Electronic Supplementary Material (ESI) for Dalton Transactions.

Transmetalation from B to Rh in the course of the catalytic asymmetric 1,4-addition reaction of phenylboronic acid to enones: A computational comparison of diphosphane and diene ligands

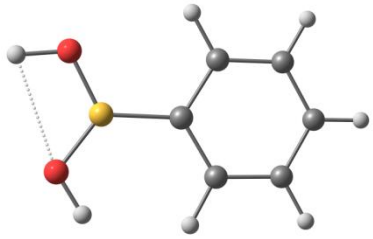
You-Gui Li,[†] He Gang,[†] Hua-Li Qin,[‡] Eric Assen B. Kantchev*[†,§]*

[†]School of Chemistry and Chemical Engineering, Hefei University of Technology, 193 Tunxi Rd, Hefei 230009 Anhui, China
[‡]School of Chemistry, Chemical Engineering and Life Science, Wuhan University of Technology, 205 Luoshi Road, Wuhan, 430070, China
[§]Institute of Materials Research and Engineering, 3 Research Link Singapore 117602

STRUTURE PLOTS, STANDARD COORDINATES, SCF ENERGIES AND THERMOCHEMISTRY, AND FIRST 3 FREQUENCIES

All at PCM(solvent=1,4-dioxane, 303.15K)/PBE0/DGDZVP level of theory

$PhB(OH)_2$–in/out (1a)

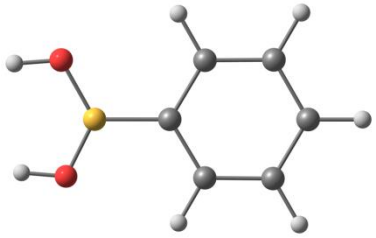


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.743583	-0.001005	0.000008
2	8	0	-2.535295	1.124108	-0.000100
3	8	0	-2.381583	-1.213190	0.000065
4	1	0	-3.341658	-1.088101	0.000019
5	6	0	-0.177288	0.017981	0.000039
6	6	0	0.567134	1.207869	0.000041
7	6	0	0.531225	-1.194581	-0.000022
8	6	0	1.960548	1.193435	0.000030
9	1	0	0.067780	2.176444	0.000065
10	6	0	1.923551	-1.219011	-0.000037
11	1	0	-0.024317	-2.128682	-0.000032
12	6	0	2.641622	-0.023216	-0.000016
13	1	0	2.515366	2.128078	0.000052
14	1	0	2.451361	-2.169350	-0.000081
15	1	0	3.728558	-0.038761	-0.000046
16	1	0	-2.024905	1.943193	0.000053

```
SCF Done:  E(RPBE1PBE) =  -407.832811411     A.U. after    1 cycles
             Convg  =    0.8788D-09             -V/T =  2.0132
Zero-point correction=                          0.125812 (Hartree/Particle)
 Thermal correction to Energy=                   0.133928
 Thermal correction to Enthalpy=                 0.134888
 Thermal correction to Gibbs Free Energy=        0.092060
 Sum of electronic and zero-point Energies=          -407.706999
 Sum of electronic and thermal Energies=             -407.698884
 Sum of electronic and thermal Enthalpies=           -407.697924
 Sum of electronic and thermal Free Energies=        -407.740752
```

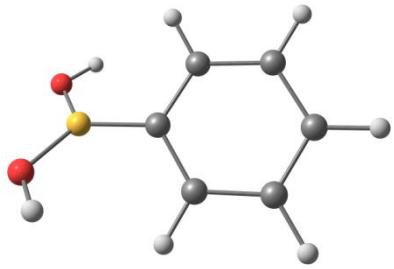
```
                     1                      2                      3
                     A                      A                      A
 Frequencies --    42.8363               138.1522               169.8693
```

PhB(OH)$_2$–out/out (1b)



```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          5           0       -1.732757   -0.000069   -0.000005
      2          8           0       -2.382372   -1.210901   -0.056616
      3          1           0       -3.346007   -1.142409   -0.071856
      4          8           0       -2.382070    1.210962    0.056805
      5          1           0       -3.345721    1.142945    0.072336
      6          6           0       -0.171107   -0.000117   -0.000252
      7          6           0        0.550226   -1.203735    0.026721
      8          6           0        0.550086    1.203601   -0.027056
      9          6           0        1.943496   -1.207096    0.030061
     10          1           0        0.009182   -2.146561    0.047132
     11          6           0        1.943358    1.207154   -0.029988
     12          1           0        0.008899    2.146335   -0.047717
     13          6           0        2.642298    0.000071    0.000173
     14          1           0        2.486762   -2.148523    0.055181
     15          1           0        2.486499    2.148656   -0.054956
     16          1           0        3.729575    0.000131    0.000438
 ---------------------------------------------------------------------SCF
Done:  E(RPBE1PBE) =  -407.829876887     A.U. after    1 cycles
            Convg  =    0.2590D-08             -V/T =  2.0132
Zero-point correction=                          0.125649 (Hartree/Particle)
 Thermal correction to Energy=                   0.133753
 Thermal correction to Enthalpy=                 0.134713
 Thermal correction to Gibbs Free Energy=        0.092214
 Sum of electronic and zero-point Energies=           -407.704228
 Sum of electronic and thermal Energies=              -407.696124
 Sum of electronic and thermal Enthalpies=            -407.695164
 Sum of electronic and thermal Free Energies=         -407.737663
                     1                      2                      3
                     A                      A                      A
 Frequencies --    66.9625               138.5665               153.9235
```

PhB(OH)$_2$–in/in (1c)



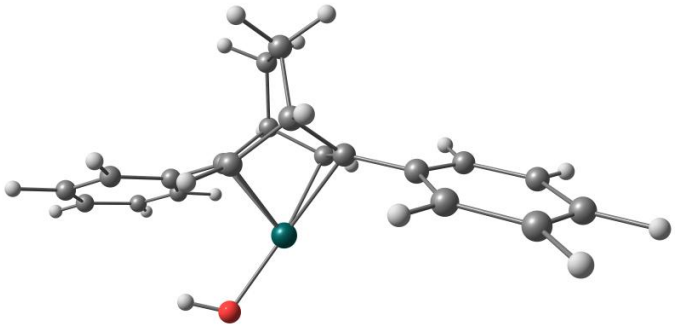
```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	5	0	-1.766950	-0.000007	-0.000012
2	8	0	-2.505515	1.079284	-0.409369
3	8	0	-2.505518	-1.079281	0.409377
4	1	0	-1.943636	-1.773602	0.774812
5	6	0	-0.193545	-0.000002	-0.000004
6	6	0	0.534029	1.180986	0.219581
7	6	0	0.534034	-1.180988	-0.219584
8	6	0	1.927448	1.184358	0.226985
9	1	0	0.009380	2.115585	0.413271
10	6	0	1.927454	-1.184355	-0.226983
11	1	0	0.009391	-2.115589	-0.413281
12	6	0	2.627412	0.000002	0.000003
13	1	0	2.468120	2.109263	0.410375
14	1	0	2.468130	-2.109258	-0.410371
15	1	0	3.714271	0.000005	0.000006
16	1	0	-1.943628	1.773603	-0.774802

SCF Done: E(RPBE1PBE) = -407.828969394 A.U. after 1 cycles
Convg = 0.1139D-08 -V/T = 2.0132
Zero-point correction= 0.126045 (Hartree/Particle)
Thermal correction to Energy= 0.134102
Thermal correction to Enthalpy= 0.135062
Thermal correction to Gibbs Free Energy= 0.092585
Sum of electronic and zero-point Energies= -407.702925
Sum of electronic and thermal Energies= -407.694867
Sum of electronic and thermal Enthalpies= -407.693907
Sum of electronic and thermal Free Energies= -407.736385

	1	2	3
	A	A	A
Frequencies --	66.0369	126.2876	163.2238

PhBOD-Rh-OH (4)

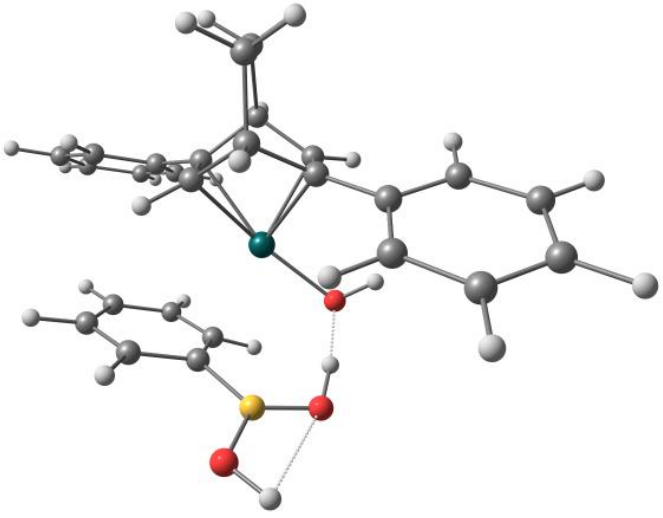


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.059020	-1.049538	-0.167674
2	6	0	-1.311481	0.542278	0.063151
3	6	0	0.770312	1.212121	1.194406
4	6	0	3.457260	-0.391700	1.095687
5	6	0	-2.760894	0.248035	0.009134
6	6	0	-3.547587	0.252194	1.169844
7	6	0	-0.503894	0.390485	1.225350
8	6	0	-0.643163	1.473981	-0.948946
9	6	0	-4.751319	-0.302398	-1.274894
10	6	0	5.595605	-0.544480	-0.020044
11	6	0	0.457502	2.704288	0.956980
12	6	0	0.668844	0.748459	-1.181517
13	6	0	-4.913225	-0.019875	1.110893

14	6	0	1.456968	0.611859	-0.031378
15	6	0	3.702479	0.451943	-1.145155
16	6	0	-3.388952	-0.032178	-1.214401
17	6	0	-0.406130	2.858709	-0.311077
18	6	0	-5.521836	-0.298106	-0.111004
19	6	0	2.883731	0.225092	-0.028209
20	6	0	5.041723	0.070809	-1.141913
21	6	0	4.795363	-0.773399	1.099388
22	1	0	2.843269	-0.596205	1.969278
23	1	0	6.641067	-0.840787	-0.016844
24	1	0	3.291318	0.949458	-2.019467
25	1	0	5.657619	0.262934	-2.016792
26	1	0	5.214055	-1.257186	1.978075
27	1	0	-3.092765	0.487449	2.128249
28	1	0	-5.213843	-0.526012	-2.232692
29	1	0	-5.503868	-0.007067	2.023267
30	1	0	-2.797553	-0.066790	-2.125706
31	1	0	-6.586617	-0.509810	-0.157804
32	1	0	1.359623	1.074422	2.102294
33	1	0	-1.226343	1.559820	-1.867389
34	1	0	-0.058781	3.102991	1.836527
35	1	0	1.400340	3.253012	0.863895
36	1	0	0.084622	3.505809	-1.045220
37	1	0	-1.374113	3.315039	-0.078780
38	1	0	1.051909	0.597085	-2.188397
39	1	0	-0.898284	0.003053	2.162491
40	8	0	-1.005066	-2.649500	0.312010
41	1	0	-1.894854	-2.450714	0.636510

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5535.12072064     A.U. after    1 cycles
             Convg  =    0.2943D-08             -V/T =  2.0038
Zero-point correction=                           0.337388 (Hartree/Particle)
 Thermal correction to Energy=                    0.356645
 Thermal correction to Enthalpy=                  0.357605
 Thermal correction to Gibbs Free Energy=         0.288070
 Sum of electronic and zero-point Energies=          -5534.783332
 Sum of electronic and thermal Energies=             -5534.764076
 Sum of electronic and thermal Enthalpies=           -5534.763116
 Sum of electronic and thermal Free Energies=        -5534.832651
                     1                      2                      3
                     A                      A                      A
 Frequencies --    26.9558                36.9755                42.3240
```

PhBOD-Rh-OH-PhB(OH)$_2$-in (5a)

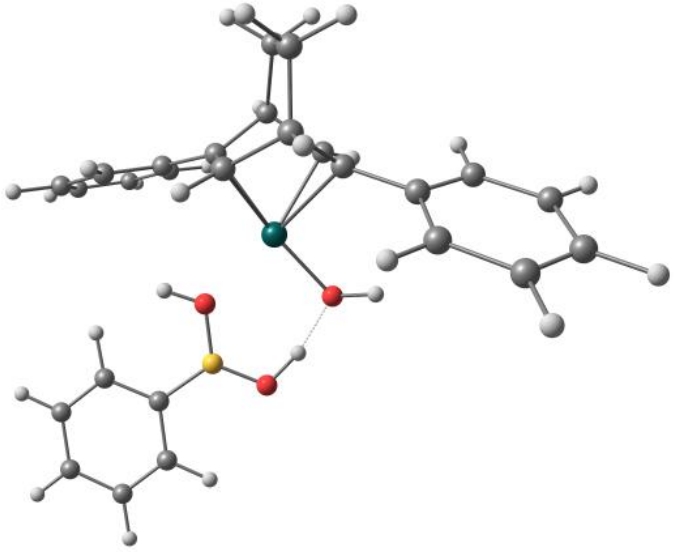


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.103046	0.111328	-0.630613
2	6	0	-1.399445	-1.363016	0.225852
3	6	0	0.699207	-2.502380	-0.328546
4	6	0	3.406220	-1.147305	-1.224331
5	6	0	-2.860403	-1.148313	0.141137
6	6	0	-3.651841	-1.919172	-0.722946
7	6	0	-0.615447	-1.925506	-0.806998
8	6	0	-0.672452	-1.415261	1.566310
9	6	0	-4.867714	0.015190	0.860870
10	6	0	5.608288	-0.756159	-0.309431
11	6	0	0.462634	-3.532949	0.798138
12	6	0	0.612513	-0.670946	1.251996
13	6	0	-5.029348	-1.723233	-0.798242
14	6	0	1.384265	-1.266427	0.250893
15	6	0	3.682472	-0.843531	1.147749
16	6	0	-3.493643	-0.180600	0.935013
17	6	0	-0.365550	-2.886565	1.925635
18	6	0	-5.643281	-0.754948	-0.006878
19	6	0	2.836030	-1.065569	0.054007
20	6	0	5.055837	-0.690068	0.968568
21	6	0	4.775994	-0.986712	-1.406573
22	1	0	2.763528	-1.310074	-2.086648
23	1	0	6.679178	-0.636134	-0.450452
24	1	0	3.261932	-0.800989	2.148959
25	1	0	5.696670	-0.522896	1.830670
26	1	0	5.197097	-1.039963	-2.407314
27	1	0	-3.190557	-2.695779	-1.327035
28	1	0	-5.335952	0.779706	1.475061
29	1	0	-5.624129	-2.335038	-1.471500
30	1	0	-2.899245	0.446545	1.594044
31	1	0	-6.717272	-0.600161	-0.064897
32	1	0	1.274617	-2.935906	-1.148319
33	1	0	-1.242272	-0.925203	2.357350
34	1	0	-0.052972	-4.402749	0.378089
35	1	0	1.431781	-3.882926	1.168288
36	1	0	0.175972	-2.910482	2.876875
37	1	0	-1.309421	-3.419218	2.081032
38	1	0	1.012570	0.081215	1.928071
39	1	0	-1.032931	-2.211796	-1.770028
40	8	0	-1.406010	0.838474	-2.039078
41	1	0	-2.136165	0.212897	-2.157758
42	5	0	-1.444142	3.120718	0.241008
43	8	0	-2.339356	2.846052	-0.731429
44	1	0	-2.015905	2.093165	-1.340183
45	8	0	-1.840960	3.855137	1.342421
46	1	0	-2.783365	4.058373	1.250595
47	6	0	0.082703	2.701476	0.205974
48	6	0	0.743030	2.373944	-1.003814
49	6	0	0.874903	2.834214	1.362734
50	6	0	2.132528	2.171269	-1.033846
51	1	0	0.196700	2.404374	-1.943378
52	6	0	2.252877	2.646976	1.325193
53	1	0	0.394040	3.121192	2.294440
54	6	0	2.886304	2.308221	0.126374
55	1	0	2.620454	1.938531	-1.976519
56	1	0	2.842603	2.772866	2.230298
57	1	0	3.961334	2.154019	0.098460

SCF Done: E(RPBE1PBE) = -5942.98751981 A.U. after 1 cycles
Convg = 0.1363D-08 -V/T = 2.0045

```
Zero-point correction=                           0.465261 (Hartree/Particle)
 Thermal correction to Energy=                    0.493587
 Thermal correction to Enthalpy=                  0.494547
 Thermal correction to Gibbs Free Energy=         0.404611
 Sum of electronic and zero-point Energies=         -5942.522259
 Sum of electronic and thermal Energies=            -5942.493933
 Sum of electronic and thermal Enthalpies=          -5942.492973
 Sum of electronic and thermal Free Energies=       -5942.582909
                     1                      2                      3
                     A                      A                      A
 Frequencies --    16.3995                28.8883                35.3641
```

PhBOD-Rh-OH-PhB(OH)$_2$-out (5b)



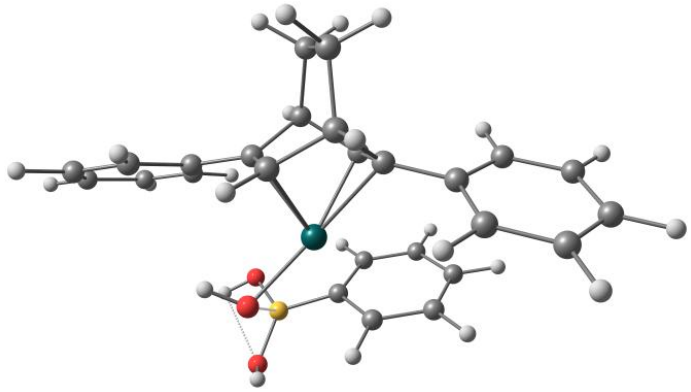
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.616919	-0.069184	-0.302238
2	6	0	0.568601	2.024462	0.196392
3	6	0	2.389973	0.998542	1.478067
4	6	0	3.436439	-1.952939	1.189245
5	6	0	-0.745919	2.665379	-0.021129
6	6	0	-1.610686	2.939503	1.051093
7	6	0	0.904580	1.267357	1.331447
8	6	0	1.807783	2.359321	-0.635617
9	6	0	-2.437165	3.548915	-1.532305
10	6	0	5.203825	-3.255259	0.180715
11	6	0	3.191326	2.317031	1.472511
12	6	0	2.324837	0.966196	-0.948028
13	6	0	-2.867371	3.502700	0.835472
14	6	0	2.669606	0.213592	0.194887
15	6	0	4.506040	-1.168432	-0.819157
16	6	0	-1.184414	2.983687	-1.316875
17	6	0	2.827411	3.139469	0.220953
18	6	0	-3.287467	3.810994	-0.457517
19	6	0	3.545922	-0.978713	0.184607
20	6	0	5.325540	-2.295704	-0.822180
21	6	0	4.253709	-3.078014	1.187482
22	1	0	2.682512	-1.842589	1.964630
23	1	0	5.842290	-4.134544	0.178436
24	1	0	4.625160	-0.420415	-1.598356
25	1	0	6.065014	-2.420649	-1.608918

26	1	0	4.143790	-3.824764	1.969523
27	1	0	-1.290363	2.730551	2.068233
28	1	0	-2.755722	3.777410	-2.545940
29	1	0	-3.514631	3.711682	1.683458
30	1	0	-0.549962	2.759083	-2.169934
31	1	0	-4.265743	4.252540	-0.626539
32	1	0	2.607085	0.408768	2.370197
33	1	0	1.557886	2.908194	-1.544868
34	1	0	2.964545	2.872182	2.388532
35	1	0	4.260711	2.083076	1.496918
36	1	0	3.714635	3.346292	-0.386301
37	1	0	2.394699	4.107279	0.494535
38	1	0	2.657987	0.700291	-1.948682
39	1	0	0.229311	1.115526	2.170591
40	8	0	-1.553250	-0.539841	-0.112955
41	1	0	-2.110391	0.167755	0.239208
42	5	0	-2.232082	-1.760395	-0.337712
43	8	0	-1.540044	-2.783123	-0.848174
44	1	0	-0.574148	-2.503341	-1.088189
45	8	0	0.707079	-1.784249	-1.415567
46	1	0	1.568134	-2.221685	-1.369773
47	6	0	-3.754837	-1.887610	0.024176
48	6	0	-4.359847	-3.153010	-0.043288
49	6	0	-4.557289	-0.801495	0.407528
50	6	0	-5.705482	-3.329908	0.268426
51	1	0	-3.755424	-4.004112	-0.346365
52	6	0	-5.906737	-0.967679	0.715143
53	1	0	-4.146678	0.207384	0.460046
54	6	0	-6.482757	-2.235628	0.648979
55	1	0	-6.151863	-4.319688	0.212364
56	1	0	-6.509392	-0.110229	1.003985
57	1	0	-7.534416	-2.369567	0.889889

SCF Done: E(RPBE1PBE) = -5942.99174004 A.U. after 1 cycles
Convg = 0.4136D-08 -V/T = 2.0045
Zero-point correction= 0.464460 (Hartree/Particle)
Thermal correction to Energy= 0.493162
Thermal correction to Enthalpy= 0.494122
Thermal correction to Gibbs Free Energy= 0.400594
Sum of electronic and zero-point Energies= -5942.527280
Sum of electronic and thermal Energies= -5942.498578
Sum of electronic and thermal Enthalpies= -5942.497618
Sum of electronic and thermal Free Energies= -5942.591146

	1	2	3
	A	A	A
Frequencies --	9.4302	19.5955	26.3257

PhBOD-Rh-OH-PhB(OH)$_2$-in-TS (6a)

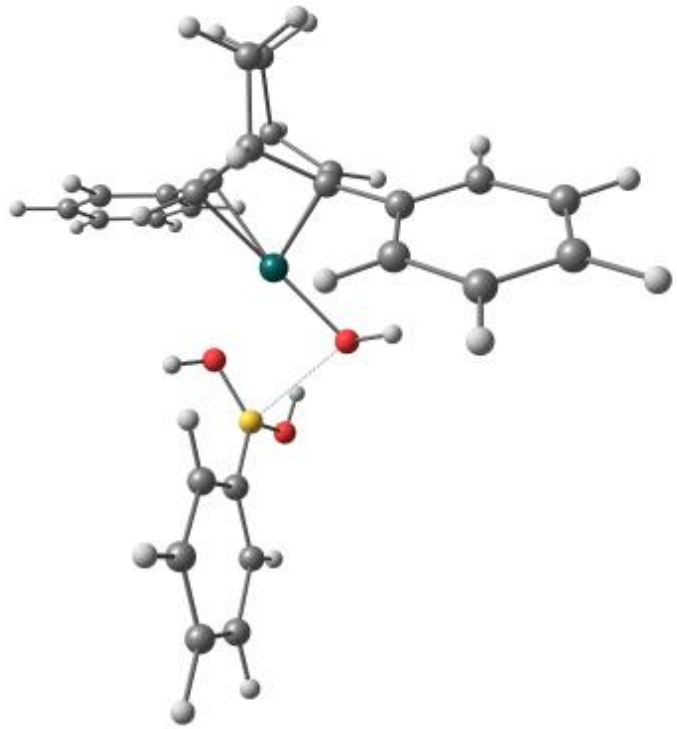


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.081420	0.180799	-0.514979
2	6	0	-1.368837	-1.414459	0.147992
3	6	0	0.724577	-2.443465	-0.600689
4	6	0	3.399379	-0.986172	-1.364587
5	6	0	-2.829886	-1.185352	0.123736
6	6	0	-3.643276	-1.812506	-0.831908
7	6	0	-0.606162	-1.820605	-0.966141
8	6	0	-0.611828	-1.646832	1.453207
9	6	0	-4.815648	-0.138740	1.052856
10	6	0	5.613477	-0.621085	-0.468181
11	6	0	0.519277	-3.626119	0.371804
12	6	0	0.662036	-0.854225	1.225695
13	6	0	-5.020856	-1.603315	-0.848300
14	6	0	1.416222	-1.295852	0.133952
15	6	0	3.728721	-0.905755	1.017854
16	6	0	-3.440750	-0.344949	1.066783
17	6	0	-0.289282	-3.152031	1.595346
18	6	0	-5.613727	-0.767002	0.095594
19	6	0	2.858991	-1.045813	-0.071500
20	6	0	5.091888	-0.693683	0.822473
21	6	0	4.759556	-0.770655	-1.562292
22	1	0	2.741040	-1.081047	-2.225059
23	1	0	6.676791	-0.456983	-0.621660
24	1	0	3.334594	-0.972731	2.028428
25	1	0	5.749838	-0.591459	1.681912
26	1	0	5.155622	-0.715617	-2.573172
27	1	0	-3.198408	-2.487790	-1.557813
28	1	0	-5.266480	0.523889	1.787215
29	1	0	-5.632450	-2.102918	-1.595126
30	1	0	-2.828862	0.186784	1.789188
31	1	0	-6.688281	-0.604896	0.085783
32	1	0	1.283228	-2.751413	-1.486059
33	1	0	-1.168668	-1.279101	2.316279
34	1	0	0.000496	-4.432986	-0.156267
35	1	0	1.498311	-4.015494	0.669677
36	1	0	0.272486	-3.304252	2.522678
37	1	0	-1.226585	-3.709583	1.692699
38	1	0	1.067878	-0.207152	2.000199
39	1	0	-1.039543	-1.960472	-1.953956
40	8	0	-1.377041	1.146268	-1.743625
41	1	0	-2.210263	0.656517	-1.805267
42	5	0	-1.488665	2.929982	-0.160318
43	8	0	-1.840651	3.688546	-1.266167
44	1	0	-1.491919	3.209289	-2.036096
45	8	0	-2.412812	2.815209	0.855354
46	1	0	-3.262799	3.147039	0.531551
47	6	0	0.009374	2.569543	0.232491
48	6	0	1.026958	2.368305	-0.729394
49	6	0	0.406308	2.655564	1.585735
50	6	0	2.378330	2.292412	-0.352362
51	1	0	0.778804	2.391151	-1.789116
52	6	0	1.743982	2.590003	1.954222
53	1	0	-0.356825	2.814573	2.343272
54	6	0	2.736920	2.412173	0.982543
55	1	0	3.142346	2.149450	-1.111574
56	1	0	2.023170	2.688519	3.000887
57	1	0	3.783288	2.364320	1.270995

SCF Done: E(RPBE1PBE) = -5942.97265092 A.U. after 1 cycles
Convg = 0.5073D-08 -V/T = 2.0045

Zero-point correction=			0.464007 (Hartree/Particle)
Thermal correction to Energy=			0.492144
Thermal correction to Enthalpy=			0.493104
Thermal correction to Gibbs Free Energy=			0.404057
Sum of electronic and zero-point Energies=			-5942.508644
Sum of electronic and thermal Energies=			-5942.480507
Sum of electronic and thermal Enthalpies=			-5942.479547
Sum of electronic and thermal Free Energies=			-5942.568594
	1	2	3
	A	A	A
Frequencies --	-156.1408	13.7193	24.1833

PhBOD-Rh-OH-PhB(OH)$_2$-out-TS (6b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.341863	0.098634	-0.417517
2	6	0	-2.367931	0.084471	0.370809
3	6	0	-1.119260	1.842631	1.533000
4	6	0	1.800023	2.834320	0.819287
5	6	0	-3.122605	-1.180332	0.242352
6	6	0	-3.422775	-1.966271	1.364423
7	6	0	-1.454051	0.368342	1.396101
8	6	0	-2.774726	1.350490	-0.383101
9	6	0	-4.260790	-2.823233	-1.144189
10	6	0	2.934627	4.661634	-0.280623
11	6	0	-2.402777	2.678144	1.728913
12	6	0	-1.427384	1.841200	-0.875291
13	6	0	-4.123572	-3.163481	1.235457
14	6	0	-0.515508	2.140220	0.159227
15	6	0	0.700331	4.033474	-0.954192
16	6	0	-3.559436	-1.628967	-1.013881
17	6	0	-3.400947	2.367471	0.594723
18	6	0	-4.545415	-3.598810	-0.019652

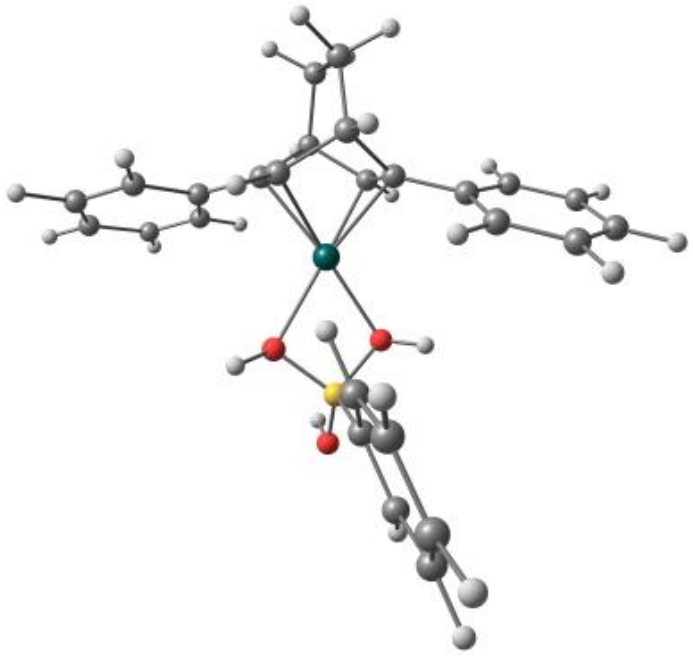
19	6	0	0.672259	3.009871	0.002963
20	6	0	1.820977	4.850248	-1.096201
21	6	0	2.918436	3.648318	0.679418
22	1	0	1.810790	2.029104	1.549743
23	1	0	3.809094	5.297150	-0.391377
24	1	0	-0.168415	4.202015	-1.585027
25	1	0	1.820243	5.639773	-1.843294
26	1	0	3.785986	3.485985	1.313663
27	1	0	-3.122543	-1.626536	2.352311
28	1	0	-4.581301	-3.154762	-2.128545
29	1	0	-4.349657	-3.753006	2.120419
30	1	0	-3.325101	-1.047250	-1.902137
31	1	0	-5.094052	-4.531296	-0.121239
32	1	0	-0.402444	2.023423	2.336320
33	1	0	-3.451766	1.131902	-1.210543
34	1	0	-2.832741	2.442110	2.707821
35	1	0	-2.137663	3.740575	1.743459
36	1	0	-3.664430	3.275629	0.042548
37	1	0	-4.333450	1.951914	0.990553
38	1	0	-1.295516	2.201902	-1.893184
39	1	0	-1.231621	-0.330059	2.200963
40	8	0	0.420390	-2.015651	-0.333376
41	1	0	0.464357	-2.277176	0.596953
42	5	0	1.684672	-2.201635	-0.959021
43	8	0	1.728684	-2.498562	-2.284332
44	1	0	0.953028	-2.127975	-2.731241
45	8	0	1.194654	0.124110	-1.709947
46	1	0	1.594488	1.001269	-1.795446
47	6	0	2.970671	-2.383792	-0.084409
48	6	0	4.082292	-3.061148	-0.608890
49	6	0	3.058715	-1.898496	1.229562
50	6	0	5.230992	-3.260678	0.152878
51	1	0	4.038842	-3.433557	-1.629184
52	6	0	4.207049	-2.087457	1.996562
53	1	0	2.231242	-1.334709	1.659820
54	6	0	5.294869	-2.774941	1.459254
55	1	0	6.079693	-3.792165	-0.270475
56	1	0	4.257510	-1.696668	3.009877
57	1	0	6.191674	-2.926488	2.054852

SCF Done: E(RPBE1PBE) = -5942.96739476 A.U. after 16 cycles
Convg = 0.7300D-08 -V/T = 2.0045

Zero-point correction= 0.463734 (Hartree/Particle)
Thermal correction to Energy= 0.492198
Thermal correction to Enthalpy= 0.493158
Thermal correction to Gibbs Free Energy= 0.401058
Sum of electronic and zero-point Energies= -5942.503661
Sum of electronic and thermal Energies= -5942.475197
Sum of electronic and thermal Enthalpies= -5942.474237
Sum of electronic and thermal Free Energies= -5942.566337

	1	2	3
	A	A	A
Frequencies --	-105.5959	14.0065	20.0169

PhBOD-Rh-PhB(OH)$_3$-out (7)

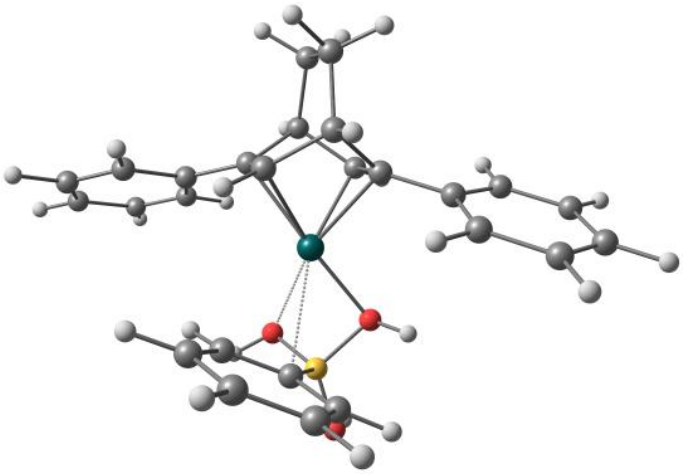


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.385520	-0.011723	-0.424802
2	6	0	-2.287667	0.629635	0.352707
3	6	0	-0.540489	1.931924	1.479372
4	6	0	2.533920	1.888799	0.694744
5	6	0	-3.399690	-0.340361	0.257270
6	6	0	-3.911390	-0.971921	1.399318
7	6	0	-1.313540	0.631871	1.366600
8	6	0	-2.295180	1.950981	-0.414452
9	6	0	-5.014770	-1.563859	-1.084737
10	6	0	4.185559	3.201953	-0.481553
11	6	0	-1.502713	3.122979	1.674872
12	6	0	-0.868419	1.990690	-0.922436
13	6	0	-4.956044	-1.888227	1.301550
14	6	0	0.102855	2.005217	0.094610
15	6	0	1.851407	3.360014	-1.085900
16	6	0	-3.972220	-0.648671	-0.985860
17	6	0	-2.564080	3.121412	0.556303
18	6	0	-5.511813	-2.189017	0.059365
19	6	0	1.509451	2.422371	-0.101505
20	6	0	3.176741	3.746294	-1.274288
21	6	0	3.857878	2.270195	0.504259
22	1	0	2.297002	1.142063	1.448083
23	1	0	5.219829	3.500158	-0.630459
24	1	0	1.071859	3.802219	-1.700582
25	1	0	3.420646	4.477929	-2.040163
26	1	0	4.637604	1.829895	1.119915
27	1	0	-3.501395	-0.731797	2.376822
28	1	0	-5.436970	-1.796354	-2.058832
29	1	0	-5.341799	-2.362775	2.200103
30	1	0	-3.578566	-0.187001	-1.888011
31	1	0	-6.326981	-2.903432	-0.017332
32	1	0	0.208537	1.891676	2.272005
33	1	0	-3.017103	1.941207	-1.232457

34	1	0	-1.969797	3.040936	2.661527
35	1	0	-0.922936	4.051581	1.671140
36	1	0	-2.543724	4.059378	-0.007731
37	1	0	-3.573253	3.016311	0.967352
38	1	0	-0.642737	2.257600	-1.952597
39	1	0	-1.301434	-0.099824	2.171740
40	8	0	-0.253118	-2.138794	-0.526670
41	1	0	-0.369539	-2.760692	0.202479
42	5	0	1.145595	-2.202949	-1.143663
43	8	0	1.233303	-3.170222	-2.189006
44	1	0	0.549902	-2.974838	-2.844146
45	8	0	1.145695	-0.765594	-1.703438
46	1	0	2.027822	-0.372134	-1.664905
47	6	0	2.305970	-2.436946	-0.045590
48	6	0	3.453952	-3.177870	-0.366511
49	6	0	2.232341	-1.912355	1.254627
50	6	0	4.481475	-3.377390	0.556073
51	1	0	3.530612	-3.612451	-1.360379
52	6	0	3.249834	-2.107877	2.189681
53	1	0	1.354833	-1.334210	1.548453
54	6	0	4.383742	-2.841189	1.840340
55	1	0	5.358886	-3.956829	0.276490
56	1	0	3.159038	-1.693162	3.191804
57	1	0	5.180395	-2.998188	2.563828

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5942.99861284     A.U. after    1 cycles
             Convg  =    0.2206D-08             -V/T =  2.0045
Zero-point correction=                           0.465506 (Hartree/Particle)
 Thermal correction to Energy=                    0.493646
 Thermal correction to Enthalpy=                  0.494606
 Thermal correction to Gibbs Free Energy=         0.404618
 Sum of electronic and zero-point Energies=          -5942.533107
 Sum of electronic and thermal Energies=             -5942.504967
 Sum of electronic and thermal Enthalpies=           -5942.504007
 Sum of electronic and thermal Free Energies=        -5942.593994
                     1                      2                      3
                     A                      A                      A
 Frequencies --    19.0342                27.4443                32.5885
```

PhBOD-Rh-PhB(OH)$_3$-out-to-in-TS (8)



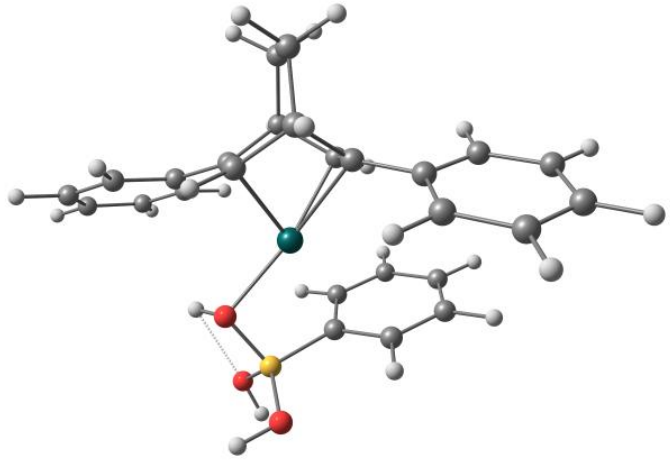
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.037829	0.053273	-0.438595

2	6	0	1.527165	-1.355178	0.251536
3	6	0	-0.541694	-1.810434	1.480913
4	6	0	-3.331680	-0.456350	0.968748
5	6	0	2.933586	-0.932141	0.079420
6	6	0	3.734077	-0.629896	1.189914
7	6	0	0.707334	-0.968393	1.319944
8	6	0	0.923480	-2.526070	-0.524638
9	6	0	4.823871	-0.435373	-1.362146
10	6	0	-5.452529	-0.819158	-0.131724
11	6	0	-0.187383	-3.306888	1.600535
12	6	0	-0.398280	-1.916351	-0.948682
13	6	0	5.059991	-0.234890	1.027752
14	6	0	-1.226277	-1.531486	0.143731
15	6	0	-3.451008	-1.887148	-0.964767
16	6	0	3.500610	-0.832164	-1.199824
17	6	0	0.705868	-3.727999	0.417079
18	6	0	5.610262	-0.135504	-0.249015
19	6	0	-2.682773	-1.292524	0.046034
20	6	0	-4.821515	-1.652677	-1.053205
21	6	0	-4.699708	-0.221140	0.880068
22	1	0	-2.753649	0.038989	1.744987
23	1	0	-6.521293	-0.635462	-0.200966
24	1	0	-2.976159	-2.550250	-1.682586
25	1	0	-5.398203	-2.126617	-1.843228
26	1	0	-5.180301	0.436884	1.599428
27	1	0	3.321268	-0.723355	2.191007
28	1	0	5.241921	-0.352916	-2.361934
29	1	0	5.666663	-0.011798	1.901590
30	1	0	2.890246	-1.035017	-2.075759
31	1	0	6.644629	0.172147	-0.376671
32	1	0	-1.146893	-1.477084	2.325088
33	1	0	1.535702	-2.800813	-1.384987
34	1	0	0.319885	-3.474906	2.556053
35	1	0	-1.114587	-3.888566	1.624578
36	1	0	0.247721	-4.542503	-0.153069
37	1	0	1.679575	-4.089059	0.763874
38	1	0	-0.779876	-2.053002	-1.957898
39	1	0	1.038637	-0.292499	2.104204
40	8	0	1.008160	1.801668	-2.059884
41	1	0	1.724349	2.421396	-1.871787
42	5	0	-0.274674	2.372850	-1.601660
43	8	0	-0.749658	3.528476	-2.306561
44	1	0	-0.702897	3.333317	-3.253090
45	8	0	-1.161294	1.135621	-1.845950
46	1	0	-2.059510	1.304204	-1.527464
47	6	0	-0.259502	2.632139	0.017605
48	6	0	-1.430112	3.019086	0.705700
49	6	0	0.894569	2.446037	0.800870
50	6	0	-1.447751	3.213537	2.081381
51	1	0	-2.342748	3.197932	0.138709
52	6	0	0.887588	2.637405	2.190804
53	1	0	1.840203	2.188659	0.324600
54	6	0	-0.282904	3.018174	2.834251
55	1	0	-2.364876	3.526816	2.575799
56	1	0	1.804949	2.501834	2.760010
57	1	0	-0.293047	3.176317	3.910048

SCF Done: E(RPBE1PBE) = -5942.98410812 A.U. after 1 cycles
Convg = 0.4503D-08 -V/T = 2.0045
Zero-point correction= 0.465440 (Hartree/Particle)
Thermal correction to Energy= 0.492775
Thermal correction to Enthalpy= 0.493735
Thermal correction to Gibbs Free Energy= 0.406771

```
 Sum of electronic and zero-point Energies=          -5942.518668
 Sum of electronic and thermal Energies=             -5942.491334
 Sum of electronic and thermal Enthalpies=           -5942.490373
 Sum of electronic and thermal Free Energies=        -5942.577337
                     1                      2                      3
                     A                      A                      A
 Frequencies --   -35.9459               26.9762                30.4633
```

PhBOD-Rh-PhB(OH)$_3$-in (9a)



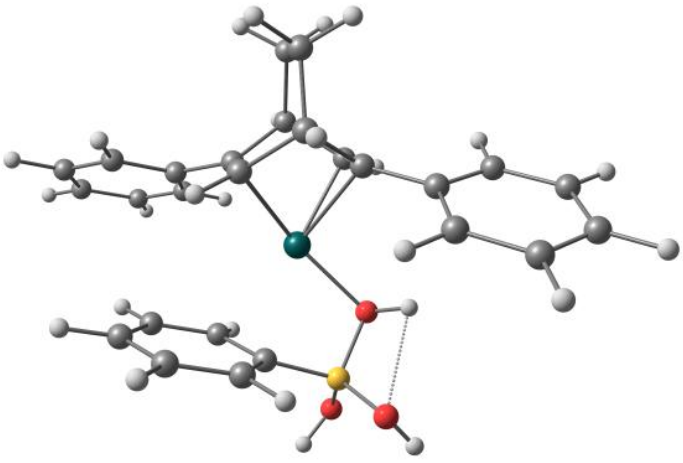
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.192948	0.236040	-0.215491
2	6	0	-1.581060	-1.378346	0.004133
3	6	0	0.418784	-2.305240	-1.066068
4	6	0	3.163073	-0.827387	-1.473752
5	6	0	-3.006045	-0.994186	0.094243
6	6	0	-3.876571	-1.180475	-0.989641
7	6	0	-0.861082	-1.510103	-1.202470
8	6	0	-0.839435	-2.029210	1.168308
9	6	0	-4.859476	-0.050968	1.355030
10	6	0	5.406519	-0.829031	-0.578186
11	6	0	0.136763	-3.695840	-0.455550
12	6	0	0.487159	-1.291039	1.132941
13	6	0	-5.215514	-0.807268	-0.903875
14	6	0	1.196667	-1.458540	-0.060650
15	6	0	3.537194	-1.434736	0.827078
16	6	0	-3.522908	-0.425964	1.269518
17	6	0	-0.622161	-3.530744	0.875170
18	6	0	-5.713325	-0.240235	0.267926
19	6	0	2.645910	-1.225776	-0.232836
20	6	0	4.905825	-1.238644	0.656322
21	6	0	4.528168	-0.623937	-1.643782
22	1	0	2.484712	-0.641517	-2.302919
23	1	0	6.473885	-0.674123	-0.711842
24	1	0	3.157410	-1.765372	1.789970
25	1	0	5.583170	-1.410332	1.489019
26	1	0	4.908921	-0.299102	-2.608560
27	1	0	-3.507588	-1.635046	-1.904735
28	1	0	-5.235083	0.398177	2.270554
29	1	0	-5.872781	-0.964022	-1.755114
30	1	0	-2.866051	-0.250908	2.117751
31	1	0	-6.757422	0.053129	0.334073

32	1	0	0.946602	-2.389861	-2.017164
33	1	0	-1.358762	-1.884550	2.116656
34	1	0	-0.446477	-4.281903	-1.172976
35	1	0	1.086303	-4.220504	-0.308863
36	1	0	-0.062216	-3.971812	1.706074
37	1	0	-1.595255	-4.031277	0.843127
38	1	0	0.948651	-0.908635	2.040222
39	1	0	-1.304332	-1.318690	-2.176505
40	8	0	-1.379651	1.663097	-1.217527
41	1	0	-2.281516	1.733695	-0.868586
42	5	0	-0.608849	2.941542	-0.831674
43	8	0	0.049191	3.502010	-1.986325
44	1	0	-0.633394	3.742706	-2.627356
45	8	0	-1.637613	3.778383	-0.223652
46	1	0	-1.283767	4.669751	-0.115873
47	6	0	0.547010	2.429615	0.223908
48	6	0	1.912146	2.317734	-0.121783
49	6	0	0.208922	2.154531	1.570752
50	6	0	2.888837	2.024557	0.827439
51	1	0	2.196805	2.513687	-1.152565
52	6	0	1.186040	1.864522	2.530911
53	1	0	-0.828056	2.272145	1.881093
54	6	0	2.527617	1.809335	2.159721
55	1	0	3.932641	1.956124	0.530802
56	1	0	0.898767	1.700120	3.567384
57	1	0	3.292000	1.594949	2.902953

SCF Done: E(RPBE1PBE) = -5942.99272427 A.U. after 1 cycles
Convg = 0.4804D-08 -V/T = 2.0045
Zero-point correction= 0.464871 (Hartree/Particle)
Thermal correction to Energy= 0.493329
Thermal correction to Enthalpy= 0.494289
Thermal correction to Gibbs Free Energy= 0.404650
Sum of electronic and zero-point Energies= -5942.527853
Sum of electronic and thermal Energies= -5942.499395
Sum of electronic and thermal Enthalpies= -5942.498435
Sum of electronic and thermal Free Energies= -5942.588074

	1	2	3
	A	A	A
Frequencies --	25.0527	27.9986	32.1061

PhBOD-Rh-PhB(OH)$_3$-out-to-in (9b)



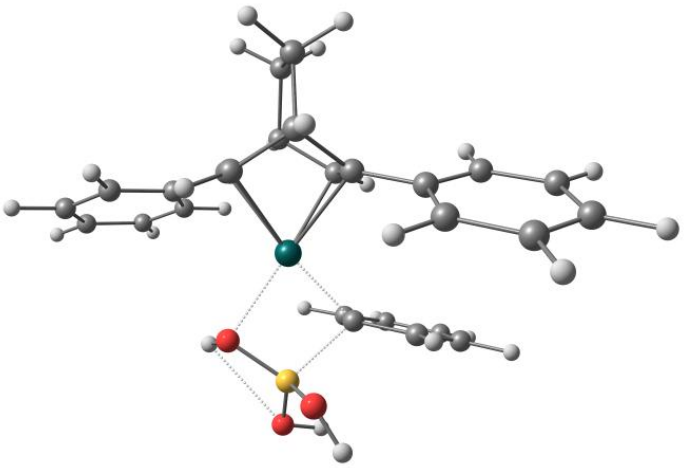
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	45	0	-0.088553	0.178568	-0.393586
2	6	0	1.397485	-1.358752	0.034249
3	6	0	-0.596516	-1.842784	1.363397
4	6	0	-3.380889	-0.369069	1.130171
5	6	0	2.828831	-1.063605	-0.190711
6	6	0	3.742448	-1.086660	0.870563
7	6	0	0.674519	-1.032588	1.188628
8	6	0	0.687371	-2.424336	-0.798486
9	6	0	4.651994	-0.506719	-1.695202
10	6	0	-5.591409	-0.671447	0.204487
11	6	0	-0.280417	-3.355507	1.336730
12	6	0	-0.648020	-1.761666	-1.063315
13	6	0	5.092312	-0.818275	0.654310
14	6	0	-1.376922	-1.468513	0.105267
15	6	0	-3.689083	-1.752938	-0.819016
16	6	0	3.305629	-0.782763	-1.478984
17	6	0	0.501313	-3.699625	0.054131
18	6	0	5.551832	-0.522320	-0.628145
19	6	0	-2.829601	-1.194016	0.137744
20	6	0	-5.057555	-1.494598	-0.785370
21	6	0	-4.746174	-0.107535	1.160830
22	1	0	-2.728016	0.102171	1.860567
23	1	0	-6.658236	-0.466475	0.228550
24	1	0	-3.286475	-2.409224	-1.585860
25	1	0	-5.708022	-1.941215	-1.532753
26	1	0	-5.150521	0.549417	1.925921
27	1	0	3.393418	-1.321186	1.872735
28	1	0	5.000830	-0.273992	-2.697934
29	1	0	5.787482	-0.842748	1.489617
30	1	0	2.608354	-0.748980	-2.313100
31	1	0	6.603952	-0.309085	-0.797053
32	1	0	-1.135078	-1.564541	2.270451
33	1	0	1.226093	-2.638168	-1.723001
34	1	0	0.296378	-3.609973	2.231598
35	1	0	-1.219915	-3.914660	1.391195
36	1	0	-0.028944	-4.448861	-0.542508
37	1	0	1.486483	-4.115431	0.288958
38	1	0	-1.103849	-1.777919	-2.050627
39	1	0	1.102003	-0.458473	2.008080
40	8	0	-0.802710	3.629299	-1.944238
41	1	0	-0.383418	4.423224	-1.589793
42	5	0	-1.171216	2.764559	-0.838113
43	8	0	-2.369021	3.173540	-0.125213
44	1	0	-2.869308	3.743034	-0.724378
45	8	0	-1.430850	1.382407	-1.481811
46	1	0	-2.346557	1.151695	-1.262937
47	6	0	0.062523	2.501833	0.215598
48	6	0	-0.091992	2.606129	1.618104
49	6	0	1.364492	2.228430	-0.262564
50	6	0	0.992684	2.510060	2.480320
51	1	0	-1.084708	2.816985	2.008902
52	6	0	2.466634	2.133785	0.608007
53	1	0	1.539560	2.218362	-1.338899
54	6	0	2.281915	2.282308	1.973699
55	1	0	0.847875	2.627256	3.552445
56	1	0	3.460090	1.951926	0.205648
57	1	0	3.131719	2.223562	2.649546

SCF Done: E(RPBE1PBE) = -5942.99158166 A.U. after 1 cycles
Convg = 0.2769D-08 -V/T = 2.0045
Zero-point correction= 0.464923 (Hartree/Particle)
Thermal correction to Energy= 0.493320
Thermal correction to Enthalpy= 0.494280

```
 Thermal correction to Gibbs Free Energy=          0.405287
 Sum of electronic and zero-point Energies=         -5942.526659
 Sum of electronic and thermal Energies=            -5942.498262
 Sum of electronic and thermal Enthalpies=          -5942.497302
 Sum of electronic and thermal Free Energies=       -5942.586295
                     1                      2                      3
                     A                      A                      A
 Frequencies --    27.9992                34.8857                39.9964
```

PhBOD-Rh-PhB(OH)$_3$-in-TS (10)



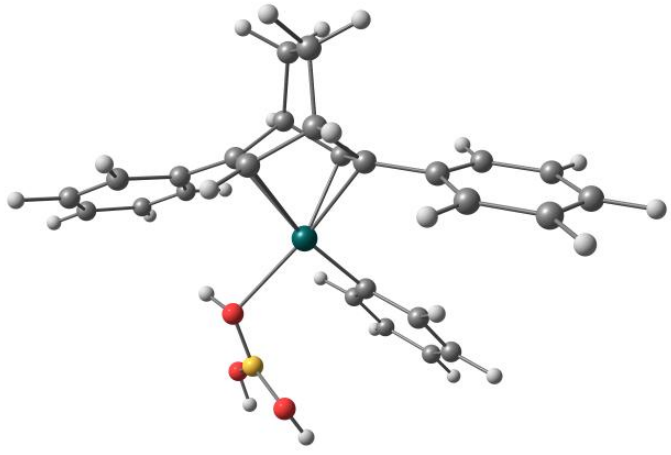
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.288195	0.179165	-0.324101
2	6	0	-1.912892	-1.193111	0.170708
3	6	0	-0.068238	-2.540240	-0.689109
4	6	0	2.826303	-1.556697	-1.380772
5	6	0	-3.249872	-0.561416	0.186082
6	6	0	-4.170643	-0.781549	-0.848898
7	6	0	-1.259166	-1.651515	-0.975119
8	6	0	-1.226875	-1.685462	1.444671
9	6	0	-4.877546	0.903285	1.248333
10	6	0	5.077349	-1.638010	-0.506237
11	6	0	-0.489348	-3.742571	0.185747
12	6	0	0.180177	-1.140921	1.276855
13	6	0	-5.420248	-0.167564	-0.838891
14	6	0	0.834447	-1.618219	0.130107
15	6	0	3.185937	-1.694198	0.996472
16	6	0	-3.628832	0.289331	1.237106
17	6	0	-1.205684	-3.231372	1.450678
18	6	0	-5.780472	0.678587	0.209002
19	6	0	2.296606	-1.616457	-0.083012
20	6	0	4.563100	-1.703481	0.787757
21	6	0	4.201424	-1.563835	-1.590570
22	1	0	2.154295	-1.465257	-2.230380
23	1	0	6.151821	-1.645875	-0.669732
24	1	0	2.796721	-1.754821	2.009181
25	1	0	5.236331	-1.766531	1.638919
26	1	0	4.591754	-1.503673	-2.603274
27	1	0	-3.911937	-1.451265	-1.664152
28	1	0	-5.145960	1.562702	2.069680
29	1	0	-6.118230	-0.356514	-1.650368
30	1	0	-2.931076	0.490853	2.045930
31	1	0	-6.756522	1.156090	0.217488

32	1	0	0.418929	-2.872133	-1.607115
33	1	0	-1.705977	-1.298461	2.345039
34	1	0	-1.142846	-4.395226	-0.401931
35	1	0	0.401654	-4.325299	0.441507
36	1	0	-0.697242	-3.573186	2.358035
37	1	0	-2.235204	-3.600673	1.500957
38	1	0	0.710730	-0.682337	2.107988
39	1	0	-1.681066	-1.578772	-1.974224
40	8	0	-1.063426	1.709641	-1.622535
41	1	0	-1.736348	2.249066	-1.181559
42	5	0	0.211173	2.405573	-1.532882
43	8	0	1.090641	1.971212	-2.541502
44	1	0	1.728920	2.670311	-2.726332
45	8	0	0.035163	3.790273	-1.273228
46	1	0	0.733231	4.130403	-0.701131
47	6	0	1.067986	1.804352	0.229837
48	6	0	2.467012	1.726596	0.106723
49	6	0	0.576239	2.452097	1.386410
50	6	0	3.327785	2.262514	1.065538
51	1	0	2.888510	1.242315	-0.771413
52	6	0	1.423308	2.978911	2.360478
53	1	0	-0.498973	2.568553	1.519541
54	6	0	2.807862	2.886833	2.199485
55	1	0	4.404773	2.189047	0.930385
56	1	0	1.008485	3.470712	3.238008
57	1	0	3.474824	3.305322	2.949738

SCF Done: E(RPBE1PBE) = -5942.97277441 A.U. after 1 cycles
Convg = 0.3982D-08 -V/T = 2.0045
Zero-point correction= 0.463338 (Hartree/Particle)
Thermal correction to Energy= 0.491785
Thermal correction to Enthalpy= 0.492745
Thermal correction to Gibbs Free Energy= 0.402634
Sum of electronic and zero-point Energies= -5942.509436
Sum of electronic and thermal Energies= -5942.480989
Sum of electronic and thermal Enthalpies= -5942.480029
Sum of electronic and thermal Free Energies= -5942.570140

	1	2	3
	A	A	A
Frequencies --	-237.5210	16.5759	29.9283

PhBOD-Rh-Ph-B(OH)$_3$ (11)



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

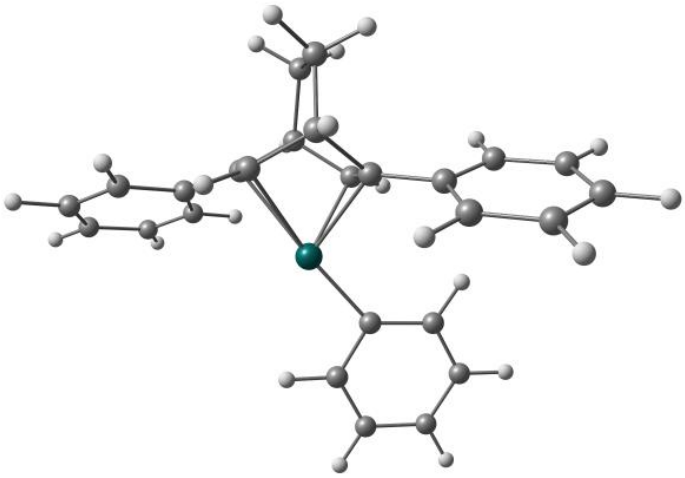
1	45	0	-0.136746	0.080521	-0.217161
2	6	0	-1.663737	-1.570251	0.108985
3	6	0	0.336908	-2.592643	-0.816262
4	6	0	3.177847	-1.509063	-1.378386
5	6	0	-3.048758	-1.057725	0.157123
6	6	0	-3.971060	-1.350845	-0.859000
7	6	0	-0.973371	-1.870789	-1.047970
8	6	0	-0.913339	-2.032659	1.357156
9	6	0	-4.764001	0.285844	1.247115
10	6	0	5.391090	-1.282650	-0.434786
11	6	0	0.083828	-3.894092	-0.018509
12	6	0	0.416579	-1.306683	1.244329
13	6	0	-5.263292	-0.832710	-0.825956
14	6	0	1.131632	-1.622641	0.062909
15	6	0	3.452444	-1.391929	1.005472
16	6	0	-3.472231	-0.234442	1.214730
17	6	0	-0.690439	-3.560994	1.271613
18	6	0	-5.666808	-0.010536	0.225694
19	6	0	2.597024	-1.505701	-0.100001
20	6	0	4.830083	-1.278123	0.841519
21	6	0	4.555279	-1.399361	-1.545398
22	1	0	2.542150	-1.570275	-2.258007
23	1	0	6.466958	-1.196952	-0.562792
24	1	0	3.037260	-1.396271	2.009023
25	1	0	5.469308	-1.189579	1.716384
26	1	0	4.976953	-1.397446	-2.547515
27	1	0	-3.675378	-2.002991	-1.676152
28	1	0	-5.064645	0.927614	2.071230
29	1	0	-5.960794	-1.077421	-1.622901
30	1	0	-2.774497	0.018953	2.009235
31	1	0	-6.675489	0.392633	0.251059
32	1	0	0.847303	-2.807622	-1.755923
33	1	0	-1.442634	-1.767023	2.274106
34	1	0	-0.478362	-4.593834	-0.645612
35	1	0	1.046624	-4.364897	0.206364
36	1	0	-0.139071	-3.887163	2.159587
37	1	0	-1.661818	-4.066224	1.292921
38	1	0	0.900301	-0.912064	2.134520
39	1	0	-1.391672	-1.755415	-2.044862
40	8	0	-1.629589	1.633120	-1.071670
41	1	0	-2.443683	1.517500	-0.556333
42	5	0	-1.260100	2.972387	-1.138931
43	8	0	-0.280307	3.267306	-2.038738
44	1	0	0.127789	4.131542	-1.910720
45	8	0	-1.970931	3.850917	-0.361391
46	1	0	-1.714118	4.773611	-0.479022
47	6	0	1.098448	1.589637	0.381505
48	6	0	2.354558	1.866881	-0.186791
49	6	0	0.648058	2.483037	1.372947
50	6	0	3.108364	2.978361	0.194928
51	1	0	2.761063	1.205931	-0.949941
52	6	0	1.399788	3.594129	1.769569
53	1	0	-0.317008	2.319443	1.852847
54	6	0	2.635902	3.851340	1.177360
55	1	0	4.074634	3.160325	-0.272802
56	1	0	1.017912	4.257018	2.544644
57	1	0	3.226806	4.712135	1.482560

SCF Done: E(RPBE1PBE) = -5942.98914683 A.U. after 1 cycles
Convg = 0.5391D-08 -V/T = 2.0045

Zero-point correction= 0.464108 (Hartree/Particle)
Thermal correction to Energy= 0.493548
Thermal correction to Enthalpy= 0.494508
Thermal correction to Gibbs Free Energy= 0.400719

```
 Sum of electronic and zero-point Energies=          -5942.525039
 Sum of electronic and thermal Energies=             -5942.495599
 Sum of electronic and thermal Enthalpies=           -5942.494639
 Sum of electronic and thermal Free Energies=        -5942.588428
                      1                      2                      3
                      A                      A                      A
 Frequencies --    19.0104                30.0973                32.6092
```

PhBOD-Rh-Ph (12)

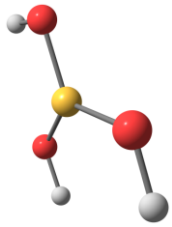


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.206391	0.508569	-0.360793
2	6	0	-1.919075	-0.971760	0.028852
3	6	0	-0.008237	-2.219900	-0.809244
4	6	0	2.978501	-1.243103	-1.304830
5	6	0	-3.252368	-0.335247	0.028684
6	6	0	-4.181926	-0.595643	-0.989945
7	6	0	-1.243196	-1.394024	-1.096825
8	6	0	-1.229751	-1.427720	1.313028
9	6	0	-4.868621	1.173896	1.043725
10	6	0	5.133987	-1.608886	-0.275883
11	6	0	-0.390623	-3.447589	0.051363
12	6	0	0.162587	-0.835253	1.188144
13	6	0	-5.429733	0.021688	-0.995378
14	6	0	0.862404	-1.285893	0.035046
15	6	0	3.122521	-1.649469	1.062530
16	6	0	-3.621282	0.556396	1.048727
17	6	0	-1.142688	-2.973779	1.310881
18	6	0	-5.779587	0.910409	0.021023
19	6	0	2.335743	-1.382457	-0.066046
20	6	0	4.509087	-1.758718	0.959934
21	6	0	4.360389	-1.351542	-1.409819
22	1	0	2.386345	-1.012487	-2.187377
23	1	0	6.214607	-1.690837	-0.357321
24	1	0	2.644193	-1.782052	2.029621
25	1	0	5.100385	-1.965521	1.848445
26	1	0	4.839657	-1.223968	-2.377087
27	1	0	-3.931180	-1.304841	-1.774315
28	1	0	-5.128766	1.867230	1.839347
29	1	0	-6.136467	-0.200535	-1.790850
30	1	0	-2.914948	0.788133	1.841948
31	1	0	-6.754950	1.389469	0.018522
32	1	0	0.501317	-2.522778	-1.725947

33	1	0	-1.746060	-1.068554	2.204609
34	1	0	-1.010242	-4.122925	-0.547334
35	1	0	0.520840	-3.994476	0.314468
36	1	0	-0.630663	-3.298834	2.222578
37	1	0	-2.155655	-3.387773	1.347244
38	1	0	0.682136	-0.458532	2.067384
39	1	0	-1.638325	-1.296215	-2.105511
40	6	0	1.107228	1.975282	0.021708
41	6	0	2.376015	2.009187	0.617381
42	6	0	0.575198	3.192791	-0.436048
43	6	0	3.079812	3.208063	0.746788
44	1	0	2.835793	1.090605	0.976686
45	6	0	1.271647	4.397606	-0.313413
46	1	0	-0.416454	3.218282	-0.901028
47	6	0	2.532466	4.405942	0.282692
48	1	0	4.065463	3.208343	1.208416
49	1	0	0.832638	5.323936	-0.678548
50	1	0	3.084911	5.337059	0.383274

```
SCF Done:  E(RPBE1PBE) =  -5690.72654201     A.U. after    1 cycles
             Convg  =    0.3070D-08             -V/T =  2.0042
 Zero-point correction=                           0.413724 (Hartree/Particle)
 Thermal correction to Energy=                    0.436916
 Thermal correction to Enthalpy=                  0.437876
 Thermal correction to Gibbs Free Energy=         0.358606
 Sum of electronic and zero-point Energies=          -5690.312818
 Sum of electronic and thermal Energies=             -5690.289626
 Sum of electronic and thermal Enthalpies=           -5690.288666
 Sum of electronic and thermal Free Energies=        -5690.367936
                      1                      2                      3
                      A                      A                      A
 Frequencies --    26.0587                31.1725                40.5342
```

B(OH)$_2$-syn (13a)

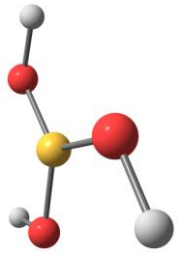


1	5	0	-0.008070	-0.029684	-0.000527
2	8	0	1.074746	-0.873132	-0.000064
3	8	0	0.052563	1.350358	0.000024
4	1	0	0.948228	1.708352	0.000122
5	8	0	-1.239382	-0.625783	0.000267
6	1	0	-1.934475	0.044597	0.000476
7	1	0	1.923179	-0.416067	0.000216

```
SCF Done:  E(RPBE1PBE) =  -252.246653096     A.U. after    1 cycles
             Convg  =    0.4789D-09             -V/T =  2.0107
Zero-point correction=                           0.048888 (Hartree/Particle)
 Thermal correction to Energy=                    0.053508
 Thermal correction to Enthalpy=                  0.054468
 Thermal correction to Gibbs Free Energy=         0.021812
 Sum of electronic and zero-point Energies=           -252.197765
 Sum of electronic and thermal Energies=              -252.193145
 Sum of electronic and thermal Enthalpies=            -252.192185
```

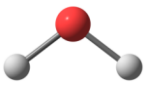
```
 Sum of electronic and thermal Free Energies=         -252.224841
                      1                      2                      3
                      A                      A                      A
 Frequencies --    306.8622               445.0252               467.4989
```

$B(OH)_2$-anti (13b)



```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          8           0        1.026881   -0.910284   -0.000014
      2          5           0       -0.000037    0.000024   -0.000015
      3          8           0       -1.301808   -0.434164   -0.000007
      4          8           0        0.274926    1.344458   -0.000003
      5          1           0        0.684231   -1.813882    0.000124
      6          1           0        1.228820    1.499155    0.000072
      7          1           0       -1.912857    0.314527    0.000066
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -252.253311712     A.U. after    1 cycles
             Convg  =    0.4909D-09             -V/T =  2.0107
Zero-point correction=                           0.049045 (Hartree/Particle)
 Thermal correction to Energy=                    0.053563
 Thermal correction to Enthalpy=                  0.054523
 Thermal correction to Gibbs Free Energy=         0.022070
 Sum of electronic and zero-point Energies=           -252.204266
 Sum of electronic and thermal Energies=              -252.199749
 Sum of electronic and thermal Enthalpies=            -252.198789
 Sum of electronic and thermal Free Energies=         -252.231242
                      1                      2                      3
                      A                      A                      A
 Frequencies --    416.1739               425.9798               427.0889
```

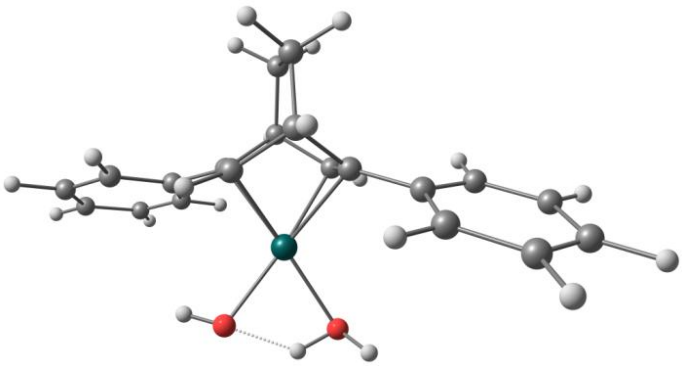
H_2O



```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          8           0        0.000000    0.000000    0.117139
      2          1           0        0.000000    0.767242   -0.468555
      3          1           0        0.000000   -0.767242   -0.468555
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -76.3516415090     A.U. after    1 cycles
             Convg  =    0.2157D-09             -V/T =  2.0095
Zero-point correction=                           0.021555 (Hartree/Particle)
 Thermal correction to Energy=                    0.024437
 Thermal correction to Enthalpy=                  0.025397
 Thermal correction to Gibbs Free Energy=         0.003544
 Sum of electronic and zero-point Energies=           -76.330087
 Sum of electronic and thermal Energies=              -76.327204
```

```
 Sum of electronic and thermal Enthalpies=            -76.326244
 Sum of electronic and thermal Free Energies=         -76.348098
                     1                    2                    3
                    A1                   A1                   B2
 Frequencies --  1686.5450            3820.9379            3953.8733
```

PhBOD-Rh-OH-OH_2 (14)



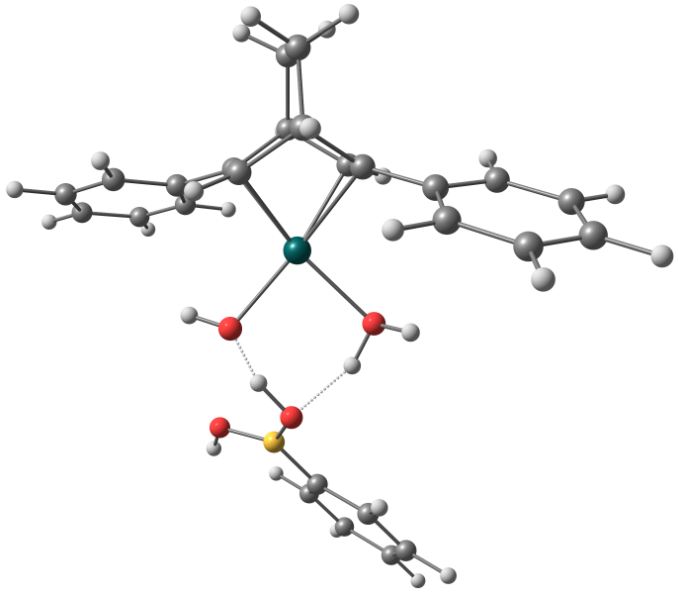
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.011703	-0.899482	-0.024101
2	6	0	1.376101	0.716296	-0.027183
3	6	0	-0.698198	1.539990	-1.042594
4	6	0	-3.394731	-0.055326	-1.184745
5	6	0	2.813907	0.367091	0.002265
6	6	0	3.631270	0.560777	-1.119982
7	6	0	0.583981	0.744177	-1.193874
8	6	0	0.705432	1.473431	1.120176
9	6	0	4.746234	-0.499729	1.196867
10	6	0	-5.551807	-0.294288	-0.121284
11	6	0	-0.399371	2.979900	-0.573213
12	6	0	-0.605778	0.719396	1.238833
13	6	0	4.983830	0.226577	-1.087195
14	6	0	-1.390486	0.760237	0.076151
15	6	0	-3.653165	0.511785	1.139568
16	6	0	3.396636	-0.165913	1.162574
17	6	0	0.462141	2.940079	0.704466
18	6	0	5.547717	-0.305418	0.070651
19	6	0	-2.824526	0.405018	0.013151
20	6	0	-5.000570	0.164493	1.074184
21	6	0	-4.740742	-0.401838	-1.251718
22	1	0	-2.770913	-0.163962	-2.068609
23	1	0	-6.603642	-0.562356	-0.173249
24	1	0	-3.242370	0.886006	2.073349
25	1	0	-5.624228	0.260571	1.959343
26	1	0	-5.158322	-0.760838	-2.189002
27	1	0	3.208945	0.991200	-2.023944
28	1	0	5.174066	-0.921210	2.102848
29	1	0	5.599579	0.388299	-1.968243
30	1	0	2.777271	-0.347841	2.037293
31	1	0	6.602258	-0.566544	0.096904
32	1	0	-1.284811	1.540640	-1.962807
33	1	0	1.290705	1.415665	2.039568
34	1	0	0.114146	3.516480	-1.377863
35	1	0	-1.346998	3.499017	-0.396037
36	1	0	-0.032020	3.463447	1.529491
37	1	0	1.428434	3.430599	0.546928
38	1	0	-0.995750	0.421897	2.209422

39	1	0	0.975595	0.485050	-2.175077
40	8	0	1.007831	-2.490928	-0.787695
41	1	0	1.961906	-2.351487	-0.855572
42	8	0	-0.944633	-2.786051	0.774340
43	1	0	-0.206565	-3.223917	0.268968
44	1	0	-1.773461	-3.028586	0.335080

SCF Done: E(RPBE1PBE) = -5611.50140288 A.U. after 1 cycles
Convg = 0.4336D-08 -V/T = 2.0039
Zero-point correction= 0.362925 (Hartree/Particle)
Thermal correction to Energy= 0.384708
Thermal correction to Enthalpy= 0.385668
Thermal correction to Gibbs Free Energy= 0.311068
Sum of electronic and zero-point Energies= -5611.138477
Sum of electronic and thermal Energies= -5611.116695
Sum of electronic and thermal Enthalpies= -5611.115735
Sum of electronic and thermal Free Energies= -5611.190335

	1	2	3
	A	A	A
Frequencies --	30.1012	36.2597	44.2826

PhBOD-Rh-OH-OH_2-PhB$(OH)_2$-conf1 (15a)



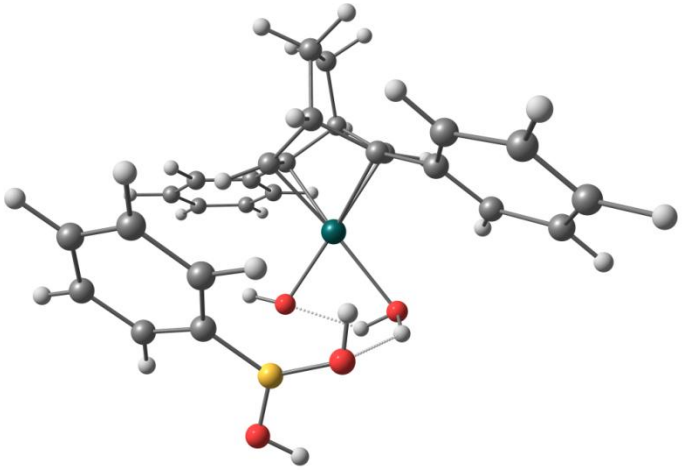
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.796503	0.067149	-0.228168
2	6	0	2.339930	-1.353441	0.168251
3	6	0	3.417839	0.701381	-0.625403
4	6	0	1.967513	3.419423	-1.181492
5	6	0	1.974745	-2.786451	0.120215
6	6	0	2.441418	-3.619953	-0.905771
7	6	0	2.664767	-0.573479	-0.959494
8	6	0	2.798432	-0.680761	1.463273
9	6	0	0.805150	-4.693823	1.070797
10	6	0	1.426081	5.574073	-0.229434
11	6	0	4.692227	0.385321	0.186163
12	6	0	2.055984	0.640379	1.382031
13	6	0	2.094041	-4.968983	-0.945274
14	6	0	2.395349	1.415143	0.259987
15	6	0	1.855241	3.678676	1.208830

16	6	0	1.152438	-3.347816	1.109224
17	6	0	4.324617	-0.456865	1.423543
18	6	0	1.275070	-5.512155	0.042556
19	6	0	2.076119	2.850306	0.098227
20	6	0	1.532585	5.024149	1.047211
21	6	0	1.645544	4.763640	-1.343829
22	1	0	2.113763	2.797551	-2.061068
23	1	0	1.176416	6.624088	-0.355557
24	1	0	1.949840	3.269696	2.210981
25	1	0	1.370108	5.646848	1.923184
26	1	0	1.561157	5.179387	-2.344606
27	1	0	3.094797	-3.213388	-1.673097
28	1	0	0.157154	-5.104730	1.840519
29	1	0	2.469665	-5.597966	-1.748197
30	1	0	0.756443	-2.715177	1.899639
31	1	0	1.003089	-6.563778	0.011771
32	1	0	3.655330	1.275886	-1.522036
33	1	0	2.505923	-1.255448	2.343687
34	1	0	5.398483	-0.148348	-0.458242
35	1	0	5.171331	1.326521	0.475000
36	1	0	4.631727	0.044548	2.347058
37	1	0	4.827119	-1.429578	1.404956
38	1	0	1.529127	1.041750	2.244437
39	1	0	2.641921	-0.967313	-1.973036
40	8	0	-0.487207	-1.048581	-1.404366
41	1	0	-0.291058	-1.995395	-1.397508
42	8	0	-0.943529	1.365142	0.235490
43	1	0	-1.763169	0.965957	-0.163993
44	1	0	-0.853370	2.262067	-0.118689
45	5	0	-3.782964	-0.944091	-0.559823
46	6	0	-5.119518	-0.243111	-0.099880
47	6	0	-5.351707	1.099910	-0.435897
48	6	0	-6.106667	-0.902536	0.649146
49	6	0	-6.520078	1.754678	-0.052389
50	1	0	-4.600694	1.631350	-1.015368
51	6	0	-7.275967	-0.254731	1.045941
52	1	0	-5.965444	-1.939170	0.955311
53	6	0	-7.486364	1.077319	0.691847
54	1	0	-6.679758	2.793500	-0.331327
55	1	0	-8.021661	-0.786119	1.632167
56	1	0	-8.397976	1.585431	0.996464
57	8	0	-2.734589	-0.184467	-0.960414
58	1	0	-1.829562	-0.708907	-1.204302
59	8	0	-3.648468	-2.319840	-0.574772
60	1	0	-4.476929	-2.760294	-0.349247

SCF Done: E(RPBE1PBE) = -6019.35921966 A.U. after 1 cycles
Convg = 0.1672D-08 -V/T = 2.0045
Zero-point correction= 0.489248 (Hartree/Particle)
Thermal correction to Energy= 0.520358
Thermal correction to Enthalpy= 0.521318
Thermal correction to Gibbs Free Energy= 0.422576
Sum of electronic and zero-point Energies= -6018.869972
Sum of electronic and thermal Energies= -6018.838861
Sum of electronic and thermal Enthalpies= -6018.837901
Sum of electronic and thermal Free Energies= -6018.936644

	1	2	3
	A	A	A
Frequencies --	13.6566	19.8347	21.8872

PhBOD-Rh-OH-OH_2-PhB$(OH)_2$-conf1 (15a)

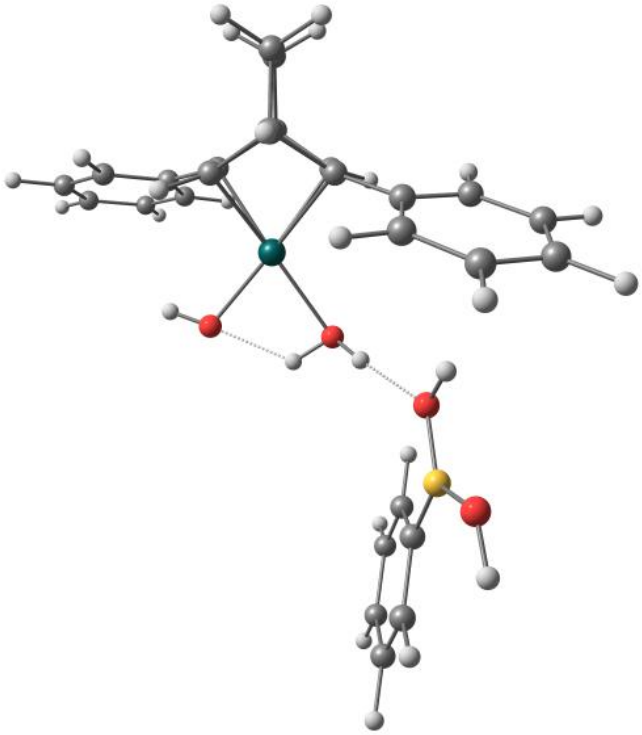


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.000467	-0.569448	-0.843252
2	6	0	1.438647	-1.402189	0.500564
3	6	0	-0.580751	-0.929312	1.811372
4	6	0	-3.597922	-0.736398	1.394805
5	6	0	2.861913	-1.259297	0.123395
6	6	0	3.695227	-0.339237	0.775807
7	6	0	0.678341	-0.406161	1.144939
8	6	0	0.753668	-2.765404	0.591900
9	6	0	4.751526	-1.912480	-1.260251
10	6	0	-5.536589	-0.845128	-0.046067
11	6	0	-0.240119	-2.062309	2.801973
12	6	0	-0.582849	-2.468466	-0.061860
13	6	0	5.033953	-0.204844	0.414448
14	6	0	-1.331254	-1.478652	0.601068
15	6	0	-3.371170	-1.553596	-0.857301
16	6	0	3.415139	-2.045213	-0.899134
17	6	0	0.565565	-3.157071	2.073774
18	6	0	5.568846	-0.990593	-0.604775
19	6	0	-2.774585	-1.249010	0.380303
20	6	0	-4.730683	-1.354892	-1.066255
21	6	0	-4.962182	-0.538730	1.184768
22	1	0	-3.180176	-0.505610	2.370449
23	1	0	-6.598799	-0.687341	-0.211654
24	1	0	-2.755529	-1.929705	-1.670047
25	1	0	-5.164413	-1.592890	-2.034181
26	1	0	-5.577448	-0.146357	1.990485
27	1	0	3.296827	0.268634	1.583395
28	1	0	5.156402	-2.525056	-2.061616
29	1	0	5.662695	0.511957	0.936412
30	1	0	2.784226	-2.747803	-1.437294
31	1	0	6.613302	-0.886863	-0.886363
32	1	0	-1.116987	-0.113874	2.299016
33	1	0	1.303081	-3.536620	0.049637
34	1	0	0.331096	-1.643927	3.637302
35	1	0	-1.167671	-2.468485	3.219222
36	1	0	0.049653	-4.121597	2.119182
37	1	0	1.549472	-3.297257	2.533527
38	1	0	-1.031479	-3.176904	-0.754240
39	1	0	1.075199	0.573867	1.399682
40	8	0	0.963152	0.906439	-1.846792
41	1	0	1.871370	1.084310	-1.567329

42	8	0	-1.040485	-0.287273	-2.842451
43	1	0	-0.221423	0.217675	-3.070048
44	1	0	-1.680324	0.424381	-2.648584
45	5	0	-0.783673	2.988761	-1.332188
46	6	0	-0.171322	3.280351	0.083014
47	6	0	1.130485	3.793097	0.191680
48	6	0	-0.884135	3.053459	1.269178
49	6	0	1.704774	4.051784	1.434071
50	1	0	1.697743	3.986019	-0.715370
51	6	0	-0.320682	3.316853	2.518032
52	1	0	-1.907952	2.681108	1.233158
53	6	0	0.979666	3.812372	2.602813
54	1	0	2.717235	4.443889	1.494490
55	1	0	-0.896458	3.141830	3.423732
56	1	0	1.422960	4.018999	3.573887
57	8	0	-0.342112	3.716084	-2.402103
58	1	0	-0.776908	3.428770	-3.216886
59	8	0	-1.882484	2.157514	-1.520064
60	1	0	-2.103926	1.684510	-0.704954

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6019.34235675     A.U. after    1 cycles
            Convg  =    0.4042D-08             -V/T =  2.0045
Zero-point correction=                           0.490329 (Hartree/Particle)
 Thermal correction to Energy=                    0.522111
 Thermal correction to Enthalpy=                  0.523071
 Thermal correction to Gibbs Free Energy=         0.423019
 Sum of electronic and zero-point Energies=          -6018.852028
 Sum of electronic and thermal Energies=             -6018.820245
 Sum of electronic and thermal Enthalpies=           -6018.819285
 Sum of electronic and thermal Free Energies=        -6018.919338
                      1                      2                      3
                      A                      A                      A
 Frequencies --    11.3714                18.3433                24.2280
```

PhBOD-Rh-OH-OH_2-PhB$(OH)_2$-conf3 (15c)

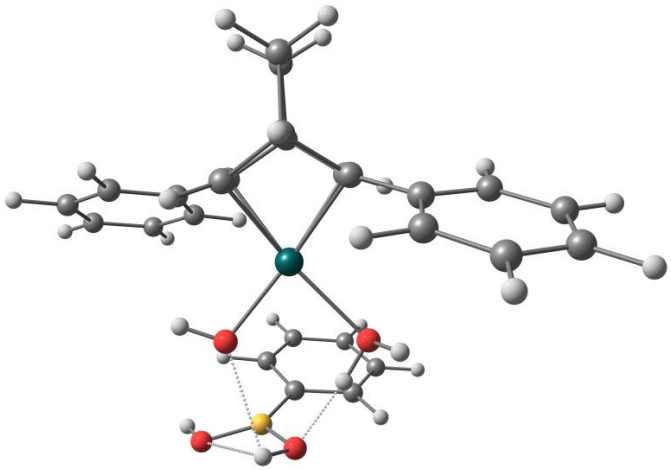


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.961263	-0.225323	0.032045
2	6	0	3.084860	-0.069696	-0.086269
3	6	0	2.158991	1.999750	-1.018733
4	6	0	-0.831196	2.877321	-1.011678
5	6	0	3.856373	-1.332192	-0.120002
6	6	0	4.491189	-1.764569	-1.292941
7	6	0	2.485027	0.530667	-1.212324
8	6	0	3.209416	0.920404	1.073045
9	6	0	4.700329	-3.316169	1.004838
10	6	0	-2.517357	4.132790	0.188048
11	6	0	3.416281	2.791506	-0.601535
12	6	0	1.758266	1.315619	1.274182
13	6	0	5.215207	-2.955244	-1.319608
14	6	0	1.174258	1.922217	0.149043
15	6	0	-0.584969	3.258286	1.349631
16	6	0	3.976445	-2.129110	1.029134
17	6	0	4.056436	2.134030	0.636725
18	6	0	5.324028	-3.736462	-0.171040
19	6	0	-0.085610	2.694451	0.165156
20	6	0	-1.785377	3.964116	1.363126
21	6	0	-2.030759	3.586443	-1.002107
22	1	0	-0.486053	2.434948	-1.942319
23	1	0	-3.454539	4.682226	0.196159
24	1	0	-0.022440	3.150370	2.272601
25	1	0	-2.149080	4.387914	2.295559
26	1	0	-2.593393	3.704927	-1.924565
27	1	0	4.431641	-1.156045	-2.191301
28	1	0	4.771384	-3.922009	1.904533
29	1	0	5.701576	-3.268764	-2.239829
30	1	0	3.471118	-1.829972	1.943868
31	1	0	5.889558	-4.664255	-0.190194
32	1	0	1.705017	2.431424	-1.912148
33	1	0	3.626433	0.449545	1.964960
34	1	0	4.117299	2.812999	-1.442605
35	1	0	3.131261	3.828798	-0.396451
36	1	0	4.117468	2.840581	1.470990
37	1	0	5.077760	1.800057	0.425047
38	1	0	1.329746	1.369756	2.272036
39	1	0	2.524216	0.088647	-2.205421
40	8	0	0.552816	-2.065731	-0.701629
41	1	0	1.338345	-2.563588	-0.965740
42	8	0	-0.976202	-0.821124	0.935865
43	1	0	-0.922498	-1.674900	0.450661
44	1	0	-1.769194	-0.345049	0.611014
45	5	0	-4.423586	0.269982	-0.491268
46	6	0	-5.029374	-1.129140	-0.143624
47	6	0	-4.575377	-1.839485	0.979568
48	6	0	-6.032847	-1.718225	-0.929577
49	6	0	-5.107493	-3.083435	1.309920
50	1	0	-3.798819	-1.408870	1.606781
51	6	0	-6.565190	-2.965179	-0.609835
52	1	0	-6.400452	-1.215988	-1.823992
53	6	0	-6.103713	-3.648898	0.514480
54	1	0	-4.743473	-3.614728	2.185420
55	1	0	-7.335765	-3.405985	-1.236890
56	1	0	-6.517226	-4.621805	0.767524
57	8	0	-3.233101	0.642268	0.090828
58	1	0	-2.967445	1.540368	-0.177059
59	8	0	-5.004833	1.174717	-1.343789
60	1	0	-5.867866	0.879192	-1.660251

```
 ---------------------------------------------------------------------

 SCF Done:  E(RPBE1PBE) =  -6019.34620848     A.U. after    1 cycles
            Convg  =    0.1544D-08             -V/T =  2.0045
Zero-point correction=                          0.490439 (Hartree/Particle)
 Thermal correction to Energy=                  0.522177
 Thermal correction to Enthalpy=                0.523137
 Thermal correction to Gibbs Free Energy=       0.421577
 Sum of electronic and zero-point Energies=          -6018.855769
 Sum of electronic and thermal Energies=             -6018.824032
 Sum of electronic and thermal Enthalpies=           -6018.823072
 Sum of electronic and thermal Free Energies=        -6018.924632
                     1                      2                      3
                     A                      A                      A
 Frequencies --     8.8608                15.6322                16.5993
```

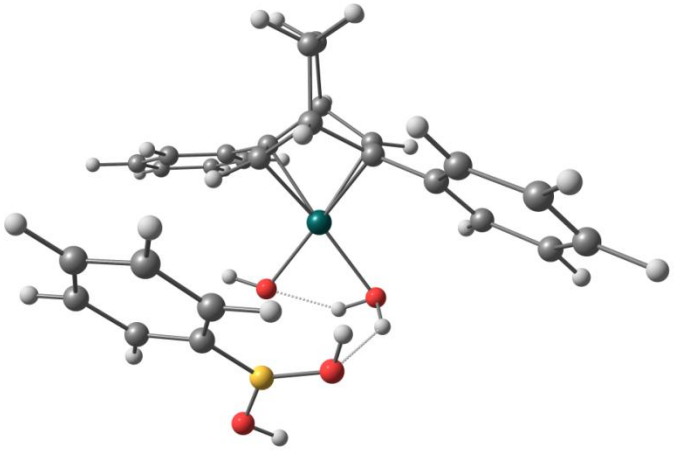
PhBOD-Rh-OH-PhB(OH)$_2$-OH$_2$-TS-conf1 (16a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.567431	0.112009	-0.460732
2	6	0	-0.231585	2.092042	0.257283
3	6	0	-2.629263	1.881022	-0.213667
4	6	0	-4.109698	-0.758443	-1.019182
5	6	0	1.124282	2.663569	0.095697
6	6	0	1.371020	3.697520	-0.818274
7	6	0	-1.223110	2.091210	-0.745959
8	6	0	-0.836590	1.835849	1.639032
9	6	0	3.472443	2.727347	0.721323
10	6	0	-5.384700	-2.628381	-0.169119
11	6	0	-2.968373	2.933864	0.862789
12	6	0	-1.500308	0.489550	1.420873
13	6	0	2.648520	4.235436	-0.965701
14	6	0	-2.492719	0.498615	0.426127
15	6	0	-3.860072	-1.431333	1.276840
16	6	0	2.198544	2.188416	0.864009
17	6	0	-1.883559	2.923047	1.959580
18	6	0	3.705204	3.754186	-0.195644
19	6	0	-3.498775	-0.567357	0.231641
20	6	0	-4.788930	-2.450375	1.078748
21	6	0	-5.039641	-1.774886	-1.217795
22	1	0	-3.835018	-0.118047	-1.853606
23	1	0	-6.111707	-3.421339	-0.322711
24	1	0	-3.418838	-1.296345	2.260434

```
     25          1           0       -5.054178   -3.103680    1.906193
     26          1           0       -5.493884   -1.904508   -2.196935
     27          1           0        0.551381    4.097717   -1.409146
     28          1           0        4.290573    2.340847    1.324184
     29          1           0        2.815376    5.039481   -1.678005
     30          1           0        2.038470    1.367011    1.557700
     31          1           0        4.700783    4.175840   -0.306354
     32          1           0       -3.368852    1.890466   -1.016006
     33          1           0       -0.068796    1.786139    2.413150
     34          1           0       -3.037591    3.918149    0.387578
     35          1           0       -3.955933    2.710176    1.279789
     36          1           0       -2.319289    2.716556    2.942685
     37          1           0       -1.381388    3.893865    2.029405
     38          1           0       -1.391511   -0.312086    2.147328
     39          1           0       -1.053691    2.498198   -1.740604
     40          8           0        0.868370   -0.098103   -1.866651
     41          1           0        1.298763    0.744983   -2.066234
     42          8           0       -0.537346   -2.108135   -0.466195
     43          1           0        0.195389   -2.371208   -1.075027
     44          1           0       -1.353409   -2.497066   -0.813880
     45          5           0        2.744261   -2.106331   -1.614227
     46          6           0        3.138288   -2.383483   -0.121280
     47          6           0        2.557031   -3.448208    0.584103
     48          6           0        4.078500   -1.590654    0.555505
     49          6           0        2.907030   -3.719722    1.904957
     50          1           0        1.820549   -4.076377    0.089205
     51          6           0        4.428386   -1.848427    1.879369
     52          1           0        4.536912   -0.736736    0.057405
     53          6           0        3.844436   -2.918977    2.556466
     54          1           0        2.446950   -4.553649    2.429221
     55          1           0        5.154888   -1.216448    2.384322
     56          1           0        4.117226   -3.125795    3.588357
     57          8           0        1.605794   -2.707359   -2.130953
     58          1           0        1.347643   -2.173280   -2.902043
     59          8           0        3.543400   -1.417280   -2.490441
     60          1           0        4.342380   -1.083185   -2.064750
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6019.34074062     A.U. after    1 cycles
             Convg  =    0.3044D-08             -V/T =  2.0045
Zero-point correction=                           0.489700 (Hartree/Particle)
 Thermal correction to Energy=                    0.520804
 Thermal correction to Enthalpy=                  0.521764
 Thermal correction to Gibbs Free Energy=         0.422773
 Sum of electronic and zero-point Energies=          -6018.851041
 Sum of electronic and thermal Energies=             -6018.819937
 Sum of electronic and thermal Enthalpies=           -6018.818977
 Sum of electronic and thermal Free Energies=        -6018.917967
                     1                      2                      3
                     A                      A                      A
 Frequencies --  -105.8320               11.4032                15.5517
```

PhBOD-Rh-OH-PhB(OH)$_2$-OH$_2$-TS-conf2 (16b)

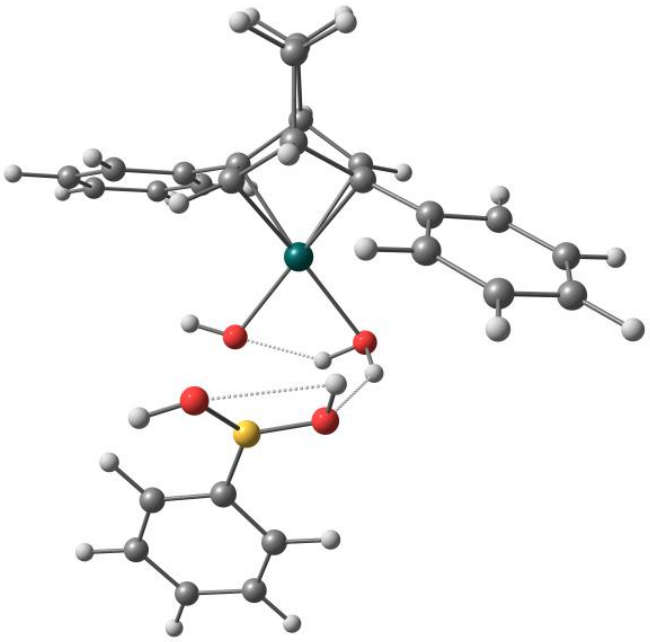


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.059018	-0.550289	-0.837725
2	6	0	1.320658	-1.478351	0.501780
3	6	0	-0.681970	-0.920472	1.805815
4	6	0	-3.681965	-0.579904	1.378907
5	6	0	2.749828	-1.402363	0.126856
6	6	0	3.629457	-0.534394	0.789591
7	6	0	0.608873	-0.454152	1.157950
8	6	0	0.565179	-2.804824	0.566319
9	6	0	4.600717	-2.128005	-1.273285
10	6	0	-5.611672	-0.549253	-0.077923
11	6	0	-0.410468	-2.086428	2.779569
12	6	0	-0.749077	-2.427140	-0.092240
13	6	0	4.972339	-0.461653	0.425287
14	6	0	-1.449969	-1.410304	0.580842
15	6	0	-3.477125	-1.339351	-0.895324
16	6	0	3.260522	-2.199454	-0.909246
17	6	0	0.343838	-3.209836	2.039896
18	6	0	5.464732	-1.257824	-0.607184
19	6	0	-2.877354	-1.102223	0.355093
20	6	0	-4.823525	-1.067257	-1.107691
21	6	0	-5.032929	-0.308782	1.165773
22	1	0	-3.260550	-0.398626	2.363579
23	1	0	-6.663383	-0.333857	-0.245852
24	1	0	-2.873532	-1.720690	-1.714667
25	1	0	-5.260267	-1.253880	-2.085508
26	1	0	-5.634714	0.089360	1.978803
27	1	0	3.263864	0.081528	1.606612
28	1	0	4.972062	-2.747596	-2.085435
29	1	0	5.637309	0.215565	0.955135
30	1	0	2.593599	-2.860466	-1.456502
31	1	0	6.512205	-1.201771	-0.891051
32	1	0	-1.179678	-0.086452	2.303281
33	1	0	1.077305	-3.595218	0.015289
34	1	0	0.173631	-1.712847	3.627091
35	1	0	-1.362123	-2.450428	3.181169
36	1	0	-0.221606	-4.146939	2.065255
37	1	0	1.315106	-3.408406	2.504984
38	1	0	-1.228660	-3.098740	-0.800805
39	1	0	1.054915	0.499596	1.430312
40	8	0	1.010430	0.876409	-1.809405
41	1	0	1.929589	0.965623	-1.522462
42	8	0	-1.042843	-0.188070	-2.856431

43	1	0	-0.177837	0.239835	-3.070503
44	1	0	-1.612893	0.583952	-2.676814
45	5	0	-0.442400	3.039909	-1.344915
46	6	0	0.123015	3.265115	0.103781
47	6	0	1.460017	3.652413	0.281906
48	6	0	-0.664429	3.098443	1.252186
49	6	0	1.995883	3.843263	1.553329
50	1	0	2.085353	3.801749	-0.594645
51	6	0	-0.139653	3.294471	2.530035
52	1	0	-1.716367	2.826126	1.165228
53	6	0	1.196552	3.661384	2.683370
54	1	0	3.036605	4.137574	1.666741
55	1	0	-0.772619	3.166086	3.404883
56	1	0	1.610570	3.813983	3.677092
57	8	0	0.123629	3.727684	-2.383493
58	1	0	-0.297910	3.490950	-3.221047
59	8	0	-1.632483	2.356673	-1.584706
60	1	0	-1.950866	1.927186	-0.778041

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6019.34236619     A.U. after    1 cycles
            Convg  =    0.1563D-08             -V/T =  2.0045
Zero-point correction=                          0.490224 (Hartree/Particle)
 Thermal correction to Energy=                  0.521095
 Thermal correction to Enthalpy=                0.522055
 Thermal correction to Gibbs Free Energy=       0.425707
 Sum of electronic and zero-point Energies=         -6018.852142
 Sum of electronic and thermal Energies=            -6018.821271
 Sum of electronic and thermal Enthalpies=          -6018.820311
 Sum of electronic and thermal Free Energies=       -6018.916659
                     1                      2                      3
                     A                      A                      A
 Frequencies --   -30.5422               18.8466                25.2700
```

PhBOD-Rh-OH-PhB(OH)$_2$-OH$_2$-TS-conf3 (16c)



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

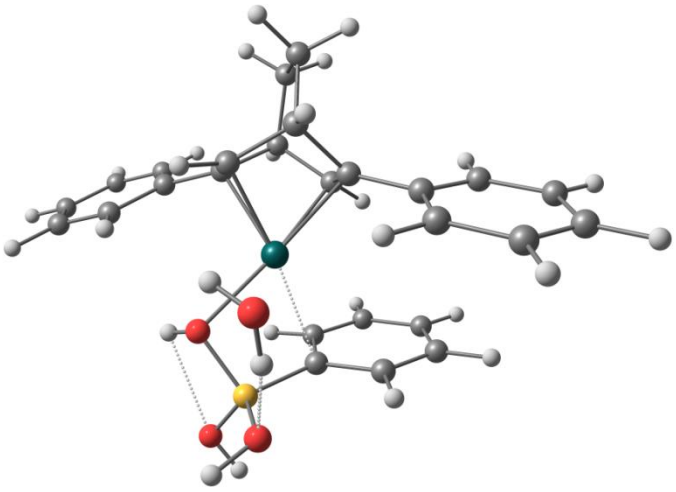
1	45	0	0.513884	0.046463	-0.452639
2	6	0	1.851902	1.595100	0.148960
3	6	0	2.475162	-0.419404	1.397383
4	6	0	1.382134	-3.284904	1.082754
5	6	0	1.377939	2.987749	-0.007940
6	6	0	1.060784	3.774781	1.108007
7	6	0	1.538843	0.764240	1.243467
8	6	0	3.044622	1.051042	-0.639576
9	6	0	0.797112	4.867731	-1.435693
10	6	0	1.381858	-5.360922	-0.155683
11	6	0	3.943157	0.047145	1.487201
12	6	0	2.534672	-0.325324	-1.024454
13	6	0	0.615046	5.086549	0.955961
14	6	0	2.229560	-1.147422	0.074758
15	6	0	2.257926	-3.340071	-1.154809
16	6	0	1.241336	3.558905	-1.282462
17	6	0	4.277806	0.946917	0.281969
18	6	0	0.481043	5.639153	-0.316184
19	6	0	1.966727	-2.600449	0.002680
20	6	0	1.968852	-4.698772	-1.233642
21	6	0	1.092548	-4.645012	1.004908
22	1	0	1.146313	-2.753196	2.000883
23	1	0	1.156450	-6.421929	-0.218296
24	1	0	2.723848	-2.850021	-2.004422
25	1	0	2.207127	-5.245174	-2.142607
26	1	0	0.637883	-5.146053	1.855722
27	1	0	1.181056	3.362789	2.106497
28	1	0	0.688849	5.286412	-2.432875
29	1	0	0.380089	5.680859	1.835353
30	1	0	1.458098	2.960432	-2.163735
31	1	0	0.134580	6.662162	-0.435859
32	1	0	2.210133	-1.024685	2.264338
33	1	0	3.259812	1.659773	-1.519577
34	1	0	4.086018	0.583849	2.430912
35	1	0	4.594238	-0.832690	1.517911
36	1	0	5.114980	0.539728	-0.294150
37	1	0	4.569644	1.951912	0.604627
38	1	0	2.662768	-0.697583	-2.037409
39	1	0	0.893431	1.081250	2.059482
40	8	0	-1.356420	0.826753	-0.302662
41	1	0	-1.396495	1.740608	0.011058
42	8	0	-0.772775	-1.055159	-1.944017
43	1	0	-1.408072	-0.309711	-1.835308
44	1	0	-1.179321	-1.746883	-1.384373
45	5	0	-2.592779	-0.990601	1.043907
46	6	0	-3.971447	-0.499232	0.477127
47	6	0	-4.682064	-1.286678	-0.440046
48	6	0	-4.557713	0.706807	0.889864
49	6	0	-5.927150	-0.888962	-0.926177
50	1	0	-4.253221	-2.228993	-0.772791
51	6	0	-5.799967	1.114127	0.409651
52	1	0	-4.030488	1.362927	1.582083
53	6	0	-6.490013	0.313365	-0.501204
54	1	0	-6.460019	-1.517322	-1.635813
55	1	0	-6.229921	2.056802	0.739391
56	1	0	-7.460213	0.626988	-0.878469
57	8	0	-1.965461	-2.057015	0.414451
58	1	0	-1.194310	-2.340660	0.929756
59	8	0	-2.099502	-0.634915	2.280965
60	1	0	-2.644930	0.044521	2.696046

SCF Done: E(RPBE1PBE) = -6019.34143123 A.U. after 1 cycles
Convg = 0.4311D-08 -V/T = 2.0045
Zero-point correction= 0.490056 (Hartree/Particle)

Thermal correction to Energy=	0.520989
Thermal correction to Enthalpy=	0.521949
Thermal correction to Gibbs Free Energy=	0.424785
Sum of electronic and zero-point Energies=	-6018.851376
Sum of electronic and thermal Energies=	-6018.820442
Sum of electronic and thermal Enthalpies=	-6018.819482
Sum of electronic and thermal Free Energies=	-6018.916646

	1	2	3
	A	A	A
Frequencies --	-64.9525	16.2819	22.7493

PhBOD-Rh-PhB(OH)$_3$-OH$_2$-conf1 (17a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.231424	0.240351	-0.049579
2	6	0	-1.737887	-1.312210	-0.092667
3	6	0	0.242562	-2.165185	-1.272119
4	6	0	3.062826	-0.723165	-1.370120
5	6	0	-3.144381	-0.871113	0.019039
6	6	0	-3.714600	-0.025725	-0.950527
7	6	0	-0.995958	-1.295625	-1.295510
8	6	0	-1.052025	-2.178525	0.957604
9	6	0	-5.290072	-0.884464	1.170751
10	6	0	5.285931	-1.085388	-0.486230
11	6	0	-0.121899	-3.618244	-0.893199
12	6	0	0.309160	-1.513108	1.054732
13	6	0	-5.038494	0.385096	-0.856410
14	6	0	1.040287	-1.532324	-0.137324
15	6	0	3.355494	-1.852925	0.744434
16	6	0	-3.960628	-1.291908	1.079156
17	6	0	-0.903207	-3.624999	0.434747
18	6	0	-5.836225	-0.041261	0.206922
19	6	0	2.503382	-1.353873	-0.248852
20	6	0	4.737567	-1.721586	0.626220
21	6	0	4.442917	-0.585517	-1.480594
22	1	0	2.413371	-0.292174	-2.131503
23	1	0	6.363850	-0.980901	-0.579678
24	1	0	2.934139	-2.359217	1.609223
25	1	0	5.386441	-2.120262	1.401951
26	1	0	4.862541	-0.079443	-2.346252
27	1	0	-3.112109	0.327052	-1.782565
28	1	0	-5.899804	-1.229959	2.001433

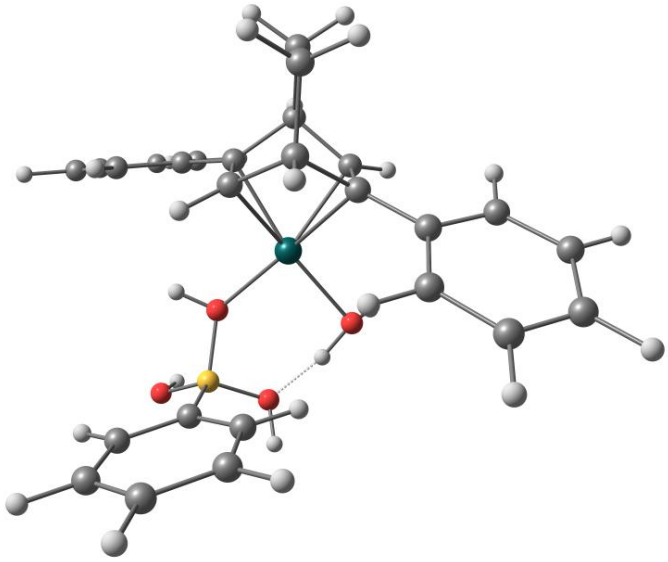
29	1	0	-5.450315	1.044290	-1.616065
30	1	0	-3.568389	-1.955239	1.843556
31	1	0	-6.871157	0.281068	0.280849
32	1	0	0.783898	-2.119181	-2.217964
33	1	0	-1.559907	-2.149247	1.921420
34	1	0	-0.715423	-4.053290	-1.703485
35	1	0	0.797745	-4.207123	-0.817028
36	1	0	-0.386144	-4.221030	1.193646
37	1	0	-1.898465	-4.062974	0.306454
38	1	0	0.766356	-1.303147	2.018660
39	1	0	-1.435354	-0.991743	-2.242817
40	8	0	-1.183784	1.952973	-0.887713
41	1	0	-2.046868	2.157686	-0.496538
42	8	0	0.926362	1.212499	-3.202836
43	1	0	0.964844	2.015321	-2.633004
44	1	0	0.026611	0.895525	-3.046378
45	5	0	-0.177471	3.010131	-0.397349
46	8	0	0.667917	3.417085	-1.514325
47	1	0	0.167430	4.066824	-2.027814
48	8	0	-1.014904	4.067797	0.137934
49	1	0	-0.469562	4.699561	0.622586
50	6	0	0.754299	2.244695	0.719879
51	6	0	0.173537	1.817433	1.939794
52	6	0	2.152853	2.088263	0.593493
53	6	0	0.955001	1.317739	2.991100
54	1	0	-0.890648	1.979968	2.106355
55	6	0	2.931709	1.588697	1.631198
56	1	0	2.625055	2.397460	-0.335204
57	6	0	2.333342	1.209009	2.837606
58	1	0	0.484118	1.032113	3.929096
59	1	0	4.006274	1.485976	1.502800
60	1	0	2.945208	0.830090	3.652827

SCF Done: E(RPBE1PBE) = -6019.36118094 A.U. after 1 cycles
Convg = 0.1585D-08 -V/T = 2.0046

Zero-point correction= 0.490255 (Hartree/Particle)
Thermal correction to Energy= 0.521697
Thermal correction to Enthalpy= 0.522657
Thermal correction to Gibbs Free Energy= 0.426530
Sum of electronic and zero-point Energies= -6018.870926
Sum of electronic and thermal Energies= -6018.839484
Sum of electronic and thermal Enthalpies= -6018.838524
Sum of electronic and thermal Free Energies= -6018.934651

	1	2	3
	A	A	A
Frequencies --	20.1101	26.8028	33.7541

PhBOD-Rh-PhB(OH)$_3$-OH$_2$-conf2 (17b)



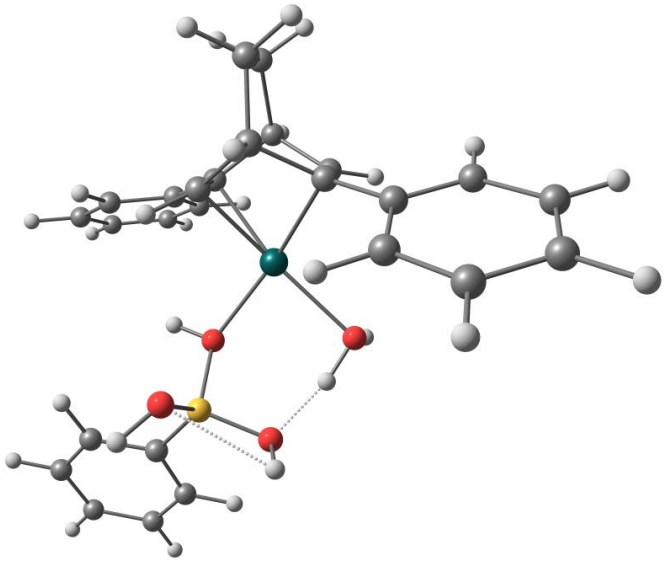
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.033913	-0.430863	-0.616704
2	6	0	1.140450	-1.781382	0.555775
3	6	0	-0.995211	-1.458052	1.722261
4	6	0	-3.490980	0.087498	0.633595
5	6	0	2.604739	-1.692535	0.365825
6	6	0	3.419717	-1.035925	1.300398
7	6	0	0.387241	-0.933290	1.389816
8	6	0	0.335405	-3.017986	0.156539
9	6	0	4.589392	-2.148946	-0.963702
10	6	0	-5.636831	-0.241599	-0.426661
11	6	0	-0.912960	-2.868318	2.343310
12	6	0	-0.865284	-2.377889	-0.517131
13	6	0	4.795064	-0.932772	1.103993
14	6	0	-1.615672	-1.541229	0.327963
15	6	0	-3.861016	-1.847682	-0.749186
16	6	0	3.216165	-2.249234	-0.768473
17	6	0	-0.096821	-3.793057	1.420031
18	6	0	5.386721	-1.488867	-0.028424
19	6	0	-3.001080	-1.097201	0.064174
20	6	0	-5.165134	-1.424281	-0.993587
21	6	0	-4.792642	0.512155	0.389118
22	1	0	-2.837890	0.697298	1.253021
23	1	0	-6.654458	0.089163	-0.616072
24	1	0	-3.514324	-2.782960	-1.180846
25	1	0	-5.817648	-2.024728	-1.622260
26	1	0	-5.149083	1.438310	0.832589
27	1	0	2.979413	-0.613780	2.199449
28	1	0	5.038952	-2.580442	-1.854134
29	1	0	5.405871	-0.420280	1.842346
30	1	0	2.609006	-2.743941	-1.521768
31	1	0	6.459382	-1.408886	-0.181746
32	1	0	-1.540209	-0.770570	2.370262
33	1	0	0.885653	-3.663731	-0.528966
34	1	0	-0.452408	-2.792532	3.333450
35	1	0	-1.928532	-3.249541	2.490571
36	1	0	-0.684618	-4.664502	1.114308
37	1	0	0.797051	-4.171467	1.926381

38	1	0	-1.252604	-2.767854	-1.455987
39	1	0	0.824329	-0.116570	1.959590
40	8	0	1.442930	1.053903	-0.990994
41	1	0	2.236987	0.956660	-0.446195
42	8	0	-1.086112	0.448665	-2.315077
43	1	0	-1.067381	-0.083412	-3.123107
44	1	0	-0.559683	1.303103	-2.498165
45	5	0	1.262732	2.560371	-1.258403
46	6	0	0.570537	3.292360	0.011060
47	6	0	1.313484	4.088723	0.895643
48	6	0	-0.796602	3.137096	0.293894
49	6	0	0.731062	4.689637	2.013244
50	1	0	2.370784	4.245448	0.692620
51	6	0	-1.393486	3.735531	1.405041
52	1	0	-1.416461	2.537415	-0.372560
53	6	0	-0.628252	4.513914	2.274213
54	1	0	1.335468	5.302619	2.679147
55	1	0	-2.458159	3.603324	1.590389
56	1	0	-1.087926	4.985048	3.140135
57	8	0	2.561270	3.131440	-1.518572
58	1	0	2.868243	2.778799	-2.364929
59	8	0	0.384253	2.533805	-2.469113
60	1	0	-0.024117	3.402442	-2.576147

SCF Done: E(RPBE1PBE) = -6019.36768049 A.U. after 1 cycles
Convg = 0.1476D-08 -V/T = 2.0045
Zero-point correction= 0.491155 (Hartree/Particle)
Thermal correction to Energy= 0.521733
Thermal correction to Enthalpy= 0.522693
Thermal correction to Gibbs Free Energy= 0.426796
Sum of electronic and zero-point Energies= -6018.876526
Sum of electronic and thermal Energies= -6018.845947
Sum of electronic and thermal Enthalpies= -6018.844987
Sum of electronic and thermal Free Energies= -6018.940884

	1	2	3
	A	A	A
Frequencies --	12.4101	18.9589	29.8989

PhBOD-Rh-PhB(OH)$_3$-OH$_2$-conf3 (17c)



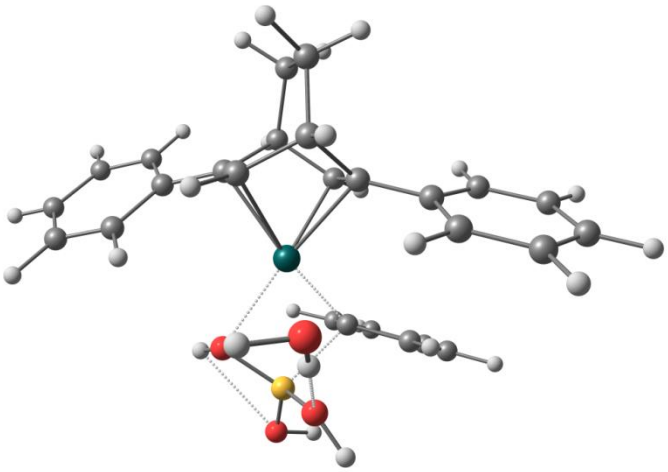
Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	45	0	0.633009	0.023092	-0.412070
2	6	0	0.561464	2.081155	0.164703
3	6	0	2.354806	1.016342	1.454446
4	6	0	3.353335	-1.931981	1.042024
5	6	0	-0.737945	2.755837	-0.043665
6	6	0	-1.595514	3.028405	1.032765
7	6	0	0.873044	1.272870	1.273302
8	6	0	1.821572	2.468919	-0.610556
9	6	0	-2.384477	3.741229	-1.537364
10	6	0	5.178753	-3.187857	0.079636
11	6	0	3.134638	2.345524	1.539934
12	6	0	2.373592	1.100763	-0.970214
13	6	0	-2.828566	3.643462	0.827481
14	6	0	2.687174	0.303891	0.144098
15	6	0	4.573742	-1.032845	-0.829431
16	6	0	-1.154113	3.126174	-1.332010
17	6	0	2.795537	3.223940	0.320117
18	6	0	-3.228919	4.002836	-0.458082
19	6	0	3.546279	-0.898642	0.113295
20	6	0	5.382710	-2.166595	-0.846584
21	6	0	4.158840	-3.065562	1.023915
22	1	0	2.546304	-1.860366	1.767227
23	1	0	5.809862	-4.072466	0.066779
24	1	0	4.753500	-0.235926	-1.546451
25	1	0	6.178897	-2.249324	-1.581962
26	1	0	3.986546	-3.860095	1.745267
27	1	0	-1.289540	2.772306	2.043380
28	1	0	-2.690494	4.009654	-2.545013
29	1	0	-3.475369	3.847669	1.676650
30	1	0	-0.520155	2.905620	-2.186811
31	1	0	-4.191083	4.481217	-0.618805
32	1	0	2.552260	0.384166	2.321142
33	1	0	1.590591	3.058107	-1.499359
34	1	0	2.871926	2.850499	2.474966
35	1	0	4.206038	2.125098	1.585186
36	1	0	3.697095	3.478900	-0.246079
37	1	0	2.332600	4.167512	0.626769
38	1	0	2.747805	0.888581	-1.969277
39	1	0	0.165082	1.057895	2.069943
40	8	0	-1.429326	-0.515194	-0.268853
41	1	0	-1.991035	0.203004	0.054893
42	8	0	0.769481	-1.749768	-1.695901
43	1	0	0.521114	-1.538658	-2.607996
44	1	0	-0.010731	-2.281375	-1.307104
45	5	0	-1.892771	-1.830554	0.352544
46	6	0	-3.509758	-1.911741	0.242433
47	6	0	-4.141467	-2.710126	-0.722153
48	6	0	-4.343671	-1.175641	1.101643
49	6	0	-5.531292	-2.775712	-0.828056
50	1	0	-3.519880	-3.296279	-1.395671
51	6	0	-5.735590	-1.227855	1.004808
52	1	0	-3.899530	-0.541598	1.870509
53	6	0	-6.335777	-2.031793	0.036095
54	1	0	-5.990821	-3.408717	-1.584671
55	1	0	-6.352782	-0.644935	1.685577
56	1	0	-7.419376	-2.080060	-0.042970
57	8	0	-1.208628	-2.855722	-0.490465
58	1	0	-0.893290	-3.536525	0.118017
59	8	0	-1.409717	-1.911419	1.726932
60	1	0	-2.121930	-2.223428	2.297126

SCF Done: E(RPBE1PBE) = -6019.36536131   A.U. after   1 cycles

```
            Convg  =    0.3253D-08             -V/T =  2.0045
Zero-point correction=                           0.490873 (Hartree/Particle)
 Thermal correction to Energy=                   0.521654
 Thermal correction to Enthalpy=                 0.522614
 Thermal correction to Gibbs Free Energy=        0.425822
 Sum of electronic and zero-point Energies=         -6018.874488
 Sum of electronic and thermal Energies=            -6018.843708
 Sum of electronic and thermal Enthalpies=          -6018.842748
 Sum of electronic and thermal Free Energies=       -6018.939539
                     1                      2                      3
                     A                      A                      A
 Frequencies --    15.6806                19.1025                28.6698
```

PhBOD-Rh-Ph-B(OH)$_3$-OH$_2$-TS-conf1 (18a)



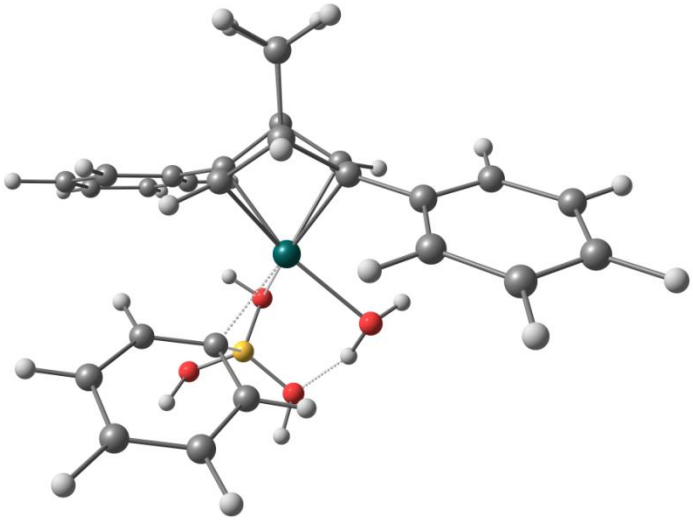
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.319671	0.250876	0.148337
2	6	0	2.007918	-1.119582	-0.213688
3	6	0	0.161055	-2.443664	0.682579
4	6	0	-2.790987	-1.604384	1.209002
5	6	0	3.344261	-0.488560	-0.208934
6	6	0	3.788025	0.244244	0.906582
7	6	0	1.327328	-1.516315	0.938694
8	6	0	1.366702	-1.705288	-1.468242
9	6	0	5.488557	-0.045098	-1.272446
10	6	0	-5.001039	-1.779974	0.241007
11	6	0	0.638101	-3.691205	-0.098337
12	6	0	-0.055866	-1.180768	-1.371715
13	6	0	5.052732	0.819575	0.929997
14	6	0	-0.740307	-1.608343	-0.222143
15	6	0	-3.049129	-1.779846	-1.182069
16	6	0	4.218462	-0.619297	-1.297287
17	6	0	1.364969	-3.249046	-1.383799
18	6	0	5.912752	0.678744	-0.161099
19	6	0	-2.208930	-1.656632	-0.067265
20	6	0	-4.432097	-1.840021	-1.030532
21	6	0	-4.173521	-1.661407	1.358785
22	1	0	-2.160720	-1.479257	2.087154
23	1	0	-6.080400	-1.828081	0.360613
24	1	0	-2.617650	-1.837577	-2.177616
25	1	0	-5.066518	-1.938569	-1.907787
26	1	0	-4.606274	-1.607970	2.354597
27	1	0	3.125467	0.379039	1.757154

28	1	0	6.148708	-0.167458	-2.127266
29	1	0	5.369061	1.385514	1.802588
30	1	0	3.918932	-1.188478	-2.172369
31	1	0	6.901192	1.129732	-0.143264
32	1	0	-0.339099	-2.721741	1.610427
33	1	0	1.845220	-1.351224	-2.382218
34	1	0	1.299312	-4.278211	0.547026
35	1	0	-0.228848	-4.319447	-0.327581
36	1	0	0.870562	-3.650456	-2.274458
37	1	0	2.397993	-3.612281	-1.398210
38	1	0	-0.567275	-0.796933	-2.251109
39	1	0	1.744249	-1.412834	1.937101
40	8	0	1.000536	1.910998	1.383892
41	1	0	1.636022	2.461984	0.902196
42	8	0	-1.018117	-0.344578	3.784774
43	1	0	-1.064354	0.470287	3.244987
44	1	0	-0.210292	-0.247230	4.305711
45	5	0	-0.308130	2.505257	1.247269
46	8	0	-1.170889	2.046941	2.268805
47	1	0	-1.894641	2.670990	2.403188
48	8	0	-0.262513	3.873488	0.911247
49	1	0	-0.971162	4.115962	0.303033
50	6	0	-1.110218	1.731149	-0.530747
51	6	0	-0.644981	2.383549	-1.695881
52	6	0	-2.505944	1.626999	-0.389754
53	6	0	-1.514358	2.890674	-2.660299
54	1	0	0.425811	2.517928	-1.845967
55	6	0	-3.388327	2.145769	-1.338755
56	1	0	-2.912412	1.134425	0.490992
57	6	0	-2.895091	2.776156	-2.480724
58	1	0	-1.119085	3.384555	-3.545536
59	1	0	-4.461726	2.051956	-1.188988
60	1	0	-3.579163	3.180323	-3.223251

SCF Done: E(RPBE1PBE) = -6019.33897699   A.U. after   1 cycles
             Convg =   0.3020D-08   -V/T = 2.0046
Zero-point correction=   0.488139 (Hartree/Particle)
 Thermal correction to Energy=   0.519956
 Thermal correction to Enthalpy=   0.520916
 Thermal correction to Gibbs Free Energy=   0.423783
 Sum of electronic and zero-point Energies=   -6018.850838
 Sum of electronic and thermal Energies=   -6018.819021
 Sum of electronic and thermal Enthalpies=   -6018.818061
 Sum of electronic and thermal Free Energies=   -6018.915194

	1	2	3
	A	A	A
Frequencies --	-247.1817	18.2004	28.3485

PhBOD-Rh-Ph-B(OH)$_3$-OH$_2$-TS-conf2 (18b)

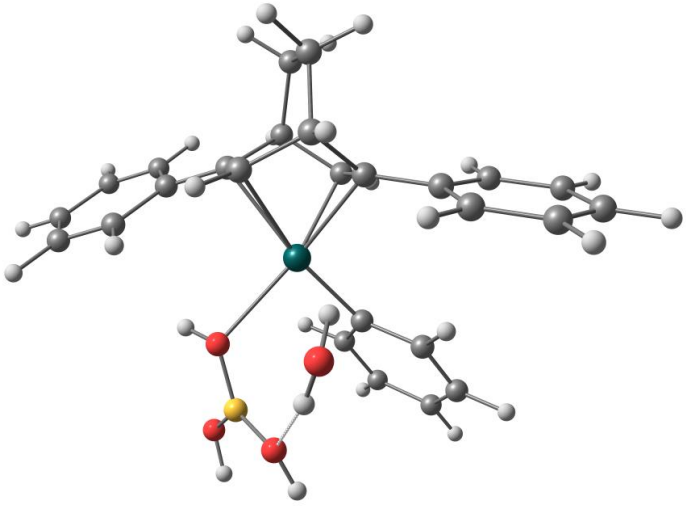


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.241556	0.075001	-0.421995
2	6	0	0.920399	-1.599652	0.317085
3	6	0	-1.191550	-1.552470	1.560999
4	6	0	-3.641883	0.315009	0.949868
5	6	0	2.392607	-1.602218	0.178322
6	6	0	3.229221	-1.397302	1.285004
7	6	0	0.200427	-0.986162	1.361493
8	6	0	0.075912	-2.659724	-0.389847
9	6	0	4.381342	-1.863177	-1.203042
10	6	0	-5.823933	0.291520	-0.088564
11	6	0	-1.136652	-3.078844	1.780197
12	6	0	-1.111589	-1.839583	-0.848196
13	6	0	4.615476	-1.416198	1.150152
14	6	0	-1.822970	-1.239698	0.208150
15	6	0	-4.101269	-1.226974	-0.840376
16	6	0	2.996477	-1.850477	-1.065584
17	6	0	-0.357626	-3.739023	0.625769
18	6	0	5.199125	-1.642054	-0.094924
19	6	0	-3.200129	-0.710889	0.100854
20	6	0	-5.400021	-0.730225	-0.935748
21	6	0	-4.937232	0.811270	0.855863
22	1	0	-2.952940	0.748712	1.670416
23	1	0	-6.836853	0.678513	-0.160651
24	1	0	-3.791197	-2.041069	-1.490578
25	1	0	-6.084957	-1.150340	-1.667931
26	1	0	-5.255919	1.612652	1.517517
27	1	0	2.790990	-1.235805	2.265934
28	1	0	4.822913	-2.043079	-2.179723
29	1	0	5.242159	-1.257660	2.024035
30	1	0	2.375900	-2.032074	-1.939868
31	1	0	6.280417	-1.652113	-0.200793
32	1	0	-1.715202	-1.052967	2.377392
33	1	0	0.604487	-3.106547	-1.233000
34	1	0	-0.659983	-3.280651	2.745124
35	1	0	-2.158977	-3.466334	1.841578
36	1	0	-0.973503	-4.482137	0.108628
37	1	0	0.531876	-4.261069	0.994137
38	1	0	-1.520038	-1.955926	-1.849745
39	1	0	0.676850	-0.393235	2.137083

40	8	0	1.513481	0.756236	-2.344483
41	1	0	2.302050	0.279744	-2.049684
42	8	0	-1.509029	1.307854	-1.761089
43	1	0	-1.873610	0.800806	-2.500893
44	1	0	-0.869457	1.973824	-2.144438
45	5	0	1.507375	2.014057	-1.699967
46	6	0	0.802605	1.935232	0.288913
47	6	0	1.874675	1.861808	1.207256
48	6	0	-0.222240	2.842978	0.635172
49	6	0	1.934424	2.634613	2.364528
50	1	0	2.708210	1.196369	0.989088
51	6	0	-0.188818	3.616965	1.799723
52	1	0	-1.086107	2.952660	-0.019258
53	6	0	0.894382	3.517605	2.669804
54	1	0	2.791218	2.552940	3.031043
55	1	0	-1.007676	4.297842	2.024375
56	1	0	0.933205	4.122021	3.573165
57	8	0	2.795805	2.539660	-1.451201
58	1	0	2.785160	3.212663	-0.760352
59	8	0	0.507424	2.851848	-2.308612
60	1	0	0.525723	3.738161	-1.927151

```
SCF Done:  E(RPBE1PBE) =  -6019.33015301     A.U. after    1 cycles
             Convg  =    0.1549D-08             -V/T =  2.0046
Zero-point correction=                           0.489791 (Hartree/Particle)
 Thermal correction to Energy=                    0.520291
 Thermal correction to Enthalpy=                  0.521251
 Thermal correction to Gibbs Free Energy=         0.428267
 Sum of electronic and zero-point Energies=          -6018.840362
 Sum of electronic and thermal Energies=             -6018.809862
 Sum of electronic and thermal Enthalpies=           -6018.808902
 Sum of electronic and thermal Free Energies=        -6018.901886
                     1                      2                      3
                     A                      A                      A
 Frequencies --  -288.1092               25.9898                35.9459
```

PhBOD-Rh-Ph-B(OH)$_3$-OH$_2$- (19)



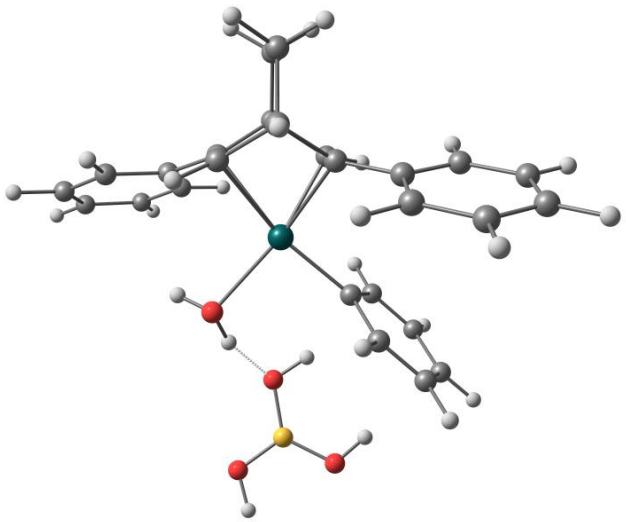
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.186961	0.097647	0.050707
2	6	0	1.755360	-1.567421	-0.063327
3	6	0	-0.254506	-2.507349	0.940451

4	6	0	-3.163175	-1.504402	1.300151
5	6	0	3.142161	-1.060039	-0.129981
6	6	0	3.728274	-0.406843	0.972167
7	6	0	1.039711	-1.743288	1.105409
8	6	0	1.023523	-2.173440	-1.259536
9	6	0	5.235401	-0.733338	-1.336445
10	6	0	-5.343436	-1.491419	0.257130
11	6	0	0.037167	-3.887146	0.301324
12	6	0	-0.320408	-1.462703	-1.242600
13	6	0	5.031811	0.073787	0.917707
14	6	0	-1.056471	-1.666811	-0.053006
15	6	0	-3.344564	-1.648225	-1.092117
16	6	0	3.927035	-1.211411	-1.283020
17	6	0	0.808810	-3.686234	-1.017597
18	6	0	5.796492	-0.084996	-0.239779
19	6	0	-2.531419	-1.600368	0.049991
20	6	0	-4.731665	-1.591903	-0.991697
21	6	0	-4.550051	-1.447815	1.403168
22	1	0	-2.570336	-1.445450	2.208941
23	1	0	-6.426493	-1.448156	0.336617
24	1	0	-2.888574	-1.737307	-2.073644
25	1	0	-5.337371	-1.630600	-1.893548
26	1	0	-5.010935	-1.361172	2.383711
27	1	0	3.155630	-0.268583	1.885095
28	1	0	5.817491	-0.870488	-2.244054
29	1	0	5.453500	0.575507	1.785039
30	1	0	3.524332	-1.717201	-2.154629
31	1	0	6.814909	0.291020	-0.282699
32	1	0	-0.769672	-2.623888	1.894782
33	1	0	1.537795	-1.992964	-2.203605
34	1	0	0.615769	-4.489571	1.008804
35	1	0	-0.910994	-4.408177	0.132660
36	1	0	0.255952	-4.103090	-1.865765
37	1	0	1.780944	-4.189649	-0.988390
38	1	0	-0.791346	-1.175910	-2.179576
39	1	0	1.443506	-1.551535	2.095525
40	8	0	1.496733	1.794748	0.920209
41	1	0	2.380110	1.722025	0.524593
42	8	0	-1.127090	0.864683	3.007933
43	1	0	-0.845998	1.765764	2.775841
44	1	0	-1.045628	0.395911	2.157480
45	5	0	1.068110	3.114840	0.978546
46	8	0	-0.022719	3.339975	1.774490
47	1	0	-0.464842	4.185827	1.632767
48	8	0	1.818114	4.049174	0.319892
49	1	0	1.520950	4.958722	0.445909
50	6	0	-1.059873	1.520280	-0.705692
51	6	0	-0.502813	2.420703	-1.635547
52	6	0	-2.396862	1.746823	-0.335900
53	6	0	-1.233739	3.488751	-2.165097
54	1	0	0.528617	2.294572	-1.966112
55	6	0	-3.130791	2.817891	-0.850520
56	1	0	-2.886648	1.083915	0.374214
57	6	0	-2.554980	3.696651	-1.769821
58	1	0	-0.768650	4.156414	-2.888625
59	1	0	-4.162033	2.963660	-0.533571
60	1	0	-3.130055	4.525030	-2.177390

SCF Done: E(RPBE1PBE) = -6019.35238351 A.U. after 1 cycles
Convg = 0.4166D-08 -V/T = 2.0046
Zero-point correction= 0.489133 (Hartree/Particle)
Thermal correction to Energy= 0.521668
Thermal correction to Enthalpy= 0.522628

```
 Thermal correction to Gibbs Free Energy=         0.423081
 Sum of electronic and zero-point Energies=          -6018.863250
 Sum of electronic and thermal Energies=             -6018.830716
 Sum of electronic and thermal Enthalpies=           -6018.829756
 Sum of electronic and thermal Free Energies=        -6018.929302
                     1                      2                      3
                     A                      A                      A
 Frequencies --    23.5169                30.8695                33.2464
```

PhBOD-Rh-Ph-OH_2-$B(OH)_3$-syn (20a)



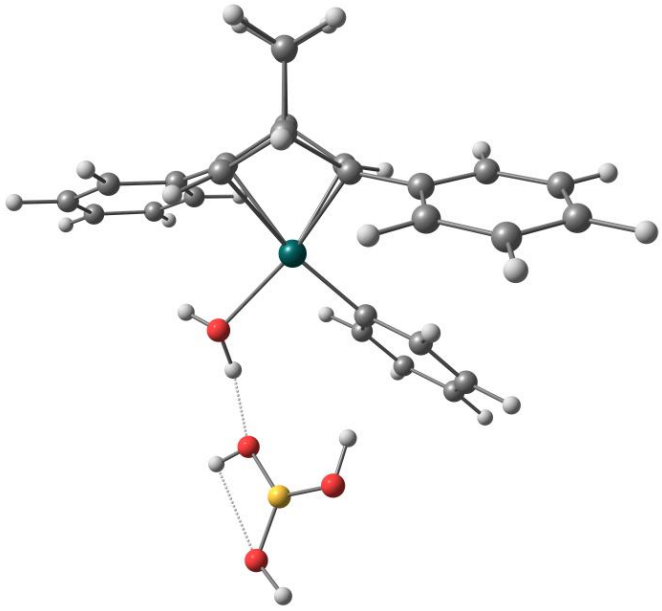
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.272519	-0.157172	-0.228747
2	6	0	0.536323	-2.121598	0.001568
3	6	0	-1.560582	-2.060017	1.277541
4	6	0	-3.645539	0.270551	1.216475
5	6	0	1.989820	-2.347268	-0.161961
6	6	0	2.565996	-2.385391	-1.441245
7	6	0	-0.091011	-1.683053	1.191268
8	6	0	-0.463003	-2.833290	-0.913553
9	6	0	4.197370	-2.756003	0.775894
10	6	0	-5.682715	1.081664	0.198243
11	6	0	-1.720098	-3.592164	1.134648
12	6	0	-1.548342	-1.797204	-1.118229
13	6	0	3.929651	-2.602951	-1.610604
14	6	0	-2.162602	-1.380430	0.047653
15	6	0	-4.304498	-0.537035	-0.953114
16	6	0	2.831335	-2.541802	0.942089
17	6	0	-1.042762	-4.058552	-0.169055
18	6	0	4.754745	-2.789217	-0.501186
19	6	0	-3.383442	-0.550202	0.106712
20	6	0	-5.438170	0.270937	-0.909564
21	6	0	-4.779775	1.076362	1.261569
22	1	0	-2.940237	0.298201	2.042892
23	1	0	-6.568551	1.709855	0.233896
24	1	0	-4.140382	-1.180310	-1.813317
25	1	0	-6.138480	0.259483	-1.740780
26	1	0	-4.955615	1.708626	2.127986
27	1	0	1.942460	-2.218366	-2.316158
28	1	0	4.828156	-2.904653	1.648739
29	1	0	4.351890	-2.620967	-2.612348

30	1	0	2.413036	-2.534697	1.944702
31	1	0	5.820162	-2.959736	-0.631493
32	1	0	-2.015381	-1.707320	2.204821
33	1	0	-0.010669	-3.132510	-1.860073
34	1	0	-1.270224	-4.075599	2.007968
35	1	0	-2.785570	-3.844881	1.140727
36	1	0	-1.757360	-4.567616	-0.824058
37	1	0	-0.232013	-4.765753	0.035046
38	1	0	-1.914731	-1.551552	-2.112052
39	1	0	0.467821	-1.445987	2.093923
40	8	0	-0.038272	5.810442	-0.996270
41	1	0	0.533959	6.508432	-1.340488
42	8	0	-1.178557	1.648545	-1.184956
43	1	0	-2.141155	1.657733	-1.066575
44	1	0	-0.846937	2.505607	-0.832147
45	5	0	0.718267	4.848216	-0.382451
46	6	0	1.380145	0.910588	0.332295
47	6	0	2.427445	1.179920	-0.571690
48	6	0	1.530823	1.445487	1.630774
49	6	0	3.549860	1.926979	-0.210428
50	1	0	2.372370	0.791427	-1.587117
51	6	0	2.648511	2.202994	2.003300
52	1	0	0.760034	1.266435	2.379932
53	6	0	3.667322	2.450635	1.081674
54	1	0	4.337835	2.106142	-0.939403
55	1	0	2.721615	2.599935	3.014018
56	1	0	4.545334	3.024283	1.368954
57	8	0	2.076968	5.006393	-0.299890
58	1	0	2.540906	4.235916	0.069847
59	8	0	0.020161	3.767369	0.122488
60	1	0	0.590486	3.127906	0.591018

SCF Done: E(RPBE1PBE) = -6019.37088720 A.U. after 1 cycles
Convg = 0.2004D-08 -V/T = 2.0045
Zero-point correction= 0.490546 (Hartree/Particle)
Thermal correction to Energy= 0.522276
Thermal correction to Enthalpy= 0.523236
Thermal correction to Gibbs Free Energy= 0.423017
Sum of electronic and zero-point Energies= -6018.880341
Sum of electronic and thermal Energies= -6018.848612
Sum of electronic and thermal Enthalpies= -6018.847652
Sum of electronic and thermal Free Energies= -6018.947870

	1	2	3
	A	A	A
Frequencies --	12.5144	19.6414	24.5794

PhBOD-Rh-Ph-OH_2-$B(OH)_3$-anti (20b)

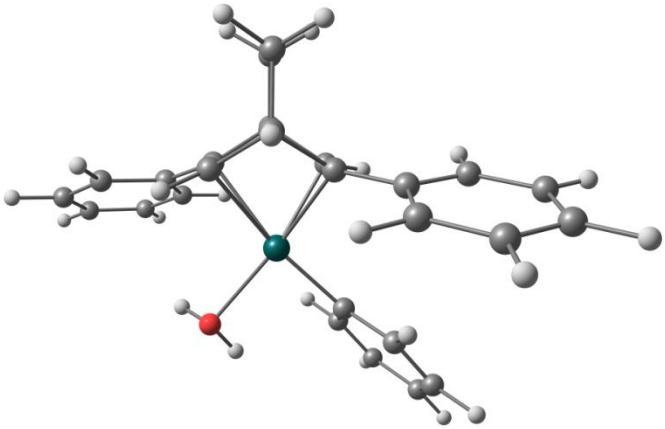


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.266958	-0.109574	-0.109281
2	6	0	0.546466	-2.102220	-0.140681
3	6	0	-1.581669	-2.206962	1.073827
4	6	0	-3.646777	0.127755	1.290777
5	6	0	1.998288	-2.339826	-0.288802
6	6	0	2.619349	-2.217003	-1.542140
7	6	0	-0.110060	-1.828180	1.081156
8	6	0	-0.429053	-2.669306	-1.175609
9	6	0	4.164033	-2.923688	0.655882
10	6	0	-5.667442	1.075546	0.360449
11	6	0	-1.739488	-3.702638	0.711999
12	6	0	-1.505440	-1.609715	-1.261773
13	6	0	3.984561	-2.439735	-1.694560
14	6	0	-2.146118	-1.355534	-0.063253
15	6	0	-4.272566	-0.377975	-0.977343
16	6	0	2.797133	-2.702670	0.804879
17	6	0	-1.028975	-3.984856	-0.626155
18	6	0	4.766249	-2.794522	-0.594585
19	6	0	-3.367792	-0.536718	0.084377
20	6	0	-5.406293	0.420473	-0.842566
21	6	0	-4.781079	0.923235	1.427387
22	1	0	-2.954243	0.038759	2.123729
23	1	0	-6.554514	1.693909	0.467679
24	1	0	-4.094549	-0.900674	-1.913100
25	1	0	-6.094080	0.522204	-1.678131
26	1	0	-4.971877	1.429848	2.370064
27	1	0	2.032242	-1.911938	-2.404730
28	1	0	4.760545	-3.202397	1.520932
29	1	0	4.441885	-2.327932	-2.674510
30	1	0	2.344313	-2.818588	1.785269
31	1	0	5.832606	-2.968629	-0.711823
32	1	0	-2.060980	-1.984925	2.028795
33	1	0	0.049856	-2.834542	-2.141838
34	1	0	-1.314299	-4.306655	1.520326
35	1	0	-2.805377	-3.947631	0.655010

36	1	0	-1.726649	-4.394903	-1.363775
37	1	0	-0.224177	-4.716990	-0.501667
38	1	0	-1.845416	-1.223982	-2.219707
39	1	0	0.424024	-1.723812	2.022532
40	8	0	1.174978	5.843672	-1.779675
41	1	0	2.062764	5.959888	-2.144163
42	8	0	-1.187417	1.771616	-0.857871
43	1	0	-2.137293	1.817565	-0.671880
44	1	0	-0.801586	2.646137	-0.629018
45	5	0	1.079356	4.638237	-1.130286
46	6	0	1.256340	0.954234	0.756053
47	6	0	2.625286	0.877095	0.432309
48	6	0	0.916119	1.850878	1.792239
49	6	0	3.592746	1.630871	1.106641
50	1	0	2.956120	0.210641	-0.361409
51	6	0	1.875251	2.598924	2.479259
52	1	0	-0.128648	1.968679	2.079611
53	6	0	3.224511	2.491266	2.140262
54	1	0	4.638278	1.544858	0.816938
55	1	0	1.567310	3.272440	3.277154
56	1	0	3.975054	3.075963	2.666604
57	8	0	2.131838	3.781972	-1.099664
58	1	0	1.996771	2.986774	-0.553671
59	8	0	-0.131717	4.330521	-0.524136
60	1	0	-0.754694	5.060962	-0.645556

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6019.36762898     A.U. after    1 cycles
             Convg  =    0.3752D-08             -V/T =  2.0045
Zero-point correction=                           0.490116 (Hartree/Particle)
 Thermal correction to Energy=                    0.521148
 Thermal correction to Enthalpy=                  0.522108
 Thermal correction to Gibbs Free Energy=         0.425263
 Sum of electronic and zero-point Energies=          -6018.877513
 Sum of electronic and thermal Energies=             -6018.846481
 Sum of electronic and thermal Enthalpies=           -6018.845520
 Sum of electronic and thermal Free Energies=        -6018.942366
                     1                      2                      3
                     A                      A                      A
 Frequencies --    -3.6688                24.8159                28.0530
```

PhBOD-Rh-Ph-OH_2 (21)



```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         45           0       -0.193182    0.361445   -0.375348
      2          6           0       -1.862822   -1.068394    0.143249
```

3	6	0	0.036939	-2.401318	-0.579553
4	6	0	2.969691	-1.641805	-1.231833
5	6	0	-3.191529	-0.423628	0.080880
6	6	0	-4.115039	-0.754571	-0.923129
7	6	0	-1.191033	-1.594808	-0.943892
8	6	0	-1.176408	-1.421903	1.462489
9	6	0	-4.796724	1.193067	0.942674
10	6	0	5.187186	-1.502552	-0.281591
11	6	0	-0.353770	-3.546236	0.384316
12	6	0	0.220366	-0.851983	1.281346
13	6	0	-5.352997	-0.120567	-0.997223
14	6	0	0.912022	-1.396345	0.174453
15	6	0	3.236315	-1.263254	1.126311
16	6	0	-3.558429	0.559967	1.015098
17	6	0	-1.104492	-2.961289	1.596673
18	6	0	-5.701082	0.856779	-0.065311
19	6	0	2.382774	-1.431998	0.026474
20	6	0	4.620123	-1.294362	0.974730
21	6	0	4.352444	-1.676668	-1.385735
22	1	0	2.336605	-1.751418	-2.108750
23	1	0	6.267239	-1.528658	-0.399622
24	1	0	2.814482	-1.110228	2.115451
25	1	0	5.258645	-1.159083	1.844080
26	1	0	4.780276	-1.832526	-2.372994
27	1	0	-3.866065	-1.529343	-1.643112
28	1	0	-5.055923	1.953130	1.675378
29	1	0	-6.053035	-0.398053	-1.781106
30	1	0	-2.856642	0.846090	1.794558
31	1	0	-6.668886	1.347734	-0.120476
32	1	0	0.535876	-2.795008	-1.466103
33	1	0	-1.685331	-0.979842	2.320792
34	1	0	-0.977097	-4.267918	-0.153789
35	1	0	0.553998	-4.073511	0.695913
36	1	0	-0.595970	-3.209782	2.533980
37	1	0	-2.120647	-3.363607	1.666170
38	1	0	0.729705	-0.376096	2.115743
39	1	0	-1.586621	-1.587472	-1.956533
40	6	0	1.133199	1.868711	0.005696
41	6	0	2.449878	1.948199	-0.482999
42	6	0	0.669851	2.984797	0.734647
43	6	0	3.251914	3.070506	-0.265101
44	1	0	2.868326	1.114866	-1.044320
45	6	0	1.469229	4.109209	0.966925
46	1	0	-0.334470	2.974690	1.162267
47	6	0	2.767635	4.158797	0.462602
48	1	0	4.264914	3.093303	-0.663151
49	1	0	1.076962	4.943905	1.545601
50	1	0	3.394968	5.029786	0.637196
51	8	0	-1.338127	1.911569	-1.535467
52	1	0	-0.946240	2.769290	-1.295868
53	1	0	-2.268295	1.942089	-1.260085

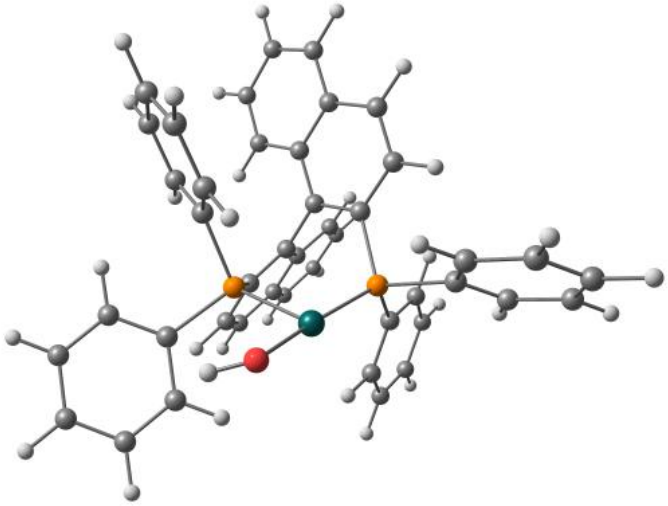
SCF Done: E(RPBE1PBE) = -5767.10118679 A.U. after 1 cycles
Convg = 0.4630D-08 -V/T = 2.0043

Zero-point correction= 0.439309 (Hartree/Particle)
Thermal correction to Energy= 0.465285
Thermal correction to Enthalpy= 0.466245
Thermal correction to Gibbs Free Energy= 0.381218
Sum of electronic and zero-point Energies= -5766.661878
Sum of electronic and thermal Energies= -5766.635902
Sum of electronic and thermal Enthalpies= -5766.634942
Sum of electronic and thermal Free Energies= -5766.719969

1	2	3
A	A	A

Frequencies -- 25.4482 29.9284 33.5906

BINAP-Rh-OH (22)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.495269	-0.642886	-2.012848
2	6	0	-5.337739	-1.576399	-3.036108
3	6	0	-4.426714	-0.334484	-1.172379
4	6	0	-4.107328	-2.208442	-3.211626
5	6	0	-3.557938	1.781812	2.553747
6	6	0	-3.772277	0.873492	3.589238
7	6	0	-2.923690	1.369305	1.383733
8	6	0	-3.185695	-0.956818	-1.347126
9	6	0	-3.040762	-1.906059	-2.367868
10	6	0	-3.351397	-0.449216	3.451752
11	6	0	-2.488651	0.047393	1.245978
12	6	0	-0.668446	4.576161	2.402270
13	6	0	-2.708409	-0.861872	2.287152
14	6	0	-1.313611	1.118991	-2.464643
15	6	0	-0.190513	4.445907	3.726303
16	6	0	-0.670371	2.061647	-3.222628
17	6	0	-0.428684	3.593776	1.471558
18	6	0	-0.929609	0.851513	-1.122842
19	6	0	0.523099	3.328712	4.085631
20	6	0	0.412539	2.797677	-2.691201
21	6	0	0.304454	2.423248	1.808223
22	6	0	0.121892	1.572197	-0.557251
23	6	0	1.100137	3.763876	-3.468692
24	6	0	0.788574	2.301462	3.144435
25	6	0	0.812032	2.554830	-1.344261
26	6	0	0.571888	1.383992	0.858385
27	6	0	2.151115	4.473214	-2.940647
28	6	0	1.540792	1.157610	3.497884
29	6	0	1.909504	3.301259	-0.834822
30	6	0	1.299694	0.263820	1.249883
31	6	0	2.557632	4.234179	-1.608595
32	6	0	1.786469	0.170757	2.578784
33	6	0	1.984305	-1.030543	-2.593274
34	6	0	2.661489	-0.609301	-3.736307
35	6	0	2.365636	-0.561296	-1.332617
36	6	0	3.725812	0.284110	-3.626506
37	6	0	3.433560	0.337954	-1.229998

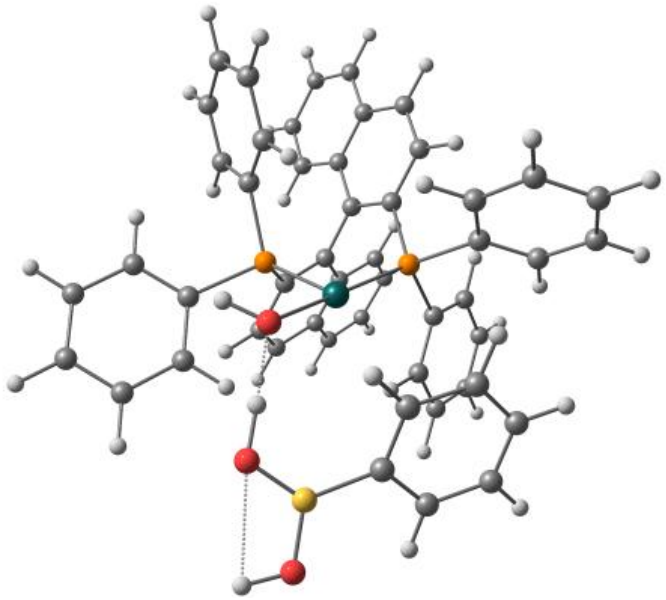
38	6	0	4.111908	0.756182	-2.371692
39	6	0	2.659002	-2.309915	0.950241
40	6	0	2.165228	-3.136292	1.973115
41	6	0	3.994329	-2.451910	0.557452
42	6	0	2.993665	-4.060977	2.603506
43	6	0	4.821338	-3.381707	1.186577
44	6	0	4.326314	-4.185001	2.212104
45	1	0	-6.455292	-0.156065	-1.861618
46	1	0	-6.173870	-1.818351	-3.687007
47	1	0	-4.569225	0.386552	-0.372725
48	1	0	-3.878204	2.815301	2.657021
49	1	0	-3.979468	-2.948178	-3.997636
50	1	0	-4.264314	1.196958	4.502966
51	1	0	-2.765696	2.082506	0.578485
52	1	0	-1.230687	5.461843	2.117627
53	1	0	-2.137745	0.566454	-2.903284
54	1	0	-3.519207	-1.161282	4.255706
55	1	0	-0.989267	2.247343	-4.245971
56	1	0	-0.387234	5.229230	4.453509
57	1	0	-2.084759	-2.411739	-2.486585
58	1	0	-0.803314	3.715464	0.460194
59	1	0	-2.374306	-1.890821	2.168445
60	1	0	0.779107	3.932636	-4.494080
61	1	0	0.897800	3.215771	5.100397
62	1	0	2.671576	5.213390	-3.542682
63	1	0	1.926850	1.067796	4.510951
64	1	0	1.143454	-1.717780	-2.667922
65	1	0	2.246489	3.127075	0.181548
66	1	0	2.353837	-0.974402	-4.712842
67	1	0	3.394189	4.789899	-1.192964
68	1	0	2.369250	-0.695960	2.874476
69	1	0	1.124096	-3.050548	2.282815
70	1	0	4.251392	0.617540	-4.517613
71	1	0	3.731207	0.720926	-0.256301
72	1	0	4.935508	1.459818	-2.283140
73	1	0	4.393763	-1.845539	-0.250003
74	1	0	2.593813	-4.689727	3.394634
75	1	0	5.855941	-3.480767	0.868240
76	1	0	4.973231	-4.910434	2.698357
77	15	0	-1.719950	-0.596704	-0.285991
78	15	0	1.452814	-1.192161	0.123655
79	45	0	-0.458825	-2.380564	-0.023242
80	8	0	-1.966166	-3.703494	0.127115
81	1	0	-2.797268	-3.480331	-0.313104

SCF Done: E(RPBE1PBE) = -7139.48147756 A.U. after 1 cycles
Convg = 0.4109D-08 -V/T = 2.0054

Zero-point correction= 0.640500 (Hartree/Particle)
Thermal correction to Energy= 0.703113
Thermal correction to Enthalpy= 0.704295
Thermal correction to Gibbs Free Energy= 0.532912
Sum of electronic and zero-point Energies= -7138.840978
Sum of electronic and thermal Energies= -7138.778364
Sum of electronic and thermal Enthalpies= -7138.777182
Sum of electronic and thermal Free Energies= -7138.948565

	1	2	3
	A	A	A
Frequencies --	10.0187	25.2999	31.2691

BINAP-Rh-OH-PhB(OH)$_2$–in (23)



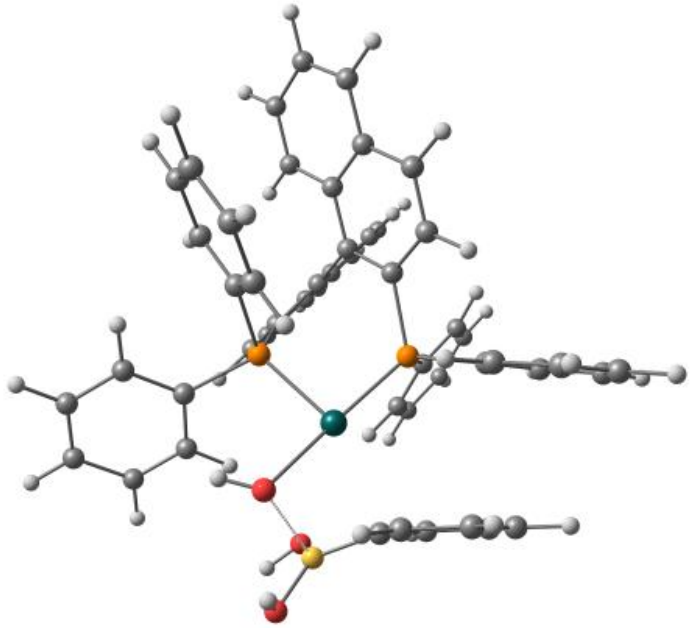
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.311234	5.868609	0.508429
2	6	0	0.894380	6.041167	1.185218
3	6	0	-0.705265	4.599826	0.084910
4	6	0	1.712877	4.938865	1.427493
5	6	0	-3.976589	2.745821	-1.881454
6	6	0	-3.717244	2.595029	-3.243519
7	6	0	-2.980472	2.474752	-0.947362
8	6	0	0.102571	3.484623	0.337125
9	6	0	1.323961	3.672633	1.000015
10	6	0	-2.459285	2.170657	-3.668071
11	6	0	-1.714070	2.049981	-1.366705
12	6	0	-5.989520	0.079355	0.192748
13	6	0	-1.462309	1.898494	-2.733435
14	6	0	-0.734112	1.557744	2.577552
15	6	0	-6.473803	-0.499336	-1.002516
16	6	0	-1.101163	0.949809	3.748907
17	6	0	-4.655705	0.004822	0.516454
18	6	0	-1.095327	1.015982	1.315558
19	6	0	-5.603615	-1.139754	-1.850688
20	6	0	-1.847377	-0.250936	3.736645
21	6	0	-3.727705	-0.654174	-0.334942
22	6	0	-1.852633	-0.152305	1.263189
23	6	0	-2.225347	-0.896789	4.940889
24	6	0	-4.222641	-1.231140	-1.540969
25	6	0	-2.230393	-0.808728	2.481808
26	6	0	-2.329373	-0.735650	-0.028467
27	6	0	-2.958628	-2.058130	4.915554
28	6	0	-3.317469	-1.889192	-2.404436
29	6	0	-2.980862	-2.015626	2.493920
30	6	0	-1.465390	-1.371049	-0.914565
31	6	0	-3.336762	-2.620564	3.675664
32	6	0	-1.982431	-1.954040	-2.100372
33	6	0	1.541576	-1.806125	1.829678
34	6	0	1.757979	-2.480973	3.029574
35	6	0	0.579843	-2.267284	0.926328
36	6	0	1.018215	-3.622241	3.332220

37	6	0	-0.164838	-3.411566	1.238184
38	6	0	0.057629	-4.088429	2.433786
39	6	0	1.003300	-2.473460	-1.942602
40	6	0	1.171451	-1.931802	-3.226662
41	6	0	1.396700	-3.794736	-1.711383
42	6	0	1.702247	-2.700243	-4.259176
43	6	0	1.936840	-4.561295	-2.744179
44	6	0	2.088621	-4.019121	-4.019054
45	1	0	-0.948231	6.724290	0.299816
46	1	0	1.202084	7.032328	1.508327
47	1	0	-1.640254	4.491295	-0.455000
48	1	0	-4.958921	3.064926	-1.543523
49	1	0	2.668818	5.061597	1.928732
50	1	0	-4.496840	2.803273	-3.971717
51	1	0	-3.193510	2.587294	0.112975
52	1	0	-6.678098	0.589339	0.861456
53	1	0	-0.160784	2.477439	2.620261
54	1	0	-2.253608	2.048178	-4.728310
55	1	0	-0.817621	1.390419	4.702169
56	1	0	-7.530918	-0.435151	-1.246532
57	1	0	1.984818	2.825806	1.160661
58	1	0	-4.305053	0.461437	1.436319
59	1	0	-0.479168	1.559522	-3.053972
60	1	0	-1.922592	-0.454485	5.887239
61	1	0	-5.961805	-1.586390	-2.775416
62	1	0	-3.246489	-2.546014	5.843043
63	1	0	-3.691053	-2.346644	-3.317978
64	1	0	2.114782	-0.912612	1.590911
65	1	0	-3.274577	-2.470205	1.553584
66	1	0	2.503855	-2.110794	3.728012
67	1	0	-3.910686	-3.543411	3.655912
68	1	0	-1.311721	-2.468949	-2.779797
69	1	0	0.889336	-0.896702	-3.412871
70	1	0	1.183751	-4.146281	4.270084
71	1	0	-0.928097	-3.769683	0.550643
72	1	0	-0.528814	-4.972255	2.671169
73	1	0	1.302024	-4.227267	-0.719918
74	1	0	1.825665	-2.264716	-5.247274
75	1	0	2.244488	-5.585253	-2.547752
76	1	0	2.513196	-4.618340	-4.820179
77	15	0	-0.335961	1.773599	-0.192744
78	15	0	0.363691	-1.344023	-0.637668
79	45	0	1.426865	0.641079	-0.922558
80	8	0	2.542436	2.284476	-1.472903
81	1	0	2.036326	3.099201	-1.596508
82	5	0	5.041888	1.771293	0.755859
83	8	0	4.451132	2.825502	0.150616
84	1	0	3.709894	2.598883	-0.521931
85	8	0	5.902758	2.011898	1.813838
86	1	0	5.938914	2.967543	1.964732
87	6	0	4.839125	0.260379	0.353555
88	6	0	4.349793	-0.116650	-0.912584
89	6	0	5.202691	-0.760729	1.242900
90	6	0	4.231786	-1.461992	-1.267531
91	1	0	4.122084	0.650130	-1.651415
92	6	0	5.070652	-2.106167	0.898809
93	1	0	5.604313	-0.491919	2.217070
94	6	0	4.583915	-2.459845	-0.357772
95	1	0	3.883874	-1.733775	-2.260512
96	1	0	5.353047	-2.880048	1.608892
97	1	0	4.485132	-3.506555	-0.633840

SCF Done: E(RPBE1PBE) = -7547.34219990 A.U. after 22 cycles
Convg = 0.4692D-08 -V/T = 2.0058

```
Zero-point correction=                           0.768057 (Hartree/Particle)
 Thermal correction to Energy=                    0.844116
 Thermal correction to Enthalpy=                  0.845298
 Thermal correction to Gibbs Free Energy=         0.642962
 Sum of electronic and zero-point Energies=      -7546.574143
 Sum of electronic and thermal Energies=         -7546.498084
 Sum of electronic and thermal Enthalpies=       -7546.496902
 Sum of electronic and thermal Free Energies=    -7546.699238
                     1                      2                      3
                     A                      A                      A
 Frequencies --     7.8465                13.3294                25.3691
```

BINAP-Rh-OH-PhB(OH)$_2$–TS-in (24)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.539770	5.892419	0.127135
2	6	0	0.363703	6.153666	1.154019
3	6	0	-0.760880	4.583543	-0.302141
4	6	0	1.061399	5.098313	1.740991
5	6	0	-3.494646	2.472328	-2.735517
6	6	0	-2.935181	2.238564	-3.991853
7	6	0	-2.725183	2.305600	-1.587516
8	6	0	-0.078169	3.515958	0.290940
9	6	0	0.852442	3.792705	1.305569
10	6	0	-1.604543	1.837262	-4.096545
11	6	0	-1.388409	1.901388	-1.685355
12	6	0	-5.752065	-0.241886	-1.045929
13	6	0	-0.834168	1.668163	-2.947521
14	6	0	-1.352611	1.684785	2.393828
15	6	0	-5.914886	-0.912618	-2.279370
16	6	0	-1.969014	1.118967	3.478801
17	6	0	-4.530550	-0.219780	-0.415761
18	6	0	-1.346063	1.046634	1.124798
19	6	0	-4.841064	-1.546775	-2.855149
20	6	0	-2.617639	-0.132341	3.371044
21	6	0	-3.398804	-0.869681	-0.979368
22	6	0	-1.997646	-0.174039	0.976189

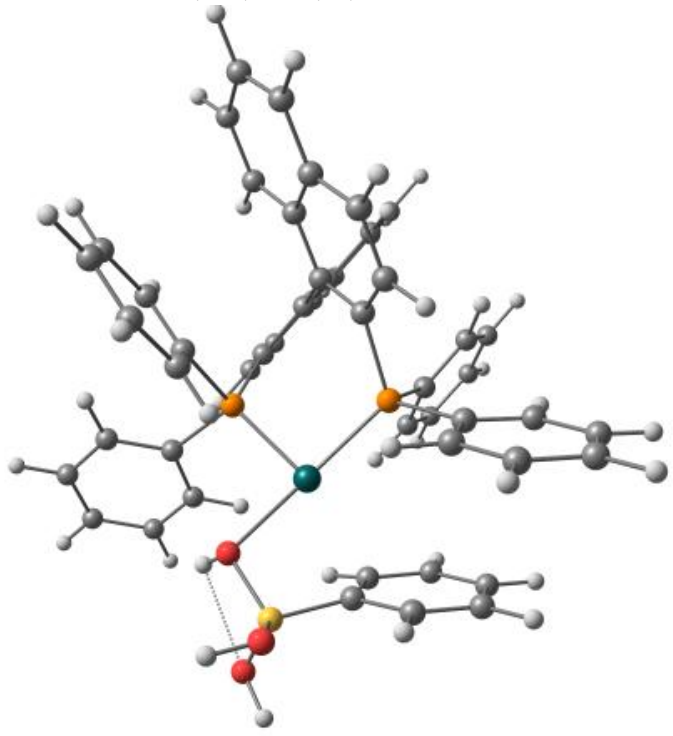
23	6	0	-3.254140	-0.734863	4.485536
24	6	0	-3.571008	-1.540292	-2.224468
25	6	0	-2.637308	-0.785925	2.105039
26	6	0	-2.109649	-0.853807	-0.348499
27	6	0	-3.894297	-1.943967	4.360244
28	6	0	-2.459001	-2.195984	-2.797961
29	6	0	-3.299355	-2.040127	2.014795
30	6	0	-1.026684	-1.481394	-0.957127
31	6	0	-3.913792	-2.600463	3.109154
32	6	0	-1.233931	-2.164940	-2.184564
33	6	0	1.089415	-1.326917	2.489216
34	6	0	0.985021	-1.819316	3.788960
35	6	0	0.521348	-2.027889	1.420971
36	6	0	0.315297	-3.016894	4.032236
37	6	0	-0.168257	-3.220375	1.675102
38	6	0	-0.263407	-3.715957	2.972441
39	6	0	1.583622	-2.634054	-1.224450
40	6	0	1.924368	-2.324001	-2.549357
41	6	0	1.941294	-3.885990	-0.717860
42	6	0	2.555122	-3.260303	-3.363005
43	6	0	2.591862	-4.818934	-1.526902
44	6	0	2.889106	-4.515356	-2.853406
45	1	0	-1.075319	6.709091	-0.349979
46	1	0	0.534706	7.174434	1.485740
47	1	0	-1.461515	4.405308	-1.111472
48	1	0	-4.534362	2.776269	-2.648012
49	1	0	1.783570	5.292733	2.529945
50	1	0	-3.538278	2.365846	-4.887178
51	1	0	-3.168386	2.488074	-0.611405
52	1	0	-6.600414	0.264131	-0.592301
53	1	0	-0.871005	2.648458	2.512120
54	1	0	-1.165244	1.652827	-5.073517
55	1	0	-1.964490	1.635289	4.436304
56	1	0	-6.885939	-0.923332	-2.767380
57	1	0	1.428551	2.978299	1.738812
58	1	0	-4.429379	0.308083	0.526689
59	1	0	0.205282	1.353376	-3.015961
60	1	0	-3.227646	-0.220004	5.443256
61	1	0	-4.948943	-2.064888	-3.805357
62	1	0	-4.383426	-2.397385	5.218434
63	1	0	-2.582690	-2.733340	-3.735836
64	1	0	1.600284	-0.386218	2.296511
65	1	0	-3.315298	-2.566004	1.065985
66	1	0	1.422842	-1.260533	4.612237
67	1	0	-4.414035	-3.560627	3.012768
68	1	0	-0.409639	-2.690628	-2.651260
69	1	0	1.691566	-1.337187	-2.944991
70	1	0	0.231451	-3.399577	5.046204
71	1	0	-0.646482	-3.758667	0.859721
72	1	0	-0.804226	-4.640306	3.158369
73	1	0	1.727594	-4.140007	0.315578
74	1	0	2.796696	-3.004674	-4.391700
75	1	0	2.866496	-5.786330	-1.113944
76	1	0	3.387991	-5.247045	-3.483750
77	15	0	-0.293492	1.755794	-0.224975
78	15	0	0.701818	-1.331548	-0.265909
79	45	0	1.691515	0.716947	-0.502228
80	8	0	2.647656	2.503115	-0.878008
81	1	0	2.113352	3.285260	-0.685067
82	5	0	4.019613	1.851046	0.968688
83	8	0	4.823053	2.903787	0.555267
84	1	0	4.641132	3.005723	-0.394011
85	8	0	3.523495	1.928470	2.260306
86	1	0	3.764566	2.796324	2.616101

87	6	0	4.047177	0.411195	0.305942
88	6	0	4.227322	0.205318	-1.080377
89	6	0	4.244396	-0.705542	1.154536
90	6	0	4.648739	-1.035850	-1.578251
91	1	0	4.141872	1.048157	-1.760719
92	6	0	4.658453	-1.932159	0.657900
93	1	0	4.121633	-0.574513	2.226389
94	6	0	4.881011	-2.096035	-0.715021
95	1	0	4.811929	-1.158557	-2.645714
96	1	0	4.826253	-2.763767	1.338236
97	1	0	5.220317	-3.052698	-1.102955

SCF Done: E(RPBE1PBE) = -7547.32512075 A.U. after 1 cycles
Convg = 0.6397D-08 -V/T = 2.0059
Zero-point correction= 0.768210 (Hartree/Particle)
Thermal correction to Energy= 0.843302
Thermal correction to Enthalpy= 0.844484
Thermal correction to Gibbs Free Energy= 0.649946
Sum of electronic and zero-point Energies= -7546.556910
Sum of electronic and thermal Energies= -7546.481818
Sum of electronic and thermal Enthalpies= -7546.480637
Sum of electronic and thermal Free Energies= -7546.675175

	1	2	3
	A	A	A
Frequencies --	-160.0887	19.6284	27.5737

BINAP-Rh-PhB(OH)$_2$–in (25)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.272026	5.611619	-1.672129
2	6	0	-1.069392	5.431444	-2.799217
3	6	0	0.117279	4.516846	-0.899464
4	6	0	-1.485417	4.147161	-3.151434

5	6	0	2.722224	3.523427	2.415561
6	6	0	1.965125	3.525009	3.587132
7	6	0	2.199560	2.972442	1.248748
8	6	0	-0.285268	3.224763	-1.248957
9	6	0	-1.101977	3.055320	-2.378129
10	6	0	0.683325	2.977136	3.589119
11	6	0	0.914782	2.417492	1.246497
12	6	0	5.461709	0.766678	1.957745
13	6	0	0.158512	2.424187	2.423020
14	6	0	1.711401	1.328714	-2.571656
15	6	0	5.420294	0.393428	3.320299
16	6	0	2.592366	0.659149	-3.380678
17	6	0	4.409784	0.480730	1.120503
18	6	0	1.510650	0.945383	-1.219307
19	6	0	4.318029	-0.261082	3.813140
20	6	0	3.327262	-0.445125	-2.891706
21	6	0	3.254841	-0.199269	1.594791
22	6	0	2.238589	-0.118750	-0.694926
23	6	0	4.233550	-1.155226	-3.719361
24	6	0	3.220437	-0.570791	2.970191
25	6	0	3.155822	-0.835874	-1.531254
26	6	0	2.138928	-0.503662	0.745898
27	6	0	4.953133	-2.215903	-3.225160
28	6	0	2.085520	-1.254867	3.459754
29	6	0	3.911819	-1.941378	-1.056031
30	6	0	1.024811	-1.155283	1.268560
31	6	0	4.787379	-2.609492	-1.878039
32	6	0	1.027142	-1.536646	2.635893
33	6	0	-0.325339	-1.992364	-2.458043
34	6	0	0.101786	-2.712695	-3.571720
35	6	0	0.077012	-2.370392	-1.174318
36	6	0	0.931883	-3.820341	-3.410216
37	6	0	0.925862	-3.473769	-1.020664
38	6	0	1.344013	-4.199133	-2.132566
39	6	0	-1.479293	-2.591602	1.279977
40	6	0	-2.137313	-2.078140	2.407411
41	6	0	-1.599841	-3.954157	0.993184
42	6	0	-2.851710	-2.916889	3.257145
43	6	0	-2.331773	-4.791723	1.835433
44	6	0	-2.947783	-4.279334	2.974877
45	1	0	0.044272	6.610185	-1.382160
46	1	0	-1.377053	6.287366	-3.393871
47	1	0	0.725177	4.680688	-0.015044
48	1	0	3.725268	3.941673	2.412264
49	1	0	-2.122030	3.995359	-4.018882
50	1	0	2.376946	3.950131	4.498813
51	1	0	2.796682	2.966544	0.339850
52	1	0	6.332759	1.287394	1.568443
53	1	0	1.167381	2.175623	-2.975439
54	1	0	0.090490	2.977428	4.499999
55	1	0	2.734457	0.978358	-4.410902
56	1	0	6.258488	0.625252	3.972072
57	1	0	-1.444570	2.057394	-2.645413
58	1	0	4.462085	0.783605	0.079985
59	1	0	-0.841565	1.996158	2.414567
60	1	0	4.350354	-0.842868	-4.754597
61	1	0	4.270746	-0.553125	4.859728
62	1	0	5.648321	-2.752669	-3.865304
63	1	0	2.057648	-1.561453	4.503119
64	1	0	-0.965212	-1.121706	-2.573914
65	1	0	3.791811	-2.265333	-0.027369
66	1	0	-0.209477	-2.404328	-4.566545
67	1	0	5.353390	-3.452346	-1.490006
68	1	0	0.178352	-2.072642	3.044555

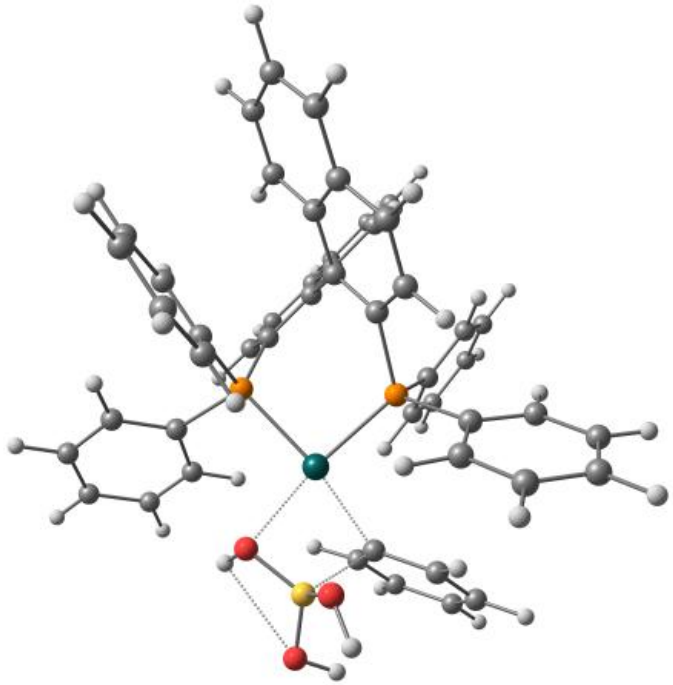
69	1	0	-2.091411	-1.012090	2.620051
70	1	0	1.267250	-4.381886	-4.278270
71	1	0	1.272802	-3.761294	-0.030755
72	1	0	2.004481	-5.052434	-2.002728
73	1	0	-1.133647	-4.371678	0.106348
74	1	0	-3.346772	-2.500930	4.130686
75	1	0	-2.419562	-5.848328	1.595572
76	1	0	-3.511860	-4.935277	3.633029
77	15	0	0.141065	1.730226	-0.259655
78	15	0	-0.519319	-1.401628	0.259437
79	45	0	-1.723232	0.487616	-0.035239
80	8	0	-2.926157	2.245607	0.101260
81	1	0	-2.925814	2.839783	-0.663913
82	5	0	-4.320631	1.641975	0.243448
83	8	0	-4.798378	1.775439	1.604274
84	1	0	-4.879611	2.722050	1.783307
85	8	0	-5.103142	2.379231	-0.754595
86	1	0	-6.027308	2.112878	-0.674350
87	6	0	-4.178425	0.042612	-0.101857
88	6	0	-4.713594	-0.959164	0.736434
89	6	0	-3.693216	-0.378254	-1.361044
90	6	0	-4.804969	-2.283881	0.333280
91	1	0	-5.092669	-0.659348	1.710381
92	6	0	-3.763716	-1.723375	-1.767361
93	1	0	-3.396860	0.371883	-2.094585
94	6	0	-4.323488	-2.671855	-0.924182
95	1	0	-5.241233	-3.027447	0.996232
96	1	0	-3.407761	-2.014606	-2.752897
97	1	0	-4.392646	-3.710495	-1.238815

SCF Done: E(RPBE1PBE) = -7547.35171627 A.U. after 1 cycles
Convg = 0.5501D-08 -V/T = 2.0058

Zero-point correction= 0.768343 (Hartree/Particle)
Thermal correction to Energy= 0.844162
Thermal correction to Enthalpy= 0.845344
Thermal correction to Gibbs Free Energy= 0.647597
Sum of electronic and zero-point Energies= -7546.583373
Sum of electronic and thermal Energies= -7546.507554
Sum of electronic and thermal Enthalpies= -7546.506372
Sum of electronic and thermal Free Energies= -7546.704119

	1	2	3
	A	A	A
Frequencies --	11.5544	20.1285	31.8531

BINAP-Rh-PhB(OH)$_3$–TS-in (26)

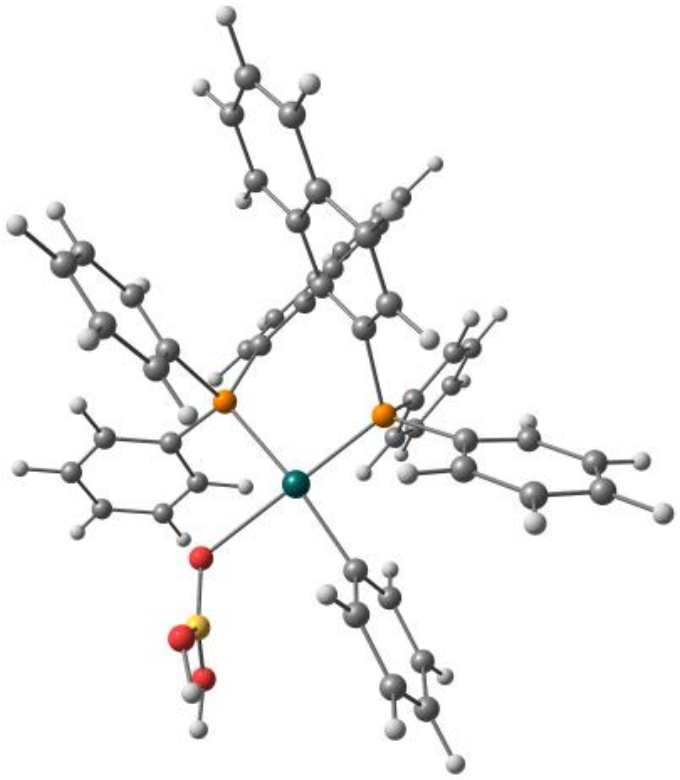


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.296172	5.613668	1.820843
2	6	0	0.666876	5.499371	2.819806
3	6	0	-0.668854	4.499897	1.066743
4	6	0	1.265939	4.261980	3.059959
5	6	0	-3.692466	3.255516	-1.758306
6	6	0	-3.170284	3.404444	-3.043595
7	6	0	-2.896788	2.741873	-0.737887
8	6	0	-0.081372	3.253791	1.302874
9	6	0	0.900877	3.153682	2.301206
10	6	0	-1.850503	3.040840	-3.305920
11	6	0	-1.571140	2.373971	-0.995731
12	6	0	-5.776204	0.016540	-1.171757
13	6	0	-1.052562	2.526208	-2.285649
14	6	0	-1.517436	0.967579	2.800057
15	6	0	-5.882332	-0.253987	-2.554934
16	6	0	-2.124227	0.106930	3.678206
17	6	0	-4.576625	-0.135418	-0.518014
18	6	0	-1.477410	0.695860	1.407819
19	6	0	-4.775734	-0.672070	-3.252931
20	6	0	-2.737398	-1.081367	3.218990
21	6	0	-3.412279	-0.573017	-1.206622
22	6	0	-2.086585	-0.455281	0.917380
23	6	0	-3.374701	-1.978690	4.113461
24	6	0	-3.527467	-0.841803	-2.601644
25	6	0	-2.729445	-1.362329	1.821127
26	6	0	-2.147103	-0.737316	-0.549827
27	6	0	-3.995314	-3.112521	3.648464
28	6	0	-2.382812	-1.279484	-3.304529
29	6	0	-3.377032	-2.546444	1.376470
30	6	0	-1.034550	-1.155259	-1.276918
31	6	0	-3.995773	-3.394319	2.263405
32	6	0	-1.181227	-1.429709	-2.662544

33	6	0	1.158830	-2.199064	2.026754
34	6	0	1.061161	-3.102265	3.083474
35	6	0	0.485899	-2.441228	0.826223
36	6	0	0.291894	-4.256238	2.948066
37	6	0	-0.289370	-3.600709	0.698139
38	6	0	-0.381476	-4.505300	1.752099
39	6	0	1.615774	-2.121330	-1.830109
40	6	0	2.111243	-1.354567	-2.895399
41	6	0	1.883293	-3.492503	-1.803406
42	6	0	2.820955	-1.955934	-3.931035
43	6	0	2.610233	-4.091251	-2.833296
44	6	0	3.070817	-3.328674	-3.904435
45	1	0	-0.759390	6.575902	1.618416
46	1	0	0.956620	6.369505	3.402872
47	1	0	-1.412530	4.613503	0.283803
48	1	0	-4.723813	3.529990	-1.552651
49	1	0	2.023880	4.161235	3.832682
50	1	0	-3.794806	3.800166	-3.840432
51	1	0	-3.310474	2.620230	0.260670
52	1	0	-6.650623	0.352103	-0.620088
53	1	0	-1.067787	1.878188	3.181468
54	1	0	-1.441147	3.154275	-4.306351
55	1	0	-2.144896	0.338970	4.740879
56	1	0	-6.836095	-0.128991	-3.060849
57	1	0	1.377265	2.191874	2.483355
58	1	0	-4.517929	0.086992	0.542320
59	1	0	-0.021859	2.237210	-2.480934
60	1	0	-3.367355	-1.749454	5.176697
61	1	0	-4.840607	-0.880467	-4.318459
62	1	0	-4.486200	-3.792098	4.340185
63	1	0	-2.462362	-1.500148	-4.366853
64	1	0	1.758208	-1.297667	2.122984
65	1	0	-3.382773	-2.783087	0.317423
66	1	0	1.585853	-2.902037	4.014212
67	1	0	-4.486469	-4.292308	1.896961
68	1	0	-0.324990	-1.771999	-3.232536
69	1	0	1.970536	-0.275028	-2.891770
70	1	0	0.211287	-4.958622	3.773772
71	1	0	-0.833664	-3.793711	-0.223675
72	1	0	-0.992129	-5.398034	1.644700
73	1	0	1.542715	-4.101610	-0.971732
74	1	0	3.194863	-1.346300	-4.749713
75	1	0	2.817568	-5.157649	-2.793508
76	1	0	3.633969	-3.798142	-4.707074
77	15	0	-0.439897	1.749598	0.298261
78	15	0	0.670405	-1.223449	-0.528630
79	45	0	1.582730	0.798053	-0.160912
80	8	0	2.683058	2.663152	-0.413857
81	1	0	2.898591	3.106521	0.419926
82	5	0	3.824944	1.891133	-0.841064
83	8	0	3.786827	1.568543	-2.209818
84	1	0	4.693510	1.544165	-2.539626
85	8	0	5.036024	2.350251	-0.260821
86	1	0	5.619797	1.611223	-0.050683
87	6	0	3.636546	0.080250	0.198346
88	6	0	4.384470	-0.906493	-0.469135
89	6	0	3.904880	0.218525	1.581078
90	6	0	5.319110	-1.711705	0.186974
91	1	0	4.246671	-1.038763	-1.539043
92	6	0	4.825991	-0.581207	2.254344
93	1	0	3.393256	0.993878	2.151399
94	6	0	5.538697	-1.558391	1.554866
95	1	0	5.875573	-2.461648	-0.371855
96	1	0	4.996805	-0.439603	3.319825

```
     97          1           0        6.263417   -2.184751    2.069858
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -7547.33157569     A.U. after    1 cycles
            Convg  =    0.6144D-08             -V/T =  2.0058
Zero-point correction=                           0.766442 (Hartree/Particle)
 Thermal correction to Energy=                    0.842286
 Thermal correction to Enthalpy=                  0.843468
 Thermal correction to Gibbs Free Energy=         0.645094
 Sum of electronic and zero-point Energies=          -7546.565133
 Sum of electronic and thermal Energies=             -7546.489289
 Sum of electronic and thermal Enthalpies=           -7546.488108
 Sum of electronic and thermal Free Energies=        -7546.686482
                     1                      2                      3
                     A                      A                      A
 Frequencies --  -250.7813               13.9975                26.2132
```

BINAP-Rh-Ph-B(OH)$_3$ (27)



```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        2.056236   -5.292815   -1.005556
      2          6           0        2.754915   -5.060721   -2.186892
      3          6           0        1.360098   -4.256070   -0.382106
      4          6           0        2.769802   -3.777629   -2.734113
      5          6           0       -1.520665   -3.791391    2.636752
      6          6           0       -0.986077   -3.330394    3.839767
      7          6           0       -1.098372   -3.242730    1.428764
      8          6           0        1.355593   -2.969866   -0.929914
      9          6           0        2.090184   -2.742026   -2.102601
     10          6           0       -0.027454   -2.318770    3.828538
     11          6           0       -0.132932   -2.228252    1.406887
     12          6           0       -5.035226   -2.548033    1.587254
```

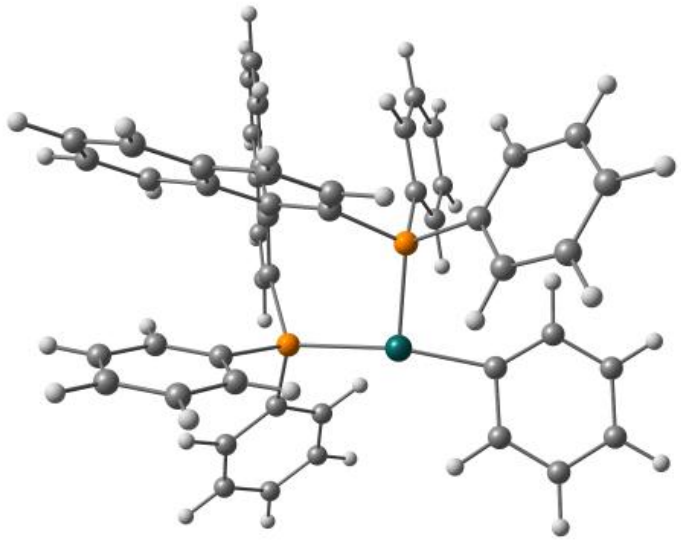
13	6	0	0.395953	-1.772930	2.617846
14	6	0	-0.946604	-1.774726	-2.560426
15	6	0	-5.328923	-2.112524	2.899688
16	6	0	-1.935772	-1.509045	-3.469296
17	6	0	-4.078491	-1.908753	0.835678
18	6	0	-1.004450	-1.299007	-1.222912
19	6	0	-4.656839	-1.036929	3.427312
20	6	0	-3.057814	-0.730010	-3.106859
21	6	0	-3.361012	-0.795165	1.350338
22	6	0	-2.118050	-0.562886	-0.818857
23	6	0	-4.085685	-0.436006	-4.037966
24	6	0	-3.669361	-0.355015	2.671023
25	6	0	-3.152256	-0.252203	-1.767048
26	6	0	-2.346968	-0.121160	0.593107
27	6	0	-5.178189	0.309910	-3.667558
28	6	0	-2.989449	0.770294	3.190759
29	6	0	-4.293547	0.522955	-1.422264
30	6	0	-1.678243	0.963123	1.149793
31	6	0	-5.276332	0.795053	-2.344179
32	6	0	-2.027351	1.408492	2.451389
33	6	0	-0.295629	2.522964	-2.388229
34	6	0	-0.802931	3.159918	-3.519678
35	6	0	-1.010346	2.543307	-1.186183
36	6	0	-2.030551	3.816791	-3.458919
37	6	0	-2.245872	3.200010	-1.133502
38	6	0	-2.752471	3.834358	-2.264860
39	6	0	0.238622	3.107015	1.359411
40	6	0	0.947213	2.790050	2.532023
41	6	0	0.045747	4.453792	1.040138
42	6	0	1.428404	3.793803	3.369415
43	6	0	0.535399	5.459577	1.875766
44	6	0	1.224324	5.135463	3.041536
45	1	0	2.053976	-6.283367	-0.557209
46	1	0	3.297932	-5.868987	-2.670211
47	1	0	0.833995	-4.460578	0.544711
48	1	0	-2.277392	-4.571578	2.638646
49	1	0	3.330600	-3.576340	-3.643417
50	1	0	-1.320807	-3.755394	4.782662
51	1	0	-1.529019	-3.603926	0.497783
52	1	0	-5.568916	-3.398086	1.169927
53	1	0	-0.105529	-2.383843	-2.872424
54	1	0	0.389954	-1.951629	4.762887
55	1	0	-1.863193	-1.900643	-4.481849
56	1	0	-6.086250	-2.627314	3.485284
57	1	0	2.139403	-1.736801	-2.513295
58	1	0	-3.863241	-2.261104	-0.167935
59	1	0	1.138500	-0.977718	2.597303
60	1	0	-3.992116	-0.813297	-5.053944
61	1	0	-4.874602	-0.689828	4.434993
62	1	0	-5.963188	0.529770	-4.386564
63	1	0	-3.241345	1.131252	4.185807
64	1	0	0.657248	1.998917	-2.428415
65	1	0	-4.391089	0.910668	-0.413647
66	1	0	-0.241107	3.137577	-4.449911
67	1	0	-6.136735	1.391820	-2.051879
68	1	0	-1.527700	2.275392	2.871171
69	1	0	1.122854	1.745912	2.786456
70	1	0	-2.430236	4.307999	-4.342484
71	1	0	-2.816662	3.212200	-0.207401
72	1	0	-3.715664	4.336240	-2.217277
73	1	0	-0.479041	4.726921	0.129418
74	1	0	1.970243	3.527030	4.273259
75	1	0	0.379781	6.501330	1.606881
76	1	0	1.607477	5.920499	3.688016

77	15	0	0.512135	-1.516048	-0.159647
78	15	0	-0.247470	1.710704	0.256129
79	45	0	1.677111	0.375153	-0.041928
80	8	0	2.910077	2.376624	0.082818
81	1	0	2.834962	2.616114	1.020164
82	5	0	4.231839	2.450030	-0.328799
83	8	0	4.438635	2.486547	-1.681942
84	1	0	5.354693	2.311051	-1.928854
85	8	0	5.187363	2.578116	0.647554
86	1	0	6.086107	2.671992	0.308841
87	6	0	3.478722	-0.618983	-0.052442
88	6	0	4.340198	-0.573170	-1.166628
89	6	0	4.004241	-1.224275	1.105463
90	6	0	5.641124	-1.083408	-1.128639
91	1	0	3.986270	-0.133264	-2.098359
92	6	0	5.303797	-1.734514	1.157945
93	1	0	3.385407	-1.310103	1.997823
94	6	0	6.134527	-1.665705	0.039267
95	1	0	6.267428	-1.038202	-2.019508
96	1	0	5.667880	-2.193244	2.076106
97	1	0	7.143905	-2.070171	0.073114

SCF Done: E(RPBE1PBE) = -7547.34371237 A.U. after 1 cycles
Convg = 0.4842D-08 -V/T = 2.0058
Zero-point correction= 0.767095 (Hartree/Particle)
Thermal correction to Energy= 0.841825
Thermal correction to Enthalpy= 0.843007
Thermal correction to Gibbs Free Energy= 0.646156
Sum of electronic and zero-point Energies= -7546.576618
Sum of electronic and thermal Energies= -7546.501887
Sum of electronic and thermal Enthalpies= -7546.500705
Sum of electronic and thermal Free Energies= -7546.697556

	1	2	3
	A	A	A
Frequencies --	7.2181	11.5849	18.2264

BINAP-Rh-Ph (28)



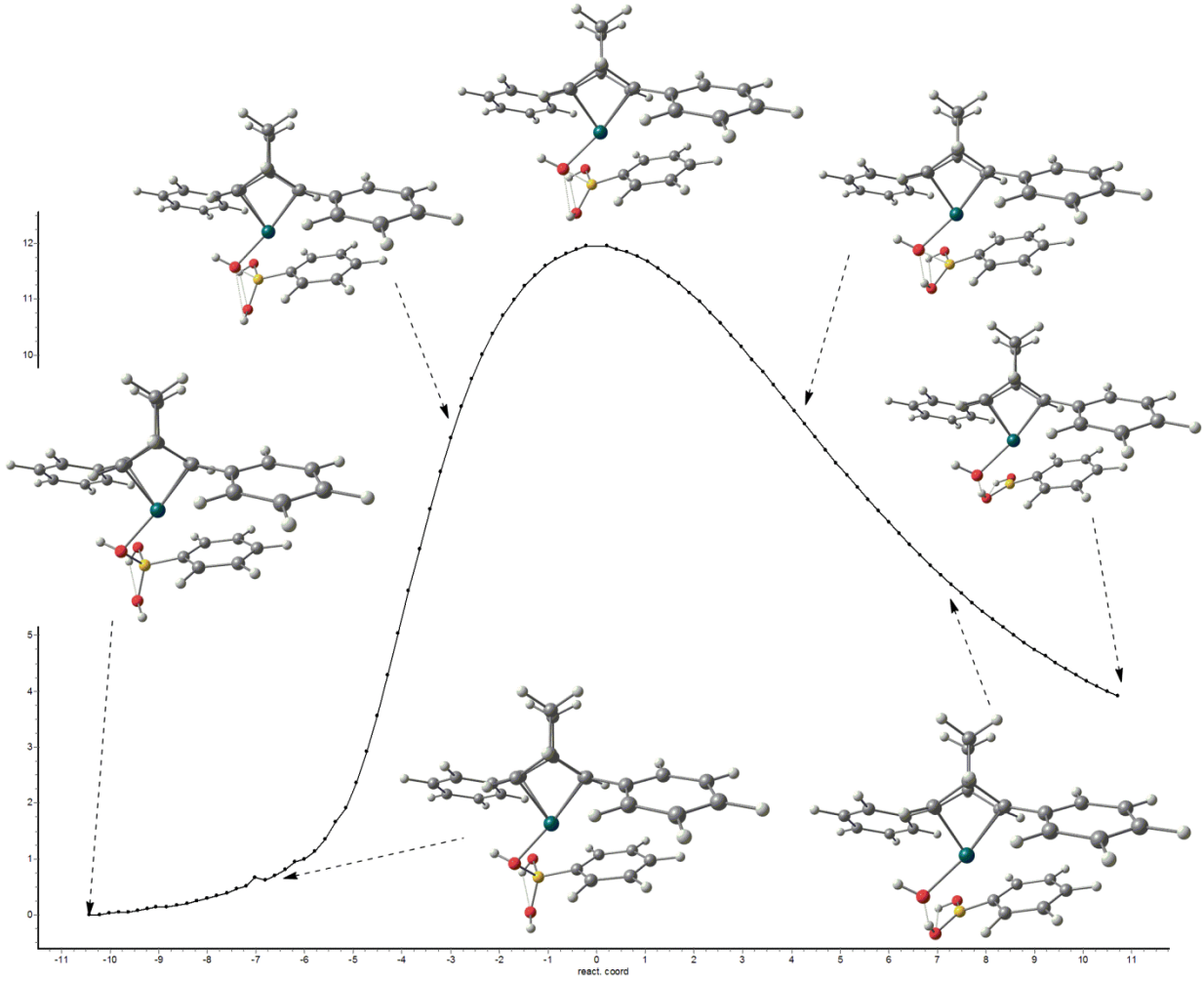
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.338118	-4.269971	-1.871885

2	6	0	3.961492	-3.668413	-2.962862
3	6	0	2.480477	-3.531545	-1.056053
4	6	0	3.734823	-2.317655	-3.226862
5	6	0	0.213938	-3.922664	2.591229
6	6	0	0.846614	-3.398222	3.717666
7	6	0	0.271971	-3.242126	1.377841
8	6	0	2.239528	-2.179124	-1.317828
9	6	0	2.891200	-1.578061	-2.403311
10	6	0	1.535082	-2.189676	3.626239
11	6	0	0.966580	-2.030767	1.275731
12	6	0	-3.541042	-3.449196	2.394810
13	6	0	1.593781	-1.508509	2.411944
14	6	0	-0.509378	-1.782768	-2.489608
15	6	0	-3.686108	-3.019538	3.733688
16	6	0	-1.652446	-1.838438	-3.242622
17	6	0	-2.947785	-2.635737	1.459328
18	6	0	-0.519842	-1.330043	-1.142521
19	6	0	-3.238360	-1.774112	4.101895
20	6	0	-2.894147	-1.439458	-2.698766
21	6	0	-2.472211	-1.341557	1.804694
22	6	0	-1.729589	-0.935083	-0.569932
23	6	0	-4.086003	-1.489823	-3.465109
24	6	0	-2.633134	-0.909532	3.154259
25	6	0	-2.935317	-0.984958	-1.348366
26	6	0	-1.848226	-0.474177	0.850033
27	6	0	-5.288388	-1.107379	-2.921949
28	6	0	-2.200008	0.387768	3.513033
29	6	0	-4.195635	-0.588472	-0.823247
30	6	0	-1.432976	0.795276	1.242151
31	6	0	-5.337910	-0.651485	-1.585474
32	6	0	-1.624432	1.214954	2.583467
33	6	0	-1.007973	2.179411	-2.596542
34	6	0	-1.795862	2.462266	-3.710778
35	6	0	-1.563181	2.198877	-1.312897
36	6	0	-3.147170	2.763449	-3.549829
37	6	0	-2.922528	2.497079	-1.159649
38	6	0	-3.709254	2.780007	-2.272932
39	6	0	-0.277464	3.456730	0.954868
40	6	0	0.727581	3.549304	1.931444
41	6	0	-1.017591	4.602084	0.643430
42	6	0	0.966143	4.748385	2.597529
43	6	0	-0.772329	5.805159	1.305315
44	6	0	0.214795	5.881538	2.285813
45	1	0	3.521732	-5.317665	-1.647390
46	1	0	4.631640	-4.244703	-3.595606
47	1	0	2.016258	-4.018145	-0.204092
48	1	0	-0.338275	-4.856284	2.659057
49	1	0	4.231636	-1.832455	-4.062995
50	1	0	0.794871	-3.926651	4.666178
51	1	0	-0.241807	-3.650719	0.510892
52	1	0	-3.898876	-4.433440	2.103581
53	1	0	0.426412	-2.100543	-2.936543
54	1	0	2.023485	-1.771877	4.502893
55	1	0	-1.610720	-2.194663	-4.269738
56	1	0	-4.153276	-3.673325	4.465518
57	1	0	2.745434	-0.515237	-2.583987
58	1	0	-2.839860	-2.985710	0.437694
59	1	0	2.120935	-0.560086	2.331491
60	1	0	-4.030170	-1.839122	-4.493698
61	1	0	-3.346967	-1.429481	5.127828
62	1	0	-6.198352	-1.152062	-3.514615
63	1	0	-2.336427	0.729326	4.536881
64	1	0	0.043974	1.924673	-2.713828
65	1	0	-4.257467	-0.226300	0.197588

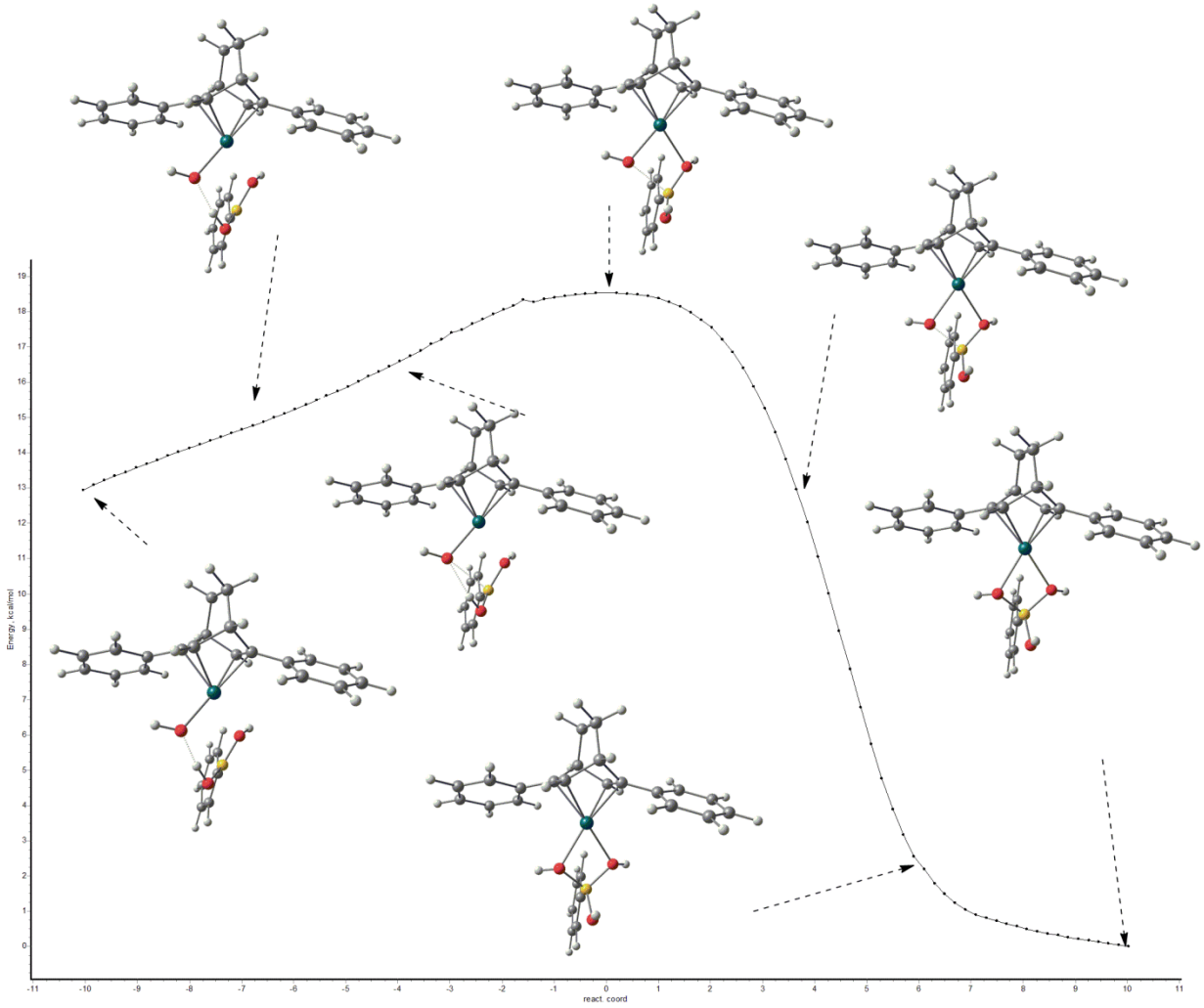
```
     66          1           0       -1.356204    2.438376   -4.704560
     67          1           0       -6.287894   -0.342945   -1.156608
     68          1           0       -1.310027    2.210168    2.881565
     69          1           0        1.323998    2.670211    2.174414
     70          1           0       -3.764979    2.977781   -4.418064
     71          1           0       -3.371409    2.498414   -0.168786
     72          1           0       -4.765419    3.002513   -2.144783
     73          1           0       -1.782562    4.565413   -0.126378
     74          1           0        1.746195    4.798656    3.352717
     75          1           0       -1.354436    6.686583    1.048588
     76          1           0        0.404224    6.820908    2.798588
     77         15           0        1.125606   -1.109671   -0.303258
     78         15           0       -0.442255    1.841146    0.087904
     79         45           0        1.738273    1.008809   -0.169016
     80          6           0        3.727407    0.685655   -0.107941
     81          6           0        4.624695   -0.315826    0.291884
     82          6           0        4.270213    1.939684   -0.438218
     83          6           0        5.995884   -0.064366    0.377377
     84          1           0        4.260039   -1.309820    0.544963
     85          6           0        5.640396    2.201160   -0.362333
     86          1           0        3.612778    2.752705   -0.774007
     87          6           0        6.510898    1.191502    0.049832
     88          1           0        6.669737   -0.855761    0.700941
     89          1           0        6.027209    3.183009   -0.628837
     90          1           0        7.580077    1.380091    0.111237
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -7295.08926670     A.U. after    2 cycles
            Convg  =    0.7524D-08             -V/T =  2.0057
Zero-point correction=                           0.716749 (Hartree/Particle)
 Thermal correction to Energy=                    0.785057
 Thermal correction to Enthalpy=                  0.786239
 Thermal correction to Gibbs Free Energy=         0.602026
 Sum of electronic and zero-point Energies=          -7294.372518
 Sum of electronic and thermal Energies=             -7294.304209
 Sum of electronic and thermal Enthalpies=           -7294.303028
 Sum of electronic and thermal Free Energies=        -7294.487240
                     1                      2                      3
                     A                      A                      A
 Frequencies --    16.4291                24.3499                24.9496
```

IRC PLOTS

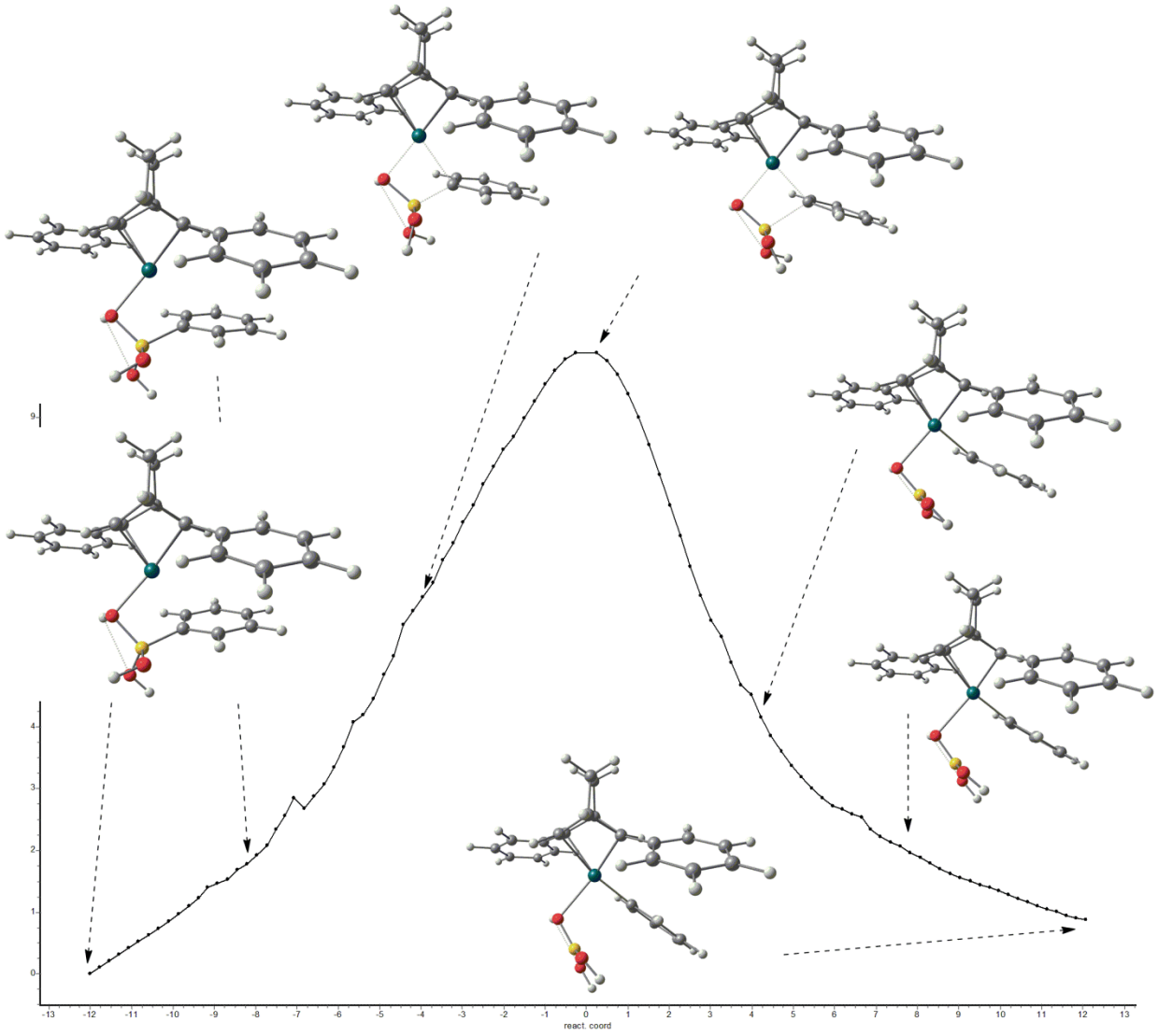
PhBOD-Rh-OH-PhB(OH)$_2$-in-TS (6a)



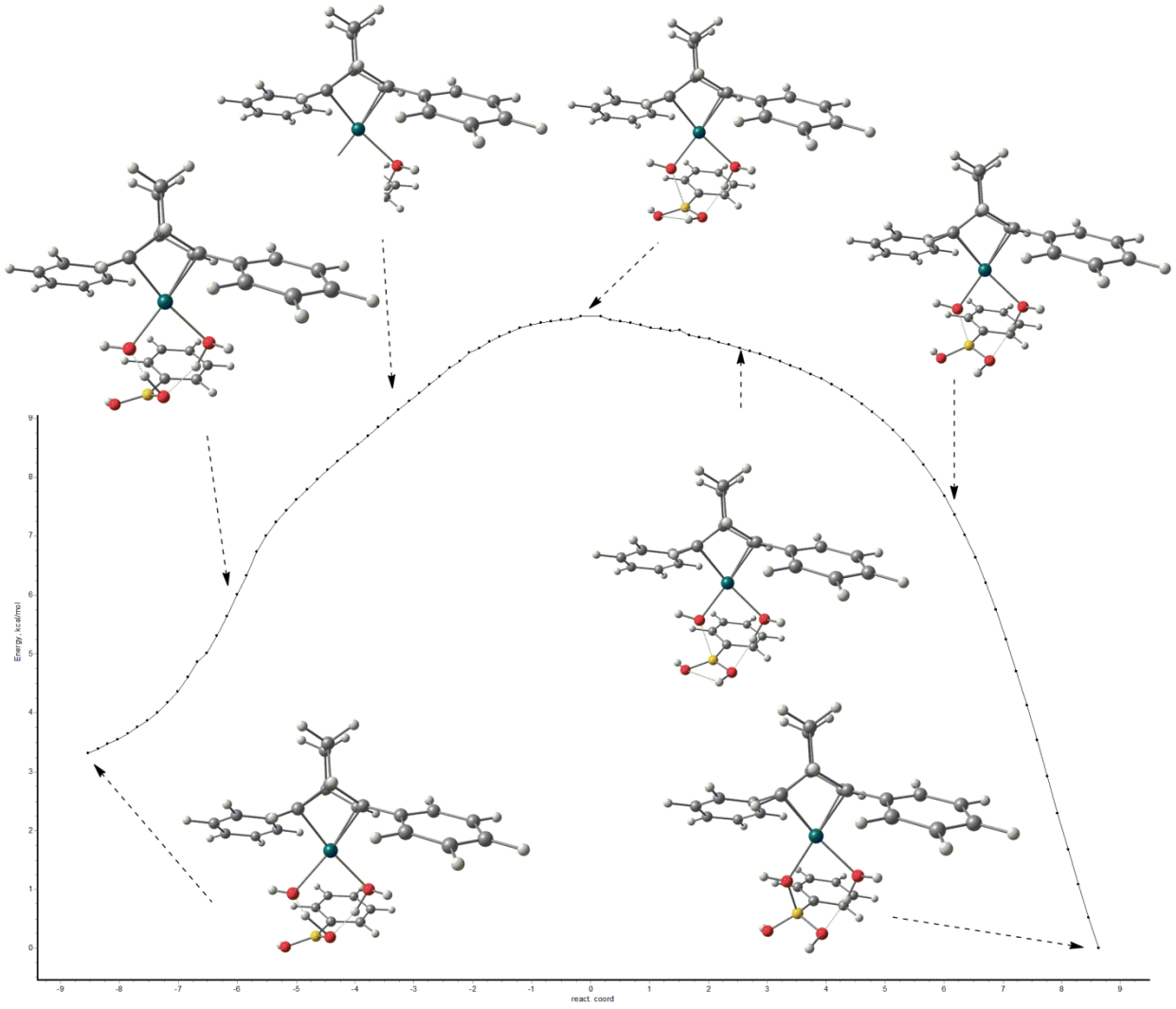
PhBOD-Rh-OH-PhB(OH)$_2$-in-TS (6b)



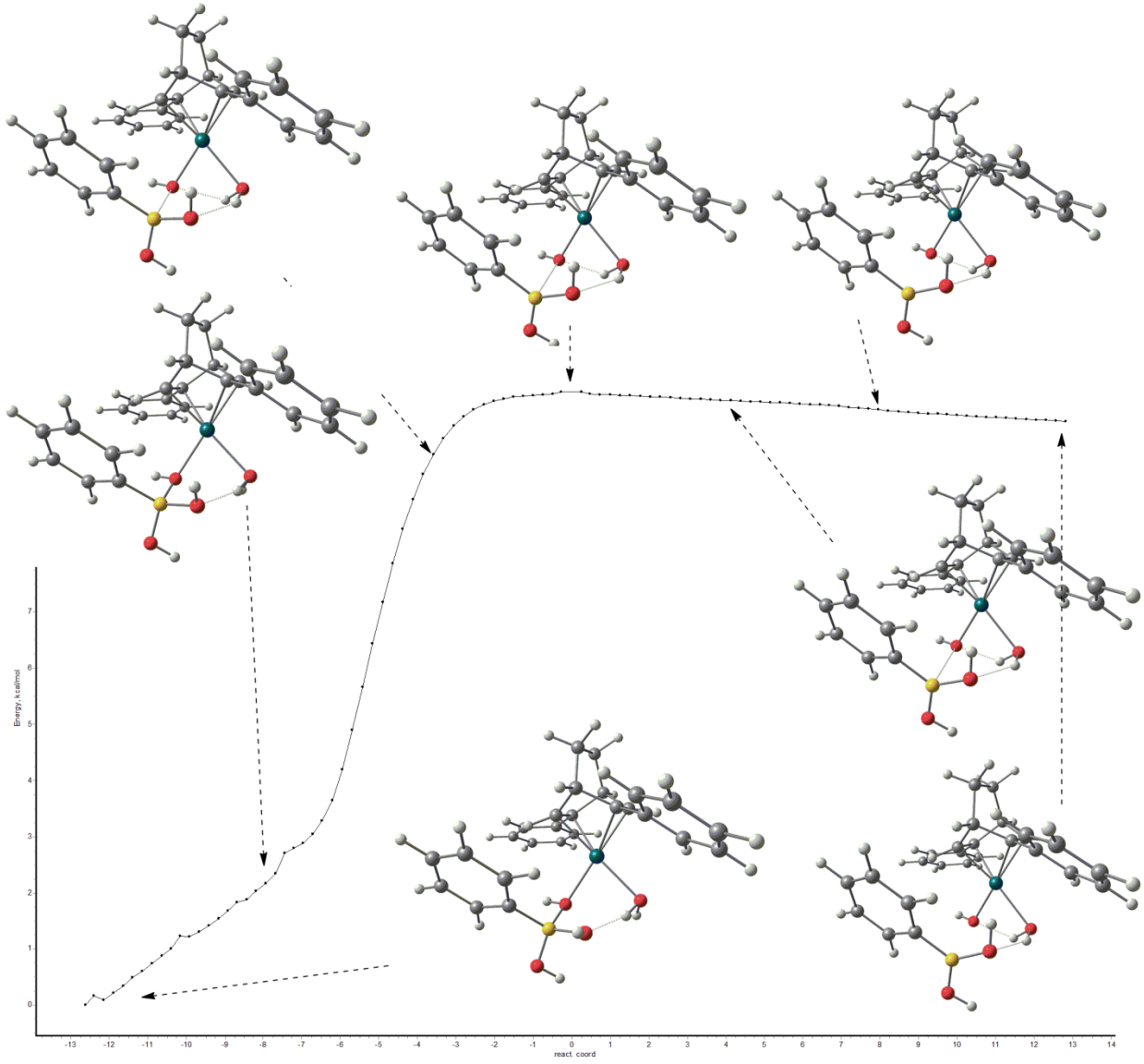
PhBOD-Rh-PhB(OH)$_3$-in-TS (10)



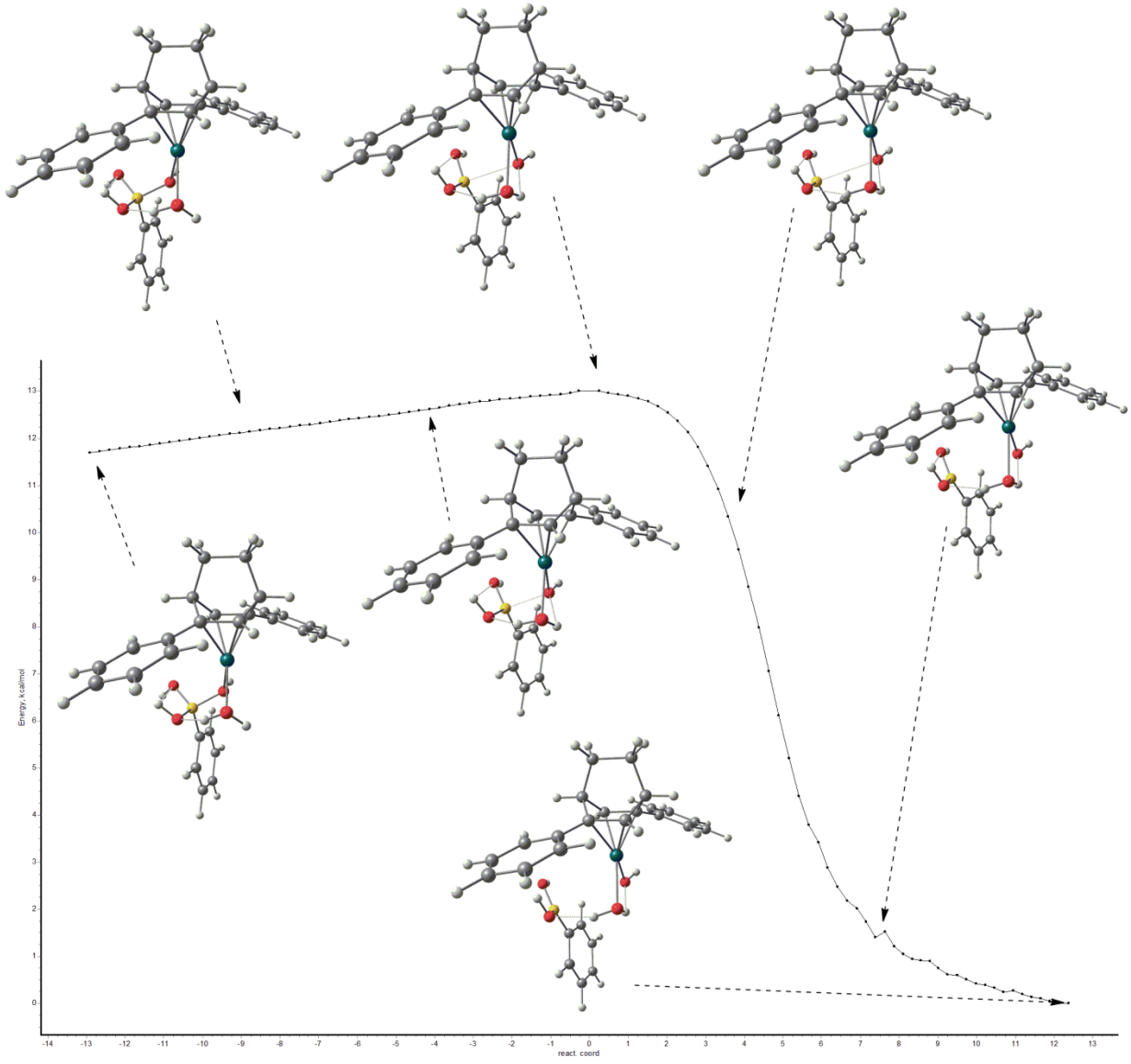
PhBOD-Rh-OH-H_2O-PhB$(OH)_2$-conf1-TS (16a)



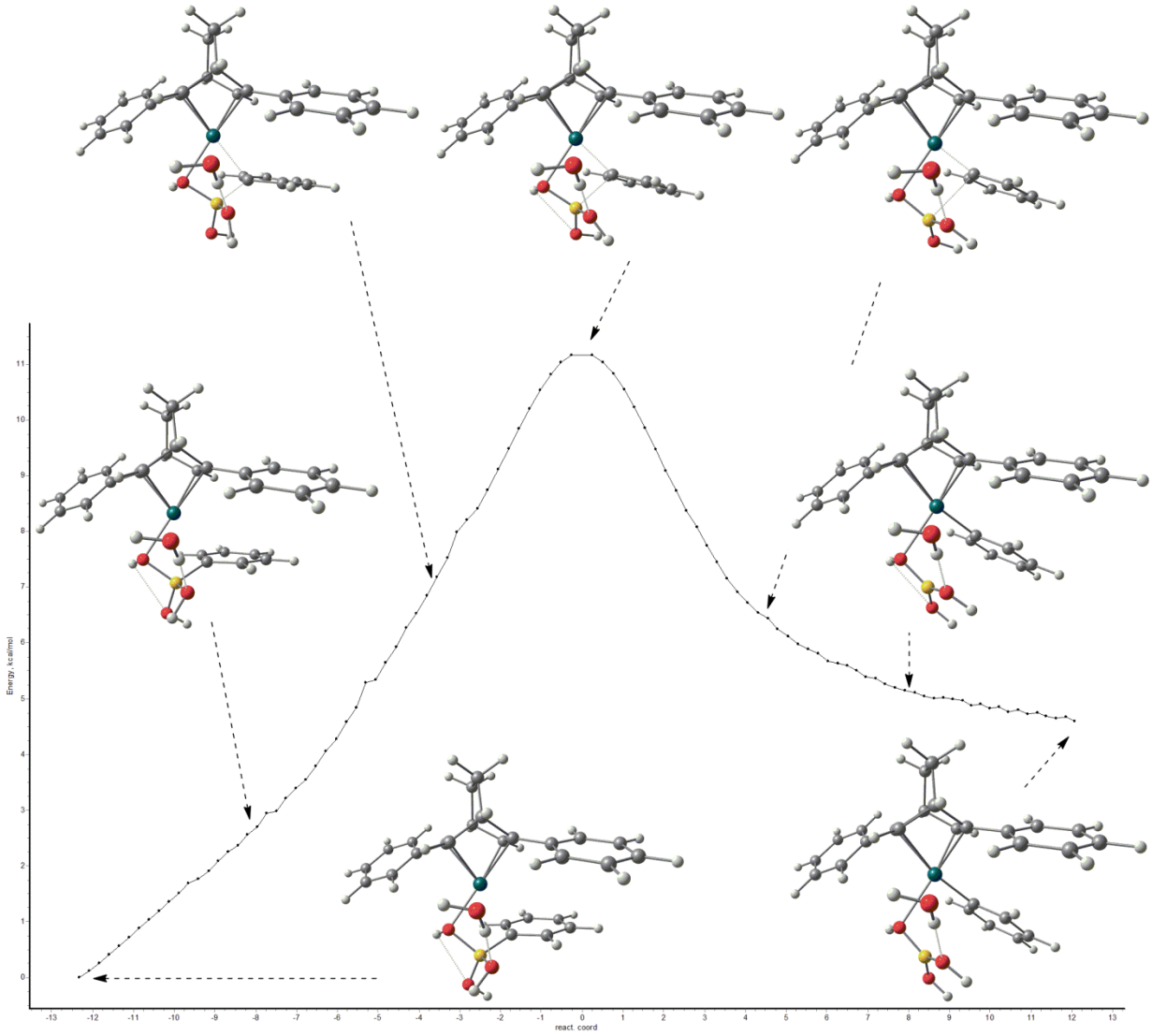
PhBOD-Rh-OH-H_2O-PhB$(OH)_2$-conf2-TS (16b)



PhBOD-Rh-OH-H_2O-PhB$(OH)_2$-conf3-TS (16c)



PhBOD-Rh-PhB(OH)$_3$-H$_2$O-conf1-TS (18a)



PhBOD-Rh-PhB(OH)$_3$-H$_2$O-conf1-TS (18b)