Computational modelling of the enantioselectivity in the asymmetric 1,4-addition of phenylboronic acid to a bulky, doubly pro-chiral maleimide catalyzed by a Rh/chiral diene complex

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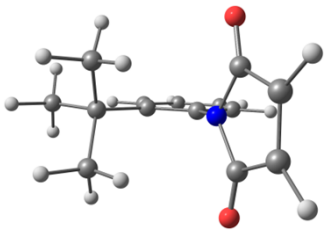
STRUTURE PLOTS, STANDARD COORDINATES, SCF ENERGIES AND THERMOCHEMISTRY, AND FIRST 3 FREQUENCIES

All at PCM(solvent=1,4dioxane, 333.15K)/PBE0/DGDZVP level of theory

(S)-*N*-(2-*tert*-butylphenyl)maleimide (3)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-3.299846	-0.310048	-0.678489
3	6	0	-3.306244	-0.315593	0.655429
4	1	0	-4.103766	-0.525000	-1.372451
5	1	0	-4.116836	-0.536333	1.339739
6	8	0	-1.572332	0.267530	-2.287257
7	6	0	-1.946909	0.069651	1.141226
8	8	0	-1.595710	0.245119	2.287811
9	7	0	-1.141757	0.205245	0.002316
10	6	0	0.160905	0.803947	0.005304
11	6	0	0.169567	2.199337	0.014050
12	6	0	1.355553	0.054419	-0.007410
13	6	0	1.361377	2.911295	0.010064
14	1	0	-0.782113	2.724253	0.023071
15	6	0	2.538876	0.807988	-0.014109
16	6	0	2.554783	2.200037	-0.005633
17	1	0	1.353617	3.997362	0.017157
18	1	0	3.493835	0.297166	-0.027062
19	1	0	3.507060	2.723942	-0.011678
20	6	0	1.423091	-1.483045	-0.000323

21	6	0	0.830171	-2.038110	1.305688
22	1	0	1.346289	-1.626506	2.178649
23	1	0	-0.231651	-1.814682	1.412528
24	1	0	0.942985	-3.127791	1.326004
25	6	0	0.677798	-2.080037	-1.206209
26	1	0	-0.401684	-1.940042	-1.142683
27	1	0	1.020932	-1.637230	-2.146082
28	1	0	0.861478	-3.159043	-1.250614
29	6	0	2.872329	-1.984634	-0.082317
30	1	0	3.372020	-1.660522	-1.001111
31	1	0	3.473693	-1.665462	0.774886
32	1	0	2.867903	-3.079047	-0.082518

SCF Done: E(RPBE1PBE) = -746.921709243 A.U. after 1 cycles
Convg = 0.4680D-08 -V/T = 2.0138
Zero-point correction= 0.263587 (Hartree/Particle)
Thermal correction to Energy= 0.282523
Thermal correction to Enthalpy= 0.283578
Thermal correction to Gibbs Free Energy= 0.213833
Sum of electronic and zero-point Energies= -746.658122
Sum of electronic and thermal Energies= -746.639187
Sum of electronic and thermal Enthalpies= -746.638131
Sum of electronic and thermal Free Energies= -746.707876

	1	2	3
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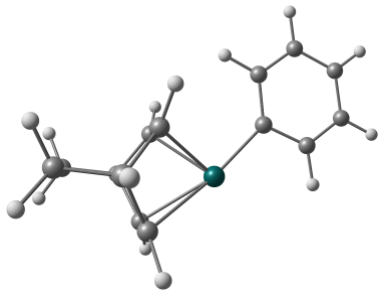
Frequencies --	28.4228	60.4094	75.1633

BOD-Rh-Ph (5)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.019697	-0.719009	-0.001758
2	6	0	-2.196178	-1.108018	-0.682888
3	6	0	-2.262464	0.285093	1.294340
4	6	0	-2.192516	-1.105348	0.689009
5	6	0	-2.268006	0.280928	-1.292135
6	6	0	-3.535723	0.999976	0.774417
7	6	0	-1.037507	0.959637	-0.711923
8	6	0	-1.034495	0.962224	0.706802
9	6	0	-3.538806	0.997892	-0.768877
10	1	0	-2.233649	0.259822	2.385366
11	1	0	-2.243874	0.252658	-2.383205
12	1	0	-4.419580	0.488892	1.169801
13	1	0	-3.553489	2.021938	1.167048
14	1	0	-3.557420	2.018808	-1.164217
15	1	0	-4.424738	0.486624	-1.159374
16	1	0	-0.470900	1.677757	-1.300851
17	1	0	-2.309448	-2.003670	1.290705
18	6	0	1.847622	0.007697	-0.002125
19	6	0	2.292789	1.339120	-0.003666

20	6	0	2.831572	-0.996314	0.001784
21	6	0	3.653283	1.652116	-0.001378
22	1	0	1.572351	2.156639	-0.006616
23	6	0	4.195668	-0.695420	0.004004
24	1	0	2.537244	-2.049587	0.003551
25	6	0	4.610877	0.636206	0.002380
26	1	0	3.970408	2.693301	-0.002621
27	1	0	4.932311	-1.496417	0.007079
28	1	0	5.670349	0.880527	0.003995
29	1	0	-0.464790	1.681839	1.290828
30	1	0	-2.315094	-2.008444	-1.280859

```
SCF Done:  E(RPBE1PBE) =  -5229.13925717     A.U. after    1 cycles
             Convg  =    0.1512D-08             -V/T =  2.0032
Zero-point correction=                           0.251300 (Hartree/Particle)
 Thermal correction to Energy=                    0.266977
 Thermal correction to Enthalpy=                  0.268032
 Thermal correction to Gibbs Free Energy=         0.204957
 Sum of electronic and zero-point Energies=          -5228.887957
 Sum of electronic and thermal Energies=             -5228.872280
 Sum of electronic and thermal Enthalpies=           -5228.871225
 Sum of electronic and thermal Free Energies=        -5228.934300
                     1                      2                      3
                     A                      A                      A
 Frequencies --    47.8894                61.2498                68.6460
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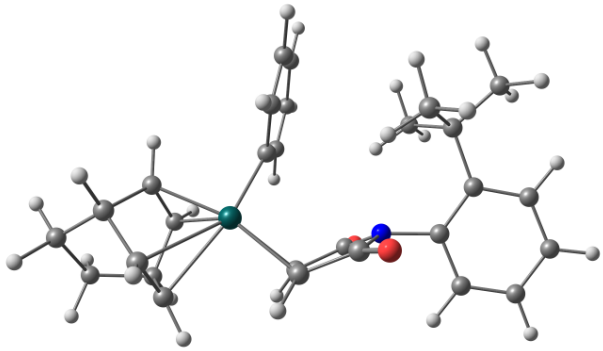
BOD-Rh-Ph-maleimide-syn-MB-“close” (6)



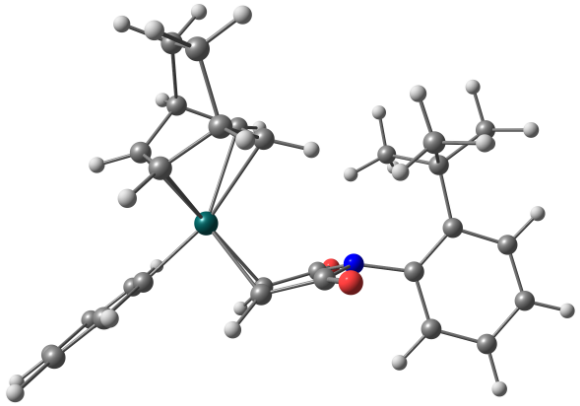
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.803612	-0.214465	-0.292305
2	6	0	3.563036	-1.849500	-0.135636
3	6	0	4.490669	0.156137	-1.096657
4	6	0	3.748180	-1.154454	-1.293438
5	6	0	4.127651	-1.163265	1.090845
6	6	0	5.866695	-0.170565	-0.454188
7	6	0	3.460394	0.198997	1.102013
8	6	0	3.663692	0.918174	-0.070255
9	6	0	5.649544	-0.945332	0.860359
10	1	0	4.605081	0.711079	-2.029050
11	1	0	3.936076	-1.726358	2.005690
12	1	0	6.460770	-0.755626	-1.163256
13	1	0	6.403095	0.766556	-0.276696
14	1	0	6.058455	-0.397343	1.714665
15	1	0	6.148306	-1.918971	0.832901
16	1	0	3.141808	0.663529	2.030388
17	1	0	3.526707	-1.557362	-2.278333
18	6	0	0.775337	1.441636	0.189564

19	6	0	0.473567	2.246838	-0.917369
20	6	0	0.577470	1.969184	1.470161
21	6	0	0.023284	3.557984	-0.750453
22	1	0	0.601376	1.862579	-1.930850
23	6	0	0.122045	3.279670	1.638123
24	1	0	0.770712	1.360689	2.350599
25	6	0	-0.144599	4.083395	0.530929
26	1	0	-0.197735	4.166856	-1.624753
27	1	0	-0.026220	3.670570	2.642549
28	1	0	-0.492833	5.104571	0.664107
29	6	0	0.433610	-1.535635	0.738944
30	6	0	0.342030	-1.801223	-0.638392
31	1	0	1.035377	-2.062882	1.473748
32	1	0	0.871478	-2.572061	-1.190208
33	6	0	-1.052896	-1.516038	-1.064186
34	8	0	-1.553528	-1.735465	-2.149724
35	6	0	-0.916166	-1.066347	1.188815
36	8	0	-1.276525	-0.854030	2.328558
37	7	0	-1.753075	-1.021483	0.056388
38	6	0	-3.180323	-1.204525	0.165153
39	6	0	-4.150054	-0.214414	-0.089521
40	6	0	-3.555215	-2.499884	0.533925
41	6	0	-5.487151	-0.622061	0.036398
42	6	0	-4.887404	-2.867095	0.659766
43	1	0	-2.773103	-3.231261	0.721565
44	6	0	-5.862029	-1.911365	0.400383
45	1	0	-6.277176	0.094230	-0.153814
46	1	0	-5.153488	-3.879942	0.948892
47	1	0	-6.916774	-2.161675	0.481262
48	6	0	-3.827183	1.241095	-0.446396
49	6	0	-3.062229	1.885216	0.719024
50	1	0	-3.651005	1.835629	1.641448
51	1	0	-2.103039	1.402041	0.903688
52	1	0	-2.859401	2.937796	0.497088
53	6	0	-3.002903	1.317919	-1.740233
54	1	0	-2.019709	0.861821	-1.632129
55	1	0	-3.522003	0.820019	-2.565707
56	1	0	-2.848464	2.367555	-2.013930
57	6	0	-5.095507	2.075110	-0.673607
58	1	0	-5.727318	2.128784	0.219284
59	1	0	-4.799975	3.099881	-0.920451
60	1	0	-5.699037	1.700528	-1.507570
61	1	0	3.176164	-2.864753	-0.100957
62	1	0	3.520028	1.992870	-0.136285

SCF Done: E(RPBE1PBE) = -5976.08813232 A.U. after 1 cycles
Convg = 0.2946D-08 -V/T = 2.0046
Zero-point correction= 0.516739 (Hartree/Particle)
Thermal correction to Energy= 0.552877
Thermal correction to Enthalpy= 0.553932
Thermal correction to Gibbs Free Energy= 0.445683
Sum of electronic and zero-point Energies= -5975.571393
Sum of electronic and thermal Energies= -5975.535255
Sum of electronic and thermal Enthalpies= -5975.534200
Sum of electronic and thermal Free Energies= -5975.642450

	1	2	3
	A	A	A
Frequencies --	15.6599	32.0058	46.8603

BOD-Rh-Ph-maleimide-syn-MB-“far” (7)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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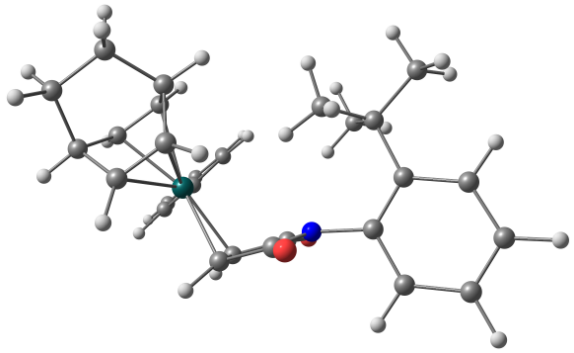
3	6	0	-2.227826	2.792001	-0.964238
4	6	0	-0.822270	2.229298	-1.057892
5	6	0	-1.108142	2.418923	1.331138
6	6	0	-2.140962	4.145573	-0.203985
7	6	0	-2.375573	1.611618	1.153174
8	6	0	-2.981503	1.812372	-0.077854
9	6	0	-1.481013	3.921541	1.170102
10	1	0	-2.696308	2.910403	-1.942477
11	1	0	-0.618538	2.221732	2.285592
12	1	0	-1.567170	4.856267	-0.806822
13	1	0	-3.150968	4.552798	-0.096412
14	1	0	-2.154587	4.206649	1.983996
15	1	0	-0.573390	4.523363	1.276126
16	1	0	-2.892944	1.177698	2.003437
17	1	0	-0.293182	2.128750	-2.002304
18	6	0	-3.170898	-1.210915	-0.050154
19	6	0	-3.693408	-1.735328	-1.241562
20	6	0	-3.800173	-1.552615	1.152851
21	6	0	-4.823376	-2.556167	-1.234372
22	1	0	-3.219427	-1.507867	-2.197534
23	6	0	-4.924837	-2.381947	1.163510
24	1	0	-3.419617	-1.174553	2.100118
25	6	0	-5.443967	-2.883692	-0.029107
26	1	0	-5.212001	-2.946811	-2.172425
27	1	0	-5.396965	-2.634970	2.110490
28	1	0	-6.319114	-3.528240	-0.019641
29	6	0	-0.369105	-1.663461	-0.553973
30	6	0	-0.440039	-1.333189	0.811623
31	1	0	-0.973365	-2.405257	-1.067629
32	1	0	-1.069858	-1.798833	1.562125
33	6	0	0.930819	-0.901967	1.236651
34	8	0	1.299673	-0.599589	2.355414
35	6	0	1.032405	-1.477698	-0.995848
36	8	0	1.527215	-1.753808	-2.070315
37	7	0	1.765861	-0.966981	0.106534
38	6	0	3.186219	-1.203202	0.199860
39	6	0	4.189919	-0.252337	-0.075780
40	6	0	3.517996	-2.512616	0.559034
41	6	0	5.512553	-0.709983	0.019098
42	6	0	4.837926	-2.930179	0.655165
43	1	0	2.712007	-3.214052	0.759131

44	6	0	5.843671	-2.013853	0.373688
45	1	0	6.325147	-0.024633	-0.190008
46	1	0	5.070653	-3.953330	0.936272
47	1	0	6.888920	-2.306754	0.429018
48	6	0	3.917711	1.222359	-0.398128
49	6	0	2.943988	1.369895	-1.578306
50	1	0	3.353027	0.895810	-2.475761
51	1	0	1.971153	0.919881	-1.388236
52	1	0	2.787157	2.432784	-1.794891
53	6	0	3.375726	1.898581	0.873895
54	1	0	2.531948	1.360619	1.310563
55	1	0	4.154281	1.932036	1.643369
56	1	0	3.068645	2.928861	0.658720
57	6	0	5.193519	1.977394	-0.799299
58	1	0	5.666833	1.545051	-1.687118
59	1	0	4.930311	3.012988	-1.038489
60	1	0	5.931708	2.014407	0.007692
61	1	0	0.803663	1.774331	0.278621
62	1	0	-4.016045	1.544169	-0.274077

SCF Done: E(RPBE1PBE) = -5976.09306788 A.U. after 1 cycles
Convg = 0.4745D-08 -V/T = 2.0046
Zero-point correction= 0.517268 (Hartree/Particle)
Thermal correction to Energy= 0.553286
Thermal correction to Enthalpy= 0.554341
Thermal correction to Gibbs Free Energy= 0.446240
Sum of electronic and zero-point Energies= -5975.575800
Sum of electronic and thermal Energies= -5975.539782
Sum of electronic and thermal Enthalpies= -5975.538727
Sum of electronic and thermal Free Energies= -5975.646827

	1	2	3
	A	A	A
Frequencies --	18.2025	35.5729	40.0233

BOD-Rh-Ph-maleimide-3*S*-syn-MB-“parallel” (8)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-2.345628	-2.125536	-1.164226
3	6	0	-1.863516	-2.296081	1.199489
4	6	0	-1.362689	-2.367949	-0.229657
5	6	0	-3.706291	-1.844753	-0.556559
6	6	0	-3.014357	-3.322882	1.371751
7	6	0	-3.436631	-0.659012	0.348628
8	6	0	-2.443391	-0.898123	1.285799
9	6	0	-4.112338	-3.055144	0.324526
10	1	0	-1.066001	-2.459754	1.924267

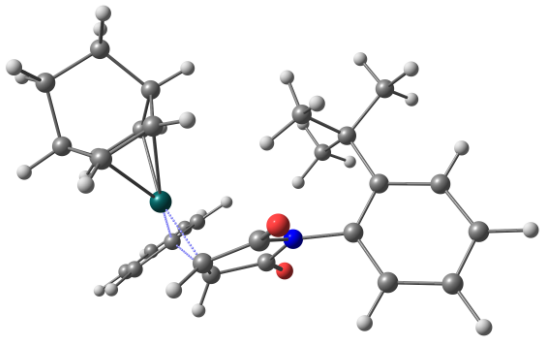
11	1	0	-4.460205	-1.622970	-1.313244
12	1	0	-2.604662	-4.332096	1.265324
13	1	0	-3.410362	-3.241122	2.388738
14	1	0	-5.071602	-2.836105	0.803783
15	1	0	-4.265475	-3.926609	-0.319667
16	1	0	-4.117027	0.184348	0.412496
17	1	0	-0.387803	-2.773800	-0.485608
18	6	0	-1.902654	1.822384	0.075710
19	6	0	-1.386029	2.343912	1.267581
20	6	0	-2.843194	2.593221	-0.622588
21	6	0	-1.797947	3.589670	1.748583
22	1	0	-0.642172	1.787817	1.834616
23	6	0	-3.261124	3.836231	-0.142525
24	1	0	-3.261945	2.227279	-1.559540
25	6	0	-2.739849	4.340979	1.048609
26	1	0	-1.373214	3.974237	2.673574
27	1	0	-3.993094	4.412497	-0.704904
28	1	0	-3.058464	5.310886	1.422115
29	6	0	-0.107209	1.131633	-1.762460
30	6	0	-0.079712	-0.200033	-2.179860
31	1	0	-0.635330	1.955035	-2.226003
32	1	0	-0.576133	-0.624353	-3.046543
33	6	0	1.200092	-0.802236	-1.704704
34	8	0	1.624380	-1.920156	-1.927396
35	6	0	1.171936	1.407423	-1.045396
36	8	0	1.595634	2.472416	-0.649279
37	7	0	1.872255	0.185126	-0.969389
38	6	0	3.266997	0.080045	-0.650580
39	6	0	3.763682	-0.242989	0.628579
40	6	0	4.127074	0.302285	-1.728279
41	6	0	5.160311	-0.328080	0.735455
42	6	0	5.504727	0.214402	-1.585720
43	1	0	3.692099	0.546405	-2.693796
44	6	0	6.020291	-0.107719	-0.336087
45	1	0	5.605271	-0.579356	1.690772
46	1	0	6.158015	0.391423	-2.435344
47	1	0	7.093887	-0.190379	-0.187494
48	6	0	2.891996	-0.451422	1.876782
49	6	0	2.362331	0.911992	2.352400
50	1	0	3.189293	1.577203	2.621664
51	1	0	1.773715	1.416803	1.584555
52	1	0	1.732023	0.777834	3.239826
53	6	0	1.713258	-1.399386	1.604773
54	1	0	0.952891	-0.945466	0.965911
55	1	0	2.048209	-2.330389	1.135808
56	1	0	1.230186	-1.652945	2.555224
57	6	0	3.693751	-1.065698	3.034015
58	1	0	4.485729	-0.403957	3.397403
59	1	0	3.018842	-1.242152	3.877495
60	1	0	4.140577	-2.027313	2.759730
61	1	0	-2.223964	-2.339577	-2.222345
62	1	0	-2.279435	-0.255604	2.145751

SCF Done: E(RPBE1PBE) = -5976.09666762 A.U. after 1 cycles
Convg = 0.3347D-08 -V/T = 2.0046
Zero-point correction= 0.517865 (Hartree/Particle)
Thermal correction to Energy= 0.553696
Thermal correction to Enthalpy= 0.554751
Thermal correction to Gibbs Free Energy= 0.447427
Sum of electronic and zero-point Energies= -5975.578803
Sum of electronic and thermal Energies= -5975.542971
Sum of electronic and thermal Enthalpies= -5975.541916

1	2	3
A	A	A

Frequencies -- 22.4883 30.8721 46.3834 Sum of electronic and thermal Free Energies= -5975.649240

BOD-Rh-Ph-maleimide-3*S*-syn-CR-TS (9)



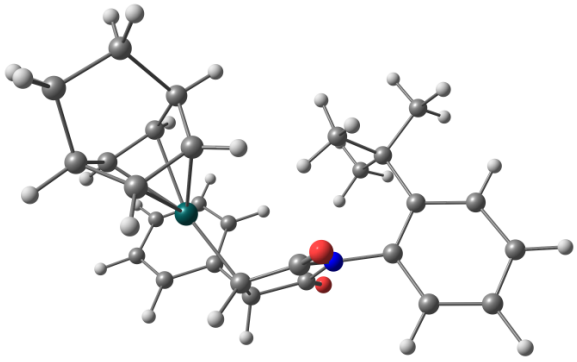
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.509921	-0.090414	-0.579194
2	6	0	-2.486874	-1.873744	-1.378969
3	6	0	-1.962618	-2.411478	0.928322
4	6	0	-1.488492	-2.289632	-0.508785
5	6	0	-3.818912	-1.631211	-0.690009
6	6	0	-3.150512	-3.408587	0.977700
7	6	0	-3.473734	-0.603691	0.373756
8	6	0	-2.481173	-1.018948	1.234787
9	6	0	-4.258764	-2.943441	0.011715
10	1	0	-1.158712	-2.710438	1.602009
11	1	0	-4.580787	-1.267977	-1.381766
12	1	0	-2.786800	-4.405649	0.709899
13	1	0	-3.522273	-3.466019	2.005620
14	1	0	-5.197266	-2.762720	0.545233
15	1	0	-4.461789	-3.702375	-0.750514
16	1	0	-4.091796	0.271219	0.555111
17	1	0	-0.555562	-2.731917	-0.848887
18	6	0	-1.564848	1.947926	0.082090
19	6	0	-1.146926	2.279327	1.375833
20	6	0	-2.614940	2.683388	-0.493198
21	6	0	-1.800299	3.279259	2.096406
22	1	0	-0.311546	1.757484	1.833834
23	6	0	-3.272700	3.673832	0.231547
24	1	0	-2.921514	2.478412	-1.517726
25	6	0	-2.868756	3.975923	1.533476
26	1	0	-1.465549	3.516826	3.103460
27	1	0	-4.092932	4.221427	-0.227019
28	1	0	-3.369656	4.759741	2.095386
29	6	0	-0.117488	1.582920	-1.298465
30	6	0	-0.103106	0.366026	-2.065915
31	1	0	-0.399767	2.524834	-1.756006
32	1	0	-0.530620	0.276838	-3.061770
33	6	0	1.175964	-0.320732	-1.809190
34	8	0	1.625825	-1.322425	-2.332275
35	6	0	1.212948	1.634861	-0.572117
36	8	0	1.663040	2.559058	0.073073
37	7	0	1.876173	0.437390	-0.833017
38	6	0	3.274652	0.241066	-0.577945
39	6	0	3.788667	-0.446827	0.540016
40	6	0	4.120942	0.777481	-1.550524
41	6	0	5.186331	-0.554699	0.599711
42	6	0	5.500427	0.656769	-1.457431

43	1	0	3.674049	1.295877	-2.394661
44	6	0	6.032689	-0.020946	-0.367326
45	1	0	5.642983	-1.077448	1.431397
46	1	0	6.142362	1.081184	-2.224118
47	1	0	7.108156	-0.139422	-0.263092
48	6	0	2.930808	-1.025941	1.675704
49	6	0	2.368696	0.128997	2.521190
50	1	0	3.177939	0.702610	2.984862
51	1	0	1.779069	0.824663	1.922108
52	1	0	1.730513	-0.267802	3.319645
53	6	0	1.775947	-1.884212	1.135499
54	1	0	0.999057	-1.282463	0.659975
55	1	0	2.130740	-2.622529	0.409632
56	1	0	1.306630	-2.422569	1.966617
57	6	0	3.753597	-1.923772	2.611235
58	1	0	4.538157	-1.374054	3.140052
59	1	0	3.090355	-2.341656	3.375230
60	1	0	4.213439	-2.762019	2.077209
61	1	0	-2.410904	-1.977273	-2.458331
62	1	0	-2.242818	-0.502417	2.160410

SCF Done: E(RPBE1PBE) = -5976.08012742 A.U. after 1 cycles
Convg = 0.5341D-08 -V/T = 2.0046
Zero-point correction= 0.516796 (Hartree/Particle)
Thermal correction to Energy= 0.551968
Thermal correction to Enthalpy= 0.553023
Thermal correction to Gibbs Free Energy= 0.447361
Sum of electronic and zero-point Energies= -5975.563331
Sum of electronic and thermal Energies= -5975.528160
Sum of electronic and thermal Enthalpies= -5975.527105
Sum of electronic and thermal Free Energies= -5975.632766

	1	2	3
	A	A	A
Frequencies --	-299.0730	25.5626	33.0361

BOD-Rh-α-Rh-(3*S*,*S*$_a$)-Phsuccinimide (10)



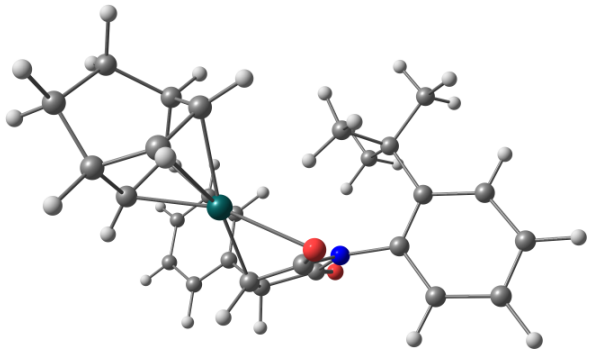
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.682680	0.141072	-0.423270
2	6	0	-2.517451	-1.489189	-1.513377
3	6	0	-2.241497	-2.306830	0.765825
4	6	0	-1.601314	-1.985622	-0.572855
5	6	0	-3.929680	-1.383120	-0.965598
6	6	0	-3.385293	-3.330770	0.551808
7	6	0	-3.743024	-0.478421	0.242353
8	6	0	-2.845401	-0.970048	1.164047
9	6	0	-4.392211	-2.779784	-0.477955

10	1	0	-1.511282	-2.662592	1.494805
11	1	0	-4.624513	-0.959381	-1.693117
12	1	0	-2.952350	-4.276907	0.211540
13	1	0	-3.872880	-3.527066	1.512291
14	1	0	-5.392595	-2.691103	-0.041840
15	1	0	-4.476266	-3.446577	-1.342143
16	1	0	-4.400277	0.363725	0.442651
17	1	0	-0.630581	-2.382195	-0.860422
18	6	0	-0.909990	2.290130	-0.029045
19	6	0	-0.753379	2.051662	1.350795
20	6	0	-2.173249	2.733091	-0.482725
21	6	0	-1.785413	2.338973	2.247620
22	1	0	0.203249	1.711772	1.734095
23	6	0	-3.197963	3.024194	0.420804
24	1	0	-2.318714	2.930232	-1.542243
25	6	0	-3.001448	2.841470	1.788914
26	1	0	-1.625513	2.180144	3.310622
27	1	0	-4.145977	3.403313	0.048637
28	1	0	-3.793655	3.083488	2.492011
29	6	0	0.191571	2.054285	-1.059782
30	6	0	-0.133990	0.731793	-1.731109
31	1	0	0.250906	2.913021	-1.740026
32	1	0	-0.534492	0.763037	-2.746993
33	6	0	1.068966	-0.095858	-1.629716
34	8	0	1.325667	-1.171305	-2.145887
35	6	0	1.579798	1.858688	-0.465633
36	8	0	2.217920	2.679926	0.169574
37	7	0	2.000570	0.580348	-0.780139
38	6	0	3.352170	0.125176	-0.629677
39	6	0	3.818500	-0.638905	0.460371
40	6	0	4.198306	0.475097	-1.683810
41	6	0	5.168671	-1.017216	0.404808
42	6	0	5.531553	0.089883	-1.702322
43	1	0	3.786087	1.058909	-2.502412
44	6	0	6.015124	-0.668558	-0.643246
45	1	0	5.586258	-1.611216	1.208824
46	1	0	6.174182	0.372739	-2.531250
47	1	0	7.052010	-0.994406	-0.626054
48	6	0	2.975274	-1.017209	1.689210
49	6	0	2.774602	0.236580	2.557868
50	1	0	3.733535	0.593270	2.948627
51	1	0	2.333686	1.061919	1.996598
52	1	0	2.125729	0.004109	3.410858
53	6	0	1.613488	-1.615213	1.299446
54	1	0	0.935233	-0.884857	0.854923
55	1	0	1.732542	-2.441306	0.591385
56	1	0	1.121483	-2.005928	2.197611
57	6	0	3.678230	-2.068947	2.561539
58	1	0	4.609535	-1.698963	3.000814
59	1	0	3.020211	-2.334610	3.395188
60	1	0	3.894839	-2.986855	2.004758
61	1	0	-2.317665	-1.496303	-2.582036
62	1	0	-2.724487	-0.551058	2.159577

SCF Done: E(RPBE1PBE) = -5976.13420320 A.U. after 1 cycles
Convg = 0.4278D-08 -V/T = 2.0046
Zero-point correction= 0.519116 (Hartree/Particle)
Thermal correction to Energy= 0.554342
Thermal correction to Enthalpy= 0.555397
Thermal correction to Gibbs Free Energy= 0.449584
Sum of electronic and zero-point Energies= -5975.615087
Sum of electronic and thermal Energies= -5975.579861
Sum of electronic and thermal Enthalpies= -5975.578806
Sum of electronic and thermal Free Energies= -5975.684619

	1	2	3
	A	A	A
Frequencies --	23.6864	30.0919	42.2668

BOD-Rh-(3*S*,*S*$_a$)-Rh-oxa-π-allyl (10)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.286816	-0.959042	-0.788354
2	6	0	-2.642553	-2.685291	-0.678265
3	6	0	-2.754846	-1.562056	1.470389
4	6	0	-2.034351	-2.538603	0.558420
5	6	0	-3.895218	-1.839710	-0.837943
6	6	0	-4.221589	-2.019207	1.663187
7	6	0	-3.343327	-0.442356	-0.611991
8	6	0	-2.723980	-0.293276	0.636657
9	6	0	-4.899438	-2.189380	0.287696
10	1	0	-2.241331	-1.438296	2.425704
11	1	0	-4.342038	-1.951249	-1.827563
12	1	0	-4.231694	-2.958609	2.225406
13	1	0	-4.746875	-1.275686	2.271408
14	1	0	-5.775467	-1.538929	0.197215
15	1	0	-5.247735	-3.217572	0.145641
16	1	0	-3.671884	0.405584	-1.207668
17	1	0	-1.263806	-3.212040	0.924951
18	6	0	-0.659541	2.899806	-0.364391
19	6	0	-0.666080	2.663226	1.013913
20	6	0	-1.518522	3.874912	-0.877097
21	6	0	-1.512065	3.380486	1.856052
22	1	0	-0.001713	1.915620	1.440698
23	6	0	-2.374314	4.589217	-0.039244
24	1	0	-1.517678	4.081301	-1.945561
25	6	0	-2.373912	4.344491	1.332422
26	1	0	-1.495499	3.189062	2.926099
27	1	0	-3.034689	5.343698	-0.458941
28	1	0	-3.032732	4.905507	1.989907
29	6	0	0.222859	2.108769	-1.303885
30	6	0	-0.266767	0.735131	-1.720996
31	1	0	0.385732	2.722788	-2.199477
32	1	0	-0.784550	0.633458	-2.675940
33	6	0	0.801259	-0.173356	-1.471327
34	8	0	0.729761	-1.419828	-1.648780
35	6	0	1.627664	1.842116	-0.749249
36	8	0	2.412417	2.668527	-0.329462
37	7	0	1.866474	0.471498	-0.812894
38	6	0	3.149940	-0.142362	-0.619833
39	6	0	3.600739	-0.684638	0.602299
40	6	0	3.943474	-0.181174	-1.768571

41	6	0	4.882227	-1.255739	0.575021
42	6	0	5.208176	-0.752593	-1.757262
43	1	0	3.546093	0.249610	-2.683789
44	6	0	5.676222	-1.295549	-0.567084
45	1	0	5.285889	-1.693744	1.479703
46	1	0	5.810658	-0.772778	-2.660890
47	1	0	6.660604	-1.754055	-0.519707
48	6	0	2.813785	-0.652818	1.923144
49	6	0	2.804513	0.781558	2.478131
50	1	0	3.823603	1.118701	2.694573
51	1	0	2.371254	1.499430	1.780356
52	1	0	2.231122	0.815057	3.412132
53	6	0	1.374427	-1.160233	1.741382
54	1	0	0.753404	-0.481727	1.153658
55	1	0	1.358216	-2.137629	1.249375
56	1	0	0.897522	-1.263818	2.722609
57	6	0	3.458903	-1.549345	2.991582
58	1	0	4.454204	-1.204035	3.287489
59	1	0	2.836631	-1.527639	3.891804
60	1	0	3.533145	-2.592349	2.665637
61	1	0	-2.392376	-3.484481	-1.371665
62	1	0	-2.530138	0.679443	1.080035

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SCF Done:  E(RPBE1PBE) =  -5976.12542495     A.U. after    1 cycles
             Convg  =    0.1757D-08             -V/T =  2.0045
Zero-point correction=                           0.519126 (Hartree/Particle)
 Thermal correction to Energy=                    0.554363
 Thermal correction to Enthalpy=                  0.555418
 Thermal correction to Gibbs Free Energy=         0.447431
 Sum of electronic and zero-point Energies=          -5975.606299
 Sum of electronic and thermal Energies=             -5975.571062
 Sum of electronic and thermal Enthalpies=           -5975.570007
 Sum of electronic and thermal Free Energies=        -5975.677994
                     1                      2                      3
                     A                      A                      A
 Frequencies --     7.0088                25.4167                33.4538
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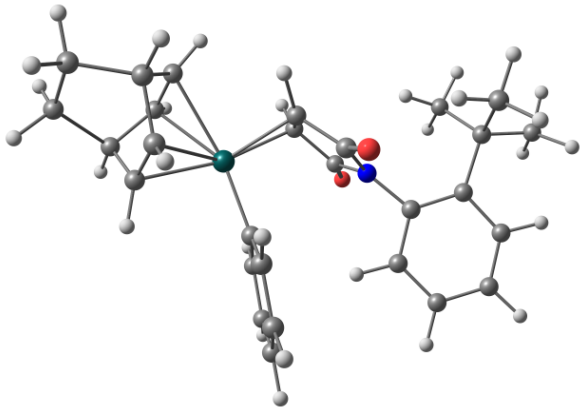
BOD-Rh-Ph-maleimide-anti-MB-“close” (12)



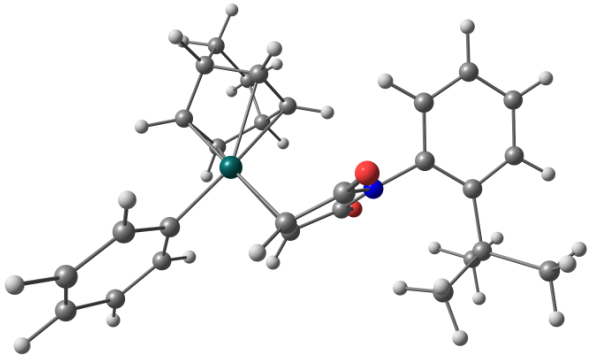
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.877430	-0.128034	-0.397977
2	6	0	3.412113	-1.992684	-0.160533
3	6	0	4.697272	-0.042942	-0.753337
4	6	0	3.861598	-1.231538	-1.194962
5	6	0	3.836761	-1.486832	1.203225

6	6	0	5.905437	-0.591013	0.055366
7	6	0	3.334552	-0.056762	1.256901
8	6	0	3.802333	0.726198	0.208941
9	6	0	5.391213	-1.445682	1.230519
10	1	0	5.023021	0.570321	-1.594938
11	1	0	3.436757	-2.096276	2.015178
12	1	0	6.544107	-1.179789	-0.610480
13	1	0	6.500908	0.254669	0.412616
14	1	0	5.715102	-1.033787	2.191062
15	1	0	5.773960	-2.469188	1.172378
16	1	0	2.925604	0.361071	2.171835
17	1	0	3.756470	-1.514646	-2.239182
18	6	0	0.920777	1.579238	0.015112
19	6	0	0.699554	2.364471	-1.126483
20	6	0	0.649013	2.133491	1.270450
21	6	0	0.249349	3.682025	-1.014304
22	1	0	0.868236	1.951483	-2.122279
23	6	0	0.185834	3.447194	1.382263
24	1	0	0.775134	1.539544	2.172422
25	6	0	-0.006353	4.229619	0.243604
26	1	0	0.083556	4.273195	-1.912248
27	1	0	-0.029900	3.857149	2.366483
28	1	0	-0.364830	5.251859	0.333690
29	6	0	0.331870	-1.424955	0.347072
30	6	0	0.206441	-1.373220	-1.053984
31	1	0	0.809759	-2.202859	0.934824
32	1	0	0.588025	-2.096574	-1.768608
33	6	0	-1.076496	-0.688171	-1.362973
34	8	0	-1.549308	-0.429407	-2.452434
35	6	0	-0.878805	-0.771302	0.934724
36	8	0	-1.137494	-0.616293	2.113234
37	7	0	-1.707733	-0.421698	-0.133312
38	6	0	-2.939278	0.300703	-0.019233
39	6	0	-4.195954	-0.336887	0.082596
40	6	0	-2.825881	1.690744	-0.039726
41	6	0	-5.303780	0.521075	0.164197
42	6	0	-3.946164	2.506272	0.046587
43	1	0	-1.836329	2.126092	-0.127934
44	6	0	-5.195900	1.908624	0.149085
45	1	0	-6.298720	0.099610	0.239562
46	1	0	-3.837824	3.587227	0.030592
47	1	0	-6.095281	2.515995	0.214628
48	6	0	-4.419485	-1.859521	0.161507
49	6	0	-3.595914	-2.642489	-0.876295
50	1	0	-3.696590	-2.214170	-1.877761
51	1	0	-2.534900	-2.683375	-0.626495
52	1	0	-3.952985	-3.677483	-0.912442
53	6	0	-4.065167	-2.348107	1.577135
54	1	0	-3.027437	-2.136095	1.841311
55	1	0	-4.700247	-1.861535	2.324910
56	1	0	-4.225251	-3.430585	1.648225
57	6	0	-5.891836	-2.223900	-0.092671
58	1	0	-6.242855	-1.862256	-1.065086
59	1	0	-5.992887	-3.313661	-0.086981
60	1	0	-6.562125	-1.843399	0.683556
61	1	0	2.911068	-2.947834	-0.295331
62	1	0	3.792045	1.812395	0.233583

SCF Done: E(RPBE1PBE) = -5976.09757709 A.U. after 1 cycles
Convg = 0.4837D-08 -V/T = 2.0046
Zero-point correction= 0.517108 (Hartree/Particle)
Thermal correction to Energy= 0.553170
Thermal correction to Enthalpy= 0.554225
Thermal correction to Gibbs Free Energy= 0.445957

```
 Sum of electronic and zero-point Energies=          -5975.580469
 Sum of electronic and thermal Energies=             -5975.544407
 Sum of electronic and thermal Enthalpies=           -5975.543352
 Sum of electronic and thermal Free Energies=        -5975.651620
                      1                      2                      3
                      A                      A                      A
 Frequencies --    20.7189                27.5478                39.4409
```

BOD-Rh-Ph-maleimide-anti-MB-“far” (13)



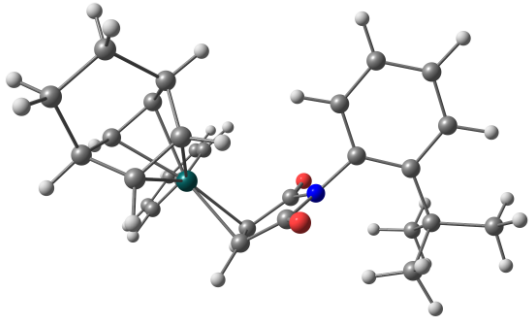
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.713320	0.091265	-0.308307
2	6	0	1.138963	2.398675	-0.914287
3	6	0	1.293298	2.347367	1.492470
4	6	0	0.461451	2.176268	0.241569
5	6	0	2.588675	2.790009	-0.693702
6	6	0	1.835040	3.806944	1.493290
7	6	0	3.181840	1.665592	0.139923
8	6	0	2.479245	1.424160	1.309516
9	6	0	2.596790	4.075638	0.181160
10	1	0	0.724351	2.122705	2.395011
11	1	0	3.126889	2.939066	-1.631057
12	1	0	0.992984	4.495677	1.610325
13	1	0	2.485083	3.940642	2.363320
14	1	0	3.635208	4.359733	0.377383
15	1	0	2.137229	4.893388	-0.382556
16	1	0	4.196545	1.310594	-0.020058
17	1	0	-0.612168	2.034041	0.299151
18	6	0	3.053686	-1.376810	-0.069919
19	6	0	3.506842	-1.895932	1.148697
20	6	0	3.634315	-1.859158	-1.252009
21	6	0	4.519069	-2.858689	1.185477
22	1	0	3.072808	-1.555056	2.086742
23	6	0	4.653074	-2.814024	-1.216886
24	1	0	3.292658	-1.494394	-2.221677
25	6	0	5.099469	-3.318729	0.004381
26	1	0	4.854354	-3.249584	2.143886
27	1	0	5.090650	-3.169851	-2.147177
28	1	0	5.886889	-4.067400	0.034172
29	6	0	0.248896	-1.214912	0.563674
30	6	0	0.264410	-1.448556	-0.824435
31	1	0	0.705501	-1.829254	1.332145
32	1	0	0.779353	-2.258637	-1.330978
33	6	0	-0.998025	-0.924435	-1.393270
34	8	0	-1.386415	-0.952590	-2.546037
35	6	0	-1.027190	-0.504063	0.880547
36	8	0	-1.417871	-0.107108	1.963319

37	7	0	-1.737367	-0.390527	-0.319642
38	6	0	-2.978323	0.298696	-0.465891
39	6	0	-4.204155	-0.204595	0.010448
40	6	0	-2.907984	1.537014	-1.115589
41	6	0	-5.302533	0.666517	-0.106275
42	6	0	-4.023648	2.346269	-1.257723
43	1	0	-1.951660	1.854224	-1.520834
44	6	0	-5.230250	1.911203	-0.716591
45	1	0	-6.263112	0.355507	0.290212
46	1	0	-3.948449	3.302311	-1.768073
47	1	0	-6.120301	2.531629	-0.781188
48	6	0	-4.472366	-1.586529	0.638805
49	6	0	-3.380757	-2.640717	0.400758
50	1	0	-3.113232	-2.727130	-0.656733
51	1	0	-2.477771	-2.460830	0.985024
52	1	0	-3.766554	-3.614563	0.720736
53	6	0	-4.665747	-1.412717	2.155049
54	1	0	-3.765153	-0.999929	2.617836
55	1	0	-5.500951	-0.740087	2.375896
56	1	0	-4.882389	-2.382301	2.618301
57	6	0	-5.761101	-2.177618	0.030018
58	1	0	-5.676513	-2.270740	-1.057659
59	1	0	-5.930885	-3.177096	0.443304
60	1	0	-6.653887	-1.588217	0.250822
61	1	0	0.668214	2.441238	-1.893378
62	1	0	2.892870	0.867437	2.144961

SCF Done: E(RPBE1PBE) = -5976.09916605 A.U. after 1 cycles
Convg = 0.2326D-08 -V/T = 2.0046
Zero-point correction= 0.517350 (Hartree/Particle)
Thermal correction to Energy= 0.553411
Thermal correction to Enthalpy= 0.554466
Thermal correction to Gibbs Free Energy= 0.445995
Sum of electronic and zero-point Energies= -5975.581816
Sum of electronic and thermal Energies= -5975.545755
Sum of electronic and thermal Enthalpies= -5975.544700
Sum of electronic and thermal Free Energies= -5975.653171

	1	2	3
	A	A	A
Frequencies --	24.8081	34.1540	35.5878

BOD-Rh-Ph-maleimide-anti-MB-“parallel” (14)



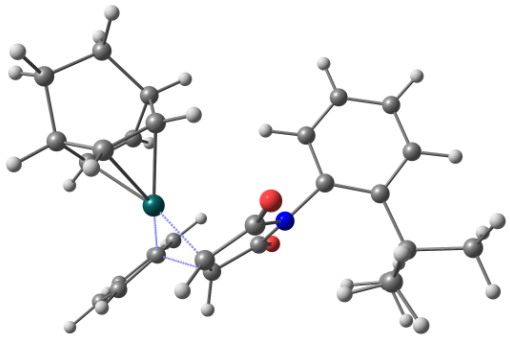
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.713320	0.091265	-0.308307
2	6	0	1.138963	2.398675	-0.914287
3	6	0	1.293298	2.347367	1.492470
4	6	0	0.461451	2.176268	0.241569

5	6	0	2.588675	2.790009	-0.693702
6	6	0	1.835040	3.806944	1.493290
7	6	0	3.181840	1.665592	0.139923
8	6	0	2.479245	1.424160	1.309516
9	6	0	2.596790	4.075638	0.181160
10	1	0	0.724351	2.122705	2.395011
11	1	0	3.126889	2.939066	-1.631057
12	1	0	0.992984	4.495677	1.610325
13	1	0	2.485083	3.940642	2.363320
14	1	0	3.635208	4.359733	0.377383
15	1	0	2.137229	4.893388	-0.382556
16	1	0	4.196545	1.310594	-0.020058
17	1	0	-0.612168	2.034041	0.299151
18	6	0	3.053686	-1.376810	-0.069919
19	6	0	3.506842	-1.895932	1.148697
20	6	0	3.634315	-1.859158	-1.252009
21	6	0	4.519069	-2.858689	1.185477
22	1	0	3.072808	-1.555056	2.086742
23	6	0	4.653074	-2.814024	-1.216886
24	1	0	3.292658	-1.494394	-2.221677
25	6	0	5.099469	-3.318729	0.004381
26	1	0	4.854354	-3.249584	2.143886
27	1	0	5.090650	-3.169851	-2.147177
28	1	0	5.886889	-4.067400	0.034172
29	6	0	0.248896	-1.214912	0.563674
30	6	0	0.264410	-1.448556	-0.824435
31	1	0	0.705501	-1.829254	1.332145
32	1	0	0.779353	-2.258637	-1.330978
33	6	0	-0.998025	-0.924435	-1.393270
34	8	0	-1.386415	-0.952590	-2.546037
35	6	0	-1.027190	-0.504063	0.880547
36	8	0	-1.417871	-0.107108	1.963319
37	7	0	-1.737367	-0.390527	-0.319642
38	6	0	-2.978323	0.298696	-0.465891
39	6	0	-4.204155	-0.204595	0.010448
40	6	0	-2.907984	1.537014	-1.115589
41	6	0	-5.302533	0.666517	-0.106275
42	6	0	-4.023648	2.346269	-1.257723
43	1	0	-1.951660	1.854224	-1.520834
44	6	0	-5.230250	1.911203	-0.716591
45	1	0	-6.263112	0.355507	0.290212
46	1	0	-3.948449	3.302311	-1.768073
47	1	0	-6.120301	2.531629	-0.781188
48	6	0	-4.472366	-1.586529	0.638805
49	6	0	-3.380757	-2.640717	0.400758
50	1	0	-3.113232	-2.727130	-0.656733
51	1	0	-2.477771	-2.460830	0.985024
52	1	0	-3.766554	-3.614563	0.720736
53	6	0	-4.665747	-1.412717	2.155049
54	1	0	-3.765153	-0.999929	2.617836
55	1	0	-5.500951	-0.740087	2.375896
56	1	0	-4.882389	-2.382301	2.618301
57	6	0	-5.761101	-2.177618	0.030018
58	1	0	-5.676513	-2.270740	-1.057659
59	1	0	-5.930885	-3.177096	0.443304
60	1	0	-6.653887	-1.588217	0.250822
61	1	0	0.668214	2.441238	-1.893378
62	1	0	2.892870	0.867437	2.144961

SCF Done: E(RPBE1PBE) = -5976.09916605 A.U. after 1 cycles
Convg = 0.2326D-08 -V/T = 2.0046
Zero-point correction= 0.517350 (Hartree/Particle)
Thermal correction to Energy= 0.553411
Thermal correction to Enthalpy= 0.554466

```
 Thermal correction to Gibbs Free Energy=          0.445995
 Sum of electronic and zero-point Energies=         -5975.581816
 Sum of electronic and thermal Energies=            -5975.545755
 Sum of electronic and thermal Enthalpies=          -5975.544700
 Sum of electronic and thermal Free Energies=       -5975.653171
                      1                      2                      3
                      A                      A                      A
 Frequencies --    24.8081                34.1540                35.5878
```

BOD-Rh-Ph-maleimide-3*S*-anti-CR-TS" (15)



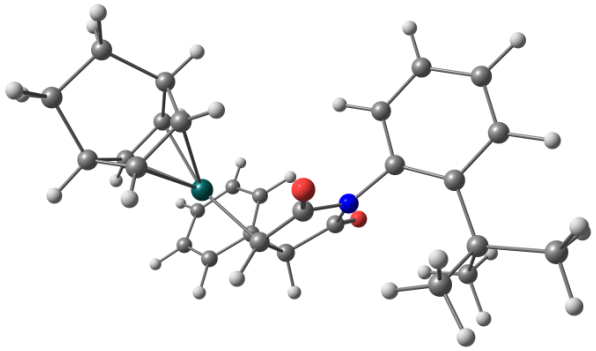
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.593240	-0.074091	-0.522146
2	6	0	-2.314580	-1.927966	-1.428572
3	6	0	-1.919930	-2.472477	0.903102
4	6	0	-1.351687	-2.269039	-0.489367
5	6	0	-3.713413	-1.831353	-0.842052
6	6	0	-3.005646	-3.579817	0.840414
7	6	0	-3.554655	-0.803927	0.266281
8	6	0	-2.592858	-1.144466	1.193562
9	6	0	-4.075823	-3.197888	-0.201892
10	1	0	-1.147054	-2.713965	1.635017
11	1	0	-4.452514	-1.525033	-1.584141
12	1	0	-2.526451	-4.529897	0.584198
13	1	0	-3.447769	-3.698785	1.834584
14	1	0	-5.066179	-3.123296	0.258230
15	1	0	-4.142681	-3.951992	-0.992420
16	1	0	-4.268166	0.001692	0.416637
17	1	0	-0.356033	-2.609035	-0.764034
18	6	0	-1.877815	1.917869	0.170572
19	6	0	-1.798907	2.280190	1.520041
20	6	0	-2.799307	2.578551	-0.658485
21	6	0	-2.669968	3.237225	2.039935
22	1	0	-1.054194	1.825694	2.166588
23	6	0	-3.679116	3.521843	-0.129784
24	1	0	-2.832618	2.355145	-1.723835
25	6	0	-3.619071	3.854379	1.224069
26	1	0	-2.602523	3.504111	3.092115
27	1	0	-4.400996	4.009252	-0.781090
28	1	0	-4.291865	4.602212	1.635352
29	6	0	-0.100433	1.629249	-0.793671
30	6	0	-0.029802	0.588147	-1.782162
31	1	0	-0.200862	2.672821	-1.070809
32	1	0	-0.312804	0.715940	-2.823678
33	6	0	1.122660	-0.270366	-1.464054
34	8	0	1.540987	-1.249031	-2.055101
35	6	0	1.006119	1.344404	0.197729
36	8	0	1.263035	1.952128	1.218444

37	7	0	1.729286	0.259528	-0.295134
38	6	0	2.675628	-0.481223	0.483254
39	6	0	4.072611	-0.327245	0.368338
40	6	0	2.113084	-1.402428	1.367905
41	6	0	4.842092	-1.171228	1.184067
42	6	0	2.905184	-2.214979	2.167218
43	1	0	1.028623	-1.465662	1.414200
44	6	0	4.286036	-2.096149	2.063335
45	1	0	5.922835	-1.112696	1.138940
46	1	0	2.452330	-2.926871	2.851759
47	1	0	4.939623	-2.720497	2.667167
48	6	0	4.767204	0.712712	-0.528377
49	6	0	4.278503	0.646827	-1.985220
50	1	0	4.327318	-0.371783	-2.380630
51	1	0	3.254542	1.003360	-2.098365
52	1	0	4.913949	1.286438	-2.607698
53	6	0	4.514947	2.120556	0.039053
54	1	0	3.453404	2.369534	0.077140
55	1	0	4.909401	2.207855	1.056778
56	1	0	5.018618	2.867135	-0.585917
57	6	0	6.288170	0.501541	-0.565065
58	1	0	6.557758	-0.488519	-0.948133
59	1	0	6.731746	1.245151	-1.234427
60	1	0	6.756143	0.637096	0.414909
61	1	0	-2.142067	-1.996143	-2.499421
62	1	0	-2.478241	-0.634290	2.145720

SCF Done: E(RPBE1PBE) = -5976.08170052 A.U. after 1 cycles
Convg = 0.3667D-08 -V/T = 2.0046
Zero-point correction= 0.516723 (Hartree/Particle)
Thermal correction to Energy= 0.551912
Thermal correction to Enthalpy= 0.552967
Thermal correction to Gibbs Free Energy= 0.446238
Sum of electronic and zero-point Energies= -5975.564977
Sum of electronic and thermal Energies= -5975.529788
Sum of electronic and thermal Enthalpies= -5975.528733
Sum of electronic and thermal Free Energies= -5975.635462

	1	2	3
	A	A	A
Frequencies --	-296.5431	16.7602	24.9420

BOD-α-Rh-(3*S*,*R*$_a$)- Phsuccinimide (16)



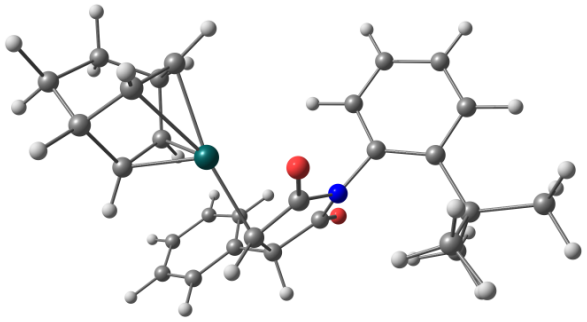
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.829900	0.104589	-0.357659
2	6	0	-2.536850	-1.601197	-1.427642
3	6	0	-2.731724	-2.189128	0.929789

4	6	0	-1.839080	-2.030290	-0.288503
5	6	0	-4.016288	-1.382985	-1.166480
6	6	0	-3.873196	-3.185234	0.600867
7	6	0	-4.003206	-0.367503	-0.034433
8	6	0	-3.320209	-0.796454	1.082295
9	6	0	-4.641716	-2.702551	-0.646454
10	1	0	-2.170345	-2.498470	1.813388
11	1	0	-4.541175	-1.008933	-2.047476
12	1	0	-3.439124	-4.176698	0.437005
13	1	0	-4.538548	-3.263773	1.466748
14	1	0	-5.697492	-2.528182	-0.414818
15	1	0	-4.606422	-3.450426	-1.445033
16	1	0	-4.636426	0.515906	-0.040642
17	1	0	-0.855569	-2.489907	-0.350792
18	6	0	0.275271	1.830340	-0.683429
19	6	0	-0.037713	0.527715	-1.399292
20	1	0	0.594421	2.654346	-1.335842
21	1	0	-0.253959	0.567362	-2.469129
22	6	0	1.031995	-0.410837	-1.062269
23	8	0	1.235117	-1.545639	-1.463950
24	6	0	1.448703	1.489975	0.222457
25	8	0	1.926577	2.196740	1.093115
26	7	0	1.890340	0.225902	-0.114996
27	6	0	2.878446	-0.494251	0.630033
28	6	0	4.244356	-0.539490	0.281048
29	6	0	2.385146	-1.186017	1.737529
30	6	0	5.057139	-1.318400	1.118988
31	6	0	3.220189	-1.943804	2.547096
32	1	0	1.321144	-1.121107	1.951686
33	6	0	4.570972	-2.006780	2.226877
34	1	0	6.115837	-1.400847	0.904952
35	1	0	2.821050	-2.475737	3.406217
36	1	0	5.254564	-2.593707	2.835046
37	6	0	4.872789	0.219646	-0.901464
38	6	0	4.122461	-0.039556	-2.219391
39	1	0	3.983241	-1.109391	-2.398109
40	1	0	3.140939	0.434192	-2.242688
41	1	0	4.701379	0.374944	-3.052189
42	6	0	4.884807	1.727998	-0.598901
43	1	0	3.882794	2.131324	-0.446328
44	1	0	5.464322	1.940688	0.305405
45	1	0	5.346281	2.268430	-1.433648
46	6	0	6.330140	-0.206550	-1.135341
47	1	0	6.419135	-1.277894	-1.344795
48	1	0	6.720353	0.332532	-2.004259
49	1	0	6.981313	0.039734	-0.290831
50	1	0	-2.142736	-1.723008	-2.433376
51	1	0	-3.358732	-0.282265	2.039086
52	6	0	-0.997697	2.220821	0.065209
53	6	0	-2.106291	2.659678	-0.694931
54	6	0	-1.148994	2.136069	1.463678
55	6	0	-3.279828	3.090472	-0.069249
56	1	0	-2.011485	2.746523	-1.774822
57	6	0	-2.327900	2.561372	2.079429
58	1	0	-0.314750	1.807858	2.075493
59	6	0	-3.387840	3.054762	1.319481
60	1	0	-4.102416	3.461404	-0.674787
61	1	0	-2.407046	2.517846	3.162394
62	1	0	-4.294307	3.403718	1.806481

SCF Done: E(RPBE1PBE) = -5976.13478880 A.U. after 1 cycles
Convg = 0.2642D-08 -V/T = 2.0046
Zero-point correction= 0.519211 (Hartree/Particle)
Thermal correction to Energy= 0.554448

```
 Thermal correction to Enthalpy=                  0.555503
 Thermal correction to Gibbs Free Energy=         0.448721
 Sum of electronic and zero-point Energies=          -5975.615578
 Sum of electronic and thermal Energies=             -5975.580341
 Sum of electronic and thermal Enthalpies=           -5975.579286
 Sum of electronic and thermal Free Energies=        -5975.686068
                     1                      2                      3
                     A                      A                      A
 Frequencies --    18.4501                28.0808                33.5935
```

BOD-α-Rh-(3*S*,R_a)- Rh-oxa-π-allyl (17)



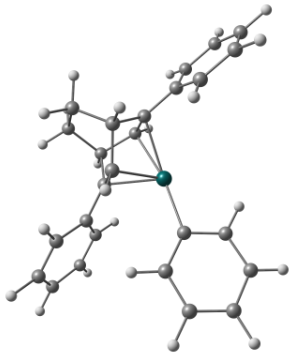
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.257552	-0.966628	-0.749689
2	6	0	-2.616306	-2.702643	-0.794493
3	6	0	-2.883769	-1.651709	1.376350
4	6	0	-2.098672	-2.597165	0.485445
5	6	0	-3.853529	-1.848216	-1.016240
6	6	0	-4.359841	-2.116262	1.445746
7	6	0	-3.323643	-0.459233	-0.702696
8	6	0	-2.797569	-0.353832	0.591888
9	6	0	-4.937859	-2.233317	0.020172
10	1	0	-2.442219	-1.561330	2.370602
11	1	0	-4.226774	-1.925518	-2.039080
12	1	0	-4.406455	-3.076709	1.969184
13	1	0	-4.929071	-1.397225	2.043626
14	1	0	-5.802125	-1.573880	-0.109192
15	1	0	-5.278828	-3.253499	-0.183756
16	1	0	-3.611517	0.410616	-1.287318
17	1	0	-1.349782	-3.278856	0.880742
18	6	0	0.168254	2.097962	-0.733257
19	6	0	-0.156542	0.793662	-1.434780
20	1	0	0.602805	2.800141	-1.461410
21	1	0	-0.479758	0.803060	-2.475416
22	6	0	0.850975	-0.140021	-1.059971
23	8	0	0.845898	-1.364965	-1.369804
24	6	0	1.327510	1.724900	0.190209
25	8	0	1.835705	2.412824	1.054304
26	7	0	1.737115	0.432739	-0.129852
27	6	0	2.613228	-0.347047	0.693654
28	6	0	3.982768	-0.525539	0.412348
29	6	0	2.008130	-0.942519	1.801068
30	6	0	4.685782	-1.333028	1.318878
31	6	0	2.736199	-1.734335	2.678742
32	1	0	0.945352	-0.775074	1.959581
33	6	0	4.089567	-1.926904	2.428063
34	1	0	5.742018	-1.514688	1.161295
35	1	0	2.253809	-2.191373	3.538243

36	1	0	4.690351	-2.541946	3.093161
37	6	0	4.714390	0.111469	-0.781813
38	6	0	4.038231	-0.250363	-2.115596
39	1	0	3.903162	-1.331594	-2.214664
40	1	0	3.063462	0.223948	-2.234938
41	1	0	4.666914	0.091162	-2.945383
42	6	0	4.761221	1.639776	-0.617016
43	1	0	3.768227	2.089652	-0.592380
44	1	0	5.270481	1.917571	0.311301
45	1	0	5.312825	2.083673	-1.453706
46	6	0	6.168045	-0.375184	-0.877479
47	1	0	6.234002	-1.460331	-1.009978
48	1	0	6.639729	0.090327	-1.748539
49	1	0	6.762061	-0.092692	-0.002575
50	1	0	-2.314355	-3.477213	-1.495049
51	1	0	-2.643108	0.603145	1.083146
52	6	0	-1.006150	2.796595	-0.074319
53	6	0	-2.039504	3.252341	-0.902317
54	6	0	-1.127142	2.982625	1.304736
55	6	0	-3.169827	3.865637	-0.369920
56	1	0	-1.959465	3.121733	-1.979855
57	6	0	-2.260747	3.596666	1.840890
58	1	0	-0.330360	2.663414	1.968158
59	6	0	-3.287106	4.038309	1.009860
60	1	0	-3.958926	4.211748	-1.032766
61	1	0	-2.335081	3.733639	2.916842
62	1	0	-4.166759	4.518606	1.430185

SCF Done: E(RPBE1PBE) = -5976.12835925 A.U. after 1 cycles
Convg = 0.6450D-08 -V/T = 2.0045
Zero-point correction= 0.519080 (Hartree/Particle)
Thermal correction to Energy= 0.554361
Thermal correction to Enthalpy= 0.555416
Thermal correction to Gibbs Free Energy= 0.447178
Sum of electronic and zero-point Energies= -5975.609279
Sum of electronic and thermal Energies= -5975.573998
Sum of electronic and thermal Enthalpies= -5975.572943
Sum of electronic and thermal Free Energies= -5975.681181

	1	2	3
	A	A	A
Frequencies --	15.7714	21.9614	24.5421

(*S*)-PhBOD-Rh-Ph (18)



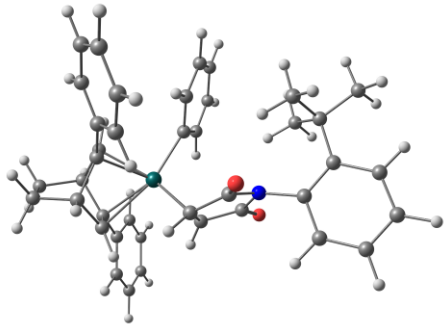
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.206720	0.509214	-0.361142
2	6	0	-1.919445	-0.971722	0.029043

3	6	0	-0.008440	-2.219558	-0.809043
4	6	0	2.978251	-1.243142	-1.305008
5	6	0	-3.252792	-0.335344	0.028785
6	6	0	-4.182054	-0.595421	-0.990222
7	6	0	-1.243611	-1.394031	-1.096611
8	6	0	-1.229743	-1.427028	1.313236
9	6	0	-4.869489	1.173279	1.043925
10	6	0	5.133589	-1.610521	-0.276318
11	6	0	-0.390485	-3.447085	0.051914
12	6	0	0.162420	-0.834257	1.187896
13	6	0	-5.429887	0.021822	-0.995787
14	6	0	0.862201	-1.285173	0.034858
15	6	0	3.122187	-1.650330	1.062215
16	6	0	-3.622090	0.555868	1.049054
17	6	0	-1.142098	-2.973038	1.311624
18	6	0	-5.780125	0.910126	0.020866
19	6	0	2.335503	-1.382465	-0.066229
20	6	0	4.508674	-1.760384	0.959495
21	6	0	4.360075	-1.352388	-1.410129
22	1	0	2.386125	-1.011893	-2.187425
23	1	0	6.214156	-1.693074	-0.357845
24	1	0	2.643806	-1.782997	2.029274
25	1	0	5.099908	-1.967814	1.847903
26	1	0	4.839362	-1.224829	-2.377390
27	1	0	-3.931071	-1.304339	-1.774764
28	1	0	-5.129890	1.866262	1.839768
29	1	0	-6.136375	-0.200126	-1.791555
30	1	0	-2.916015	0.787432	1.842554
31	1	0	-6.755542	1.389075	0.018235
32	1	0	0.501015	-2.522579	-1.725766
33	1	0	-1.745945	-1.067754	2.204835
34	1	0	-1.010371	-4.122453	-0.546474
35	1	0	0.521022	-3.994006	0.314789
36	1	0	-0.629415	-3.297442	2.223188
37	1	0	-2.154836	-3.387527	1.348735
38	1	0	0.682074	-0.457130	2.066909
39	1	0	-1.638908	-1.296549	-2.105266
40	6	0	1.107521	1.975398	0.021753
41	6	0	2.375971	2.008517	0.618208
42	6	0	0.576748	3.193417	-0.436214
43	6	0	3.080672	3.206842	0.747818
44	1	0	2.834927	1.089703	0.977934
45	6	0	1.274055	4.397697	-0.313374
46	1	0	-0.414605	3.219782	-0.901693
47	6	0	2.534604	4.405119	0.283287
48	1	0	4.066080	3.206320	1.209961
49	1	0	0.835891	5.324315	-0.678792
50	1	0	3.087767	5.335793	0.384050

SCF Done: E(RPBE1PBE) = -5690.72654212 A.U. after 1 cycles
Convg = 0.5485D-08 -V/T = 2.0042
Zero-point correction= 0.413722 (Hartree/Particle)
Thermal correction to Energy= 0.441537
Thermal correction to Enthalpy= 0.442592
Thermal correction to Gibbs Free Energy= 0.350523
Sum of electronic and zero-point Energies= -5690.312820
Sum of electronic and thermal Energies= -5690.285005
Sum of electronic and thermal Enthalpies= -5690.283950
Sum of electronic and thermal Free Energies= -5690.376019

	1	2	3
	A	A	A
Frequencies --	25.9052	31.2170	40.3296

(*S*)-PhBOD-Rh-Ph-maleimide-syn-MB-“close” (19)



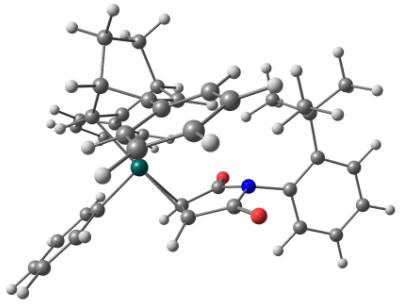
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.178466	-0.122706	0.106995
2	6	0	3.419653	-0.928417	-0.266040
3	6	0	3.133263	1.029020	-1.672891
4	6	0	0.816330	3.176023	-1.797815
5	6	0	3.557998	-2.351213	0.097957
6	6	0	3.801889	-3.326020	-0.881361
7	6	0	2.971667	-0.459270	-1.469949
8	6	0	3.945202	0.202071	0.614660
9	6	0	3.538936	-4.109284	1.775833
10	6	0	0.437220	5.470259	-1.142874
11	6	0	4.638049	1.378209	-1.507022
12	6	0	2.816904	1.215623	0.709707
13	6	0	3.906246	-4.670641	-0.538385
14	6	0	2.393373	1.705198	-0.522221
15	6	0	1.965225	4.085242	0.114643
16	6	0	3.437273	-2.764438	1.433049
17	6	0	5.128927	0.863266	-0.142160
18	6	0	3.773368	-5.068512	0.791685
19	6	0	1.712302	2.998104	-0.733572
20	6	0	1.333182	5.309872	-0.087420
21	6	0	0.180091	4.396607	-1.996802
22	1	0	0.577551	2.339585	-2.448737
23	1	0	-0.059804	6.424012	-1.298831
24	1	0	2.669723	3.973671	0.934174
25	1	0	1.543539	6.140973	0.580691
26	1	0	-0.529019	4.504984	-2.812890
27	1	0	3.931797	-3.025417	-1.917613
28	1	0	3.429194	-4.409999	2.814193
29	1	0	4.101276	-5.409689	-1.310905
30	1	0	3.237835	-2.032266	2.211763
31	1	0	3.855032	-6.118303	1.059392
32	1	0	2.757826	1.353297	-2.644731
33	1	0	4.260562	-0.150375	1.597354
34	1	0	5.198194	0.921331	-2.328507
35	1	0	4.761391	2.462246	-1.593621
36	1	0	5.520770	1.679609	0.472324
37	1	0	5.933100	0.129830	-0.258557
38	1	0	2.602767	1.726361	1.645236
39	1	0	2.662230	-1.111793	-2.282218
40	6	0	-0.099016	0.680798	1.416519
41	6	0	-0.624265	1.974357	1.467001
42	6	0	-0.201092	-0.130437	2.558641
43	6	0	-1.196254	2.459979	2.646166
44	1	0	-0.584905	2.619165	0.592692
45	6	0	-0.751016	0.363849	3.743230
46	1	0	0.148179	-1.163989	2.535960

47	6	0	-1.246917	1.666480	3.791619
48	1	0	-1.597215	3.471358	2.667414
49	1	0	-0.810656	-0.278469	4.619306
50	1	0	-1.685086	2.052710	4.708657
51	6	0	-0.084570	-1.688620	-0.719085
52	6	0	-0.151443	-0.537606	-1.528106
53	1	0	0.569901	-2.546146	-0.854075
54	1	0	0.416637	-0.341991	-2.432627
55	6	0	-1.578793	-0.088392	-1.557196
56	8	0	-2.051280	0.794297	-2.246445
57	6	0	-1.462650	-1.963954	-0.226455
58	8	0	-1.844158	-2.917036	0.421957
59	7	0	-2.316172	-0.953643	-0.732944
60	6	0	-3.706826	-1.235024	-1.001760
61	6	0	-4.802603	-0.726017	-0.276154
62	6	0	-3.902737	-2.092945	-2.088611
63	6	0	-6.071108	-1.134570	-0.716990
64	6	0	-5.171415	-2.478137	-2.497764
65	1	0	-3.029034	-2.463622	-2.618993
66	6	0	-6.267018	-1.987964	-1.797825
67	1	0	-6.950592	-0.775405	-0.196367
68	1	0	-5.296424	-3.146721	-3.344903
69	1	0	-7.277294	-2.266634	-2.086665
70	6	0	-4.682929	0.221591	0.922873
71	6	0	-3.825265	-0.422747	2.020915
72	1	0	-4.249230	-1.383802	2.331305
73	1	0	-2.798289	-0.591378	1.700888
74	1	0	-3.787407	0.235489	2.894961
75	6	0	-4.072601	1.556136	0.468221
76	1	0	-3.065117	1.438314	0.070822
77	1	0	-4.690887	2.018783	-0.308649
78	1	0	-4.013505	2.244689	1.318234
79	6	0	-6.048542	0.538137	1.548305
80	1	0	-6.555819	-0.360190	1.916329
81	1	0	-5.893704	1.199157	2.407134
82	1	0	-6.718033	1.060108	0.856379

SCF Done: E(RPBE1PBE) = -6437.67511086 A.U. after 1 cycles
Convg = 0.2670D-08 -V/T = 2.0053
Zero-point correction= 0.679358 (Hartree/Particle)
Thermal correction to Energy= 0.727512
Thermal correction to Enthalpy= 0.728567
Thermal correction to Gibbs Free Energy= 0.593026
Sum of electronic and zero-point Energies= -6436.995752
Sum of electronic and thermal Energies= -6436.947599
Sum of electronic and thermal Enthalpies= -6436.946544
Sum of electronic and thermal Free Energies= -6437.082085

	1	2	3
	A	A	A
Frequencies --	14.4170	25.4347	28.5128

(*S*)-PhBOD-Rh-Ph-maleimide-syn-MB-“far” (20)



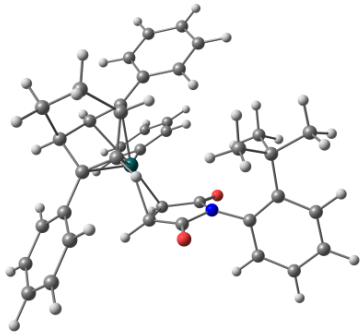
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.189689	0.440184	0.427823
2	6	0	-0.531147	2.047121	-1.261883
3	6	0	-0.738377	-0.111552	-2.345588
4	6	0	-1.884222	-2.865040	-1.352023
5	6	0	0.088092	3.249195	-0.671012
6	6	0	1.415862	3.595459	-0.954913
7	6	0	0.103720	0.876208	-1.570491
8	6	0	-1.971902	2.057873	-1.761514
9	6	0	-0.066937	5.200560	0.769079
10	6	0	-3.863686	-4.227437	-1.614549
11	6	0	-1.204400	0.581437	-3.657162
12	6	0	-2.629227	0.823477	-1.171294
13	6	0	1.996365	4.721424	-0.379726
14	6	0	-1.994314	-0.369183	-1.517488
15	6	0	-4.016203	-1.821952	-1.774997
16	6	0	-0.648442	4.077057	0.190184
17	6	0	-1.926004	1.893808	-3.305437
18	6	0	1.259257	5.526554	0.487374
19	6	0	-2.639334	-1.697386	-1.540492
20	6	0	-4.622957	-3.075130	-1.811412
21	6	0	-2.491945	-4.116071	-1.382826
22	1	0	-0.821183	-2.796558	-1.136424
23	1	0	-4.336702	-5.205540	-1.641589
24	1	0	-4.616214	-0.931322	-1.940423
25	1	0	-5.691033	-3.150876	-1.998210
26	1	0	-1.891690	-5.006723	-1.217150
27	1	0	1.991816	2.986421	-1.644946
28	1	0	-0.649425	5.822015	1.443999
29	1	0	3.027773	4.972568	-0.611820
30	1	0	-1.681452	3.831914	0.426319
31	1	0	1.714128	6.404377	0.938038
32	1	0	-0.194204	-1.032796	-2.557248
33	1	0	-2.497028	2.972178	-1.483039
34	1	0	-0.328094	0.765933	-4.285910
35	1	0	-1.860109	-0.101450	-4.206375
36	1	0	-2.953013	1.896035	-3.683497
37	1	0	-1.416921	2.759215	-3.741544
38	1	0	-3.655579	0.858214	-0.815832
39	1	0	1.164352	0.715302	-1.411015
40	6	0	-2.672907	-0.033637	1.701811
41	6	0	-3.446255	-1.198211	1.745735
42	6	0	-2.979672	1.002075	2.597323
43	6	0	-4.509337	-1.315316	2.645306
44	1	0	-3.229141	-2.028380	1.076906
45	6	0	-4.046854	0.888780	3.491842
46	1	0	-2.387146	1.918080	2.607444
47	6	0	-4.817706	-0.273015	3.518413

48	1	0	-5.098614	-2.229823	2.660672
49	1	0	-4.268090	1.707659	4.173219
50	1	0	-5.644807	-0.367429	4.217457
51	6	0	-0.105315	-1.086230	1.506462
52	6	0	0.307454	0.164426	1.998644
53	1	0	-0.839025	-1.751205	1.947069
54	1	0	-0.087006	0.674946	2.872674
55	6	0	1.754921	0.311895	1.698843
56	8	0	2.514387	1.188011	2.058743
57	6	0	1.077361	-1.725179	0.855319
58	8	0	1.148118	-2.842531	0.379121
59	7	0	2.160269	-0.831803	0.957298
60	6	0	3.511531	-1.336199	1.039461
61	6	0	4.460097	-1.304523	-0.003065
62	6	0	3.827230	-1.904807	2.276813
63	6	0	5.708222	-1.877693	0.282204
64	6	0	5.074479	-2.458631	2.528871
65	1	0	3.066977	-1.908920	3.053783
66	6	0	6.022294	-2.444865	1.513128
67	1	0	6.473811	-1.884451	-0.484396
68	1	0	5.295336	-2.893824	3.499382
69	1	0	7.008678	-2.872941	1.671997
70	6	0	4.209884	-0.672179	-1.377084
71	6	0	3.031338	-1.362578	-2.081003
72	1	0	3.253529	-2.420299	-2.254217
73	1	0	2.110701	-1.318625	-1.501308
74	1	0	2.848756	-0.889623	-3.053263
75	6	0	3.950520	0.831595	-1.198061
76	1	0	3.129142	1.039744	-0.511646
77	1	0	4.837612	1.327147	-0.790218
78	1	0	3.723620	1.289417	-2.168556
79	6	0	5.418640	-0.806830	-2.313508
80	1	0	5.671094	-1.852411	-2.518049
81	1	0	5.174490	-0.337894	-3.272371
82	1	0	6.307988	-0.301383	-1.923658

SCF Done: E(RPBE1PBE) = -6437.67968340 A.U. after 1 cycles
Convg = 0.2153D-08 -V/T = 2.0053
Zero-point correction= 0.679869 (Hartree/Particle)
Thermal correction to Energy= 0.727876
Thermal correction to Enthalpy= 0.728931
Thermal correction to Gibbs Free Energy= 0.593804
Sum of electronic and zero-point Energies= -6436.999814
Sum of electronic and thermal Energies= -6436.951807
Sum of electronic and thermal Enthalpies= -6436.950752
Sum of electronic and thermal Free Energies= -6437.085880

	1	2	3
	A	A	A
Frequencies --	14.0882	28.4859	31.0440

(*S*)-PhBOD-Rh-Ph-maleimide-3*S*-syn-MB-“parallel” (21)



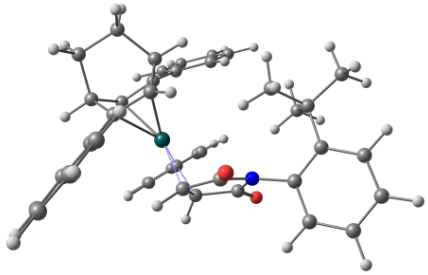
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.052714	0.173800	0.435497
2	6	0	-2.236996	1.581283	-0.959579
3	6	0	-1.442251	-0.267429	-2.330860
4	6	0	-0.214722	-3.041477	-1.717382
5	6	0	-2.384093	2.985561	-0.525393
6	6	0	-1.688387	4.017820	-1.171055
7	6	0	-1.161323	1.058402	-1.657690
8	6	0	-3.427846	0.633220	-0.979467
9	6	0	-3.365368	4.641941	0.960594
10	6	0	-0.759591	-5.361382	-1.326422
11	6	0	-2.667346	-0.100997	-3.268130
12	6	0	-2.882178	-0.674511	-0.446840
13	6	0	-1.826387	5.339261	-0.756388
14	6	0	-1.843605	-1.210656	-1.203883
15	6	0	-2.358231	-3.629187	-0.798438
16	6	0	-3.227734	3.321074	0.545026
17	6	0	-3.860386	0.432560	-2.455309
18	6	0	-2.665535	5.658252	0.310210
19	6	0	-1.465082	-2.636876	-1.229011
20	6	0	-2.009518	-4.974868	-0.844463
21	6	0	0.136804	-4.386852	-1.762980
22	1	0	0.504043	-2.294402	-2.039939
23	1	0	-0.487047	-6.412722	-1.362952
24	1	0	-3.340984	-3.349315	-0.431078
25	1	0	-2.718413	-5.725436	-0.505133
26	1	0	1.116175	-4.676137	-2.135540
27	1	0	-1.034700	3.786882	-2.006574
28	1	0	-4.017172	4.878112	1.797581
29	1	0	-1.277211	6.122894	-1.271272
30	1	0	-3.762531	2.539198	1.078039
31	1	0	-2.773285	6.690277	0.632749
32	1	0	-0.574553	-0.626874	-2.883938
33	1	0	-4.258700	0.998850	-0.375574
34	1	0	-2.397904	0.586726	-4.075666
35	1	0	-2.897243	-1.067254	-3.728151
36	1	0	-4.701798	-0.266984	-2.479228
37	1	0	-4.221068	1.386200	-2.853691
38	1	0	-3.454096	-1.264808	0.262381
39	1	0	-0.283199	1.645092	-1.914321
40	6	0	-1.207626	-1.309359	1.878192
41	6	0	-0.448053	-2.482650	1.887390
42	6	0	-2.209896	-1.167370	2.849704
43	6	0	-0.690575	-3.489501	2.824998
44	1	0	0.348323	-2.630055	1.161636
45	6	0	-2.459480	-2.174522	3.784683
46	1	0	-2.810422	-0.258926	2.886584

47	6	0	-1.699352	-3.344110	3.775210
48	1	0	-0.081675	-4.390947	2.809932
49	1	0	-3.246248	-2.039975	4.524580
50	1	0	-1.886233	-4.127762	4.505341
51	6	0	0.379016	0.792336	2.016800
52	6	0	0.194349	1.813634	1.085690
53	1	0	-0.085332	0.700141	2.990103
54	1	0	-0.446899	2.682752	1.187895
55	6	0	1.439143	1.919848	0.268826
56	8	0	1.701556	2.742896	-0.587412
57	6	0	1.753321	0.245766	1.822580
58	8	0	2.344782	-0.558981	2.509848
59	7	0	2.311279	0.908743	0.705243
60	6	0	3.728687	0.986837	0.481433
61	6	0	4.425013	0.220786	-0.474556
62	6	0	4.394316	1.908920	1.292435
63	6	0	5.806612	0.450391	-0.554824
64	6	0	5.763894	2.109414	1.189571
65	1	0	3.813999	2.475433	2.016110
66	6	0	6.472249	1.369121	0.250931
67	1	0	6.396733	-0.105847	-1.273138
68	1	0	6.263120	2.830631	1.830398
69	1	0	7.545546	1.500940	0.140585
70	6	0	3.769949	-0.832554	-1.379110
71	6	0	3.238318	-1.989138	-0.517781
72	1	0	4.039134	-2.421345	0.090431
73	1	0	2.444756	-1.672770	0.160055
74	1	0	2.838254	-2.781626	-1.159835
75	6	0	2.631073	-0.210878	-2.203312
76	1	0	1.785709	0.082058	-1.578787
77	1	0	2.975222	0.674474	-2.747169
78	1	0	2.269638	-0.937747	-2.940565
79	6	0	4.769735	-1.432354	-2.377486
80	1	0	5.588852	-1.961928	-1.880802
81	1	0	4.248317	-2.163928	-3.003129
82	1	0	5.195865	-0.675895	-3.044948

SCF Done: E(RPBE1PBE) = -6437.68135099 A.U. after 1 cycles
Convg = 0.4646D-08 -V/T = 2.0053
Zero-point correction= 0.680550 (Hartree/Particle)
Thermal correction to Energy= 0.728355
Thermal correction to Enthalpy= 0.729410
Thermal correction to Gibbs Free Energy= 0.595949
Sum of electronic and zero-point Energies= -6437.000801
Sum of electronic and thermal Energies= -6436.952996
Sum of electronic and thermal Enthalpies= -6436.951941
Sum of electronic and thermal Free Energies= -6437.085402

	1	2	3
	A	A	A
Frequencies --	24.0078	29.4282	35.4341

(*S*)-PhBOD-Rh-Ph-maleimide-(3S,S_a)-CR-TS-conf"pp" (22)



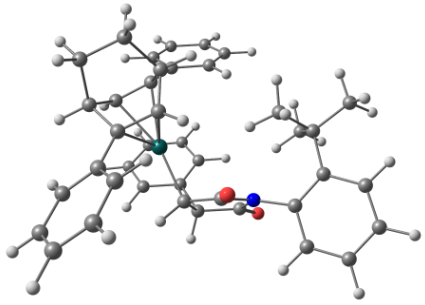
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.038039	0.218107	0.355822
2	6	0	-2.349486	1.493195	-0.876033
3	6	0	-1.676047	-0.361968	-2.314141
4	6	0	-0.273200	-3.064616	-1.645189
5	6	0	-2.480658	2.910587	-0.472961
6	6	0	-1.873952	3.935608	-1.211597
7	6	0	-1.331204	0.967437	-1.673484
8	6	0	-3.537909	0.539858	-0.794538
9	6	0	-3.356210	4.594999	1.048568
10	6	0	-0.693360	-5.390453	-1.146342
11	6	0	-2.979827	-0.203789	-3.138840
12	6	0	-2.941161	-0.764514	-0.308903
13	6	0	-2.000358	5.267089	-0.824580
14	6	0	-1.970716	-1.292134	-1.141206
15	6	0	-2.359481	-3.715209	-0.641362
16	6	0	-3.227304	3.264959	0.661572
17	6	0	-4.096597	0.335814	-2.226695
18	6	0	-2.742454	5.604281	0.306026
19	6	0	-1.527212	-2.699549	-1.134629
20	6	0	-1.946841	-5.044010	-0.643410
21	6	0	0.141453	-4.392875	-1.648823
22	1	0	0.397467	-2.297346	-2.020979
23	1	0	-0.371733	-6.428522	-1.151093
24	1	0	-3.346871	-3.465267	-0.263689
25	1	0	-2.610152	-5.813624	-0.257293
26	1	0	1.122329	-4.650956	-2.040108
27	1	0	-1.299777	3.691448	-2.100491
28	1	0	-3.933715	4.845063	1.934903
29	1	0	-1.518842	6.044451	-1.411843
30	1	0	-3.692067	2.488611	1.264314
31	1	0	-2.842368	6.643833	0.606375
32	1	0	-0.862299	-0.731128	-2.939522
33	1	0	-4.314241	0.904691	-0.121180
34	1	0	-2.786541	0.477859	-3.973168
35	1	0	-3.250082	-1.173459	-3.569106
36	1	0	-4.939772	-0.360432	-2.178244
37	1	0	-4.485936	1.290295	-2.595250
38	1	0	-3.411321	-1.337448	0.485822
39	1	0	-0.501570	1.566761	-2.040944
40	6	0	-0.751368	-1.092977	2.035254
41	6	0	-0.092679	-2.316564	1.885299
42	6	0	-1.774346	-0.993677	2.995108
43	6	0	-0.483754	-3.428163	2.631992
44	1	0	0.725747	-2.419202	1.179389
45	6	0	-2.171631	-2.106753	3.730359
46	1	0	-2.262323	-0.036045	3.170059
47	6	0	-1.525999	-3.332718	3.551374
48	1	0	0.033946	-4.373495	2.489459
49	1	0	-2.975069	-2.012726	4.457639
50	1	0	-1.822775	-4.198955	4.137010
51	6	0	0.436933	0.563007	2.079741
52	6	0	0.209759	1.676494	1.201308
53	1	0	0.192884	0.628026	3.134463
54	1	0	-0.372702	2.553609	1.471430
55	6	0	1.433545	1.891178	0.406728
56	8	0	1.694205	2.786643	-0.373641
57	6	0	1.859408	0.105159	1.816036
58	8	0	2.495459	-0.718103	2.440186
59	7	0	2.350916	0.863296	0.752798
60	6	0	3.749877	0.976784	0.452528

61	6	0	4.382279	0.332669	-0.629293
62	6	0	4.461778	1.815887	1.312285
63	6	0	5.751721	0.596499	-0.782142
64	6	0	5.818566	2.049807	1.136892
65	1	0	3.926765	2.292551	2.129371
66	6	0	6.464122	1.432350	0.072407
67	1	0	6.293694	0.136315	-1.599566
68	1	0	6.355505	2.705641	1.816320
69	1	0	7.524604	1.597466	-0.099834
70	6	0	3.680878	-0.646489	-1.581681
71	6	0	3.349150	-1.934817	-0.811114
72	1	0	4.259390	-2.394304	-0.412454
73	1	0	2.679985	-1.750531	0.031100
74	1	0	2.868418	-2.659488	-1.477737
75	6	0	2.400510	-0.040427	-2.180916
76	1	0	1.594641	0.046646	-1.449059
77	1	0	2.589641	0.953512	-2.597985
78	1	0	2.040641	-0.683001	-2.993302
79	6	0	4.580984	-1.037641	-2.762763
80	1	0	5.481925	-1.571674	-2.445662
81	1	0	4.026250	-1.712677	-3.422219
82	1	0	4.881136	-0.168579	-3.357911

SCF Done: E(RPBE1PBE) = -6437.66625470 A.U. after 1 cycles
Convg = 0.5104D-08 -V/T = 2.0053
Zero-point correction= 0.679526 (Hartree/Particle)
Thermal correction to Energy= 0.726683
Thermal correction to Enthalpy= 0.727738
Thermal correction to Gibbs Free Energy= 0.594713
Sum of electronic and zero-point Energies= -6436.986728
Sum of electronic and thermal Energies= -6436.939571
Sum of electronic and thermal Enthalpies= -6436.938516
Sum of electronic and thermal Free Energies= -6437.071541

	1	2	3
	A	A	A
Frequencies --	-299.1892	19.4147	26.1217

(*S*)-PhBOD-α-Rh-(3S,S_a)-Phsuccinimide (23)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.126881	0.239622	0.391327
2	6	0	-2.118007	1.648100	-0.913184
3	6	0	-1.740256	-0.386757	-2.231210
4	6	0	-0.834924	-3.209017	-1.181053
5	6	0	-1.999320	3.090588	-0.607395
6	6	0	-1.092660	3.910099	-1.294756
7	6	0	-1.168293	0.880594	-1.623603
8	6	0	-3.475813	0.951450	-0.889892
9	6	0	-2.694564	5.035839	0.681568

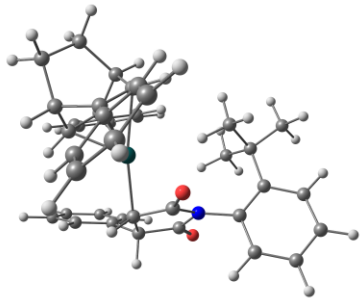
10	6	0	-1.695303	-5.394110	-0.610971
11	6	0	-2.936112	-0.035154	-3.149196
12	6	0	-3.171445	-0.408271	-0.295172
13	6	0	-0.987348	5.266283	-0.999530
14	6	0	-2.268702	-1.159316	-1.023750
15	6	0	-3.115448	-3.445495	-0.451035
16	6	0	-2.797494	3.680118	0.386272
17	6	0	-3.971016	0.775995	-2.347536
18	6	0	-1.788595	5.838245	-0.012679
19	6	0	-2.068643	-2.615216	-0.876810
20	6	0	-2.930993	-4.819359	-0.316800
21	6	0	-0.647858	-4.580808	-1.045659
22	1	0	-0.004101	-2.584550	-1.497616
23	1	0	-1.551064	-6.466575	-0.510259
24	1	0	-4.089729	-3.012694	-0.240633
25	1	0	-3.758588	-5.444758	0.008552
26	1	0	0.320451	-5.018423	-1.275638
27	1	0	-0.455124	3.482723	-2.061538
28	1	0	-3.320079	5.467199	1.459085
29	1	0	-0.274080	5.878644	-1.544937
30	1	0	-3.491557	3.067275	0.955579
31	1	0	-1.707056	6.897694	0.215482
32	1	0	-0.979937	-0.949294	-2.775152
33	1	0	-4.210780	1.494486	-0.295007
34	1	0	-2.563924	0.535593	-4.005900
35	1	0	-3.372352	-0.959556	-3.541670
36	1	0	-4.942256	0.271016	-2.330807
37	1	0	-4.129349	1.765495	-2.788409
38	1	0	-3.779474	-0.825996	0.503286
39	1	0	-0.232212	1.299397	-1.985981
40	6	0	-0.277397	-0.480337	2.495600
41	6	0	-0.085982	-1.860193	2.294243
42	6	0	-1.558330	-0.036486	2.895673
43	6	0	-1.117616	-2.763891	2.530661
44	1	0	0.888855	-2.229131	1.992556
45	6	0	-2.584721	-0.954160	3.147806
46	1	0	-1.716361	1.017867	3.111003
47	6	0	-2.364464	-2.316425	2.970550
48	1	0	-0.946020	-3.824217	2.368367
49	1	0	-3.550326	-0.593564	3.492964
50	1	0	-3.159754	-3.029674	3.169082
51	6	0	0.814612	0.574552	2.338514
52	6	0	0.424947	1.450710	1.160266
53	1	0	0.932641	1.118204	3.285562
54	1	0	0.017636	2.439597	1.379174
55	6	0	1.602304	1.519596	0.288162
56	8	0	1.819884	2.225703	-0.683123
57	6	0	2.191431	0.033651	1.984415
58	8	0	2.867472	-0.726522	2.654980
59	7	0	2.565206	0.576212	0.766566
60	6	0	3.921392	0.572001	0.296105
61	6	0	4.418688	-0.293193	-0.700094
62	6	0	4.742234	1.526727	0.899686
63	6	0	5.770936	-0.126065	-1.034336
64	6	0	6.078216	1.661980	0.548373
65	1	0	4.308634	2.173159	1.657994
66	6	0	6.591930	0.823134	-0.432885
67	1	0	6.211992	-0.757722	-1.795922
68	1	0	6.700151	2.411000	1.030361
69	1	0	7.632563	0.902103	-0.736947
70	6	0	3.591009	-1.386758	-1.392650
71	6	0	3.214101	-2.471677	-0.371211
72	1	0	4.109740	-2.930708	0.059619
73	1	0	2.622256	-2.072187	0.452692

74	1	0	2.629484	-3.259932	-0.860287
75	6	0	2.321978	-0.801188	-2.033536
76	1	0	1.584613	-0.490174	-1.290942
77	1	0	2.556366	0.065791	-2.658443
78	1	0	1.853062	-1.560370	-2.671003
79	6	0	4.379020	-2.076631	-2.515753
80	1	0	5.268926	-2.595466	-2.145705
81	1	0	3.738998	-2.832113	-2.982678
82	1	0	4.683118	-1.375001	-3.299626

SCF Done: E(RPBE1PBE) = -6437.72098084 A.U. after 1 cycles
Convg = 0.2476D-08 -V/T = 2.0053
Zero-point correction= 0.681848 (Hartree/Particle)
Thermal correction to Energy= 0.729101
Thermal correction to Enthalpy= 0.730156
Thermal correction to Gibbs Free Energy= 0.597286
Sum of electronic and zero-point Energies= -6437.039133
Sum of electronic and thermal Energies= -6436.991880
Sum of electronic and thermal Enthalpies= -6436.990825
Sum of electronic and thermal Free Energies= -6437.123695

	1	2	3
	A	A	A
Frequencies --	24.7250	27.7338	34.9810

(*S*)-PhBOD-(3S,*S*$_a$)-Rh-oxa-π-allyl (24)



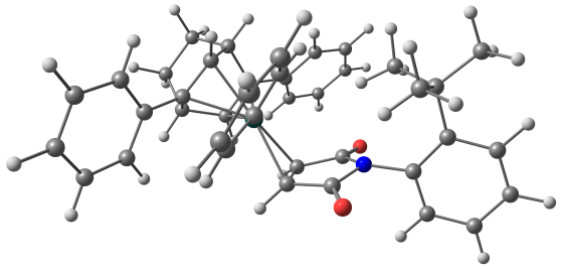
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.163572	-0.145294	-0.272454
2	6	0	3.254389	-0.338091	0.384820
3	6	0	1.850357	-1.283870	2.138823
4	6	0	-1.227809	-1.918429	2.105302
5	6	0	4.198084	0.613965	-0.237828
6	6	0	4.769341	1.656371	0.505402
7	6	0	2.452072	-0.057873	1.489590
8	6	0	3.289342	-1.833551	0.076767
9	6	0	5.434626	1.389262	-2.182058
10	6	0	-2.618785	-3.892470	2.073769
11	6	0	2.964022	-2.279821	2.538093
12	6	0	1.820226	-2.158648	-0.125185
13	6	0	5.655533	2.553177	-0.084961
14	6	0	1.025501	-1.893265	1.005058
15	6	0	-0.495031	-3.880691	0.923207
16	6	0	4.550441	0.492994	-1.590450
17	6	0	3.836853	-2.593473	1.308015
18	6	0	5.992052	2.424517	-1.431608
19	6	0	-0.257769	-2.558834	1.321581
20	6	0	-1.661803	-4.542090	1.297704
21	6	0	-2.398148	-2.573976	2.472091
22	1	0	-1.071691	-0.891075	2.421926

23	1	0	-3.530886	-4.407255	2.363939
24	1	0	0.250375	-4.404190	0.330803
25	1	0	-1.823166	-5.568943	0.980629
26	1	0	-3.143424	-2.053068	3.067916
27	1	0	4.528973	1.757910	1.560186
28	1	0	5.685753	1.283501	-3.234251
29	1	0	6.089677	3.351874	0.510805
30	1	0	4.107408	-0.295677	-2.193519
31	1	0	6.684175	3.124023	-1.892622
32	1	0	1.225411	-1.023645	2.994518
33	1	0	3.880636	-2.052205	-0.813597
34	1	0	3.559962	-1.839244	3.343789
35	1	0	2.500907	-3.187168	2.939434
36	1	0	3.838077	-3.665807	1.087252
37	1	0	4.878165	-2.298689	1.473983
38	1	0	1.498859	-2.835253	-0.913557
39	1	0	2.438300	0.910497	1.983408
40	6	0	-2.250340	-1.761939	-2.027992
41	6	0	-3.512267	-2.139238	-1.562629
42	6	0	-1.391486	-2.755820	-2.512892
43	6	0	-3.902429	-3.478815	-1.584839
44	1	0	-4.199638	-1.383000	-1.198781
45	6	0	-1.785943	-4.090309	-2.547561
46	1	0	-0.404452	-2.479357	-2.875958
47	6	0	-3.048741	-4.458551	-2.084814
48	1	0	-4.887436	-3.753036	-1.215217
49	1	0	-1.106257	-4.843823	-2.938551
50	1	0	-3.362146	-5.499081	-2.112558
51	6	0	-1.806603	-0.318035	-2.158563
52	6	0	-0.362207	0.031919	-1.874938
53	1	0	-1.996058	-0.053041	-3.213249
54	1	0	0.373029	-0.095995	-2.670058
55	6	0	-0.372360	1.304164	-1.241479
56	8	0	0.664780	1.934490	-0.892218
57	6	0	-2.596370	0.763178	-1.421427
58	8	0	-3.804334	0.880108	-1.345524
59	7	0	-1.683979	1.677527	-0.890898
60	6	0	-2.051544	3.015290	-0.513133
61	6	0	-2.326430	3.434092	0.805381
62	6	0	-2.133410	3.904952	-1.587047
63	6	0	-2.686670	4.782456	0.951391
64	6	0	-2.487642	5.234365	-1.404791
65	1	0	-1.913051	3.531515	-2.583675
66	6	0	-2.769411	5.670849	-0.116508
67	1	0	-2.914231	5.166601	1.938223
68	1	0	-2.544332	5.909740	-2.253697
69	1	0	-3.054721	6.703668	0.066287
70	6	0	-2.235063	2.532639	2.046337
71	6	0	-3.191616	1.335042	1.927916
72	1	0	-4.216049	1.667821	1.734402
73	1	0	-2.909437	0.647131	1.131716
74	1	0	-3.190243	0.771498	2.868365
75	6	0	-0.789777	2.043657	2.229294
76	1	0	-0.458934	1.399926	1.411738
77	1	0	-0.094920	2.887850	2.287470
78	1	0	-0.706344	1.472023	3.161540
79	6	0	-2.620127	3.283524	3.329122
80	1	0	-3.652809	3.646817	3.304687
81	1	0	-2.538835	2.595322	4.176437
82	1	0	-1.955442	4.128849	3.534717

SCF Done: E(RPBE1PBE) = -6437.70604142 A.U. after 1 cycles
Convg = 0.1533D-08 -V/T = 2.0053
Zero-point correction= 0.681427 (Hartree/Particle)

Thermal correction to Energy=	0.728700
Thermal correction to Enthalpy=	0.729755
Thermal correction to Gibbs Free Energy=	0.595528
Sum of electronic and zero-point Energies=	-6437.024614
Sum of electronic and thermal Energies=	-6436.977341
Sum of electronic and thermal Enthalpies=	-6436.976286
Sum of electronic and thermal Free Energies=	-6437.110513

(*S*)-PhBOD-Rh-Ph-maleimide-(3*R*)-syn-MB-"parallel" (25)



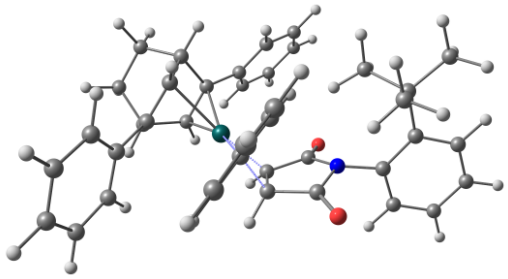
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.984559	0.282382	-0.323297
2	6	0	-1.241148	2.539123	0.206034
3	6	0	-3.345114	1.790122	-0.768709
4	6	0	-4.466162	-0.989127	-1.519021
5	6	0	-0.018588	3.357513	0.316380
6	6	0	0.273830	4.339592	-0.641415
7	6	0	-1.930799	2.281879	-0.961508
8	6	0	-2.077704	2.173237	1.428261
9	6	0	2.004576	3.985963	1.505059
10	6	0	-5.857792	-2.783828	-0.698396
11	6	0	-4.118786	2.819859	0.097885
12	6	0	-2.479072	0.727440	1.211969
13	6	0	1.416594	5.124496	-0.533589
14	6	0	-3.210969	0.510594	0.042429
15	6	0	-4.660963	-1.367175	0.849769
16	6	0	0.862558	3.199645	1.395474
17	6	0	-3.351042	3.057845	1.410029
18	6	0	2.288315	4.950339	0.539802
19	6	0	-4.112923	-0.630396	-0.209230
20	6	0	-5.522486	-2.432950	0.608330
21	6	0	-5.325376	-2.055583	-1.762457
22	1	0	-4.041900	-0.447567	-2.360655
23	1	0	-6.529572	-3.616928	-0.887046
24	1	0	-4.416567	-1.101522	1.874034
25	1	0	-5.934166	-2.991361	1.444795
26	1	0	-5.576122	-2.323246	-2.785671
27	1	0	-0.411065	4.506737	-1.468370
28	1	0	2.680511	3.839007	2.343239
29	1	0	1.624110	5.880130	-1.286629
30	1	0	0.667381	2.438706	2.146616
31	1	0	3.182020	5.562540	0.624228
32	1	0	-3.848896	1.625634	-1.721362
33	1	0	-1.524991	2.303538	2.359062
34	1	0	-4.227870	3.747297	-0.472813
35	1	0	-5.126244	2.436335	0.287488
36	1	0	-3.964697	2.804410	2.280185
37	1	0	-3.056380	4.106957	1.514830
38	1	0	-2.472316	0.021885	2.036963
39	1	0	-1.599638	2.635013	-1.933963
40	6	0	-1.018349	-1.658626	0.391595

41	6	0	-1.636010	-2.745224	-0.236889
42	6	0	-0.492312	-1.859170	1.674944
43	6	0	-1.734438	-3.985484	0.394043
44	1	0	-2.057754	-2.638064	-1.233808
45	6	0	-0.589976	-3.099525	2.311471
46	1	0	0.000803	-1.043033	2.201375
47	6	0	-1.213487	-4.169865	1.673885
48	1	0	-2.220042	-4.811238	-0.121582
49	1	0	-0.171665	-3.226137	3.308236
50	1	0	-1.287206	-5.136610	2.165878
51	6	0	0.200508	-0.764515	-1.867060
52	1	0	-0.518458	-1.241222	-2.523669
53	6	0	0.553856	0.585676	-1.839769
54	1	0	0.194159	1.367562	-2.498955
55	6	0	1.962341	0.678428	-1.352526
56	8	0	2.665426	1.665307	-1.294317
57	6	0	1.394405	-1.553802	-1.432506
58	8	0	1.553684	-2.754367	-1.486848
59	7	0	2.381535	-0.628156	-1.041138
60	6	0	3.777869	-0.955882	-0.958837
61	6	0	4.483365	-1.125264	0.248690
62	6	0	4.420605	-1.067399	-2.194243
63	6	0	5.854569	-1.397359	0.121873
64	6	0	5.776749	-1.347336	-2.284140
65	1	0	3.832806	-0.925424	-3.097404
66	6	0	6.497714	-1.508223	-1.106782
67	1	0	6.453832	-1.530226	1.014708
68	1	0	6.257973	-1.431462	-3.254451
69	1	0	7.563279	-1.721049	-1.137269
70	6	0	3.839237	-1.097879	1.641799
71	6	0	2.928113	0.125018	1.835540
72	1	0	3.445330	1.053978	1.576717
73	1	0	2.019639	0.067226	1.234824
74	1	0	2.621544	0.185862	2.886452
75	6	0	3.035703	-2.395820	1.827212
76	1	0	2.242681	-2.506658	1.085759
77	1	0	3.692004	-3.269027	1.746959
78	1	0	2.571254	-2.410602	2.820161
79	6	0	4.894119	-1.043299	2.757196
80	1	0	5.518477	-1.941251	2.790859
81	1	0	5.546068	-0.167571	2.666701
82	1	0	4.384062	-0.978479	3.723658

SCF Done: E(RPBE1PBE) = -6437.67307553 A.U. after 1 cycles
Convg = 0.1917D-08 -V/T = 2.0053
Zero-point correction= 0.679886 (Hartree/Particle)
Thermal correction to Energy= 0.727839
Thermal correction to Enthalpy= 0.728894
Thermal correction to Gibbs Free Energy= 0.594246
Sum of electronic and zero-point Energies= -6436.993189
Sum of electronic and thermal Energies= -6436.945237
Sum of electronic and thermal Enthalpies= -6436.944182
Sum of electronic and thermal Free Energies= -6437.078829

	1	2	3
	A	A	A
Frequencies --	12.8607	19.2434	34.3127

(*S*)-PhBOD-Rh-Ph-maleimide-(3*R*,S_a)-CR-TS-conf“pp” (26)



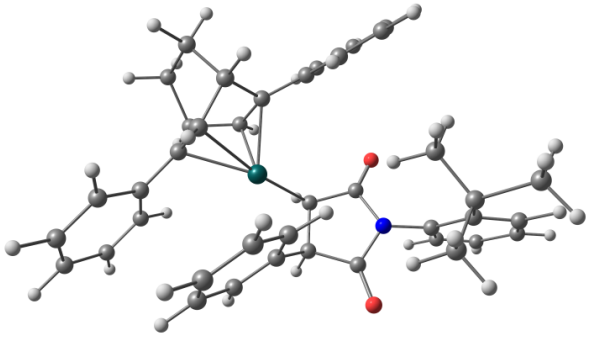
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.106462	0.308356	-0.340929
2	6	0	-1.332728	2.473964	0.135010
3	6	0	-3.449388	1.744800	-0.836904
4	6	0	-4.503785	-1.090288	-1.497035
5	6	0	-0.102359	3.287308	0.229628
6	6	0	0.236453	4.204312	-0.775587
7	6	0	-2.013972	2.177352	-1.043323
8	6	0	-2.208561	2.214612	1.359392
9	6	0	1.891260	3.966297	1.444602
10	6	0	-5.873363	-2.892517	-0.653920
11	6	0	-4.205405	2.841391	-0.044432
12	6	0	-2.637693	0.768806	1.210941
13	6	0	1.385311	4.982327	-0.677886
14	6	0	-3.344303	0.505016	0.045491
15	6	0	-4.774802	-1.378413	0.875989
16	6	0	0.743337	3.186971	1.344164
17	6	0	-3.454331	3.131466	1.267218
18	6	0	2.219418	4.867043	0.432657
19	6	0	-4.208978	-0.667640	-0.191394
20	6	0	-5.595205	-2.479733	0.648239
21	6	0	-5.323248	-2.190862	-1.727091
22	1	0	-4.066210	-0.568604	-2.344416
23	1	0	-6.515906	-3.750656	-0.832054
24	1	0	-4.579222	-1.060987	1.896248
25	1	0	-6.023629	-3.014544	1.491881
26	1	0	-5.530159	-2.504920	-2.746979
27	1	0	-0.413492	4.322678	-1.638147
28	1	0	2.536065	3.864696	2.313602
29	1	0	1.628493	5.684698	-1.470780
30	1	0	0.514812	2.475259	2.133449
31	1	0	3.117572	5.473851	0.509197
32	1	0	-3.948284	1.535481	-1.783767
33	1	0	-1.669908	2.382297	2.292653
34	1	0	-4.277073	3.738715	-0.667291
35	1	0	-5.227560	2.499985	0.148262
36	1	0	-4.091815	2.946607	2.137572
37	1	0	-3.131083	4.176223	1.318577
38	1	0	-2.609878	0.083975	2.054447
39	1	0	-1.667873	2.501950	-2.021349
40	6	0	-0.861457	-1.724184	0.245594
41	6	0	-1.703378	-2.800321	-0.057661
42	6	0	-0.160036	-1.741857	1.461892
43	6	0	-1.874956	-3.843962	0.848707
44	1	0	-2.239158	-2.826447	-1.003801
45	6	0	-0.350583	-2.775379	2.377082
46	1	0	0.532567	-0.939458	1.706493
47	6	0	-1.206147	-3.834021	2.072655
48	1	0	-2.537148	-4.668267	0.595233

49	1	0	0.189243	-2.762770	3.321310
50	1	0	-1.336865	-4.652639	2.775604
51	6	0	0.163119	-1.207950	-1.469872
52	1	0	-0.442276	-1.828432	-2.123246
53	6	0	0.446998	0.163961	-1.774545
54	1	0	0.057392	0.675938	-2.651051
55	6	0	1.867661	0.412665	-1.457529
56	8	0	2.528029	1.411179	-1.657325
57	6	0	1.486472	-1.836292	-1.073970
58	8	0	1.739688	-3.018229	-0.981336
59	7	0	2.410317	-0.797736	-0.939957
60	6	0	3.831219	-1.022507	-0.950250
61	6	0	4.658180	-0.954523	0.189002
62	6	0	4.362640	-1.294202	-2.213025
63	6	0	6.027190	-1.163889	-0.035813
64	6	0	5.721620	-1.505083	-2.399046
65	1	0	3.684595	-1.334501	-3.061367
66	6	0	6.559513	-1.432620	-1.292853
67	1	0	6.714633	-1.117454	0.800084
68	1	0	6.114644	-1.715675	-3.389652
69	1	0	7.630378	-1.584960	-1.400864
70	6	0	4.146810	-0.728655	1.618629
71	6	0	3.247944	0.513957	1.709506
72	1	0	3.760064	1.401291	1.325656
73	1	0	2.317772	0.407710	1.151857
74	1	0	2.985927	0.698666	2.757983
75	6	0	3.386816	-1.985893	2.072832
76	1	0	2.567920	-2.248242	1.401653
77	1	0	4.061988	-2.847105	2.115490
78	1	0	2.971791	-1.831534	3.076240
79	6	0	5.296849	-0.508302	2.613313
80	1	0	5.947608	-1.383428	2.704446
81	1	0	5.911905	0.358671	2.349062
82	1	0	4.874233	-0.322488	3.606122

SCF Done: E(RPBE1PBE) = -6437.66037512 A.U. after 1 cycles
Convg = 0.3232D-08 -V/T = 2.0053
Zero-point correction= 0.679677 (Hartree/Particle)
Thermal correction to Energy= 0.726618
Thermal correction to Enthalpy= 0.727673
Thermal correction to Gibbs Free Energy= 0.596308
Sum of electronic and zero-point Energies= -6436.980698
Sum of electronic and thermal Energies= -6436.933757
Sum of electronic and thermal Enthalpies= -6436.932702
Sum of electronic and thermal Free Energies= -6437.064068

	1	2	3
	A	A	A
Frequencies --	-274.9520	16.4929	29.7998

(*S*)-PhBOD-α-Rh-(3*R*,*S*$_a$)-Phsuccinimide (27)



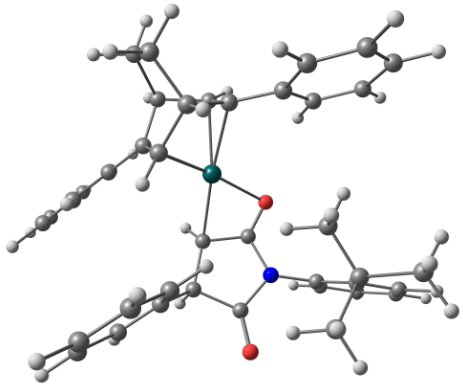
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.190826	0.166317	-0.249499
2	6	0	-1.153345	2.345350	-0.005695
3	6	0	-3.308520	1.759671	-1.011268
4	6	0	-4.605501	-1.049940	-1.365825
5	6	0	0.105220	3.116451	0.054976
6	6	0	0.522667	3.901749	-1.028510
7	6	0	-1.817010	1.964913	-1.187963
8	6	0	-2.113434	2.361822	1.181225
9	6	0	2.028598	3.920221	1.306829
10	6	0	-6.253043	-2.529363	-0.398910
11	6	0	-3.946938	3.037050	-0.413317
12	6	0	-2.714091	0.972502	1.188049
13	6	0	1.672168	4.680692	-0.948797
14	6	0	-3.391348	0.643615	0.025543
15	6	0	-5.099690	-0.918889	0.985255
16	6	0	0.879704	3.141119	1.224364
17	6	0	-3.222974	3.405129	0.894692
18	6	0	2.430241	4.696204	0.220136
19	6	0	-4.365346	-0.458335	-0.116462
20	6	0	-6.032941	-1.943565	0.846707
21	6	0	-5.533741	-2.076360	-1.505925
22	1	0	-4.040056	-0.720224	-2.233923
23	1	0	-6.984158	-3.325933	-0.508951
24	1	0	-4.952725	-0.456191	1.957361
25	1	0	-6.597046	-2.279013	1.713366
26	1	0	-5.697323	-2.525802	-2.482131
27	1	0	-0.066346	3.916738	-1.940933
28	1	0	2.616103	3.918506	2.221432
29	1	0	1.975765	5.280828	-1.802577
30	1	0	0.592710	2.526850	2.074125
31	1	0	3.328147	5.305103	0.283731
32	1	0	-3.793300	1.483232	-1.948636
33	1	0	-1.601704	2.585521	2.117916
34	1	0	-3.872151	3.844876	-1.148421
35	1	0	-5.012941	2.856113	-0.240809
36	1	0	-3.917569	3.421178	1.740697
37	1	0	-2.766652	4.398347	0.831760
38	1	0	-2.800433	0.396933	2.105995
39	1	0	-1.397913	2.151418	-2.174048
40	6	0	-0.574719	-2.173708	-0.168345
41	6	0	-1.697953	-2.993665	-0.380631
42	6	0	-0.330818	-1.693152	1.136174
43	6	0	-2.533343	-3.343042	0.670026
44	1	0	-1.898929	-3.367912	-1.381451
45	6	0	-1.177842	-2.055471	2.193940
46	1	0	0.578567	-1.137634	1.353231
47	6	0	-2.272288	-2.877640	1.963739
48	1	0	-3.397466	-3.974534	0.484511
49	1	0	-0.957899	-1.700716	3.197515
50	1	0	-2.924723	-3.162649	2.784589
51	6	0	0.399165	-1.855317	-1.294916
52	1	0	0.117832	-2.428059	-2.184654
53	6	0	0.432499	-0.352114	-1.517169
54	1	0	0.084413	-0.014029	-2.497960
55	6	0	1.835344	0.054402	-1.333149
56	8	0	2.377018	1.117301	-1.569843
57	6	0	1.826659	-2.245326	-0.931384
58	8	0	2.242644	-3.372138	-0.734862
59	7	0	2.574046	-1.082683	-0.860933
60	6	0	4.009532	-1.090582	-0.835276

61	6	0	4.783976	-0.924915	0.331624
62	6	0	4.610661	-1.269022	-2.082604
63	6	0	6.174856	-0.952263	0.150331
64	6	0	5.991029	-1.293776	-2.225888
65	1	0	3.968925	-1.386541	-2.951654
66	6	0	6.776940	-1.131891	-1.091491
67	1	0	6.824480	-0.827577	1.008428
68	1	0	6.439437	-1.434065	-3.205423
69	1	0	7.861416	-1.142992	-1.165407
70	6	0	4.200762	-0.744137	1.741807
71	6	0	3.226019	0.443038	1.785239
72	1	0	3.709069	1.361620	1.440108
73	1	0	2.342369	0.293627	1.165176
74	1	0	2.886496	0.601373	2.815878
75	6	0	3.497887	-2.037433	2.186186
76	1	0	2.698273	-2.340252	1.509709
77	1	0	4.210119	-2.867653	2.233992
78	1	0	3.068318	-1.901657	3.185874
79	6	0	5.293123	-0.449987	2.780309
80	1	0	6.000870	-1.277925	2.888760
81	1	0	5.853633	0.461113	2.545595
82	1	0	4.820934	-0.303035	3.757097

SCF Done: E(RPBE1PBE) = -6437.71271481 A.U. after 1 cycles
Convg = 0.3207D-08 -V/T = 2.0053
Zero-point correction= 0.681468 (Hartree/Particle)
Thermal correction to Energy= 0.728764
Thermal correction to Enthalpy= 0.729819
Thermal correction to Gibbs Free Energy= 0.597062
Sum of electronic and zero-point Energies= -6437.031247
Sum of electronic and thermal Energies= -6436.983951
Sum of electronic and thermal Enthalpies= -6436.982896
Sum of electronic and thermal Free Energies= -6437.115652

	1	2	3
	A	A	A
Frequencies --	15.9548	27.0499	34.0734

(*S*)-PhBOD-(3*R*,*S*$_a$)-Rh-oxa-π-allyl (28)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.681064	0.787474	-0.679122
2	6	0	-0.550345	2.854059	0.153942
3	6	0	-2.733212	2.579999	-0.914895
4	6	0	-4.107218	0.038961	-2.052637
5	6	0	0.796849	3.433995	0.322038
6	6	0	1.718550	3.436039	-0.738688

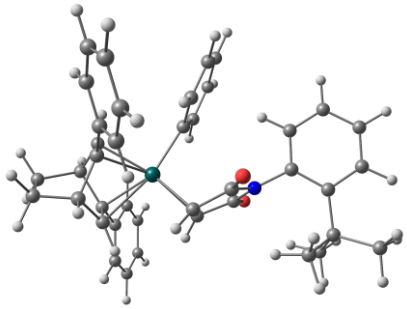
7	6	0	-1.248929	2.854471	-1.053368
8	6	0	-1.468057	2.521207	1.325211
9	6	0	2.436910	4.618063	1.674348
10	6	0	-5.604982	-1.779923	-1.519737
11	6	0	-3.369068	3.593284	0.066562
12	6	0	-2.021843	1.168302	0.916792
13	6	0	2.971057	4.019921	-0.595224
14	6	0	-2.751772	1.188413	-0.287787
15	6	0	-4.328247	-0.700018	0.226113
16	6	0	1.180819	4.030438	1.530956
17	6	0	-2.612605	3.556884	1.408450
18	6	0	3.338486	4.616364	0.613011
19	6	0	-3.737483	0.166268	-0.704364
20	6	0	-5.249525	-1.663024	-0.177169
21	6	0	-5.027489	-0.922667	-2.457059
22	1	0	-3.651565	0.683444	-2.800082
23	1	0	-6.325737	-2.530323	-1.833647
24	1	0	-4.069832	-0.621190	1.278228
25	1	0	-5.692460	-2.323344	0.563808
26	1	0	-5.292480	-1.006228	-3.507973
27	1	0	1.465165	2.940464	-1.671956
28	1	0	2.709050	5.078927	2.620519
29	1	0	3.671482	3.996232	-1.426032
30	1	0	0.491117	4.055152	2.370044
31	1	0	4.320348	5.068329	0.725776
32	1	0	-3.237316	2.605202	-1.881715
33	1	0	-0.922173	2.445720	2.267025
34	1	0	-3.326966	4.590366	-0.383014
35	1	0	-4.426756	3.343532	0.198968
36	1	0	-3.280605	3.278183	2.229900
37	1	0	-2.195346	4.539490	1.652426
38	1	0	-2.121658	0.370980	1.648450
39	1	0	-0.845747	3.300134	-1.959782
40	6	0	-1.200004	-2.862082	0.874078
41	6	0	-2.169045	-3.850988	1.047564
42	6	0	-0.883524	-2.036972	1.958448
43	6	0	-2.817196	-4.010851	2.272392
44	1	0	-2.424127	-4.502918	0.215112
45	6	0	-1.522027	-2.197010	3.184820
46	1	0	-0.132775	-1.258627	1.840711
47	6	0	-2.496088	-3.183959	3.346193
48	1	0	-3.570515	-4.786105	2.387055
49	1	0	-1.256456	-1.553211	4.019916
50	1	0	-2.994448	-3.310138	4.303871
51	6	0	-0.498637	-2.702571	-0.457525
52	1	0	-0.874538	-3.486064	-1.126647
53	6	0	-0.573505	-1.359704	-1.156060
54	1	0	-1.274623	-1.253826	-1.984621
55	6	0	0.766897	-0.944012	-1.392163
56	8	0	1.083235	0.162933	-1.908052
57	6	0	1.010010	-2.963975	-0.338291
58	8	0	1.542812	-3.970228	0.080877
59	7	0	1.683106	-1.833208	-0.801644
60	6	0	3.097716	-1.779126	-1.040525
61	6	0	4.044245	-1.300554	-0.109805
62	6	0	3.486052	-2.245927	-2.298222
63	6	0	5.380470	-1.330313	-0.537313
64	6	0	4.818363	-2.259386	-2.686886
65	1	0	2.715504	-2.604934	-2.975428
66	6	0	5.771864	-1.794645	-1.789574
67	1	0	6.157081	-0.974772	0.128893
68	1	0	5.100960	-2.626768	-3.669310
69	1	0	6.825291	-1.789769	-2.057608
70	6	0	3.708201	-0.787159	1.300385

71	6	0	2.631936	0.307233	1.252616
72	1	0	2.935231	1.137588	0.608382
73	1	0	1.671510	-0.062406	0.888774
74	1	0	2.468550	0.705731	2.260369
75	6	0	3.239026	-1.953208	2.187000
76	1	0	2.334873	-2.433478	1.813282
77	1	0	4.012275	-2.725135	2.257851
78	1	0	3.033392	-1.585010	3.198843
79	6	0	4.933135	-0.164753	1.986831
80	1	0	5.729830	-0.893523	2.166972
81	1	0	5.345188	0.673468	1.415216
82	1	0	4.628348	0.222874	2.964036

SCF Done: E(RPBE1PBE) = -6437.71422421 A.U. after 1 cycles
Convg = 0.4319D-08 -V/T = 2.0053
Zero-point correction= 0.681941 (Hartree/Particle)
Thermal correction to Energy= 0.729199
Thermal correction to Enthalpy= 0.730254
Thermal correction to Gibbs Free Energy= 0.596006
Sum of electronic and zero-point Energies= -6437.032283
Sum of electronic and thermal Energies= -6436.985025
Sum of electronic and thermal Enthalpies= -6436.983970
Sum of electronic and thermal Free Energies= -6437.118218

	1	2	3
	A	A	A
Frequencies --	15.8661	21.1107	25.8998

(*S*)-PhBOD-Rh-Ph-maleimide-anti-MB-“close” (29)

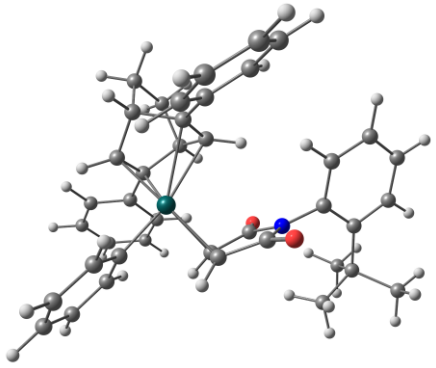


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.181042	0.175620	0.135256
2	6	0	-3.120010	1.496181	-0.245133
3	6	0	-3.311569	-0.438089	-1.700388
4	6	0	-1.661451	-3.073666	-1.929062
5	6	0	-2.907383	2.900233	0.154322
6	6	0	-2.892740	3.927972	-0.800600
7	6	0	-2.778199	0.953657	-1.455047
8	6	0	-3.930683	0.513504	0.597674
9	6	0	-2.462041	4.556609	1.876385
10	6	0	-1.730230	-5.399067	-1.281965
11	6	0	-4.858270	-0.397936	-1.563311
12	6	0	-3.094814	-0.754423	0.679590
13	6	0	-2.660168	5.247382	-0.423532
14	6	0	-2.786025	-1.305312	-0.561441
15	6	0	-2.831220	-3.727886	0.071363
16	6	0	-2.697845	3.238116	1.499798
17	6	0	-5.229501	0.189988	-0.190024
18	6	0	-2.441422	5.567260	0.916135
19	6	0	-2.418659	-2.713294	-0.804181

20	6	0	-2.490316	-5.056941	-0.164607
21	6	0	-1.315683	-4.400080	-2.163172
22	1	0	-1.303705	-2.305395	-2.608933
23	1	0	-1.460464	-6.435798	-1.464453
24	1	0	-3.432793	-3.476587	0.940210
25	1	0	-2.821798	-5.827801	0.526092
26	1	0	-0.709674	-4.652790	-3.028880
27	1	0	-3.085346	3.694479	-1.844419
28	1	0	-2.286415	4.794664	2.921882
29	1	0	-2.657970	6.030307	-1.177244
30	1	0	-2.694265	2.459891	2.259091
31	1	0	-2.258736	6.597181	1.209875
32	1	0	-3.015908	-0.821272	-2.677904
33	1	0	-4.163987	0.911721	1.585860
34	1	0	-5.268139	0.206775	-2.377986
35	1	0	-5.250833	-1.412514	-1.683174
36	1	0	-5.825115	-0.516473	0.396128
37	1	0	-5.820576	1.105363	-0.294644
38	1	0	-3.030260	-1.320854	1.605003
39	1	0	-2.298728	1.521496	-2.248589
40	6	0	-0.126663	-0.991875	1.382847
41	6	0	0.222103	-2.338045	1.237334
42	6	0	0.101639	-0.373577	2.623520
43	6	0	0.752193	-3.056548	2.312656
44	1	0	0.095118	-2.838305	0.280975
45	6	0	0.619922	-1.094433	3.701992
46	1	0	-0.112803	0.687150	2.761192
47	6	0	0.942052	-2.443959	3.551294
48	1	0	1.021384	-4.101603	2.175072
49	1	0	0.787248	-0.594392	4.653577
50	1	0	1.352950	-3.006368	4.386075
51	6	0	0.351695	0.308460	-1.377121
52	1	0	-0.125337	0.185002	-2.344682
53	6	0	0.393388	1.476493	-0.595212
54	1	0	-0.062486	2.436060	-0.823348
55	6	0	1.680315	1.471780	0.154299
56	8	0	2.080786	2.290180	0.960211
57	6	0	1.626294	-0.437691	-1.140571
58	8	0	1.976457	-1.488895	-1.638020
59	7	0	2.402603	0.350016	-0.278897
60	6	0	3.669141	-0.062002	0.249335
61	6	0	4.899866	0.293646	-0.346735
62	6	0	3.615877	-0.859743	1.391848
63	6	0	6.046026	-0.216249	0.282389
64	6	0	4.773423	-1.339176	1.990300
65	1	0	2.643707	-1.102728	1.806457
66	6	0	5.998371	-1.013504	1.422493
67	1	0	7.022976	0.010577	-0.126677
68	1	0	4.711423	-1.959673	2.880041
69	1	0	6.924832	-1.377135	1.860226
70	6	0	5.062067	1.222216	-1.566088
71	6	0	4.114776	0.862323	-2.724217
72	1	0	4.137163	-0.208091	-2.948001
73	1	0	3.081552	1.147722	-2.522662
74	1	0	4.423580	1.404892	-3.624435
75	6	0	4.810524	2.676026	-1.128160
76	1	0	3.807761	2.818702	-0.721687
77	1	0	5.524288	2.977391	-0.354356
78	1	0	4.933595	3.348951	-1.985157
79	6	0	6.488351	1.157050	-2.135997
80	1	0	7.240193	1.534522	-1.436611
81	1	0	6.766310	0.139892	-2.432076
82	1	0	6.543173	1.789326	-3.027673

```
SCF Done:  E(RPBE1PBE) =  -6437.68532881     A.U. after    1 cycles
             Convg  =    0.6236D-08             -V/T =  2.0053
Zero-point correction=                           0.679524 (Hartree/Particle)
 Thermal correction to Energy=                    0.727723
 Thermal correction to Enthalpy=                  0.728778
 Thermal correction to Gibbs Free Energy=         0.591422
 Sum of electronic and zero-point Energies=           -6437.005805
 Sum of electronic and thermal Energies=              -6436.957606
 Sum of electronic and thermal Enthalpies=            -6436.956551
 Sum of electronic and thermal Free Energies=         -6437.093906
                     1                      2                      3
                     A                      A                      A
 Frequencies --     6.7812                17.1291                27.5190
```

(*S*)-PhBOD-Rh-Ph-maleimide-anti-MB-"far" (30)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.191426	0.402627	0.514061
2	6	0	-0.533017	2.304302	-0.979560
3	6	0	-1.000735	0.392927	-2.386907
4	6	0	-2.198521	-2.420226	-1.893268
5	6	0	0.239640	3.372629	-0.317506
6	6	0	1.458861	3.812021	-0.850750
7	6	0	-0.019245	1.181436	-1.553650
8	6	0	-2.015466	2.475054	-1.289871
9	6	0	0.479002	4.999472	1.469147
10	6	0	-4.269664	-3.658311	-2.051474
11	6	0	-1.546162	1.343091	-3.492870
12	6	0	-2.698303	1.187123	-0.871165
13	6	0	2.182267	4.826150	-0.227788
14	6	0	-2.184838	0.049268	-1.492229
15	6	0	-4.307219	-1.273060	-1.670861
16	6	0	-0.247002	3.992566	0.841970
17	6	0	-2.138526	2.602021	-2.834769
18	6	0	1.698124	5.419032	0.936989
19	6	0	-2.905846	-1.225594	-1.681264
20	6	0	-4.982662	-2.476917	-1.852689
21	6	0	-2.874814	-3.623452	-2.071112
22	1	0	-1.110928	-2.415191	-1.886332
23	1	0	-4.796193	-4.598403	-2.193459
24	1	0	-4.875713	-0.358622	-1.527281
25	1	0	-6.069379	-2.491039	-1.842175
26	1	0	-2.308829	-4.539116	-2.221720
27	1	0	1.825378	3.372792	-1.775325
28	1	0	0.095480	5.456289	2.377420
29	1	0	3.123663	5.158460	-0.657350
30	1	0	-1.194470	3.669624	1.268593

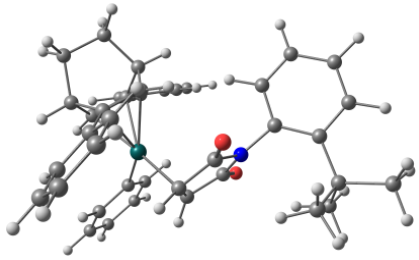
31	1	0	2.264492	6.207568	1.424703
32	1	0	-0.537158	-0.493649	-2.818261
33	1	0	-2.439792	3.346183	-0.787856
34	1	0	-0.726063	1.597548	-4.170935
35	1	0	-2.298351	0.807427	-4.080356
36	1	0	-3.195873	2.723809	-3.089342
37	1	0	-1.618845	3.507738	-3.163351
38	1	0	-3.684256	1.210355	-0.414068
39	1	0	1.039832	0.939312	-1.560442
40	6	0	-2.573217	-0.363140	1.745056
41	6	0	-3.248442	-1.582207	1.644951
42	6	0	-2.900362	0.494978	2.805877
43	6	0	-4.235553	-1.927911	2.572618
44	1	0	-3.021997	-2.274063	0.836680
45	6	0	-3.894020	0.156172	3.726293
46	1	0	-2.373114	1.441999	2.930375
47	6	0	-4.566245	-1.061291	3.612646
48	1	0	-4.749421	-2.881991	2.475756
49	1	0	-4.133399	0.839894	4.537969
50	1	0	-5.334402	-1.333115	4.332127
51	6	0	-0.038824	-1.346254	0.855637
52	6	0	0.287523	-0.447718	1.891497
53	1	0	-0.698729	-2.204923	0.922530
54	1	0	-0.128423	-0.453027	2.893770
55	6	0	1.693388	-0.026296	1.702971
56	8	0	2.380215	0.688354	2.406474
57	6	0	1.150062	-1.434954	-0.047583
58	8	0	1.255329	-2.062162	-1.088476
59	7	0	2.160212	-0.669576	0.534140
60	6	0	3.450028	-0.458802	-0.038065
61	6	0	4.436998	-1.460784	-0.118192
62	6	0	3.683219	0.828198	-0.535428
63	6	0	5.592763	-1.113864	-0.841335
64	6	0	4.859070	1.148643	-1.194340
65	1	0	2.921421	1.585835	-0.379555
66	6	0	5.810512	0.148722	-1.376008
67	1	0	6.366246	-1.860502	-0.986281
68	1	0	5.023132	2.155364	-1.568907
69	1	0	6.731144	0.352603	-1.916646
70	6	0	4.391539	-2.873980	0.497027
71	6	0	3.344337	-3.069697	1.604126
72	1	0	3.398336	-2.285866	2.365709
73	1	0	2.323999	-3.127544	1.223917
74	1	0	3.541545	-4.024698	2.102820
75	6	0	4.130019	-3.898043	-0.620671
76	1	0	3.168966	-3.708888	-1.106579
77	1	0	4.912900	-3.858284	-1.385162
78	1	0	4.117023	-4.912174	-0.204382
79	6	0	5.752491	-3.184756	1.154209
80	1	0	5.999044	-2.442728	1.920693
81	1	0	5.705403	-4.166553	1.636293
82	1	0	6.578723	-3.222457	0.440732

SCF Done: E(RPBE1PBE) = -6437.68601967 A.U. after 1 cycles
Convg = 0.6042D-08 -V/T = 2.0053
Zero-point correction= 0.679790 (Hartree/Particle)
Thermal correction to Energy= 0.727900
Thermal correction to Enthalpy= 0.728955
Thermal correction to Gibbs Free Energy= 0.592775
Sum of electronic and zero-point Energies= -6437.006230
Sum of electronic and thermal Energies= -6436.958120
Sum of electronic and thermal Enthalpies= -6436.957065
Sum of electronic and thermal Free Energies= -6437.093245

1 2 3

	A	A	A
Frequencies --	16.8713	21.7046	28.1317

(*S*)-PhBOD-Rh-Ph-maleimide-(3*S*,*R*$_a$)-MB-"parallel" (31)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.128590	0.313802	0.406335
2	6	0	-1.645583	1.981523	-1.095383
3	6	0	-1.244725	-0.024216	-2.413686
4	6	0	-0.827982	-3.002934	-1.524492
5	6	0	-1.434234	3.345739	-0.570778
6	6	0	-0.422456	4.172223	-1.077780
7	6	0	-0.689876	1.184834	-1.694754
8	6	0	-3.046821	1.408544	-1.284936
9	6	0	-2.057101	5.124122	0.966192
10	6	0	-2.024160	-5.094152	-1.357580
11	6	0	-2.263313	0.454850	-3.483253
12	6	0	-2.971348	-0.001854	-0.733187
13	6	0	-0.229723	5.453438	-0.569462
14	6	0	-2.018763	-0.804788	-1.358090
15	6	0	-3.212204	-2.997606	-1.190724
16	6	0	-2.251051	3.844524	0.456120
17	6	0	-3.330046	1.334166	-2.807873
18	6	0	-1.045228	5.935852	0.453264
19	6	0	-2.018284	-2.280861	-1.352591
20	6	0	-3.215661	-4.389620	-1.193457
21	6	0	-0.828816	-4.393720	-1.521177
22	1	0	0.118029	-2.477592	-1.622177
23	1	0	-2.025554	-6.180854	-1.355158
24	1	0	-4.149009	-2.461501	-1.069368
25	1	0	-4.152855	-4.925247	-1.067381
26	1	0	0.108719	-4.931086	-1.634749
27	1	0	0.218886	3.811486	-1.875811
28	1	0	-2.694452	5.487656	1.767987
29	1	0	0.561461	6.077626	-0.975848
30	1	0	-3.030468	3.215967	0.879892
31	1	0	-0.893667	6.936832	0.848161
32	1	0	-0.458002	-0.625317	-2.871206
33	1	0	-3.806849	2.000636	-0.774844
34	1	0	-1.723152	1.008731	-4.257064
35	1	0	-2.711147	-0.420675	-3.963749
36	1	0	-4.333873	0.923593	-2.955128
37	1	0	-3.330251	2.348551	-3.219316
38	1	0	-3.780511	-0.406631	-0.133134
39	1	0	0.340140	1.501885	-1.831293
40	6	0	-2.000266	-0.876212	1.839900
41	6	0	-1.869578	-2.261836	1.969820
42	6	0	-2.859219	-0.203855	2.721561
43	6	0	-2.595986	-2.959095	2.938901
44	1	0	-1.185109	-2.811464	1.328254
45	6	0	-3.589680	-0.900848	3.687620

46	1	0	-2.970245	0.878859	2.662312
47	6	0	-3.462603	-2.285364	3.798505
48	1	0	-2.475138	-4.037123	3.022856
49	1	0	-4.255205	-0.357762	4.355802
50	1	0	-4.025251	-2.830465	4.552366
51	6	0	0.494206	0.023676	1.869376
52	6	0	0.603903	1.299816	1.313586
53	1	0	0.116960	-0.234941	2.849289
54	1	0	0.289173	2.238616	1.758692
55	6	0	1.745496	1.282211	0.357560
56	8	0	2.192643	2.195969	-0.309970
57	6	0	1.511433	-0.850743	1.217873
58	8	0	1.703818	-2.039958	1.380025
59	7	0	2.275981	-0.018088	0.381339
60	6	0	3.267424	-0.472639	-0.543754
61	6	0	4.645234	-0.528382	-0.243093
62	6	0	2.784175	-0.842297	-1.799689
63	6	0	5.472306	-0.986986	-1.280600
64	6	0	3.630806	-1.293263	-2.802615
65	1	0	1.715787	-0.761034	-1.977428
66	6	0	4.991578	-1.365104	-2.530743
67	1	0	6.541184	-1.051676	-1.117720
68	1	0	3.234959	-1.577563	-3.773643
69	1	0	5.688014	-1.710701	-3.290377
70	6	0	5.266853	-0.166601	1.118642
71	6	0	4.749034	1.176679	1.661826
72	1	0	4.798458	1.964638	0.904833
73	1	0	3.721480	1.114199	2.021604
74	1	0	5.366173	1.483559	2.513101
75	6	0	4.963859	-1.285629	2.130282
76	1	0	3.893030	-1.439111	2.272591
77	1	0	5.391279	-2.237292	1.797372
78	1	0	5.407183	-1.035505	3.101217
79	6	0	6.795504	-0.039711	1.021586
80	1	0	7.100918	0.714421	0.288346
81	1	0	7.187063	0.267759	1.996133
82	1	0	7.282224	-0.987346	0.772183

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SCF Done:  E(RPBE1PBE) =  -6437.68408419     A.U. after    1 cycles
             Convg  =    0.4878D-08             -V/T =  2.0053
Zero-point correction=                           0.680129 (Hartree/Particle)
 Thermal correction to Energy=                    0.728237
 Thermal correction to Enthalpy=                  0.729292
 Thermal correction to Gibbs Free Energy=         0.592459
 Sum of electronic and zero-point Energies=          -6437.003955
 Sum of electronic and thermal Energies=             -6436.955847
 Sum of electronic and thermal Enthalpies=           -6436.954792
 Sum of electronic and thermal Free Energies=        -6437.091625
                      1                      2                      3
                      A                      A                      A
 Frequencies --    13.7345                21.4420                27.3272
```
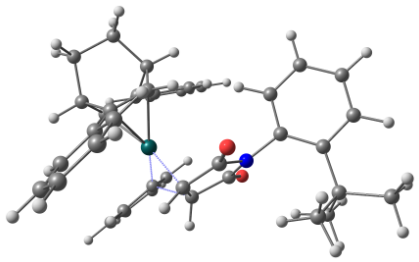

(*S*)-PhBOD-Rh-Ph-(R_a)-maleimide-(3*S*,R_a)-CR-TS-conf"pp" (32)



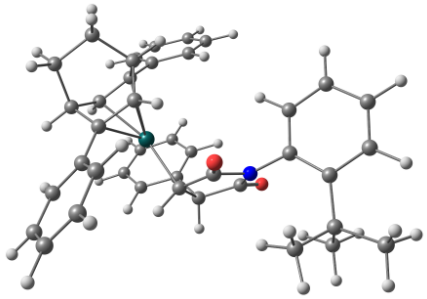
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.097466	0.290780	0.346738
2	6	0	-2.043142	1.795776	-0.954147
3	6	0	-1.563696	-0.125790	-2.385463
4	6	0	-0.670583	-3.027897	-1.609815
5	6	0	-1.946902	3.189959	-0.469378
6	6	0	-1.031735	4.094773	-1.026139
7	6	0	-1.062625	1.118013	-1.680318
8	6	0	-3.380385	1.060754	-1.016952
9	6	0	-2.680548	4.947577	1.046041
10	6	0	-1.523200	-5.257636	-1.242546
11	6	0	-2.739653	0.257113	-3.320043
12	6	0	-3.063289	-0.334052	-0.515285
13	6	0	-0.939030	5.400266	-0.553057
14	6	0	-2.115945	-1.006632	-1.267722
15	6	0	-2.950811	-3.337448	-0.908461
16	6	0	-2.771044	3.642003	0.573535
17	6	0	-3.824256	0.979094	-2.499803
18	6	0	-1.763221	5.835225	0.483879
19	6	0	-1.907271	-2.467673	-1.257071
20	6	0	-2.761460	-4.716341	-0.899597
21	6	0	-0.477485	-4.405557	-1.597557
22	1	0	0.164589	-2.382228	-1.865687
23	1	0	-1.373916	-6.334042	-1.234827
24	1	0	-3.925077	-2.930884	-0.652482
25	1	0	-3.586110	-5.370705	-0.629007
26	1	0	0.495823	-4.813558	-1.856503
27	1	0	-0.381655	3.776355	-1.834909
28	1	0	-3.325439	5.272017	1.858772
29	1	0	-0.219066	6.081233	-0.999116
30	1	0	-3.476887	2.960039	1.040728
31	1	0	-1.691617	6.855657	0.850714
32	1	0	-0.769620	-0.622405	-2.944994
33	1	0	-4.146787	1.541480	-0.408949
34	1	0	-2.356744	0.897240	-4.121007
35	1	0	-3.132260	-0.650227	-3.790122
36	1	0	-4.779407	0.447104	-2.551728
37	1	0	-3.997140	1.993260	-2.873824
38	1	0	-3.698614	-0.827917	0.215293
39	1	0	-0.111526	1.570179	-1.950724
40	6	0	-1.209055	-1.013709	2.030263
41	6	0	-1.079327	-2.404551	1.977932
42	6	0	-2.067276	-0.442133	2.985865
43	6	0	-1.842892	-3.208689	2.824198
44	1	0	-0.382702	-2.864395	1.284239
45	6	0	-2.844182	-1.251798	3.812524
46	1	0	-2.128551	0.640450	3.087042
47	6	0	-2.734025	-2.641330	3.735013
48	1	0	-1.738236	-4.289500	2.765921
49	1	0	-3.520849	-0.795499	4.531588
50	1	0	-3.323372	-3.274898	4.392853
51	6	0	0.537671	0.040992	1.902936
52	6	0	0.486955	1.337612	1.285917
53	1	0	0.541883	-0.078775	2.980758
54	1	0	0.178875	2.246385	1.795883
55	6	0	1.586830	1.421227	0.309739
56	8	0	1.923565	2.351480	-0.399840
57	6	0	1.629826	-0.725459	1.187763
58	8	0	1.942285	-1.890657	1.335910
59	7	0	2.267663	0.176519	0.337993
60	6	0	3.237851	-0.191038	-0.647129

61	6	0	4.630443	-0.134814	-0.427301
62	6	0	2.711735	-0.586232	-1.877714
63	6	0	5.429730	-0.522529	-1.514108
64	6	0	3.532345	-0.960950	-2.932278
65	1	0	1.631287	-0.582060	-1.993629
66	6	0	4.908092	-0.930132	-2.738457
67	1	0	6.508101	-0.503144	-1.413755
68	1	0	3.105264	-1.265630	-3.883742
69	1	0	5.584206	-1.215496	-3.540311
70	6	0	5.295998	0.292434	0.894014
71	6	0	4.739112	1.629615	1.412733
72	1	0	4.757380	2.400250	0.636594
73	1	0	3.716000	1.543258	1.779456
74	1	0	5.353841	1.975207	2.251079
75	6	0	5.095463	-0.800953	1.957381
76	1	0	4.042706	-0.988462	2.171439
77	1	0	5.537860	-1.747992	1.631355
78	1	0	5.585353	-0.500583	2.890835
79	6	0	6.810917	0.485473	0.723583
80	1	0	7.049020	1.237217	-0.036571
81	1	0	7.231843	0.831487	1.672732
82	1	0	7.327498	-0.445124	0.469027

SCF Done: E(RPBE1PBE) = -6437.66838399 A.U. after 1 cycles
Convg = 0.5232D-08 -V/T = 2.0053
Zero-point correction= 0.679582 (Hartree/Particle)
Thermal correction to Energy= 0.726781
Thermal correction to Enthalpy= 0.727836
Thermal correction to Gibbs Free Energy= 0.593899
Sum of electronic and zero-point Energies= -6436.988802
Sum of electronic and thermal Energies= -6436.941603
Sum of electronic and thermal Enthalpies= -6436.940548
Sum of electronic and thermal Free Energies= -6437.074485

	1	2	3
	A	A	A
Frequencies --	-297.6111	14.9590	24.8116

(*S*)-PhBOD-α-Rh-(3*S*,*R*$_a$)-Phsuccinimide (33)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.202414	0.297602	0.337932
2	6	0	-1.997621	1.919743	-0.840163
3	6	0	-2.141560	-0.090827	-2.237185
4	6	0	-1.672870	-3.052252	-1.340318
5	6	0	-1.564644	3.292876	-0.500411
6	6	0	-0.537138	3.933116	-1.209026
7	6	0	-1.280529	1.011418	-1.650953
8	6	0	-3.460201	1.500681	-0.711976
9	6	0	-1.774473	5.286660	0.883114

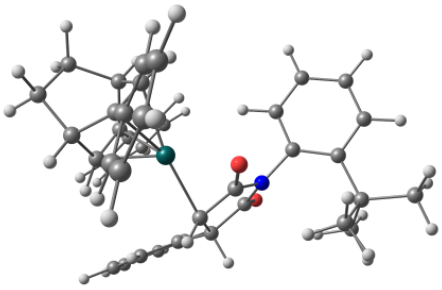
10	6	0	-2.825215	-5.074732	-0.694438
11	6	0	-3.317556	0.523920	-3.033524
12	6	0	-3.383277	0.083053	-0.180049
13	6	0	-0.134689	5.223489	-0.876816
14	6	0	-2.704258	-0.794931	-1.004276
15	6	0	-3.870750	-2.920137	-0.369758
16	6	0	-2.174364	3.995961	0.551351
17	6	0	-4.100320	1.487460	-2.122737
18	6	0	-0.751624	5.909804	0.168391
19	6	0	-2.748519	-2.267228	-0.899190
20	6	0	-3.908842	-4.308333	-0.267094
21	6	0	-1.706161	-4.438880	-1.233634
22	1	0	-0.788347	-2.569362	-1.748164
23	1	0	-2.854456	-6.158195	-0.615494
24	1	0	-4.728278	-2.334579	-0.049645
25	1	0	-4.791639	-4.794252	0.140767
26	1	0	-0.855392	-5.026253	-1.569250
27	1	0	-0.037940	3.414914	-2.021175
28	1	0	-2.260794	5.806755	1.704636
29	1	0	0.665941	5.695230	-1.440564
30	1	0	-2.958280	3.522481	1.136531
31	1	0	-0.438395	6.918547	0.424158
32	1	0	-1.556588	-0.766284	-2.863112
33	1	0	-4.021468	2.149739	-0.039466
34	1	0	-2.913386	1.045489	-3.906881
35	1	0	-3.959139	-0.281164	-3.406419
36	1	0	-5.147562	1.181854	-2.030930
37	1	0	-4.095321	2.506231	-2.523445
38	1	0	-3.991261	-0.242921	0.660206
39	1	0	-0.307836	1.246900	-2.076312
40	6	0	-0.365902	-0.651438	2.350462
41	6	0	-0.573718	-2.029822	2.152402
42	6	0	-1.430983	0.115091	2.876592
43	6	0	-1.778652	-2.625469	2.515446
44	1	0	0.227995	-2.641819	1.752726
45	6	0	-2.632545	-0.495504	3.252845
46	1	0	-1.277214	1.170873	3.086732
47	6	0	-2.805055	-1.865413	3.078312
48	1	0	-1.915253	-3.691172	2.355062
49	1	0	-3.423618	0.106860	3.691962
50	1	0	-3.735607	-2.341437	3.375787
51	6	0	0.945321	0.079700	2.062740
52	6	0	0.662828	1.087631	0.960443
53	1	0	1.333489	0.517554	2.992755
54	1	0	0.540690	2.135401	1.240013
55	6	0	1.684415	0.880859	-0.069797
56	8	0	1.907183	1.502479	-1.097470
57	6	0	2.042574	-0.807669	1.498103
58	8	0	2.481163	-1.831897	1.993556
59	7	0	2.472614	-0.245979	0.313182
60	6	0	3.389621	-0.881985	-0.583590
61	6	0	4.776893	-0.628230	-0.602105
62	6	0	2.801079	-1.776121	-1.479252
63	6	0	5.507048	-1.332254	-1.572434
64	6	0	3.555166	-2.458194	-2.423986
65	1	0	1.725902	-1.924890	-1.419986
66	6	0	4.924850	-2.226806	-2.465705
67	1	0	6.577164	-1.180366	-1.645256
68	1	0	3.080958	-3.151422	-3.113182
69	1	0	5.548512	-2.738391	-3.194337
70	6	0	5.512924	0.307791	0.373650
71	6	0	4.831105	1.681541	0.492807
72	1	0	4.633294	2.119296	-0.489584
73	1	0	3.886552	1.635302	1.035285

74	1	0	5.486880	2.362441	1.046527
75	6	0	5.586293	-0.356954	1.759469
76	1	0	4.598861	-0.572900	2.170669
77	1	0	6.133969	-1.303835	1.708863
78	1	0	6.112764	0.303327	2.458705
79	6	0	6.955847	0.574496	-0.082538
80	1	0	6.995057	1.021857	-1.081535
81	1	0	7.422052	1.278818	0.613482
82	1	0	7.574300	-0.328204	-0.079056

SCF Done: E(RPBE1PBE) = -6437.72125745 A.U. after 1 cycles
Convg = 0.3019D-08 -V/T = 2.0053
Zero-point correction= 0.681675 (Hartree/Particle)
Thermal correction to Energy= 0.729122
Thermal correction to Enthalpy= 0.730177
Thermal correction to Gibbs Free Energy= 0.594102
Sum of electronic and zero-point Energies= -6437.039583
Sum of electronic and thermal Energies= -6436.992136
Sum of electronic and thermal Enthalpies= -6436.991081
Sum of electronic and thermal Free Energies= -6437.127155

	1	2	3
	A	A	A
Frequencies --	8.6983	12.6200	23.9941

(*S*)-PhBOD-(3*S*,R_a)-Rh-oxa-α-allyl (34)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.140012	-0.363557	-0.175811
2	6	0	-3.137035	-1.182915	0.259912
3	6	0	-2.590945	0.375191	2.051270
4	6	0	-0.195480	2.337136	2.306380
5	6	0	-3.426751	-2.489774	-0.366755
6	6	0	-3.532684	-3.654364	0.406550
7	6	0	-2.448069	-1.008446	1.458038
8	6	0	-3.836790	0.101192	-0.182104
9	6	0	-3.876348	-3.823991	-2.348583
10	6	0	0.314438	4.686931	2.108271
11	6	0	-4.084647	0.725175	2.246643
12	6	0	-2.686722	1.088928	-0.265713
13	6	0	-3.802621	-4.884337	-0.186984
14	6	0	-2.009515	1.267078	0.955477
15	6	0	-1.423217	3.699482	0.750344
16	6	0	-3.608691	-2.595235	-1.754003
17	6	0	-4.836211	0.536324	0.915294
18	6	0	-3.974992	-4.975397	-1.567328
19	6	0	-1.191678	2.442655	1.324312
20	6	0	-0.679111	4.809927	1.139428
21	6	0	0.555647	3.442414	2.689769
22	1	0	0.002014	1.373309	2.768499

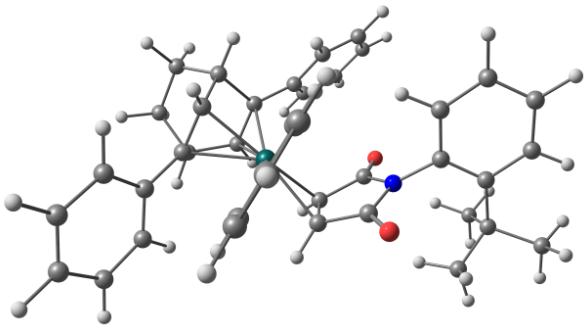
23	1	0	0.898947	5.553111	2.406785
24	1	0	-2.202405	3.813646	0.002464
25	1	0	-0.875442	5.774875	0.680453
26	1	0	1.334138	3.331991	3.440047
27	1	0	-3.417202	-3.594621	1.485299
28	1	0	-4.002836	-3.885043	-3.426375
29	1	0	-3.884387	-5.774193	0.431736
30	1	0	-3.513918	-1.710245	-2.378375
31	1	0	-4.185768	-5.935362	-2.030938
32	1	0	-2.040736	0.472362	2.987934
33	1	0	-4.338251	-0.019762	-1.143460
34	1	0	-4.498613	0.081062	3.029058
35	1	0	-4.162173	1.756950	2.604673
36	1	0	-5.322258	1.465333	0.600405
37	1	0	-5.620293	-0.222621	1.005131
38	1	0	-2.631650	1.812988	-1.074783
39	1	0	-2.037670	-1.834454	2.033524
40	6	0	1.171279	2.700452	-1.767363
41	6	0	2.002061	3.751761	-1.366706
42	6	0	-0.023049	3.008689	-2.428422
43	6	0	1.642467	5.074246	-1.624105
44	1	0	2.930635	3.532606	-0.851322
45	6	0	-0.376257	4.329322	-2.696371
46	1	0	-0.681006	2.203913	-2.745280
47	6	0	0.458826	5.371286	-2.296548
48	1	0	2.299732	5.877753	-1.300567
49	1	0	-1.304285	4.543508	-3.221422
50	1	0	0.189603	6.403368	-2.506961
51	6	0	1.576026	1.246367	-1.650453
52	6	0	0.495130	0.190288	-1.588006
53	1	0	2.171188	1.035535	-2.557830
54	1	0	-0.029034	-0.095070	-2.499521
55	6	0	1.012665	-0.868878	-0.794574
56	8	0	0.383698	-1.929534	-0.513805
57	6	0	2.537964	0.827617	-0.537732
58	8	0	3.443776	1.463407	-0.035221
59	7	0	2.237594	-0.496870	-0.215295
60	6	0	2.852445	-1.219854	0.856877
61	6	0	3.879419	-2.165036	0.654155
62	6	0	2.354474	-0.943783	2.129464
63	6	0	4.353075	-2.802281	1.810644
64	6	0	2.850372	-1.590173	3.253629
65	1	0	1.563811	-0.204601	2.219031
66	6	0	3.859540	-2.530319	3.083877
67	1	0	5.138248	-3.543976	1.726276
68	1	0	2.454060	-1.364226	4.239720
69	1	0	4.269601	-3.058659	3.940812
70	6	0	4.499438	-2.493557	-0.715284
71	6	0	3.431146	-2.903024	-1.744529
72	1	0	2.776117	-3.686669	-1.352651
73	1	0	2.805832	-2.066302	-2.058170
74	1	0	3.924303	-3.289244	-2.643478
75	6	0	5.285461	-1.278065	-1.235773
76	1	0	4.653673	-0.399881	-1.375884
77	1	0	6.083511	-1.001211	-0.539408
78	1	0	5.744694	-1.520865	-2.200931
79	6	0	5.489216	-3.664023	-0.620855
80	1	0	5.011300	-4.581640	-0.261667
81	1	0	5.887805	-3.871051	-1.618909
82	1	0	6.344663	-3.439502	0.024047

SCF Done: E(RPBE1PBE) = -6437.71007709 A.U. after 1 cycles
Convg = 0.6467D-08 -V/T = 2.0053
Zero-point correction= 0.681549 (Hartree/Particle)

Thermal correction to Energy=		0.728908	
Thermal correction to Enthalpy=		0.729963	
Thermal correction to Gibbs Free Energy=		0.594958	
Sum of electronic and zero-point Energies=		-6437.028528	
Sum of electronic and thermal Energies=		-6436.981169	
Sum of electronic and thermal Enthalpies=		-6436.980114	
Sum of electronic and thermal Free Energies=		-6437.11511	

	1	2	3
	A	A	A
Frequencies --	17.0314	18.5518	27.1695

(*S*)-PhBOD-Rh-Ph-maleimide-(3*R*,*R*$_a$)-MB-"parallel" (35)



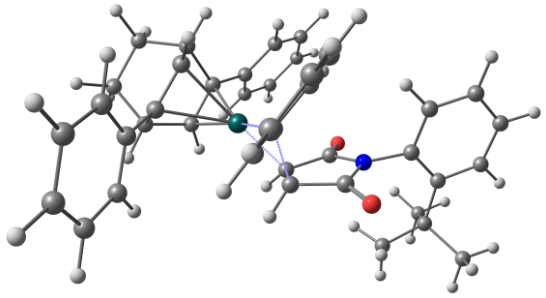
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.104416	0.174904	-0.217215
2	6	0	-1.275034	2.488893	0.057691
3	6	0	-3.242569	1.757085	-1.171410
4	6	0	-4.360491	-1.059311	-1.822340
5	6	0	-0.010669	3.202960	0.315141
6	6	0	0.480085	4.151887	-0.590650
7	6	0	-1.786019	2.162096	-1.180663
8	6	0	-2.315626	2.307610	1.156160
9	6	0	1.901025	3.640008	1.747671
10	6	0	-5.990733	-2.680304	-1.082565
11	6	0	-4.078274	2.903860	-0.543094
12	6	0	-2.764675	0.867991	1.020202
13	6	0	1.664455	4.834698	-0.331597
14	6	0	-3.312264	0.560791	-0.230838
15	6	0	-5.006885	-1.137358	0.495033
16	6	0	0.712896	2.964391	1.492919
17	6	0	-3.506867	3.248312	0.844449
18	6	0	2.380948	4.579100	0.835563
19	6	0	-4.230284	-0.558494	-0.517731
20	6	0	-5.877187	-2.187405	0.216137
21	6	0	-5.226900	-2.110779	-2.102158
22	1	0	-3.755011	-0.642332	-2.623251
23	1	0	-6.668727	-3.501274	-1.299872
24	1	0	-4.932507	-0.761146	1.511092
25	1	0	-6.468983	-2.622026	1.017331
26	1	0	-5.302978	-2.491345	-3.117422
27	1	0	-0.077330	4.366477	-1.498575
28	1	0	2.459275	3.428655	2.655782
29	1	0	2.030444	5.567827	-1.045393
30	1	0	0.354013	2.224618	2.205112
31	1	0	3.309766	5.107070	1.033394
32	1	0	-3.601363	1.516100	-2.172398
33	1	0	-1.903192	2.510939	2.144902
34	1	0	-4.044235	3.769259	-1.212222

35	1	0	-5.123802	2.586371	-0.477897
36	1	0	-4.262554	3.124065	1.626456
37	1	0	-3.163255	4.286861	0.887663
38	1	0	-2.936360	0.256884	1.900784
39	1	0	-1.271554	2.392224	-2.109201
40	6	0	-1.282242	-1.583105	0.855239
41	6	0	-1.982166	-2.729197	0.469563
42	6	0	-0.709589	-1.560167	2.134078
43	6	0	-2.107378	-3.819225	1.334259
44	1	0	-2.439405	-2.789681	-0.516082
45	6	0	-0.834166	-2.646598	3.002063
46	1	0	-0.158152	-0.682936	2.472263
47	6	0	-1.534919	-3.784503	2.604277
48	1	0	-2.653582	-4.701538	1.006984
49	1	0	-0.377426	-2.602743	3.988745
50	1	0	-1.627911	-4.635523	3.274378
51	6	0	0.232176	-1.208060	-1.312991
52	1	0	-0.390204	-1.922661	-1.838921
53	6	0	0.517834	0.103456	-1.695520
54	1	0	0.169919	0.606181	-2.591014
55	6	0	1.851771	0.471032	-1.139733
56	8	0	2.464189	1.509772	-1.292673
57	6	0	1.392889	-1.708456	-0.513404
58	8	0	1.577972	-2.814652	-0.056216
59	7	0	2.319918	-0.649847	-0.445094
60	6	0	3.476454	-0.668214	0.396273
61	6	0	4.762429	-1.047063	-0.044087
62	6	0	3.240859	-0.298707	1.721991
63	6	0	5.767238	-1.023240	0.936551
64	6	0	4.259652	-0.284688	2.663693
65	1	0	2.227644	-0.023723	2.001546
66	6	0	5.536555	-0.654226	2.258016
67	1	0	6.777235	-1.308144	0.667980
68	1	0	4.057268	0.002288	3.691864
69	1	0	6.360168	-0.661648	2.967461
70	6	0	5.136844	-1.413612	-1.492615
71	6	0	4.099474	-2.323130	-2.173362
72	1	0	3.825241	-3.171434	-1.540208
73	1	0	3.187585	-1.788831	-2.443192
74	1	0	4.522838	-2.715950	-3.104050
75	6	0	5.294815	-0.117602	-2.307391
76	1	0	4.378291	0.475981	-2.314193
77	1	0	6.091638	0.508362	-1.891722
78	1	0	5.559185	-0.361139	-3.343256
79	6	0	6.477682	-2.164993	-1.550106
80	1	0	7.325131	-1.544554	-1.244386
81	1	0	6.467645	-3.070197	-0.933557
82	1	0	6.670354	-2.468413	-2.583772

SCF Done: E(RPBE1PBE) = -6437.67428651 A.U. after 1 cycles
Convg = 0.3535D-08 -V/T = 2.0053
Zero-point correction= 0.679731 (Hartree/Particle)
Thermal correction to Energy= 0.727749
Thermal correction to Enthalpy= 0.728804
Thermal correction to Gibbs Free Energy= 0.592884
Sum of electronic and zero-point Energies= -6436.994556
Sum of electronic and thermal Energies= -6436.946537
Sum of electronic and thermal Enthalpies= -6436.945482
Sum of electronic and thermal Free Energies= -6437.081403

	1	2	3
	A	A	A
Frequencies --	11.4116	14.8447	26.9460

(*S*)-PhBOD-Rh-Ph-(3*R*,R_a)-CR-TS-conf"pp" (36)



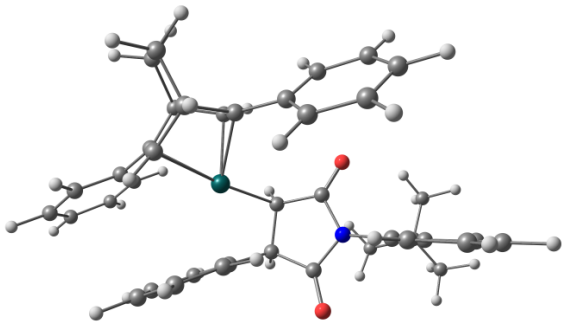
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.201437	0.290470	-0.167037
2	6	0	-1.773007	2.427755	0.037135
3	6	0	-3.547109	1.355514	-1.248095
4	6	0	-4.044342	-1.656208	-1.823768
5	6	0	-0.672139	3.378831	0.296407
6	6	0	-0.262184	4.296505	-0.680228
7	6	0	-2.162897	1.967840	-1.217934
8	6	0	-2.842267	2.140340	1.091447
9	6	0	1.013687	4.291503	1.790812
10	6	0	-5.313721	-3.578743	-1.096466
11	6	0	-4.576003	2.386990	-0.719978
12	6	0	-3.056860	0.642518	1.002646
13	6	0	0.772839	5.192519	-0.429099
14	6	0	-3.468659	0.203598	-0.249562
15	6	0	-4.792851	-1.803479	0.458300
16	6	0	-0.019849	3.395922	1.538119
17	6	0	-4.143916	2.870247	0.676447
18	6	0	1.415680	5.194631	0.807293
19	6	0	-4.103856	-1.097351	-0.537452
20	6	0	-5.388493	-3.031574	0.183443
21	6	0	-4.638914	-2.883292	-2.100536
22	1	0	-3.503424	-1.138117	-2.611776
23	1	0	-5.780177	-4.536307	-1.311923
24	1	0	-4.871142	-1.383595	1.457102
25	1	0	-5.918309	-3.560435	0.971472
26	1	0	-4.571679	-3.301286	-3.101691
27	1	0	-0.768956	4.320816	-1.641260
28	1	0	1.514901	4.278473	2.755123
29	1	0	1.074807	5.895955	-1.200662
30	1	0	-0.307920	2.682851	2.306907
31	1	0	2.225119	5.892607	1.002970
32	1	0	-3.816708	1.014291	-2.248324
33	1	0	-2.523048	2.444359	2.089157
34	1	0	-4.633839	3.220452	-1.427314
35	1	0	-5.565548	1.919478	-0.691605
36	1	0	-4.916896	2.663736	1.423489
37	1	0	-3.964820	3.950282	0.686253
38	1	0	-3.119235	0.027147	1.896358
39	1	0	-1.661410	2.261247	-2.137090
40	6	0	-0.780246	-1.601114	0.667881
41	6	0	-1.440817	-2.818328	0.471686
42	6	0	-0.183449	-1.345361	1.914316
43	6	0	-1.540783	-3.739542	1.511269
44	1	0	-1.886680	-3.049459	-0.492758
45	6	0	-0.312023	-2.255917	2.961471
46	1	0	0.370417	-0.421074	2.074310
47	6	0	-0.984140	-3.461677	2.760474

48	1	0	-2.057964	-4.681129	1.343162
49	1	0	0.133440	-2.033226	3.928522
50	1	0	-1.059638	-4.186470	3.566785
51	6	0	0.342527	-1.155191	-1.013213
52	1	0	-0.152441	-1.807205	-1.726884
53	6	0	0.610091	0.228645	-1.276527
54	1	0	0.370251	0.722888	-2.214309
55	6	0	1.922327	0.551793	-0.673168
56	8	0	2.525497	1.607551	-0.668309
57	6	0	1.600031	-1.728455	-0.395091
58	8	0	1.880469	-2.896959	-0.230043
59	7	0	2.441634	-0.650053	-0.144996
60	6	0	3.708352	-0.749669	0.510248
61	6	0	4.938786	-0.811211	-0.170452
62	6	0	3.651728	-0.755853	1.908048
63	6	0	6.083306	-0.821124	0.648294
64	6	0	4.800215	-0.796682	2.681935
65	1	0	2.674257	-0.726480	2.379331
66	6	0	6.032797	-0.814973	2.035151
67	1	0	7.062942	-0.833519	0.181477
68	1	0	4.734184	-0.803289	3.766255
69	1	0	6.956973	-0.828204	2.607183
70	6	0	5.183151	-0.837110	-1.691790
71	6	0	3.948770	-1.078894	-2.570013
72	1	0	3.422523	-1.998404	-2.299455
73	1	0	3.250115	-0.240902	-2.559691
74	1	0	4.284762	-1.190587	-3.606880
75	6	0	5.796259	0.513936	-2.101420
76	1	0	5.110262	1.334171	-1.869177
77	1	0	6.741046	0.705229	-1.582999
78	1	0	5.996444	0.524077	-3.179142
79	6	0	6.167903	-1.974529	-2.028777
80	1	0	7.145455	-1.853139	-1.556459
81	1	0	5.762574	-2.944404	-1.722794
82	1	0	6.335334	-2.003216	-3.110738

SCF Done: E(RPBE1PBE) = -6437.66130027 A.U. after 1 cycles
Convg = 0.4196D-08 -V/T = 2.0053
Zero-point correction= 0.678981 (Hartree/Particle)
Thermal correction to Energy= 0.726156
Thermal correction to Enthalpy= 0.727211
Thermal correction to Gibbs Free Energy= 0.593810
Sum of electronic and zero-point Energies= -6436.982320
Sum of electronic and thermal Energies= -6436.935145
Sum of electronic and thermal Enthalpies= -6436.934090
Sum of electronic and thermal Free Energies= -6437.067490

	1	2	3
	A	A	A
Frequencies --	-277.1578	13.0166	21.4310

(*S*)-PhBOD-α-Rh-(3*R*,*R*$_a$)-Phsuccinimide (37)



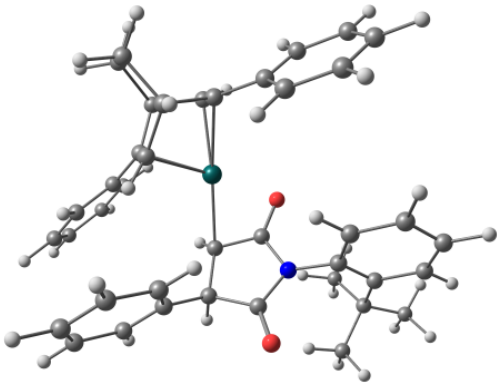
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.325953	0.060024	-0.125232
2	6	0	-1.079471	2.218804	-0.183787
3	6	0	-3.066879	1.683053	-1.511037
4	6	0	-4.466994	-1.112647	-1.680502
5	6	0	0.243458	2.832908	0.050533
6	6	0	0.978731	3.403317	-0.996197
7	6	0	-1.552823	1.719895	-1.417497
8	6	0	-2.233235	2.530584	0.766284
9	6	0	1.998722	3.519423	1.588683
10	6	0	-6.387778	-2.336105	-0.873963
11	6	0	-3.650361	3.091367	-1.241715
12	6	0	-2.989697	1.223674	0.857423
13	6	0	2.202165	4.022658	-0.756345
14	6	0	-3.461272	0.761005	-0.358745
15	6	0	-5.459504	-0.527940	0.433202
16	6	0	0.775890	2.903718	1.347918
17	6	0	-3.131273	3.609392	0.112112
18	6	0	2.718294	4.084867	0.535319
19	6	0	-4.467950	-0.306125	-0.532375
20	6	0	-6.409143	-1.532772	0.265203
21	6	0	-5.411499	-2.120170	-1.847638
22	1	0	-3.702996	-0.964853	-2.440073
23	1	0	-7.130400	-3.118363	-1.007123
24	1	0	-5.497223	0.104097	1.316374
25	1	0	-7.174068	-1.683389	1.022839
26	1	0	-5.386838	-2.739779	-2.740475
27	1	0	0.589866	3.365847	-2.009165
28	1	0	2.395495	3.555475	2.600211
29	1	0	2.757605	4.452171	-1.585735
30	1	0	0.235044	2.452754	2.176721
31	1	0	3.676219	4.562989	0.721198
32	1	0	-3.403765	1.296352	-2.474174
33	1	0	-1.878144	2.861886	1.742963
34	1	0	-3.354477	3.756057	-2.059701
35	1	0	-4.743753	3.033824	-1.252555
36	1	0	-3.958298	3.838666	0.791834
37	1	0	-2.549063	4.528642	-0.009467
38	1	0	-3.309546	0.814805	1.811974
39	1	0	-0.938466	1.711671	-2.314603
40	6	0	-0.773690	-2.112857	0.772810
41	6	0	-1.876251	-2.942777	0.493423
42	6	0	-0.809466	-1.323071	1.940715
43	6	0	-2.952675	-3.020237	1.367548
44	1	0	-1.865921	-3.551204	-0.407975
45	6	0	-1.890879	-1.419438	2.826619
46	1	0	0.057751	-0.731091	2.223140
47	6	0	-2.956189	-2.265698	2.544610
48	1	0	-3.791212	-3.670029	1.133834

49	1	0	-1.880726	-0.838986	3.745569
50	1	0	-3.790043	-2.343297	3.237076
51	6	0	0.440041	-2.088970	-0.142524
52	1	0	0.464869	-3.010164	-0.738683
53	6	0	0.404064	-0.823958	-0.981665
54	1	0	0.096910	-0.944831	-2.025461
55	6	0	1.743435	-0.235488	-0.897361
56	8	0	2.244282	0.661966	-1.554267
57	6	0	1.763266	-2.015172	0.610004
58	8	0	2.147965	-2.762793	1.491329
59	7	0	2.471642	-0.949679	0.094059
60	6	0	3.767584	-0.561913	0.553513
61	6	0	4.962467	-0.864358	-0.124850
62	6	0	3.772182	0.178438	1.739716
63	6	0	6.133028	-0.328940	0.442247
64	6	0	4.949429	0.661836	2.287628
65	1	0	2.819048	0.377855	2.220548
66	6	0	6.142954	0.412750	1.615995
67	1	0	7.083120	-0.496592	-0.054085
68	1	0	4.933824	1.232930	3.211831
69	1	0	7.084771	0.792535	2.003945
70	6	0	5.121429	-1.669121	-1.429193
71	6	0	3.913259	-2.528856	-1.827170
72	1	0	3.602044	-3.197748	-1.019101
73	1	0	3.060387	-1.932461	-2.154153
74	1	0	4.202549	-3.156437	-2.677349
75	6	0	5.403405	-0.676208	-2.570751
76	1	0	4.572461	0.026473	-2.682030
77	1	0	6.314738	-0.099444	-2.382324
78	1	0	5.534690	-1.216230	-3.515934
79	6	0	6.307300	-2.645011	-1.295815
80	1	0	7.267623	-2.142750	-1.158297
81	1	0	6.159849	-3.331109	-0.455361
82	1	0	6.390037	-3.242156	-2.209968

SCF Done: E(RPBE1PBE) = -6437.71440511 A.U. after 1 cycles
Convg = 0.2306D-08 -V/T = 2.0053
Zero-point correction= 0.681427 (Hartree/Particle)
Thermal correction to Energy= 0.728858
Thermal correction to Enthalpy= 0.729913
Thermal correction to Gibbs Free Energy= 0.594981
Sum of electronic and zero-point Energies= -6437.032979
Sum of electronic and thermal Energies= -6436.985547
Sum of electronic and thermal Enthalpies= -6436.984492
Sum of electronic and thermal Free Energies= -6437.119424

	1	2	3
	A	A	A
Frequencies --	10.2676	22.1782	24.6748

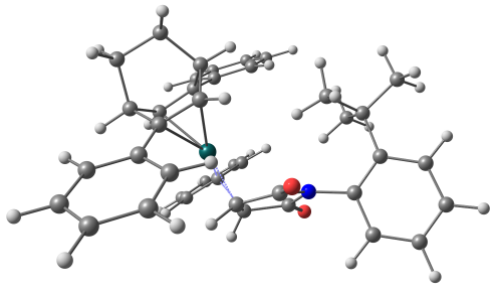
(*S*)-PhBOD-(3*R*,R_a)-Rh-oxa-π-allyl (37)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.754973	0.681279	-0.635680
2	6	0	-1.072133	2.801506	-0.018315
3	6	0	-2.993428	2.084527	-1.348599
4	6	0	-3.724043	-0.745352	-2.406775
5	6	0	0.142329	3.575062	0.315409
6	6	0	0.730045	4.444966	-0.616317
7	6	0	-1.564667	2.590623	-1.305348
8	6	0	-2.102774	2.412006	1.038953
9	6	0	1.875492	4.207202	1.904513
10	6	0	-5.059749	-2.699646	-1.925422
11	6	0	-3.926019	3.049229	-0.580182
12	6	0	-2.376889	0.958161	0.706766
13	6	0	1.869973	5.175495	-0.297957
14	6	0	-2.897069	0.763429	-0.587240
15	6	0	-4.278391	-1.284071	-0.127949
16	6	0	0.738140	3.472713	1.582285
17	6	0	-3.381827	3.259143	0.844965
18	6	0	2.449508	5.062198	0.965369
19	6	0	-3.637379	-0.434964	-1.040167
20	6	0	-4.981435	-2.403677	-0.565909
21	6	0	-4.423645	-1.864625	-2.845216
22	1	0	-3.217275	-0.117290	-3.135157
23	1	0	-5.610918	-3.572009	-2.266631
24	1	0	-4.232547	-1.067924	0.935687
25	1	0	-5.472192	-3.045472	0.161185
26	1	0	-4.470608	-2.088524	-3.907918
27	1	0	0.283842	4.563868	-1.599316
28	1	0	2.315243	4.110410	2.894081
29	1	0	2.303908	5.843051	-1.037779
30	1	0	0.318723	2.801461	2.326553
31	1	0	3.337082	5.637005	1.215588
32	1	0	-3.336930	1.942982	-2.374055
33	1	0	-1.718824	2.522290	2.053252
34	1	0	-3.980734	3.996231	-1.126495
35	1	0	-4.936592	2.628287	-0.563022
36	1	0	-4.118200	2.959110	1.597440
37	1	0	-3.144031	4.311913	1.028968
38	1	0	-2.467154	0.213806	1.492768
39	1	0	-1.081694	2.974525	-2.200163
40	6	0	-0.978517	-2.665625	1.461227
41	6	0	-1.920164	-3.695461	1.423215
42	6	0	-1.005093	-1.775458	2.539944
43	6	0	-2.876416	-3.830936	2.428987
44	1	0	-1.909843	-4.400416	0.594643

```
     45          6           0       -1.956037   -1.907383    3.548347
     46          1           0       -0.268049   -0.977622    2.599812
     47          6           0       -2.899294   -2.935214    3.495435
     48          1           0       -3.599689   -4.641020    2.380676
     49          1           0       -1.955605   -1.212416    4.384562
     50          1           0       -3.637700   -3.041342    4.285981
     51          6           0        0.029871   -2.525147    0.345758
     52          1           0        0.100973   -3.498756   -0.160758
     53          6           0       -0.202691   -1.449277   -0.700879
     54          1           0       -0.776188   -1.701776   -1.592324
     55          6           0        1.047423   -0.788219   -0.884724
     56          8           0        1.210210    0.243403   -1.592474
     57          6           0        1.449419   -2.239010    0.843528
     58          8           0        2.004406   -2.726661    1.806514
     59          7           0        2.021584   -1.298790   -0.012305
     60          6           0        3.273179   -0.649988    0.243749
     61          6           0        4.485034   -1.057214   -0.351901
     62          6           0        3.215814    0.432039    1.121058
     63          6           0        5.617344   -0.313967    0.011981
     64          6           0        4.356663    1.149865    1.452757
     65          1           0        2.251237    0.709892    1.537681
     66          6           0        5.567721    0.763479    0.892487
     67          1           0        6.582087   -0.574678   -0.406088
     68          1           0        4.295069    1.996075    2.130797
     69          1           0        6.481688    1.301276    1.131672
     70          6           0        4.618387   -2.228229   -1.341088
     71          6           0        4.285891   -3.560805   -0.649600
     72          1           0        4.933441   -3.725171    0.217320
     73          1           0        3.253609   -3.607706   -0.302310
     74          1           0        4.440406   -4.388225   -1.351604
     75          6           0        3.701577   -2.028678   -2.561105
     76          1           0        2.643341   -2.111637   -2.310282
     77          1           0        3.863393   -1.050281   -3.023904
     78          1           0        3.918190   -2.799391   -3.309321
     79          6           0        6.050536   -2.350549   -1.882101
     80          1           0        6.371402   -1.449281   -2.414992
     81          1           0        6.777839   -2.568443   -1.093384
     82          1           0        6.088957   -3.181608   -2.593394
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6437.71491255     A.U. after    1 cycles
             Convg  =    0.6209D-08             -V/T =  2.0053
Zero-point correction=                           0.681768 (Hartree/Particle)
 Thermal correction to Energy=                    0.729123
 Thermal correction to Enthalpy=                  0.730178
 Thermal correction to Gibbs Free Energy=         0.595027
 Sum of electronic and zero-point Energies=          -6437.033145
 Sum of electronic and thermal Energies=             -6436.985790
 Sum of electronic and thermal Enthalpies=           -6436.984735
 Sum of electronic and thermal Free Energies=        -6437.119885
                     1                      2                      3
                     A                      A                      A
 Frequencies --    17.2740                22.9638                25.0834
```

(*S*)-PhBOD-Rh-Ph-maleimide-(3*S*,*S*$_a$)-CR-TS-conf"pm" (22a)

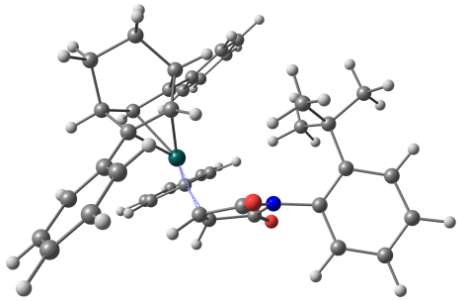


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.033590	-0.173087	0.402351
2	6	0	2.479091	-1.402678	-0.776539
3	6	0	1.723623	0.400562	-2.249484
4	6	0	0.177676	3.046127	-1.716170
5	6	0	2.690889	-2.820108	-0.400329
6	6	0	1.669622	-3.774698	-0.555077
7	6	0	1.449550	-0.942382	-1.603198
8	6	0	3.592097	-0.367122	-0.671579
9	6	0	4.143192	-4.606982	0.400848
10	6	0	0.457607	5.394536	-1.224326
11	6	0	3.057939	0.316904	-3.036680
12	6	0	2.892590	0.895560	-0.215030
13	6	0	1.880582	-5.109713	-0.234635
14	6	0	1.922281	1.361484	-1.084183
15	6	0	2.162443	3.804508	-0.590229
16	6	0	3.929391	-3.265820	0.084569
17	6	0	4.182677	-0.131352	-2.085507
18	6	0	3.120447	-5.537588	0.244879
19	6	0	1.411484	2.745125	-1.121258
20	6	0	1.690599	5.112307	-0.637496
21	6	0	-0.296307	4.353515	-1.764853
22	1	0	-0.432177	2.245857	-2.125112
23	1	0	0.089757	6.416357	-1.264484
24	1	0	3.132631	3.606230	-0.143975
25	1	0	2.291498	5.915946	-0.219885
26	1	0	-1.260398	4.560949	-2.222359
27	1	0	0.684434	-3.473877	-0.899520
28	1	0	5.116155	-4.920926	0.770118
29	1	0	1.067283	-5.820432	-0.356328
30	1	0	4.753202	-2.571338	0.212972
31	1	0	3.283668	-6.582568	0.494625
32	1	0	0.905943	0.702819	-2.904510
33	1	0	4.365679	-0.649396	0.041387
34	1	0	2.932767	-0.390433	-3.862436
35	1	0	3.274255	1.295328	-3.477525
36	1	0	4.968773	0.627264	-2.016422
37	1	0	4.653526	-1.055584	-2.435721
38	1	0	3.308763	1.501559	0.585007
39	1	0	0.696344	-1.603153	-2.024253
40	6	0	0.623243	1.189614	2.015101
41	6	0	-0.113927	2.357776	1.803309
42	6	0	1.615176	1.192051	3.011898
43	6	0	0.166414	3.515104	2.530134
44	1	0	-0.911139	2.380718	1.066621
45	6	0	1.903272	2.351533	3.726080
46	1	0	2.163414	0.277749	3.233635
47	6	0	1.177570	3.521511	3.488008

48	1	0	-0.413397	4.415137	2.341201
49	1	0	2.683765	2.336626	4.483628
50	1	0	1.388523	4.422678	4.057944
51	6	0	-0.470844	-0.537633	2.101113
52	6	0	-0.179479	-1.661490	1.258381
53	1	0	-0.230447	-0.557235	3.158295
54	1	0	0.435994	-2.502011	1.567921
55	6	0	-1.380790	-1.950236	0.451880
56	8	0	-1.588037	-2.874701	-0.313226
57	6	0	-1.909932	-0.155819	1.811002
58	8	0	-2.596191	0.645849	2.408571
59	7	0	-2.347754	-0.960803	0.757874
60	6	0	-3.732111	-1.133541	0.421560
61	6	0	-4.349495	-0.551311	-0.702955
62	6	0	-4.442501	-1.964284	1.290437
63	6	0	-5.703214	-0.869318	-0.889244
64	6	0	-5.784413	-2.250838	1.081918
65	1	0	-3.918309	-2.391063	2.141395
66	6	0	-6.414622	-1.696964	-0.025937
67	1	0	-6.233136	-0.459551	-1.740667
68	1	0	-6.321455	-2.898423	1.769097
69	1	0	-7.462626	-1.905508	-0.225290
70	6	0	-3.653291	0.422065	-1.665278
71	6	0	-3.422612	1.754793	-0.933823
72	1	0	-4.372492	2.184533	-0.599442
73	1	0	-2.789217	1.634285	-0.053104
74	1	0	-2.942002	2.475910	-1.604574
75	6	0	-2.316550	-0.137268	-2.181782
76	1	0	-1.536382	-0.133766	-1.416992
77	1	0	-2.428524	-1.162040	-2.548495
78	1	0	-1.962356	0.481082	-3.014983
79	6	0	-4.517992	0.718395	-2.899632
80	1	0	-5.454296	1.224528	-2.645237
81	1	0	-3.965853	1.388415	-3.566279
82	1	0	-4.753852	-0.189260	-3.465272

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6437.66582044     A.U. after    1 cycles
             Convg  =    0.8448D-08             -V/T =  2.0053
Zero-point correction=                           0.679977 (Hartree/Particle)
 Thermal correction to Energy=                    0.727031
 Thermal correction to Enthalpy=                  0.728086
 Thermal correction to Gibbs Free Energy=         0.595706
 Sum of electronic and zero-point Energies=          -6436.985844
 Sum of electronic and thermal Energies=             -6436.938790
 Sum of electronic and thermal Enthalpies=           -6436.937735
 Sum of electronic and thermal Free Energies=        -6437.070115
                     1                      2                      3
                     A                      A                      A
 Frequencies --  -293.1785               17.2379                25.3233
```

(*S*)-PhBOD-Rh-Ph-maleimide-(3*S*,*S*$_a$)-CR-TS-conf"mp" (22b)



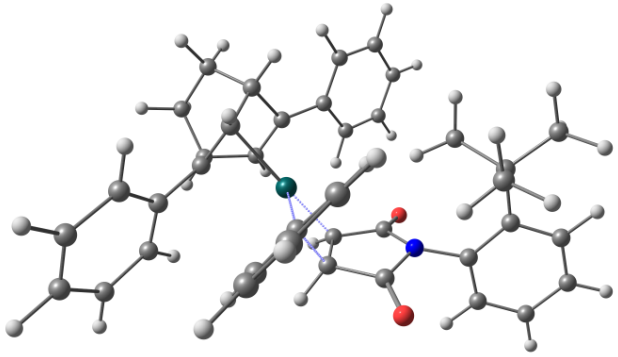
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.021979	-0.107390	0.334246
2	6	0	2.466892	-1.126501	-0.976829
3	6	0	1.446426	0.614802	-2.357331
4	6	0	0.095912	3.315328	-2.153759
5	6	0	2.835415	-2.510054	-0.604111
6	6	0	2.300263	-3.612883	-1.284941
7	6	0	1.346161	-0.757219	-1.723030
8	6	0	3.481457	0.008061	-0.924576
9	6	0	4.073352	-4.053950	0.812468
10	6	0	-0.167100	5.485338	-1.124608
11	6	0	2.723153	0.675745	-3.234061
12	6	0	2.697983	1.191703	-0.395319
13	6	0	2.641047	-4.912646	-0.921569
14	6	0	1.625374	1.574208	-1.184793
15	6	0	1.268929	3.820433	-0.119916
16	6	0	3.730499	-2.755195	0.449085
17	6	0	3.946738	0.316987	-2.371165
18	6	0	3.529963	-5.140963	0.127779
19	6	0	0.978475	2.901946	-1.143608
20	6	0	0.705015	5.089706	-0.109365
21	6	0	-0.467504	4.589483	-2.147159
22	1	0	-0.156502	2.645951	-2.969351
23	1	0	-0.605564	6.479655	-1.117019
24	1	0	1.936699	3.539566	0.687905
25	1	0	0.946534	5.774614	0.699357
26	1	0	-1.142902	4.880815	-2.947471
27	1	0	1.609480	-3.456042	-2.107757
28	1	0	4.763622	-4.218428	1.635907
29	1	0	2.210470	-5.750662	-1.463154
30	1	0	4.147308	-1.922770	1.010088
31	1	0	3.796893	-6.155915	0.409740
32	1	0	0.554249	0.823631	-2.945244
33	1	0	4.333042	-0.223729	-0.284454
34	1	0	2.609048	-0.023555	-4.068364
35	1	0	2.818818	1.678935	-3.661981
36	1	0	4.665215	1.141983	-2.339551
37	1	0	4.473434	-0.556473	-2.768770
38	1	0	3.132614	1.831740	0.366732
39	1	0	0.612137	-1.476555	-2.077336
40	6	0	0.668529	1.010885	2.148978
41	6	0	-0.175125	2.122377	2.238685
42	6	0	1.791717	0.955474	2.996703
43	6	0	0.115875	3.166705	3.118100
44	1	0	-1.071844	2.188453	1.631130
45	6	0	2.096091	2.010653	3.851057
46	1	0	2.431549	0.074393	2.990902
47	6	0	1.253193	3.123844	3.919876
48	1	0	-0.556146	4.020093	3.168384
49	1	0	2.980494	1.954452	4.481825
50	1	0	1.474068	3.937264	4.606142
51	6	0	-0.296339	-0.778217	2.100140
52	6	0	0.063011	-1.788195	1.145270
53	1	0	-0.018869	-0.874005	3.144067
54	1	0	0.770978	-2.587717	1.345965
55	6	0	-1.138157	-2.118732	0.352380
56	8	0	-1.290890	-2.996469	-0.476627
57	6	0	-1.772467	-0.507514	1.884481
58	8	0	-2.507553	0.163029	2.577442
59	7	0	-2.170313	-1.238332	0.763389
60	6	0	-3.549265	-1.441986	0.426340

61	6	0	-4.226767	-0.728208	-0.583569
62	6	0	-4.198544	-2.416334	1.186344
63	6	0	-5.577793	-1.060364	-0.762824
64	6	0	-5.537018	-2.721674	0.980530
65	1	0	-3.630680	-2.937507	1.952447
66	6	0	-6.228907	-2.030647	-0.006596
67	1	0	-6.155688	-0.545503	-1.520856
68	1	0	-6.025767	-3.482882	1.581978
69	1	0	-7.278681	-2.241330	-0.194097
70	6	0	-3.576635	0.344352	-1.471602
71	6	0	-2.961958	1.465668	-0.619372
72	1	0	-3.680248	1.853167	0.109720
73	1	0	-2.076414	1.123969	-0.082365
74	1	0	-2.644908	2.293859	-1.261883
75	6	0	-2.488905	-0.293426	-2.350064
76	1	0	-1.667799	-0.695566	-1.755130
77	1	0	-2.898039	-1.108959	-2.954898
78	1	0	-2.074952	0.461557	-3.029041
79	6	0	-4.596231	1.000102	-2.413354
80	1	0	-5.404507	1.498241	-1.867820
81	1	0	-4.085696	1.763504	-3.009179
82	1	0	-5.037291	0.285605	-3.116027

SCF Done: E(RPBE1PBE) = -6437.66528889 A.U. after 1 cycles
Convg = 0.3402D-08 -V/T = 2.0053
Zero-point correction= 0.679892 (Hartree/Particle)
Thermal correction to Energy= 0.727018
Thermal correction to Enthalpy= 0.728073
Thermal correction to Gibbs Free Energy= 0.595545
Sum of electronic and zero-point Energies= -6436.985396
Sum of electronic and thermal Energies= -6436.938271
Sum of electronic and thermal Enthalpies= -6436.937216
Sum of electronic and thermal Free Energies= -6437.069744

	1	2	3
	A	A	A
Frequencies --	-301.8955	21.2576	26.1200

(*S*)-PhBOD-Rh-Ph-maleimide-(3*R*,*S*$_a$)-CR-TS-conf"pm" (26a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.068934	0.258452	-0.363825
2	6	0	-1.231298	2.481695	-0.004633
3	6	0	-3.331370	1.745750	-1.010262
4	6	0	-4.416781	-1.116545	-1.545246
5	6	0	0.012383	3.278076	0.074840
6	6	0	0.890882	3.362273	-1.017000
7	6	0	-1.878908	2.132585	-1.189483

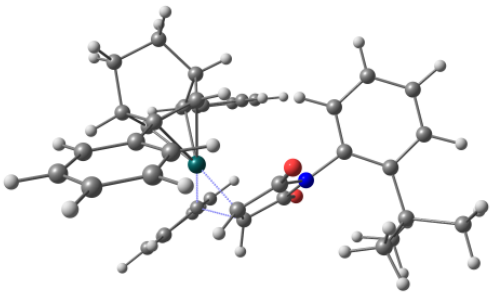
8	6	0	-2.154295	2.307818	1.196639
9	6	0	1.474239	4.806434	1.283250
10	6	0	-5.923944	-2.779749	-0.652693
11	6	0	-4.084100	2.904012	-0.306163
12	6	0	-2.609413	0.865225	1.109026
13	6	0	2.036789	4.144510	-0.959433
14	6	0	-3.289036	0.554154	-0.062243
15	6	0	-4.858296	-1.187721	0.819995
16	6	0	0.329058	4.014435	1.226990
17	6	0	-3.379234	3.239991	1.021031
18	6	0	2.335545	4.875193	0.191315
19	6	0	-4.189523	-0.598195	-0.260973
20	6	0	-5.714834	-2.268429	0.627036
21	6	0	-5.270423	-2.197569	-1.739778
22	1	0	-3.897229	-0.686868	-2.398385
23	1	0	-6.593228	-3.622477	-0.803764
24	1	0	-4.712297	-0.791958	1.821112
25	1	0	-6.224541	-2.709750	1.479528
26	1	0	-5.424038	-2.590246	-2.741642
27	1	0	0.701579	2.782605	-1.913928
28	1	0	1.691351	5.370655	2.186671
29	1	0	2.708722	4.167210	-1.812669
30	1	0	-0.326398	3.992084	2.091906
31	1	0	3.234244	5.484551	0.237624
32	1	0	-3.803063	1.498512	-1.962123
33	1	0	-1.644658	2.486589	2.143026
34	1	0	-4.099109	3.769096	-0.976589
35	1	0	-5.124295	2.605040	-0.141336
36	1	0	-4.052425	3.099702	1.872774
37	1	0	-3.045736	4.282814	1.039500
38	1	0	-2.626879	0.229321	1.990089
39	1	0	-1.508619	2.429791	-2.167090
40	6	0	-0.924260	-1.695833	0.470019
41	6	0	-1.808656	-2.766544	0.304403
42	6	0	-0.221156	-1.586075	1.680524
43	6	0	-2.022312	-3.676594	1.337665
44	1	0	-2.346880	-2.894371	-0.632102
45	6	0	-0.450535	-2.485775	2.719411
46	1	0	0.498460	-0.783785	1.826530
47	6	0	-1.350608	-3.538323	2.551686
48	1	0	-2.718174	-4.498741	1.189096
49	1	0	0.091844	-2.372871	3.655469
50	1	0	-1.513751	-4.253472	3.353709
51	6	0	0.098560	-1.450038	-1.305118
52	1	0	-0.539796	-2.143345	-1.843606
53	6	0	0.422084	-0.158198	-1.838793
54	1	0	-0.003461	0.223994	-2.763666
55	6	0	1.866116	0.058049	-1.647947
56	8	0	2.566776	0.950199	-2.085644
57	6	0	1.410478	-2.052152	-0.828872
58	8	0	1.621949	-3.204035	-0.516526
59	7	0	2.372992	-1.045810	-0.913783
60	6	0	3.784938	-1.298848	-0.851445
61	6	0	4.602504	-0.922490	0.232804
62	6	0	4.318956	-1.919118	-1.982536
63	6	0	5.971178	-1.195907	0.087512
64	6	0	5.676533	-2.188001	-2.087221
65	1	0	3.645182	-2.186627	-2.792127
66	6	0	6.507828	-1.812285	-1.038726
67	1	0	6.654772	-0.920752	0.881723
68	1	0	6.074184	-2.673070	-2.974182
69	1	0	7.577775	-1.997261	-1.090203
70	6	0	4.079466	-0.323732	1.547120
71	6	0	3.130357	0.865214	1.319428

72	1	0	3.577904	1.616438	0.662237
73	1	0	2.174885	0.572200	0.883130
74	1	0	2.913012	1.345117	2.280099
75	6	0	3.365599	-1.441086	2.327597
76	1	0	2.565819	-1.906316	1.748349
77	1	0	4.072817	-2.231308	2.600935
78	1	0	2.932110	-1.039002	3.251495
79	6	0	5.222843	0.198244	2.430942
80	1	0	5.900512	-0.595993	2.758613
81	1	0	5.810363	0.972886	1.926488
82	1	0	4.796200	0.643912	3.335249

SCF Done: E(RPBE1PBE) = -6437.66025751 A.U. after 1 cycles
Convg = 0.5248D-08 -V/T = 2.0053
Zero-point correction= 0.679618 (Hartree/Particle)
Thermal correction to Energy= 0.726683
Thermal correction to Enthalpy= 0.727738
Thermal correction to Gibbs Free Energy= 0.595520
Sum of electronic and zero-point Energies= -6436.980639
Sum of electronic and thermal Energies= -6436.933574
Sum of electronic and thermal Enthalpies= -6436.932519
Sum of electronic and thermal Free Energies= -6437.064738

	1	2	3
	A	A	A
Frequencies --	-271.3087	15.7694	27.8783

(*S*)-PhBOD-Rh-Ph-maleimide-(3*S*,*R*$_a$)-CR-TS-conf"pm" (32a)



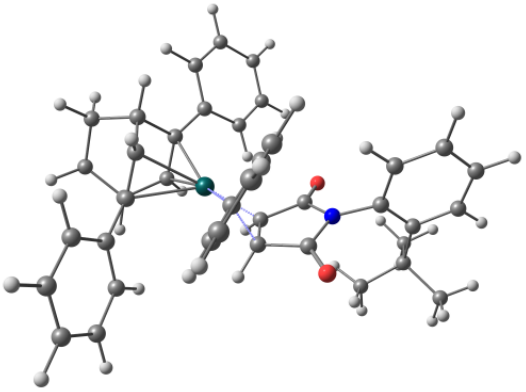
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.109379	0.169333	0.386011
2	6	0	-2.353397	1.539083	-0.858133
3	6	0	-1.583004	-0.246160	-2.342864
4	6	0	-0.163688	-2.966679	-1.629295
5	6	0	-2.504027	2.941389	-0.404293
6	6	0	-1.410294	3.825303	-0.400204
7	6	0	-1.287902	1.052056	-1.619880
8	6	0	-3.533818	0.572154	-0.895377
9	6	0	-3.901806	4.773130	0.391318
10	6	0	-0.631302	-5.320474	-1.360677
11	6	0	-2.837994	-0.052382	-3.234693
12	6	0	-2.956187	-0.752275	-0.438952
13	6	0	-1.561130	5.148537	-0.005750
14	6	0	-1.933852	-1.234514	-1.238128
15	6	0	-2.367726	-3.683781	-0.981882
16	6	0	-3.750030	3.443541	-0.000191
17	6	0	-4.011546	0.432064	-2.363153
18	6	0	-2.808517	5.634071	0.392548
19	6	0	-1.481423	-2.638753	-1.279411
20	6	0	-1.947497	-5.010450	-1.021209

21	6	0	0.260136	-4.291114	-1.664035
22	1	0	0.552219	-2.177072	-1.838253
23	1	0	-0.301830	-6.355704	-1.388560
24	1	0	-3.398837	-3.456229	-0.726132
25	1	0	-2.652021	-5.805096	-0.789589
26	1	0	1.292328	-4.517950	-1.916678
27	1	0	-0.421119	3.476763	-0.682414
28	1	0	-4.881621	5.133260	0.694327
29	1	0	-0.695123	5.805497	-0.007221
30	1	0	-4.626991	2.804390	0.004294
31	1	0	-2.923738	6.670165	0.699643
32	1	0	-0.732705	-0.580914	-2.939666
33	1	0	-4.346912	0.875847	-0.237532
34	1	0	-2.600320	0.673901	-4.018131
35	1	0	-3.072816	-0.999645	-3.730750
36	1	0	-4.846362	-0.275224	-2.395262
37	1	0	-4.391357	1.398127	-2.711296
38	1	0	-3.474038	-1.367725	0.292044
39	1	0	-0.459182	1.679820	-1.937261
40	6	0	-1.040643	-1.177999	2.031095
41	6	0	-0.750154	-2.542952	1.956791
42	6	0	-1.941337	-0.720366	3.008308
43	6	0	-1.400491	-3.440699	2.803718
44	1	0	-0.015240	-2.908707	1.246996
45	6	0	-2.605098	-1.625569	3.834509
46	1	0	-2.127621	0.346043	3.125456
47	6	0	-2.336374	-2.991848	3.735492
48	1	0	-1.171017	-4.501050	2.729328
49	1	0	-3.318044	-1.259510	4.569886
50	1	0	-2.837443	-3.697235	4.393372
51	6	0	0.581630	0.063920	1.889745
52	6	0	0.377361	1.368899	1.323615
53	1	0	0.623628	-0.091586	2.962150
54	1	0	-0.012499	2.217356	1.879101
55	6	0	1.451519	1.606528	0.344128
56	8	0	1.691880	2.602362	-0.317380
57	6	0	1.731074	-0.556781	1.125710
58	8	0	2.167780	-1.687055	1.220744
59	7	0	2.250771	0.439209	0.301237
60	6	0	3.254820	0.229433	-0.696050
61	6	0	4.635151	0.399289	-0.458380
62	6	0	2.772750	-0.125573	-1.956865
63	6	0	5.471933	0.153127	-1.558477
64	6	0	3.629270	-0.356262	-3.023902
65	1	0	1.697007	-0.204464	-2.087776
66	6	0	4.996044	-0.220040	-2.811803
67	1	0	6.543601	0.262570	-1.444782
68	1	0	3.235827	-0.631444	-3.998505
69	1	0	5.699592	-0.392844	-3.622147
70	6	0	5.257123	0.800991	0.892122
71	6	0	4.524645	1.988017	1.542964
72	1	0	4.385452	2.812244	0.837319
73	1	0	3.546803	1.712041	1.938899
74	1	0	5.118146	2.357946	2.385834
75	6	0	5.241103	-0.404684	1.847596
76	1	0	4.231193	-0.768930	2.041293
77	1	0	5.817002	-1.238148	1.431757
78	1	0	5.694740	-0.123483	2.805130
79	6	0	6.723411	1.232224	0.725986
80	1	0	6.831171	2.062448	0.019811
81	1	0	7.104416	1.569577	1.694856
82	1	0	7.370704	0.411650	0.402173

SCF Done: E(RPBE1PBE) = -6437.66804187 A.U. after 1 cycles

```
            Convg  =    0.5160D-08             -V/T =  2.0053
Zero-point correction=                          0.679712 (Hartree/Particle)
 Thermal correction to Energy=                  0.726879
 Thermal correction to Enthalpy=                0.727934
 Thermal correction to Gibbs Free Energy=       0.594069
 Sum of electronic and zero-point Energies=         -6436.988330
 Sum of electronic and thermal Energies=            -6436.941163
 Sum of electronic and thermal Enthalpies=          -6436.940108
 Sum of electronic and thermal Free Energies=       -6437.073972
                     1                      2                      3
                     A                      A                      A
 Frequencies --  -293.0236               19.3270                21.3928
```

(*S*)-PhBOD-Rh-Ph-maleimide-(3*R*,R_a)-CR-TS-conf"pm" (36a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.204593	0.225468	-0.118511
2	6	0	-2.188796	2.265114	-0.160598
3	6	0	-3.541373	0.756452	-1.517747
4	6	0	-3.375314	-2.343681	-1.817852
5	6	0	-1.347068	3.451223	0.106502
6	6	0	-0.132612	3.658584	-0.565170
7	6	0	-2.319688	1.643265	-1.399506
8	6	0	-3.304109	1.847811	0.792321
9	6	0	-1.017530	5.579623	1.240403
10	6	0	-4.414151	-4.385763	-1.052144
11	6	0	-4.810271	1.592213	-1.210099
12	6	0	-3.192688	0.336701	0.832423
13	6	0	0.625257	4.800843	-0.336180
14	6	0	-3.363066	-0.274669	-0.408327
15	6	0	-4.441374	-2.409666	0.339198
16	6	0	-1.772262	4.430004	1.017823
17	6	0	-4.669077	2.244688	0.178413
18	6	0	0.186224	5.770815	0.565864
19	6	0	-3.726599	-1.688920	-0.627094
20	6	0	-4.779819	-3.744488	0.130185
21	6	0	-3.710317	-3.677541	-2.027410
22	1	0	-2.809044	-1.809810	-2.577344
23	1	0	-4.677056	-5.427464	-1.215036
24	1	0	-4.741098	-1.918584	1.260660
25	1	0	-5.335135	-4.284254	0.892852
26	1	0	-3.417153	-4.168419	-2.951795
27	1	0	0.249865	2.901593	-1.241653
28	1	0	-1.372652	6.326357	1.946033
29	1	0	1.573385	4.921658	-0.852859
30	1	0	-2.711282	4.311710	1.550475

31	1	0	0.782099	6.661253	0.747855
32	1	0	-3.609532	0.292478	-2.502678
33	1	0	-3.168684	2.268371	1.789296
34	1	0	-4.929621	2.348790	-1.992019
35	1	0	-5.687145	0.938347	-1.256206
36	1	0	-5.466697	1.916206	0.852593
37	1	0	-4.733735	3.335589	0.108412
38	1	0	-3.255182	-0.204824	1.772608
39	1	0	-1.798856	1.998046	-2.285694
40	6	0	-0.568903	-1.428428	1.000466
41	6	0	-1.070844	-2.731209	1.075150
42	6	0	0.029729	-0.856651	2.134798
43	6	0	-1.018011	-3.430069	2.278191
44	1	0	-1.503569	-3.204227	0.197366
45	6	0	0.046141	-1.546859	3.346506
46	1	0	0.466845	0.140761	2.080440
47	6	0	-0.469740	-2.840387	3.418799
48	1	0	-1.408351	-4.443914	2.325011
49	1	0	0.483535	-1.081855	4.227134
50	1	0	-0.428974	-3.393120	4.353642
51	6	0	0.441391	-1.180416	-0.813194
52	1	0	-0.045012	-1.947625	-1.409062
53	6	0	0.625783	0.167592	-1.260498
54	1	0	0.318432	0.522727	-2.240343
55	6	0	1.941184	0.624113	-0.769412
56	8	0	2.492459	1.696549	-0.945874
57	6	0	1.745107	-1.603162	-0.168401
58	8	0	2.094290	-2.723116	0.139265
59	7	0	2.536991	-0.461229	-0.098291
60	6	0	3.819814	-0.403843	0.531119
61	6	0	5.040147	-0.485669	-0.165800
62	6	0	3.786679	-0.228312	1.918627
63	6	0	6.196419	-0.319203	0.618343
64	6	0	4.948614	-0.099074	2.662306
65	1	0	2.817063	-0.193914	2.405475
66	6	0	6.168843	-0.130798	1.993246
67	1	0	7.166403	-0.336305	0.132398
68	1	0	4.901126	0.034979	3.739280
69	1	0	7.101603	-0.012995	2.538731
70	6	0	5.257979	-0.700380	-1.676218
71	6	0	4.028693	-1.162135	-2.470186
72	1	0	3.580535	-2.065649	-2.047526
73	1	0	3.267870	-0.385338	-2.560047
74	1	0	4.349321	-1.403466	-3.489636
75	6	0	5.748518	0.625394	-2.284586
76	1	0	5.002362	1.413264	-2.144440
77	1	0	6.684465	0.958954	-1.825256
78	1	0	5.925943	0.502217	-3.359303
79	6	0	6.328692	-1.789757	-1.887687
80	1	0	7.304352	-1.522378	-1.475326
81	1	0	6.017721	-2.736868	-1.434950
82	1	0	6.469990	-1.957367	-2.960627

SCF Done: E(RPBE1PBE) = -6437.66057671 A.U. after 1 cycles
Convg = 0.4343D-08 -V/T = 2.0053
Zero-point correction= 0.679152 (Hartree/Particle)
Thermal correction to Energy= 0.726302
Thermal correction to Enthalpy= 0.727357
Thermal correction to Gibbs Free Energy= 0.594146
Sum of electronic and zero-point Energies= -6436.981425
Sum of electronic and thermal Energies= -6436.934274
Sum of electronic and thermal Enthalpies= -6436.933219
Sum of electronic and thermal Free Energies= -6437.066430

1 2 3

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                      A                   A                   A
Frequencies --    -270.3280           17.7424             20.9578
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