-0.745793	2.832195
53	1	0	4.784845	1.236686	3.420934
54	1	0	5.722774	-2.724614	2.045392
55	1	0	6.250346	-0.766982	3.487015
56	6	0	2.251166	-0.918445	-2.354354
57	8	0	2.890755	-0.502319	-3.466453
58	6	0	1.440306	-2.153371	-2.474762
59	6	0	2.049479	-3.303058	-2.993216
60	6	0	0.090796	-2.180590	-2.102737
61	6	0	1.323734	-4.484950	-3.103001
62	1	0	3.095714	-3.276117	-3.287264
63	6	0	-0.625958	-3.370478	-2.213487
64	1	0	-0.409710	-1.269436	-1.770253
65	6	0	-0.012112	-4.521339	-2.705796
66	1	0	1.802321	-5.377653	-3.493610
67	1	0	-1.672350	-3.394890	-1.921994
68	1	0	-0.576601	-5.445459	-2.786777
69	6	0	-5.863261	-0.184991	-1.563610
70	6	0	-5.413841	0.899360	-0.803630
71	6	0	-4.056953	1.135407	-0.614969
72	6	0	-3.052742	0.280482	-1.170078
73	6	0	-3.546326	-0.802761	-1.961464
74	6	0	-4.906715	-1.024510	-2.142618
75	8	0	-1.794823	0.472585	-0.961025

76	1	0	2.559239	-0.997006	-4.237836
77	1	0	-6.137063	1.576796	-0.352471
78	1	0	-3.727147	1.987210	-0.021295
79	1	0	-2.815947	-1.458419	-2.431949
80	1	0	-5.228381	-1.869129	-2.749668
81	1	0	-6.924109	-0.364976	-1.707349

TS3b/P_PhOH(*R*RS)

SCF Done: E(RM062X) = -1896.57188526

Imaginary Frequencies = -118.0270

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.421516	-1.026591	0.872702
2	6	0	0.540704	-1.965295	1.084504
3	1	0	2.789090	-0.033384	0.735716
4	1	0	0.264687	-2.993196	1.303779
5	1	0	1.559393	-1.680704	1.324780
6	6	0	0.044695	0.347535	0.762779
7	8	0	1.209173	0.722657	0.747599
8	8	0	-0.971532	1.249091	0.689009
9	6	0	-0.718764	2.590296	0.419640
10	6	0	0.077103	2.982483	-0.652839
11	6	0	-1.406420	3.513931	1.196102

12	6	0	0.176304	4.339965	-0.946228
13	1	0	0.595360	2.240860	-1.250713
14	6	0	-1.298935	4.868743	0.888614
15	1	0	-2.027428	3.165884	2.016050
16	6	0	-0.510669	5.284151	-0.182393
17	1	0	0.787149	4.657107	-1.786145
18	1	0	-1.838288	5.597185	1.486311
19	1	0	-0.431856	6.339656	-0.423521
20	6	0	3.278783	-3.698123	-2.178020
21	6	0	2.732740	-3.391192	-0.751732
22	1	0	3.612477	-4.738004	-2.254222
23	1	0	4.128756	-3.050959	-2.418682
24	1	0	2.597572	-4.307448	-0.166867
25	1	0	3.397701	-2.719329	-0.199136
26	6	0	1.038220	-4.228423	-2.806014
27	1	0	0.299770	-4.144914	-3.610044
28	1	0	1.324146	-5.281802	-2.716899
29	6	0	0.463964	-3.687010	-1.465931
30	1	0	-0.477007	-3.148615	-1.615404
31	1	0	0.293253	-4.494183	-0.745505
32	6	0	1.552371	-1.566598	-1.745947
33	1	0	0.612922	-1.003666	-1.706265
34	1	0	2.349257	-0.939924	-1.332284
35	6	0	1.889770	-2.035464	-3.187464
36	1	0	1.035053	-1.897179	-3.858789
37	1	0	2.734830	-1.470220	-3.593921

38	7	0	2.234597	-3.465322	-3.187050
39	7	0	1.422182	-2.741763	-0.877490
40	6	0	-2.863319	-0.591039	0.004420
41	6	0	-1.882557	-1.475531	0.835698
42	1	0	-1.878163	-2.454746	0.345824
43	6	0	-4.142041	-1.296696	-0.148170
44	7	0	-5.142403	-1.862032	-0.275994
45	6	0	-2.464932	-1.661049	2.230264
46	6	0	-2.347514	-0.657217	3.197583
47	6	0	-3.153002	-2.832845	2.551750
48	6	0	-2.908519	-0.823118	4.460382
49	1	0	-1.810423	0.259070	2.962326
50	6	0	-3.715017	-3.001697	3.817383
51	1	0	-3.248710	-3.617692	1.804631
52	6	0	-3.593965	-1.997347	4.774081
53	1	0	-2.807667	-0.036682	5.202665
54	1	0	-4.244998	-3.919767	4.053757
55	1	0	-4.029533	-2.127403	5.760317
56	6	0	-2.326358	-0.305462	-1.414190
57	8	0	-1.784073	-1.209999	-2.017578
58	6	0	-2.480140	1.050855	-2.006445
59	6	0	-3.291499	2.038626	-1.437270
60	6	0	-1.763525	1.331212	-3.177590
61	6	0	-3.377735	3.294978	-2.030640
62	1	0	-3.868614	1.840945	-0.539228
63	6	0	-1.845542	2.587973	-3.763153

64	1	0	-1.138152	0.556363	-3.611151
65	6	0	-2.652534	3.571753	-3.188306
66	1	0	-4.008411	4.058180	-1.585345
67	1	0	-1.280470	2.805178	-4.664295
68	1	0	-2.715338	4.555911	-3.643416
69	6	0	6.467383	2.411721	2.036229
70	6	0	6.841971	1.088578	1.799760
71	6	0	5.904577	0.150650	1.380032
72	6	0	4.573401	0.534010	1.193063
73	6	0	4.188835	1.858821	1.424516
74	6	0	5.138751	2.786603	1.845573
75	8	0	3.693715	-0.414473	0.781564
76	1	0	-3.070446	0.332374	0.545215
77	1	0	7.874168	0.781457	1.943739
78	1	0	6.183835	-0.882182	1.193533
79	1	0	3.152825	2.151048	1.274172
80	1	0	4.832366	3.813526	2.024989
81	1	0	7.201585	3.139760	2.366551

TS3b/P_PhOH(*R*SR)

SCF Done: E(RM062X) = -1896.56790669

Imaginary Frequencies = -150.9194

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

1	6	0	6.717182	0.745641	-0.595070
2	6	0	6.996304	0.482322	0.746734
3	6	0	5.961577	0.529904	1.679531
4	6	0	4.660085	0.830850	1.283891
5	6	0	4.386406	1.078254	-0.065449
6	6	0	5.421184	1.043160	-1.005379
7	8	0	3.134792	1.347666	-0.512910
8	8	0	1.239246	0.752319	1.389194
9	6	0	0.047822	0.598559	1.125078
10	8	0	-0.770568	1.682602	0.957973
11	6	0	-0.188822	2.937868	0.852758
12	6	0	0.563902	3.255053	-0.274122
13	6	0	1.077955	4.543149	-0.399510
14	6	0	0.831678	5.497382	0.587749
15	6	0	0.069335	5.161699	1.705384
16	6	0	-0.445067	3.873578	1.845838
17	6	0	-0.634785	-0.663534	0.972684
18	6	0	0.089203	-1.787118	1.300446
19	6	0	-2.076123	-0.693375	0.491720
20	6	0	-2.972628	-1.578524	1.358887
21	6	0	-3.934614	-2.457253	0.855063
22	6	0	-4.753666	-3.191557	1.716853
23	6	0	-4.632966	-3.054138	3.094199
24	6	0	-3.683052	-2.170739	3.609797
25	6	0	-2.864430	-1.447277	2.751508

26	6	0	-2.171685	-0.958918	-1.047326
27	6	0	-3.492380	-0.485406	-1.680417
28	6	0	-3.787216	0.977965	-1.648150
29	6	0	-2.795108	1.951226	-1.479070
30	6	0	-3.139155	3.299938	-1.460869
31	6	0	-4.471707	3.681808	-1.604956
32	6	0	-5.463547	2.715359	-1.778110
33	6	0	-5.122235	1.369014	-1.805511
34	6	0	-1.924479	-2.361926	-1.388978
35	7	0	-1.711790	-3.468404	-1.647637
36	8	0	-4.270774	-1.277096	-2.171576
37	7	0	1.560466	-2.378544	-0.141337
38	6	0	1.529346	-3.797256	-0.534209
39	6	0	2.611568	-4.030382	-1.628794
40	7	0	3.513990	-2.873432	-1.716559
41	6	0	2.747338	-1.711247	-2.187866
42	6	0	1.456671	-1.538654	-1.341669
43	6	0	4.011701	-2.573449	-0.368164
44	6	0	2.841965	-2.101904	0.533091
45	1	0	-2.461271	0.324084	0.607879
46	1	0	-4.072374	-2.584947	-0.212823
47	1	0	-2.125042	-0.765319	3.162752
48	1	0	-5.488231	-3.873366	1.298264
49	1	0	-3.578642	-2.046424	4.683882
50	1	0	-5.270126	-3.626923	3.761433
51	1	0	-1.751348	1.673359	-1.370973

52	1	0	-5.882160	0.605653	-1.939257
53	1	0	-2.364508	4.050858	-1.335607
54	1	0	-6.501377	3.013410	-1.890264
55	1	0	-4.738551	4.734267	-1.584108
56	1	0	2.490079	1.280125	0.224678
57	1	0	-0.399924	-2.759567	1.304623
58	1	0	0.946580	-1.681216	1.955808
59	1	0	0.736479	2.501568	-1.038100
60	1	0	-1.041070	3.590614	2.707684
61	1	0	1.669052	4.800601	-1.273015
62	1	0	-0.125101	5.902406	2.474958
63	1	0	1.232572	6.500805	0.484531
64	1	0	2.146323	-4.169369	-2.609847
65	1	0	3.202806	-4.922999	-1.402813
66	1	0	0.527805	-4.039336	-0.898504
67	1	0	1.726691	-4.391975	0.363532
68	1	0	3.386637	-0.826416	-2.098257
69	1	0	2.499482	-1.852335	-3.244450
70	1	0	1.313527	-0.499936	-1.025181
71	1	0	0.571952	-1.859522	-1.899219
72	1	0	2.874336	-1.026745	0.722767
73	1	0	2.840923	-2.619762	1.498126
74	1	0	4.781692	-1.796616	-0.436583
75	1	0	4.476168	-3.480438	0.031766
76	1	0	-1.358865	-0.385765	-1.510808
77	1	0	6.164343	0.332096	2.728338

78	1	0	3.850884	0.867745	2.009635
79	1	0	5.191772	1.247347	-2.047201
80	1	0	7.514843	0.716521	-1.332268
81	1	0	8.008075	0.245827	1.060355

TS3b/P_PhOH(*S*RS)

SCF Done: E(RM062X) = -1896.55976751

Imaginary Frequencies = -142.8607

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.485520	1.265919	-1.151630
2	6	0	0.808800	1.545403	0.353016
3	1	0	-0.178067	1.712711	0.795002
4	6	0	1.674797	1.049543	-1.979502
5	7	0	2.602482	0.866422	-2.644940
6	6	0	1.590778	2.831400	0.617036
7	6	0	2.257155	3.580315	-0.353610
8	6	0	1.628072	3.284678	1.944613
9	6	0	2.949355	4.744493	-0.005504
10	1	0	2.241290	3.287760	-1.397171
11	6	0	2.309511	4.443503	2.291843
12	1	0	1.112391	2.711056	2.711902
13	6	0	2.980848	5.180035	1.313029

14	1	0	3.462643	5.307229	-0.779792
15	1	0	2.318232	4.774169	3.326413
16	1	0	3.519558	6.084275	1.580048
17	6	0	-0.371722	2.379615	-1.783944
18	8	0	0.083322	3.093581	-2.653535
19	6	0	-1.766320	2.566637	-1.282386
20	6	0	-2.453519	1.581439	-0.565617
21	6	0	-2.408019	3.774232	-1.584409
22	6	0	-3.768164	1.797014	-0.162855
23	1	0	-1.976723	0.635989	-0.331512
24	6	0	-3.714924	3.994048	-1.168411
25	1	0	-1.868262	4.532409	-2.142951
26	6	0	-4.397431	3.004383	-0.459353
27	1	0	-4.298691	1.020159	0.380064
28	1	0	-4.205476	4.934931	-1.397680
29	1	0	-5.421400	3.174583	-0.140313
30	6	0	1.404066	0.364295	1.107241
31	6	0	2.753144	0.126856	1.242251
32	1	0	-1.207725	-1.348393	-0.019903
33	1	0	3.471766	0.819894	0.808562
34	1	0	3.095264	-0.438463	2.102579
35	6	0	0.552930	-0.526594	1.868171
36	8	0	0.891054	-1.393789	2.647697
37	8	0	-0.800559	-0.306169	1.596027
38	6	0	-1.778294	-0.975931	2.325379
39	6	0	-2.792207	-0.192049	2.864447

40	6	0	-1.816346	-2.366720	2.390830
41	6	0	-3.872885	-0.815616	3.485043
42	1	0	-2.730127	0.888843	2.778848
43	6	0	-2.899475	-2.975251	3.021949
44	1	0	-1.018156	-2.956496	1.952892
45	6	0	-3.926978	-2.206220	3.566420
46	1	0	-4.671723	-0.211014	3.903647
47	1	0	-2.940939	-4.058680	3.079228
48	1	0	-4.769429	-2.690223	4.050328
49	6	0	4.569180	-1.207875	-0.770950
50	6	0	4.948924	-2.474083	-1.591168
51	1	0	4.252619	-0.386427	-1.417698
52	1	0	5.403255	-0.861069	-0.152254
53	1	0	4.657080	-2.358911	-2.640143
54	1	0	6.028317	-2.650686	-1.555432
55	6	0	2.346266	-2.130401	-0.618296
56	1	0	1.505631	-2.267922	0.069130
57	1	0	2.043659	-1.415215	-1.386754
58	6	0	2.813544	-3.477532	-1.241355
59	1	0	2.305999	-4.324020	-0.768168
60	1	0	2.591504	-3.503935	-2.312456
61	6	0	4.538025	-3.747425	0.381377
62	1	0	4.113805	-4.681085	0.763156
63	1	0	5.623669	-3.788696	0.514298
64	6	0	3.932963	-2.525110	1.127610
65	1	0	3.073513	-2.801879	1.745632

66	1	0	4.672900	-2.034069	1.768358
67	7	0	3.459751	-1.543341	0.136087
68	7	0	4.259641	-3.655067	-1.056661
69	6	0	-4.735229	-2.641121	-2.694581
70	6	0	-3.527914	-2.863808	-3.357869
71	6	0	-2.316749	-2.551061	-2.749401
72	6	0	-2.311915	-2.011193	-1.462760
73	6	0	-3.513028	-1.787902	-0.786645
74	6	0	-4.719028	-2.102967	-1.409935
75	8	0	-1.095881	-1.710859	-0.916213
76	1	0	-0.075990	0.322177	-1.189431
77	1	0	-3.526702	-3.282888	-4.359940
78	1	0	-1.369986	-2.715912	-3.254911
79	1	0	-3.504930	-1.370961	0.219004
80	1	0	-5.650416	-1.923243	-0.880617
81	1	0	-5.677363	-2.883888	-3.175615

TS3b/P_PhOH(*S*SR)

SCF Done: E(RM062X) = -1896.57256262

Imaginary Frequencies = -113.5076

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.091489	-0.321147	-1.629011

2	6	0	1.151062	-0.791604	-2.353714
3	1	0	-0.555693	1.391163	0.796899
4	1	0	1.339137	-1.855880	-2.449736
5	1	0	1.588163	-0.152755	-3.114893
6	6	0	-0.193456	1.097492	-1.757172
7	8	0	0.397651	1.926960	-2.412014
8	8	0	-1.301723	1.467514	-0.979770
9	6	0	-1.909319	2.700913	-1.198006
10	6	0	-2.273924	3.107421	-2.478270
11	6	0	-2.224862	3.460023	-0.076713
12	6	0	-2.957391	4.310377	-2.628367
13	1	0	-2.026739	2.492882	-3.337090
14	6	0	-2.915482	4.659337	-0.242136
15	1	0	-1.938594	3.111850	0.912295
16	6	0	-3.279369	5.088591	-1.515923
17	1	0	-3.245312	4.636873	-3.622984
18	1	0	-3.166918	5.254141	0.630381
19	1	0	-3.813908	6.024593	-1.643590
20	6	0	3.491924	-1.883173	-0.690675
21	6	0	4.848686	-1.650378	0.034002
22	1	0	2.729026	-2.251450	0.001275
23	1	0	3.585794	-2.599017	-1.514241
24	1	0	4.837372	-2.108573	1.028314
25	1	0	5.678281	-2.086379	-0.531891
26	6	0	2.704127	0.314681	-0.139112
27	1	0	2.459686	1.285354	-0.583595

28	1	0	1.806978	-0.052399	0.373585
29	6	0	3.928465	0.408149	0.809267
30	1	0	4.157201	1.453409	1.043930
31	1	0	3.737098	-0.116698	1.751651
32	6	0	5.279069	0.364027	-1.162483
33	1	0	5.364200	1.450259	-1.055574
34	1	0	6.215913	-0.010631	-1.586154
35	6	0	4.071696	-0.010039	-2.071886
36	1	0	3.658359	0.869552	-2.575841
37	1	0	4.348844	-0.745957	-2.833833
38	7	0	3.017652	-0.602573	-1.236683
39	7	0	5.105074	-0.211268	0.178218
40	6	0	-2.127024	-1.541218	-1.388090
41	6	0	-0.764339	-1.169132	-0.703072
42	1	0	-1.062594	-0.551403	0.144659
43	6	0	-1.933765	-2.197460	-2.683441
44	7	0	-1.760626	-2.684978	-3.716949
45	6	0	-0.054961	-2.363312	-0.088358
46	6	0	0.246860	-3.534276	-0.793312
47	6	0	0.311646	-2.280832	1.260671
48	6	0	0.920467	-4.582931	-0.168684
49	1	0	-0.036878	-3.638970	-1.836498
50	6	0	0.986389	-3.327722	1.885859
51	1	0	0.068095	-1.378874	1.819520
52	6	0	1.296790	-4.482109	1.169508
53	1	0	1.150372	-5.482278	-0.732506

54	1	0	1.264394	-3.241869	2.932396
55	1	0	1.820952	-5.301303	1.652673
56	6	0	-2.978394	-2.420436	-0.466548
57	8	0	-3.203419	-3.578595	-0.750950
58	6	0	-3.457452	-1.817219	0.813020
59	6	0	-3.476627	-0.435816	1.042338
60	6	0	-3.903043	-2.690872	1.812094
61	6	0	-3.934832	0.061385	2.258992
62	1	0	-3.147691	0.264016	0.278250
63	6	0	-4.354686	-2.191799	3.027384
64	1	0	-3.883106	-3.759353	1.621821
65	6	0	-4.370581	-0.814560	3.251471
66	1	0	-3.951751	1.133313	2.429949
67	1	0	-4.693887	-2.873786	3.800880
68	1	0	-4.724346	-0.424244	4.201010
69	6	0	2.967474	3.617256	2.755391
70	6	0	2.562827	2.560392	3.571604
71	6	0	1.500388	1.742575	3.198061
72	6	0	0.832631	1.985414	1.996424
73	6	0	1.234040	3.035236	1.166802
74	6	0	2.300219	3.845490	1.552685
75	8	0	-0.208078	1.163613	1.678830
76	1	0	-2.653967	-0.601386	-1.593878
77	1	0	3.077910	2.368080	4.508432
78	1	0	1.176229	0.916265	3.823834
79	1	0	0.722838	3.207662	0.220790

80	1	0	2.607584	4.660853	0.904210
81	1	0	3.796359	4.252384	3.051086
