Electronic Supplementary Material (ESI) for Green Chemistry.

Computational and experimental comparison of diphosphane and diene ligands in the Rh-catalysed carboxylation of organoboron compounds with CO_2

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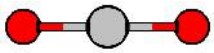
Computational results

CO_2



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 Number     Number       Type              X           Y           Z
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      2          6           0        0.000000    0.000000    0.000000
      3          8           0        0.000000    0.000000   -1.167248
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SCF Done:  E(RPBE1PBE) =  -188.412243201     A.U. after    1 cycles
             Convg  =    0.4939D-09             -V/T =  2.0120
Zero-point correction=                           0.011837 (Hartree/Particle)
 Thermal correction to Energy=                    0.014844
 Thermal correction to Enthalpy=                  0.015899
 Thermal correction to Gibbs Free Energy=        -0.011742
 Sum of electronic and zero-point Energies=           -188.400407
 Sum of electronic and thermal Energies=              -188.397400
 Sum of electronic and thermal Enthalpies=            -188.396344
 Sum of electronic and thermal Free Energies=         -188.423985
                    1                    2                    3
                  PIU                  PIU                  SGG
 Frequencies --   673.7536             673.7536            1393.8676
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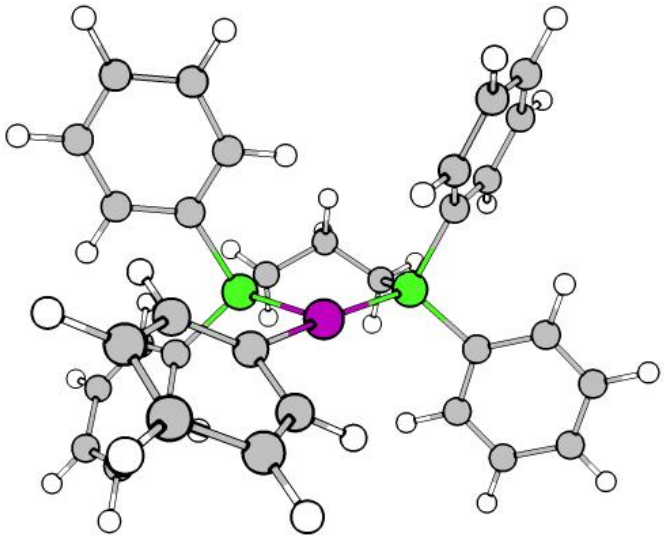
DPPP-Rh catalyst

syn-pathway

DPPP-Rh-Ph (3)



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 Number     Number       Type              X           Y           Z
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      2         15           0       -1.347048    0.155730   -0.929109
      3         15           0        2.037434   -0.088980   -0.557995
      4          6           0        1.862271    0.150579   -2.378284
      5          6           0       -0.667347    0.487018   -2.634107
      6          1           0        1.666351   -0.837719   -2.809514
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9	6	0	2.903545	-2.707208	-0.859775
10	6	0	4.612191	-1.232815	-0.011411
11	6	0	3.795072	-3.774883	-0.811061
12	1	0	1.878310	-2.877678	-1.184369
13	6	0	5.501278	-2.306643	0.049855
14	1	0	4.941274	-0.249222	0.312373
15	6	0	5.099378	-3.577166	-0.355654
16	1	0	3.467520	-4.765347	-1.116507
17	1	0	6.511798	-2.146166	0.417171
18	1	0	5.794105	-4.411634	-0.308653
19	6	0	2.940170	1.424417	-0.028792
20	6	0	3.951580	2.036242	-0.781838
21	6	0	2.585194	1.992354	1.201171
22	6	0	4.588431	3.184802	-0.316549
23	1	0	4.258913	1.616914	-1.736478
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25	1	0	1.788955	1.537122	1.788086
26	6	0	4.228078	3.737407	0.912717
27	1	0	5.369627	3.647486	-0.914281
28	1	0	2.936460	3.562183	2.630130
29	1	0	4.726122	4.633244	1.274284
30	6	0	-2.725632	-0.980637	-1.386684
31	6	0	-2.971312	-2.116210	-0.608810
32	6	0	-3.509865	-0.770100	-2.532209
33	6	0	-3.981522	-3.013185	-0.956222
34	1	0	-2.360956	-2.290562	0.273264
35	6	0	-4.516080	-1.667134	-2.881692
36	1	0	-3.346240	0.099204	-3.163626
37	6	0	-4.756098	-2.792043	-2.092423
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39	1	0	-5.113371	-1.486144	-3.771850
40	1	0	-5.541245	-3.492589	-2.365176
41	6	0	-2.179529	1.763258	-0.565486
42	6	0	-3.555808	1.983665	-0.688325
43	6	0	-1.367700	2.816698	-0.120639
44	6	0	-4.103534	3.232633	-0.391633
45	1	0	-4.214125	1.176787	-0.997035
46	6	0	-1.911423	4.067924	0.155485
47	1	0	-0.305205	2.642333	0.038120
48	6	0	-3.283928	4.280358	0.020913
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51	1	0	-3.712557	5.252299	0.251198
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53	6	0	-0.829625	-1.735928	2.916512
54	6	0	-2.552583	-0.134704	2.441723
55	6	0	-1.417079	-2.026213	4.150587
56	1	0	0.079457	-2.282055	2.639208
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59	6	0	-2.586255	-1.366638	4.531427
60	1	0	-0.970415	-2.770578	4.807226
61	1	0	-4.056880	0.102361	3.965702
62	1	0	-3.055600	-1.589383	5.486704
63	6	0	0.724432	1.111181	-2.729959
64	1	0	0.864158	1.436254	-3.767946
65	1	0	0.787420	2.024137	-2.125384
66	1	0	-1.383797	1.134451	-3.150726
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SCF Done: E(RPBE1PBE) = -6644.38270067   A.U. after   1 cycles

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            Convg  =    0.2048D-08             -V/T =  2.0048
Zero-point correction=                           0.546383 (Hartree/Particle)
 Thermal correction to Energy=                    0.587556
 Thermal correction to Enthalpy=                  0.588611
 Thermal correction to Gibbs Free Energy=         0.463153
 Sum of electronic and zero-point Energies=          -6643.836317
 Sum of electronic and thermal Energies=             -6643.795145
 Sum of electronic and thermal Enthalpies=           -6643.794090
 Sum of electronic and thermal Free Energies=        -6643.919548
                    1                      2                      3
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 Frequencies --     7.9298                14.2718                22.6496
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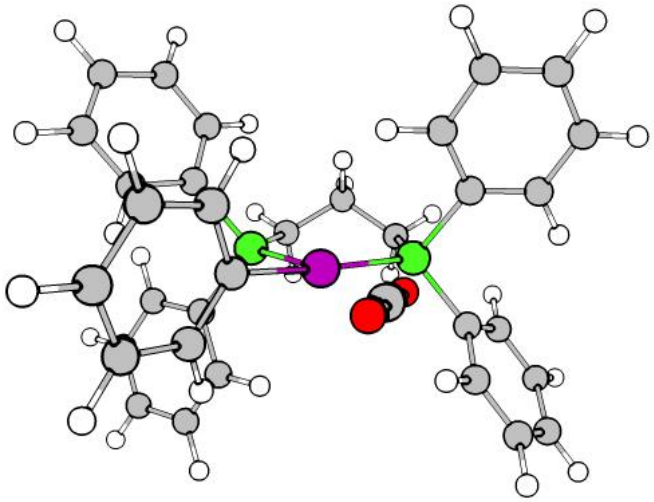
DPPP-Rh-Ph-O=C=O-conf1 (4)



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3	15	0	-2.052015	0.343282	-0.658549
4	6	0	-1.898345	1.087374	-2.350180
5	6	0	0.638745	1.341002	-2.527023
6	1	0	-1.904128	2.177688	-2.235048
7	1	0	-2.775904	0.812463	-2.945155
8	6	0	-3.300704	1.437626	0.130304
9	6	0	-4.252743	2.172361	-0.589398
10	6	0	-3.284571	1.548063	1.526161
11	6	0	-5.167913	2.990474	0.071008
12	1	0	-4.289362	2.112136	-1.674014
13	6	0	-4.203641	2.359526	2.188580
14	1	0	-2.538414	0.999595	2.095671
15	6	0	-5.147530	3.083837	1.462013
16	1	0	-5.898425	3.554958	-0.502970
17	1	0	-4.176558	2.432892	3.272721
18	1	0	-5.860920	3.722380	1.976364
19	6	0	-3.000037	-1.196484	-1.026557
20	6	0	-4.397599	-1.269765	-1.055485
21	6	0	-2.258441	-2.354246	-1.301485
22	6	0	-5.037591	-2.468574	-1.366981
23	1	0	-4.995591	-0.392541	-0.822475
24	6	0	-2.898516	-3.549423	-1.624508
25	1	0	-1.171349	-2.314368	-1.247189

26	6	0	-4.290869	-3.609760	-1.657923
27	1	0	-6.123887	-2.511135	-1.378628
28	1	0	-2.307867	-4.436953	-1.837338
29	1	0	-4.792217	-4.543358	-1.899798
30	6	0	2.323051	2.115049	-0.421067
31	6	0	1.827060	2.901890	0.623526
32	6	0	3.481577	2.528783	-1.090351
33	6	0	2.474552	4.079867	0.993795
34	1	0	0.925956	2.578675	1.142088
35	6	0	4.132701	3.702294	-0.716681
36	1	0	3.885219	1.929501	-1.903001
37	6	0	3.630312	4.481149	0.325994
38	1	0	2.078477	4.680919	1.808512
39	1	0	5.034475	4.009026	-1.240730
40	1	0	4.140272	5.395595	0.618134
41	6	0	2.659087	-0.485639	-1.586605
42	6	0	3.790940	-0.752985	-0.803626
43	6	0	2.525837	-1.144958	-2.814596
44	6	0	4.769344	-1.637321	-1.248929
45	1	0	3.909926	-0.267039	0.160787
46	6	0	3.500976	-2.039038	-3.256080
47	1	0	1.658309	-0.970589	-3.444987
48	6	0	4.628738	-2.285469	-2.476172
49	1	0	5.641606	-1.825232	-0.628161
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51	1	0	5.391811	-2.978834	-2.820380
52	6	0	1.521213	-0.864570	1.591510
53	6	0	2.081003	-0.141642	2.661660
54	6	0	1.925272	-2.208387	1.460667
55	6	0	2.976267	-0.728051	3.561835
56	1	0	1.823297	0.907756	2.797638
57	6	0	2.813791	-2.804610	2.358487
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63	6	0	-0.620005	0.660666	-3.072535
64	1	0	-0.722724	0.933418	-4.129791
65	1	0	-0.524066	-0.431515	-3.048317
66	1	0	1.433973	1.346558	-3.280915
67	1	0	0.415928	2.392580	-2.312925
68	6	0	-0.950913	-1.962910	3.156941
69	8	0	-0.573222	-2.628236	4.031740
70	8	0	-1.378911	-1.298242	2.290402

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SCF Done:  E(RPBE1PBE) =  -6832.80184169     A.U. after    1 cycles
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Zero-point correction=                           0.559483 (Hartree/Particle)
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 Thermal correction to Enthalpy=                  0.606381
 Thermal correction to Gibbs Free Energy=         0.469443
 Sum of electronic and zero-point Energies=          -6832.242359
 Sum of electronic and thermal Energies=             -6832.196515
 Sum of electronic and thermal Enthalpies=           -6832.195460
 Sum of electronic and thermal Free Energies=        -6832.332399
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 Frequencies --    12.2907              18.0576              19.1910
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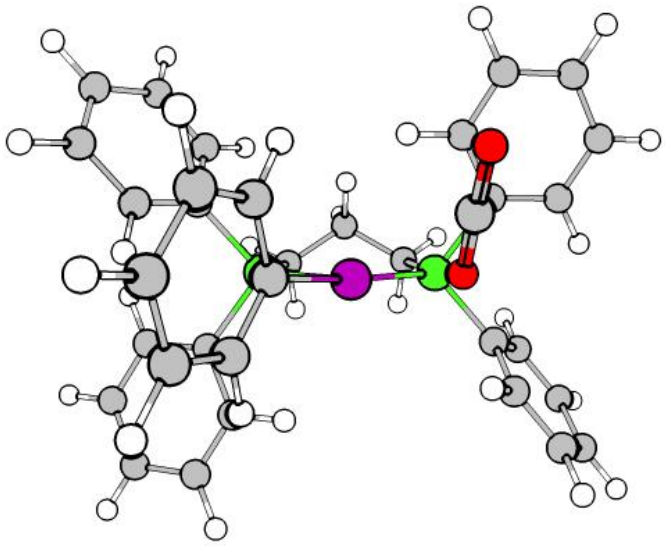
DPPP-Rh-Ph-O=C=O-conf2 (5)



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7	1	0	-2.689163	0.859435	-2.954740
8	6	0	-3.222158	1.586868	0.111288
9	6	0	-4.150429	2.331654	-0.628766
10	6	0	-3.208799	1.725418	1.504784
11	6	0	-5.045290	3.188483	0.009935
12	1	0	-4.184614	2.247694	-1.711940
13	6	0	-4.108093	2.575695	2.145355
14	1	0	-2.481937	1.168096	2.090631
15	6	0	-5.028095	3.310422	1.398879
16	1	0	-5.757724	3.760518	-0.579068
17	1	0	-4.083733	2.670628	3.227836
18	1	0	-5.725723	3.979181	1.896169
19	6	0	-2.996853	-1.081579	-0.972622
20	6	0	-4.395941	-1.123368	-0.959536
21	6	0	-2.290042	-2.262066	-1.245866
22	6	0	-5.071466	-2.313373	-1.227722
23	1	0	-4.966698	-0.228004	-0.727343
24	6	0	-2.966048	-3.448710	-1.524443
25	1	0	-1.201194	-2.246721	-1.224857
26	6	0	-4.359921	-3.477371	-1.515760
27	1	0	-6.158302	-2.330923	-1.207056
28	1	0	-2.401933	-4.353707	-1.735370
29	1	0	-4.889140	-4.403959	-1.722390
30	6	0	2.443736	2.053915	-0.394806
31	6	0	1.951696	2.898999	0.605445
32	6	0	3.642795	2.387443	-1.035881
33	6	0	2.643358	4.056297	0.959756
34	1	0	1.019195	2.636448	1.102715
35	6	0	4.338024	3.540548	-0.677574
36	1	0	4.042622	1.741793	-1.814124
37	6	0	3.839654	4.378019	0.320450

38	1	0	2.250362	4.703100	1.740197
39	1	0	5.271094	3.785378	-1.178923
40	1	0	4.384089	5.276198	0.600589
41	6	0	2.672940	-0.579209	-1.522613
42	6	0	3.760307	-0.924733	-0.707169
43	6	0	2.547008	-1.206588	-2.768018
44	6	0	4.701859	-1.855595	-1.136588
45	1	0	3.873433	-0.464225	0.270296
46	6	0	3.484758	-2.147374	-3.193560
47	1	0	1.715080	-0.970697	-3.425454
48	6	0	4.567944	-2.472903	-2.380502
49	1	0	5.540041	-2.103634	-0.490504
50	1	0	3.367628	-2.621727	-4.164746
51	1	0	5.301922	-3.202850	-2.712072
52	6	0	1.492195	-0.819327	1.690732
53	6	0	2.103075	-0.059416	2.704808
54	6	0	1.798964	-2.193987	1.663183
55	6	0	2.952253	-0.639029	3.652031
56	1	0	1.921255	1.012607	2.761373
57	6	0	2.639314	-2.784464	2.610690
58	1	0	1.384242	-2.823941	0.875887
59	6	0	3.223007	-2.007355	3.611919
60	1	0	3.407128	-0.018316	4.422284
61	1	0	2.846817	-3.851987	2.559866
62	1	0	3.884997	-2.460184	4.346521
63	6	0	-0.533969	0.665006	-3.047200
64	1	0	-0.611885	0.923032	-4.110232
65	1	0	-0.464675	-0.428493	-3.004391
66	1	0	1.534389	1.318302	-3.234863
67	1	0	0.524880	2.378231	-2.274098
68	6	0	-1.409743	-2.413241	2.441708
69	8	0	-1.371528	-3.557682	2.645586
70	8	0	-1.478824	-1.259692	2.246583

SCF Done: E(RPBE1PBE) = -6832.80192876   A.U. after   1 cycles
             Convg =   0.1810D-08   -V/T = 2.0050
Zero-point correction=   0.559559 (Hartree/Particle)
 Thermal correction to Energy=   0.605390
 Thermal correction to Enthalpy=   0.606445
 Thermal correction to Gibbs Free Energy=   0.469258
 Sum of electronic and zero-point Energies=   -6832.242370
 Sum of electronic and thermal Energies=   -6832.196539
 Sum of electronic and thermal Enthalpies=   -6832.195484
 Sum of electronic and thermal Free Energies=   -6832.332671

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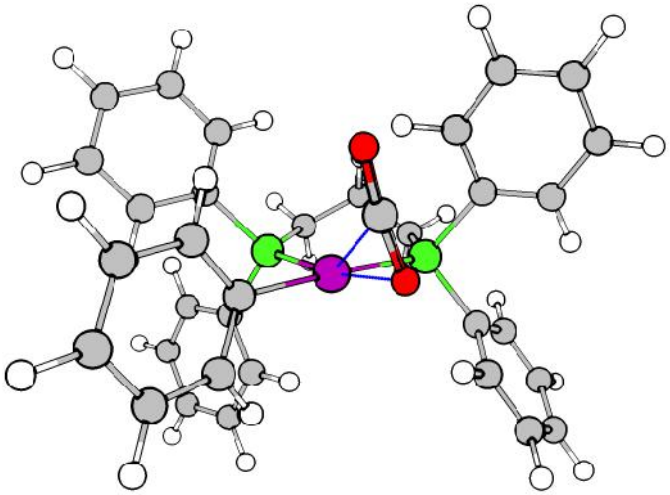
	A	A	A
Frequencies --	12.5166	14.6910	16.9084

DPPP-Rh-Ph-O=C=O-TS1 (6)



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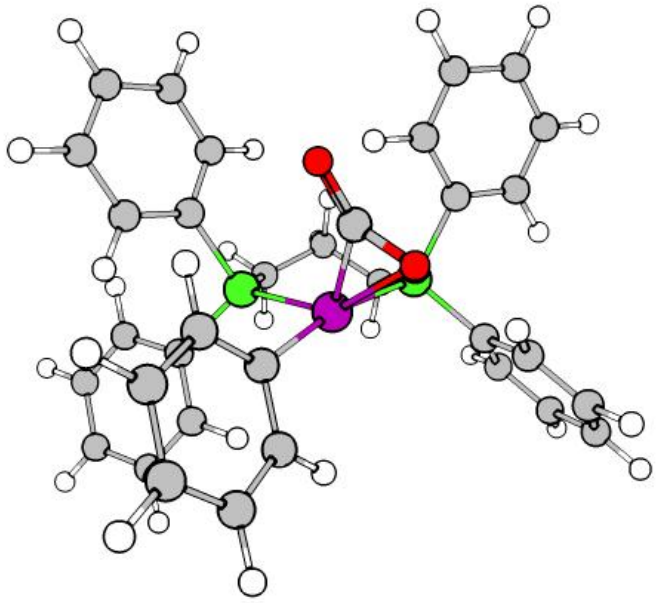
3	15	0	-2.047962	0.193974	-0.594682
4	6	0	-1.899857	0.530227	-2.408963
5	6	0	0.630926	0.488932	-2.759882
6	1	0	-1.783301	1.612351	-2.541142
7	1	0	-2.831119	0.234404	-2.903439
8	6	0	-3.165048	1.529886	-0.014238
9	6	0	-4.001301	2.266988	-0.862313
10	6	0	-3.169626	1.822503	1.356091
11	6	0	-4.821866	3.272264	-0.352242
12	1	0	-4.024459	2.060834	-1.928904
13	6	0	-3.996680	2.820048	1.867591
14	1	0	-2.520765	1.264429	2.026437
15	6	0	-4.823173	3.549641	1.013855
16	1	0	-5.463037	3.837031	-1.024215
17	1	0	-3.989507	3.031999	2.933564
18	1	0	-5.463634	4.332736	1.410988
19	6	0	-3.139603	-1.291721	-0.603035
20	6	0	-4.533820	-1.224719	-0.495444
21	6	0	-2.532952	-2.547806	-0.742285
22	6	0	-5.303335	-2.385979	-0.540931
23	1	0	-5.025133	-0.263980	-0.365585
24	6	0	-3.304119	-3.707511	-0.798217
25	1	0	-1.448098	-2.618703	-0.789859
26	6	0	-4.692133	-3.629386	-0.698027
27	1	0	-6.384499	-2.318159	-0.449595
28	1	0	-2.816555	-4.673077	-0.904679
29	1	0	-5.294228	-4.533635	-0.730888
30	6	0	2.272131	1.877224	-0.955374
31	6	0	1.745239	2.899627	-0.159894
32	6	0	3.405552	2.139749	-1.735149
33	6	0	2.340831	4.159673	-0.136859
34	1	0	0.859744	2.698716	0.440118
35	6	0	4.005373	3.396749	-1.706908
36	1	0	3.829504	1.359642	-2.362887
37	6	0	3.474755	4.409486	-0.907477
38	1	0	1.921602	4.943802	0.488425
39	1	0	4.889259	3.585486	-2.310950

```
     40          1           0        3.945580    5.388908   -0.884922
     41          6           0        2.668289   -0.961196   -1.335057
     42          6           0        3.881520   -0.899185   -0.638369
     43          6           0        2.443034   -2.040018   -2.198672
     44          6           0        4.854665   -1.878336   -0.824563
     45          1           0        4.068619   -0.085027    0.055975
     46          6           0        3.412916   -3.024570   -2.377562
     47          1           0        1.503631   -2.125560   -2.739006
     48          6           0        4.625311   -2.943489   -1.694265
     49          1           0        5.792263   -1.810266   -0.279002
     50          1           0        3.220021   -3.854208   -3.052939
     51          1           0        5.384516   -3.708355   -1.835544
     52          6           0        1.586987   -0.295555    1.864161
     53          6           0        1.895620    0.753694    2.750824
     54          6           0        2.288155   -1.500242    2.048206
     55          6           0        2.839810    0.607851    3.769633
     56          1           0        1.390404    1.714080    2.652317
     57          6           0        3.227070   -1.660253    3.071193
     58          1           0        2.103425   -2.339406    1.379543
     59          6           0        3.510503   -0.604698    3.936807
     60          1           0        3.053070    1.443284    4.434277
     61          1           0        3.742734   -2.612160    3.185972
     62          1           0        4.245272   -0.723040    4.730003
     63          6           0       -0.709475   -0.187809   -3.049034
     64          1           0       -0.856985   -0.183188   -4.135627
     65          1           0       -0.695508   -1.243005   -2.751774
     66          1           0        1.390227    0.155829   -3.475813
     67          1           0        0.521922    1.568723   -2.911540
     68          6           0       -0.877102   -1.994613    2.136457
     69          8           0       -0.587769   -3.117804    1.990248
     70          8           0       -1.305257   -0.937887    2.464209
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.79974542     A.U. after    1 cycles
             Convg  =    0.7080D-08             -V/T =  2.0050
Zero-point correction=                           0.559114 (Hartree/Particle)
 Thermal correction to Energy=                    0.603836
 Thermal correction to Enthalpy=                  0.604891
 Thermal correction to Gibbs Free Energy=         0.472820
 Sum of electronic and zero-point Energies=          -6832.240632
 Sum of electronic and thermal Energies=             -6832.195909
 Sum of electronic and thermal Enthalpies=           -6832.194854
 Sum of electronic and thermal Free Energies=        -6832.326926
                     1                      2                      3
                     A                      A                      A
 Frequencies --   -94.1523               10.4477               19.3084
```

DPPP-Rh-Ph-CO_2 (7)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.042945	-0.567610	-0.539864
2	15	0	1.342267	0.448703	0.941357
3	15	0	-2.079173	-0.051675	0.635452
4	6	0	-1.877048	0.324754	2.426681
5	6	0	0.605039	0.984501	2.569039
6	1	0	-1.549465	-0.589646	2.935597
7	1	0	-2.846071	0.614821	2.847170
8	6	0	-3.193662	-1.502571	0.590706
9	6	0	-3.782922	-2.067313	1.727503
10	6	0	-3.436974	-2.082161	-0.663540
11	6	0	-4.605107	-3.188338	1.612871
12	1	0	-3.611672	-1.639283	2.711072
13	6	0	-4.265397	-3.195028	-0.775229
14	1	0	-2.974370	-1.658569	-1.552399
15	6	0	-4.849635	-3.752511	0.362657
16	1	0	-5.056124	-3.618151	2.503568
17	1	0	-4.448249	-3.632356	-1.753125
18	1	0	-5.490912	-4.625530	0.274997
19	6	0	-3.153940	1.332759	0.092398
20	6	0	-4.535003	1.323850	0.327213
21	6	0	-2.573749	2.445970	-0.525695
22	6	0	-5.318409	2.414106	-0.040898
23	1	0	-5.004452	0.457655	0.787689
24	6	0	-3.360373	3.538794	-0.889743
25	1	0	-1.509656	2.456189	-0.746853
26	6	0	-4.731828	3.525698	-0.647419
27	1	0	-6.389969	2.393576	0.140365
28	1	0	-2.898184	4.392739	-1.377669
29	1	0	-5.345818	4.373480	-0.939948
30	6	0	2.774300	-0.471560	1.631662
31	6	0	2.784057	-1.867926	1.594174
32	6	0	3.802047	0.197715	2.310426
33	6	0	3.803624	-2.585846	2.217943
34	1	0	2.000776	-2.397157	1.060320
35	6	0	4.822479	-0.519095	2.929112

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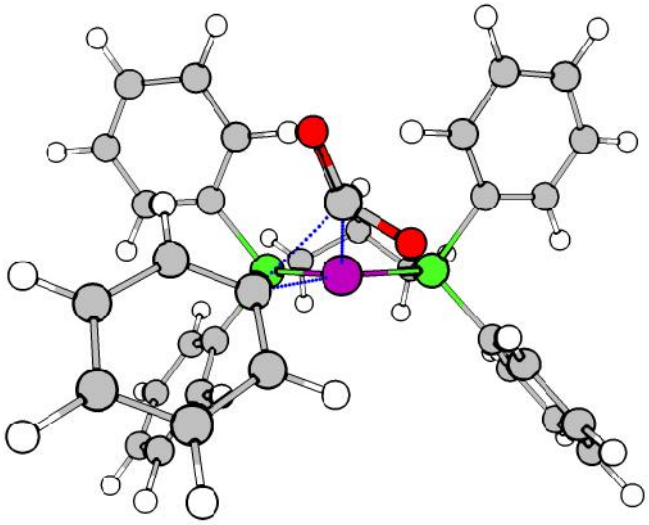
     36          1           0        3.814877    1.284275    2.348702
     37          6           0        4.825177   -1.913604    2.884664
     38          1           0        3.802830   -3.671612    2.172011
     39          1           0        5.617835    0.012788    3.444830
     40          1           0        5.624442   -2.472501    3.364331
     41          6           0        2.100833    1.978709    0.282496
     42          6           0        3.313250    1.922479   -0.415776
     43          6           0        1.453165    3.211913    0.412512
     44          6           0        3.863814    3.076551   -0.967411
     45          1           0        3.837926    0.977226   -0.520962
     46          6           0        2.004807    4.365286   -0.139800
     47          1           0        0.510376    3.287029    0.945950
     48          6           0        3.211171    4.300849   -0.833951
     49          1           0        4.806598    3.015580   -1.504781
     50          1           0        1.487848    5.314828   -0.028712
     51          1           0        3.640574    5.199839   -1.267949
     52          6           0        1.541677   -1.373067   -1.563240
     53          6           0        1.540660   -2.778805   -1.545275
     54          6           0        2.482629   -0.739444   -2.383960
     55          6           0        2.454157   -3.520837   -2.295767
     56          1           0        0.808774   -3.320679   -0.942700
     57          6           0        3.399235   -1.476333   -3.139823
     58          1           0        2.491472    0.345457   -2.460430
     59          6           0        3.395082   -2.869232   -3.094058
     60          1           0        2.427468   -4.608319   -2.260847
     61          1           0        4.114551   -0.956394   -3.774405
     62          1           0        4.108661   -3.442222   -3.681294
     63          6           0       -0.852891    1.439494    2.653152
     64          1           0       -1.001930    1.832765    3.665646
     65          1           0       -1.058560    2.279921    1.981353
     66          1           0        1.261810    1.769227    2.962181
     67          1           0        0.737976    0.119190    3.228875
     68          6           0       -0.381204    0.549349   -2.220399
     69          8           0        0.056792    1.623205   -2.538059
     70          8           0       -1.116496   -0.383425   -2.564466
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.80859017     A.U. after    1 cycles
             Convg  =    0.4941D-08             -V/T =  2.0050
Zero-point correction=                           0.560199 (Hartree/Particle)
 Thermal correction to Energy=                    0.605021
 Thermal correction to Enthalpy=                  0.606076
 Thermal correction to Gibbs Free Energy=         0.475136
 Sum of electronic and zero-point Energies=          -6832.248392
 Sum of electronic and thermal Energies=             -6832.203569
 Sum of electronic and thermal Enthalpies=           -6832.202514
 Sum of electronic and thermal Free Energies=        -6832.333455
                     1                      2                      3
                     A                      A                      A
 Frequencies --    12.2737               24.0209               30.2365
```

DPPP-Rh-Ph-CO_2-TS2 (8)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.135087	-0.149066	0.626295
2	15	0	-1.304725	0.171639	-1.100771
3	15	0	2.046155	-0.101775	-0.702032
4	6	0	1.882901	0.098027	-2.522555
5	6	0	-0.614963	0.490242	-2.803081
6	1	0	1.635864	-0.876619	-2.958543
7	1	0	2.845436	0.415663	-2.936808
8	6	0	3.102827	-1.581659	-0.481748
9	6	0	3.704970	-2.273017	-1.538503
10	6	0	3.307175	-2.031014	0.830874
11	6	0	4.496659	-3.394348	-1.288398
12	1	0	3.569048	-1.945738	-2.565499
13	6	0	4.104796	-3.144166	1.077847
14	1	0	2.841979	-1.502671	1.660103
15	6	0	4.699283	-3.831118	0.018594
16	1	0	4.957219	-3.923700	-2.118564
17	1	0	4.258291	-3.479417	2.100219
18	1	0	5.317455	-4.703772	0.212090
19	6	0	3.182781	1.277600	-0.273382
20	6	0	4.534859	1.243209	-0.638451
21	6	0	2.687076	2.399252	0.397056
22	6	0	5.369416	2.319241	-0.350484
23	1	0	4.944855	0.367299	-1.136575
24	6	0	3.523198	3.478124	0.683659
25	1	0	1.647062	2.418755	0.711680
26	6	0	4.863805	3.440991	0.308721
27	1	0	6.418050	2.279792	-0.634010
28	1	0	3.125824	4.340560	1.212089
29	1	0	5.517956	4.278163	0.537991
30	6	0	-2.511940	-1.163764	-1.480414
31	6	0	-2.735323	-2.178376	-0.544426
32	6	0	-3.201967	-1.210287	-2.702045
33	6	0	-3.631549	-3.211127	-0.817512
34	1	0	-2.203269	-2.162070	0.401742
35	6	0	-4.095814	-2.242699	-2.974559
36	1	0	-3.050696	-0.439116	-3.452786
37	6	0	-4.313411	-3.246936	-2.031180
38	1	0	-3.791865	-3.990093	-0.076803

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     39          1           0       -4.622336   -2.261723   -3.925330
     40          1           0       -5.009569   -4.053859   -2.244698
     41          6           0       -2.330319    1.683159   -0.865678
     42          6           0       -3.695240    1.746736   -1.166155
     43          6           0       -1.689548    2.830129   -0.380416
     44          6           0       -4.399201    2.938696   -0.998753
     45          1           0       -4.223208    0.862618   -1.511455
     46          6           0       -2.391184    4.022747   -0.223823
     47          1           0       -0.642663    2.777149   -0.091605
     48          6           0       -3.749158    4.080799   -0.534522
     49          1           0       -5.461896    2.970001   -1.225442
     50          1           0       -1.879543    4.900851    0.161016
     51          1           0       -4.301424    5.007188   -0.400648
     52          6           0       -1.382003   -0.403200    2.117694
     53          6           0       -1.201118   -1.628654    2.782926
     54          6           0       -2.646462    0.200592    2.182497
     55          6           0       -2.263835   -2.264350    3.427617
     56          1           0       -0.214781   -2.088150    2.802378
     57          6           0       -3.709360   -0.426610    2.826243
     58          1           0       -2.793564    1.180503    1.736836
     59          6           0       -3.523766   -1.667196    3.441931
     60          1           0       -2.104993   -3.216917    3.928270
     61          1           0       -4.684648    0.053868    2.855549
     62          1           0       -4.353347   -2.154583    3.948490
     63          6           0        0.782503    1.102931   -2.873545
     64          1           0        0.943655    1.445941   -3.901754
     65          1           0        0.854852    1.998106   -2.243294
     66          1           0       -1.327271    1.141893   -3.319359
     67          1           0       -0.609709   -0.468461   -3.333876
     68          6           0        0.153922    0.874035    2.519102
     69          8           0       -0.252710    1.919710    2.954506
     70          8           0        1.169812    0.145366    2.535067
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.79546039     A.U. after    1 cycles
             Convg  =    0.2182D-08             -V/T =  2.0050
Zero-point correction=                           0.559540 (Hartree/Particle)
 Thermal correction to Energy=                    0.603683
 Thermal correction to Enthalpy=                  0.604738
 Thermal correction to Gibbs Free Energy=         0.474945
 Sum of electronic and zero-point Energies=          -6832.235921
 Sum of electronic and thermal Energies=             -6832.191777
 Sum of electronic and thermal Enthalpies=           -6832.190722
 Sum of electronic and thermal Free Energies=        -6832.320516
                    1                      2                      3
                    A                      A                      A
 Frequencies --  -290.1578               13.1068               19.1949
```
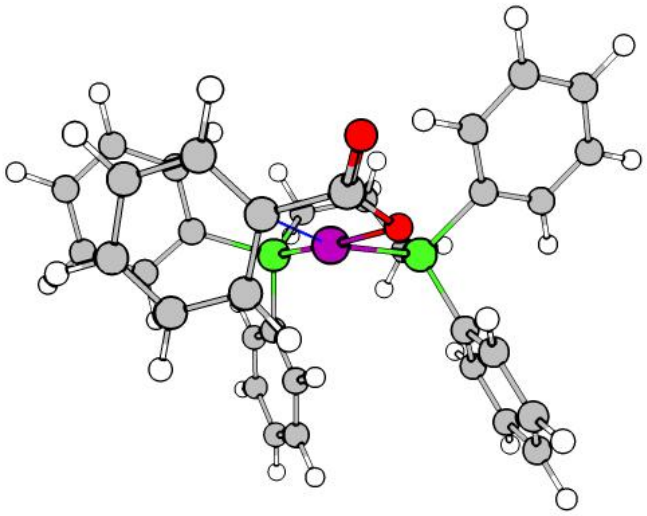

DPPP-Rh-OOCPh-conf1 (9)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.004630	-0.711948	-0.399905
2	15	0	-1.355141	0.569623	0.876700
3	15	0	1.805156	0.255098	0.577092
4	6	0	1.517765	1.297890	2.066427
5	6	0	-0.903866	0.702377	2.681654
6	1	0	1.074412	2.255122	1.770120
7	1	0	2.478438	1.508316	2.547515
8	6	0	2.753367	1.296438	-0.589760
9	6	0	3.068690	2.636394	-0.343343
10	6	0	3.162265	0.704196	-1.794507
11	6	0	3.783661	3.376224	-1.286191
12	1	0	2.763732	3.118443	0.580820
13	6	0	3.882030	1.443958	-2.727206
14	1	0	2.907696	-0.334146	-1.997367
15	6	0	4.193006	2.782116	-2.477352
16	1	0	4.021791	4.417480	-1.084453
17	1	0	4.198072	0.974961	-3.655373
18	1	0	4.752330	3.358367	-3.209780
19	6	0	3.059741	-0.930454	1.196646
20	6	0	4.346143	-0.494761	1.539483
21	6	0	2.723340	-2.275456	1.367460
22	6	0	5.275408	-1.390127	2.060253
23	1	0	4.630528	0.544406	1.387059
24	6	0	3.654896	-3.171298	1.891237
25	1	0	1.737969	-2.620089	1.066821
26	6	0	4.929110	-2.730509	2.240164
27	1	0	6.272953	-1.044396	2.318926
28	1	0	3.386269	-4.217327	2.011644
29	1	0	5.657229	-3.430705	2.641417
30	6	0	-1.437069	2.330736	0.343229
31	6	0	-0.827459	2.687453	-0.864282
32	6	0	-2.075389	3.326312	1.097333
33	6	0	-0.847043	4.009588	-1.308552
34	1	0	-0.325651	1.918488	-1.447903
35	6	0	-2.096806	4.645839	0.654255
36	1	0	-2.575255	3.075948	2.030132
37	6	0	-1.479931	4.990891	-0.549764
38	1	0	-0.361396	4.269951	-2.245249

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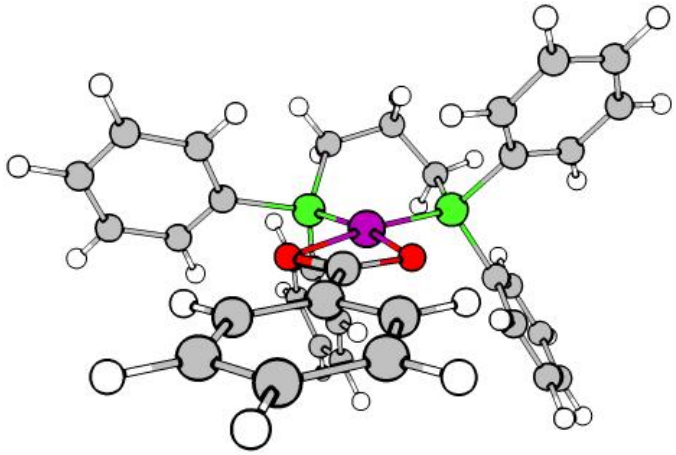
     39          1           0       -2.597241    5.406010    1.248522
     40          1           0       -1.494369    6.022309   -0.892242
     41          6           0       -3.118939    0.073163    1.024334
     42          6           0       -4.173147    0.835188    0.511471
     43          6           0       -3.410416   -1.145727    1.651388
     44          6           0       -5.492245    0.403675    0.651531
     45          1           0       -3.971830    1.771141   -0.001739
     46          6           0       -4.727191   -1.573343    1.795591
     47          1           0       -2.605126   -1.777541    2.020639
     48          6           0       -5.774312   -0.796551    1.299815
     49          1           0       -6.300118    1.010786    0.250923
     50          1           0       -4.934483   -2.518938    2.289883
     51          1           0       -6.802796   -1.129409    1.412363
     52          6           0       -1.014126   -2.397086   -1.776153
     53          6           0       -1.330867   -1.144515   -2.349981
     54          6           0       -2.055147   -3.215733   -1.294498
     55          6           0       -2.676696   -0.740510   -2.445841
     56          1           0       -0.564193   -0.581682   -2.879668
     57          6           0       -3.370229   -2.795684   -1.379269
     58          1           0       -1.801037   -4.190121   -0.886588
     59          6           0       -3.684386   -1.555883   -1.961347
     60          1           0       -2.917332    0.206685   -2.921843
     61          1           0       -4.168473   -3.430946   -1.004870
     62          1           0       -4.721827   -1.242390   -2.035708
     63          6           0        0.580367    0.542954    3.014980
     64          1           0        0.737525    0.899645    4.038737
     65          1           0        0.842548   -0.521167    3.020577
     66          1           0       -1.479039   -0.063699    3.209467
     67          1           0       -1.267737    1.668094    3.047149
     68          6           0        0.411701   -2.910117   -1.828460
     69          8           0        0.651031   -4.081506   -2.112142
     70          8           0        1.272777   -1.988820   -1.526056
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.84096857     A.U. after    1 cycles
             Convg  =    0.2071D-08             -V/T =  2.0050
Zero-point correction=                           0.562137 (Hartree/Particle)
 Thermal correction to Energy=                    0.606236
 Thermal correction to Enthalpy=                  0.607291
 Thermal correction to Gibbs Free Energy=         0.477769
 Sum of electronic and zero-point Energies=          -6832.278832
 Sum of electronic and thermal Energies=             -6832.234733
 Sum of electronic and thermal Enthalpies=           -6832.233678
 Sum of electronic and thermal Free Energies=        -6832.363200
                     1                      2                      3
                     A                      A                      A
 Frequencies --    14.8645               22.5574               29.4812
```

DPPP-Rh-OOCPh-conf2 (10)

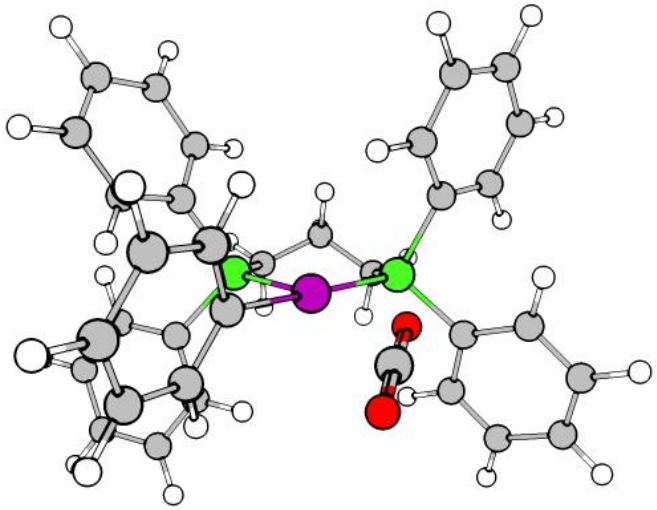


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.408096	0.000242	-0.164874
2	15	0	-0.724609	1.850298	-0.670145
3	15	0	-1.434763	-1.203109	-0.521209
4	6	0	-2.827591	-0.398336	-1.424439
5	6	0	-1.756096	1.803843	-2.218058
6	1	0	-3.375023	0.253104	-0.733001
7	1	0	-3.522004	-1.167024	-1.779141
8	6	0	-2.182872	-1.906281	0.995476
9	6	0	-3.554813	-1.895722	1.266190
10	6	0	-1.306043	-2.476649	1.929751
11	6	0	-4.044210	-2.448918	2.450089
12	1	0	-4.255416	-1.455322	0.562126
13	6	0	-1.797707	-3.035933	3.105166
14	1	0	-0.235485	-2.472332	1.733289
15	6	0	-3.168484	-3.021917	3.369311
16	1	0	-5.112315	-2.431310	2.651291
17	1	0	-1.108895	-3.477059	3.820912
18	1	0	-3.551087	-3.453605	4.290497
19	6	0	-1.123323	-2.693994	-1.551516
20	6	0	-2.061168	-3.730000	-1.645509
21	6	0	0.069676	-2.784243	-2.274755
22	6	0	-1.815780	-4.829173	-2.463365
23	1	0	-2.981861	-3.687789	-1.067220
24	6	0	0.314583	-3.885858	-3.094655
25	1	0	0.809577	-1.992691	-2.177871
26	6	0	-0.627483	-4.907254	-3.192123
27	1	0	-2.548372	-5.629743	-2.527347
28	1	0	1.246612	-3.947707	-3.650375
29	1	0	-0.435326	-5.767972	-3.827559
30	6	0	-1.904710	2.424041	0.618590
31	6	0	-1.859739	1.805893	1.873189
32	6	0	-2.835333	3.450656	0.403334
33	6	0	-2.729378	2.198346	2.890019
34	1	0	-1.138675	1.008178	2.040514
35	6	0	-3.703565	3.843459	1.418770
36	1	0	-2.881966	3.962746	-0.554881
37	6	0	-3.653587	3.215829	2.664467
38	1	0	-2.684492	1.703835	3.856674
39	1	0	-4.418294	4.642233	1.237936
40	1	0	-4.333934	3.521453	3.455115

```
     41          6           0        0.373993    3.289693   -0.965043
     42          6           0        0.335761    4.461598   -0.204492
     43          6           0        1.342888    3.161933   -1.969663
     44          6           0        1.231337    5.499313   -0.464197
     45          1           0       -0.387365    4.569405    0.598903
     46          6           0        2.228825    4.201290   -2.233864
     47          1           0        1.417130    2.235843   -2.536157
     48          6           0        2.173588    5.375747   -1.482344
     49          1           0        1.191898    6.404777    0.135926
     50          1           0        2.974161    4.088261   -3.016831
     51          1           0        2.870734    6.185115   -1.682796
     52          6           0        4.158271   -0.901845    0.953287
     53          6           0        4.512344   -2.231759    1.198918
     54          6           0        5.110014    0.111157    1.103133
     55          6           0        5.810212   -2.546367    1.592471
     56          1           0        3.759790   -3.005009    1.075732
     57          6           0        6.407402   -0.205055    1.497056
     58          1           0        4.816035    1.138437    0.908441
     59          6           0        6.758851   -1.533501    1.742174
     60          1           0        6.084628   -3.580696    1.783201
     61          1           0        7.146720    0.583033    1.614474
     62          1           0        7.772088   -1.779470    2.049923
     63          6           0       -2.268766    0.411977   -2.600975
     64          1           0       -3.051672    0.534398   -3.357637
     65          1           0       -1.462450   -0.152808   -3.083209
     66          1           0       -1.133793    2.200612   -3.026068
     67          1           0       -2.597805    2.494510   -2.101401
     68          6           0        2.770075   -0.564285    0.533474
     69          8           0        2.456690    0.643715    0.296242
     70          8           0        1.904569   -1.492491    0.413380
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.85317999     A.U. after    1 cycles
             Convg  =    0.3001D-08             -V/T =  2.0049
Zero-point correction=                           0.562538 (Hartree/Particle)
 Thermal correction to Energy=                    0.606684
 Thermal correction to Enthalpy=                  0.607739
 Thermal correction to Gibbs Free Energy=         0.475426
 Sum of electronic and zero-point Energies=          -6832.290642
 Sum of electronic and thermal Energies=             -6832.246496
 Sum of electronic and thermal Enthalpies=           -6832.245441
 Sum of electronic and thermal Free Energies=        -6832.377754
                     1                      2                      3
                     A                      A                      A
 Frequencies --    11.8767               16.3803               23.3084
```

anti-pathway

DPPP-Rh-Ph-O=C=O-conf1 (11)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.081789	-0.429064	0.371958
2	15	0	-1.359406	0.546917	-0.990382
3	15	0	2.022137	0.298439	-0.709264
4	6	0	1.842421	0.997143	-2.409155
5	6	0	-0.694536	1.343489	-2.536530
6	1	0	1.661009	0.175499	-3.110183
7	1	0	2.782583	1.473538	-2.705625
8	6	0	3.322232	-0.985451	-0.908729
9	6	0	3.212145	-1.937847	-1.931146
10	6	0	4.354784	-1.126021	0.027162
11	6	0	4.128634	-2.981566	-2.035134
12	1	0	2.399519	-1.878618	-2.651085
13	6	0	5.268379	-2.173890	-0.073448
14	1	0	4.449591	-0.412849	0.841924
15	6	0	5.162889	-3.102364	-1.107467
16	1	0	4.030180	-3.705638	-2.839949
17	1	0	6.065198	-2.263244	0.660685
18	1	0	5.876935	-3.917788	-1.186841
19	6	0	2.909391	1.675220	0.128928
20	6	0	4.136944	2.172808	-0.329791
21	6	0	2.311357	2.271961	1.243445
22	6	0	4.751293	3.243311	0.313356
23	1	0	4.625541	1.714129	-1.186959
24	6	0	2.925340	3.346319	1.888593
25	1	0	1.353815	1.890780	1.594984
26	6	0	4.144963	3.833153	1.424481
27	1	0	5.704650	3.618111	-0.050494
28	1	0	2.448394	3.802067	2.752470
29	1	0	4.625017	4.669678	1.925775
30	6	0	-2.611847	-0.527005	-1.809279
31	6	0	-2.239460	-1.840498	-2.117821
32	6	0	-3.858903	-0.059782	-2.237791
33	6	0	-3.093685	-2.671113	-2.839806
34	1	0	-1.270581	-2.205701	-1.779781
35	6	0	-4.719295	-0.894071	-2.950219
36	1	0	-4.167108	0.958138	-2.012852
37	6	0	-4.339222	-2.200479	-3.254344

```
     38          1           0       -2.790881   -3.689801   -3.069166
     39          1           0       -5.688806   -0.520075   -3.269722
     40          1           0       -5.012108   -2.849582   -3.808773
     41          6           0       -2.375174    1.880276   -0.236056
     42          6           0       -3.422899    1.542653    0.633145
     43          6           0       -2.092620    3.234955   -0.448554
     44          6           0       -4.175562    2.534496    1.255315
     45          1           0       -3.652653    0.498378    0.825204
     46          6           0       -2.839633    4.228216    0.184673
     47          1           0       -1.284268    3.534373   -1.109458
     48          6           0       -3.886142    3.881740    1.036311
     49          1           0       -4.988324    2.250779    1.919029
     50          1           0       -2.602631    5.274189    0.006719
     51          1           0       -4.471633    4.655084    1.526821
     52          6           0       -1.488308   -1.081887    1.530504
     53          6           0       -2.201727   -2.280064    1.345324
     54          6           0       -1.697199   -0.413991    2.755634
     55          6           0       -3.059710   -2.791802    2.324031
     56          1           0       -2.095744   -2.834201    0.414676
     57          6           0       -2.549500   -0.917660    3.740925
     58          1           0       -1.190969    0.532971    2.945075
     59          6           0       -3.238204   -2.113307    3.528740
     60          1           0       -3.592214   -3.723736    2.141839
     61          1           0       -2.681618   -0.372133    4.673912
     62          1           0       -3.906423   -2.507886    4.290698
     63          6           0        0.686683    1.998718   -2.475860
     64          1           0        0.808699    2.599182   -3.385249
     65          1           0        0.756789    2.703500   -1.638538
     66          1           0       -1.445994    2.061064   -2.886721
     67          1           0       -0.674468    0.541931   -3.283757
     68          8           0        1.451204   -1.632182    2.015303
     69          6           0        1.020949   -2.450544    2.737375
     70          8           0        0.641093   -3.274728    3.463578
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.80255545     A.U. after    1 cycles
             Convg  =    0.7257D-08             -V/T =  2.0050
Zero-point correction=                           0.559538 (Hartree/Particle)
 Thermal correction to Energy=                    0.605300
 Thermal correction to Enthalpy=                  0.606355
 Thermal correction to Gibbs Free Energy=         0.470142
 Sum of electronic and zero-point Energies=          -6832.243018
 Sum of electronic and thermal Energies=             -6832.197255
 Sum of electronic and thermal Enthalpies=           -6832.196200
 Sum of electronic and thermal Free Energies=        -6832.332414
                     1                      2                      3
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 Frequencies --    11.6072               19.6730               22.1158
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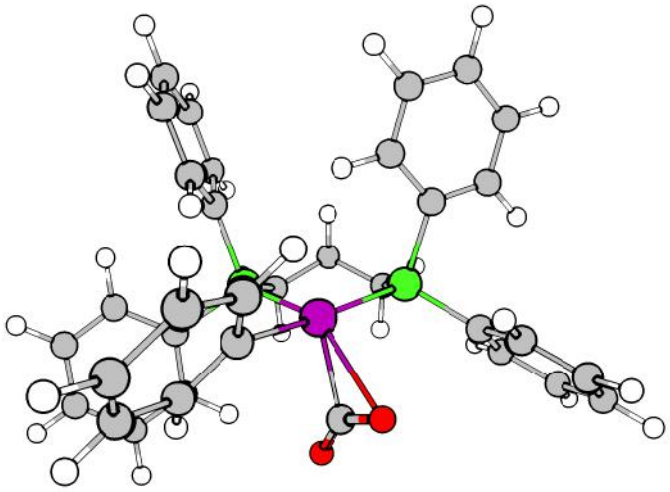
DPPP-Rh-Ph-CO_2 (12)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.041133	-0.707516	0.504077
2	15	0	-1.313868	0.406049	-0.922893
3	15	0	2.077392	0.050135	-0.549874
4	6	0	1.967407	0.473527	-2.338700
5	6	0	-0.583121	0.689743	-2.594375
6	1	0	1.872642	-0.465818	-2.895654
7	1	0	2.900101	0.956836	-2.650718
8	6	0	3.522966	-1.063730	-0.441491
9	6	0	4.286765	-1.451569	-1.547469
10	6	0	3.864768	-1.555120	0.825572
11	6	0	5.378239	-2.305249	-1.387542
12	1	0	4.043519	-1.094627	-2.543799
13	6	0	4.959791	-2.397403	0.985131
14	1	0	3.266698	-1.284158	1.691813
15	6	0	5.719816	-2.775669	-0.122061
16	1	0	5.961225	-2.600559	-2.256031
17	1	0	5.211415	-2.771124	1.973948
18	1	0	6.570123	-3.441127	0.001114
19	6	0	2.713263	1.613970	0.174754
20	6	0	4.054739	1.997126	0.048264
21	6	0	1.825449	2.460296	0.847983
22	6	0	4.494224	3.207295	0.577805
23	1	0	4.763149	1.340868	-0.451995
24	6	0	2.264783	3.674911	1.373844
25	1	0	0.782639	2.171084	0.961036
26	6	0	3.599682	4.049863	1.239743
27	1	0	5.538641	3.491575	0.478598
28	1	0	1.562654	4.322762	1.891984
29	1	0	3.945773	4.992820	1.654817
30	6	0	-2.890178	-0.381669	-1.429657
31	6	0	-2.831378	-1.652779	-2.017807
32	6	0	-4.129254	0.247890	-1.281127
33	6	0	-3.995986	-2.273202	-2.462229
34	1	0	-1.880625	-2.175449	-2.097994
35	6	0	-5.293810	-0.382127	-1.719196
36	1	0	-4.194801	1.229503	-0.820494
37	6	0	-5.230327	-1.640145	-2.313981
38	1	0	-3.938179	-3.260891	-2.912169
39	1	0	-6.252342	0.114625	-1.592987

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     40          1           0       -6.139213   -2.129293   -2.654546
     41          6           0       -1.818864    2.072043   -0.342433
     42          6           0       -2.204347    2.213511    0.998260
     43          6           0       -1.838388    3.200086   -1.171723
     44          6           0       -2.607012    3.451528    1.493528
     45          1           0       -2.200120    1.346483    1.654456
     46          6           0       -2.228803    4.441194   -0.671087
     47          1           0       -1.553103    3.126946   -2.216746
     48          6           0       -2.615067    4.570536    0.661596
     49          1           0       -2.912076    3.539693    2.532930
     50          1           0       -2.233098    5.307467   -1.327416
     51          1           0       -2.922051    5.538348    1.049151
     52          6           0       -1.539844   -1.237611    1.693500
     53          6           0       -2.625887   -2.087223    1.456112
     54          6           0       -1.371887   -0.746992    2.999995
     55          6           0       -3.510637   -2.432666    2.481329
     56          1           0       -2.789127   -2.499004    0.463527
     57          6           0       -2.257191   -1.080304    4.027213
     58          1           0       -0.528869   -0.094142    3.238112
     59          6           0       -3.335427   -1.926993    3.768583
     60          1           0       -4.342272   -3.102055    2.270357
     61          1           0       -2.100141   -0.684710    5.028812
     62          1           0       -4.027184   -2.194210    4.563820
     63          6           0        0.779972    1.382648   -2.659619
     64          1           0        0.913538    1.748807   -3.684098
     65          1           0        0.800744    2.273813   -2.021002
     66          1           0       -1.324067    1.236702   -3.187933
     67          1           0       -0.517082   -0.304509   -3.051234
     68          6           0        0.324200   -2.642022   -0.048504
     69          8           0        0.952116   -2.769421    1.007305
     70          8           0       -0.036405   -3.221001   -1.045665
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.81587874     A.U. after    1 cycles
             Convg  =    0.3841D-08             -V/T =  2.0050
Zero-point correction=                           0.560023 (Hartree/Particle)
 Thermal correction to Energy=                    0.604951
 Thermal correction to Enthalpy=                  0.606006
 Thermal correction to Gibbs Free Energy=         0.473833
 Sum of electronic and zero-point Energies=          -6832.255855
 Sum of electronic and thermal Energies=             -6832.210928
 Sum of electronic and thermal Enthalpies=           -6832.209873
 Sum of electronic and thermal Free Energies=        -6832.342046
                     1                      2                      3
                     A                      A                      A
 Frequencies --    16.5405               20.8018               24.9145
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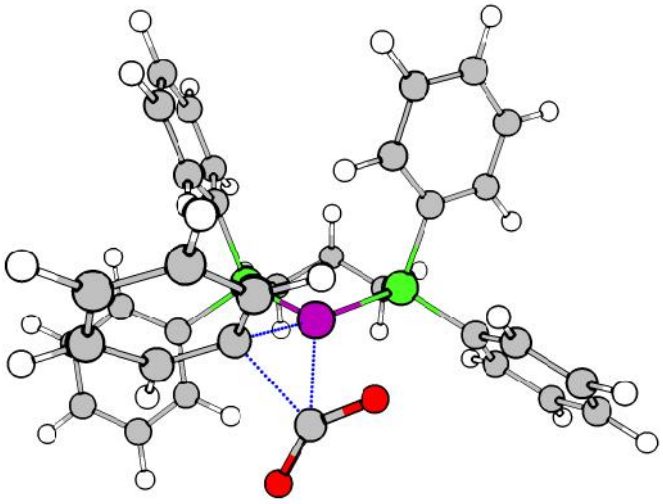
DPPP-Rh-Ph-CO_2-TS2 (13)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.131509	-0.776702	0.346261
2	15	0	-1.240861	0.374108	-1.030819
3	15	0	2.037133	0.095708	-0.669291
4	6	0	1.968956	0.578111	-2.443683
5	6	0	-0.569123	0.775854	-2.704241
6	1	0	1.889297	-0.339249	-3.038116
7	1	0	2.907508	1.074386	-2.715154
8	6	0	3.500353	-0.995297	-0.553356
9	6	0	4.226207	-1.433788	-1.665989
10	6	0	3.889953	-1.421184	0.723615
11	6	0	5.327267	-2.274625	-1.503409
12	1	0	3.947276	-1.126131	-2.669398
13	6	0	4.992959	-2.252780	0.883994
14	1	0	3.323320	-1.106752	1.595806
15	6	0	5.714784	-2.683221	-0.229620
16	1	0	5.882131	-2.608141	-2.376523
17	1	0	5.281947	-2.575809	1.880487
18	1	0	6.572397	-3.338889	-0.104446
19	6	0	2.628499	1.646406	0.118080
20	6	0	3.924045	2.130909	-0.105380
21	6	0	1.761142	2.373035	0.939668
22	6	0	4.338934	3.325277	0.476345
23	1	0	4.619070	1.565349	-0.722437
24	6	0	2.176443	3.571777	1.519897
25	1	0	0.758698	1.994670	1.128159
26	6	0	3.464247	4.049359	1.288773
27	1	0	5.347920	3.689560	0.301028
28	1	0	1.492275	4.127335	2.155894
29	1	0	3.790719	4.980374	1.744847
30	6	0	-2.758175	-0.509315	-1.568896
31	6	0	-2.624421	-1.843473	-1.974905
32	6	0	-4.012308	0.103621	-1.636714
33	6	0	-3.725847	-2.547567	-2.453702
34	1	0	-1.661626	-2.342949	-1.883055
35	6	0	-5.116375	-0.607104	-2.107814
36	1	0	-4.136575	1.133360	-1.311766
37	6	0	-4.975590	-1.930581	-2.520635
38	1	0	-3.610286	-3.584764	-2.756691
39	1	0	-6.089054	-0.123473	-2.148454

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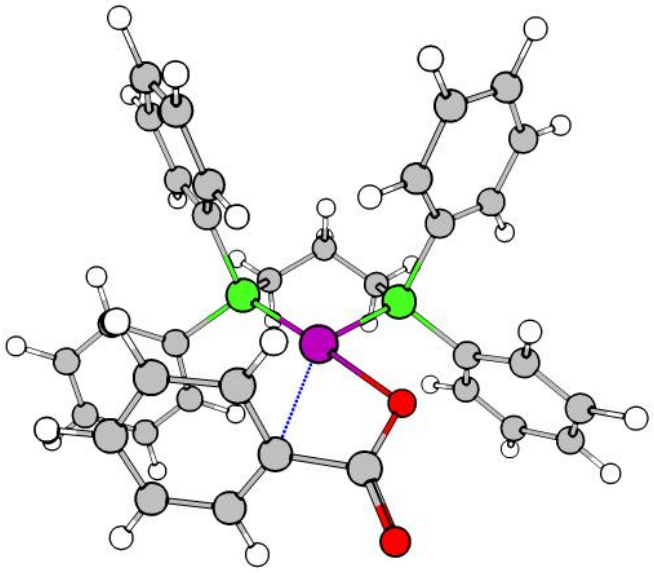
     40          1           0       -5.837920   -2.483367   -2.884024
     41          6           0       -1.860434    1.977866   -0.384950
     42          6           0       -2.257865    2.030041    0.958890
     43          6           0       -1.947631    3.141682   -1.158492
     44          6           0       -2.743825    3.213562    1.508502
     45          1           0       -2.183773    1.139251    1.577833
     46          6           0       -2.420872    4.329990   -0.602810
     47          1           0       -1.648637    3.139409   -2.202373
     48          6           0       -2.823151    4.368462    0.730406
     49          1           0       -3.054535    3.232829    2.549819
     50          1           0       -2.475574    5.225615   -1.216193
     51          1           0       -3.193889    5.294551    1.161915
     52          6           0       -1.369307   -1.424440    1.727539
     53          6           0       -2.717073   -1.750410    1.522161
     54          6           0       -0.990370   -0.960639    2.999670
     55          6           0       -3.664637   -1.551269    2.523322
     56          1           0       -3.026210   -2.184221    0.576119
     57          6           0       -1.935976   -0.752988    4.005270
     58          1           0        0.059728   -0.767055    3.210469
     59          6           0       -3.279489   -1.039421    3.764622
     60          1           0       -4.706422   -1.803450    2.338909
     61          1           0       -1.621339   -0.383632    4.978830
     62          1           0       -4.019564   -0.887964    4.546757
     63          6           0        0.781657    1.490077   -2.754879
     64          1           0        0.917496    1.879929   -3.770304
     65          1           0        0.789974    2.364973   -2.093695
     66          1           0       -1.331409    1.342228   -3.250458
     67          1           0       -0.497080   -0.190274   -3.217707
     68          6           0       -0.088555   -2.830753    1.010683
     69          8           0        1.030429   -2.468793    1.426367
     70          8           0       -0.684728   -3.808256    0.641388
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.79896595     A.U. after    1 cycles
             Convg  =    0.7670D-08             -V/T =  2.0050
Zero-point correction=                           0.559659 (Hartree/Particle)
 Thermal correction to Energy=                    0.603715
 Thermal correction to Enthalpy=                  0.604770
 Thermal correction to Gibbs Free Energy=         0.475628
 Sum of electronic and zero-point Energies=          -6832.239307
 Sum of electronic and thermal Energies=             -6832.195251
 Sum of electronic and thermal Enthalpies=           -6832.194196
 Sum of electronic and thermal Free Energies=        -6832.323338
                    1                      2                      3
                    A                      A                      A
 Frequencies --  -286.4499               18.6753                22.5339
```

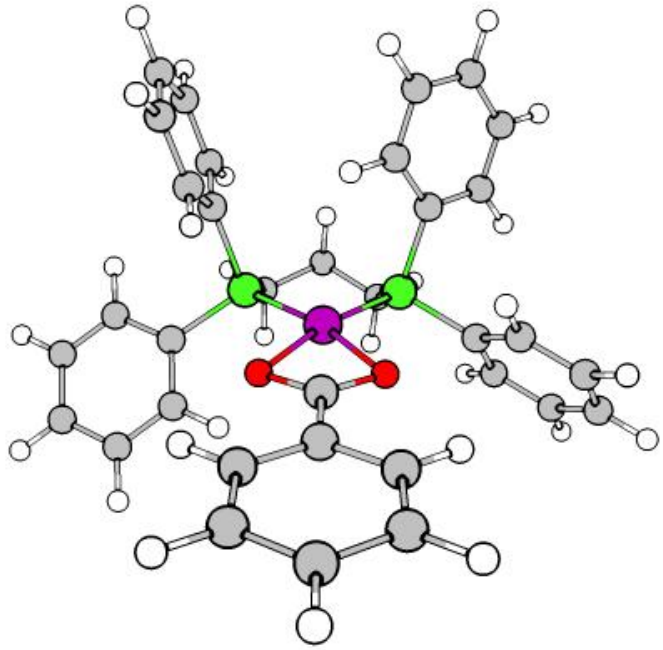
DPPP-Rh-OOCPh-conf1 (14)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.113284	-0.575093	-0.451653
2	15	0	1.404499	0.578467	0.778276
3	15	0	-1.874592	0.251253	0.719486
4	6	0	-1.618364	0.840491	2.445675
5	6	0	0.913463	1.092010	2.484941
6	1	0	-1.443441	-0.030727	3.085201
7	1	0	-2.544319	1.314707	2.787705
8	6	0	-3.252711	-0.943630	0.870637
9	6	0	-3.452376	-1.712874	2.022630
10	6	0	-4.087139	-1.150760	-0.235433
11	6	0	-4.479812	-2.653376	2.076090
12	1	0	-2.810159	-1.596144	2.890557
13	6	0	-5.110596	-2.091226	-0.180204
14	1	0	-3.930005	-0.583850	-1.147615
15	6	0	-5.312783	-2.843884	0.975857
16	1	0	-4.624272	-3.239946	2.979714
17	1	0	-5.744041	-2.244564	-1.049665
18	1	0	-6.110437	-3.580958	1.016045
19	6	0	-2.686102	1.712967	-0.043113
20	6	0	-3.896265	2.211045	0.458979
21	6	0	-2.083352	2.356503	-1.125633
22	6	0	-4.483489	3.337578	-0.108421
23	1	0	-4.394333	1.707405	1.284663
24	6	0	-2.671207	3.486079	-1.695095
25	1	0	-1.152364	1.958768	-1.521314
26	6	0	-3.869903	3.979054	-1.186263
27	1	0	-5.424356	3.712695	0.285889
28	1	0	-2.192809	3.977233	-2.538434
29	1	0	-4.331371	4.857184	-1.630409
30	6	0	2.947700	-0.332681	1.192003
31	6	0	2.805162	-1.568562	1.836735
32	6	0	4.233153	0.142363	0.916666
33	6	0	3.924666	-2.297313	2.228569
34	1	0	1.810731	-1.972745	2.017364
35	6	0	5.354652	-0.594398	1.298746
36	1	0	4.367975	1.086369	0.396121

```
     37          6           0        5.204603   -1.810547    1.961745
     38          1           0        3.796927   -3.252186    2.731955
     39          1           0        6.348278   -0.213712    1.075871
     40          1           0        6.079686   -2.380760    2.262521
     41          6           0        1.989695    2.160109    0.035865
     42          6           0        1.739137    2.394725   -1.320699
     43          6           0        2.677391    3.139687    0.765762
     44          6           0        2.164545    3.570720   -1.936325
     45          1           0        1.199743    1.645272   -1.894051
     46          6           0        3.098760    4.318579    0.154999
     47          1           0        2.901766    2.990565    1.818233
     48          6           0        2.843933    4.537489   -1.198525
     49          1           0        1.959572    3.732299   -2.991491
     50          1           0        3.629045    5.066766    0.738395
     51          1           0        3.172306    5.458150   -1.673527
     52          6           0       -0.436634    1.799364    2.582571
     53          1           0       -0.501113    2.276101    3.567215
     54          1           0       -0.506996    2.612018    1.849240
     55          1           0        1.707633    1.715199    2.906625
     56          1           0        0.898792    0.176283    3.087139
     57          6           0       -0.727545   -2.722545   -1.928394
     58          8           0       -1.464151   -1.704370   -1.615796
     59          8           0       -1.111922   -3.826533   -2.305922
     60          6           0        0.750681   -2.423909   -1.780052
     61          6           0        1.631664   -3.378374   -1.235813
     62          6           0        1.275321   -1.229930   -2.321557
     63          6           0        2.995215   -3.146186   -1.231251
     64          1           0        1.218997   -4.306413   -0.850182
     65          6           0        2.668929   -1.018603   -2.327930
     66          1           0        0.626771   -0.572009   -2.899432
     67          6           0        3.518596   -1.964817   -1.782960
     68          1           0        3.669924   -3.886004   -0.808906
     69          1           0        3.073435   -0.117650   -2.782090
     70          1           0        4.592265   -1.799612   -1.786436
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.83978814     A.U. after    1 cycles
             Convg  =    0.1645D-08             -V/T =  2.0050
Zero-point correction=                           0.562289 (Hartree/Particle)
 Thermal correction to Energy=                    0.605298
 Thermal correction to Enthalpy=                  0.606353
 Thermal correction to Gibbs Free Energy=         0.480903
 Sum of electronic and zero-point Energies=          -6832.277499
 Sum of electronic and thermal Energies=             -6832.234490
 Sum of electronic and thermal Enthalpies=           -6832.233435
 Sum of electronic and thermal Free Energies=        -6832.358886
                     1                      2                      3
                     A                      A                      A
 Frequencies --    -4.1075               19.8391               21.7526
```

DPPP-Rh-OOCPh-conf2 (15)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.290521	0.250499	-0.229054
2	15	0	0.060853	-1.920714	-0.682373
3	15	0	-1.856152	0.645092	-0.684503
4	6	0	-2.681028	-0.370781	-1.982987
5	6	0	-1.217005	-2.473708	-1.889104
6	1	0	-2.188389	-0.156498	-2.938626
7	1	0	-3.727810	-0.057632	-2.068184
8	6	0	-2.158171	2.373420	-1.213203
9	6	0	-2.661393	2.716723	-2.472404
10	6	0	-1.832163	3.394185	-0.309896
11	6	0	-2.846857	4.055475	-2.818409
12	1	0	-2.917540	1.948571	-3.195977
13	6	0	-2.023751	4.727976	-0.654470
14	1	0	-1.417039	3.143528	0.662681
15	6	0	-2.531616	5.063461	-1.910427
16	1	0	-3.240295	4.307850	-3.799777
17	1	0	-1.768298	5.508867	0.056583
18	1	0	-2.676892	6.106145	-2.180369
19	6	0	-3.023883	0.461683	0.724257
20	6	0	-4.339743	0.936819	0.643266
21	6	0	-2.599098	-0.176772	1.892998
22	6	0	-5.217312	0.765593	1.709731
23	1	0	-4.677518	1.458941	-0.249597
24	6	0	-3.479823	-0.349506	2.961668
25	1	0	-1.572621	-0.531277	1.961254
26	6	0	-4.788330	0.119723	2.871220
27	1	0	-6.234725	1.141919	1.639146
28	1	0	-3.138408	-0.847471	3.865424
29	1	0	-5.473541	-0.010473	3.705012
30	6	0	1.565998	-2.678925	-1.412382
31	6	0	2.473572	-1.865524	-2.097489
32	6	0	1.793568	-4.059135	-1.349693
33	6	0	3.585510	-2.427146	-2.724154

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     34          1           0        2.313124   -0.790483   -2.123324
     35          6           0        2.905391   -4.617787   -1.974741
     36          1           0        1.108362   -4.701488   -0.801079
     37          6           0        3.802180   -3.802186   -2.665680
     38          1           0        4.287442   -1.785928   -3.250643
     39          1           0        3.075245   -5.689922   -1.918197
     40          1           0        4.671967   -4.238558   -3.150079
     41          6           0       -0.214847   -2.943219    0.816896
     42          6           0        0.636942   -2.701920    1.905422
     43          6           0       -1.219294   -3.906937    0.945273
     44          6           0        0.495142   -3.421843    3.087103
     45          1           0        1.410713   -1.941067    1.822763
     46          6           0       -1.369041   -4.619729    2.136214
     47          1           0       -1.899310   -4.113704    0.123650
     48          6           0       -0.511376   -4.382380    3.206944
     49          1           0        1.166801   -3.228360    3.919329
     50          1           0       -2.158625   -5.361670    2.223020
     51          1           0       -0.627473   -4.939419    4.132901
     52          6           0       -2.611056   -1.872904   -1.698172
     53          1           0       -3.291643   -2.378675   -2.392957
     54          1           0       -2.996431   -2.082317   -0.693199
     55          1           0       -1.259714   -3.568783   -1.892616
     56          1           0       -0.821053   -2.182378   -2.869383
     57          6           0        2.257373    1.650368    0.523381
     58          8           0        1.120509    2.198098    0.362173
     59          8           0        2.407415    0.404749    0.310351
     60          6           0        3.415774    2.475016    0.966329
     61          6           0        4.666921    1.879371    1.153852
     62          6           0        3.255813    3.845255    1.194251
     63          6           0        5.751233    2.648903    1.567681
     64          1           0        4.772915    0.814224    0.970381
     65          6           0        4.341430    4.613551    1.607707
     66          1           0        2.277697    4.291537    1.041134
     67          6           0        5.589081    4.016683    1.795133
     68          1           0        6.723048    2.184677    1.712799
     69          1           0        4.216079    5.678777    1.783928
     70          1           0        6.435737    4.617354    2.117705
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6832.85652132     A.U. after    1 cycles
             Convg  =    0.4032D-08             -V/T =  2.0049
Zero-point correction=                           0.562463 (Hartree/Particle)
 Thermal correction to Energy=                    0.606653
 Thermal correction to Enthalpy=                  0.607708
 Thermal correction to Gibbs Free Energy=         0.473235
 Sum of electronic and zero-point Energies=          -6832.294058
 Sum of electronic and thermal Energies=             -6832.249868
 Sum of electronic and thermal Enthalpies=           -6832.248813
 Sum of electronic and thermal Free Energies=        -6832.383286
                     1                      2                      3
                     A                      A                      A
 Frequencies --     3.0884                17.5704                18.5238
```
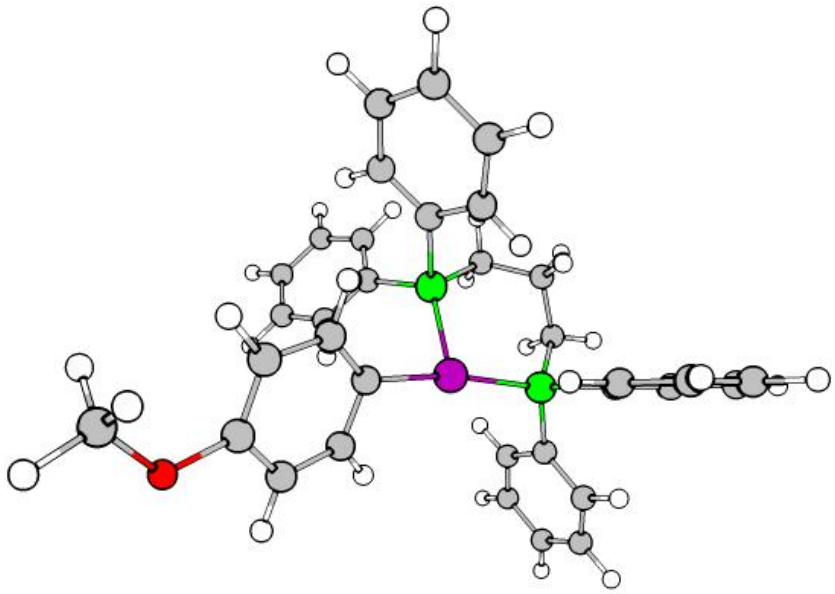
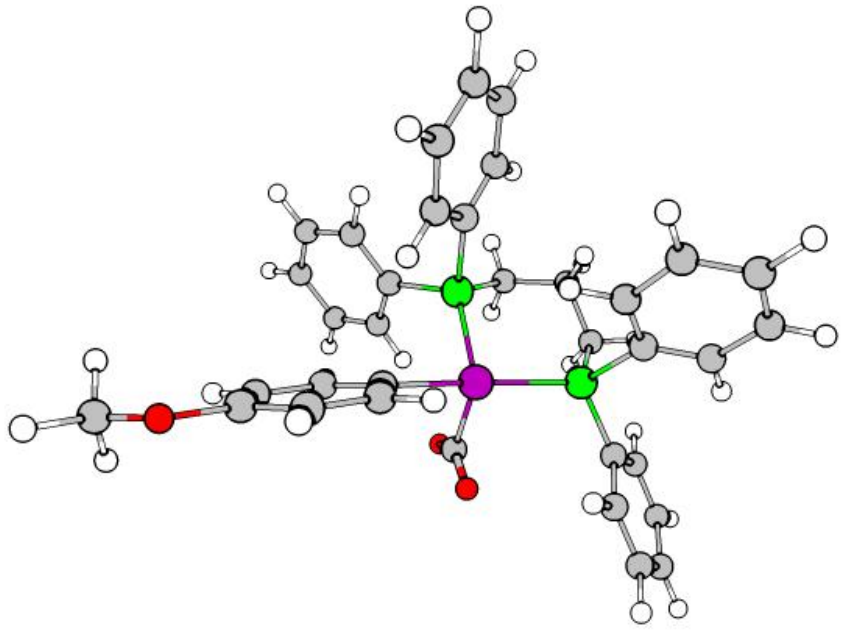

DPPP-Rh-(*p*-MeOPh) (16)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.166291	0.539532	-0.005158
2	15	0	-0.807854	-1.311186	0.700333
3	15	0	2.382398	-0.161691	0.270733
4	6	0	2.654722	-1.739448	1.189996
5	6	0	0.274908	-2.678460	1.366020
6	1	0	2.532549	-1.528853	2.258008
7	1	0	3.686428	-2.077316	1.050555
8	6	0	3.467242	1.018122	1.173492
9	6	0	3.177034	1.275563	2.521933
10	6	0	4.492935	1.743988	0.557977
11	6	0	3.917584	2.206749	3.244231
12	1	0	2.354688	0.755801	3.009779
13	6	0	5.227561	2.685328	1.279797
14	1	0	4.722373	1.580347	-0.491444
15	6	0	4.948381	2.914825	2.624903
16	1	0	3.681826	2.388199	4.289732
17	1	0	6.020802	3.240322	0.785302
18	1	0	5.522965	3.646823	3.186275
19	6	0	3.286819	-0.477760	-1.300518
20	6	0	4.579318	-1.018218	-1.347192
21	6	0	2.643409	-0.170468	-2.504697
22	6	0	5.209669	-1.246701	-2.567538
23	1	0	5.109469	-1.253085	-0.427101
24	6	0	3.273878	-0.395826	-3.728674
25	1	0	1.635441	0.241430	-2.478276
26	6	0	4.557144	-0.936511	-3.761900
27	1	0	6.212832	-1.664936	-2.587136
28	1	0	2.759553	-0.150354	-4.654164
29	1	0	5.049967	-1.115764	-4.713923
30	6	0	-2.032941	-1.195830	2.074955
31	6	0	-2.538138	0.053918	2.445794
32	6	0	-2.455562	-2.328598	2.788277
33	6	0	-3.449835	0.171532	3.494633
34	1	0	-2.211682	0.934998	1.900205
35	6	0	-3.362157	-2.211431	3.839290

```
     36          1           0       -2.085467   -3.316213    2.526616
     37          6           0       -3.863304   -0.959199    4.195210
     38          1           0       -3.833421    1.152134    3.764410
     39          1           0       -3.678132   -3.100559    4.379260
     40          1           0       -4.570588   -0.867682    5.015586
     41          6           0       -1.717103   -2.218496   -0.626480
     42          6           0       -3.015408   -2.720228   -0.485893
     43          6           0       -1.055475   -2.401837   -1.849236
     44          6           0       -3.629682   -3.403858   -1.536216
     45          1           0       -3.564981   -2.564925    0.438091
     46          6           0       -1.660991   -3.100105   -2.890351
     47          1           0       -0.068447   -1.966317   -1.992515
     48          6           0       -2.952925   -3.604577   -2.736956
     49          1           0       -4.644001   -3.775382   -1.413145
     50          1           0       -1.129855   -3.234639   -3.829326
     51          1           0       -3.433064   -4.137589   -3.553523
     52          6           0       -1.585065    1.454983   -0.449573
     53          6           0       -1.481141    2.818590   -0.098520
     54          6           0       -2.671822    1.105568   -1.259846
     55          6           0       -2.382176    3.777381   -0.552349
     56          1           0       -0.671668    3.154948    0.555194
     57          6           0       -3.593641    2.052280   -1.725469
     58          1           0       -2.815880    0.069154   -1.559286
     59          6           0       -3.449385    3.395515   -1.372856
     60          1           0       -2.282797    4.824566   -0.275239
     61          1           0       -4.411013    1.725504   -2.361585
     62          6           0        1.668553   -2.825482    0.754819
     63          1           0        2.065927   -3.795008    1.077957
     64          1           0        1.612543   -2.879003   -0.339422
     65          1           0       -0.270594   -3.619710    1.238648
     66          1           0        0.371813   -2.505292    2.444302
     67          8           0       -4.291327    4.399821   -1.768403
     68          6           0       -5.383771    4.046575   -2.591559
     69          1           0       -6.055026    3.338388   -2.090491
     70          1           0       -5.925056    4.972524   -2.789491
     71          1           0       -5.049949    3.615823   -3.543551
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6758.79559746     A.U. after    1 cycles
             Convg  =    0.2738D-08             -V/T =  2.0049
Zero-point correction=                           0.579678 (Hartree/Particle)
 Thermal correction to Energy=                    0.623861
 Thermal correction to Enthalpy=                  0.624916
 Thermal correction to Gibbs Free Energy=         0.493525
 Sum of electronic and zero-point Energies=          -6758.215919
 Sum of electronic and thermal Energies=             -6758.171737
 Sum of electronic and thermal Enthalpies=           -6758.170682
 Sum of electronic and thermal Free Energies=        -6758.302072
                     1                      2                      3
                     A                      A                      A
 Frequencies --    13.9620                17.7490                23.2419
```

DPPP-Rh-(*p*-MeOPh)-CO_2 (17)

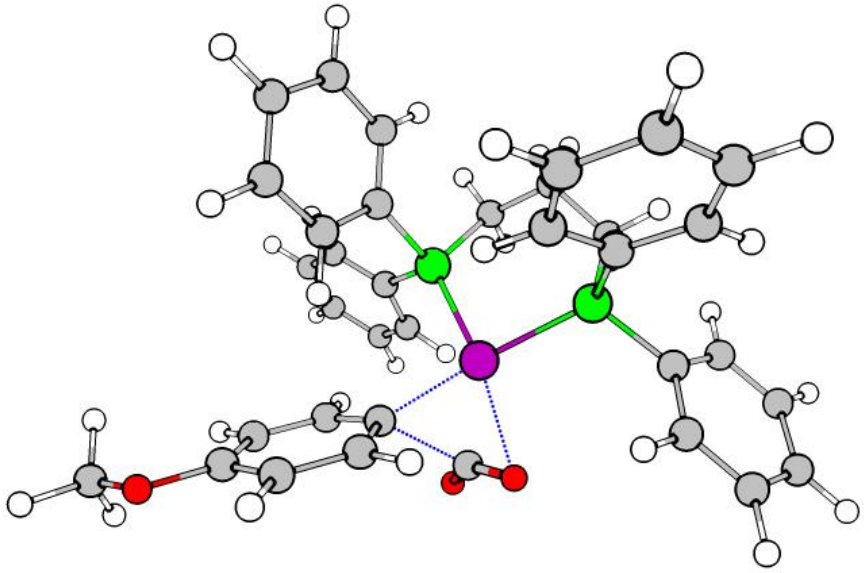


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.127817	-0.689085	-0.106677
2	15	0	0.772874	1.017286	1.070751
3	15	0	-2.402085	-0.054853	0.379527
4	6	0	-2.687682	0.867865	1.947010
5	6	0	-0.283969	1.625273	2.457542
6	1	0	-2.567642	0.160887	2.776207
7	1	0	-3.719924	1.235117	1.964897
8	6	0	-3.642622	-1.397040	0.413752
9	6	0	-4.548671	-1.592788	1.461346
10	6	0	-3.662732	-2.278349	-0.675399
11	6	0	-5.466039	-2.642725	1.413849
12	1	0	-4.551081	-0.933218	2.324252
13	6	0	-4.584669	-3.318148	-0.726427
14	1	0	-2.946175	-2.157088	-1.483673
15	6	0	-5.488899	-3.504020	0.319640
16	1	0	-6.162394	-2.785419	2.236073
17	1	0	-4.586859	-3.994140	-1.577197
18	1	0	-6.202889	-4.322611	0.284990
19	6	0	-3.090750	1.100727	-0.872477
20	6	0	-4.470451	1.291950	-1.022180
21	6	0	-2.212385	1.829463	-1.681578
22	6	0	-4.958291	2.200249	-1.957543
23	1	0	-5.168205	0.718160	-0.416402
24	6	0	-2.701000	2.742277	-2.616058
25	1	0	-1.138257	1.686691	-1.581692
26	6	0	-4.074313	2.928718	-2.755350
27	1	0	-6.030991	2.336276	-2.068523
28	1	0	-2.005732	3.302285	-3.235854
29	1	0	-4.457743	3.634941	-3.487115
30	6	0	2.320910	0.726262	2.008157
31	6	0	2.341305	-0.334314	2.924559
32	6	0	3.450996	1.537272	1.871576
33	6	0	3.473070	-0.565348	3.702176
34	1	0	1.486934	-1.003555	3.005001

35	6	0	4.585394	1.295573	2.646352
36	1	0	3.454970	2.356969	1.158607
37	6	0	4.597774	0.248762	3.565576
38	1	0	3.479488	-1.393647	4.405876
39	1	0	5.460508	1.929463	2.528577
40	1	0	5.482594	0.063029	4.168908
41	6	0	1.134941	2.507979	0.064543
42	6	0	1.727841	2.323296	-1.192541
43	6	0	0.849023	3.810551	0.491251
44	6	0	2.033423	3.416879	-1.999292
45	1	0	1.958900	1.317270	-1.535268
46	6	0	1.143289	4.903014	-0.323208
47	1	0	0.397435	3.991036	1.462049
48	6	0	1.736853	4.709805	-1.569207
49	1	0	2.501220	3.255414	-2.966907
50	1	0	0.910006	5.907268	0.020727
51	1	0	1.967500	5.563177	-2.201404
52	6	0	1.698698	-1.223704	-0.866893
53	6	0	2.881050	-1.661830	-0.270688
54	6	0	1.654820	-1.244499	-2.274052
55	6	0	3.980675	-2.092177	-1.024932
56	1	0	2.972139	-1.683694	0.811992
57	6	0	2.737106	-1.657309	-3.043785
58	1	0	0.749368	-0.935557	-2.801085
59	6	0	3.914564	-2.082564	-2.418291
60	1	0	2.687060	-1.666322	-4.130106
61	6	0	-1.719150	2.038180	2.123979
62	1	0	-2.087506	2.648453	2.956685
63	1	0	-1.747539	2.689347	1.242318
64	1	0	0.252937	2.448254	2.942124
65	1	0	-0.292403	0.808820	3.189174
66	6	0	-0.233456	-2.411439	0.965147
67	8	0	-0.647502	-2.941811	-0.070553
68	8	0	0.026675	-2.614425	2.127830
69	1	0	4.874318	-2.428316	-0.507778
70	8	0	4.929897	-2.467349	-3.249494
71	6	0	6.128904	-2.912879	-2.647921
72	1	0	5.963030	-3.801698	-2.027523
73	1	0	6.800732	-3.169760	-3.467611
74	1	0	6.590212	-2.126587	-2.038058

```
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6947.22901206     A.U. after    1 cycles
             Convg  =    0.6687D-08             -V/T =  2.0051
Zero-point correction=                           0.593324 (Hartree/Particle)
 Thermal correction to Energy=                    0.641291
 Thermal correction to Enthalpy=                  0.642346
 Thermal correction to Gibbs Free Energy=         0.503435
 Sum of electronic and zero-point Energies=          -6946.635688
 Sum of electronic and thermal Energies=             -6946.587721
 Sum of electronic and thermal Enthalpies=           -6946.586666
 Sum of electronic and thermal Free Energies=        -6946.725577
                     1                      2                      3
                     A                      A                      A
 Frequencies --    15.4873               20.9635               22.8648
```

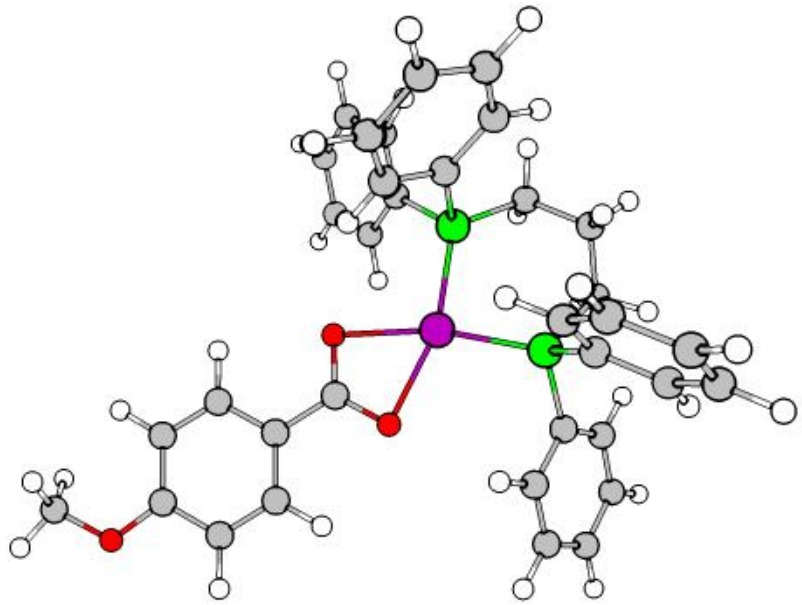
DPPP-Rh-(*p*-MeOPh)-CO_2-TS2 (18)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.290423	-0.748234	-0.075582
2	15	0	0.732501	0.720493	1.300498
3	15	0	-2.413775	0.091145	0.423206
4	6	0	-2.700330	0.887981	2.058707
5	6	0	-0.272964	1.348751	2.717488
6	1	0	-2.678449	0.104397	2.824837
7	1	0	-3.698695	1.339586	2.067240
8	6	0	-3.765801	-1.131345	0.272821
9	6	0	-4.661364	-1.421629	1.307380
10	6	0	-3.884874	-1.819411	-0.942390
11	6	0	-5.663576	-2.374998	1.126974
12	1	0	-4.592157	-0.909772	2.262379
13	6	0	-4.889567	-2.763989	-1.122784
14	1	0	-3.184497	-1.620152	-1.748783
15	6	0	-5.781809	-3.045666	-0.087876
16	1	0	-6.352629	-2.590719	1.939436
17	1	0	-4.968309	-3.290272	-2.070257
18	1	0	-6.562473	-3.788855	-0.227037
19	6	0	-2.939928	1.419008	-0.732922
20	6	0	-4.282483	1.802234	-0.848547
21	6	0	-1.973284	2.082706	-1.495227
22	6	0	-4.647615	2.836953	-1.704904
23	1	0	-5.049431	1.280415	-0.280167
24	6	0	-2.339289	3.122054	-2.350598
25	1	0	-0.930760	1.779932	-1.420181
26	6	0	-3.675604	3.500459	-2.456068
27	1	0	-5.692697	3.122990	-1.791535
28	1	0	-1.578110	3.630624	-2.936439
29	1	0	-3.962953	4.306277	-3.126491
30	6	0	2.148795	0.064628	2.266972
31	6	0	2.002849	-1.202028	2.847439
32	6	0	3.321460	0.790310	2.493566
33	6	0	3.009440	-1.727643	3.652901
34	1	0	1.112841	-1.792529	2.637427
35	6	0	4.332652	0.257268	3.293343
36	1	0	3.455939	1.768956	2.040008

```
     37          6           0        4.177704   -0.998577    3.877474
     38          1           0        2.887397   -2.715153    4.089856
     39          1           0        5.244101    0.826506    3.457597
     40          1           0        4.968000   -1.412422    4.498334
     41          6           0        1.391400    2.237109    0.499181
     42          6           0        2.035746    2.094167   -0.738063
     43          6           0        1.276689    3.517637    1.053793
     44          6           0        2.566442    3.202378   -1.393336
     45          1           0        2.117165    1.109599   -1.191671
     46          6           0        1.795912    4.628698    0.389806
     47          1           0        0.781548    3.667594    2.008323
     48          6           0        2.445527    4.473878   -0.832923
     49          1           0        3.068920    3.070566   -2.348030
     50          1           0        1.691814    5.616072    0.832171
     51          1           0        2.851597    5.340188   -1.348570
     52          6           0        1.482878   -1.465243   -1.009683
     53          6           0        2.776625   -1.655191   -0.513895
     54          6           0        1.354657   -1.266425   -2.399396
     55          6           0        3.903087   -1.582567   -1.332521
     56          1           0        2.919706   -1.887517    0.537013
     57          6           0        2.462157   -1.181318   -3.232777
     58          1           0        0.364102   -1.180707   -2.842458
     59          6           0        3.749248   -1.329120   -2.699906
     60          1           0        4.885184   -1.732890   -0.895565
     61          1           0        2.353459   -1.020535   -4.302460
     62          6           0       -1.641302    1.942567    2.381516
     63          1           0       -1.986754    2.508253    3.254490
     64          1           0       -1.566362    2.668278    1.562851
     65          1           0        0.337484    2.064323    3.279173
     66          1           0       -0.396578    0.484231    3.380416
     67          6           0        0.152531   -2.853910   -0.280577
     68          8           0       -0.865273   -2.674349   -0.977536
     69          8           0        0.710510   -3.689639    0.381021
     70          8           0        4.776720   -1.231119   -3.586438
     71          6           0        6.092202   -1.410978   -3.093562
     72          1           0        6.226297   -2.410724   -2.665260
     73          1           0        6.752331   -1.297815   -3.953674
     74          1           0        6.346168   -0.654412   -2.342123
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6947.21397238     A.U. after    1 cycles
             Convg  =    0.4344D-08             -V/T =  2.0051
Zero-point correction=                           0.592662 (Hartree/Particle)
 Thermal correction to Energy=                    0.639813
 Thermal correction to Enthalpy=                  0.640868
 Thermal correction to Gibbs Free Energy=         0.505021
 Sum of electronic and zero-point Energies=          -6946.621311
 Sum of electronic and thermal Energies=             -6946.574159
 Sum of electronic and thermal Enthalpies=           -6946.573104
 Sum of electronic and thermal Free Energies=        -6946.708952
                    1                    2                    3
                    A                    A                    A
 Frequencies --  -277.5621              16.6261              24.4423
```

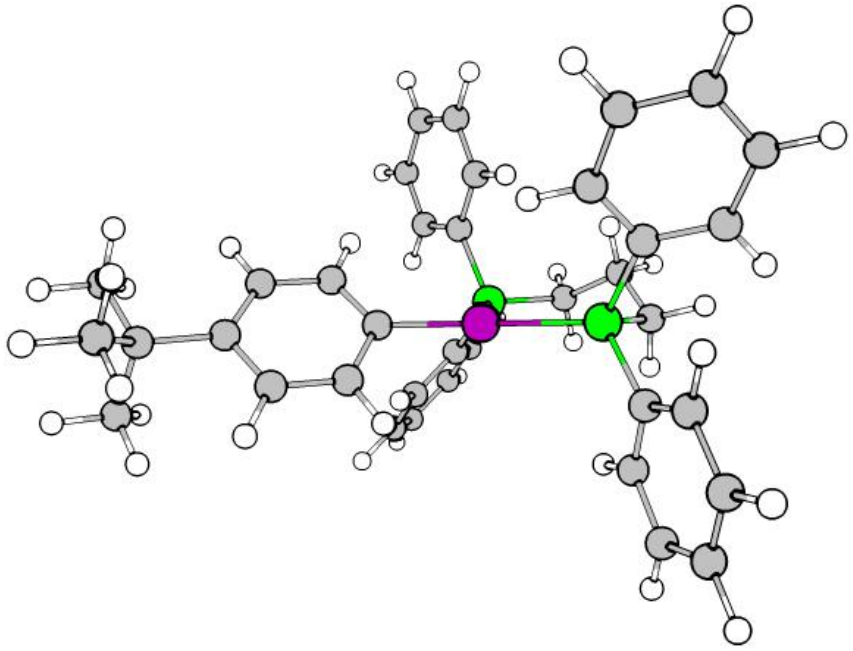
DPPP-Rh-OOC(*p*-MeOPh)-conf2 (19)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.099003	-0.081971	-0.332371
2	15	0	1.311548	1.764376	-0.619445
3	15	0	1.894248	-1.395853	-0.550710
4	6	0	3.296516	-0.827813	-1.602869
5	6	0	2.891537	1.702456	-1.564597
6	1	0	2.944581	-0.798360	-2.640814
7	1	0	4.104642	-1.565192	-1.542086
8	6	0	1.496431	-3.058450	-1.212222
9	6	0	2.114017	-3.613607	-2.338250
10	6	0	0.504630	-3.794220	-0.548928
11	6	0	1.754287	-4.884644	-2.787184
12	1	0	2.880763	-3.065635	-2.878079
13	6	0	0.153543	-5.064641	-0.993775
14	1	0	-0.005119	-3.363889	0.308649
15	6	0	0.776802	-5.614261	-2.114677
16	1	0	2.242335	-5.303186	-3.663698
17	1	0	-0.616537	-5.623791	-0.468785
18	1	0	0.498070	-6.604828	-2.464547
19	6	0	2.760045	-1.795927	1.023425
20	6	0	3.684759	-2.845457	1.104807
21	6	0	2.508149	-1.019250	2.158491
22	6	0	4.353875	-3.103470	2.297924
23	1	0	3.872727	-3.476973	0.238689
24	6	0	3.180816	-1.276815	3.353291
25	1	0	1.776849	-0.215642	2.099519
26	6	0	4.104455	-2.317070	3.424389
27	1	0	5.065040	-3.923856	2.352311
28	1	0	2.976248	-0.665878	4.228673
29	1	0	4.624785	-2.522226	4.356475
30	6	0	0.415836	3.080693	-1.534197
31	6	0	-0.612999	2.715348	-2.408196
32	6	0	0.770774	4.430033	-1.417514
33	6	0	-1.266520	3.684767	-3.167695
34	1	0	-0.909285	1.671152	-2.475571

```
     35          6           0        0.115562    5.397236   -2.175759
     36          1           0        1.552492    4.730958   -0.723461
     37          6           0       -0.902616    5.025272   -3.054401
     38          1           0       -2.068090    3.391732   -3.840736
     39          1           0        0.395897    6.442837   -2.076576
     40          1           0       -1.416386    5.781348   -3.642634
     41          6           0        1.730830    2.587538    0.967247
     42          6           0        0.678038    2.776415    1.875849
     43          6           0        3.016229    3.003724    1.326740
     44          6           0        0.907337    3.381215    3.107338
     45          1           0       -0.324028    2.442668    1.613708
     46          6           0        3.247140    3.599076    2.568114
     47          1           0        3.854610    2.868601    0.649256
     48          6           0        2.194713    3.792041    3.458973
     49          1           0        0.080516    3.525948    3.797795
     50          1           0        4.253111    3.912724    2.835036
     51          1           0        2.375193    4.257591    4.424341
     52          6           0        3.827599    0.549034   -1.199714
     53          1           0        4.778197    0.709847   -1.721570
     54          1           0        4.066031    0.558155   -0.129456
     55          1           0        3.405079    2.666679   -1.476851
     56          1           0        2.590080    1.614506   -2.615178
     57          6           0       -2.365455   -0.421922    0.123759
     58          8           0       -1.598523   -1.435198    0.060388
     59          8           0       -1.891505    0.751057   -0.040571
     60          6           0       -3.812940   -0.600693    0.386986
     61          6           0       -4.656682    0.506116    0.476340
     62          6           0       -4.354969   -1.882760    0.549318
     63          6           0       -6.018600    0.353852    0.725544
     64          1           0       -4.233597    1.498112    0.347329
     65          6           0       -5.706776   -2.050025    0.796282
     66          1           0       -3.697048   -2.743702    0.476876
     67          6           0       -6.548370   -0.931346    0.886977
     68          1           0       -6.649486    1.233857    0.790321
     69          1           0       -6.140403   -3.037963    0.923848
     70          8           0       -7.857122   -1.196249    1.132854
     71          6           0       -8.747417   -0.099182    1.239902
     72          1           0       -9.729195   -0.529353    1.437023
     73          1           0       -8.469853    0.561366    2.069013
     74          1           0       -8.786539    0.476813    0.308525
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6947.27219627     A.U. after    1 cycles
             Convg  =    0.1924D-08             -V/T =  2.0050
Zero-point correction=                           0.595948 (Hartree/Particle)
 Thermal correction to Energy=                    0.643049
 Thermal correction to Enthalpy=                  0.644104
 Thermal correction to Gibbs Free Energy=         0.505453
 Sum of electronic and zero-point Energies=          -6946.676248
 Sum of electronic and thermal Energies=             -6946.629148
 Sum of electronic and thermal Enthalpies=           -6946.628093
 Sum of electronic and thermal Free Energies=        -6946.766743
                     1                      2                      3
                     A                      A                      A
 Frequencies --    11.4081               16.5989                19.2256
```

DPPP-Rh-(*p*-*t*-BuPh) (20)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.303830	-0.346580	-0.131739
2	15	0	-0.124965	1.804289	-0.386905
3	15	0	2.644131	-0.197033	-0.212658
4	6	0	3.367684	1.421887	-0.728137
5	6	0	1.309190	2.951108	-0.717117
6	1	0	3.284926	1.490910	-1.818508
7	1	0	4.435955	1.440861	-0.490298
8	6	0	3.451059	-1.373878	-1.373767
9	6	0	3.151173	-1.243859	-2.738455
10	6	0	4.261224	-2.438428	-0.964090
11	6	0	3.679260	-2.131488	-3.671325
12	1	0	2.484296	-0.451644	-3.073801
13	6	0	4.780866	-3.334893	-1.898764
14	1	0	4.489529	-2.576918	0.089143
15	6	0	4.499123	-3.180947	-3.254011
16	1	0	3.440330	-2.010799	-4.724859
17	1	0	5.408266	-4.156423	-1.562231
18	1	0	4.906564	-3.878727	-3.980806
19	6	0	3.492555	-0.499427	1.391888
20	6	0	4.874961	-0.350439	1.570014
21	6	0	2.711617	-0.886169	2.486706
22	6	0	5.459620	-0.583500	2.812049
23	1	0	5.508170	-0.064017	0.733502
24	6	0	3.295133	-1.121867	3.731795
25	1	0	1.635450	-0.993541	2.358819
26	6	0	4.669942	-0.969513	3.896428
27	1	0	6.533369	-0.465931	2.934140
28	1	0	2.673601	-1.421936	4.571420
29	1	0	5.127304	-1.150267	4.865726
30	6	0	-1.244362	2.328161	-1.757246
31	6	0	-2.015744	1.370575	-2.422269
32	6	0	-1.322774	3.664464	-2.180432
33	6	0	-2.852954	1.736236	-3.476128

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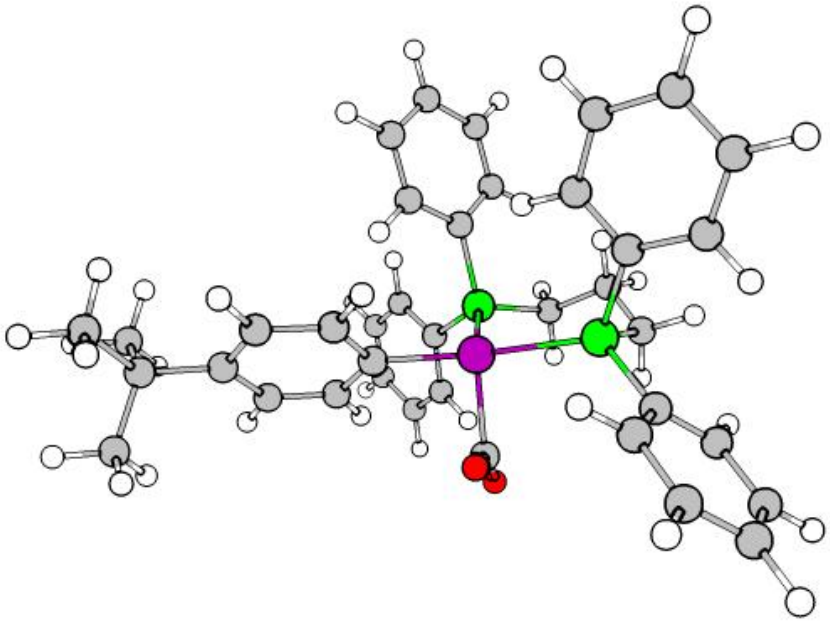
     34          1           0       -1.954395    0.333890   -2.103269
     35          6           0       -2.154383    4.029603   -3.236432
     36          1           0       -0.739207    4.436485   -1.685867
     37          6           0       -2.924047    3.065138   -3.887155
     38          1           0       -3.447187    0.976668   -3.977588
     39          1           0       -2.202091    5.069691   -3.549284
     40          1           0       -3.573388    3.350078   -4.711062
     41          6           0       -0.857452    2.601047    1.109542
     42          6           0       -1.983745    3.430628    1.082168
     43          6           0       -0.244509    2.342430    2.344048
     44          6           0       -2.471939    4.003793    2.257283
     45          1           0       -2.500054    3.620612    0.145696
     46          6           0       -0.719961    2.929456    3.513385
     47          1           0        0.594989    1.651863    2.390235
     48          6           0       -1.837266    3.764305    3.473731
     49          1           0       -3.355869    4.635579    2.218371
     50          1           0       -0.228318    2.719533    4.459995
     51          1           0       -2.218690    4.212084    4.387746
     52          6           0       -1.644115   -0.856719    0.060705
     53          6           0       -1.840309   -2.103119   -0.567946
     54          6           0       -2.684115   -0.412506    0.886781
     55          6           0       -2.987701   -2.866862   -0.358997
     56          1           0       -1.080326   -2.498907   -1.248525
     57          6           0       -3.837440   -1.176607    1.094181
     58          1           0       -2.602766    0.544334    1.399464
     59          6           0       -4.019950   -2.420139    0.479779
     60          1           0       -3.077666   -3.824031   -0.870575
     61          1           0       -4.601531   -0.779866    1.757728
     62          6           0        2.649578    2.602305   -0.071006
     63          1           0        3.295123    3.484228   -0.159740
     64          1           0        2.532783    2.429395    1.005636
     65          1           0        1.007606    3.952730   -0.392533
     66          1           0        1.433781    2.989718   -1.805758
     67          6           0       -5.270717   -3.279068    0.683160
     68          6           0       -5.967408   -3.506275   -0.669046
     69          1           0       -6.270894   -2.553830   -1.116197
     70          1           0       -5.313338   -4.016752   -1.382510
     71          1           0       -6.864275   -4.123430   -0.538433
     72          6           0       -6.278323   -2.622073    1.631043
     73          1           0       -7.152326   -3.272196    1.747342
     74          1           0       -5.854523   -2.458556    2.627543
     75          1           0       -6.632585   -1.659637    1.246915
     76          6           0       -4.871099   -4.638992    1.279688
     77          1           0       -4.181231   -5.181858    0.626453
     78          1           0       -4.380104   -4.510062    2.249931
     79          1           0       -5.757163   -5.268241    1.425426
 --------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6801.44970826     A.U. after    1 cycles
             Convg  =    0.3822D-08             -V/T =  2.0050
Zero-point correction=                           0.660012 (Hartree/Particle)
 Thermal correction to Energy=                    0.707846
 Thermal correction to Enthalpy=                  0.708901
 Thermal correction to Gibbs Free Energy=         0.570379
 Sum of electronic and zero-point Energies=          -6800.789696
 Sum of electronic and thermal Energies=             -6800.741863
 Sum of electronic and thermal Enthalpies=           -6800.740808
 Sum of electronic and thermal Free Energies=        -6800.879329
                     1                      2                      3
                     A                      A                      A
 Frequencies --    12.6668               18.4123               20.4313
```

DPPP-Rh-(*p*-*t*-BuPh)-CO_2 (21)



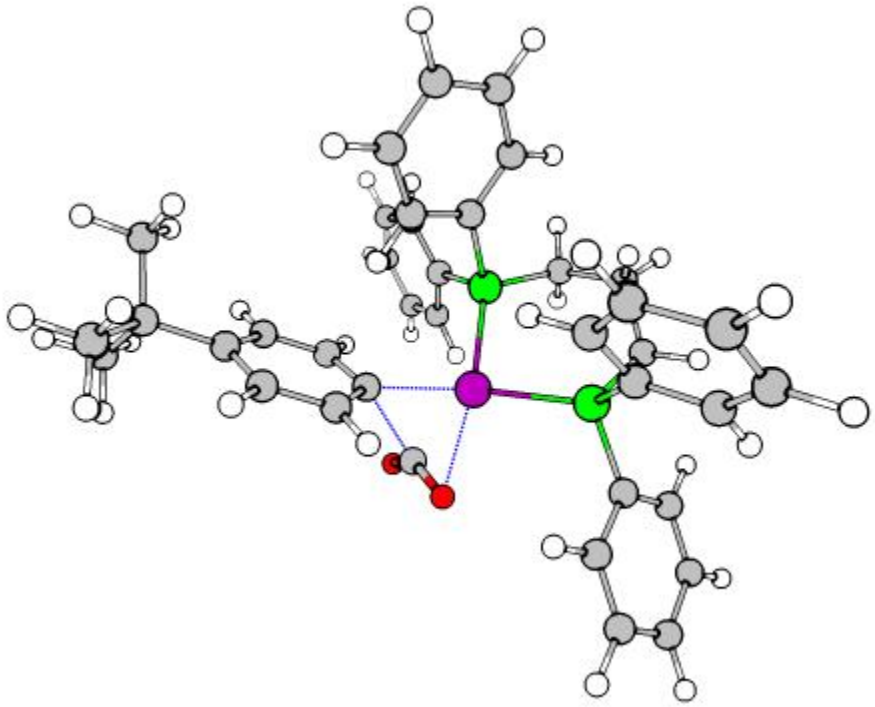
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.301916	-0.581412	0.160311
2	15	0	0.204377	1.476956	0.946490
3	15	0	-2.687373	-0.215785	0.225342
4	6	0	-3.298859	1.002737	1.463559
5	6	0	-1.104102	2.223368	2.014078
6	1	0	-3.209439	0.542474	2.454523
7	1	0	-4.360996	1.198643	1.278082
8	6	0	-3.736838	-1.688813	0.494142
9	6	0	-4.736647	-1.762406	1.469988
10	6	0	-3.504069	-2.802286	-0.324098
11	6	0	-5.496284	-2.923205	1.616261
12	1	0	-4.936460	-0.920339	2.125998
13	6	0	-4.268664	-3.955358	-0.183855
14	1	0	-2.713747	-2.770475	-1.069512
15	6	0	-5.267369	-4.019396	0.788206
16	1	0	-6.267872	-2.967573	2.380471
17	1	0	-4.074583	-4.810814	-0.825177
18	1	0	-5.858956	-4.923598	0.904319
19	6	0	-3.353704	0.475605	-1.342056
20	6	0	-4.709213	0.364547	-1.678272
21	6	0	-2.493377	1.158658	-2.208638
22	6	0	-5.193021	0.932653	-2.853450
23	1	0	-5.388211	-0.180492	-1.026656
24	6	0	-2.979146	1.731651	-3.383746
25	1	0	-1.436569	1.247881	-1.966471
26	6	0	-4.329122	1.619298	-3.708029
27	1	0	-6.245787	0.835298	-3.105789
28	1	0	-2.298608	2.260721	-4.045666
29	1	0	-4.708040	2.059505	-4.626656
30	6	0	1.630958	1.661891	2.082473
31	6	0	1.649830	0.878847	3.244784
32	6	0	2.666497	2.571394	1.850643
33	6	0	2.683750	1.019852	4.166623
34	1	0	0.875801	0.133218	3.414475

35	6	0	3.704766	2.701906	2.772753
36	1	0	2.671864	3.177608	0.949173
37	6	0	3.713483	1.931794	3.933539
38	1	0	2.690537	0.404255	5.062347
39	1	0	4.508246	3.408083	2.579825
40	1	0	4.523368	2.035715	4.650957
41	6	0	0.509815	2.728127	-0.361436
42	6	0	1.265594	2.343424	-1.477957
43	6	0	0.024615	4.040179	-0.294850
44	6	0	1.534055	3.251908	-2.499246
45	1	0	1.654773	1.329750	-1.540928
46	6	0	0.283251	4.944067	-1.323987
47	1	0	-0.556191	4.376363	0.558755
48	6	0	1.038711	4.553329	-2.428015
49	1	0	2.129725	2.938909	-3.352742
50	1	0	-0.105252	5.957019	-1.259067
51	1	0	1.241350	5.260509	-3.227990
52	6	0	1.667216	-0.983725	-0.227513
53	6	0	2.770411	-1.143629	0.618270
54	6	0	1.867770	-1.279703	-1.583040
55	6	0	4.003758	-1.572737	0.129719
56	1	0	2.678802	-0.942784	1.682648
57	6	0	3.106799	-1.702708	-2.074619
58	1	0	1.042781	-1.193045	-2.294828
59	6	0	4.208278	-1.858283	-1.227400
60	1	0	3.194501	-1.918175	-3.136101
61	6	0	-2.517358	2.316927	1.435643
62	1	0	-3.072827	3.042828	2.040635
63	1	0	-2.501168	2.727979	0.419414
64	1	0	-0.747906	3.210549	2.328277
65	1	0	-1.114391	1.612225	2.924112
66	6	0	-0.341691	-1.987501	1.626468
67	8	0	-0.522575	-2.811128	0.724016
68	8	0	-0.235667	-1.858530	2.823258
69	1	0	4.824146	-1.685926	0.836280
70	6	0	5.580913	-2.323884	-1.718286
71	6	0	5.973371	-3.622552	-0.994263
72	1	0	6.027892	-3.483229	0.089484
73	1	0	5.244201	-4.415175	-1.191846
74	1	0	6.955921	-3.969017	-1.335981
75	6	0	6.629793	-1.239881	-1.417650
76	1	0	6.377162	-0.301075	-1.922091
77	1	0	6.703286	-1.032705	-0.345786
78	1	0	7.619802	-1.558153	-1.765177
79	6	0	5.596864	-2.597415	-3.225263
80	1	0	6.595869	-2.928934	-3.528614
81	1	0	4.890246	-3.386247	-3.504271
82	1	0	5.357636	-1.700609	-3.806978

SCF Done: E(RPBE1PBE) = -6989.88322624   A.U. after   1 cycles
             Convg =   0.6744D-08   -V/T = 2.0052
Zero-point correction=   0.673733 (Hartree/Particle)
 Thermal correction to Energy=   0.725265
 Thermal correction to Enthalpy=   0.726320
 Thermal correction to Gibbs Free Energy=   0.581038
 Sum of electronic and zero-point Energies=   -6989.209493
 Sum of electronic and thermal Energies=   -6989.157961
 Sum of electronic and thermal Enthalpies=   -6989.156906
 Sum of electronic and thermal Free Energies=   -6989.302189

	1	2	3
	A	A	A
Frequencies --	16.8218	21.5709	22.8010

DPPP-Rh-(*p*-*t*-BuPh)-CO_2-TS2 (22)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.515016	-0.619478	0.393410
2	15	0	0.204446	1.433166	1.000250
3	15	0	-2.715407	0.112223	0.145585
4	6	0	-3.307136	1.545295	1.137483
5	6	0	-1.044498	2.538905	1.794644
6	1	0	-3.387468	1.224031	2.182259
7	1	0	-4.308745	1.827650	0.794481
8	6	0	-3.973296	-1.184242	0.432553
9	6	0	-5.021048	-1.051036	1.349747
10	6	0	-3.857433	-2.373835	-0.299131
11	6	0	-5.941538	-2.084267	1.525142
12	1	0	-5.135860	-0.144054	1.935521
13	6	0	-4.781034	-3.399637	-0.128432
14	1	0	-3.036393	-2.500684	-0.999306
15	6	0	-5.825632	-3.258650	0.785550
16	1	0	-6.750906	-1.967084	2.241131
17	1	0	-4.677481	-4.316630	-0.702256
18	1	0	-6.542775	-4.063470	0.923627
19	6	0	-3.091432	0.667191	-1.565778
20	6	0	-4.410657	0.791385	-2.020886
21	6	0	-2.039429	0.998014	-2.426132
22	6	0	-4.670542	1.246725	-3.310199
23	1	0	-5.239337	0.515825	-1.372051
24	6	0	-2.300754	1.458164	-3.716822
25	1	0	-1.011878	0.890008	-2.084498
26	6	0	-3.615272	1.583227	-4.160116
27	1	0	-5.697528	1.333577	-3.655575
28	1	0	-1.474378	1.712838	-4.375198
29	1	0	-3.819938	1.935582	-5.167764
30	6	0	1.464457	1.474754	2.334866

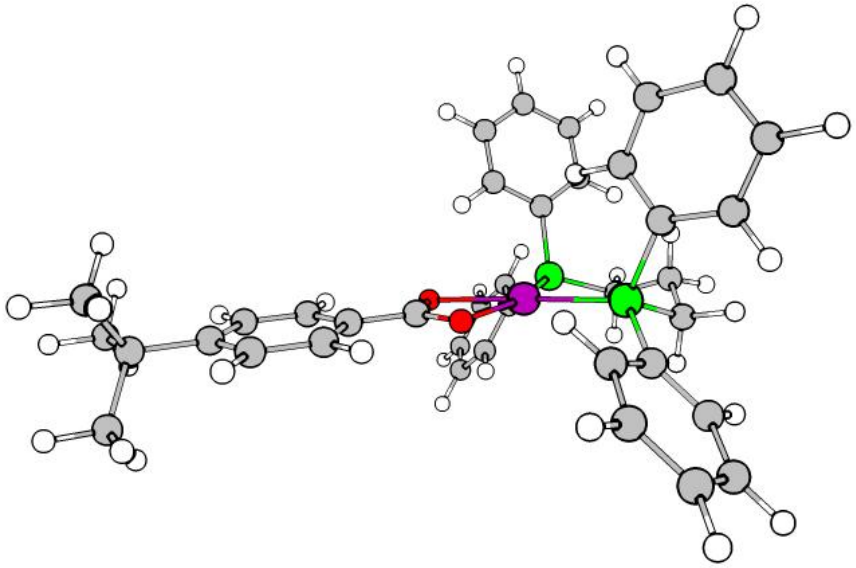
31	6	0	1.257527	0.644105	3.443894
32	6	0	2.576180	2.321415	2.312008
33	6	0	2.141774	0.671124	4.518664
34	1	0	0.420122	-0.051321	3.449802
35	6	0	3.466080	2.339620	3.386213
36	1	0	2.759649	2.960498	1.452225
37	6	0	3.249191	1.519609	4.491924
38	1	0	1.975007	0.014955	5.368714
39	1	0	4.332373	2.995564	3.355108
40	1	0	3.945790	1.533490	5.326090
41	6	0	0.933928	2.454122	-0.342150
42	6	0	1.793594	1.820305	-1.251063
43	6	0	0.671805	3.819892	-0.504737
44	6	0	2.387821	2.540283	-2.284249
45	1	0	1.997042	0.757135	-1.149511
46	6	0	1.255943	4.536240	-1.549018
47	1	0	0.009539	4.344546	0.177288
48	6	0	2.118415	3.899991	-2.439058
49	1	0	3.058211	2.033361	-2.973555
50	1	0	1.035838	5.594468	-1.663537
51	1	0	2.575443	4.459952	-3.250749
52	6	0	1.417292	-1.488863	0.144267
53	6	0	2.626370	-1.251520	0.813709
54	6	0	1.502434	-1.985614	-1.164234
55	6	0	3.849120	-1.430930	0.179211
56	1	0	2.613899	-0.938964	1.853595
57	6	0	2.731979	-2.159630	-1.804518
58	1	0	0.592592	-2.252043	-1.699581
59	6	0	3.935241	-1.876633	-1.150991
60	1	0	4.757585	-1.223035	0.740912
61	1	0	2.734337	-2.535460	-2.823598
62	6	0	-2.362025	2.743842	1.046279
63	1	0	-2.871403	3.606219	1.491576
64	1	0	-2.183543	3.008518	-0.002876
65	1	0	-0.561908	3.498803	2.008892
66	1	0	-1.242043	2.084324	2.772630
67	6	0	0.058613	-2.517352	1.268768
68	8	0	-0.853581	-2.793035	0.464479
69	8	0	0.548393	-2.887563	2.303202
70	6	0	5.302358	-2.054913	-1.811662
71	6	0	6.128702	-3.077634	-1.013374
72	1	0	5.624118	-4.048715	-0.982074
73	1	0	7.110886	-3.217684	-1.479205
74	1	0	6.292578	-2.753118	0.018281
75	6	0	6.040854	-0.705618	-1.825996
76	1	0	5.477920	0.042550	-2.394680
77	1	0	6.192105	-0.312762	-0.816317
78	1	0	7.026444	-0.816561	-2.292580
79	6	0	5.191737	-2.554259	-3.255227
80	1	0	6.193758	-2.659759	-3.684456
81	1	0	4.705229	-3.533471	-3.312939
82	1	0	4.634631	-1.856070	-3.889130

SCF Done: E(RPBE1PBE) = -6989.86689370 A.U. after 1 cycles
Convg = 0.6603D-08 -V/T = 2.0052

Zero-point correction= 0.672576 (Hartree/Particle)
Thermal correction to Energy= 0.723570
Thermal correction to Enthalpy= 0.724625
Thermal correction to Gibbs Free Energy= 0.580121
Sum of electronic and zero-point Energies= -6989.194317
Sum of electronic and thermal Energies= -6989.143323
Sum of electronic and thermal Enthalpies= -6989.142268
Sum of electronic and thermal Free Energies= -6989.286773

	1	2	3
	A	A	A
Frequencies --	-278.7154	16.3166	19.0227

DPPP-Rh-OOC(*p*-*t*-BuPh)-conf2 (23)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.519152	0.039530	-0.394503
2	15	0	-1.942261	-1.664301	-0.557091
3	15	0	-2.168739	1.543267	-0.514907
4	6	0	-3.727762	1.120113	-1.405440
5	6	0	-3.576987	-1.438498	-1.372773
6	1	0	-3.499444	1.054807	-2.475807
7	1	0	-4.444350	1.937071	-1.264587
8	6	0	-1.650961	3.132190	-1.268218
9	6	0	-2.329782	3.751744	-2.323158
10	6	0	-0.499949	3.740894	-0.748753
11	6	0	-1.871593	4.962307	-2.844061
12	1	0	-3.221168	3.301798	-2.750384
13	6	0	-0.050340	4.952241	-1.264536
14	1	0	0.055217	3.254222	0.048494
15	6	0	-0.734100	5.566869	-2.314125
16	1	0	-2.408086	5.431842	-3.664669
17	1	0	0.843349	5.413119	-0.851963
18	1	0	-0.378538	6.510270	-2.720248
19	6	0	-2.821825	2.078909	1.120842
20	6	0	-3.578131	3.250145	1.258111
21	6	0	-2.574026	1.290409	2.248774
22	6	0	-4.086730	3.618707	2.500427
23	1	0	-3.755966	3.889438	0.395765
24	6	0	-3.086516	1.658836	3.492924
25	1	0	-1.968346	0.392174	2.145540
26	6	0	-3.843370	2.821423	3.620370
27	1	0	-4.667130	4.532744	2.597399
28	1	0	-2.886274	1.038575	4.362755
29	1	0	-4.237345	3.112516	4.590771
30	6	0	-1.271343	-3.086942	-1.503435
31	6	0	-0.307160	-2.850269	-2.488936

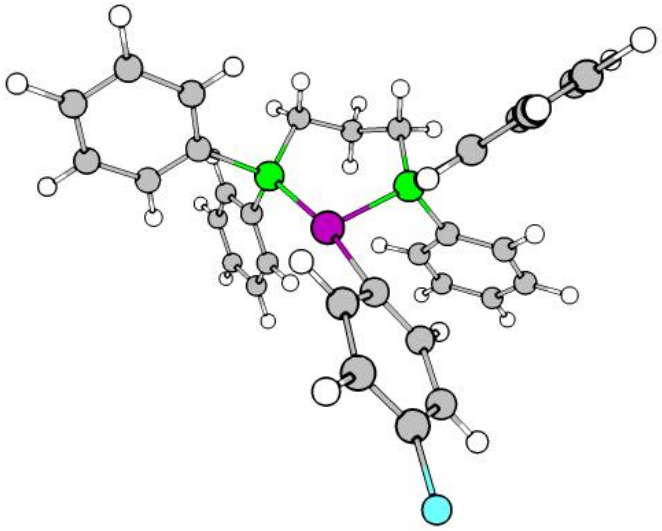
32	6	0	-1.734057	-4.391877	-1.296149
33	6	0	0.173546	-3.901460	-3.268226
34	1	0	0.075808	-1.842244	-2.631131
35	6	0	-1.250622	-5.441202	-2.073947
36	1	0	-2.464590	-4.594408	-0.516124
37	6	0	-0.298067	-5.196918	-3.063657
38	1	0	0.925800	-3.708096	-4.028525
39	1	0	-1.613347	-6.451628	-1.903097
40	1	0	0.081842	-6.017244	-3.667220
41	6	0	-2.320520	-2.404711	1.079584
42	6	0	-1.227631	-2.637482	1.928715
43	6	0	-3.605960	-2.721361	1.529242
44	6	0	-1.419249	-3.188927	3.191410
45	1	0	-0.224865	-2.377528	1.594367
46	6	0	-3.797813	-3.262446	2.801740
47	1	0	-4.473989	-2.548206	0.899125
48	6	0	-2.706602	-3.500756	3.633126
49	1	0	-0.562550	-3.368954	3.835604
50	1	0	-4.803687	-3.497797	3.139991
51	1	0	-2.857065	-3.923919	4.622857
52	6	0	-4.350889	-0.194639	-0.931712
53	1	0	-5.361621	-0.258915	-1.351251
54	1	0	-4.476569	-0.178414	0.157635
55	1	0	-4.179002	-2.343981	-1.235901
56	1	0	-3.358151	-1.379873	-2.445623
57	6	0	1.988486	0.107558	-0.065633
58	8	0	1.340501	1.200371	-0.125492
59	8	0	1.379606	-1.007047	-0.172845
60	6	0	3.461253	0.127005	0.129178
61	6	0	4.181165	-1.064224	0.210729
62	6	0	4.148245	1.340060	0.233711
63	6	0	5.561760	-1.044025	0.397760
64	1	0	3.648077	-2.006911	0.125341
65	6	0	5.524298	1.351509	0.418232
66	1	0	3.588776	2.268738	0.166976
67	6	0	6.265074	0.161410	0.507014
68	1	0	6.087874	-1.991328	0.457880
69	1	0	6.030243	2.310899	0.494791
70	6	0	7.779392	0.220830	0.713747
71	6	0	8.086384	0.964829	2.024665
72	1	0	9.169060	1.013517	2.186812
73	1	0	7.705928	1.990444	2.011183
74	1	0	7.636241	0.451836	2.880841
75	6	0	8.425273	0.973157	-0.462252
76	1	0	9.511809	1.022753	-0.328180
77	1	0	8.221865	0.465563	-1.410865
78	1	0	8.053126	1.998516	-0.544818
79	6	0	8.411632	-1.171682	0.794996
80	1	0	8.015062	-1.752997	1.633993
81	1	0	8.258807	-1.745689	-0.124943
82	1	0	9.492060	-1.074998	0.944788

SCF Done: E(RPBE1PBE) = -6989.92466710 A.U. after 1 cycles
Convg = 0.3939D-08 -V/T = 2.0052
Zero-point correction= 0.675974 (Hartree/Particle)
Thermal correction to Energy= 0.726829
Thermal correction to Enthalpy= 0.727884
Thermal correction to Gibbs Free Energy= 0.581071
Sum of electronic and zero-point Energies= -6989.248693
Sum of electronic and thermal Energies= -6989.197838
Sum of electronic and thermal Enthalpies= -6989.196783
Sum of electronic and thermal Free Energies= -6989.343596

1 2 3

	A	A	A
Frequencies --	8.8184	15.7884	17.7893

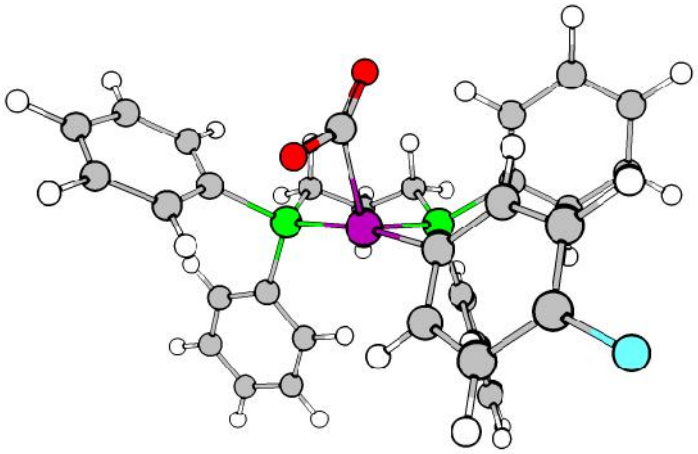
DPPP-Rh-(*p*-FPh) (24)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.101853	-0.571620	0.367563
2	15	0	-1.114599	0.640863	-1.017890
3	15	0	2.188179	0.017039	-0.512064
4	6	0	2.212531	0.799740	-2.182029
5	6	0	-0.259046	1.455925	-2.463799
6	1	0	1.991769	0.026395	-2.925596
7	1	0	3.218096	1.175395	-2.397862
8	6	0	3.370719	-1.381071	-0.676325
9	6	0	3.228179	-2.296159	-1.728989
10	6	0	4.340771	-1.631982	0.302417
11	6	0	4.055198	-3.413255	-1.817118
12	1	0	2.461548	-2.147163	-2.485519
13	6	0	5.162565	-2.754787	0.217895
14	1	0	4.460789	-0.946635	1.137474
15	6	0	5.027196	-3.646368	-0.844234
16	1	0	3.934425	-4.107120	-2.645087
17	1	0	5.911032	-2.930815	0.986304
18	1	0	5.669566	-4.520352	-0.911423
19	6	0	3.132437	1.244244	0.480971
20	6	0	4.391559	1.724573	0.095872
21	6	0	2.560119	1.721137	1.664918
22	6	0	5.059153	2.663849	0.876487
23	1	0	4.864966	1.353539	-0.810486
24	6	0	3.229082	2.660835	2.450454
25	1	0	1.580781	1.349735	1.964605
26	6	0	4.477956	3.134831	2.055600
27	1	0	6.036072	3.027201	0.567884
28	1	0	2.773116	3.019842	3.369473
29	1	0	5.001075	3.867427	2.664696
30	6	0	-2.495237	-0.158398	-1.941672
31	6	0	-2.803681	-1.500156	-1.704919
32	6	0	-3.213527	0.533402	-2.929671
33	6	0	-3.809312	-2.139012	-2.430729
34	1	0	-2.252126	-2.037918	-0.939428

```
     35          6           0       -4.215829   -0.103655   -3.656157
     36          1           0       -3.002851    1.580375   -3.132965
     37          6           0       -4.516432   -1.443729   -3.408306
     38          1           0       -4.038089   -3.182174   -2.228589
     39          1           0       -4.764405    0.448017   -4.415489
     40          1           0       -5.299709   -1.940289   -3.975295
     41          6           0       -1.916823    2.086829   -0.201188
     42          6           0       -3.301917    2.280277   -0.153092
     43          6           0       -1.088268    3.012477    0.450232
     44          6           0       -3.842285    3.383808    0.509154
     45          1           0       -3.970299    1.562467   -0.619610
     46          6           0       -1.626241    4.121738    1.095822
     47          1           0       -0.013277    2.850249    0.476214
     48          6           0       -3.008504    4.312474    1.126683
     49          1           0       -4.921306    3.511847    0.542943
     50          1           0       -0.965716    4.830346    1.589189
     51          1           0       -3.431120    5.172089    1.640204
     52          6           0       -1.517093   -1.241791    1.396406
     53          6           0       -1.431451   -2.628163    1.637085
     54          6           0       -2.473530   -0.529304    2.139192
     55          6           0       -2.230593   -3.275237    2.583465
     56          1           0       -0.722346   -3.237162    1.072631
     57          6           0       -3.287441   -1.152267    3.089376
     58          1           0       -2.590721    0.541957    1.988730
     59          6           0       -3.148775   -2.516572    3.293034
     60          1           0       -2.154293   -4.344219    2.765749
     61          1           0       -4.019035   -0.593685    3.667912
     62          6           0        1.184635    1.928640   -2.289654
     63          1           0        1.435064    2.527565   -3.173504
     64          1           0        1.276534    2.613446   -1.438425
     65          1           0       -0.876040    2.308491   -2.767561
     66          1           0       -0.300811    0.727855   -3.282413
     67          9           0       -3.939611   -3.129956    4.211237
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6743.55479041     A.U. after    1 cycles
             Convg  =    0.2036D-08             -V/T =  2.0048
Zero-point correction=                           0.538565 (Hartree/Particle)
 Thermal correction to Energy=                    0.580631
 Thermal correction to Enthalpy=                  0.581686
 Thermal correction to Gibbs Free Energy=         0.455002
 Sum of electronic and zero-point Energies=          -6743.016226
 Sum of electronic and thermal Energies=             -6742.974160
 Sum of electronic and thermal Enthalpies=           -6742.973105
 Sum of electronic and thermal Free Energies=        -6743.099789
                     1                      2                      3
                     A                      A                      A
 Frequencies --    12.5335               17.0443               23.1148
```

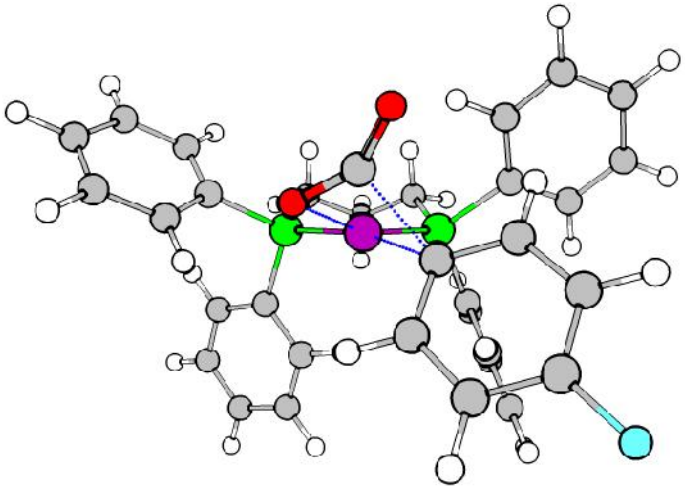
DPPP-Rh-(*p*-FPh)-CO_2 (25)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.068340	-0.711332	0.294580
2	15	0	-1.086411	0.708950	-1.034967
3	15	0	2.223703	0.039521	-0.480577
4	6	0	2.294887	0.729061	-2.186795
5	6	0	-0.204710	1.172804	-2.588019
6	1	0	2.186352	-0.106167	-2.888634
7	1	0	3.279715	1.180672	-2.350799
8	6	0	3.573994	-1.191059	-0.432421
9	6	0	4.400644	-1.480834	-1.522908
10	6	0	3.768416	-1.883468	0.770326
11	6	0	5.410886	-2.435994	-1.408470
12	1	0	4.270012	-0.968575	-2.471401
13	6	0	4.781781	-2.828635	0.885777
14	1	0	3.117872	-1.689004	1.619091
15	6	0	5.606295	-3.108031	-0.204514
16	1	0	6.044661	-2.652832	-2.264362
17	1	0	4.918954	-3.358421	1.824516
18	1	0	6.392877	-3.852806	-0.117231
19	6	0	2.902219	1.424301	0.518977
20	6	0	4.274002	1.707474	0.550455
21	6	0	2.024315	2.238675	1.242696
22	6	0	4.753495	2.788750	1.284613
23	1	0	4.973129	1.072375	0.011464
24	6	0	2.504400	3.325071	1.973634
25	1	0	0.957212	2.027652	1.236253
26	6	0	3.869344	3.601588	1.995684
27	1	0	5.820410	2.995264	1.305779
28	1	0	1.809262	3.949965	2.528178
29	1	0	4.246162	4.443859	2.569954
30	6	0	-2.665548	0.131539	-1.763857
31	6	0	-2.642000	-1.031721	-2.545851
32	6	0	-3.870685	0.819021	-1.595116
33	6	0	-3.805795	-1.486630	-3.160023
34	1	0	-1.723046	-1.605114	-2.647597
35	6	0	-5.035460	0.354218	-2.205459
36	1	0	-3.910124	1.716533	-0.984447
37	6	0	-5.005636	-0.794980	-2.992092
38	1	0	-3.775700	-2.392482	-3.759859
39	1	0	-5.967858	0.894173	-2.062462
40	1	0	-5.914595	-1.155256	-3.466685

```
     41          6           0       -1.517642    2.307215   -0.244592
     42          6           0       -1.953192    2.286671    1.087658
     43          6           0       -1.436549    3.536869   -0.909918
     44          6           0       -2.306887    3.467669    1.736036
     45          1           0       -2.026747    1.338184    1.614255
     46          6           0       -1.777942    4.719204   -0.255336
     47          1           0       -1.109961    3.589105   -1.944170
     48          6           0       -2.215135    4.687859    1.067679
     49          1           0       -2.652178    3.432276    2.765909
     50          1           0       -1.704572    5.666062   -0.783694
     51          1           0       -2.484179    5.610603    1.574820
     52          6           0       -1.640917   -1.299297    1.266144
     53          6           0       -2.752524   -2.015705    0.807800
     54          6           0       -1.564764   -1.042075    2.645651
     55          6           0       -3.752009   -2.457790    1.678703
     56          1           0       -2.853184   -2.252074   -0.247886
     57          6           0       -2.554294   -1.464708    3.536442
     58          1           0       -0.709464   -0.504999    3.059904
     59          6           0       -3.635876   -2.167393    3.028128
     60          1           0       -2.488984   -1.264348    4.602634
     61          6           0        1.199972    1.764039   -2.450764
     62          1           0        1.440325    2.263923   -3.396105
     63          1           0        1.225654    2.548205   -1.684957
     64          1           0       -0.858370    1.852508   -3.145620
     65          1           0       -0.164317    0.252255   -3.181566
     66          6           0        0.260140   -2.563802   -0.522765
     67          8           0        0.808890   -2.885039    0.535734
     68          8           0       -0.076134   -2.966441   -1.610544
     69          9           0       -4.605543   -2.586188    3.879527
     70          1           0       -4.609504   -3.020576    1.319502
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6931.98769121     A.U. after    1 cycles
             Convg  =    0.3233D-08             -V/T =  2.0050
Zero-point correction=                           0.552050 (Hartree/Particle)
 Thermal correction to Energy=                    0.597934
 Thermal correction to Enthalpy=                  0.598989
 Thermal correction to Gibbs Free Energy=         0.464574
 Sum of electronic and zero-point Energies=          -6931.435641
 Sum of electronic and thermal Energies=             -6931.389757
 Sum of electronic and thermal Enthalpies=           -6931.388702
 Sum of electronic and thermal Free Energies=        -6931.523117
                     1                      2                      3
                     A                      A                      A
 Frequencies --    14.0374                21.8634                24.6951
```

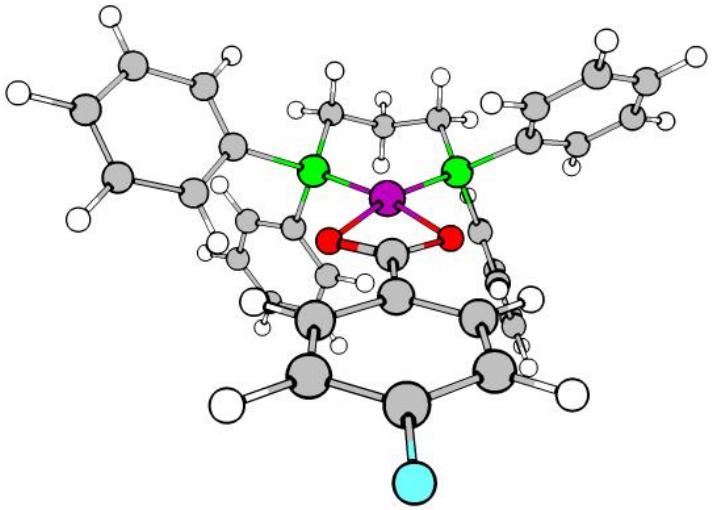
DPPP-Rh-(*p*-FPh)-CO_2-TS2 (26)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.193367	-0.769906	0.198721
2	15	0	-1.019090	0.517905	-1.207608
3	15	0	2.205793	0.110137	-0.578938
4	6	0	2.311744	0.738293	-2.305374
5	6	0	-0.185574	1.033119	-2.772908
6	1	0	2.266654	-0.122041	-2.983031
7	1	0	3.281889	1.227531	-2.447656
8	6	0	3.629211	-1.026638	-0.422248
9	6	0	4.453217	-1.384125	-1.494719
10	6	0	3.885111	-1.570371	0.843584
11	6	0	5.519289	-2.262819	-1.302175
12	1	0	4.278682	-0.983063	-2.488665
13	6	0	4.953180	-2.440239	1.034711
14	1	0	3.241847	-1.316674	1.681538
15	6	0	5.773371	-2.789960	-0.038321
16	1	0	6.151961	-2.532524	-2.143835
17	1	0	5.138642	-2.854772	2.021925
18	1	0	6.604058	-3.474823	0.109912
19	6	0	2.751887	1.576386	0.383499
20	6	0	4.070802	2.044265	0.316660
21	6	0	1.825875	2.257563	1.179680
22	6	0	4.451463	3.178879	1.027180
23	1	0	4.808850	1.511832	-0.279532
24	6	0	2.207087	3.396642	1.888990
25	1	0	0.803824	1.890111	1.246068
26	6	0	3.518854	3.858712	1.813005
27	1	0	5.478507	3.530642	0.973295
28	1	0	1.477475	3.918029	2.503000
29	1	0	3.818684	4.743024	2.369298
30	6	0	-2.488947	-0.289259	-1.953258
31	6	0	-2.338590	-1.597609	-2.431491
32	6	0	-3.718455	0.357541	-2.105952
33	6	0	-3.397829	-2.242002	-3.064714
34	1	0	-1.399241	-2.125519	-2.276579
35	6	0	-4.781128	-0.293946	-2.732337
36	1	0	-3.856478	1.367325	-1.728295
37	6	0	-4.622662	-1.591043	-3.216282
38	1	0	-3.270543	-3.259944	-3.423193
39	1	0	-5.735564	0.215258	-2.838814

```
     40          1           0       -5.453056   -2.097564   -3.701110
     41          6           0       -1.671496    2.081889   -0.498705
     42          6           0       -2.214724    2.038300    0.793389
     43          6           0       -1.646339    3.306413   -1.177207
     44          6           0       -2.733913    3.187620    1.383456
     45          1           0       -2.228881    1.098799    1.340175
     46          6           0       -2.152758    4.459944   -0.579171
     47          1           0       -1.231650    3.379858   -2.178015
     48          6           0       -2.700882    4.403257    0.700300
     49          1           0       -3.158988    3.132695    2.382192
     50          1           0       -2.118989    5.403317   -1.117872
     51          1           0       -3.097652    5.302437    1.164193
     52          6           0       -1.444921   -1.471951    1.384498
     53          6           0       -2.771569   -1.754200    1.028254
     54          6           0       -1.189661   -1.114303    2.720254
     55          6           0       -3.815725   -1.619410    1.938714
     56          1           0       -2.995946   -2.104922    0.025874
     57          6           0       -2.218564   -0.965790    3.650850
     58          1           0       -0.164633   -0.954242    3.048027
     59          6           0       -3.517633   -1.214013    3.233374
     60          1           0       -4.844722   -1.832412    1.662828
     61          1           0       -2.023816   -0.682427    4.681495
     62          6           0        1.179405    1.709518   -2.640548
     63          1           0        1.415911    2.179836   -3.601946
     64          1           0        1.148715    2.523727   -1.906608
     65          1           0       -0.882631    1.662949   -3.336512
     66          1           0       -0.085573    0.110732   -3.357293
     67          6           0       -0.121005   -2.861049    0.700358
     68          8           0        0.954994   -2.549306    1.246904
     69          8           0       -0.695385   -3.795581    0.207876
     70          9           0       -4.526109   -1.078958    4.122733
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6931.97087758     A.U. after    1 cycles
             Convg  =    0.3745D-08             -V/T =  2.0050
Zero-point correction=                           0.551289 (Hartree/Particle)
 Thermal correction to Energy=                    0.596390
 Thermal correction to Enthalpy=                  0.597446
 Thermal correction to Gibbs Free Energy=         0.465825
 Sum of electronic and zero-point Energies=          -6931.419589
 Sum of electronic and thermal Energies=             -6931.374487
 Sum of electronic and thermal Enthalpies=           -6931.373432
 Sum of electronic and thermal Free Energies=        -6931.505052
                     1                      2                      3
                     A                      A                      A
 Frequencies --  -279.9314               17.7389                21.2301
```

DPPP-Rh-OOC(*p*-FPh)-conf2 (27)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.158833	0.037455	-0.274085
2	15	0	-1.240957	-1.654613	-0.650635
3	15	0	-1.447471	1.541042	-0.644583
4	6	0	-2.775878	1.140782	-1.856016
5	6	0	-2.688076	-1.421577	-1.767197
6	1	0	-2.311999	1.057001	-2.845824
7	1	0	-3.488376	1.972721	-1.888526
8	6	0	-0.793164	3.152249	-1.223000
9	6	0	-1.153099	3.741410	-2.439755
10	6	0	0.131552	3.806713	-0.397583
11	6	0	-0.607377	4.967886	-2.819788
12	1	0	-1.862121	3.256685	-3.104571
13	6	0	0.668695	5.032950	-0.775500
14	1	0	0.439321	3.348632	0.538546
15	6	0	0.301210	5.617829	-1.988012
16	1	0	-0.896744	5.414440	-3.767647
17	1	0	1.382519	5.530566	-0.124233
18	1	0	0.724690	6.574058	-2.283919
19	6	0	-2.430435	2.029359	0.832170
20	6	0	-3.268699	3.151818	0.811319
21	6	0	-2.354894	1.256493	1.994393
22	6	0	-4.027494	3.485057	1.929521
23	1	0	-3.318353	3.780248	-0.075553
24	6	0	-3.117012	1.589651	3.114564
25	1	0	-1.689905	0.395861	2.016227
26	6	0	-3.954721	2.701934	3.083265
27	1	0	-4.671041	4.360804	1.904770
28	1	0	-3.049872	0.979877	4.011779
29	1	0	-4.545446	2.965262	3.956926
30	6	0	-0.428543	-3.097735	-1.444290
31	6	0	0.711227	-2.885203	-2.226791
32	6	0	-0.950313	-4.391860	-1.329701
33	6	0	1.310600	-3.949467	-2.898741
34	1	0	1.135315	-1.885947	-2.292196
35	6	0	-0.348742	-5.454242	-1.999977
36	1	0	-1.821784	-4.576246	-0.705572
37	6	0	0.781159	-5.233909	-2.788281
38	1	0	2.198355	-3.774900	-3.501027

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     39          1           0       -0.759036   -6.456129   -1.902342
     40          1           0        1.252194   -6.064376   -3.307919
     41          6           0       -1.925992   -2.371767    0.893734
     42          6           0       -1.010642   -2.631905    1.924946
     43          6           0       -3.280269   -2.646082    1.106526
     44          6           0       -1.441746   -3.167697    3.134106
     45          1           0        0.043783   -2.407229    1.775645
     46          6           0       -3.713395   -3.171531    2.325113
     47          1           0       -4.015569   -2.451651    0.330593
     48          6           0       -2.796574   -3.436428    3.338978
     49          1           0       -0.719976   -3.370019    3.921146
     50          1           0       -4.770299   -3.374143    2.478080
     51          1           0       -3.134659   -3.847800    4.286447
     52          6           0       -3.515292   -0.157571   -1.524352
     53          1           0       -4.403445   -0.210948   -2.164724
     54          1           0       -3.888663   -0.122537   -0.493974
     55          1           0       -3.320358   -2.315836   -1.729297
     56          1           0       -2.262096   -1.394566   -2.777250
     57          6           0        2.610516    0.147181    0.336759
     58          8           0        1.948317    1.224741    0.211704
     59          8           0        2.044962   -0.982524    0.179674
     60          6           0        4.060608    0.206217    0.661829
     61          6           0        4.791791   -0.973287    0.828703
     62          6           0        4.698658    1.442680    0.795364
     63          6           0        6.149255   -0.925779    1.128472
     64          1           0        4.282353   -1.925704    0.719123
     65          6           0        6.055618    1.508277    1.093014
     66          1           0        4.117973    2.349833    0.659334
     67          6           0        6.752938    0.318316    1.254035
     68          1           0        6.738598   -1.827725    1.263212
     69          1           0        6.574224    2.456246    1.199745
     70          9           0        8.069366    0.373258    1.543015
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6932.02815958     A.U. after    1 cycles
             Convg  =    0.6424D-08             -V/T =  2.0050
Zero-point correction=                           0.554255 (Hartree/Particle)
 Thermal correction to Energy=                    0.599409
 Thermal correction to Enthalpy=                  0.600464
 Thermal correction to Gibbs Free Energy=         0.464870
 Sum of electronic and zero-point Energies=          -6931.473905
 Sum of electronic and thermal Energies=             -6931.428750
 Sum of electronic and thermal Enthalpies=           -6931.427695
 Sum of electronic and thermal Free Energies=        -6931.563290
                     1                      2                      3
                     A                      A                      A
 Frequencies --     5.1268                18.4047                19.1167
```
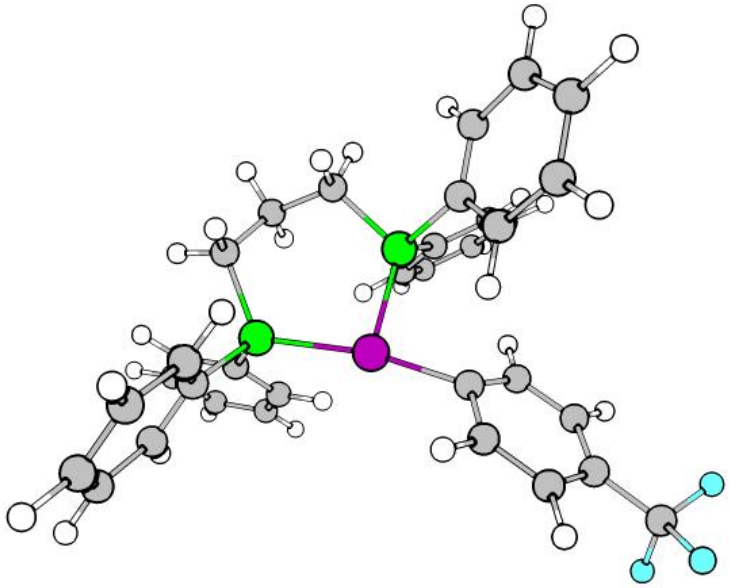
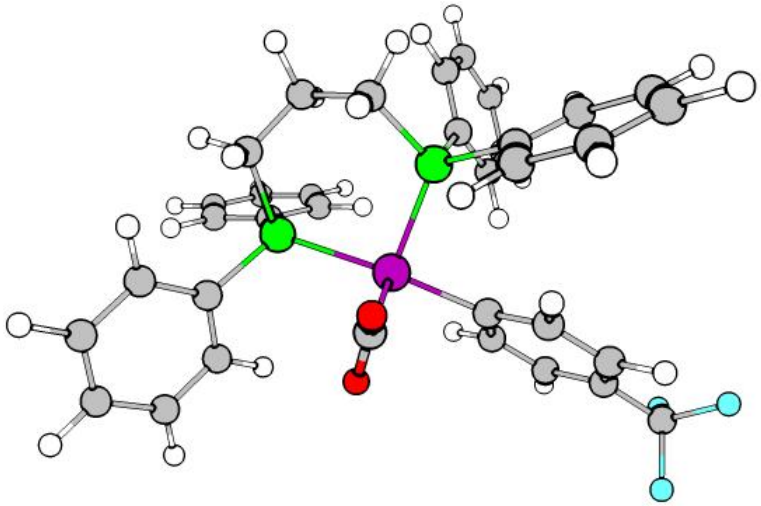

DPPP-Rh-(*p*-CF_3Ph) (28)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.305564	-0.400409	0.127277
2	15	0	0.154322	1.708636	0.601078
3	15	0	-2.642131	-0.221854	0.282795
4	6	0	-3.321299	1.286430	1.100339
5	6	0	-1.242568	2.794567	1.191123
6	1	0	-3.173464	1.174338	2.180228
7	1	0	-4.401742	1.342881	0.933942
8	6	0	-3.419211	-1.588221	1.235192
9	6	0	-3.090132	-1.701611	2.594536
10	6	0	-4.230153	-2.570137	0.655723
11	6	0	-3.589102	-2.749907	3.361922
12	1	0	-2.425027	-0.973455	3.054995
13	6	0	-4.720600	-3.626821	1.423611
14	1	0	-4.480352	-2.518133	-0.400367
15	6	0	-4.408434	-3.717013	2.778006
16	1	0	-3.328190	-2.818557	4.414852
17	1	0	-5.348466	-4.381901	0.957510
18	1	0	-4.792677	-4.540184	3.374446
19	6	0	-3.525675	-0.227682	-1.328034
20	6	0	-4.907111	-0.023940	-1.449036
21	6	0	-2.771387	-0.440106	-2.487705
22	6	0	-5.516966	-0.032570	-2.700748
23	1	0	-5.518984	0.130006	-0.563267
24	6	0	-3.380875	-0.452110	-3.742351
25	1	0	-1.695744	-0.588696	-2.401164
26	6	0	-4.754471	-0.246873	-3.850242
27	1	0	-6.589499	0.125227	-2.779925
28	1	0	-2.780945	-0.620068	-4.632868
29	1	0	-5.232419	-0.253581	-4.826326
30	6	0	1.378206	2.091775	1.924404
31	6	0	2.081796	1.055012	2.543025
32	6	0	1.584108	3.405673	2.374222
33	6	0	2.976659	1.320280	3.579794
34	1	0	1.924937	0.035572	2.202828
35	6	0	2.475128	3.671165	3.410556

```
     36          1           0        1.055889    4.236181    1.913109
     37          6           0        3.175436    2.627456    4.016485
     38          1           0        3.517641    0.500443    4.045119
     39          1           0        2.623759    4.695211    3.743689
     40          1           0        3.871720    2.835038    4.824898
     41          6           0        0.763063    2.652922   -0.861387
     42          6           0        1.972251    3.356473   -0.889198
     43          6           0       -0.022893    2.625233   -2.023218
     44          6           0        2.372899    4.034221   -2.041813
     45          1           0        2.618875    3.367486   -0.016675
     46          6           0        0.368285    3.315752   -3.166361
     47          1           0       -0.935707    2.033808   -2.042563
     48          6           0        1.569954    4.025162   -3.179448
     49          1           0        3.320412    4.567096   -2.046962
     50          1           0       -0.258290    3.285370   -4.054174
     51          1           0        1.883584    4.554499   -4.075335
     52          6           0        1.637332   -0.898784   -0.141448
     53          6           0        1.926810   -2.143938    0.455436
     54          6           0        2.595934   -0.387348   -1.034062
     55          6           0        3.089419   -2.854331    0.163333
     56          1           0        1.230470   -2.578425    1.175811
     57          6           0        3.763992   -1.084828   -1.334428
     58          1           0        2.429735    0.573485   -1.516523
     59          6           0        4.015794   -2.319407   -0.733081
     60          1           0        3.282708   -3.811560    0.641281
     61          1           0        4.483974   -0.665015   -2.033003
     62          6           0       -2.634708    2.560897    0.604978
     63          1           0       -3.256758    3.414697    0.899010
     64          1           0       -2.608309    2.582147   -0.490895
     65          1           0       -0.948062    3.832234    1.001383
     66          1           0       -1.282414    2.669136    2.279602
     67          6           0        5.248359   -3.085134   -1.089015
     68          9           0        6.294595   -2.278412   -1.367627
     69          9           0        5.644359   -3.916070   -0.101976
     70          9           0        5.074585   -3.863536   -2.187608
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6981.18634240     A.U. after    1 cycles
             Convg  =    0.2001D-08             -V/T =  2.0050
Zero-point correction=                           0.551472 (Hartree/Particle)
 Thermal correction to Energy=                    0.596965
 Thermal correction to Enthalpy=                  0.598020
 Thermal correction to Gibbs Free Energy=         0.460961
 Sum of electronic and zero-point Energies=          -6980.634871
 Sum of electronic and thermal Energies=             -6980.589377
 Sum of electronic and thermal Enthalpies=           -6980.588322
 Sum of electronic and thermal Free Energies=        -6980.725382
                    1                      2                      3
                    A                      A                      A
 Frequencies --     9.1798                13.1572                17.2868
```

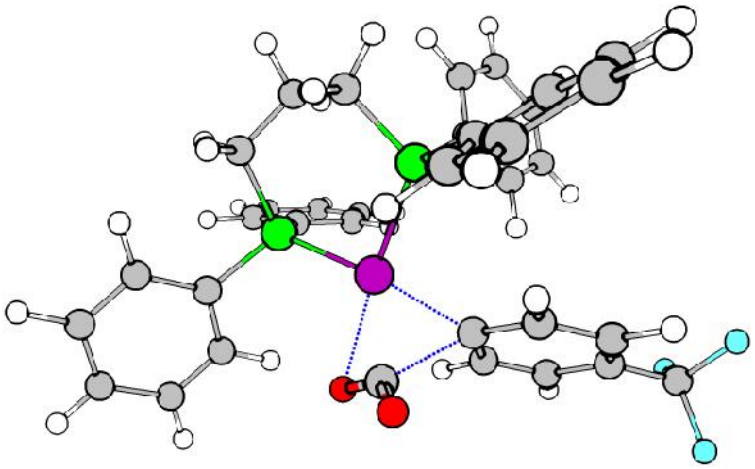
DPPP-Rh-(*p*-CF_3Ph)-CO_2 (29)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.293335	-0.583985	0.154124
2	15	0	0.220984	1.469247	0.961416
3	15	0	-2.674299	-0.203393	0.237787
4	6	0	-3.275984	0.995187	1.498591
5	6	0	-1.075691	2.202462	2.050810
6	1	0	-3.180419	0.519586	2.481622
7	1	0	-4.339110	1.194146	1.322784
8	6	0	-3.718820	-1.682386	0.486291
9	6	0	-4.705918	-1.777530	1.472983
10	6	0	-3.496845	-2.776617	-0.360437
11	6	0	-5.463741	-2.941472	1.602451
12	1	0	-4.897240	-0.950305	2.150037
13	6	0	-4.259431	-3.932708	-0.236240
14	1	0	-2.717780	-2.727536	-1.116748
15	6	0	-5.245344	-4.018619	0.747091
16	1	0	-6.225656	-3.003196	2.375038
17	1	0	-4.074222	-4.773239	-0.899465
18	1	0	-5.835626	-4.925189	0.850251
19	6	0	-3.340776	0.511145	-1.317719
20	6	0	-4.699431	0.414146	-1.645643
21	6	0	-2.480527	1.196514	-2.182337
22	6	0	-5.186321	0.999083	-2.811096
23	1	0	-5.378279	-0.133192	-0.995821
24	6	0	-2.969446	1.785777	-3.348030
25	1	0	-1.421564	1.275451	-1.946486
26	6	0	-4.322441	1.687888	-3.663994
27	1	0	-6.241433	0.913046	-3.057417
28	1	0	-2.289267	2.316547	-4.008891
29	1	0	-4.703925	2.141207	-4.575092
30	6	0	1.660646	1.621001	2.084649
31	6	0	1.677862	0.830283	3.241950
32	6	0	2.710812	2.511883	1.846024
33	6	0	2.725406	0.944940	4.151914
34	1	0	0.891207	0.099607	3.417928
35	6	0	3.762242	2.616102	2.756456
36	1	0	2.717162	3.124937	0.949242
37	6	0	3.769911	1.838105	3.911882
38	1	0	2.730703	0.323940	5.043842

```
     39          1           0        4.576745    3.307970    2.558537
     40          1           0        4.590297    1.921235    4.619880
     41          6           0        0.521494    2.736879   -0.330409
     42          6           0        1.265095    2.366002   -1.459536
     43          6           0        0.045613    4.050714   -0.238044
     44          6           0        1.531959    3.289039   -2.467911
     45          1           0        1.647824    1.351825   -1.543372
     46          6           0        0.301843    4.969450   -1.254416
     47          1           0       -0.525672    4.376817    0.625714
     48          6           0        1.045780    4.592174   -2.370816
     49          1           0        2.119302    2.986662   -3.330858
     50          1           0       -0.079233    5.983681   -1.169586
     51          1           0        1.247126    5.311206   -3.160372
     52          6           0        1.671671   -0.998743   -0.246405
     53          6           0        2.766407   -1.183442    0.606909
     54          6           0        1.870860   -1.260809   -1.614174
     55          6           0        4.005379   -1.600576    0.122418
     56          1           0        2.664838   -1.004346    1.673696
     57          6           0        3.104533   -1.670296   -2.114277
     58          1           0        1.046721   -1.149523   -2.321582
     59          6           0        4.180155   -1.834216   -1.240947
     60          1           0        3.229472   -1.857750   -3.177644
     61          6           0       -2.493032    2.308660    1.484987
     62          1           0       -3.042005    3.025750    2.105973
     63          1           0       -2.483936    2.735595    0.475298
     64          1           0       -0.712958    3.183849    2.375221
     65          1           0       -1.080625    1.579509    2.952755
     66          6           0       -0.335667   -2.013890    1.602155
     67          8           0       -0.527081   -2.814074    0.681760
     68          8           0       -0.220742   -1.902837    2.798238
     69          1           0        4.837887   -1.733784    0.808651
     70          6           0        5.498032   -2.315598   -1.758540
     71          9           0        5.597430   -3.667066   -1.739316
     72          9           0        6.536287   -1.852217   -1.032458
     73          9           0        5.714542   -1.941928   -3.037816
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -7169.61873746     A.U. after    1 cycles
             Convg  =    0.7933D-08             -V/T =  2.0052
Zero-point correction=                           0.565378 (Hartree/Particle)
 Thermal correction to Energy=                    0.614509
 Thermal correction to Enthalpy=                  0.615564
 Thermal correction to Gibbs Free Energy=         0.471786
 Sum of electronic and zero-point Energies=          -7169.053360
 Sum of electronic and thermal Energies=             -7169.004229
 Sum of electronic and thermal Enthalpies=           -7169.003174
 Sum of electronic and thermal Free Energies=        -7169.146952
                     1                      2                      3
                     A                      A                      A
 Frequencies --     4.3006                16.6651                20.8604
```

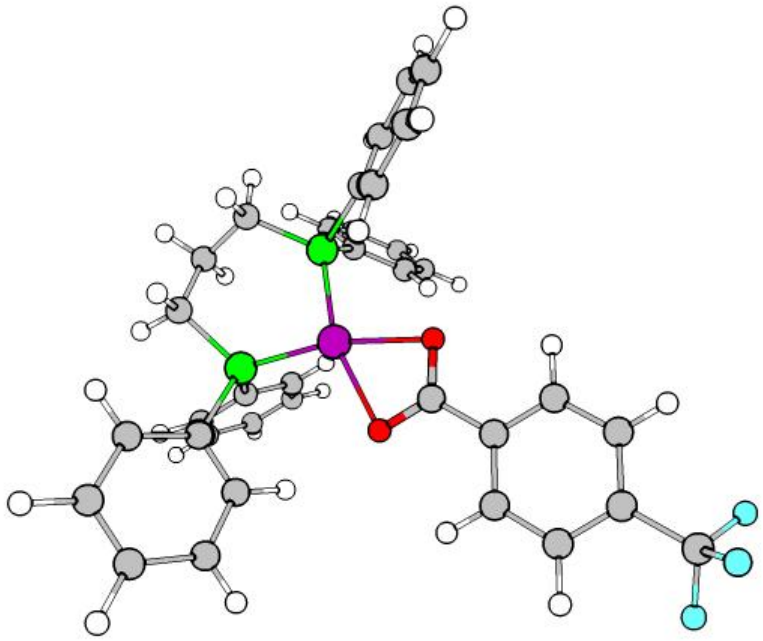
DPPP-Rh-(*p*-CF_3Ph)-CO_2-TS2 (30)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.507226	-0.670828	0.339909
2	15	0	0.221003	1.308800	1.154649
3	15	0	-2.691713	0.104844	0.186934
4	6	0	-3.273700	1.397724	1.358733
5	6	0	-1.005446	2.311795	2.100608
6	1	0	-3.338519	0.945438	2.354900
7	1	0	-4.281561	1.713260	1.066649
8	6	0	-3.946554	-1.218674	0.316754
9	6	0	-4.968726	-1.221424	1.272198
10	6	0	-3.855772	-2.287162	-0.585470
11	6	0	-5.888943	-2.268721	1.316983
12	1	0	-5.064520	-0.411144	1.988782
13	6	0	-4.779195	-3.326065	-0.543788
14	1	0	-3.055963	-2.309301	-1.320504
15	6	0	-5.798536	-3.320637	0.408720
16	1	0	-6.678281	-2.258241	2.064070
17	1	0	-4.695480	-4.148035	-1.249566
18	1	0	-6.515976	-4.136057	0.445430
19	6	0	-3.074442	0.870132	-1.437571
20	6	0	-4.397620	1.096414	-1.838986
21	6	0	-2.029126	1.259697	-2.280566
22	6	0	-4.667494	1.710217	-3.058383
23	1	0	-5.222204	0.777901	-1.204713
24	6	0	-2.300369	1.877110	-3.501774
25	1	0	-1.000063	1.075765	-1.979238
26	6	0	-3.618223	2.103757	-3.891280
27	1	0	-5.697415	1.876590	-3.363277
28	1	0	-1.479359	2.176750	-4.147742
29	1	0	-3.830656	2.580309	-4.844721
30	6	0	1.515801	1.185041	2.449716
31	6	0	1.322029	0.246941	3.472052
32	6	0	2.645550	2.006811	2.478465
33	6	0	2.239419	0.142261	4.513799
34	1	0	0.466556	-0.425222	3.433553
35	6	0	3.568187	1.893542	3.518708
36	1	0	2.816051	2.729396	1.684744
37	6	0	3.365829	0.965703	4.538441
38	1	0	2.083007	-0.595047	5.296602
39	1	0	4.448513	2.531055	3.528090
40	1	0	4.087913	0.877139	5.345850

```
     41          6           0        0.921682    2.473120   -0.080135
     42          6           0        1.756526    1.946930   -1.076399
     43          6           0        0.660263    3.848522   -0.079054
     44          6           0        2.326070    2.778290   -2.037059
     45          1           0        1.960355    0.879527   -1.101553
     46          6           0        1.219603    4.678307   -1.050284
     47          1           0        0.018922    4.292538    0.676217
     48          6           0        2.055976    4.146602   -2.029260
     49          1           0        2.977598    2.353336   -2.796083
     50          1           0        1.000548    5.742770   -1.038113
     51          1           0        2.493560    4.794538   -2.784072
     52          6           0        1.422541   -1.553941   -0.018356
     53          6           0        2.627105   -1.395947    0.681305
     54          6           0        1.494804   -1.856597   -1.389152
     55          6           0        3.853016   -1.455228    0.028930
     56          1           0        2.609169   -1.239574    1.755258
     57          6           0        2.716541   -1.915005   -2.056390
     58          1           0        0.581117   -2.054275   -1.945188
     59          6           0        3.896456   -1.697781   -1.345817
     60          1           0        4.774269   -1.309679    0.586248
     61          1           0        2.749055   -2.129731   -3.121224
     62          6           0       -2.337567    2.605244    1.410584
     63          1           0       -2.842679    3.395783    1.977332
     64          1           0       -2.181543    3.009585    0.403432
     65          1           0       -0.514537    3.238127    2.417987
     66          1           0       -1.184001    1.742856    3.020769
     67          6           0        0.076005   -2.688107    0.941997
     68          8           0       -0.860893   -2.830922    0.131693
     69          8           0        0.568788   -3.202487    1.911081
     70          6           0        5.217370   -1.800514   -2.046199
     71          9           0        6.165153   -1.040323   -1.462893
     72          9           0        5.140485   -1.414876   -3.336730
     73          9           0        5.692630   -3.066647   -2.054175
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -7169.59963045     A.U. after    1 cycles
             Convg  =    0.2722D-08             -V/T =  2.0051
Zero-point correction=                           0.564282 (Hartree/Particle)
 Thermal correction to Energy=                    0.612816
 Thermal correction to Enthalpy=                  0.613871
 Thermal correction to Gibbs Free Energy=         0.471906
 Sum of electronic and zero-point Energies=          -7169.035348
 Sum of electronic and thermal Energies=             -7168.986815
 Sum of electronic and thermal Enthalpies=           -7168.985760
 Sum of electronic and thermal Free Energies=        -7169.127724
                     1                    2                    3
                     A                    A                    A
 Frequencies --  -294.2760               12.5649              15.2575
```

DPPP-Rh-OOC(*p*-CF_3Ph)-conf2 (31)

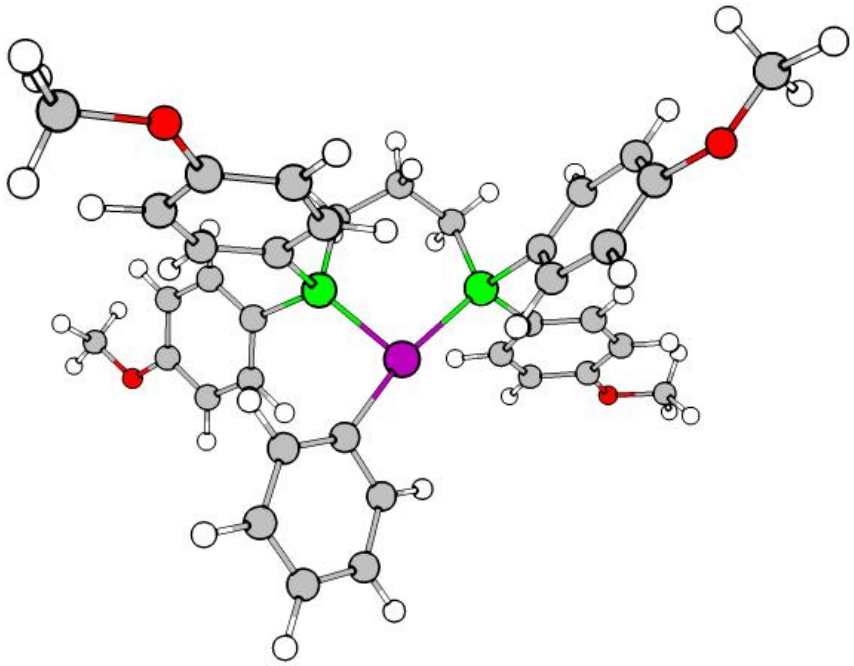


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.499455	0.042368	-0.379387
2	15	0	-1.913511	-1.665241	-0.573641
3	15	0	-2.153207	1.536019	-0.537455
4	6	0	-3.672449	1.109498	-1.491543
5	6	0	-3.520337	-1.448129	-1.444216
6	1	0	-3.398612	1.038527	-2.550737
7	1	0	-4.393991	1.927393	-1.385688
8	6	0	-1.607265	3.129836	-1.258087
9	6	0	-2.209459	3.725349	-2.371385
10	6	0	-0.512420	3.764489	-0.655364
11	6	0	-1.731270	4.938035	-2.868494
12	1	0	-3.056188	3.255283	-2.863008
13	6	0	-0.042301	4.977271	-1.148532
14	1	0	-0.018473	3.298997	0.193233
15	6	0	-0.649669	5.567842	-2.257348
16	1	0	-2.208492	5.389707	-3.734396
17	1	0	0.806655	5.459027	-0.670575
18	1	0	-0.278491	6.512868	-2.645138
19	6	0	-2.868328	2.056673	1.075654
20	6	0	-3.659274	3.208074	1.183285
21	6	0	-2.632835	1.280907	2.214820
22	6	0	-4.213155	3.569859	2.407891
23	1	0	-3.829599	3.837060	0.311863
24	6	0	-3.190247	1.642979	3.441444
25	1	0	-2.003032	0.397105	2.134850
26	6	0	-3.980721	2.785752	3.539495
27	1	0	-4.820555	4.468282	2.482293
28	1	0	-2.999530	1.032914	4.320544
29	1	0	-4.410131	3.071672	4.496262
30	6	0	-1.205123	-3.085904	-1.494217
31	6	0	-0.235337	-2.840668	-2.472336
32	6	0	-1.646208	-4.396933	-1.279145
33	6	0	0.273089	-3.889838	-3.236265

```
     34          1           0        0.129460   -1.826904   -2.621813
     35          6           0       -1.134576   -5.444352   -2.041520
     36          1           0       -2.382568   -4.605284   -0.506285
     37          6           0       -0.176210   -5.191964   -3.023372
     38          1           0        1.028865   -3.689702   -3.991285
     39          1           0       -1.480683   -6.459578   -1.865036
     40          1           0        0.225130   -6.010764   -3.614929
     41          6           0       -2.341850   -2.398388    1.053249
     42          6           0       -1.277099   -2.631572    1.937062
     43          6           0       -3.641684   -2.710893    1.462561
     44          6           0       -1.509752   -3.179596    3.194315
     45          1           0       -0.263540   -2.375507    1.634031
     46          6           0       -3.874979   -3.248303    2.729517
     47          1           0       -4.488981   -2.537995    0.804860
     48          6           0       -2.811238   -3.487308    3.595566
     49          1           0       -0.674377   -3.360675    3.865583
     50          1           0       -4.891578   -3.480732    3.036082
     51          1           0       -2.993952   -3.908127    4.580807
     52          6           0       -4.312791   -0.204182   -1.038268
     53          1           0       -5.305668   -0.271409   -1.497821
     54          1           0       -4.481691   -0.184965    0.045057
     55          1           0       -4.122976   -2.355007   -1.320712
     56          1           0       -3.266131   -1.396584   -2.509501
     57          6           0        2.005080    0.125258   -0.013911
     58          8           0        1.358600    1.215477   -0.069721
     59          8           0        1.412972   -0.993773   -0.132136
     60          6           0        3.483023    0.152135    0.190239
     61          6           0        4.202331   -1.043851    0.250665
     62          6           0        4.148911    1.372372    0.321192
     63          6           0        5.578790   -1.021776    0.442016
     64          1           0        3.669015   -1.983654    0.146743
     65          6           0        5.525690    1.400001    0.512810
     66          1           0        3.574859    2.292364    0.271686
     67          6           0        6.236819    0.201626    0.575317
     68          1           0        6.138114   -1.951296    0.494715
     69          1           0        6.043943    2.348043    0.620873
     70          6           0        7.728888    0.225556    0.735168
     71          9           0        8.182440   -0.835792    1.429552
     72          9           0        8.156245    1.331316    1.373087
     73          9           0        8.361382    0.200917   -0.460239
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -7169.65573953     A.U. after    1 cycles
             Convg  =    0.1497D-08             -V/T =  2.0051
Zero-point correction=                           0.567257 (Hartree/Particle)
 Thermal correction to Energy=                    0.615776
 Thermal correction to Enthalpy=                  0.616831
 Thermal correction to Gibbs Free Energy=         0.472425
 Sum of electronic and zero-point Energies=          -7169.088483
 Sum of electronic and thermal Energies=             -7169.039963
 Sum of electronic and thermal Enthalpies=           -7169.038908
 Sum of electronic and thermal Free Energies=        -7169.183315
                     1                      2                      3
                     A                      A                      A
 Frequencies --     9.3496                10.2189                14.2118
```

(*p*-MeO)dppp-Rh catalyst

(*p*-MeO)DPPP-Rh-Ph (32)

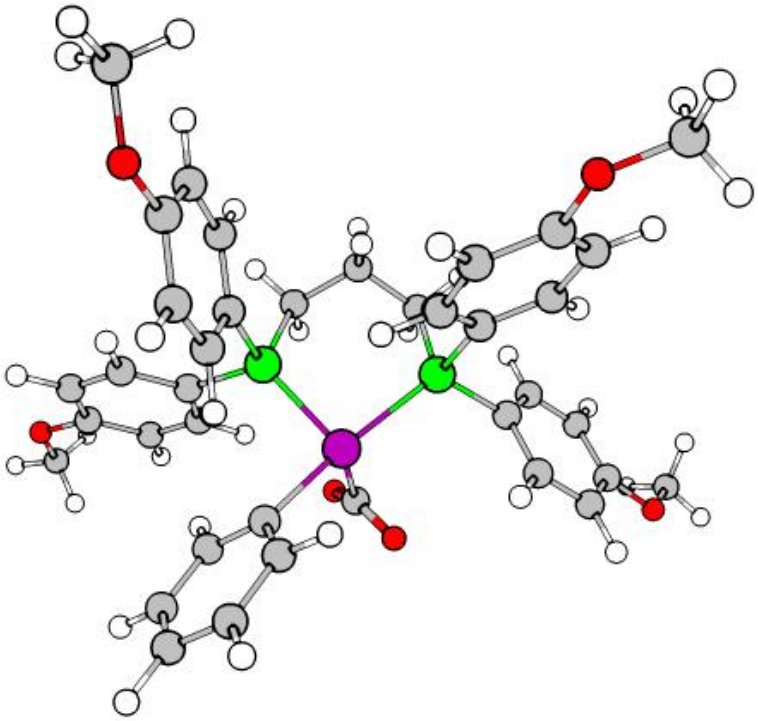


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.093360	-0.514424	0.798517
2	15	0	-1.478684	-0.125033	-0.704492
3	15	0	1.928392	-0.258009	-0.643080
4	6	0	1.575749	-0.307775	-2.453223
5	6	0	-0.977275	-0.060994	-2.499589
6	1	0	1.377362	-1.355317	-2.708132
7	1	0	2.465136	-0.014810	-3.020486
8	6	0	3.247476	-1.525264	-0.476933
9	6	0	2.847323	-2.873190	-0.467423
10	6	0	4.604520	-1.246079	-0.316950
11	6	0	3.771278	-3.896616	-0.336503
12	1	0	1.789974	-3.119960	-0.552127
13	6	0	5.547612	-2.266447	-0.170738
14	1	0	4.948537	-0.215477	-0.292589
15	6	0	5.133251	-3.599754	-0.186748
16	1	0	3.459305	-4.937427	-0.331005
17	1	0	6.592440	-2.003912	-0.042264
18	6	0	2.803396	1.341827	-0.438609
19	6	0	3.686055	1.885114	-1.375864
20	6	0	2.569907	2.073732	0.736796
21	6	0	4.320350	3.109202	-1.163827
22	1	0	3.902229	1.354954	-2.299927
23	6	0	3.195282	3.289025	0.968780
24	1	0	1.872296	1.683796	1.476316
25	6	0	4.076409	3.817948	0.016952
26	1	0	4.995316	3.492819	-1.921723
27	1	0	3.008763	3.851220	1.879528
28	6	0	-2.876195	-1.313985	-0.842902
29	6	0	-3.020987	-2.344280	0.097067
30	6	0	-3.788851	-1.270295	-1.903061
31	6	0	-4.040950	-3.278376	-0.008501

```
     32          1           0       -2.316301   -2.405803    0.921959
     33          6           0       -4.818570   -2.202282   -2.026228
     34          1           0       -3.714723   -0.497481   -2.663927
     35          6           0       -4.949986   -3.214675   -1.070573
     36          1           0       -4.148325   -4.072261    0.725526
     37          1           0       -5.501431   -2.125836   -2.865885
     38          6           0       -2.281232    1.519397   -0.492553
     39          6           0       -3.658519    1.738676   -0.528442
     40          6           0       -1.449349    2.628526   -0.259368
     41          6           0       -4.202462    3.015509   -0.364133
     42          1           0       -4.340470    0.904421   -0.666047
     43          6           0       -1.970951    3.903070   -0.114014
     44          1           0       -0.375179    2.482250   -0.165256
     45          6           0       -3.356429    4.108010   -0.167531
     46          1           0       -5.280714    3.134735   -0.385720
     47          1           0       -1.322047    4.756107    0.064827
     48          6           0       -1.193125   -0.661295    2.348161
     49          6           0       -0.523164   -1.449569    3.303482
     50          6           0       -2.368867   -0.016059    2.763045
     51          6           0       -0.983061   -1.574309    4.617001
     52          1           0        0.389142   -1.991261    3.026419
     53          6           0       -2.837691   -0.136134    4.073355
     54          1           0       -2.925473    0.604935    2.062982
     55          6           0       -2.149538   -0.914577    5.006011
     56          1           0       -0.439467   -2.190518    5.330944
     57          1           0       -3.745231    0.386125    4.371540
     58          1           0       -2.519863   -1.008530    6.024159
     59          6           0        0.377100    0.564151   -2.832802
     60          1           0        0.404102    0.727629   -3.917006
     61          1           0        0.468197    1.560020   -2.381956
     62          1           0       -1.761553    0.482320   -3.037852
     63          1           0       -0.997602   -1.096432   -2.859858
     64          8           0        5.962450   -4.668166   -0.055739
     65          8           0        4.636563    5.014774    0.324328
     66          8           0       -3.774815    5.391130   -0.006100
     67          8           0       -5.913231   -4.171925   -1.092997
     68          6           0        7.344939   -4.413389    0.119960
     69          1           0        7.532714   -3.837463    1.033261
     70          1           0        7.820347   -5.390139    0.207577
     71          1           0        7.766787   -3.882937   -0.741388
     72          6           0        5.530714    5.589307   -0.613350
     73          1           0        5.033420    5.789750   -1.569033
     74          1           0        5.858079    6.531625   -0.174843
     75          1           0        6.402677    4.946818   -0.779724
     76          6           0       -5.169210    5.638163   -0.032727
     77          1           0       -5.685257    5.107689    0.775554
     78          1           0       -5.285902    6.712186    0.111454
     79          1           0       -5.607692    5.353962   -0.996304
     80          6           0       -6.853550   -4.139586   -2.151900
     81          1           0       -7.527686   -4.978271   -1.978984
     82          1           0       -7.429627   -3.207233   -2.147280
     83          1           0       -6.365220   -4.264459   -3.125093
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -7102.04157197     A.U. after    1 cycles
             Convg  =    0.3124D-08             -V/T =  2.0052
Zero-point correction=                           0.678569 (Hartree/Particle)
 Thermal correction to Energy=                    0.732084
 Thermal correction to Enthalpy=                  0.733139
 Thermal correction to Gibbs Free Energy=         0.579962
 Sum of electronic and zero-point Energies=          -7101.363003
 Sum of electronic and thermal Energies=             -7101.309488
 Sum of electronic and thermal Enthalpies=           -7101.308433
 Sum of electronic and thermal Free Energies=        -7101.461610
```

	1	2	3
	A	A	A
Frequencies --	7.6720	12.5698	21.4306

(*p*-MeO)DPPP-Rh-Ph-CO_2 (33)



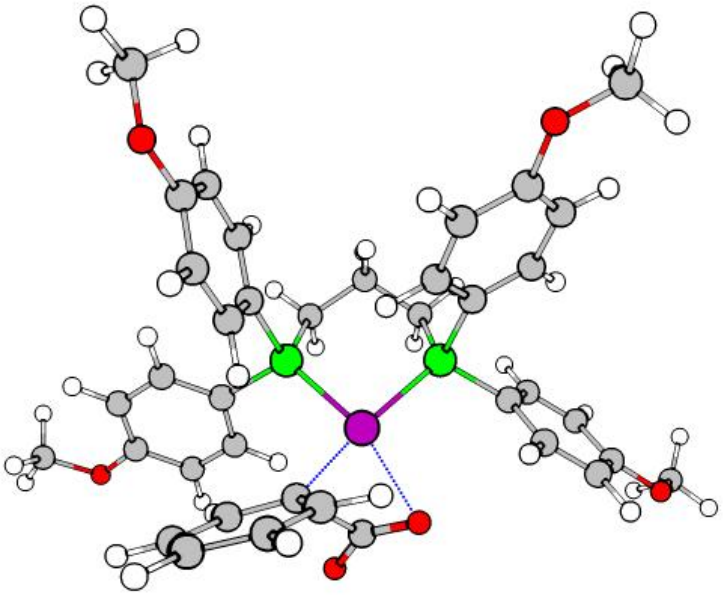
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.014750	-0.794938	0.717592
2	15	0	-1.506587	0.031554	-0.774366
3	15	0	1.905614	-0.292614	-0.654636
4	6	0	1.626422	-0.244050	-2.474554
5	6	0	-0.933113	-0.033486	-2.528309
6	1	0	1.474373	-1.274341	-2.816917
7	1	0	2.526057	0.145790	-2.964396
8	6	0	3.352905	-1.384975	-0.459867
9	6	0	4.013184	-2.004653	-1.520563
10	6	0	3.822183	-1.626954	0.842440
11	6	0	5.116782	-2.834094	-1.308282
12	1	0	3.681078	-1.855462	-2.543723
13	6	0	4.921343	-2.435170	1.067870
14	1	0	3.313276	-1.180936	1.692956
15	6	0	5.578440	-3.048577	-0.008304
16	1	0	5.597797	-3.300167	-2.161606
17	1	0	5.280202	-2.623619	2.075646
18	6	0	2.594227	1.372001	-0.317387
19	6	0	3.908626	1.712191	-0.648809
20	6	0	1.787160	2.355951	0.273141
21	6	0	4.411627	2.990011	-0.413728
22	1	0	4.567995	0.965570	-1.086119
23	6	0	2.270710	3.634021	0.509613
24	1	0	0.761778	2.124659	0.553681
25	6	0	3.588438	3.961234	0.167477

26	1	0	5.440349	3.210105	-0.678962
27	1	0	1.642797	4.393529	0.966988
28	6	0	-3.117648	-0.808897	-0.965835
29	6	0	-3.125784	-2.179939	-1.238868
30	6	0	-4.343586	-0.136029	-0.882365
31	6	0	-4.320288	-2.868672	-1.441147
32	1	0	-2.190823	-2.736732	-1.261100
33	6	0	-5.539163	-0.813126	-1.073650
34	1	0	-4.370721	0.926825	-0.658492
35	6	0	-5.537038	-2.184129	-1.357794
36	1	0	-4.284289	-3.933802	-1.643543
37	1	0	-6.491811	-0.295510	-1.002858
38	6	0	-1.940164	1.785387	-0.490182
39	6	0	-2.168777	2.214935	0.828836
40	6	0	-2.058418	2.728196	-1.513817
41	6	0	-2.503779	3.529613	1.106829
42	1	0	-2.093068	1.503380	1.647700
43	6	0	-2.383703	4.058628	-1.248502
44	1	0	-1.900434	2.445088	-2.550309
45	6	0	-2.608012	4.466518	0.069373
46	1	0	-2.686647	3.855026	2.127118
47	1	0	-2.458548	4.757405	-2.074876
48	6	0	-1.458410	-1.034902	2.151927
49	6	0	-2.606732	-1.832637	2.205250
50	6	0	-1.103472	-0.332238	3.317100
51	6	0	-3.372722	-1.921924	3.370907
52	1	0	-2.915641	-2.403187	1.333457
53	6	0	-1.868692	-0.408967	4.482778
54	1	0	-0.205524	0.290219	3.332069
55	6	0	-3.012671	-1.206895	4.512267
56	1	0	-1.567227	0.148217	5.367721
57	6	0	0.416070	0.607300	-2.858939
58	1	0	0.450701	0.762284	-3.943644
59	1	0	0.498165	1.605319	-2.412201
60	1	0	-1.728858	0.397985	-3.145859
61	1	0	-0.911594	-1.099940	-2.781388
62	6	0	0.211514	-2.802039	0.546145
63	8	0	0.958006	-2.733581	1.528946
64	8	0	-0.257036	-3.570163	-0.262866
65	1	0	-4.257827	-2.555075	3.384854
66	8	0	3.975646	5.232298	0.440860
67	8	0	6.641435	-3.828441	0.313393
68	8	0	-2.927140	5.730252	0.439778
69	8	0	-6.755699	-2.757585	-1.530061
70	6	0	7.309743	-4.502961	-0.738233
71	1	0	8.107523	-5.076032	-0.266291
72	1	0	6.635802	-5.188173	-1.264508
73	1	0	7.747614	-3.796285	-1.452553
74	6	0	5.308546	5.602002	0.129879
75	1	0	6.031338	4.995441	0.686778
76	1	0	5.506617	5.516886	-0.944528
77	1	0	5.406849	6.644513	0.431391
78	6	0	-3.044273	6.711579	-0.577301
79	1	0	-3.301482	7.639636	-0.067676
80	1	0	-2.098339	6.844184	-1.114038
81	1	0	-3.839158	6.457109	-1.287156
82	6	0	-6.800442	-4.150949	-1.786918
83	1	0	-7.856501	-4.403757	-1.879206
84	1	0	-6.286241	-4.402225	-2.721468
85	1	0	-6.362607	-4.723239	-0.961554
86	1	0	-3.612509	-1.274640	5.416734

SCF Done: E(RPBE1PBE) = -7290.47615437   A.U. after   1 cycles

```
            Convg  =    0.6163D-08             -V/T =  2.0054
Zero-point correction=                           0.692199 (Hartree/Particle)
 Thermal correction to Energy=                    0.749473
 Thermal correction to Enthalpy=                  0.750528
 Thermal correction to Gibbs Free Energy=         0.590574
 Sum of electronic and zero-point Energies=          -7289.783955
 Sum of electronic and thermal Energies=             -7289.726681
 Sum of electronic and thermal Enthalpies=           -7289.725626
 Sum of electronic and thermal Free Energies=        -7289.885580
                    1                      2                      3
                    A                      A                      A
 Frequencies --    12.9859               15.4921                24.0675
```

(*p*-MeO)DPPP-Rh-Ph-CO_2-TS2 (34)

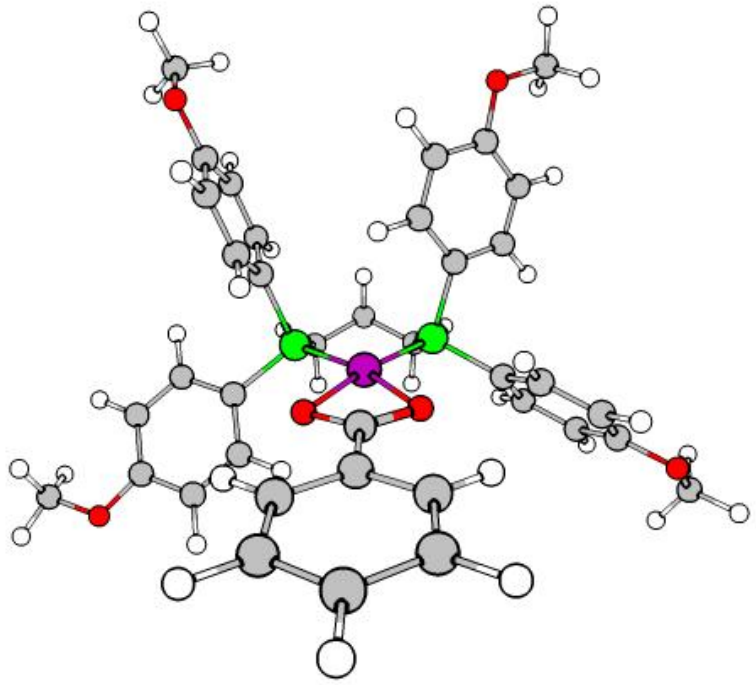


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.136703	-0.902088	0.596116
2	15	0	-1.400748	-0.137191	-0.873404
3	15	0	1.909065	-0.250706	-0.773174
4	6	0	1.665096	-0.187659	-2.597380
5	6	0	-0.891521	-0.119566	-2.649188
6	1	0	1.580296	-1.216653	-2.965949
7	1	0	2.551453	0.263557	-3.058043
8	6	0	3.424878	-1.242536	-0.562003
9	6	0	4.111372	-1.849482	-1.613538
10	6	0	3.925697	-1.409359	0.740355
11	6	0	5.271585	-2.594925	-1.392233
12	1	0	3.757933	-1.753763	-2.635919
13	6	0	5.079159	-2.135916	0.973302
14	1	0	3.399273	-0.969265	1.582519
15	6	0	5.762742	-2.737152	-0.092971
16	1	0	5.773751	-3.052217	-2.238175
17	1	0	5.463602	-2.266628	1.980834
18	6	0	2.475231	1.452690	-0.404589
19	6	0	3.729651	1.916559	-0.808460
20	6	0	1.632857	2.334138	0.287972
21	6	0	4.140224	3.221781	-0.546125

22	1	0	4.415688	1.247465	-1.323834
23	6	0	2.024896	3.637704	0.553702
24	1	0	0.658205	1.989383	0.626986
25	6	0	3.282260	4.091460	0.137422
26	1	0	5.125482	3.541640	-0.868567
27	1	0	1.372113	4.319949	1.091071
28	6	0	-2.910372	-1.158940	-1.040854
29	6	0	-2.769619	-2.555395	-1.082012
30	6	0	-4.185799	-0.615536	-1.184103
31	6	0	-3.868291	-3.375614	-1.276671
32	1	0	-1.790413	-3.003791	-0.924571
33	6	0	-5.303771	-1.430635	-1.372306
34	1	0	-4.326654	0.461533	-1.139392
35	6	0	-5.146309	-2.817870	-1.424846
36	1	0	-3.762689	-4.456613	-1.296613
37	1	0	-6.281367	-0.970785	-1.471328
38	6	0	-2.024556	1.556735	-0.562876
39	6	0	-2.293846	1.931871	0.765393
40	6	0	-2.236642	2.507033	-1.563619
41	6	0	-2.765453	3.196893	1.071652
42	1	0	-2.126891	1.221058	1.570726
43	6	0	-2.698918	3.791144	-1.269547
44	1	0	-2.042691	2.269146	-2.605400
45	6	0	-2.968153	4.141333	0.055674
46	1	0	-2.975636	3.479699	2.099377
47	1	0	-2.839836	4.498651	-2.079843
48	6	0	-1.203719	-1.202803	2.238820
49	6	0	-2.555633	-1.572577	2.257654
50	6	0	-0.715156	-0.438673	3.312987
51	6	0	-3.406106	-1.132760	3.269545
52	1	0	-2.944558	-2.226800	1.483272
53	6	0	-1.563370	0.010919	4.326353
54	1	0	0.345115	-0.197323	3.361388
55	6	0	-2.916104	-0.327512	4.300306
56	1	0	-4.454050	-1.423978	3.258826
57	1	0	-1.165530	0.612071	5.140955
58	6	0	0.414208	0.598653	-2.989520
59	1	0	0.441872	0.753181	-4.074520
60	1	0	0.441160	1.599193	-2.541519
61	1	0	-1.724690	0.284419	-3.235102
62	1	0	-0.819432	-1.176591	-2.932066
63	6	0	0.039892	-2.729395	1.746819
64	8	0	1.184364	-2.280558	1.963879
65	8	0	-0.561236	-3.770650	1.675711
66	1	0	-3.580759	0.013746	5.090362
67	8	0	3.581472	5.378936	0.445151
68	8	0	-3.419071	5.356022	0.455462
69	8	0	-6.161170	-3.701773	-1.604319
70	8	0	6.880665	-3.432952	0.236407
71	6	0	7.585184	-4.084367	-0.805796
72	1	0	8.426748	-4.586725	-0.329356
73	1	0	6.957084	-4.829170	-1.307264
74	1	0	7.963852	-3.366509	-1.542491
75	6	0	4.850131	5.877305	0.056480
76	1	0	4.972970	5.853104	-1.032208
77	1	0	4.881594	6.911656	0.398045
78	1	0	5.662745	5.316071	0.531058
79	6	0	-3.625541	6.346397	-0.537295
80	1	0	-3.979018	7.230729	-0.007778
81	1	0	-2.693486	6.587264	-1.060658
82	1	0	-4.384786	6.032765	-1.262493
83	6	0	-7.474296	-3.185361	-1.732478
84	1	0	-8.124590	-4.050871	-1.857598

```
     85          1           0       -7.776339   -2.633823   -0.834998
     86          1           0       -7.565421   -2.536069   -2.610759
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -7290.45849076     A.U. after    1 cycles
             Convg  =    0.7576D-08             -V/T =  2.0054
Zero-point correction=                           0.691794 (Hartree/Particle)
 Thermal correction to Energy=                    0.748222
 Thermal correction to Enthalpy=                  0.749277
 Thermal correction to Gibbs Free Energy=         0.591915
 Sum of electronic and zero-point Energies=          -7289.766697
 Sum of electronic and thermal Energies=             -7289.710268
 Sum of electronic and thermal Enthalpies=           -7289.709213
 Sum of electronic and thermal Free Energies=        -7289.866575
                    1                      2                      3
                    A                      A                      A
 Frequencies --  -286.7625               12.8214                16.7992
```

(*p*-MeO)DPPP-Rh-OOCPh-conf2 (35)



```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         45           0       -0.015228   -0.708770   -0.023625
      2         15           0       -1.526121    0.521743   -1.101779
      3         15           0        1.682665    0.329660   -1.041589
      4          6           0        1.431116    1.011780   -2.736989
      5          6           0       -1.121502    1.243045   -2.747592
      6          1           0        1.293589    0.169414   -3.425380
      7          1           0        2.339827    1.546430   -3.036661
      8          6           0        3.167016   -0.723435   -1.220525
      9          6           0        3.834288   -0.935558   -2.426966
     10          6           0        3.657013   -1.366927   -0.070619
     11          6           0        4.963460   -1.754790   -2.502680
     12          1           0        3.488302   -0.464876   -3.342617
     13          6           0        4.779676   -2.173451   -0.129404
```

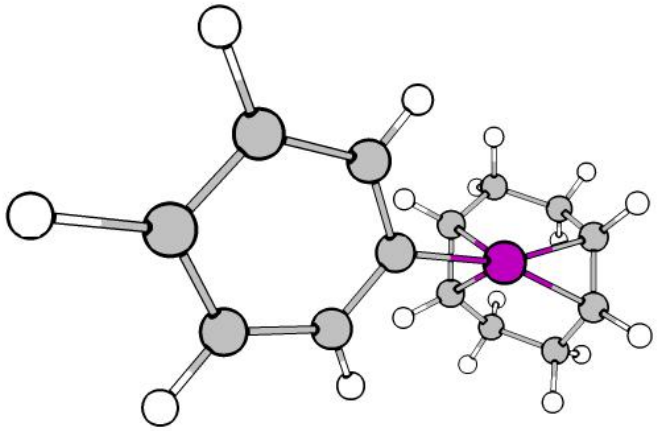
14	1	0	3.141124	-1.245774	0.877874
15	6	0	5.442943	-2.375832	-1.347941
16	1	0	5.450146	-1.894469	-3.462177
17	1	0	5.156836	-2.671915	0.759246
18	6	0	2.332931	1.797028	-0.150646
19	6	0	3.594953	2.328006	-0.428737
20	6	0	1.546979	2.430416	0.822424
21	6	0	4.067654	3.463648	0.226393
22	1	0	4.239984	1.843681	-1.159287
23	6	0	2.000889	3.564357	1.480031
24	1	0	0.569850	2.019998	1.067706
25	6	0	3.264626	4.089917	1.186253
26	1	0	5.057020	3.839818	-0.011852
27	1	0	1.392525	4.053849	2.235500
28	6	0	-3.056862	-0.407455	-1.481725
29	6	0	-2.988882	-1.795349	-1.672454
30	6	0	-4.292710	0.223498	-1.633072
31	6	0	-4.116474	-2.521289	-2.022767
32	1	0	-2.041035	-2.308536	-1.527378
33	6	0	-5.436510	-0.493990	-1.981336
34	1	0	-4.380615	1.294760	-1.466022
35	6	0	-5.349055	-1.875246	-2.181625
36	1	0	-4.068498	-3.597351	-2.164806
37	1	0	-6.380160	0.031478	-2.083348
38	6	0	-2.130628	1.931233	-0.102219
39	6	0	-2.468430	1.664085	1.237318
40	6	0	-2.251532	3.242600	-0.559389
41	6	0	-2.922014	2.668274	2.073864
42	1	0	-2.366708	0.651702	1.623314
43	6	0	-2.695912	4.270542	0.277133
44	1	0	-1.995328	3.498699	-1.583867
45	6	0	-3.036818	3.984061	1.599993
46	1	0	-3.186245	2.460103	3.106957
47	1	0	-2.767098	5.278365	-0.117812
48	6	0	0.229893	1.954560	-2.830973
49	1	0	0.281201	2.472116	-3.796194
50	1	0	0.308500	2.734864	-2.064435
51	1	0	-1.935199	1.907997	-3.059487
52	1	0	-1.138903	0.395427	-3.443046
53	6	0	-0.261817	-2.516123	1.733953
54	8	0	0.903797	-2.166326	1.368378
55	8	0	-1.291118	-1.964846	1.225887
56	6	0	-0.430166	-3.580021	2.762688
57	6	0	-1.711317	-3.964660	3.169131
58	6	0	0.691577	-4.197411	3.323440
59	6	0	-1.868621	-4.958391	4.131577
60	1	0	-2.571300	-3.476460	2.720378
61	6	0	0.532957	-5.191205	4.285546
62	1	0	1.678945	-3.888471	2.993438
63	6	0	-0.747058	-5.572447	4.691096
64	1	0	-2.865360	-5.256289	4.446692
65	1	0	1.406153	-5.670536	4.720575
66	1	0	-0.870494	-6.348411	5.442441
67	8	0	3.624576	5.198520	1.883590
68	8	0	-3.481508	4.899996	2.497810
69	8	0	6.530765	-3.188181	-1.304171
70	8	0	-6.396908	-2.669813	-2.521583
71	6	0	7.213904	-3.443662	-2.518215
72	1	0	8.034497	-4.114508	-2.264511
73	1	0	6.560628	-3.933559	-3.249186
74	1	0	7.622054	-2.522541	-2.949857
75	6	0	4.907636	5.747872	1.640055
76	1	0	5.012224	6.075967	0.599512

77	1	0	4.992634	6.612135	2.298512
78	1	0	5.701357	5.031780	1.880810
79	6	0	-3.605651	6.243851	2.066582
80	1	0	-4.327519	6.335603	1.247007
81	1	0	-3.969354	6.802085	2.928941
82	1	0	-2.639182	6.654266	1.752770
83	6	0	-7.666245	-2.060858	-2.679004
84	1	0	-8.352382	-2.864500	-2.945663
85	1	0	-8.004000	-1.592807	-1.747502
86	1	0	-7.655589	-1.314755	-3.481809

```
SCF Done:  E(RPBE1PBE) =  -7290.51568515     A.U. after    1 cycles
             Convg  =    0.2873D-08             -V/T =  2.0053
Zero-point correction=                           0.694696 (Hartree/Particle)
 Thermal correction to Energy=                    0.751181
 Thermal correction to Enthalpy=                  0.752237
 Thermal correction to Gibbs Free Energy=         0.591654
 Sum of electronic and zero-point Energies=          -7289.820989
 Sum of electronic and thermal Energies=             -7289.764504
 Sum of electronic and thermal Enthalpies=           -7289.763449
 Sum of electronic and thermal Free Energies=        -7289.924031
                    1                    2                    3
                    A                    A                    A
 Frequencies --     9.0405              14.8139              16.2014
```

COD-Rh catalyst

COD-Rh-Ph (36)

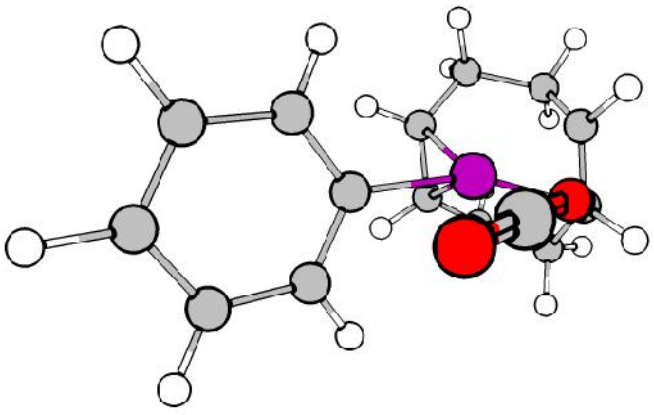


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.229064	-0.053563	-0.562665
2	6	0	0.872052	0.778126	1.249558
3	1	0	0.063346	1.374726	1.672592
4	6	0	2.209869	1.495209	1.130151
5	1	0	2.127843	2.480992	1.599302
6	1	0	2.967665	0.956516	1.707924
7	6	0	2.670879	1.686849	-0.326231
8	1	0	2.230606	2.611442	-0.713839
9	1	0	3.760506	1.833151	-0.360517
10	6	0	2.259167	0.570534	-1.258973
11	1	0	2.095809	0.865758	-2.297757
12	6	0	2.338710	-0.781521	-0.991648
13	1	0	2.207447	-1.466355	-1.830754
14	6	0	2.921078	-1.369120	0.276400

15	1	0	3.425488	-2.310534	0.034668
16	1	0	3.699798	-0.705465	0.661818
17	6	0	1.858998	-1.637549	1.357891
18	1	0	1.411156	-2.621994	1.182140
19	1	0	2.337767	-1.697248	2.347419
20	6	0	0.732473	-0.631196	1.382263
21	1	0	-0.160456	-0.979502	1.902634
22	6	0	-1.728190	0.012117	-0.078823
23	6	0	-2.417366	1.198773	0.226346
24	6	0	-2.497624	-1.156426	-0.229246
25	6	0	-3.809852	1.225268	0.342413
26	1	0	-1.865196	2.127241	0.367034
27	6	0	-3.889182	-1.137719	-0.110866
28	1	0	-2.007327	-2.107115	-0.442492
29	6	0	-4.552273	0.056540	0.174398
30	1	0	-4.316352	2.161693	0.568713
31	1	0	-4.456592	-2.058107	-0.235500
32	1	0	-5.635151	0.074255	0.270908

```
SCF Done:  E(RPBE1PBE) =  -5230.34248824     A.U. after    1 cycles
             Convg  =    0.6266D-08             -V/T =  2.0033
Zero-point correction=                           0.273993 (Hartree/Particle)
 Thermal correction to Energy=                    0.290944
 Thermal correction to Enthalpy=                  0.292000
 Thermal correction to Gibbs Free Energy=         0.225735
 Sum of electronic and zero-point Energies=          -5230.068495
 Sum of electronic and thermal Energies=             -5230.051544
 Sum of electronic and thermal Enthalpies=           -5230.050489
 Sum of electronic and thermal Free Energies=        -5230.116753
                     1                      2                      3
                     A                      A                      A
 Frequencies --    25.0591                52.5227                60.8183
```

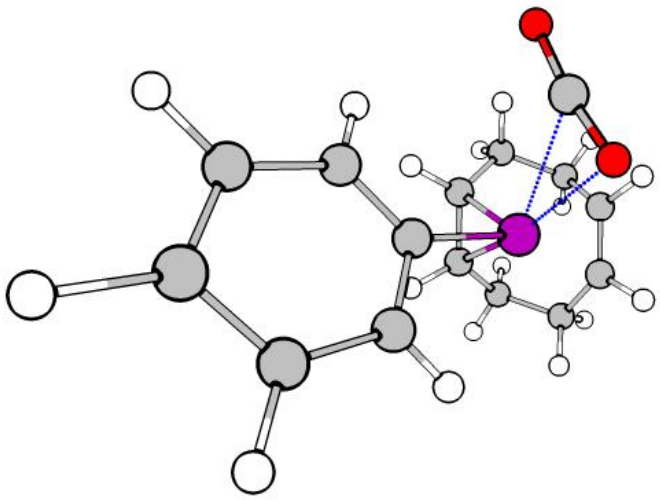
COD-Rh-Ph-O=C=O (37)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.454197	-1.172030	1.630279
2	6	0	1.853135	-0.195891	2.562593
3	6	0	2.000080	-2.459742	1.786364
4	6	0	2.733972	-0.491982	3.606328
5	1	0	1.471839	0.821713	2.477367
6	6	0	2.882486	-2.763066	2.826684
7	1	0	1.736023	-3.248591	1.081891
8	6	0	3.252371	-1.779620	3.744078

```
      9          1           0        3.018108    0.286353    4.312178
     10          1           0        3.283834   -3.770562    2.919696
     11          1           0        3.939353   -2.012866    4.553908
     12          6           0       -1.226451   -1.925916    3.091731
     13          8           0       -0.925537   -2.327180    4.138711
     14          8           0       -1.571290   -1.526590    2.042504
     15         45           0       -0.006713   -0.773214    0.276538
     16          6           0       -1.497084   -0.888284   -1.441416
     17          1           0       -2.177268   -1.681891   -1.130410
     18          6           0       -0.742599   -1.113121   -2.734135
     19          1           0       -1.258281   -1.881436   -3.319819
     20          1           0       -0.777126   -0.204215   -3.340438
     21          6           0        0.713584   -1.554338   -2.508209
     22          1           0        0.738668   -2.640255   -2.364115
     23          1           0        1.311488   -1.355968   -3.411008
     24          6           0        1.368466   -0.926433   -1.300192
     25          1           0        2.251107   -1.460268   -0.945961
     26          6           0        1.254524    0.429028   -0.902283
     27          1           0        2.054036    0.806046   -0.264303
     28          6           0        0.493603    1.490705   -1.683751
     29          1           0        0.989081    2.457047   -1.544715
     30          1           0        0.559979    1.276487   -2.755158
     31          6           0       -0.976134    1.629626   -1.248151
     32          1           0       -1.026038    2.318452   -0.398348
     33          1           0       -1.565223    2.097507   -2.050855
     34          6           0       -1.617173    0.332861   -0.810161
     35          1           0       -2.402557    0.430612   -0.058451
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5418.76103336     A.U. after    1 cycles
             Convg  =    0.2806D-08             -V/T =  2.0036
Zero-point correction=                           0.286658 (Hartree/Particle)
 Thermal correction to Energy=                    0.308515
 Thermal correction to Enthalpy=                  0.309570
 Thermal correction to Gibbs Free Energy=         0.229392
 Sum of electronic and zero-point Energies=          -5418.474376
 Sum of electronic and thermal Energies=             -5418.452518
 Sum of electronic and thermal Enthalpies=           -5418.451463
 Sum of electronic and thermal Free Energies=        -5418.531641
                     1                      2                      3
                     A                      A                      A
 Frequencies --    16.7076                32.1512                41.9985
```

COD-Rh-Ph-O=C=O-TS1 (38)

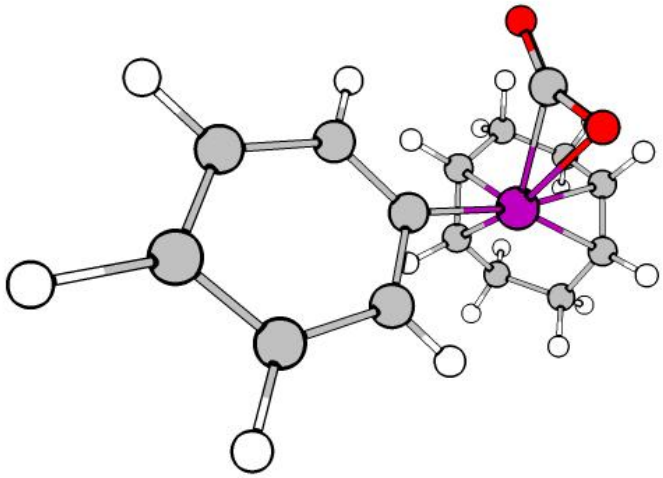


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.665727	-0.316956	0.062254
2	6	0	2.336404	-1.191629	-0.811811
3	6	0	2.431247	0.302485	1.061901
4	6	0	3.705963	-1.435675	-0.696795
5	1	0	1.785045	-1.701447	-1.604086
6	6	0	3.805039	0.068716	1.178261
7	1	0	1.963612	0.995119	1.759947
8	6	0	4.448111	-0.803607	0.302186
9	1	0	4.194352	-2.121037	-1.386747
10	1	0	4.373254	0.572392	1.957868
11	1	0	5.515222	-0.989905	0.395243
12	6	0	0.485579	2.429457	-0.668011
13	8	0	0.601142	3.127369	0.262262
14	8	0	0.410034	1.892097	-1.719701
15	45	0	-0.289356	-0.030794	-0.394791
16	6	0	-2.471671	0.702703	-0.590852
17	1	0	-2.378159	1.639095	-1.141102
18	6	0	-3.080509	0.788768	0.791471
19	1	0	-3.637654	1.727594	0.874941
20	1	0	-3.818879	-0.007514	0.915728
21	6	0	-2.031649	0.734131	1.915648
22	1	0	-1.632218	1.740550	2.081498
23	1	0	-2.511335	0.439473	2.861357
24	6	0	-0.859514	-0.171997	1.626982
25	1	0	0.012019	0.022662	2.251275
26	6	0	-0.921564	-1.452725	1.024363
27	1	0	-0.082115	-2.116250	1.231889
28	6	0	-2.213401	-2.148617	0.617570
29	1	0	-2.082409	-3.229670	0.728962
30	1	0	-3.013135	-1.875286	1.312588
31	6	0	-2.631403	-1.858151	-0.834156
32	1	0	-2.109141	-2.556498	-1.496454
33	1	0	-3.703805	-2.063285	-0.966771
34	6	0	-2.306396	-0.460924	-1.307838
35	1	0	-2.114833	-0.361870	-2.378071

SCF Done: E(RPBE1PBE) = -5418.75781384 A.U. after 1 cycles
Convg = 0.2253D-08 -V/T = 2.0036
Zero-point correction= 0.286368 (Hartree/Particle)
Thermal correction to Energy= 0.307179
Thermal correction to Enthalpy= 0.308234
Thermal correction to Gibbs Free Energy= 0.232176
Sum of electronic and zero-point Energies= -5418.471446
Sum of electronic and thermal Energies= -5418.450635
Sum of electronic and thermal Enthalpies= -5418.449580
Sum of electronic and thermal Free Energies= -5418.525637

	1	2	3
	A	A	A
Frequencies --	-78.4589	26.4537	32.5867

COD-Rh-Ph-CO_2 (39)

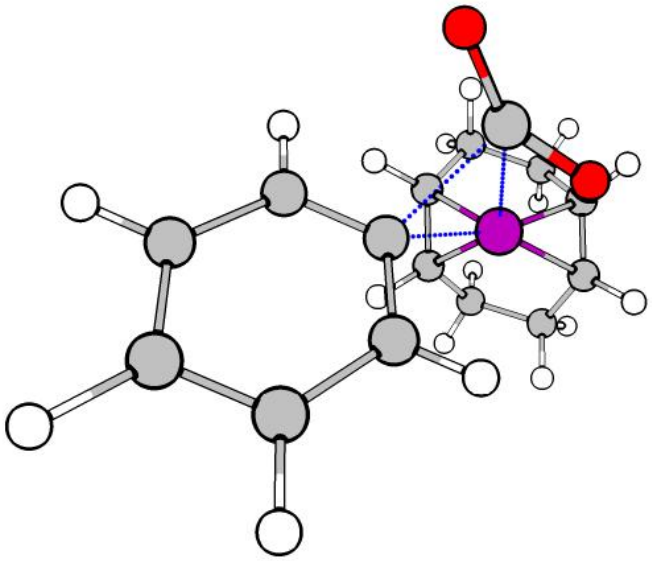


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.720499	-0.165557	0.032122
2	6	0	2.376016	-1.161257	-0.707303
3	6	0	2.475858	0.597024	0.929752
4	6	0	3.744540	-1.390800	-0.554817
5	1	0	1.822518	-1.775897	-1.419463
6	6	0	3.847332	0.372819	1.080685
7	1	0	2.007917	1.392661	1.505973
8	6	0	4.485953	-0.622182	0.343089
9	1	0	4.231067	-2.169091	-1.138871
10	1	0	4.418268	0.984896	1.775661
11	1	0	5.552473	-0.795366	0.462197
12	6	0	0.106375	2.046264	-0.666903
13	8	0	0.101657	2.914062	0.153011
14	8	0	0.233158	1.697726	-1.833250
15	45	0	-0.237846	-0.023436	-0.433027
16	6	0	-2.568528	0.471724	-0.687700
17	1	0	-2.543171	1.337858	-1.347810
18	6	0	-3.144469	0.684552	0.691880
19	1	0	-3.799652	1.560795	0.663044
20	1	0	-3.784755	-0.159994	0.956125
21	6	0	-2.073579	0.915755	1.770497
22	1	0	-1.761288	1.963352	1.748218
23	1	0	-2.507461	0.746028	2.766950
24	6	0	-0.830764	0.074726	1.623157
25	1	0	0.026542	0.448759	2.180381
26	6	0	-0.773914	-1.269428	1.216193
27	1	0	0.130559	-1.811071	1.492344
28	6	0	-1.981967	-2.136352	0.892539
29	1	0	-1.738840	-3.173619	1.142534
30	1	0	-2.815413	-1.863964	1.545493
31	6	0	-2.411334	-2.092828	-0.586248
32	1	0	-1.791783	-2.796128	-1.152846
33	1	0	-3.442230	-2.461651	-0.684924
34	6	0	-2.286666	-0.742274	-1.250748
35	1	0	-2.092296	-0.760381	-2.324039

SCF Done: E(RPBE1PBE) = -5418.76136893 A.U. after 1 cycles
Convg = 0.3942D-08 -V/T = 2.0036
Zero-point correction= 0.287424 (Hartree/Particle)

```
 Thermal correction to Energy=                    0.308399
 Thermal correction to Enthalpy=                  0.309454
 Thermal correction to Gibbs Free Energy=         0.234985
 Sum of electronic and zero-point Energies=          -5418.473944
 Sum of electronic and thermal Energies=             -5418.452970
 Sum of electronic and thermal Enthalpies=           -5418.451915
 Sum of electronic and thermal Free Energies=        -5418.526384
                     1                      2                      3
                     A                      A                      A
 Frequencies --    47.5944                54.9086                65.6464
```

COD-Rh-Ph-CO_2-TS2 (40)



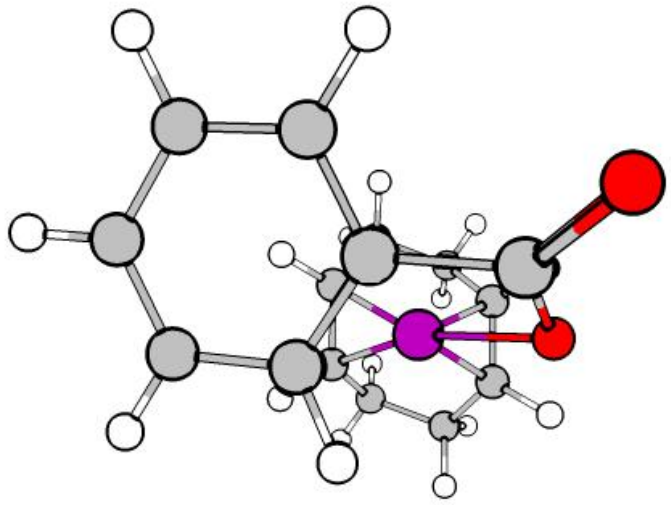
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.699705	0.050492	0.053780
2	6	0	2.305634	-0.395505	-1.131539
3	6	0	2.368890	-0.175053	1.267022
4	6	0	3.508305	-1.106208	-1.103888
5	1	0	1.841886	-0.178412	-2.093198
6	6	0	3.570058	-0.873886	1.299335
7	1	0	1.962886	0.225376	2.193138
8	6	0	4.137868	-1.351412	0.113345
9	1	0	3.957412	-1.451644	-2.031959
10	1	0	4.075087	-1.041640	2.247663
11	1	0	5.079113	-1.894506	0.141298
12	6	0	1.065753	2.023015	-0.196434
13	8	0	1.572388	2.701174	0.644491
14	8	0	0.478406	2.026141	-1.282409
15	45	0	-0.367187	0.243956	-0.318284
16	6	0	-2.530453	0.835862	-0.413944
17	1	0	-2.469858	1.883698	-0.705801
18	6	0	-3.223544	0.539404	0.897589
19	1	0	-3.845345	1.397237	1.172194
20	1	0	-3.909310	-0.302074	0.770020
21	6	0	-2.226780	0.262323	2.032254
22	1	0	-1.902500	1.214862	2.463364
23	1	0	-2.717591	-0.290923	2.846903
24	6	0	-0.986904	-0.473675	1.585278
25	1	0	-0.140713	-0.364362	2.261574

26	6	0	-0.935966	-1.553698	0.685229
27	1	0	-0.041019	-2.173647	0.729353
28	6	0	-2.156356	-2.209377	0.058805
29	1	0	-1.948198	-3.273568	-0.088529
30	1	0	-2.996434	-2.165577	0.758061
31	6	0	-2.540251	-1.591103	-1.296041
32	1	0	-1.961652	-2.082314	-2.084783
33	1	0	-3.596437	-1.794360	-1.524628
34	6	0	-2.260543	-0.109181	-1.390129
35	1	0	-2.042753	0.263332	-2.392542

SCF Done: E(RPBE1PBE) = -5418.74826557 A.U. after 1 cycles
Convg = 0.4225D-08 -V/T = 2.0036
Zero-point correction= 0.286602 (Hartree/Particle)
Thermal correction to Energy= 0.306866
Thermal correction to Enthalpy= 0.307921
Thermal correction to Gibbs Free Energy= 0.234714
Sum of electronic and zero-point Energies= -5418.461664
Sum of electronic and thermal Energies= -5418.441399
Sum of electronic and thermal Enthalpies= -5418.440344
Sum of electronic and thermal Free Energies= -5418.513552

	1	2	3
	A	A	A
Frequencies --	-280.7656	37.8432	49.2498

COD-Rh-OOCPh-conf1 (41)

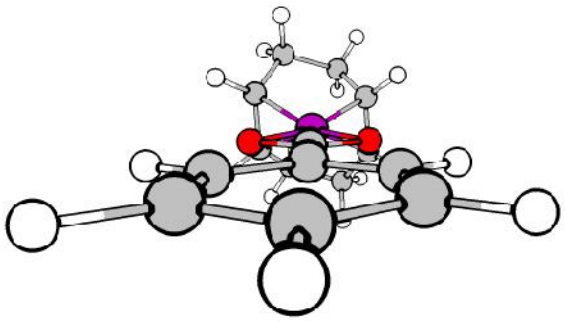


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.146013	0.403444	-0.061689
2	6	0	1.813089	-0.330165	-1.221030
3	6	0	2.783577	-0.255735	1.006261
4	6	0	2.140982	-1.695667	-1.308919
5	1	0	1.440864	0.190217	-2.104176
6	6	0	3.071544	-1.607996	0.919117
7	1	0	3.057410	0.318037	1.887003
8	6	0	2.753549	-2.332379	-0.241754
9	1	0	1.920014	-2.242012	-2.221948
10	1	0	3.559432	-2.110477	1.750167
11	1	0	3.002613	-3.387971	-0.306492
12	6	0	1.866651	1.894658	0.005880

13	8	0	2.729116	2.681307	0.375447
14	8	0	0.645455	2.179975	-0.337780
15	45	0	-0.282351	0.322561	-0.218829
16	6	0	-1.941967	1.066951	0.928743
17	1	0	-1.529172	1.941884	1.430133
18	6	0	-2.551138	0.004395	1.822715
19	1	0	-2.705951	0.425606	2.820664
20	1	0	-3.543804	-0.265269	1.451781
21	6	0	-1.649839	-1.234505	1.934900
22	1	0	-0.915389	-1.067048	2.729032
23	1	0	-2.235177	-2.114556	2.238605
24	6	0	-0.880777	-1.527573	0.666999
25	1	0	0.046524	-2.085041	0.811898
26	6	0	-1.393748	-1.489957	-0.633862
27	1	0	-0.822437	-2.014407	-1.398922
28	6	0	-2.844367	-1.199663	-0.979193
29	1	0	-3.122323	-1.781463	-1.863504
30	1	0	-3.491269	-1.555927	-0.172757
31	6	0	-3.090482	0.290228	-1.261973
32	1	0	-2.880331	0.494382	-2.316515
33	1	0	-4.149217	0.544623	-1.107488
34	6	0	-2.209384	1.201731	-0.442413
35	1	0	-2.004779	2.177330	-0.884211

```
SCF Done:  E(RPBE1PBE) =  -5418.79574295     A.U. after    1 cycles
             Convg  =    0.3083D-08             -V/T =  2.0036
SCF Done:  E(RPBE1PBE) =  -5418.79574295     A.U. after    1 cycles
             Convg  =    0.3083D-08             -V/T =  2.0036
Zero-point correction=                           0.289667 (Hartree/Particle)
 Thermal correction to Energy=                    0.309674
 Thermal correction to Enthalpy=                  0.310729
 Thermal correction to Gibbs Free Energy=         0.237899
 Sum of electronic and zero-point Energies=          -5418.506076
 Sum of electronic and thermal Energies=             -5418.486069
 Sum of electronic and thermal Enthalpies=           -5418.485014
 Sum of electronic and thermal Free Energies=        -5418.557844
                     1                      2                      3
                     A                      A                      A
 Frequencies --    29.9077               45.2967               54.9781
```

COD-Rh-OOCPh-conf1 (42)

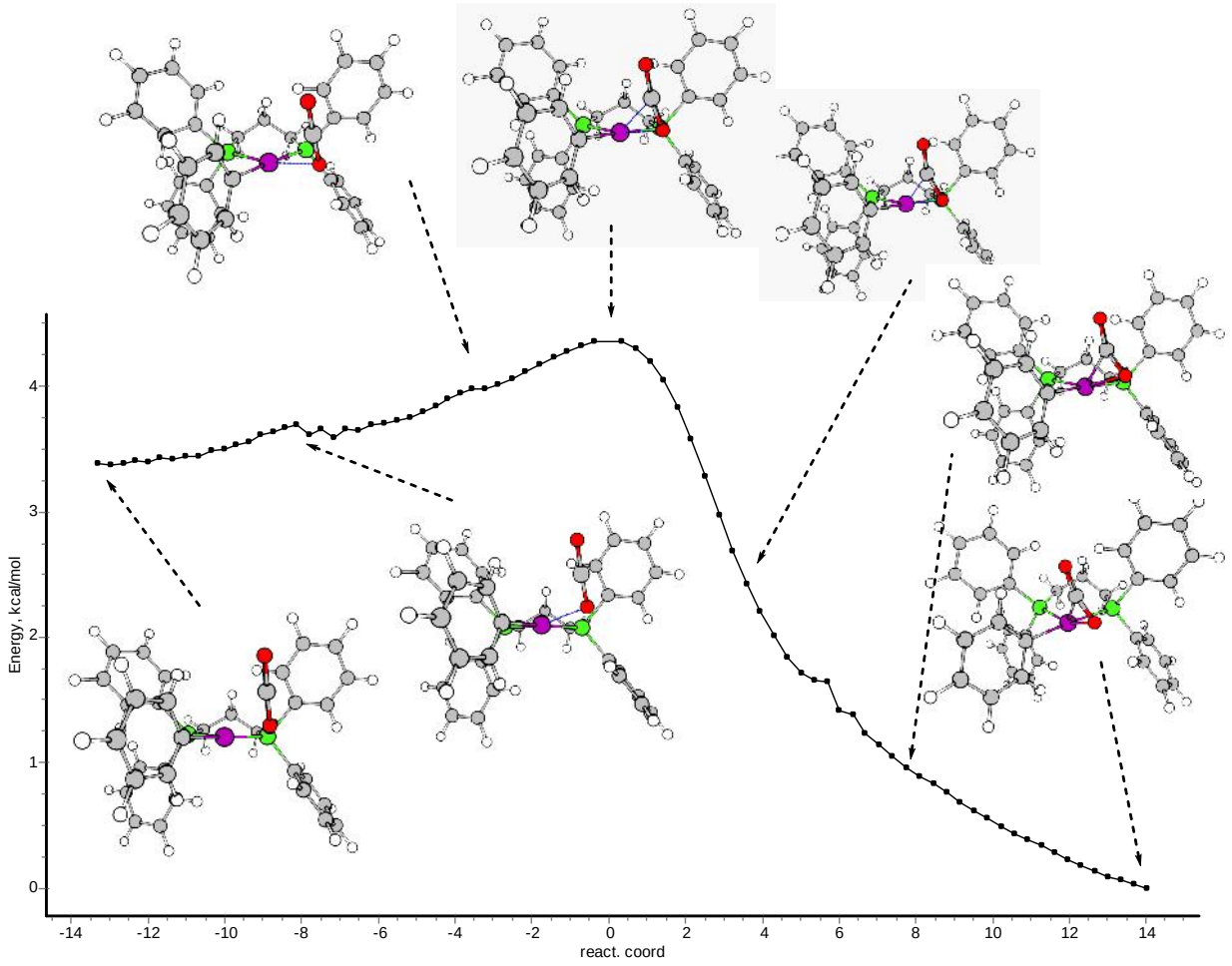


1	6	0	3.109875	0.000091	-0.000395
2	6	0	3.808665	-1.190208	-0.223451
3	6	0	3.808465	1.190399	0.223262
4	6	0	5.200381	-1.188830	-0.222470

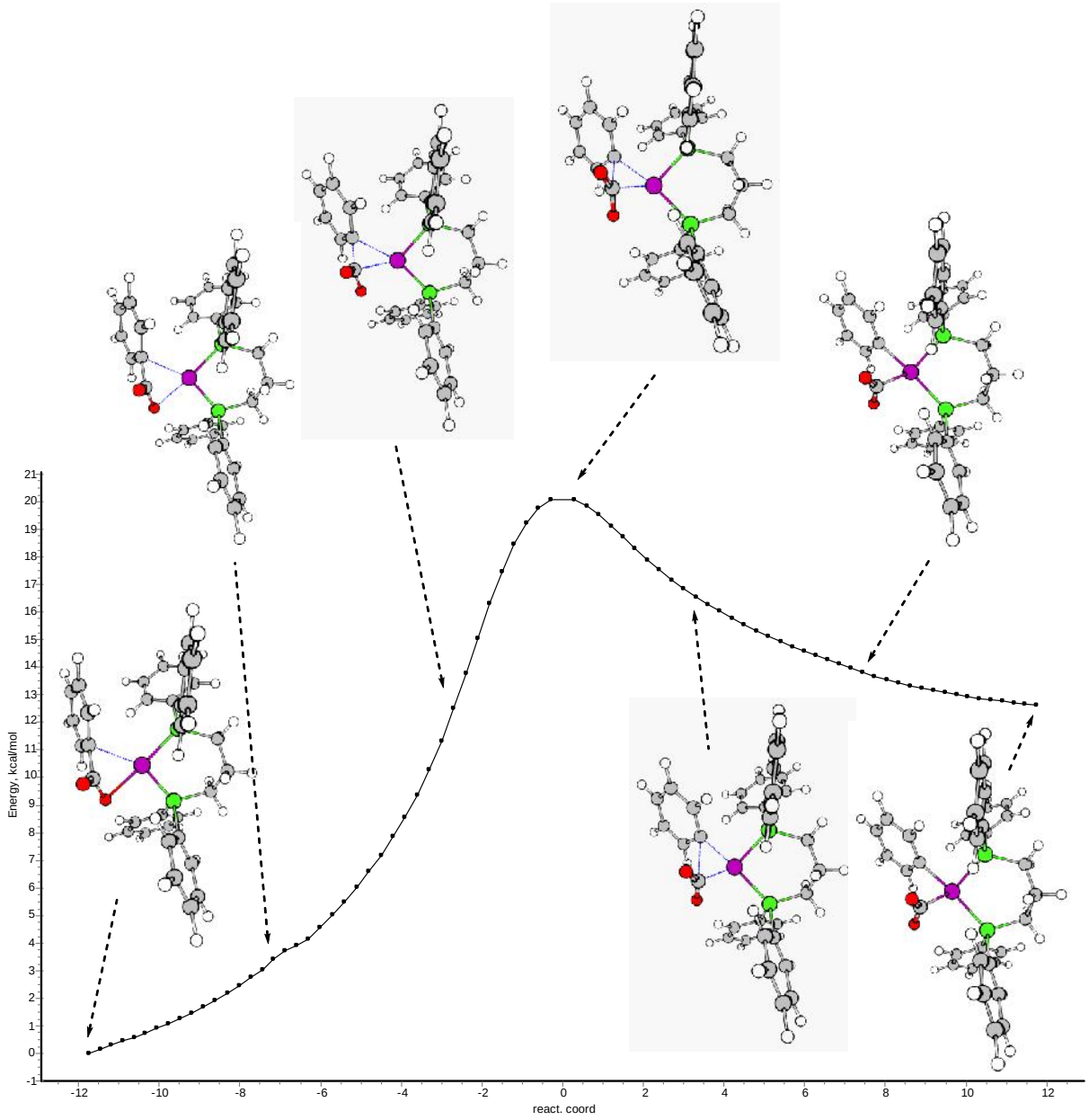
```
      5          1           0        3.248811   -2.104708   -0.394998
      6          6           0        5.200179    1.189020    0.223455
      7          1           0        3.248461    2.104887    0.394343
      8          6           0        5.896626    0.000090    0.000804
      9          1           0        5.744607   -2.113396   -0.395460
     10          1           0        5.744266    2.113581    0.396907
     11          1           0        6.983589    0.000093    0.001285
     12          6           0        1.625852    0.000085   -0.000924
     13          8           0        0.987209    1.084892    0.208302
     14          8           0        0.987428   -1.084790   -0.210495
     15         45           0       -0.878563   -0.000114   -0.000672
     16          6           0       -2.387962   -1.212839   -0.898342
     17          1           0       -1.848555   -1.843097   -1.605838
     18          6           0       -3.533514   -0.401204   -1.477969
     19          1           0       -3.768621   -0.778332   -2.478058
     20          1           0       -4.436461   -0.553662   -0.880040
     21          6           0       -3.180115    1.090528   -1.569524
     22          1           0       -2.664925    1.277041   -2.517147
     23          1           0       -4.089698    1.708394   -1.587731
     24          6           0       -2.256638    1.538556   -0.460799
     25          1           0       -1.635699    2.403281   -0.700441
     26          6           0       -2.386678    1.212720    0.899156
     27          1           0       -1.845895    1.842283    1.606206
     28          6           0       -3.531727    0.401098    1.479679
     29          1           0       -3.766982    0.778781    2.479536
     30          1           0       -4.434789    0.552490    0.881694
     31          6           0       -3.177191   -1.090211    1.571992
     32          1           0       -2.659379   -1.275237    2.518500
     33          1           0       -4.086224   -1.708794    1.593226
     34          6           0       -2.256077   -1.538576    0.461486
     35          1           0       -1.635118   -2.403592    0.700046
 -------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5418.80923241     A.U. after    1 cycles
             Convg  =    0.1770D-08             -V/T =  2.0035
Zero-point correction=                           0.289985 (Hartree/Particle)
 Thermal correction to Energy=                    0.309955
 Thermal correction to Enthalpy=                  0.311010
 Thermal correction to Gibbs Free Energy=         0.236488
 Sum of electronic and zero-point Energies=          -5418.519247
 Sum of electronic and thermal Energies=             -5418.499278
 Sum of electronic and thermal Enthalpies=           -5418.498223
 Sum of electronic and thermal Free Energies=        -5418.572745
                     1                      2                      3
                     A                      A                      A
 Frequencies --    15.0458               35.4023               39.9606
```

Intrinsic reaction coordinate (IRC) plots

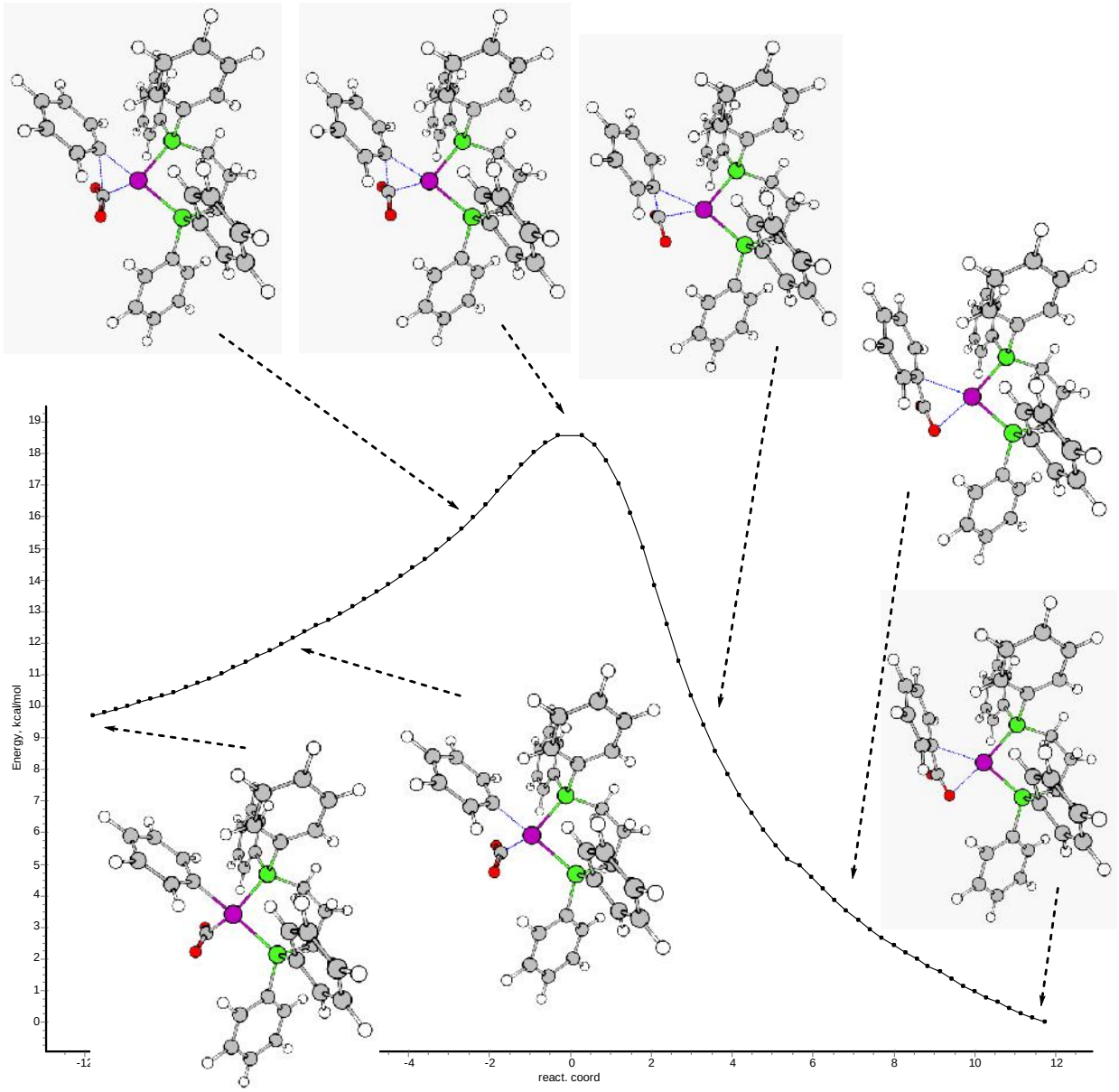
DPPP-Rh-Ph-*syn*-O=C=O-TS1 (6)



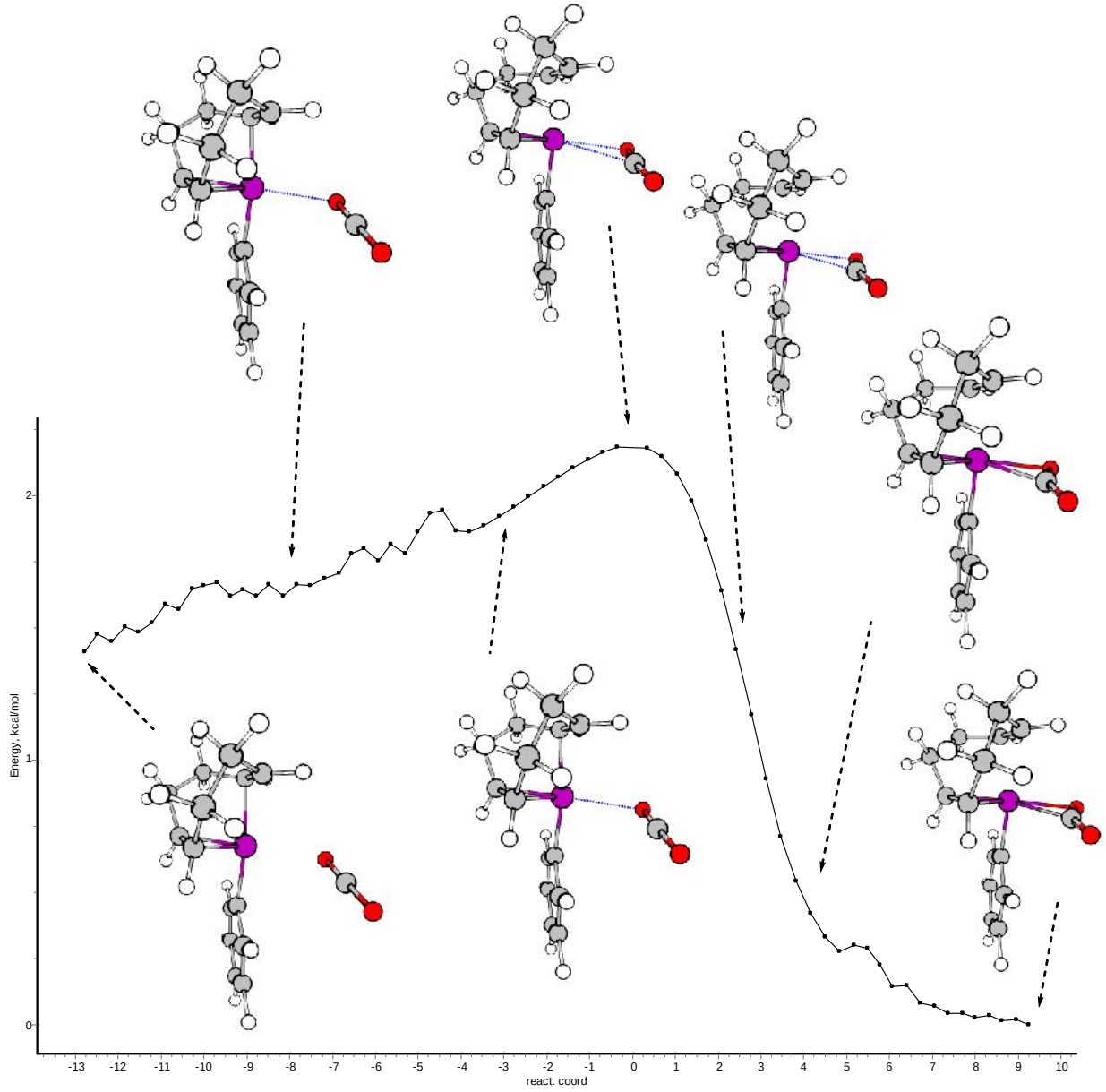
DPPP-Rh-Ph-*syn*-CO_2-TS2 (8)



DPPP-Rh-Ph-*anti*-CO_2-TS2 (13)



COD-Rh-Ph-O=C=O-TS1 (18)



COD-Rh-Ph-CO_2-TS2 (20)