

DFT modelling of a diphosphane – N-heterocyclic carbene-Rh(I) pincer complex rearrangement: A computational evaluation of the electronic effects in C-P bond activation

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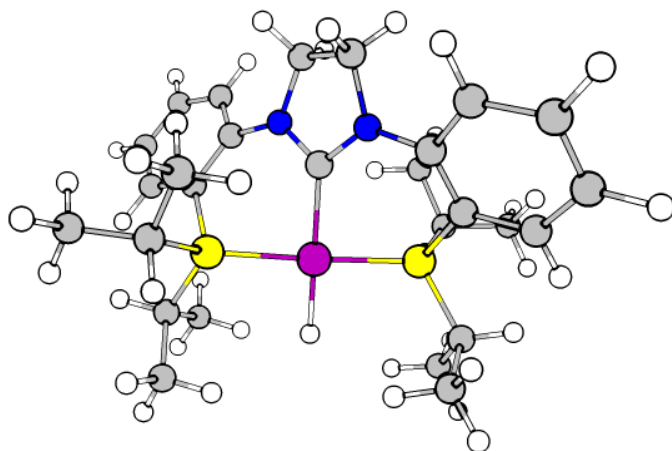
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SUPPORTING INFORMATION

1. Plots, cartesian coordinates, energies and first 3 frequencies (IEFPCM/PBE0/DGDZVP)

C-P-OA-SM (1a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.601895	-3.377150	0.447518
2	1	0	-1.391184	-4.038929	0.089121
3	1	0	-0.333654	-3.658010	1.471918
4	6	0	0.001898	-1.143268	-0.005753
5	6	0	0.612820	-3.376357	-0.453605
6	1	0	1.404224	-4.034628	-0.093402
7	1	0	0.345899	-3.660696	-1.477383
8	6	0	2.308850	-1.606913	-0.871447
9	6	0	3.010774	-0.450993	-0.454709
10	6	0	4.317696	-0.279344	-0.923702
11	1	0	4.882174	0.589786	-0.606119
12	6	0	4.935930	-1.178463	-1.786708

13	1	0	5.951222	-1.000602	-2.125108
14	6	0	4.228576	-2.296913	-2.206594
15	1	0	4.673889	-3.011055	-2.891725
16	6	0	2.933884	-2.506112	-1.747116
17	1	0	2.403754	-3.383903	-2.095068
18	6	0	-2.300275	-1.610920	0.869617
19	6	0	-3.004948	-0.454175	0.459904
20	6	0	-4.308434	-0.282929	0.938642
21	1	0	-4.874813	0.587028	0.626787
22	6	0	-4.920959	-1.183380	1.804270
23	1	0	-5.933595	-1.005591	2.150573
24	6	0	-4.211317	-2.303285	2.216313
25	1	0	-4.652099	-3.018896	2.902844
26	6	0	-2.920013	-2.512019	1.747284
27	1	0	-2.388455	-3.390990	2.089840
28	6	0	2.648951	0.284438	2.330652
29	1	0	2.233208	1.074914	2.965061
30	6	0	1.931261	-1.018060	2.698855
31	1	0	2.280919	-1.851351	2.079987
32	1	0	0.849859	-0.923603	2.574030
33	1	0	2.137487	-1.270580	3.744125
34	6	0	4.152357	0.174601	2.596246
35	1	0	4.326600	-0.125866	3.634704
36	1	0	4.673172	1.122870	2.440066
37	1	0	4.613582	-0.579082	1.950347
38	6	0	3.232229	2.361088	0.350333
39	1	0	4.288826	2.133108	0.522537
40	6	0	2.808579	3.425031	1.369710
41	1	0	3.334237	4.362305	1.160968
42	1	0	3.046956	3.136368	2.397446
43	1	0	1.732952	3.611354	1.300278
44	6	0	3.058085	2.888865	-1.077243
45	1	0	2.008526	3.138299	-1.254602
46	1	0	3.363837	2.158177	-1.831006
47	1	0	3.662432	3.791697	-1.215173
48	6	0	-3.235244	2.357564	-0.343080
49	1	0	-4.292944	2.128116	-0.506348
50	6	0	-3.049569	2.886261	1.082637
51	1	0	-1.999045	3.138105	1.250467
52	1	0	-3.346854	2.155175	1.839394
53	1	0	-3.654621	3.787823	1.225763
54	6	0	-2.822030	3.421512	-1.366621
55	1	0	-3.347606	4.357995	-1.154130
56	1	0	-3.068356	3.131642	-2.392145
57	1	0	-1.746238	3.609840	-1.306280
58	6	0	-2.667720	0.280681	-2.327689
59	1	0	-2.256580	1.070267	-2.966226
60	6	0	-4.173122	0.170863	-2.581622
61	1	0	-4.355215	-0.132089	-3.618023
62	1	0	-4.692436	1.119714	-2.423910

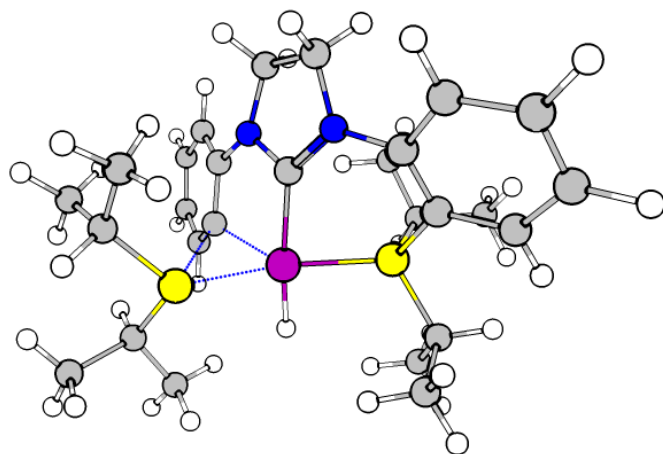
63	1	0	-4.629763	-0.581058	-1.930444
64	6	0	-1.953147	-1.022519	-2.699530
65	1	0	-2.300484	-1.855270	-2.078635
66	1	0	-0.871036	-0.929139	-2.579824
67	1	0	-2.164802	-1.275141	-3.743692
68	7	0	-1.015211	-1.971829	0.388881
69	7	0	1.021535	-1.969628	-0.398078
70	15	0	-2.207407	0.829184	-0.600034
71	15	0	2.203702	0.831796	0.598790
72	45	0	0.000384	0.883362	-0.009568
73	1	0	0.000760	2.557476	-0.012758

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SCF Done:  E(RwB97XD) = -6533.22984502      A.U. after   1 cycles
              Conv =   0.4749D-08              -V/T =   2.0047
Zero-point correction=                      0.636832 (Hartree/Particle)
Thermal correction to Energy=                0.679218
Thermal correction to Enthalpy=              0.680273
Thermal correction to Gibbs Free Energy=     0.561984
Sum of electronic and zero-point Energies=   -6532.593013
Sum of electronic and thermal Energies=      -6532.550627
Sum of electronic and thermal Enthalpies=    -6532.549572
Sum of electronic and thermal Free Energies=  -6532.667861
              1                      2                      3
              A                      A                      A
Frequencies --   24.5053              32.6495              46.8775

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C-P-OA-TS (2a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.109820	-3.420144	0.590052
2	1	0	-0.819084	-4.198096	0.301021
3	1	0	0.154717	-3.555662	1.645101
4	6	0	0.218159	-1.239402	-0.209131
5	6	0	1.127580	-3.392923	-0.313568

6	1	0	2.010410	-3.821971	0.163122
7	1	0	0.944360	-3.915482	-1.256616
8	6	0	2.542484	-1.409956	-0.982068
9	6	0	3.000368	-0.135949	-0.567929
10	6	0	4.272621	0.253035	-1.000166
11	1	0	4.666819	1.217284	-0.701149
12	6	0	5.075748	-0.553128	-1.802775
13	1	0	6.055313	-0.204255	-2.112078
14	6	0	4.607870	-1.799532	-2.198280
15	1	0	5.211918	-2.443913	-2.828440
16	6	0	3.348830	-2.220764	-1.785957
17	1	0	2.982111	-3.189805	-2.106760
18	6	0	-1.714351	-1.519305	1.119081
19	6	0	-2.007891	-0.145908	0.889140
20	6	0	-2.878845	0.442821	1.813494
21	1	0	-3.086860	1.503928	1.738770
22	6	0	-3.506243	-0.283239	2.829161
23	1	0	-4.182540	0.223100	3.511250
24	6	0	-3.274649	-1.647101	2.954456
25	1	0	-3.777305	-2.228124	3.720879
26	6	0	-2.353754	-2.264159	2.104959
27	1	0	-2.126545	-3.317811	2.234764
28	6	0	2.486430	0.531258	2.214934
29	1	0	1.937425	1.245307	2.838428
30	6	0	1.985511	-0.869382	2.579911
31	1	0	2.480470	-1.636534	1.974045
32	1	0	0.904395	-0.953082	2.441670
33	1	0	2.211345	-1.080897	3.629630
34	6	0	3.985074	0.671059	2.489127
35	1	0	4.196319	0.418129	3.533092
36	1	0	4.347005	1.688992	2.321586
37	1	0	4.567991	-0.006733	1.857970
38	6	0	2.705627	2.674977	0.218535
39	1	0	3.788957	2.617980	0.359680
40	6	0	2.154666	3.666102	1.249302
41	1	0	2.548728	4.664816	1.036631
42	1	0	2.445618	3.409166	2.271677
43	1	0	1.063422	3.707936	1.198910
44	6	0	2.407468	3.153505	-1.206071
45	1	0	1.328034	3.251875	-1.351916
46	1	0	2.789035	2.464732	-1.964670
47	1	0	2.870425	4.131421	-1.373146
48	6	0	-3.671691	1.856222	-0.854487
49	1	0	-4.319579	1.439402	-0.075677
50	6	0	-3.156644	3.220820	-0.389603
51	1	0	-2.551313	3.690014	-1.171684
52	1	0	-2.524214	3.151890	0.496108
53	1	0	-4.004487	3.878859	-0.168960
54	6	0	-4.520686	2.046524	-2.123096
55	1	0	-5.240046	2.855435	-1.959011

56	1	0	-5.094501	1.156132	-2.389033
57	1	0	-3.900575	2.324624	-2.981716
58	6	0	-3.193392	-0.803572	-1.880854
59	1	0	-3.626158	-0.344370	-2.777753
60	6	0	-4.350659	-1.366852	-1.049356
61	1	0	-4.909366	-2.101651	-1.640643
62	1	0	-5.054730	-0.590688	-0.738465
63	1	0	-3.989807	-1.865285	-0.146990
64	6	0	-2.277458	-1.920097	-2.393792
65	1	0	-1.967515	-2.584364	-1.585687
66	1	0	-1.377349	-1.519754	-2.869114
67	1	0	-2.814247	-2.525395	-3.132202
68	7	0	-0.658546	-2.085890	0.376202
69	7	0	1.309546	-1.953089	-0.551553
70	15	0	-2.260259	0.668139	-1.184688
71	15	0	1.963458	0.993644	0.484518
72	45	0	-0.246993	0.731947	-0.095577
73	1	0	-0.543021	2.301875	0.318196

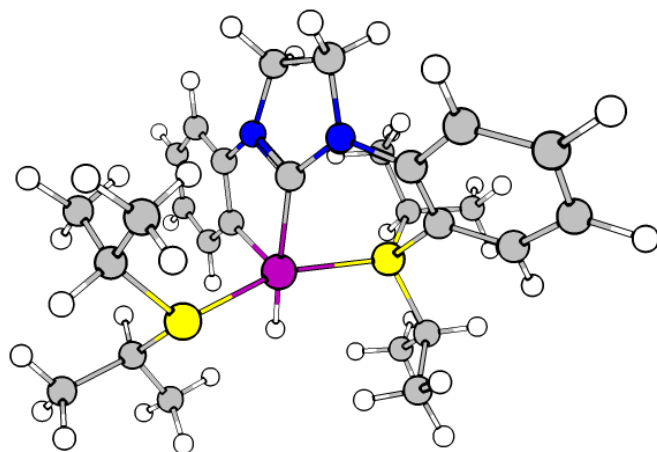
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Zero-point correction=                      0.634835 (Hartree/Particle)
Thermal correction to Energy=                0.677122
Thermal correction to Enthalpy=              0.678177
Thermal correction to Gibbs Free Energy=     0.560088
Sum of electronic and zero-point Energies=   -6532.546084
Sum of electronic and thermal Energies=      -6532.503798
Sum of electronic and thermal Enthalpies=    -6532.502743
Sum of electronic and thermal Free Energies=  -6532.620831

              1              2              3
              A              A              A
Frequencies --  -234.7056          26.2562          33.9095

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C-P-OA-PR-conf1 (3a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.285212	-3.507794	0.423611
2	1	0	-0.350375	-4.346109	0.134715
3	1	0	0.631803	-3.665368	1.450459
4	6	0	0.243932	-1.291133	-0.353058
5	6	0	1.444098	-3.292841	-0.563712
6	1	0	2.414555	-3.565504	-0.144570
7	1	0	1.290526	-3.852756	-1.489441
8	6	0	2.524222	-1.108226	-1.220831
9	6	0	2.884955	0.121151	-0.616812
10	6	0	4.088727	0.704198	-1.030115
11	1	0	4.407477	1.642411	-0.590565
12	6	0	4.916037	0.120708	-1.985510
13	1	0	5.841094	0.610008	-2.271131
14	6	0	4.544871	-1.087402	-2.563848
15	1	0	5.171308	-1.556825	-3.315066
16	6	0	3.354361	-1.693022	-2.180243
17	1	0	3.054782	-2.629766	-2.638559
18	6	0	-1.386761	-1.773570	1.255392
19	6	0	-1.558747	-0.373384	1.288468
20	6	0	-2.472141	0.122059	2.220347
21	1	0	-2.641988	1.192815	2.277990
22	6	0	-3.175627	-0.731580	3.076952
23	1	0	-3.879776	-0.314366	3.791273
24	6	0	-2.983848	-2.110136	3.016417
25	1	0	-3.534856	-2.772464	3.676440
26	6	0	-2.079098	-2.640457	2.095525
27	1	0	-1.927528	-3.714487	2.031357
28	6	0	2.460927	0.324030	2.272078
29	1	0	1.880919	0.888110	3.010736
30	6	0	2.110186	-1.155177	2.450218
31	1	0	2.618870	-1.774722	1.703374
32	1	0	1.032698	-1.318455	2.376990
33	1	0	2.436269	-1.497444	3.436971
34	6	0	3.951680	0.576660	2.503996
35	1	0	4.238046	0.214037	3.496259
36	1	0	4.206983	1.638523	2.458207
37	1	0	4.561992	0.045123	1.767690
38	6	0	2.334499	2.740696	0.596999
39	1	0	3.421338	2.808997	0.702900
40	6	0	1.699574	3.496089	1.770503
41	1	0	1.927718	4.562356	1.680278
42	1	0	2.082048	3.158220	2.737478
43	1	0	0.612345	3.377809	1.763642
44	6	0	1.920257	3.367151	-0.739066
45	1	0	0.831027	3.358698	-0.844864
46	1	0	2.349151	2.841885	-1.596665
47	1	0	2.257183	4.407677	-0.779292

48	6	0	-3.783540	1.690369	-0.720588
49	1	0	-4.131012	1.029721	0.083121
50	6	0	-3.492436	3.064063	-0.111775
51	1	0	-3.125390	3.759919	-0.874495
52	1	0	-2.736308	3.007444	0.672967
53	1	0	-4.407571	3.487113	0.318180
54	6	0	-4.906480	1.823581	-1.759551
55	1	0	-5.755263	2.363524	-1.325632
56	1	0	-5.281807	0.857147	-2.103965
57	1	0	-4.567134	2.386711	-2.636115
58	6	0	-2.943689	-0.606380	-2.270675
59	1	0	-3.625080	-0.204397	-3.031361
60	6	0	-3.746203	-1.544034	-1.363249
61	1	0	-4.206050	-2.346282	-1.953697
62	1	0	-4.547670	-1.024424	-0.831046
63	1	0	-3.102028	-2.004452	-0.611045
64	6	0	-1.856403	-1.373860	-3.026719
65	1	0	-1.151490	-1.843446	-2.335644
66	1	0	-1.284773	-0.716461	-3.688297
67	1	0	-2.304876	-2.167226	-3.635849
68	7	0	-0.429474	-2.237473	0.327736
69	7	0	1.381371	-1.843940	-0.823910
70	15	0	-2.232179	0.925328	-1.450726
71	15	0	1.812458	0.959707	0.648929
72	45	0	-0.453555	0.638590	-0.060147
73	1	0	-0.936053	2.063986	0.544554

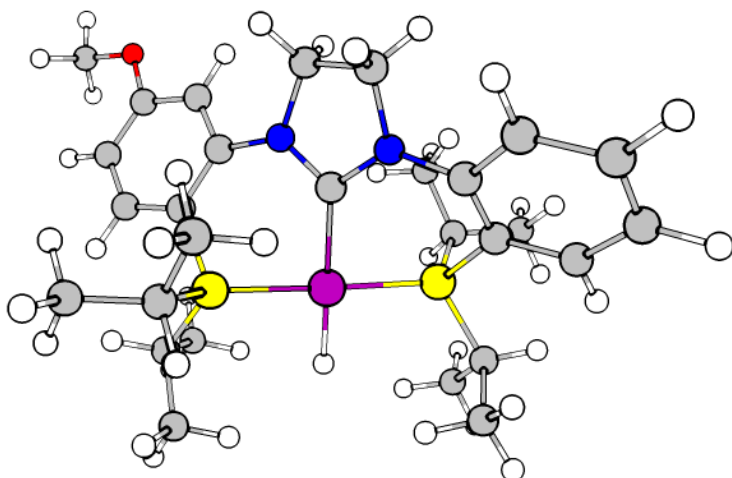
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Zero-point correction= 0.634161 (Hartree/Particle)
Thermal correction to Energy= 0.677621
Thermal correction to Enthalpy= 0.678676
Thermal correction to Gibbs Free Energy= 0.557328
Sum of electronic and zero-point Energies= -6532.564881
Sum of electronic and thermal Energies= -6532.521422
Sum of electronic and thermal Enthalpies= -6532.520367
Sum of electronic and thermal Free Energies= -6532.641714

          1          2          3
          A          A          A
Frequencies -- 25.2572 33.9637 36.4327

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C-P-OA-SM-*p*-OMe (1b)



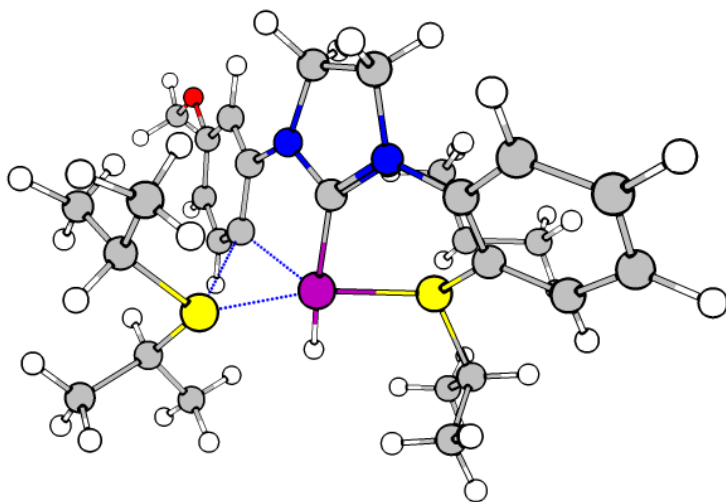
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.897724	-3.067808	0.576418
2	1	0	1.726684	-3.461764	1.164977
3	1	0	0.833660	-3.617585	-0.369064
4	6	0	-0.134522	-0.954227	0.395489
5	6	0	-0.416458	-3.104918	1.323283
6	1	0	-1.026332	-3.969985	1.060280
7	1	0	-0.254881	-3.094264	2.406743
8	6	0	-2.429093	-1.661358	1.123008
9	6	0	-3.255323	-0.802556	0.360618
10	6	0	-4.626296	-0.801890	0.640750
11	1	0	-5.283439	-0.165300	0.059795
12	6	0	-5.195412	-1.585086	1.639187
13	1	0	-6.264581	-1.547419	1.819419
14	6	0	-4.370361	-2.402720	2.399560
15	1	0	-4.777480	-3.014419	3.198178
16	6	0	-3.006388	-2.440474	2.136501
17	1	0	-2.385996	-3.083373	2.748359
18	6	0	2.321255	-1.141049	-0.083133
19	6	0	2.747361	0.201778	0.087139
20	6	0	4.067463	0.494400	-0.252243
21	1	0	4.433188	1.506048	-0.118339
22	6	0	4.968115	-0.438688	-0.761402
23	1	0	5.978990	-0.131481	-0.999422
24	6	0	4.522339	-1.742721	-0.949324
25	6	0	3.211927	-2.080184	-0.604880
26	1	0	2.916917	-3.108061	-0.773400
27	6	0	-2.661554	-0.643502	-2.476162
28	1	0	-2.291895	0.048056	-3.241269
29	6	0	-1.705718	-1.840820	-2.441364
30	1	0	-2.009129	-2.565782	-1.678309

31	1	0	-0.680477	-1.526071	-2.231588
32	1	0	-1.718490	-2.352888	-3.409008
33	6	0	-4.077165	-1.088366	-2.850891
34	1	0	-4.056487	-1.637451	-3.798099
35	1	0	-4.761065	-0.245291	-2.978713
36	1	0	-4.495187	-1.755414	-2.090437
37	6	0	-3.847477	1.660299	-1.106734
38	1	0	-4.816237	1.192104	-1.306113
39	6	0	-3.495827	2.541588	-2.310091
40	1	0	-4.221000	3.358099	-2.388255
41	1	0	-3.520138	1.988940	-3.253737
42	1	0	-2.500143	2.975985	-2.184711
43	6	0	-3.951788	2.507337	0.165492
44	1	0	-2.996193	3.000591	0.363042
45	1	0	-4.210944	1.908520	1.043055
46	1	0	-4.723444	3.274233	0.038580
47	6	0	2.370120	3.099965	0.034337
48	1	0	3.417435	3.143523	0.349808
49	6	0	2.305794	3.162900	-1.494764
50	1	0	1.262749	3.151822	-1.822527
51	1	0	2.816979	2.319322	-1.966957
52	1	0	2.776296	4.086324	-1.848998
53	6	0	1.642849	4.298639	0.653439
54	1	0	2.028429	5.226074	0.217804
55	1	0	1.786730	4.358579	1.736169
56	1	0	0.570435	4.239734	0.445920
57	6	0	1.869719	1.579672	2.489068
58	1	0	1.224753	2.399657	2.823770
59	6	0	3.310291	1.875669	2.911893
60	1	0	3.379068	1.914346	4.004156
61	1	0	3.669381	2.834740	2.529257
62	1	0	3.992274	1.093137	2.564803
63	6	0	1.358358	0.295133	3.149535
64	1	0	1.940943	-0.574499	2.826170
65	1	0	0.307751	0.116409	2.907854
66	1	0	1.454810	0.373563	4.237430
67	7	0	1.056538	-1.631571	0.327766
68	7	0	-1.044381	-1.856406	0.880237
69	15	0	1.593442	1.522763	0.642257
70	15	0	-2.545362	0.347731	-0.895861
71	45	0	-0.483156	0.971119	-0.137318
72	1	0	-0.764019	2.558136	-0.591085
73	8	0	5.271881	-2.758160	-1.453110
74	6	0	6.605031	-2.464747	-1.839396
75	1	0	7.016079	-3.394750	-2.227633
76	1	0	6.631623	-1.701828	-2.623841
77	1	0	7.203231	-2.134566	-0.983872

SCF Done: E(RwB97XD) = -6647.73626689 A.U. after 1 cycles
Convrg = 0.2495D-08 -V/T = 2.0048

Zero-point correction=	0.669165 (Hartree/Particle)
Thermal correction to Energy=	0.714936
Thermal correction to Enthalpy=	0.715991
Thermal correction to Gibbs Free Energy=	0.590096
Sum of electronic and zero-point Energies=	-6647.067101
Sum of electronic and thermal Energies=	-6647.021331
Sum of electronic and thermal Enthalpies=	-6647.020276
Sum of electronic and thermal Free Energies=	-6647.146171
	1 2 3
	A A A
Frequencies --	22.1723 28.9767 46.1961

C-P-OA-TS-*p*-OMe (2b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.342281	-3.073573	1.246862
2	1	0	1.064343	-3.479720	1.957734
3	1	0	0.307407	-3.723399	0.364844
4	6	0	-0.384860	-0.877954	0.842567
5	6	0	-1.042716	-2.875362	1.870750
6	1	0	-1.759417	-3.638445	1.563101
7	1	0	-0.988083	-2.858831	2.962986
8	6	0	-2.777617	-1.117671	1.343988
9	6	0	-3.295344	-0.269819	0.335720
10	6	0	-4.658664	0.036620	0.400337
11	1	0	-5.097141	0.679182	-0.354150
12	6	0	-5.496813	-0.458336	1.395896
13	1	0	-6.548600	-0.192675	1.401122
14	6	0	-4.970844	-1.295112	2.371631
15	1	0	-5.601909	-1.692601	3.159706
16	6	0	-3.619366	-1.619202	2.341179
17	1	0	-3.212681	-2.262761	3.113589

18	6	0	1.798882	-1.347634	0.079300
19	6	0	1.880886	0.007318	-0.350996
20	6	0	2.870647	0.257837	-1.299900
21	1	0	2.953709	1.250307	-1.727333
22	6	0	3.787926	-0.705260	-1.741047
23	1	0	4.533573	-0.423420	-2.475349
24	6	0	3.725917	-1.991953	-1.218900
25	6	0	2.706195	-2.318375	-0.315816
26	1	0	2.634467	-3.343478	0.032281
27	6	0	-2.385638	-0.878111	-2.350912
28	1	0	-1.840752	-0.439228	-3.193822
29	6	0	-1.652032	-2.162654	-1.953028
30	1	0	-2.129972	-2.639951	-1.090285
31	1	0	-0.604980	-1.963762	-1.709458
32	1	0	-1.679430	-2.877170	-2.781597
33	6	0	-3.823796	-1.172640	-2.782916
34	1	0	-3.824567	-1.906875	-3.594940
35	1	0	-4.339926	-0.280719	-3.148200
36	1	0	-4.407162	-1.590866	-1.957103
37	6	0	-3.184563	1.867384	-1.674395
38	1	0	-4.216617	1.562099	-1.870896
39	6	0	-2.581112	2.344028	-3.000372
40	1	0	-3.098914	3.250665	-3.328461
41	1	0	-2.684978	1.599268	-3.794332
42	1	0	-1.519886	2.577358	-2.878166
43	6	0	-3.180808	2.998589	-0.640945
44	1	0	-2.157189	3.340644	-0.463134
45	1	0	-3.604402	2.687746	0.317982
46	1	0	-3.769696	3.843097	-1.013222
47	6	0	2.897763	2.878339	0.400319
48	1	0	3.739732	2.283814	0.029347
49	6	0	2.356336	3.734301	-0.747593
50	1	0	1.542740	4.377900	-0.398224
51	1	0	1.951483	3.134257	-1.563191
52	1	0	3.155466	4.373014	-1.139999
53	6	0	3.424441	3.802593	1.511401
54	1	0	4.065063	4.572923	1.069856
55	1	0	4.023870	3.272781	2.255020
56	1	0	2.604733	4.311176	2.029642
57	6	0	2.493829	0.964592	2.524771
58	1	0	2.677669	1.862067	3.128251
59	6	0	3.853263	0.314337	2.246513
60	1	0	4.358887	0.091465	3.193249
61	1	0	4.511756	0.964504	1.664697
62	1	0	3.744325	-0.622671	1.695731
63	6	0	1.609451	0.063023	3.392976
64	1	0	1.522544	-0.938145	2.968214
65	1	0	0.601444	0.472974	3.505335
66	1	0	2.052258	-0.037053	4.389919
67	7	0	0.682013	-1.710800	0.854088

68	7	0	-1.432457	-1.554392	1.355217
69	15	0	1.578229	1.734096	1.078566
70	15	0	-2.224515	0.419608	-1.018780
71	45	0	-0.132591	0.863746	-0.163744
72	1	0	0.062300	2.083487	-1.260869
73	8	0	4.575888	-3.010664	-1.536801
74	6	0	5.590684	-2.743167	-2.487768
75	1	0	6.141898	-3.674346	-2.608668
76	1	0	5.164638	-2.447846	-3.452617
77	1	0	6.272914	-1.962036	-2.135385

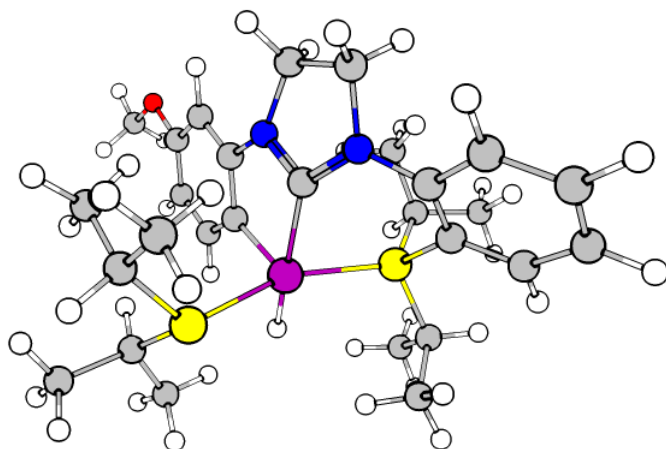
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SCF Done:  E(RwB97XD) = -6647.68580368      A.U. after   1 cycles
              Conv =   0.3688D-08              -V/T =   2.0049
Zero-point correction=                        0.667274 (Hartree/Particle)
Thermal correction to Energy=                  0.713074
Thermal correction to Enthalpy=                0.714129
Thermal correction to Gibbs Free Energy=       0.587669
Sum of electronic and zero-point Energies=    -6647.018529
Sum of electronic and thermal Energies=       -6646.972729
Sum of electronic and thermal Enthalpies=     -6646.971674
Sum of electronic and thermal Free Energies=   -6647.098135

              1              2              3
              A              A              A
Frequencies --  -222.8302          19.6111          28.2257

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C-P-OA-PR-*p*-OMe-conf1 (3b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.120003	-2.665317	2.099624
2	1	0	0.799793	-2.899621	2.919950
3	1	0	0.057039	-3.534096	1.435999
4	6	0	-0.386006	-0.567830	1.165711
5	6	0	-1.258213	-2.203569	2.600697

6	1	0	-2.044806	-2.937171	2.413938
7	1	0	-1.239221	-1.974665	3.669005
8	6	0	-2.802665	-0.510532	1.542959
9	6	0	-3.213154	-0.114376	0.246501
10	6	0	-4.557928	0.238376	0.084587
11	1	0	-4.917461	0.543496	-0.891527
12	6	0	-5.473767	0.203471	1.132314
13	1	0	-6.507398	0.481754	0.956548
14	6	0	-5.051196	-0.191862	2.396035
15	1	0	-5.747430	-0.220416	3.227620
16	6	0	-3.721591	-0.544453	2.594348
17	1	0	-3.384552	-0.841520	3.582067
18	6	0	1.626896	-1.493974	0.412174
19	6	0	1.570603	-0.460170	-0.547163
20	6	0	2.580936	-0.460786	-1.501371
21	1	0	2.592982	0.314928	-2.260848
22	6	0	3.595914	-1.430258	-1.520397
23	1	0	4.355173	-1.379590	-2.292609
24	6	0	3.614723	-2.431855	-0.551739
25	6	0	2.617266	-2.465600	0.429160
26	1	0	2.646504	-3.243984	1.185539
27	6	0	-2.183207	-1.709440	-1.978200
28	1	0	-1.548704	-1.627103	-2.867409
29	6	0	-1.569287	-2.785633	-1.079299
30	1	0	-2.129258	-2.885593	-0.143099
31	1	0	-0.524654	-2.562790	-0.850491
32	1	0	-1.603237	-3.754708	-1.586126
33	6	0	-3.603375	-2.083041	-2.406884
34	1	0	-3.597065	-3.063039	-2.894277
35	1	0	-4.025179	-1.367727	-3.117764
36	1	0	-4.273795	-2.144684	-1.544265
37	6	0	-2.842523	1.124385	-2.393483
38	1	0	-3.873230	0.804776	-2.575095
39	6	0	-2.092520	1.077296	-3.729814
40	1	0	-2.508177	1.829853	-4.406690
41	1	0	-2.183597	0.105761	-4.223001
42	1	0	-1.031132	1.297485	-3.584769
43	6	0	-2.851573	2.548541	-1.827493
44	1	0	-1.828494	2.912869	-1.693714
45	1	0	-3.363701	2.611861	-0.863627
46	1	0	-3.362881	3.219562	-2.524677
47	6	0	2.935898	2.850806	-0.312651
48	1	0	3.502046	1.926656	-0.480555
49	6	0	2.585158	3.445322	-1.679038
50	1	0	2.025809	4.380322	-1.563895
51	1	0	1.972668	2.763365	-2.271927
52	1	0	3.500672	3.666963	-2.239654
53	6	0	3.828458	3.833817	0.457631
54	1	0	4.658728	4.160806	-0.178283
55	1	0	4.264644	3.392657	1.356714

56	1	0	3.268279	4.727301	0.755727
57	6	0	2.089096	2.004908	2.329308
58	1	0	2.557130	2.948525	2.636698
59	6	0	3.155077	0.905581	2.386047
60	1	0	3.640616	0.893860	3.369778
61	1	0	3.935064	1.036390	1.630781
62	1	0	2.707338	-0.076599	2.221698
63	6	0	0.968453	1.729333	3.334802
64	1	0	0.440530	0.802305	3.093306
65	1	0	0.230986	2.537117	3.347531
66	1	0	1.381048	1.624966	4.345084
67	7	0	0.572844	-1.497126	1.348568
68	7	0	-1.494250	-0.979556	1.815569
69	15	0	1.380629	2.392135	0.635230
70	15	0	-2.032975	-0.032614	-1.187923
71	45	0	0.028875	0.823807	-0.311551
72	1	0	0.405731	1.595121	-1.689810
73	8	0	4.555879	-3.422862	-0.467448
74	6	0	5.590883	-3.423882	-1.431709
75	1	0	5.193963	-3.553952	-2.444774
76	1	0	6.180596	-2.501354	-1.388094
77	1	0	6.231088	-4.270096	-1.186173

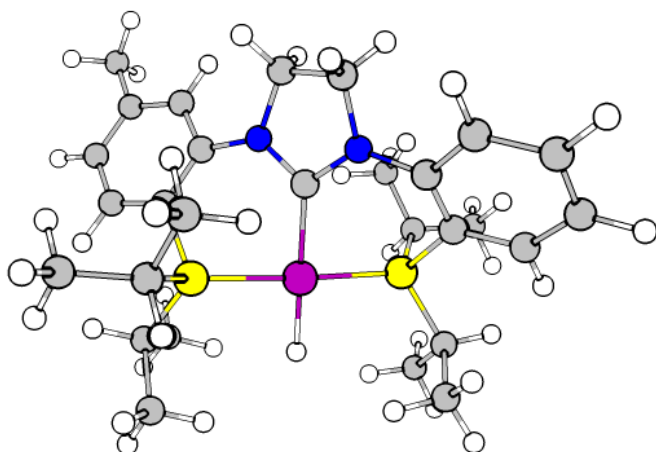
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SCF Done: E(RwB97XD) = -6647.70284536 A.U. after 1 cycles
          Conv = 0.3063D-08 -V/T = 2.0049
Zero-point correction= 0.667218 (Hartree/Particle)
Thermal correction to Energy= 0.713867
Thermal correction to Enthalpy= 0.714922
Thermal correction to Gibbs Free Energy= 0.584832
Sum of electronic and zero-point Energies= -6647.035628
Sum of electronic and thermal Energies= -6646.988978
Sum of electronic and thermal Enthalpies= -6646.987923
Sum of electronic and thermal Free Energies= -6647.118013

          1          2          3
          A          A          A
Frequencies -- 9.8061 25.0967 33.2050

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C-P-OA-SM-*p*-Me (1c)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.810108	-3.223977	0.283871
2	1	0	1.633688	-3.717509	0.801264
3	1	0	0.646515	-3.714216	-0.682006
4	6	0	-0.038036	-1.023719	0.284697
5	6	0	-0.462077	-3.195399	1.102465
6	1	0	-1.159547	-3.985588	0.822065
7	1	0	-0.246830	-3.269657	2.174024
8	6	0	-2.349520	-1.577291	1.086849
9	6	0	-3.125833	-0.602864	0.416074
10	6	0	-4.480672	-0.506855	0.751341
11	1	0	-5.101011	0.219043	0.238377
12	6	0	-5.078799	-1.305162	1.720608
13	1	0	-6.134007	-1.191491	1.945485
14	6	0	-4.299834	-2.236678	2.393633
15	1	0	-4.728948	-2.863992	3.168267
16	6	0	-2.954154	-2.370475	2.072934
17	1	0	-2.369042	-3.101035	2.617679
18	6	0	2.352375	-1.385820	-0.373857
19	6	0	2.908712	-0.106566	-0.143280
20	6	0	4.219547	0.107128	-0.580391
21	1	0	4.684262	1.070985	-0.407340
22	6	0	4.970341	-0.864148	-1.231975
23	1	0	5.986167	-0.641421	-1.545885
24	6	0	4.415266	-2.116379	-1.480656
25	6	0	3.115220	-2.354938	-1.039203
26	1	0	2.687706	-3.331151	-1.237697
27	6	0	-2.613207	-0.314632	-2.425549
28	1	0	-2.228660	0.397199	-3.164227
29	6	0	-1.742831	-1.572922	-2.506926
30	1	0	-2.057637	-2.319007	-1.769344
31	1	0	-0.689126	-1.339938	-2.334855

32	1	0	-1.839557	-2.026734	-3.498753
33	6	0	-4.071543	-0.638605	-2.758950
34	1	0	-4.131324	-1.127247	-3.737094
35	1	0	-4.699166	0.255385	-2.802381
36	1	0	-4.501493	-1.322107	-2.019995
37	6	0	-3.560536	1.987045	-0.882691
38	1	0	-4.570215	1.611584	-1.075797
39	6	0	-3.168967	2.904472	-2.046445
40	1	0	-3.804419	3.795961	-2.040569
41	1	0	-3.292279	2.418684	-3.018598
42	1	0	-2.127616	3.223501	-1.944640
43	6	0	-3.557597	2.763496	0.437819
44	1	0	-2.563080	3.177715	0.623565
45	1	0	-3.825998	2.134133	1.290827
46	1	0	-4.277990	3.586692	0.384947
47	6	0	2.822677	2.805234	0.151064
48	1	0	3.885366	2.706856	0.392973
49	6	0	2.670266	3.061386	-1.351566
50	1	0	1.613191	3.193540	-1.597357
51	1	0	3.057114	2.236777	-1.956596
52	1	0	3.213516	3.970832	-1.629880
53	6	0	2.262954	3.984550	0.954177
54	1	0	2.719668	4.915536	0.603421
55	1	0	2.473117	3.896744	2.023902
56	1	0	1.180524	4.060178	0.816024
57	6	0	2.316952	1.061880	2.446894
58	1	0	1.790379	1.901192	2.914240
59	6	0	3.805678	1.156063	2.790084
60	1	0	3.947326	1.046796	3.870411
61	1	0	4.242159	2.115377	2.499428
62	1	0	4.373919	0.359727	2.299183
63	6	0	1.709100	-0.227395	3.008353
64	1	0	2.176533	-1.110888	2.560486
65	1	0	0.633173	-0.273355	2.822085
66	1	0	1.875351	-0.275962	4.089493
67	7	0	1.078269	-1.794627	0.099614
68	7	0	-0.998082	-1.871619	0.771157
69	15	0	1.924668	1.248678	0.627880
70	15	0	-2.365477	0.564871	-0.793613
71	45	0	-0.232447	0.963039	-0.077398
72	1	0	-0.396110	2.603948	-0.370228
73	6	0	5.176676	-3.176773	-2.235257
74	1	0	6.252498	-3.078261	-2.076081
75	1	0	4.876769	-4.181742	-1.930087
76	1	0	4.992439	-3.087291	-3.309910

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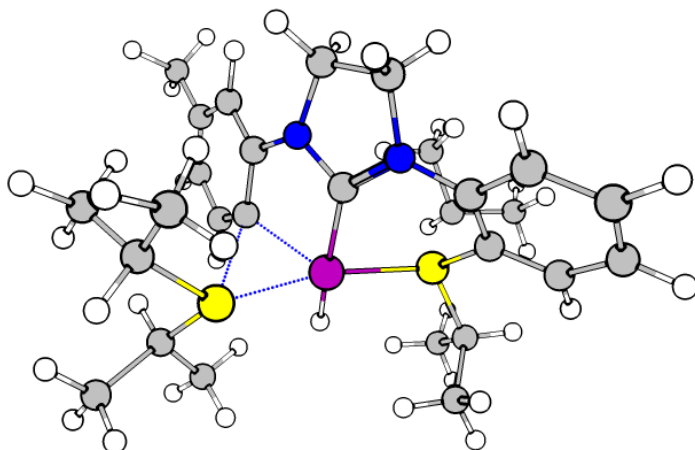
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SCF Done:  E(RwB97XD) = -6572.53899332      A.U. after   1 cycles
              Conv g =   0.2476D-08           -V/T =   2.0048
Zero-point correction=                      0.665146 (Hartree/Particle)
Thermal correction to Energy=                0.709557

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Thermal correction to Enthalpy=	0.710612
Thermal correction to Gibbs Free Energy=	0.587996
Sum of electronic and zero-point Energies=	-6571.873848
Sum of electronic and thermal Energies=	-6571.829436
Sum of electronic and thermal Enthalpies=	-6571.828381
Sum of electronic and thermal Free Energies=	-6571.950998

	1	2	3
	A	A	A
Frequencies --	26.0549	28.8721	49.1477

C-P-OA-T S-*p*-Me (2c)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.288090	-3.348460	-0.421008
2	1	0	-1.020647	-3.952565	-0.959905
3	1	0	-0.134081	-3.782108	0.573846
4	6	0	0.268942	-1.074646	-0.578438
5	6	0	1.026728	-3.201908	-1.193608
6	1	0	1.828160	-3.821628	-0.787876
7	1	0	0.894643	-3.440788	-2.252600
8	6	0	2.632718	-1.254178	-1.222360
9	6	0	3.144258	-0.170107	-0.469454
10	6	0	4.470326	0.202988	-0.713266
11	1	0	4.904164	1.025439	-0.156501
12	6	0	5.277419	-0.446069	-1.644114
13	1	0	6.300520	-0.118755	-1.795801
14	6	0	4.758221	-1.511906	-2.367671
15	1	0	5.365478	-2.032866	-3.100575
16	6	0	3.443553	-1.909269	-2.153776
17	1	0	3.038288	-2.733953	-2.729908
18	6	0	-1.801360	-1.509294	0.473250
19	6	0	-1.972247	-0.103105	0.600485
20	6	0	-2.897584	0.291115	1.570351

21	1	0	-3.031500	1.346970	1.775146
22	6	0	-3.676978	-0.620326	2.288900
23	1	0	-4.388352	-0.248241	3.021896
24	6	0	-3.564428	-1.989073	2.068152
25	6	0	-2.590840	-2.424009	1.159797
26	1	0	-2.441483	-3.490908	1.014356
27	6	0	2.472077	-0.210533	2.353946
28	1	0	1.939227	0.364934	3.118880
29	6	0	1.840048	-1.605050	2.310382
30	1	0	2.303288	-2.226074	1.535679
31	1	0	0.765085	-1.547447	2.121449
32	1	0	1.989997	-2.108638	3.270501
33	6	0	3.954715	-0.286543	2.725186
34	1	0	4.072254	-0.811875	3.678468
35	1	0	4.408208	0.701567	2.840483
36	1	0	4.523945	-0.837303	1.970115
37	6	0	2.985068	2.354849	1.021727
38	1	0	4.048578	2.170864	1.200413
39	6	0	2.425337	3.076899	2.251991
40	1	0	2.889737	4.064522	2.334761
41	1	0	2.633191	2.537336	3.180180
42	1	0	1.343979	3.210172	2.161694
43	6	0	2.826761	3.217737	-0.234304
44	1	0	1.768776	3.428322	-0.414592
45	1	0	3.230577	2.731733	-1.126648
46	1	0	3.351602	4.169058	-0.099982
47	6	0	-3.301570	2.441997	-0.656440
48	1	0	-4.055851	1.892791	-0.082445
49	6	0	-2.747063	3.572995	0.213855
50	1	0	-2.018628	4.168260	-0.345801
51	1	0	-2.233878	3.205955	1.103222
52	1	0	-3.564490	4.233139	0.524814
53	6	0	-3.993570	3.051603	-1.887661
54	1	0	-4.678439	3.842089	-1.563925
55	1	0	-4.584463	2.323892	-2.448240
56	1	0	-3.266872	3.502167	-2.571714
57	6	0	-2.917795	0.116096	-2.322869
58	1	0	-3.216014	0.830208	-3.099900
59	6	0	-4.197137	-0.520625	-1.769462
60	1	0	-4.742943	-1.017687	-2.579963
61	1	0	-4.869694	0.216607	-1.323543
62	1	0	-3.974349	-1.269716	-1.006276
63	6	0	-2.041370	-0.920388	-3.034206
64	1	0	-1.870909	-1.795902	-2.405985
65	1	0	-1.067600	-0.505557	-3.310293
66	1	0	-2.540508	-1.260252	-3.948073
67	7	0	-0.715790	-1.959267	-0.304611
68	7	0	1.332866	-1.773879	-1.023781
69	15	0	-1.950106	1.259228	-1.189828
70	15	0	2.110985	0.733635	0.784222

71	45	0	-0.063378	0.830185	0.032315
72	1	0	-0.290021	2.250763	0.841226
73	6	0	-4.445366	-2.985734	2.778812
74	1	0	-3.867967	-3.838718	3.145968
75	1	0	-4.951818	-2.529117	3.631846
76	1	0	-5.214525	-3.376277	2.105083

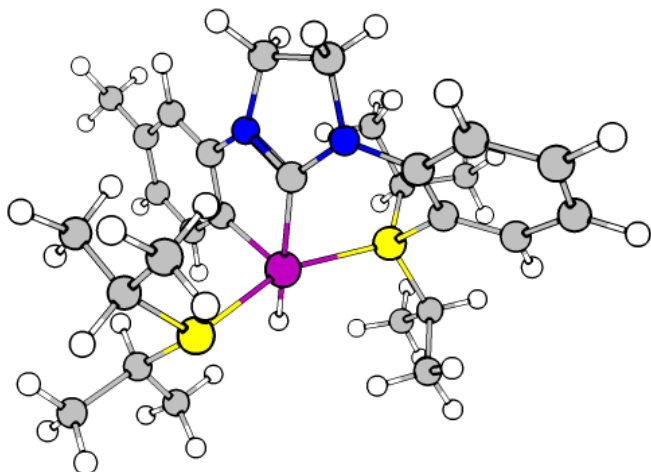
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SCF Done: E(RwB97XD) = -6572.48930774 A.U. after 1 cycles
              Conv g = 0.2248D-08 -V/T = 2.0048
Zero-point correction= 0.662853 (Hartree/Particle)
Thermal correction to Energy= 0.707435
Thermal correction to Enthalpy= 0.708490
Thermal correction to Gibbs Free Energy= 0.584525
Sum of electronic and zero-point Energies= -6571.826455
Sum of electronic and thermal Energies= -6571.781873
Sum of electronic and thermal Enthalpies= -6571.780818
Sum of electronic and thermal Free Energies= -6571.904782

              1              2              3
              A              A              A
Frequencies -- -224.6306          23.3920          25.4433

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C-P-OA-PR-*p*-Me (3c)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.017303	3.208973	1.275472
2	1	0	-0.662239	3.732408	1.949537
3	1	0	0.238283	3.859726	0.422654
4	6	0	0.271077	0.898130	0.939508
5	6	0	1.288260	2.727420	1.994193
6	1	0	2.179435	3.287105	1.703469
7	1	0	1.178059	2.782909	3.080096
8	6	0	2.633701	0.644697	1.520219

9	6	0	3.048990	-0.116395	0.400372
10	6	0	4.335711	-0.665433	0.446346
11	1	0	4.697308	-1.252256	-0.390234
12	6	0	5.191760	-0.482043	1.528644
13	1	0	6.180638	-0.927783	1.516805
14	6	0	4.766328	0.272149	2.615885
15	1	0	5.414699	0.422772	3.472645
16	6	0	3.493060	0.829107	2.605995
17	1	0	3.151417	1.407293	3.458298
18	6	0	-1.562191	1.831334	-0.177786
19	6	0	-1.605087	0.587370	-0.839566
20	6	0	-2.576513	0.452232	-1.830063
21	1	0	-2.664879	-0.490531	-2.361631
22	6	0	-3.448962	1.499841	-2.146143
23	1	0	-4.194716	1.352176	-2.924103
24	6	0	-3.386875	2.725447	-1.481719
25	6	0	-2.422878	2.881248	-0.479863
26	1	0	-2.357800	3.820541	0.065385
27	6	0	2.366121	0.978537	-2.224652
28	1	0	1.787557	0.740912	-3.124101
29	6	0	1.841777	2.310926	-1.683064
30	1	0	2.351637	2.585759	-0.753216
31	1	0	0.765218	2.270022	-1.502906
32	1	0	2.032654	3.106278	-2.409811
33	6	0	3.848414	1.071230	-2.591216
34	1	0	4.000917	1.880380	-3.312433
35	1	0	4.224724	0.152285	-3.048028
36	1	0	4.459241	1.290601	-1.710282
37	6	0	2.646198	-1.927862	-1.875467
38	1	0	3.718875	-1.790742	-2.042448
39	6	0	1.981136	-2.138113	-3.240759
40	1	0	2.335471	-3.078127	-3.674363
41	1	0	2.220466	-1.339986	-3.948630
42	1	0	0.894302	-2.198599	-3.135382
43	6	0	2.429011	-3.149014	-0.975014
44	1	0	1.359453	-3.332658	-0.834076
45	1	0	2.885816	-3.026701	0.010710
46	1	0	2.868292	-4.035698	-1.442506
47	6	0	-3.390090	-2.415156	0.093348
48	1	0	-3.854268	-1.508814	-0.314141
49	6	0	-3.047160	-3.338092	-1.078693
50	1	0	-2.575256	-4.260888	-0.723184
51	1	0	-2.357933	-2.863124	-1.779229
52	1	0	-3.959157	-3.612662	-1.621118
53	6	0	-4.406421	-3.111585	1.009835
54	1	0	-5.243182	-3.495603	0.415850
55	1	0	-4.826240	-2.440548	1.762807
56	1	0	-3.951127	-3.962119	1.529587
57	6	0	-2.582169	-1.011484	2.495937
58	1	0	-3.156423	-1.796283	3.004372

59	6	0	-3.533020	0.148209	2.183188
60	1	0	-4.031530	0.492034	3.098084
61	1	0	-4.308955	-0.130777	1.465260
62	1	0	-2.987604	0.993466	1.758253
63	6	0	-1.488564	-0.573026	3.472506
64	1	0	-0.871745	0.220603	3.042563
65	1	0	-0.826198	-1.403104	3.735064
66	1	0	-1.935057	-0.185814	4.395807
67	7	0	-0.557581	1.950730	0.806435
68	7	0	1.392567	1.324532	1.557769
69	15	0	-1.838902	-1.889850	1.012465
70	15	0	1.943411	-0.412440	-1.064705
71	45	0	-0.259578	-0.763839	-0.180555
72	1	0	-0.665065	-1.807777	-1.355383
73	6	0	-4.308979	3.865667	-1.841813
74	1	0	-3.816297	4.572560	-2.517572
75	1	0	-5.209263	3.502724	-2.343382
76	1	0	-4.620679	4.422398	-0.953703

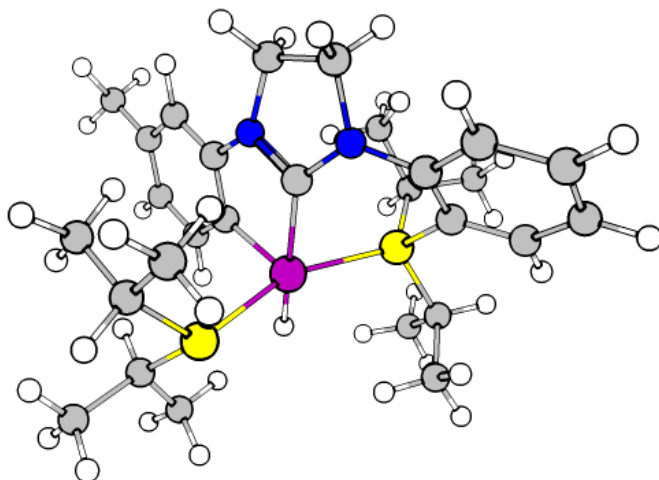
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SCF Done:  E(RwB97XD) = -6572.50700660      A.U. after   1 cycles
              Convg =   0.3105D-08              -V/T =   2.0048
Zero-point correction=                          0.662728 (Hartree/Particle)
Thermal correction to Energy=                    0.708112
Thermal correction to Enthalpy=                  0.709167
Thermal correction to Gibbs Free Energy=         0.583290
Sum of electronic and zero-point Energies=      -6571.844279
Sum of electronic and thermal Energies=         -6571.798895
Sum of electronic and thermal Enthalpies=       -6571.797840
Sum of electronic and thermal Free Energies=    -6571.923717

              1              2              3
              A              A              A
Frequencies --  22.9823          30.8291         40.4397

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C-P-OA-SM-*p*-Cl (1d)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.954915	-3.032713	0.607758
2	1	0	1.791701	-3.413806	1.193922
3	1	0	0.884178	-3.594631	-0.330113
4	6	0	-0.100041	-0.929645	0.410866
5	6	0	-0.351489	-3.070993	1.367966
6	1	0	-0.955676	-3.944649	1.121381
7	1	0	-0.180054	-3.044461	2.449406
8	6	0	-2.380957	-1.650049	1.164424
9	6	0	-3.220457	-0.808422	0.397875
10	6	0	-4.589888	-0.820416	0.685523
11	1	0	-5.257366	-0.197383	0.101729
12	6	0	-5.144289	-1.599258	1.695466
13	1	0	-6.212832	-1.572299	1.880996
14	6	0	-4.305856	-2.398904	2.460245
15	1	0	-4.701539	-3.006369	3.267710
16	6	0	-2.943023	-2.424173	2.189852
17	1	0	-2.312540	-3.053769	2.805156
18	6	0	2.350322	-1.101112	-0.094468
19	6	0	2.769204	0.244589	0.041037
20	6	0	4.080841	0.554505	-0.328488
21	1	0	4.435142	1.572535	-0.218003
22	6	0	4.978145	-0.378552	-0.836045
23	1	0	5.988358	-0.094555	-1.107054
24	6	0	4.532036	-1.680771	-0.984046
25	6	0	3.244781	-2.045378	-0.619130
26	1	0	2.944646	-3.074469	-0.764284
27	6	0	-2.650880	-0.669468	-2.445623
28	1	0	-2.293174	0.018600	-3.219428
29	6	0	-1.683961	-1.857676	-2.407125
30	1	0	-1.971978	-2.576315	-1.632202
31	1	0	-0.659402	-1.530629	-2.213521
32	1	0	-1.702859	-2.381241	-3.368401
33	6	0	-4.065550	-1.129555	-2.804983
34	1	0	-4.048215	-1.682620	-3.749835
35	1	0	-4.758588	-0.293579	-2.930192
36	1	0	-4.470126	-1.797167	-2.037844
37	6	0	-3.843838	1.638820	-1.086883
38	1	0	-4.812179	1.163283	-1.269799
39	6	0	-3.509499	2.506989	-2.304726
40	1	0	-4.237389	3.320985	-2.382670
41	1	0	-3.544737	1.943913	-3.241748
42	1	0	-2.513392	2.945040	-2.196955
43	6	0	-3.937551	2.501361	0.175715
44	1	0	-2.981672	3.000578	0.356275
45	1	0	-4.185495	1.914521	1.064410
46	1	0	-4.712883	3.264113	0.046988

47	6	0	2.367565	3.142277	-0.026548
48	1	0	3.418787	3.197855	0.273352
49	6	0	2.278685	3.194705	-1.554773
50	1	0	1.230722	3.173368	-1.865579
51	1	0	2.788955	2.352905	-2.031248
52	1	0	2.736350	4.119363	-1.921715
53	6	0	1.638684	4.338168	0.596626
54	1	0	2.010134	5.265713	0.149612
55	1	0	1.798184	4.406159	1.676586
56	1	0	0.563945	4.269542	0.405222
57	6	0	1.921542	1.630332	2.445188
58	1	0	1.277503	2.449282	2.784146
59	6	0	3.367292	1.939540	2.840461
60	1	0	3.452516	1.992544	3.930759
61	1	0	3.714570	2.895607	2.440399
62	1	0	4.049121	1.156698	2.493761
63	6	0	1.429184	0.349244	3.126595
64	1	0	2.015102	-0.519678	2.807689
65	1	0	0.376882	0.159161	2.901935
66	1	0	1.539505	0.442238	4.211842
67	7	0	1.099228	-1.597783	0.340598
68	7	0	-0.994649	-1.833405	0.915232
69	15	0	1.609984	1.565030	0.604209
70	15	0	-2.532363	0.336302	-0.875538
71	45	0	-0.466284	0.984913	-0.142231
72	1	0	-0.764190	2.561977	-0.616267
73	17	0	5.601817	-2.899516	-1.639027

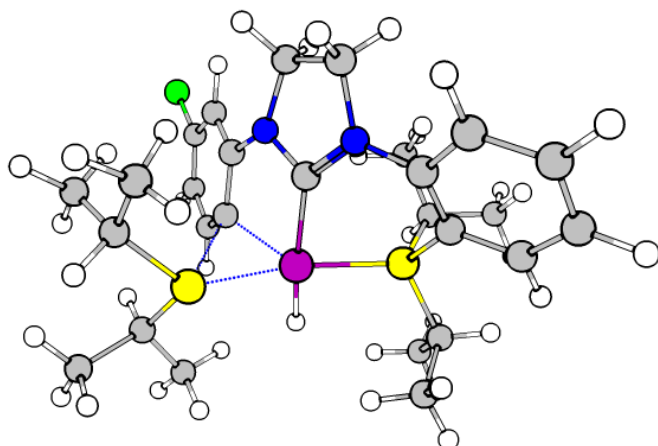
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SCF Done:  E(RwB97XD) = -6992.77562108      A.U. after   1 cycles
                Convrg =   0.4081D-08          -V/T =   2.0047
Zero-point correction=                        0.626520 (Hartree/Particle)
Thermal correction to Energy=                 0.670629
Thermal correction to Enthalpy=               0.671684
Thermal correction to Gibbs Free Energy=       0.549034
Sum of electronic and zero-point Energies=    -6992.149101
Sum of electronic and thermal Energies=       -6992.104992
Sum of electronic and thermal Enthalpies=     -6992.103937
Sum of electronic and thermal Free Energies=   -6992.226587

              1              2              3
              A              A              A
Frequencies --  21.4198      29.9201      47.8631

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C-P-OA-TS-*p*-Cl (2d)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.401695	-3.044900	1.217480
2	1	0	1.143213	-3.456382	1.904721
3	1	0	0.343192	-3.685473	0.329915
4	6	0	-0.345086	-0.848709	0.854238
5	6	0	-0.966915	-2.857448	1.880275
6	1	0	-1.689301	-3.619303	1.583569
7	1	0	-0.883525	-2.851784	2.970573
8	6	0	-2.723503	-1.105069	1.400059
9	6	0	-3.265240	-0.270867	0.393246
10	6	0	-4.630126	0.023343	0.478349
11	1	0	-5.088323	0.654165	-0.274303
12	6	0	-5.445377	-0.469565	1.493797
13	1	0	-6.499273	-0.213392	1.515249
14	6	0	-4.894909	-1.291050	2.469020
15	1	0	-5.508218	-1.685371	3.272461
16	6	0	-3.541295	-1.603832	2.417420
17	1	0	-3.113827	-2.236002	3.188125
18	6	0	1.808700	-1.306132	0.009532
19	6	0	1.874488	0.052352	-0.412265
20	6	0	2.807569	0.314387	-1.421692
21	1	0	2.863832	1.309459	-1.846763
22	6	0	3.695438	-0.645630	-1.913755
23	1	0	4.411591	-0.387586	-2.686269
24	6	0	3.654892	-1.924935	-1.386690
25	6	0	2.697529	-2.277254	-0.438059
26	1	0	2.641558	-3.299313	-0.080351
27	6	0	-2.390066	-0.883338	-2.307050
28	1	0	-1.863339	-0.442600	-3.160455
29	6	0	-1.637787	-2.159030	-1.915966
30	1	0	-2.095173	-2.635766	-1.041870
31	1	0	-0.587699	-1.950561	-1.694933

32	1	0	-1.674659	-2.878324	-2.739819
33	6	0	-3.832277	-1.193918	-2.713914
34	1	0	-3.838753	-1.930625	-3.523491
35	1	0	-4.363590	-0.308614	-3.073218
36	1	0	-4.397046	-1.615486	-1.876997
37	6	0	-3.206247	1.857391	-1.630233
38	1	0	-4.237848	1.540975	-1.810286
39	6	0	-2.627087	2.333209	-2.967470
40	1	0	-3.156654	3.234801	-3.290312
41	1	0	-2.738543	1.584984	-3.757069
42	1	0	-1.565862	2.575391	-2.863948
43	6	0	-3.198860	2.993129	-0.601823
44	1	0	-2.176453	3.346815	-0.440485
45	1	0	-3.605761	2.682600	0.364400
46	1	0	-3.801710	3.829689	-0.969393
47	6	0	2.934365	2.893888	0.323351
48	1	0	3.756750	2.304294	-0.096921
49	6	0	2.343913	3.775273	-0.780605
50	1	0	1.555508	4.419279	-0.378597
51	1	0	1.892331	3.194950	-1.585886
52	1	0	3.128636	4.413484	-1.201267
53	6	0	3.515898	3.793587	1.427194
54	1	0	4.140725	4.567787	0.970519
55	1	0	4.145143	3.246560	2.132535
56	1	0	2.724027	4.297795	1.990823
57	6	0	2.593132	0.962325	2.450832
58	1	0	2.802311	1.858416	3.047442
59	6	0	3.938930	0.304684	2.127499
60	1	0	4.475036	0.081402	3.056880
61	1	0	4.580486	0.949769	1.521658
62	1	0	3.808092	-0.633701	1.584055
63	6	0	1.730496	0.067723	3.347741
64	1	0	1.625396	-0.934396	2.929479
65	1	0	0.728942	0.483937	3.489695
66	1	0	2.202954	-0.031288	4.330882
67	7	0	0.727310	-1.676322	0.829472
68	7	0	-1.373955	-1.532138	1.389078
69	15	0	1.641478	1.739987	1.033583
70	15	0	-2.223759	0.421372	-0.983217
71	45	0	-0.133157	0.901746	-0.147154
72	1	0	0.019738	2.137696	-1.230748
73	17	0	4.787956	-3.140926	-1.942710

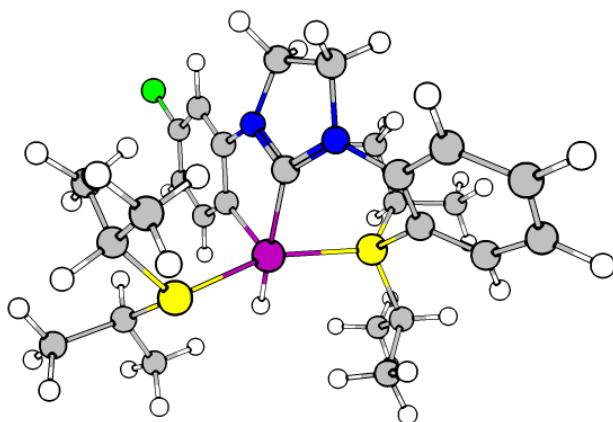
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SCF Done: E(RwB97XD) = -6992.72766407 A.U. after 1 cycles
          Conv g = 0.3103D-08 -V/T = 2.0048
Zero-point correction= 0.624565 (Hartree/Particle)
Thermal correction to Energy= 0.668618
Thermal correction to Enthalpy= 0.669673
Thermal correction to Gibbs Free Energy= 0.546806
Sum of electronic and zero-point Energies= -6992.103099

```

Sum of electronic and thermal Energies=	-6992.059046	
Sum of electronic and thermal Enthalpies=	-6992.057991	
Sum of electronic and thermal Free Energies=	-6992.180858	
1	2	3
A	A	A
Frequencies -- -237.9580	22.2829	26.2022

C-P-OA-PR-*p*-Cl (3d)



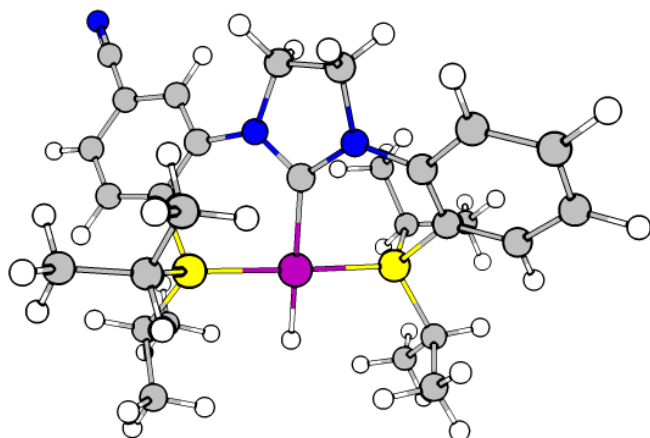
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.209431	-2.768504	1.916430
2	1	0	0.912271	-3.047171	2.702682
3	1	0	0.126776	-3.597960	1.206321
4	6	0	-0.329057	-0.624025	1.115568
5	6	0	-1.153936	-2.338989	2.482903
6	1	0	-1.944692	-3.063955	2.281384
7	1	0	-1.101982	-2.166461	3.560511
8	6	0	-2.729288	-0.585220	1.571107
9	6	0	-3.179400	-0.120436	0.311415
10	6	0	-4.524358	0.255026	0.215479
11	1	0	-4.914421	0.614608	-0.729803
12	6	0	-5.402419	0.178120	1.293045
13	1	0	-6.437475	0.477934	1.168718
14	6	0	-4.940998	-0.285573	2.519275
15	1	0	-5.607600	-0.347656	3.372975
16	6	0	-3.609963	-0.662865	2.651915
17	1	0	-3.241830	-1.013782	3.610411
18	6	0	1.661193	-1.496188	0.252235
19	6	0	1.572265	-0.412697	-0.647395
20	6	0	2.551211	-0.346447	-1.638742
21	1	0	2.531352	0.470102	-2.353243
22	6	0	3.565315	-1.304332	-1.741826
23	1	0	4.313452	-1.232097	-2.524246
24	6	0	3.607081	-2.349421	-0.829282

25	6	0	2.658455	-2.463633	0.182901
26	1	0	2.708167	-3.279350	0.896878
27	6	0	-2.226968	-1.617084	-2.016397
28	1	0	-1.634596	-1.489657	-2.928992
29	6	0	-1.572309	-2.733289	-1.199342
30	1	0	-2.093576	-2.882544	-0.247630
31	1	0	-0.519925	-2.517227	-1.001926
32	1	0	-1.623827	-3.676146	-1.751819
33	6	0	-3.664600	-1.975308	-2.397877
34	1	0	-3.678479	-2.931925	-2.929437
35	1	0	-4.119483	-1.229892	-3.055245
36	1	0	-4.294863	-2.079413	-1.509519
37	6	0	-2.892197	1.232111	-2.284446
38	1	0	-3.929969	0.923794	-2.443826
39	6	0	-2.188344	1.238528	-3.646605
40	1	0	-2.625412	2.018414	-4.277247
41	1	0	-2.298643	0.287973	-4.175254
42	1	0	-1.122117	1.451966	-3.529667
43	6	0	-2.875068	2.631481	-1.659919
44	1	0	-1.846262	2.985793	-1.545104
45	1	0	-3.355157	2.656917	-0.678078
46	1	0	-3.405462	3.332297	-2.311939
47	6	0	2.933820	2.889171	-0.248443
48	1	0	3.501514	1.977995	-0.472960
49	6	0	2.557628	3.552332	-1.576142
50	1	0	2.003680	4.481708	-1.403667
51	1	0	1.931798	2.902338	-2.190646
52	1	0	3.462471	3.799571	-2.142973
53	6	0	3.836993	3.833348	0.557364
54	1	0	4.655563	4.194240	-0.074996
55	1	0	4.289096	3.346972	1.424684
56	1	0	3.280820	4.709005	0.910442
57	6	0	2.122867	1.912619	2.363397
58	1	0	2.599980	2.838947	2.706639
59	6	0	3.181801	0.805562	2.355027
60	1	0	3.681759	0.746601	3.329600
61	1	0	3.951427	0.963177	1.594543
62	1	0	2.722565	-0.164995	2.156688
63	6	0	1.013115	1.598437	3.369738
64	1	0	0.478535	0.684127	3.096455
65	1	0	0.278786	2.407212	3.425183
66	1	0	1.437476	1.450895	4.369539
67	7	0	0.639240	-1.557487	1.220125
68	7	0	-1.415073	-1.075299	1.772168
69	15	0	1.395250	2.376948	0.698304
70	15	0	-2.047915	0.022769	-1.157317
71	45	0	0.039818	0.843821	-0.300143
72	1	0	0.378070	1.686425	-1.645430
73	17	0	4.875622	-3.557843	-0.945454

SCF Done: E(RwB97XD) = -6992.74650463 A.U. after 1 cycles
 Conv = 0.2879D-08 -V/T = 2.0048
 Zero-point correction= 0.625393 (Hartree/Particle)
 Thermal correction to Energy= 0.670101
 Thermal correction to Enthalpy= 0.671156
 Thermal correction to Gibbs Free Energy= 0.546269
 Sum of electronic and zero-point Energies= -6992.121112
 Sum of electronic and thermal Energies= -6992.076404
 Sum of electronic and thermal Enthalpies= -6992.075349
 Sum of electronic and thermal Free Energies= -6992.200236

1 2 3
 A A A
 Frequencies -- 27.0065 28.2360 32.5697

C-P-OA-SM-p-CN (1e)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.944460	-3.094620	0.536882
2	1	0	1.777478	-3.508615	1.106033
3	1	0	0.845094	-3.639118	-0.408510
4	6	0	-0.055780	-0.960903	0.382780
5	6	0	-0.353188	-3.107438	1.313551
6	1	0	-0.984905	-3.959848	1.062213
7	1	0	-0.167855	-3.100964	2.392885
8	6	0	-2.345383	-1.626677	1.153169
9	6	0	-3.169127	-0.755415	0.403197
10	6	0	-4.534963	-0.731816	0.706611
11	1	0	-5.191778	-0.085818	0.135866
12	6	0	-5.098915	-1.503692	1.716584
13	1	0	-6.164050	-1.448276	1.914712
14	6	0	-4.274600	-2.332704	2.465221
15	1	0	-4.677963	-2.935432	3.272370
16	6	0	-2.916203	-2.393738	2.178599
17	1	0	-2.295864	-3.045591	2.781016

18	6	0	2.379962	-1.189927	-0.158073
19	6	0	2.835537	0.144431	-0.010387
20	6	0	4.146834	0.436101	-0.399121
21	1	0	4.522399	1.444596	-0.275690
22	6	0	5.010318	-0.508254	-0.936001
23	1	0	6.021787	-0.242019	-1.219933
24	6	0	4.540067	-1.808453	-1.099322
25	6	0	3.242172	-2.142572	-0.712781
26	1	0	2.913604	-3.162058	-0.865392
27	6	0	-2.626921	-0.602572	-2.445808
28	1	0	-2.264019	0.085008	-3.217584
29	6	0	-1.688118	-1.813787	-2.433647
30	1	0	-1.979774	-2.532599	-1.660270
31	1	0	-0.652640	-1.513430	-2.255585
32	1	0	-1.736290	-2.328040	-3.398811
33	6	0	-4.056953	-1.025705	-2.789734
34	1	0	-4.065889	-1.567671	-3.741019
35	1	0	-4.732383	-0.172947	-2.895525
36	1	0	-4.465785	-1.692976	-2.024622
37	6	0	-3.741810	1.722541	-1.050634
38	1	0	-4.723546	1.274068	-1.230466
39	6	0	-3.396135	2.596525	-2.261226
40	1	0	-4.102615	3.430599	-2.321139
41	1	0	-3.456631	2.046739	-3.204736
42	1	0	-2.387631	3.006866	-2.159005
43	6	0	-3.803386	2.571983	0.222959
44	1	0	-2.836359	3.051299	0.397965
45	1	0	-4.052371	1.979364	1.107547
46	1	0	-4.565727	3.350321	0.111997
47	6	0	2.513641	3.055197	0.006313
48	1	0	3.567095	3.077247	0.302029
49	6	0	2.416752	3.150711	-1.519651
50	1	0	1.366879	3.163634	-1.824210
51	1	0	2.903424	2.310367	-2.022653
52	1	0	2.895015	4.073434	-1.864021
53	6	0	1.817187	4.251765	0.664993
54	1	0	2.212485	5.180752	0.242412
55	1	0	1.980963	4.286035	1.745861
56	1	0	0.740613	4.218014	0.474584
57	6	0	2.051316	1.481791	2.438988
58	1	0	1.442327	2.315324	2.805955
59	6	0	3.511383	1.727331	2.826838
60	1	0	3.607065	1.750336	3.917197
61	1	0	3.891774	2.679235	2.447789
62	1	0	4.161087	0.928074	2.456576
63	6	0	1.517682	0.203736	3.094345
64	1	0	2.068429	-0.678873	2.751475
65	1	0	0.457394	0.056812	2.875204
66	1	0	1.640272	0.268325	4.180187
67	7	0	1.125277	-1.659805	0.290532

68	7	0	-0.966931	-1.845726	0.886062
69	15	0	1.716584	1.483528	0.600231
70	15	0	-2.464771	0.382718	-0.867366
71	45	0	-0.374060	0.969011	-0.144256
72	1	0	-0.636956	2.557036	-0.597942
73	6	0	5.390496	-2.823432	-1.664298
74	7	0	6.076429	-3.643160	-2.116351

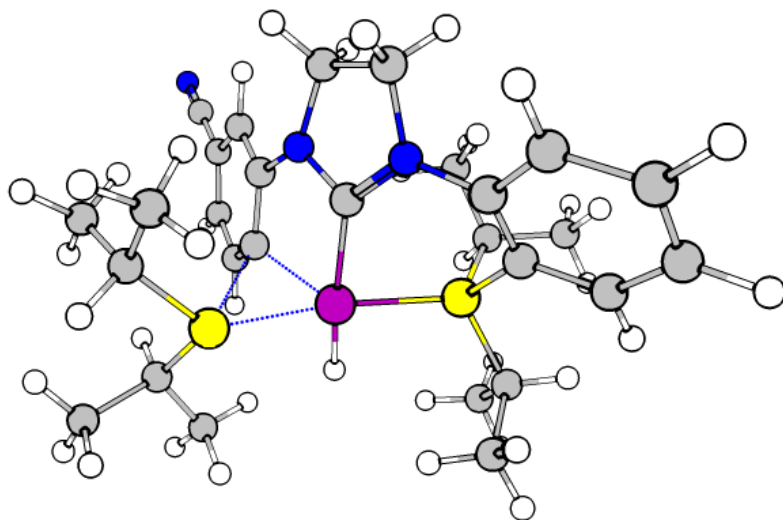
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SCF Done: E(RwB97XD) = -6625.44620733      A.U. after   1 cycles
              Convg =   0.4759D-08          -V/T =  2.0049
Zero-point correction=                      0.634716 (Hartree/Particle)
Thermal correction to Energy=                0.679586
Thermal correction to Enthalpy=              0.680641
Thermal correction to Gibbs Free Energy=      0.556088
Sum of electronic and zero-point Energies=    -6624.811492
Sum of electronic and thermal Energies=       -6624.766621
Sum of electronic and thermal Enthalpies=     -6624.765566
Sum of electronic and thermal Free Energies=   -6624.890119

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	1	2	3
	A	A	A
Frequencies --	24.3023	27.8269	43.0396

C-P-OA-TS-*p*-CN (2e)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.337348	-3.122460	-1.087753
2	1	0	-1.070557	-3.594472	-1.744075
3	1	0	-0.244693	-3.716214	-0.171199
4	6	0	0.323325	-0.883374	-0.849536
5	6	0	1.016756	-2.915729	-1.776433
6	1	0	1.774161	-3.626641	-1.442763

7	1	0	0.925050	-2.979205	-2.863923
8	6	0	2.705852	-1.073881	-1.389076
9	6	0	3.217277	-0.201070	-0.399603
10	6	0	4.571834	0.136532	-0.489163
11	1	0	5.007692	0.799158	0.249224
12	6	0	5.404337	-0.351967	-1.492662
13	1	0	6.449127	-0.061441	-1.518651
14	6	0	4.883451	-1.212607	-2.450300
15	1	0	5.511593	-1.604002	-3.243550
16	6	0	3.540640	-1.568265	-2.393927
17	1	0	3.133847	-2.231869	-3.149448
18	6	0	-1.776582	-1.390404	0.088466
19	6	0	-1.866675	-0.013155	0.464319
20	6	0	-2.755249	0.258095	1.518583
21	1	0	-2.812128	1.265482	1.913251
22	6	0	-3.587829	-0.707323	2.074661
23	1	0	-4.273416	-0.442094	2.872457
24	6	0	-3.551240	-2.015532	1.590081
25	6	0	-2.613995	-2.363992	0.604027
26	1	0	-2.544017	-3.394726	0.273727
27	6	0	2.333797	-0.771968	2.316460
28	1	0	1.798951	-0.314690	3.156042
29	6	0	1.603715	-2.071258	1.964138
30	1	0	2.073774	-2.570508	1.109726
31	1	0	0.551209	-1.887730	1.733290
32	1	0	1.647806	-2.761731	2.811762
33	6	0	3.780900	-1.044675	2.732572
34	1	0	3.799480	-1.759889	3.560811
35	1	0	4.295123	-0.140864	3.069709
36	1	0	4.354475	-1.477217	1.907352
37	6	0	3.086632	1.971979	1.572288
38	1	0	4.124686	1.688824	1.769847
39	6	0	2.481917	2.469270	2.890202
40	1	0	2.985659	3.392296	3.192592
41	1	0	2.604086	1.746419	3.701373
42	1	0	1.416251	2.682399	2.769900
43	6	0	3.058063	3.076399	0.510432
44	1	0	2.027550	3.393612	0.326117
45	1	0	3.487874	2.749887	-0.440497
46	1	0	3.629337	3.941868	0.860548
47	6	0	-3.127223	2.714055	-0.360291
48	1	0	-3.887743	2.103756	0.140055
49	6	0	-2.535091	3.693417	0.656857
50	1	0	-1.810484	4.357015	0.174878
51	1	0	-2.008442	3.190044	1.468401
52	1	0	-3.334999	4.308079	1.083342
53	6	0	-3.821853	3.510046	-1.478102
54	1	0	-4.475290	4.265038	-1.029609
55	1	0	-4.446165	2.885716	-2.120475
56	1	0	-3.095440	4.034313	-2.107561

57	6	0	-2.760202	0.702511	-2.417817
58	1	0	-3.036088	1.558742	-3.044700
59	6	0	-4.058315	-0.005733	-2.015619
60	1	0	-4.616551	-0.292713	-2.913762
61	1	0	-4.709374	0.630054	-1.410166
62	1	0	-3.860475	-0.914527	-1.443347
63	6	0	-1.884060	-0.188943	-3.305117
64	1	0	-1.744734	-1.176783	-2.863697
65	1	0	-0.896881	0.251116	-3.472694
66	1	0	-2.367500	-0.326555	-4.277942
67	7	0	-0.712137	-1.750065	-0.759258
68	7	0	1.370646	-1.546784	-1.368714
69	15	0	-1.807204	1.592992	-1.070397
70	15	0	2.151213	0.491724	0.957637
71	45	0	0.058618	0.905723	0.080743
72	1	0	-0.118826	2.181724	1.106875
73	6	0	-4.434586	-3.014418	2.117547
74	7	0	-5.148700	-3.827897	2.541305

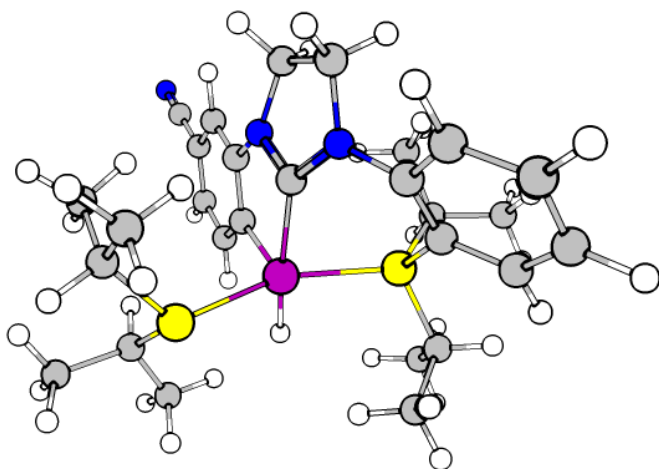
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SCF Done:  E(RwB97XD) = -6625.40230528      A.U. after   1 cycles
              Convg =   0.2062D-08              -V/T =   2.0049
Zero-point correction=                          0.633236 (Hartree/Particle)
Thermal correction to Energy=                    0.677811
Thermal correction to Enthalpy=                  0.678866
Thermal correction to Gibbs Free Energy=          0.555477
Sum of electronic and zero-point Energies=       -6624.769070
Sum of electronic and thermal Energies=          -6624.724494
Sum of electronic and thermal Enthalpies=        -6624.723439
Sum of electronic and thermal Free Energies=      -6624.846828

              1              2              3
              A              A              A
Frequencies --  -228.8381          26.3097          27.8224

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C-P-OA-PR-*p*-CN (3e)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.172862	2.878210	1.814148
2	1	0	-0.869191	3.208323	2.585986
3	1	0	-0.053242	3.680201	1.078197
4	6	0	0.290439	0.691277	1.083586
5	6	0	1.169657	2.415155	2.403764
6	1	0	1.988885	3.102470	2.185155
7	1	0	1.104266	2.277506	3.485491
8	6	0	2.681125	0.567904	1.566460
9	6	0	3.124722	0.047250	0.326900
10	6	0	4.451420	-0.393294	0.260129
11	1	0	4.836270	-0.797982	-0.668803
12	6	0	5.317595	-0.326970	1.347999
13	1	0	6.338184	-0.680375	1.247374
14	6	0	4.862907	0.192601	2.554122
15	1	0	5.520479	0.247331	3.415232
16	6	0	3.549650	0.636096	2.657228
17	1	0	3.186038	1.031334	3.600045
18	6	0	-1.662450	1.607668	0.182615
19	6	0	-1.605899	0.490540	-0.686101
20	6	0	-2.580562	0.423070	-1.686021
21	1	0	-2.577995	-0.417121	-2.372404
22	6	0	-3.557685	1.406595	-1.823679
23	1	0	-4.302807	1.332691	-2.608950
24	6	0	-3.582200	2.494385	-0.944813
25	6	0	-2.623857	2.599141	0.074081
26	1	0	-2.649729	3.438565	0.761623
27	6	0	2.254997	1.519869	-2.050592
28	1	0	1.669825	1.388761	-2.967290
29	6	0	1.633491	2.683776	-1.275404
30	1	0	2.149322	2.843727	-0.322560
31	1	0	0.571721	2.512918	-1.084167
32	1	0	1.725546	3.606511	-1.855648
33	6	0	3.710486	1.810612	-2.421682
34	1	0	3.769480	2.751499	-2.977458
35	1	0	4.142833	1.030115	-3.052982
36	1	0	4.333082	1.912662	-1.527776
37	6	0	2.808514	-1.360647	-2.237553
38	1	0	3.861192	-1.103874	-2.389777
39	6	0	2.122379	-1.368470	-3.608830
40	1	0	2.530859	-2.183708	-4.213158
41	1	0	2.283750	-0.438191	-4.159826
42	1	0	1.045968	-1.529937	-3.502378
43	6	0	2.717198	-2.741439	-1.578860
44	1	0	1.670592	-3.038032	-1.461389
45	1	0	3.191061	-2.766901	-0.594008
46	1	0	3.213007	-3.484879	-2.210439
47	6	0	-3.088213	-2.745271	-0.197598

48	1	0	-3.629722	-1.822303	-0.438256
49	6	0	-2.736517	-3.445023	-1.513098
50	1	0	-2.208055	-4.385886	-1.324591
51	1	0	-2.095363	-2.825325	-2.142944
52	1	0	-3.650487	-3.677485	-2.071106
53	6	0	-4.016130	-3.645485	0.630218
54	1	0	-4.847389	-3.994222	0.007936
55	1	0	-4.450120	-3.128073	1.488734
56	1	0	-3.485194	-4.530020	0.999234
57	6	0	-2.241650	-1.733541	2.389339
58	1	0	-2.750436	-2.634453	2.753948
59	6	0	-3.261178	-0.590868	2.352336
60	1	0	-3.756472	-0.487623	3.325358
61	1	0	-4.037929	-0.742616	1.597849
62	1	0	-2.767726	0.357065	2.127982
63	6	0	-1.121419	-1.434393	3.388588
64	1	0	-0.558981	-0.542541	3.097695
65	1	0	-0.412429	-2.264211	3.459625
66	1	0	-1.540153	-1.254754	4.385311
67	7	0	-0.644284	1.661876	1.153529
68	7	0	1.386661	1.120796	1.734087
69	15	0	-1.533219	-2.262713	0.736548
70	15	0	2.005643	-0.088308	-1.150945
71	45	0	-0.125441	-0.800674	-0.295259
72	1	0	-0.483966	-1.668558	-1.618170
73	6	0	-4.587111	3.510864	-1.080055
74	7	0	-5.397741	4.336663	-1.187540

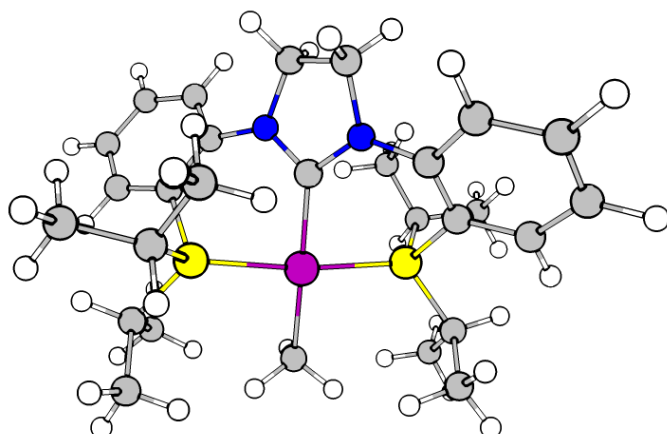
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SCF Done: E(RwB97XD) = -6625.42138525 A.U. after 1 cycles
          Conv = 0.2494D-08 -V/T = 2.0049
Zero-point correction= 0.633576 (Hartree/Particle)
Thermal correction to Energy= 0.679004
Thermal correction to Enthalpy= 0.680059
Thermal correction to Gibbs Free Energy= 0.554185
Sum of electronic and zero-point Energies= -6624.787809
Sum of electronic and thermal Energies= -6624.742381
Sum of electronic and thermal Enthalpies= -6624.741326
Sum of electronic and thermal Free Energies= -6624.867200

          1          2          3
          A          A          A
Frequencies -- 24.8968 31.5315 34.4664

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C-P-OA-SM-CH₃ (1f)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.573346	-3.355684	-0.562393
2	1	0	1.386071	-4.025188	-0.278528
3	1	0	0.234695	-3.607906	-1.573506
4	6	0	0.006247	-1.126226	-0.013617
5	6	0	-0.572868	-3.377149	0.421224
6	1	0	-1.391446	-4.025224	0.105829
7	1	0	-0.233916	-3.683826	1.417145
8	6	0	-2.247847	-1.633215	0.953524
9	6	0	-2.997277	-0.519142	0.519705
10	6	0	-4.297710	-0.385380	1.021327
11	1	0	-4.916358	0.439086	0.688888
12	6	0	-4.850561	-1.275662	1.936066
13	1	0	-5.863417	-1.126651	2.295112
14	6	0	-4.085559	-2.345320	2.382464
15	1	0	-4.480519	-3.046673	3.110224
16	6	0	-2.800193	-2.521255	1.886864
17	1	0	-2.218331	-3.362021	2.244825
18	6	0	2.266707	-1.599842	-0.991472
19	6	0	3.010966	-0.500475	-0.511428
20	6	0	4.315815	-0.346145	-0.993737
21	1	0	4.927098	0.469849	-0.628448
22	6	0	4.881462	-1.205457	-1.930615
23	1	0	5.897876	-1.042786	-2.273232
24	6	0	4.124354	-2.261898	-2.419174
25	1	0	4.529659	-2.939713	-3.163375
26	6	0	2.832724	-2.455722	-1.946005
27	1	0	2.257536	-3.285250	-2.338889
28	6	0	-2.648252	0.098720	-2.307662
29	1	0	-2.320636	0.910495	-2.967003
30	6	0	-1.813701	-1.134605	-2.667353
31	1	0	-2.090859	-1.993233	-2.046540
32	1	0	-0.745168	-0.944469	-2.542170

33	1	0	-1.995569	-1.407883	-3.711861
34	6	0	-4.135184	-0.172332	-2.552819
35	1	0	-4.281614	-0.550694	-3.569856
36	1	0	-4.750285	0.724995	-2.449487
37	1	0	-4.516435	-0.928202	-1.859134
38	6	0	-3.432954	2.179475	-0.446402
39	1	0	-4.448209	1.799414	-0.594268
40	6	0	-3.187419	3.205000	-1.563573
41	1	0	-3.776451	4.106489	-1.366699
42	1	0	-3.498872	2.819044	-2.538114
43	1	0	-2.138978	3.497189	-1.633979
44	6	0	-3.373045	2.812377	0.949955
45	1	0	-2.384108	3.215703	1.166219
46	1	0	-3.611251	2.091847	1.736083
47	1	0	-4.100590	3.628544	1.012446
48	6	0	3.446722	2.148753	0.602715
49	1	0	4.453249	1.747444	0.753987
50	6	0	3.428111	2.872764	-0.749514
51	1	0	2.474551	3.370709	-0.919535
52	1	0	3.597647	2.188817	-1.584904
53	1	0	4.220981	3.628085	-0.768742
54	6	0	3.179456	3.106533	1.774129
55	1	0	3.723441	4.042705	1.614436
56	1	0	3.522004	2.687181	2.723921
57	1	0	2.120065	3.348864	1.877372
58	6	0	2.574202	0.005447	2.331929
59	1	0	2.267796	0.812111	3.007214
60	6	0	4.046093	-0.328801	2.592763
61	1	0	4.161144	-0.736097	3.602644
62	1	0	4.699930	0.543601	2.519815
63	1	0	4.407945	-1.083396	1.887388
64	6	0	1.691996	-1.203853	2.655786
65	1	0	1.950805	-2.062760	2.027594
66	1	0	0.632823	-0.976615	2.518281
67	1	0	1.848850	-1.498643	3.698615
68	7	0	0.991725	-1.953030	-0.492177
69	7	0	-0.981292	-1.970163	0.423742
70	15	0	2.238229	0.727907	0.632607
71	15	0	-2.245029	0.749699	-0.596203
72	45	0	0.008062	0.904387	-0.029449
73	6	0	0.049217	3.055530	-0.215532
74	1	0	0.831423	3.565568	0.356780
75	1	0	0.249768	3.286474	-1.276668
76	1	0	-0.875230	3.585236	0.035419

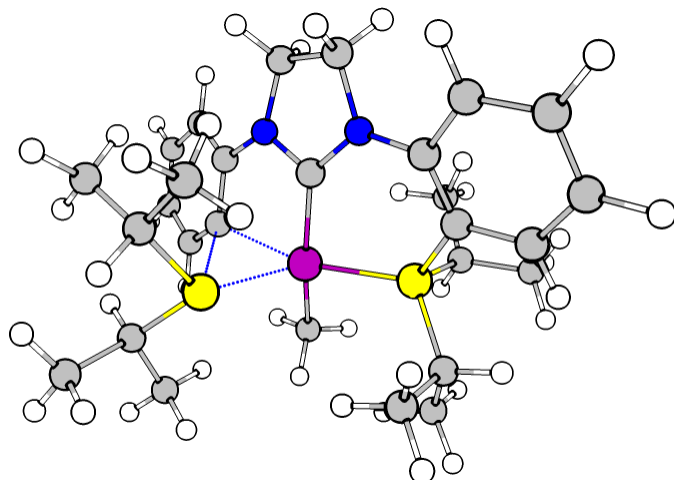
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SCF Done:  E(RwB97XD) = -6572.51904857      A.U. after   1 cycles
              Conv g =   0.2182D-08          -V/T =   2.0048
Zero-point correction=                      0.667099 (Hartree/Particle)
Thermal correction to Energy=                0.711695
Thermal correction to Enthalpy=              0.712750

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Thermal correction to Gibbs Free Energy=	0.590728		
Sum of electronic and zero-point Energies=	-6571.851950		
Sum of electronic and thermal Energies=	-6571.807353		
Sum of electronic and thermal Enthalpies=	-6571.806298		
Sum of electronic and thermal Free Energies=	-6571.928320		
	1	2	3
	A	A	A
Frequencies --	22.0275	35.4955	57.7476

C-P-OA-TS-CH₃ (2f)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.533608	3.481818	-0.852505
2	1	0	-1.267637	4.189063	-0.461734
3	1	0	-0.399585	3.663833	-1.924589
4	6	0	0.079874	1.307425	-0.201477
5	6	0	0.789161	3.537141	-0.091939
6	1	0	1.565368	4.079436	-0.633549
7	1	0	0.654893	3.995831	0.892583
8	6	0	2.383159	1.724626	0.593773
9	6	0	2.919753	0.420135	0.476763
10	6	0	4.192487	0.204154	1.022499
11	1	0	4.645853	-0.775846	0.942493
12	6	0	4.926784	1.194194	1.664753
13	1	0	5.908139	0.969653	2.068556
14	6	0	4.381173	2.465732	1.777069
15	1	0	4.922173	3.261726	2.278233
16	6	0	3.125932	2.722191	1.243628
17	1	0	2.719157	3.719179	1.352431
18	6	0	-2.077181	1.489684	-1.155859
19	6	0	-2.276307	0.121135	-0.852573
20	6	0	-3.333573	-0.496206	-1.530948
21	1	0	-3.503107	-1.558096	-1.400732

22	6	0	-4.194526	0.200340	-2.379353
23	1	0	-5.006848	-0.325226	-2.871787
24	6	0	-4.009201	1.562505	-2.590480
25	1	0	-4.679984	2.119229	-3.237098
26	6	0	-2.931693	2.209010	-1.989166
27	1	0	-2.755180	3.261846	-2.185746
28	6	0	2.896326	-1.067319	-2.013164
29	1	0	2.415518	-1.925183	-2.497096
30	6	0	2.548403	0.183499	-2.827911
31	1	0	2.958361	1.084267	-2.357685
32	1	0	1.466145	0.307297	-2.923774
33	1	0	2.977575	0.107443	-3.831823
34	6	0	4.407013	-1.302350	-1.973615
35	1	0	4.786552	-1.440545	-2.991133
36	1	0	4.677248	-2.193704	-1.400220
37	1	0	4.929438	-0.444321	-1.541145
38	6	0	2.633997	-2.462355	0.589723
39	1	0	3.718065	-2.388299	0.706948
40	6	0	2.354954	-3.775166	-0.146594
41	1	0	2.768845	-4.604238	0.436469
42	1	0	2.819069	-3.805816	-1.136236
43	1	0	1.285521	-3.944705	-0.266528
44	6	0	1.991970	-2.459846	1.980367
45	1	0	0.905217	-2.549484	1.900106
46	1	0	2.213085	-1.540695	2.530633
47	1	0	2.370220	-3.304569	2.565184
48	6	0	-3.484064	-1.664096	1.282162
49	1	0	-4.252267	-1.198032	0.657979
50	6	0	-3.214654	-3.085998	0.777483
51	1	0	-2.488756	-3.587787	1.426191
52	1	0	-2.806894	-3.110914	-0.232321
53	1	0	-4.141430	-3.670509	0.788515
54	6	0	-4.033337	-1.750194	2.715584
55	1	0	-4.815247	-2.515765	2.754946
56	1	0	-4.481735	-0.813748	3.054905
57	1	0	-3.255891	-2.040939	3.430986
58	6	0	-2.406280	0.848145	2.207267
59	1	0	-2.712680	0.338923	3.128429
60	6	0	-3.609385	1.663564	1.726662
61	1	0	-3.979514	2.300522	2.538638
62	1	0	-4.434248	1.026773	1.395441
63	1	0	-3.343571	2.313910	0.890417
64	6	0	-1.240368	1.753097	2.625600
65	1	0	-1.048428	2.526197	1.879703
66	1	0	-0.316027	1.187905	2.776290
67	1	0	-1.484034	2.263398	3.563718
68	7	0	-0.933749	2.103266	-0.619307
69	7	0	1.140021	2.114387	0.048465
70	15	0	-1.878775	-0.675609	1.241247
71	15	0	2.038471	-0.979394	-0.364563

72	45	0	-0.258544	-0.657152	-0.456200
73	6	0	-0.583351	-2.575087	-1.393941
74	1	0	-0.674012	-3.427068	-0.707487
75	1	0	-1.506566	-2.543938	-1.988344
76	1	0	0.221607	-2.832348	-2.099007

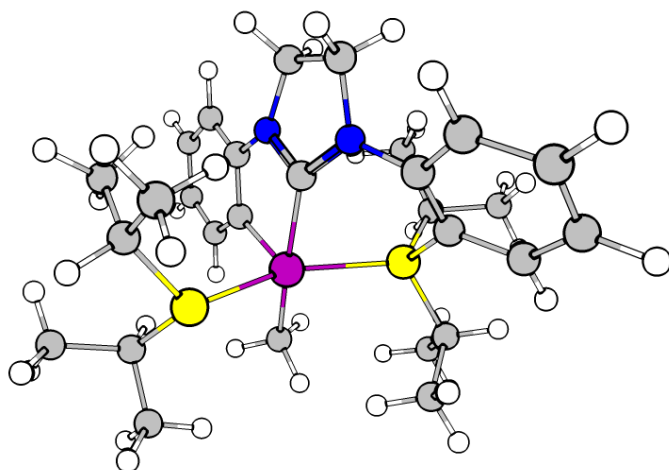
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SCF Done:  E(RwB97XD) = -6572.47191505      A.U. after   1 cycles
              Conv g =   0.3338D-08              -V/T =   2.0048
Zero-point correction=                        0.664727 (Hartree/Particle)
Thermal correction to Energy=                  0.709037
Thermal correction to Enthalpy=                0.710092
Thermal correction to Gibbs Free Energy=       0.588499
Sum of electronic and zero-point Energies=     -6571.807188
Sum of electronic and thermal Energies=        -6571.762878
Sum of electronic and thermal Enthalpies=      -6571.761823
Sum of electronic and thermal Free Energies=    -6571.883416

              1              2              3
              A              A              A
Frequencies --  -222.8847          30.6261          32.9130

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C-P-OA-PR-CH₃ (3f)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.051957	-3.502613	0.549355
2	1	0	-0.665883	-4.280306	0.283691
3	1	0	0.438137	-3.705333	1.553969
4	6	0	0.148823	-1.274509	-0.190587
5	6	0	1.167318	-3.362460	-0.497503
6	1	0	2.133046	-3.729109	-0.144053
7	1	0	0.911016	-3.883311	-1.423985
8	6	0	2.360347	-1.267210	-1.239751
9	6	0	2.853448	-0.056827	-0.699106
10	6	0	4.053501	0.427641	-1.233687

11	1	0	4.484161	1.343293	-0.847812
12	6	0	4.745126	-0.227902	-2.248410
13	1	0	5.671422	0.190934	-2.626935
14	6	0	4.238641	-1.413417	-2.767029
15	1	0	4.756113	-1.935682	-3.564843
16	6	0	3.051535	-1.926166	-2.259524
17	1	0	2.644906	-2.845496	-2.667647
18	6	0	-1.515064	-1.679309	1.410379
19	6	0	-1.655492	-0.275974	1.404540
20	6	0	-2.598470	0.249618	2.289081
21	1	0	-2.756469	1.321870	2.334466
22	6	0	-3.352829	-0.574336	3.132550
23	1	0	-4.077072	-0.128251	3.808391
24	6	0	-3.183440	-1.956051	3.112053
25	1	0	-3.770916	-2.594809	3.763826
26	6	0	-2.251941	-2.518875	2.238828
27	1	0	-2.116033	-3.596209	2.200992
28	6	0	2.662268	0.152706	2.212922
29	1	0	2.240283	0.792887	2.995589
30	6	0	2.134134	-1.263556	2.454974
31	1	0	2.491730	-1.955491	1.684950
32	1	0	1.042017	-1.286181	2.474211
33	1	0	2.496372	-1.632382	3.419453
34	6	0	4.189117	0.197813	2.298344
35	1	0	4.518911	-0.201699	3.262552
36	1	0	4.583034	1.213848	2.212622
37	1	0	4.644528	-0.411215	1.511608
38	6	0	2.715281	2.569192	0.555849
39	1	0	3.804921	2.471182	0.556216
40	6	0	2.343940	3.400116	1.790259
41	1	0	2.772579	4.401838	1.687339
42	1	0	2.742709	2.969539	2.712393
43	1	0	1.263867	3.506874	1.896814
44	6	0	2.286344	3.270796	-0.738053
45	1	0	1.202656	3.401531	-0.770780
46	1	0	2.580453	2.712346	-1.630184
47	1	0	2.750900	4.260175	-0.793264
48	6	0	-3.621748	1.770384	-1.088264
49	1	0	-3.743649	1.685193	-0.002475
50	6	0	-3.386094	3.246432	-1.445206
51	1	0	-3.369059	3.374102	-2.533156
52	1	0	-2.439726	3.622869	-1.055032
53	1	0	-4.192321	3.872708	-1.044851
54	6	0	-4.928563	1.309487	-1.743883
55	1	0	-5.742449	1.973432	-1.431501
56	1	0	-5.212374	0.292056	-1.468819
57	1	0	-4.870021	1.365104	-2.836384
58	6	0	-2.744015	-0.786046	-2.235430
59	1	0	-3.499772	-0.431908	-2.945862
60	6	0	-3.429530	-1.757499	-1.263280

61	1	0	-4.123192	-2.411562	-1.805153
62	1	0	-3.985204	-1.248784	-0.472078
63	1	0	-2.688680	-2.393032	-0.774763
64	6	0	-1.679870	-1.511353	-3.065908
65	1	0	-0.848703	-1.852128	-2.441943
66	1	0	-1.265473	-0.862872	-3.842492
67	1	0	-2.114658	-2.393172	-3.551222
68	7	0	-0.557812	-2.178511	0.507010
69	7	0	1.214209	-1.908762	-0.722291
70	15	0	-2.059495	0.805599	-1.520700
71	15	0	1.955883	0.873829	0.645566
72	45	0	-0.449153	0.683752	0.084932
73	6	0	-1.017209	2.572062	0.907163
74	1	0	-0.566207	3.439108	0.404827
75	1	0	-2.096846	2.749618	0.925681
76	1	0	-0.682855	2.596187	1.953583

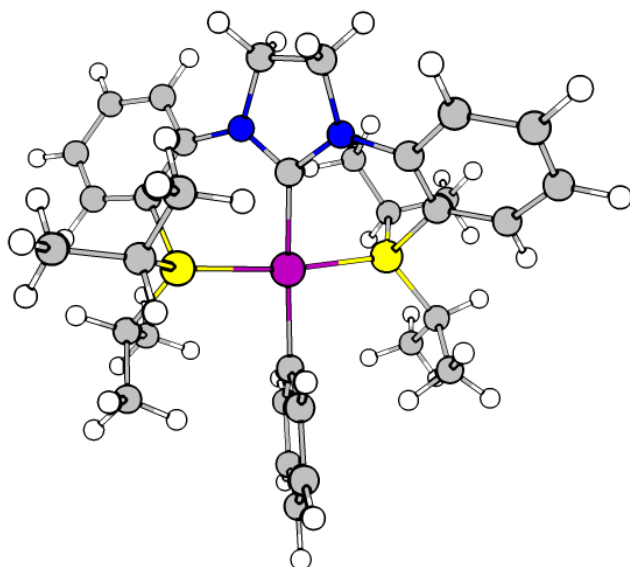
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SCF Done: E(RwB97XD) = -6572.48962460      A.U. after   1 cycles
               Conv g =   0.2150D-08          -V/T =   2.0048
Zero-point correction=                      0.665500 (Hartree/Particle)
Thermal correction to Energy=                0.710446
Thermal correction to Enthalpy=              0.711501
Thermal correction to Gibbs Free Energy=      0.588360
Sum of electronic and zero-point Energies=    -6571.824125
Sum of electronic and thermal Energies=       -6571.779178
Sum of electronic and thermal Enthalpies=     -6571.778123
Sum of electronic and thermal Free Energies=  -6571.901265

               1               2               3
               A               A               A
Frequencies --   31.2507         34.9362         41.2046

```

C-P-OA-SM-Ph (1g)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.350677	-3.702117	1.140316
2	1	0	-1.107787	-4.470629	0.981391
3	1	0	-0.033642	-3.719678	2.188974
4	6	0	0.093970	-1.602941	0.156341
5	6	0	0.828726	-3.844292	0.205475
6	1	0	1.677935	-4.352837	0.663438
7	1	0	0.543354	-4.372108	-0.711002
8	6	0	2.390461	-2.129189	-0.676922
9	6	0	3.064228	-0.905839	-0.470464
10	6	0	4.348577	-0.784731	-1.015727
11	1	0	4.909554	0.128575	-0.864373
12	6	0	4.957473	-1.794022	-1.753611
13	1	0	5.954713	-1.647103	-2.154728
14	6	0	4.268498	-2.979507	-1.972369
15	1	0	4.709095	-3.779859	-2.557812
16	6	0	3.000045	-3.141565	-1.430760
17	1	0	2.476697	-4.072833	-1.610568
18	6	0	-2.170148	-2.013452	1.160440
19	6	0	-2.954162	-1.057715	0.474332
20	6	0	-4.283406	-0.901805	0.882310
21	1	0	-4.919304	-0.193660	0.366156
22	6	0	-4.841067	-1.617901	1.936709
23	1	0	-5.877652	-1.458101	2.213799
24	6	0	-4.047630	-2.523069	2.627628
25	1	0	-4.444303	-3.080611	3.469825
26	6	0	-2.728927	-2.718769	2.235207
27	1	0	-2.126601	-3.427019	2.790824
28	6	0	2.725161	0.231726	2.193576
29	1	0	2.326473	1.120347	2.696784
30	6	0	2.006314	-0.985506	2.784108
31	1	0	2.350283	-1.912825	2.313811
32	1	0	0.923729	-0.910599	2.653361
33	1	0	2.219336	-1.058440	3.855513
34	6	0	4.231983	0.148560	2.449827
35	1	0	4.419237	-0.000996	3.518223
36	1	0	4.759044	1.058125	2.151447
37	1	0	4.676858	-0.695837	1.913877
38	6	0	3.312999	1.952646	-0.085826
39	1	0	4.355598	1.663822	0.075730
40	6	0	3.075465	3.196438	0.780158
41	1	0	3.791192	3.969736	0.481719
42	1	0	3.233371	3.001133	1.844400
43	1	0	2.071130	3.598738	0.651414
44	6	0	3.119790	2.275678	-1.570816
45	1	0	2.092718	2.590148	-1.758112
46	1	0	3.334692	1.420274	-2.216530

47	1	0	3.787132	3.094016	-1.861017
48	6	0	-3.498008	1.361003	-1.053032
49	1	0	-4.465148	0.869539	-1.193112
50	6	0	-3.601735	2.293015	0.161290
51	1	0	-2.772059	2.999586	0.180311
52	1	0	-3.597489	1.754000	1.112142
53	1	0	-4.535781	2.862012	0.100620
54	6	0	-3.221049	2.169364	-2.326524
55	1	0	-3.929375	3.002170	-2.383442
56	1	0	-3.341385	1.574666	-3.235928
57	1	0	-2.215284	2.592634	-2.315025
58	6	0	-2.419668	-0.955953	-2.401316
59	1	0	-2.099649	-0.253541	-3.178699
60	6	0	-3.862680	-1.385529	-2.684489
61	1	0	-3.906373	-1.933384	-3.631388
62	1	0	-4.549980	-0.540705	-2.769037
63	1	0	-4.235771	-2.049925	-1.898695
64	6	0	-1.484345	-2.165726	-2.483355
65	1	0	-1.733878	-2.912255	-1.722089
66	1	0	-0.439682	-1.874785	-2.357887
67	1	0	-1.593535	-2.643442	-3.462578
68	7	0	-0.855993	-2.374756	0.774601
69	7	0	1.144515	-2.442362	-0.082244
70	15	0	-2.209583	0.031458	-0.819039
71	15	0	2.244837	0.505560	0.407753
72	45	0	-0.021865	0.410173	-0.090902
73	6	0	-0.211006	2.496669	0.087286
74	6	0	-0.404893	2.997229	1.394356
75	6	0	-0.195551	3.473992	-0.925150
76	6	0	-0.573128	4.353743	1.672165
77	1	0	-0.429389	2.297689	2.229745
78	6	0	-0.361637	4.838233	-0.668819
79	1	0	-0.049181	3.168038	-1.960086
80	6	0	-0.551913	5.291182	0.636405
81	1	0	-0.720743	4.683703	2.698284
82	1	0	-0.342686	5.550036	-1.491378
83	1	0	-0.682380	6.349863	0.842618

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SCF Done: E(RwB97XD) = -6764.21449469 A.U. after 1 cycles
          Conv = 0.5741D-08 -V/T = 2.0051
Zero-point correction= 0.720750 (Hartree/Particle)
Thermal correction to Energy= 0.769549
Thermal correction to Enthalpy= 0.770604
Thermal correction to Gibbs Free Energy= 0.638225
Sum of electronic and zero-point Energies= -6763.493744
Sum of electronic and thermal Energies= -6763.444946
Sum of electronic and thermal Enthalpies= -6763.443891
Sum of electronic and thermal Free Energies= -6763.576270

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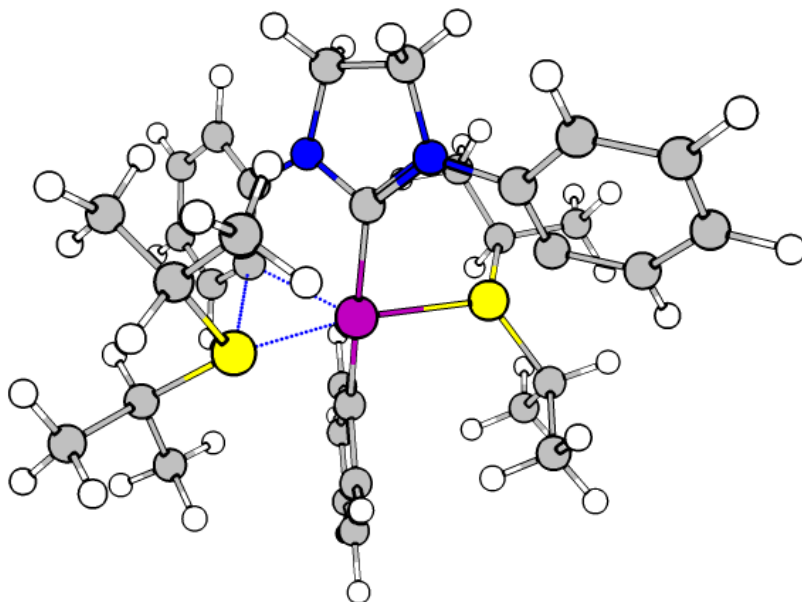
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2

3

	A	A	A
Frequencies --	23.1815	30.4284	34.4262

C-P-OA-TS-Ph (2g)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.522465	-3.554202	1.421887
2	1	0	-0.050940	-4.478135	1.325975
3	1	0	0.769973	-3.396794	2.477875
4	6	0	0.542375	-1.583049	0.141510
5	6	0	1.766854	-3.543250	0.532037
6	1	0	2.691348	-3.707940	1.087866
7	1	0	1.693979	-4.292289	-0.261975
8	6	0	2.880863	-1.606406	-0.622661
9	6	0	3.164807	-0.225209	-0.528437
10	6	0	4.382001	0.203957	-1.071644
11	1	0	4.656282	1.249472	-1.017223
12	6	0	5.283991	-0.660084	-1.685619
13	1	0	6.212728	-0.271925	-2.089989
14	6	0	4.979531	-2.011753	-1.774277
15	1	0	5.661213	-2.705044	-2.255703
16	6	0	3.783578	-2.476457	-1.241687
17	1	0	3.544980	-3.531207	-1.319660
18	6	0	-1.380722	-1.878349	1.477992
19	6	0	-1.885639	-0.693644	0.894413
20	6	0	-2.928752	-0.073907	1.591633
21	1	0	-3.319884	0.870165	1.233006
22	6	0	-3.489677	-0.624315	2.745373
23	1	0	-4.301980	-0.105565	3.245355

24	6	0	-3.017382	-1.833760	3.242426
25	1	0	-3.461060	-2.281746	4.125748
26	6	0	-1.942509	-2.459436	2.610990
27	1	0	-1.540624	-3.382869	3.016460
28	6	0	2.483995	0.974872	2.047888
29	1	0	1.867857	1.773699	2.476371
30	6	0	2.083096	-0.329294	2.743453
31	1	0	2.649675	-1.179448	2.348216
32	1	0	1.015403	-0.531181	2.626182
33	1	0	2.300586	-0.256324	3.813508
34	6	0	3.960659	1.294537	2.291260
35	1	0	4.163126	1.311389	3.366859
36	1	0	4.250101	2.268773	1.889840
37	1	0	4.607450	0.534463	1.842319
38	6	0	2.613959	2.620473	-0.365722
39	1	0	3.696421	2.632338	-0.211036
40	6	0	2.056920	3.813137	0.421472
41	1	0	2.527076	4.727322	0.044710
42	1	0	2.280718	3.748065	1.489598
43	1	0	0.978801	3.915091	0.302524
44	6	0	2.330973	2.765923	-1.864213
45	1	0	1.256135	2.807699	-2.044798
46	1	0	2.742091	1.939289	-2.449453
47	1	0	2.774246	3.695568	-2.235251
48	6	0	-3.872357	-0.054540	-1.319837
49	1	0	-4.332122	-0.484095	-0.424100
50	6	0	-4.039808	1.468668	-1.279414
51	1	0	-3.659171	1.922345	-2.199383
52	1	0	-3.512379	1.945532	-0.454713
53	1	0	-5.104072	1.714672	-1.192943
54	6	0	-4.636577	-0.586544	-2.544631
55	1	0	-5.623836	-0.114678	-2.578813
56	1	0	-4.797864	-1.666031	-2.513915
57	1	0	-4.124795	-0.338218	-3.480731
58	6	0	-2.221442	-2.365748	-1.830218
59	1	0	-2.780472	-2.242179	-2.764102
60	6	0	-3.053192	-3.280806	-0.926000
61	1	0	-3.346784	-4.182928	-1.475131
62	1	0	-3.963432	-2.795761	-0.564024
63	1	0	-2.484199	-3.597897	-0.049884
64	6	0	-0.905858	-3.034206	-2.249621
65	1	0	-0.395537	-3.486212	-1.397687
66	1	0	-0.219037	-2.326238	-2.721022
67	1	0	-1.112600	-3.837788	-2.964656
68	7	0	-0.212963	-2.408302	0.903142
69	7	0	1.735220	-2.186122	-0.034101
70	15	0	-2.053737	-0.549761	-1.380012
71	15	0	1.978252	0.981857	0.250807
72	45	0	-0.236343	0.273022	-0.179222
73	6	0	-0.974577	2.238956	-0.052850

74	6	0	-1.273514	2.808180	1.200570
75	6	0	-1.164542	3.084326	-1.162020
76	6	0	-1.723753	4.122966	1.343209
77	1	0	-1.151073	2.206318	2.099583
78	6	0	-1.609183	4.401524	-1.039063
79	1	0	-0.986190	2.693755	-2.162382
80	6	0	-1.889993	4.934328	0.219856
81	1	0	-1.938403	4.518242	2.333592
82	1	0	-1.744815	5.011788	-1.929159
83	1	0	-2.236571	5.958746	0.323596

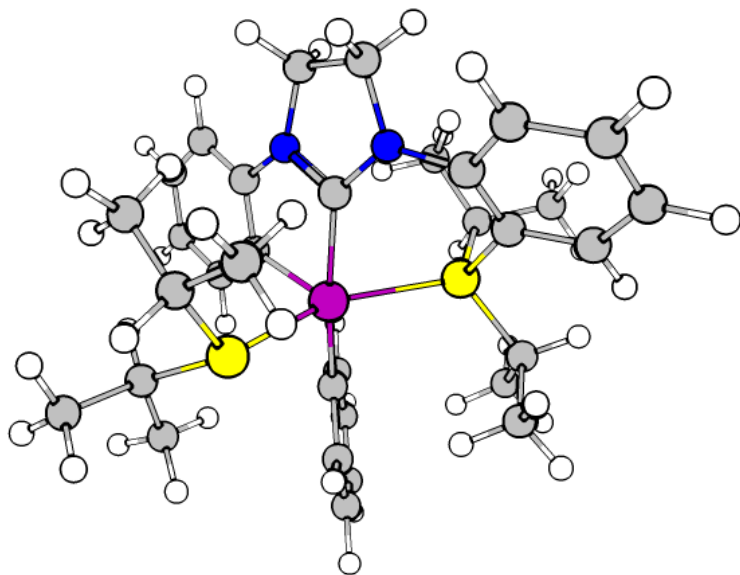
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SCF Done: E(RwB97XD) = -6764.16571611 A.U. after 1 cycles
          Conv = 0.2253D-08 -V/T = 2.0051
Zero-point correction= 0.718720 (Hartree/Particle)
Thermal correction to Energy= 0.767408
Thermal correction to Enthalpy= 0.768463
Thermal correction to Gibbs Free Energy= 0.636117
Sum of electronic and zero-point Energies= -6763.446996
Sum of electronic and thermal Energies= -6763.398308
Sum of electronic and thermal Enthalpies= -6763.397253
Sum of electronic and thermal Free Energies= -6763.529599

          1          2          3
          A          A          A
Frequencies -- -233.2724      20.5972      30.3463

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C-P-OA-PR-Ph-conf1 (3g)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.839429	-3.429595	1.693843
2	1	0	0.332281	-4.395039	1.655166

3	1	0	1.109384	-3.212944	2.733073
4	6	0	0.612672	-1.568375	0.276918
5	6	0	2.039363	-3.368692	0.742148
6	1	0	3.000036	-3.400928	1.258697
7	1	0	2.004424	-4.180082	0.009693
8	6	0	2.915424	-1.416157	-0.580295
9	6	0	3.112308	-0.018923	-0.497242
10	6	0	4.274684	0.488276	-1.091869
11	1	0	4.485474	1.548933	-1.044530
12	6	0	5.199395	-0.317320	-1.749559
13	1	0	6.084073	0.128109	-2.191738
14	6	0	4.974650	-1.685333	-1.835626
15	1	0	5.673260	-2.331519	-2.356536
16	6	0	3.837610	-2.226029	-1.249485
17	1	0	3.656560	-3.293075	-1.319819
18	6	0	-1.189098	-1.885788	1.747571
19	6	0	-1.621840	-0.634284	1.267655
20	6	0	-2.786879	-0.128751	1.847935
21	1	0	-3.180405	0.825571	1.519139
22	6	0	-3.470441	-0.821362	2.852075
23	1	0	-4.371373	-0.389413	3.278247
24	6	0	-3.010262	-2.055987	3.301160
25	1	0	-3.541965	-2.596178	4.077991
26	6	0	-1.853886	-2.598339	2.741433
27	1	0	-1.481549	-3.561832	3.078085
28	6	0	2.423953	1.190317	2.091755
29	1	0	1.761954	1.952062	2.519204
30	6	0	2.130972	-0.125224	2.819012
31	1	0	2.739215	-0.942911	2.417851
32	1	0	1.075564	-0.398223	2.742845
33	1	0	2.377144	-0.020400	3.879846
34	6	0	3.878285	1.622367	2.287744
35	1	0	4.104640	1.684106	3.356758
36	1	0	4.083600	2.604100	1.853683
37	1	0	4.567630	0.899194	1.841435
38	6	0	2.347854	2.777206	-0.378419
39	1	0	3.428670	2.894474	-0.260756
40	6	0	1.697573	3.938737	0.381779
41	1	0	2.075516	4.879021	-0.031962
42	1	0	1.941509	3.930449	1.447620
43	1	0	0.612956	3.936626	0.276634
44	6	0	2.003174	2.839669	-1.870986
45	1	0	0.923520	2.768792	-2.016837
46	1	0	2.479716	2.040889	-2.445099
47	1	0	2.336195	3.796318	-2.285499
48	6	0	-3.732197	-0.518782	-1.362512
49	1	0	-3.900644	-1.045584	-0.417228
50	6	0	-4.239681	0.918183	-1.205941
51	1	0	-4.116068	1.478097	-2.138924
52	1	0	-3.712558	1.470571	-0.429859

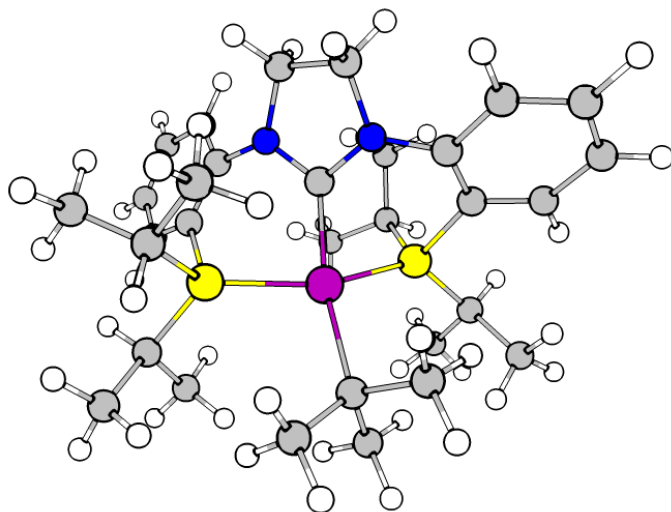
53	1	0	-5.306854	0.907789	-0.956031
54	6	0	-4.556155	-1.213937	-2.457840
55	1	0	-5.621924	-1.032020	-2.282058
56	1	0	-4.413661	-2.296423	-2.480280
57	1	0	-4.315544	-0.816261	-3.450314
58	6	0	-1.694854	-2.362598	-2.214603
59	1	0	-2.364694	-2.425555	-3.081437
60	6	0	-2.137121	-3.432436	-1.210750
61	1	0	-2.236210	-4.403716	-1.710350
62	1	0	-3.096045	-3.199446	-0.741092
63	1	0	-1.401099	-3.543001	-0.412083
64	6	0	-0.291876	-2.650668	-2.755936
65	1	0	0.460781	-2.626171	-1.965071
66	1	0	0.002264	-1.917024	-3.511821
67	1	0	-0.259713	-3.645116	-3.215945
68	7	0	-0.002259	-2.363994	1.165278
69	7	0	1.850781	-2.069562	0.076553
70	15	0	-1.885135	-0.559789	-1.730233
71	15	0	1.877196	1.115078	0.313608
72	45	0	-0.394791	0.191875	-0.142897
73	6	0	-1.279243	2.100932	-0.084306
74	6	0	-1.547482	2.875687	-1.227342
75	6	0	-1.508679	2.740451	1.149485
76	6	0	-2.020646	4.187120	-1.153111
77	1	0	-1.409202	2.434511	-2.212931
78	6	0	-1.989803	4.047795	1.242502
79	1	0	-1.302642	2.206561	2.075143
80	6	0	-2.248073	4.784973	0.086324
81	1	0	-2.220717	4.739867	-2.068056
82	1	0	-2.152159	4.496003	2.219965
83	1	0	-2.621076	5.803188	0.150989

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SCF Done:  E(RwB97XD) = -6764.18017644      A.U. after   1 cycles
              Convg =   0.3296D-08              -V/T =   2.0051
Zero-point correction=                        0.719041 (Hartree/Particle)
Thermal correction to Energy=                  0.768442
Thermal correction to Enthalpy=                 0.769497
Thermal correction to Gibbs Free Energy=        0.635915
Sum of electronic and zero-point Energies=      -6763.461135
Sum of electronic and thermal Energies=         -6763.411735
Sum of electronic and thermal Enthalpies=       -6763.410680
Sum of electronic and thermal Free Energies=    -6763.544261

              1              2              3
              A              A              A
Frequencies --   21.8482          32.2975          37.4373

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C-P-OA-SM-*t*-Bu (1h)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.627248	-3.130370	-1.727667
2	1	0	1.409662	-3.887210	-1.666656
3	1	0	0.349703	-2.987205	-2.777057
4	6	0	0.073431	-1.246577	-0.417425
5	6	0	-0.570755	-3.478617	-0.862262
6	1	0	-1.400039	-3.914932	-1.422546
7	1	0	-0.277746	-4.171873	-0.066507
8	6	0	-2.016676	-2.030775	0.578125
9	6	0	-2.694011	-0.802283	0.708987
10	6	0	-3.654727	-0.716439	1.723462
11	1	0	-4.170171	0.216068	1.912161
12	6	0	-3.995880	-1.801716	2.526587
13	1	0	-4.751365	-1.685917	3.296767
14	6	0	-3.378274	-3.027917	2.319150
15	1	0	-3.643916	-3.893093	2.917819
16	6	0	-2.386674	-3.135767	1.351005
17	1	0	-1.883075	-4.086571	1.224125
18	6	0	2.428308	-1.492150	-1.206594
19	6	0	3.066345	-0.699548	-0.220649
20	6	0	4.460379	-0.611372	-0.277595
21	1	0	4.992654	-0.072762	0.496511
22	6	0	5.215417	-1.195202	-1.292488
23	1	0	6.295228	-1.090184	-1.294680
24	6	0	4.564001	-1.888086	-2.303547
25	1	0	5.119738	-2.321624	-3.128614
26	6	0	3.183020	-2.041532	-2.249956
27	1	0	2.687291	-2.595269	-3.039097
28	6	0	-2.995441	0.037626	-2.069901
29	1	0	-3.147552	0.995191	-2.579862

30	6	0	-2.034949	-0.763886	-2.953111
31	1	0	-1.959080	-1.801205	-2.618879
32	1	0	-1.032247	-0.326910	-2.953040
33	1	0	-2.407278	-0.777062	-3.982979
34	6	0	-4.347650	-0.668528	-1.942777
35	1	0	-4.794409	-0.815771	-2.931881
36	1	0	-5.060349	-0.103236	-1.335921
37	1	0	-4.229579	-1.652096	-1.477793
38	6	0	-3.544015	1.865158	0.092361
39	1	0	-4.405327	1.295659	0.448092
40	6	0	-4.115437	2.765366	-1.013694
41	1	0	-4.707744	3.559904	-0.547981
42	1	0	-4.785669	2.211584	-1.675594
43	1	0	-3.355443	3.242434	-1.629975
44	6	0	-2.987505	2.674831	1.268201
45	1	0	-2.169376	3.319695	0.942709
46	1	0	-2.588032	2.029218	2.056018
47	1	0	-3.772382	3.302564	1.703638
48	6	0	3.352306	1.376716	1.811238
49	1	0	4.115380	0.692400	2.203075
50	6	0	4.052504	2.404193	0.910411
51	1	0	3.395625	3.237657	0.663535
52	1	0	4.413475	1.985416	-0.030340
53	1	0	4.916231	2.814533	1.444853
54	6	0	2.725585	2.087575	3.021948
55	1	0	3.435971	2.816681	3.424475
56	1	0	2.477173	1.395247	3.829048
57	1	0	1.813834	2.625291	2.748786
58	6	0	1.756543	-0.890396	2.424069
59	1	0	2.584696	-0.706624	3.118174
60	6	0	1.798491	-2.383073	2.083885
61	1	0	1.776218	-2.960761	3.013985
62	1	0	2.701099	-2.663051	1.534931
63	1	0	0.926657	-2.683313	1.498964
64	6	0	0.439553	-0.550490	3.132576
65	1	0	-0.410790	-0.767220	2.480115
66	1	0	0.372666	0.504756	3.406875
67	1	0	0.340317	-1.149548	4.044804
68	7	0	1.068615	-1.863343	-1.133958
69	7	0	-0.933533	-2.170312	-0.318854
70	15	0	2.062459	0.288320	0.978452
71	15	0	-2.259879	0.598455	-0.435545
72	45	0	0.046531	0.767722	-0.189744
73	6	0	0.373131	2.815601	-0.843503
74	6	0	1.587689	2.616241	-1.768479
75	1	0	1.371023	1.889268	-2.562589
76	1	0	1.865053	3.562612	-2.269952
77	1	0	2.477235	2.257710	-1.246470
78	6	0	-0.725306	3.421726	-1.724588
79	1	0	-1.097222	2.716244	-2.477772

80	1	0	-1.570836	3.755632	-1.120240
81	1	0	-0.357344	4.313238	-2.265397
82	6	0	0.697631	3.870701	0.216795
83	1	0	1.004842	4.827982	-0.246326
84	1	0	-0.169912	4.084840	0.851032
85	1	0	1.501245	3.562021	0.884826

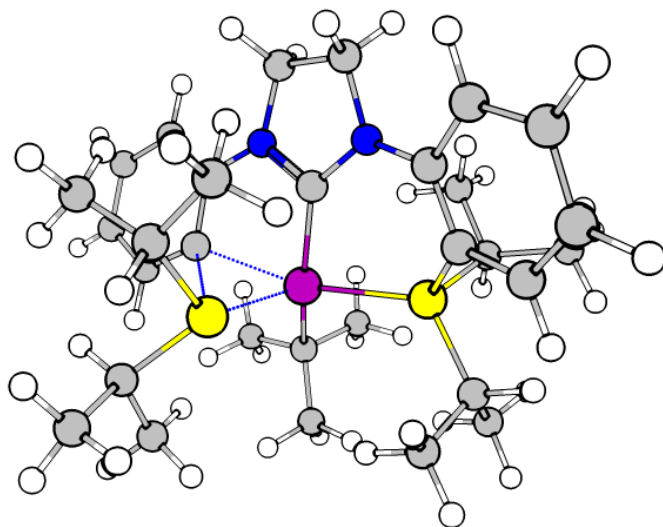
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SCF Done:  E(RwB97XD) = -6690.40740678      A.U. after   21 cycles
              Conv g =   0.8509D-08              -V/T =   2.0050
Zero-point correction=                      0.751416 (Hartree/Particle)
Thermal correction to Energy=                0.801301
Thermal correction to Enthalpy=              0.802356
Thermal correction to Gibbs Free Energy=      0.669936
Sum of electronic and zero-point Energies=    -6689.655991
Sum of electronic and thermal Energies=       -6689.606106
Sum of electronic and thermal Enthalpies=     -6689.605051
Sum of electronic and thermal Free Energies=   -6689.737470

              1              2              3
              A              A              A
Frequencies --  22.4636          39.4508          45.4368

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C-P-OA-TS-*t*-Bu (2h)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.457307	-3.063753	-2.120554
2	1	0	1.160165	-3.885125	-1.967269
3	1	0	0.379873	-2.858614	-3.192918
4	6	0	-0.117708	-1.264575	-0.721484
5	6	0	-0.904482	-3.337136	-1.480212
6	1	0	-1.678192	-3.585283	-2.208693
7	1	0	-0.827128	-4.151798	-0.754482

8	6	0	-2.314719	-1.957236	0.072679
9	6	0	-2.720943	-0.712416	0.604308
10	6	0	-3.726038	-0.741490	1.576858
11	1	0	-4.050390	0.175584	2.049314
12	6	0	-4.366706	-1.912641	1.971558
13	1	0	-5.140947	-1.876516	2.730356
14	6	0	-4.023358	-3.109330	1.360260
15	1	0	-4.529984	-4.033146	1.619432
16	6	0	-3.000245	-3.127646	0.420270
17	1	0	-2.729217	-4.075661	-0.025738
18	6	0	2.134015	-1.257851	-1.454057
19	6	0	2.375718	-0.182591	-0.562523
20	6	0	3.658160	0.372207	-0.653568
21	1	0	3.924702	1.212108	-0.027793
22	6	0	4.636161	-0.099719	-1.527088
23	1	0	5.613171	0.373209	-1.542794
24	6	0	4.353080	-1.159114	-2.382370
25	1	0	5.102447	-1.529836	-3.074414
26	6	0	3.087280	-1.735338	-2.353169
27	1	0	2.845766	-2.547821	-3.031386
28	6	0	-3.119246	1.007851	-1.629319
29	1	0	-2.975354	2.043298	-1.951262
30	6	0	-2.598261	0.113472	-2.758497
31	1	0	-2.789551	-0.942744	-2.548685
32	1	0	-1.523505	0.243325	-2.912254
33	1	0	-3.111475	0.364200	-3.692319
34	6	0	-4.615327	0.777873	-1.399434
35	1	0	-5.166113	0.993132	-2.320925
36	1	0	-5.023726	1.419928	-0.614341
37	1	0	-4.818215	-0.260909	-1.123664
38	6	0	-2.827678	2.148392	1.047102
39	1	0	-3.832096	1.800143	1.296093
40	6	0	-3.041176	3.524667	0.404789
41	1	0	-3.422605	4.212319	1.166347
42	1	0	-3.782768	3.486098	-0.397252
43	1	0	-2.130068	3.959382	-0.000433
44	6	0	-2.005817	2.216418	2.339588
45	1	0	-0.977369	2.524087	2.139478
46	1	0	-1.953878	1.243040	2.835454
47	1	0	-2.456543	2.930832	3.036136
48	6	0	3.044195	0.628504	2.330913
49	1	0	3.951954	0.279756	1.830332
50	6	0	2.961091	2.150197	2.224636
51	1	0	2.107949	2.528135	2.797731
52	1	0	2.825377	2.481989	1.196264
53	1	0	3.871048	2.614662	2.620071
54	6	0	3.151789	0.236856	3.814390
55	1	0	3.867300	0.899713	4.312401
56	1	0	3.509027	-0.785815	3.955412
57	1	0	2.191605	0.342522	4.331656

58	6	0	1.856590	-1.936655	1.965326
59	1	0	1.973497	-1.827929	3.049398
60	6	0	3.145899	-2.571795	1.439077
61	1	0	3.337458	-3.515832	1.962771
62	1	0	4.015601	-1.926032	1.585260
63	1	0	3.077314	-2.791284	0.371031
64	6	0	0.663806	-2.882128	1.796175
65	1	0	0.622926	-3.296985	0.787413
66	1	0	-0.288327	-2.388055	2.009672
67	1	0	0.764956	-3.728986	2.483626
68	7	0	0.870776	-1.868146	-1.403012
69	7	0	-1.210397	-2.070036	-0.799567
70	15	0	1.494361	-0.129872	1.572107
71	15	0	-2.058260	0.882796	-0.088899
72	45	0	0.313163	0.670635	-0.319676
73	6	0	0.770758	2.779342	-0.894838
74	6	0	-0.211083	3.038454	-2.054023
75	1	0	-0.183070	2.241405	-2.807919
76	1	0	-1.246089	3.137771	-1.721607
77	1	0	0.038960	3.979199	-2.578671
78	6	0	2.161706	2.952191	-1.526883
79	1	0	2.969823	2.923533	-0.792160
80	1	0	2.376772	2.189010	-2.281987
81	1	0	2.233846	3.936486	-2.023954
82	6	0	0.614728	3.917527	0.120654
83	1	0	-0.335506	3.891883	0.654314
84	1	0	1.397228	3.898546	0.882798
85	1	0	0.679857	4.902690	-0.377844

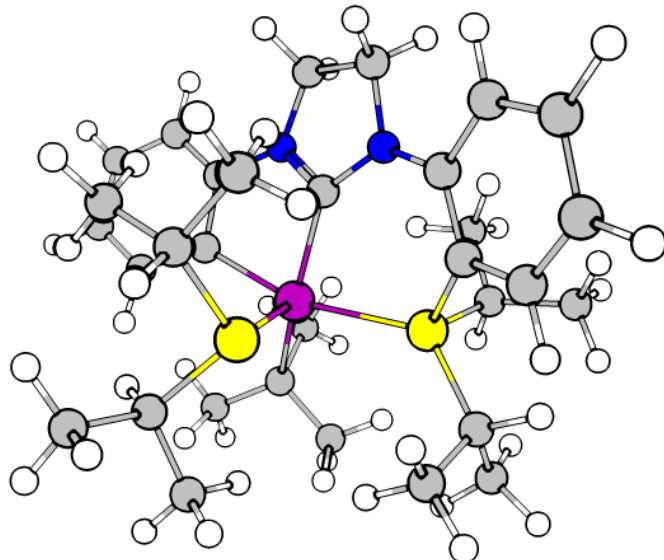
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SCF Done: E(RwB97XD) = -6690.36009176 A.U. after 1 cycles
          Conv = 0.2598D-08 -V/T = 2.0050
Zero-point correction= 0.750857 (Hartree/Particle)
Thermal correction to Energy= 0.800185
Thermal correction to Enthalpy= 0.801240
Thermal correction to Gibbs Free Energy= 0.669789
Sum of electronic and zero-point Energies= -6689.609235
Sum of electronic and thermal Energies= -6689.559907
Sum of electronic and thermal Enthalpies= -6689.558852
Sum of electronic and thermal Free Energies= -6689.690303

          1          2          3
          A          A          A
Frequencies -- -238.7098 19.2353 32.1654

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C-P-OA-PR-*t*-Bu-conf1 (3h)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.612572	3.692713	-1.298698
2	1	0	-1.303495	4.416440	-0.863018
3	1	0	-0.568916	3.853737	-2.379440
4	6	0	-0.045088	1.558922	-0.505970
5	6	0	0.764617	3.745803	-0.633283
6	1	0	1.530796	4.193724	-1.268015
7	1	0	0.710246	4.301426	0.307255
8	6	0	2.201425	1.950728	0.386296
9	6	0	2.616041	0.604946	0.549396
10	6	0	3.650352	0.377822	1.465485
11	1	0	3.973448	-0.631096	1.677779
12	6	0	4.317593	1.397276	2.136969
13	1	0	5.109106	1.154863	2.837850
14	6	0	3.973383	2.713635	1.873439
15	1	0	4.497359	3.535617	2.349843
16	6	0	2.921524	2.980400	1.007132
17	1	0	2.652298	4.014601	0.840790
18	6	0	-2.326328	1.789145	-1.079524
19	6	0	-2.435942	0.441764	-0.670243
20	6	0	-3.741194	-0.022464	-0.520578
21	1	0	-3.912349	-1.017404	-0.126606
22	6	0	-4.860017	0.760234	-0.832135
23	1	0	-5.857031	0.350166	-0.697934
24	6	0	-4.698449	2.054458	-1.313499
25	1	0	-5.560202	2.659675	-1.577142
26	6	0	-3.412224	2.585764	-1.429038
27	1	0	-3.274286	3.608720	-1.767694
28	6	0	2.766975	-0.475053	-2.112867

29	1	0	2.471342	-1.344725	-2.712317
30	6	0	2.260765	0.767996	-2.854156
31	1	0	2.600475	1.684434	-2.364777
32	1	0	1.172727	0.806185	-2.931091
33	1	0	2.667351	0.767200	-3.870365
34	6	0	4.297302	-0.422313	-2.031731
35	1	0	4.714643	-0.272109	-3.032658
36	1	0	4.738866	-1.336045	-1.629670
37	1	0	4.623334	0.414438	-1.406461
38	6	0	2.898178	-2.260180	0.166466
39	1	0	3.902418	-1.869368	0.340343
40	6	0	3.097066	-3.439187	-0.801670
41	1	0	3.950346	-4.025702	-0.446147
42	1	0	3.317069	-3.142641	-1.829152
43	1	0	2.235262	-4.104428	-0.818033
44	6	0	2.337569	-2.783037	1.492943
45	1	0	1.349053	-3.222458	1.343116
46	1	0	2.223858	-2.003506	2.248192
47	1	0	3.002137	-3.560020	1.886724
48	6	0	-2.066903	-1.931039	2.207048
49	1	0	-2.897056	-1.778049	1.510212
50	6	0	-1.503168	-3.340343	1.998779
51	1	0	-0.754244	-3.567877	2.765578
52	1	0	-1.025138	-3.441516	1.024308
53	1	0	-2.295940	-4.094990	2.066403
54	6	0	-2.612587	-1.829628	3.637410
55	1	0	-3.286036	-2.671501	3.835722
56	1	0	-3.176741	-0.911973	3.815785
57	1	0	-1.802780	-1.879278	4.374703
58	6	0	-1.307298	0.822971	2.728666
59	1	0	-1.365235	0.416747	3.747267
60	6	0	-2.673571	1.431577	2.401749
61	1	0	-2.988340	2.105185	3.209181
62	1	0	-3.449677	0.674765	2.268106
63	1	0	-2.634891	2.013686	1.478334
64	6	0	-0.239294	1.919865	2.783735
65	1	0	-0.214446	2.491381	1.852303
66	1	0	0.761478	1.512507	2.956257
67	1	0	-0.464991	2.629262	3.588412
68	7	0	-1.020385	2.326482	-1.006892
69	7	0	1.064119	2.327198	-0.366879
70	15	0	-0.695692	-0.703132	1.811245
71	15	0	1.911265	-0.789249	-0.466244
72	45	0	-0.563522	-0.442535	-0.534443
73	6	0	-1.204787	-2.268603	-1.505753
74	6	0	-1.123935	-1.406837	-2.770497
75	1	0	-0.506991	-0.475941	-2.629524
76	1	0	-0.611873	-1.910517	-3.600862
77	1	0	-2.097908	-1.047165	-3.107998
78	6	0	-2.576036	-2.925031	-1.363911

79	1	0	-2.762494	-3.286039	-0.347782
80	1	0	-3.387461	-2.249871	-1.633952
81	1	0	-2.656886	-3.797516	-2.031482
82	6	0	-0.149019	-3.368610	-1.591786
83	1	0	0.809536	-2.964578	-1.921219
84	1	0	0.012421	-3.875852	-0.636521
85	1	0	-0.437682	-4.140726	-2.324322

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SCF Done:  E(RwB97XD) = -6690.38719059      A.U. after   1 cycles
              Conv g =   0.2135D-08          -V/T =   2.0050
Zero-point correction=                      0.752201 (Hartree/Particle)
Thermal correction to Energy=                0.801484
Thermal correction to Enthalpy=              0.802539
Thermal correction to Gibbs Free Energy=      0.672111
Sum of electronic and zero-point Energies=    -6689.634989
Sum of electronic and thermal Energies=       -6689.585706
Sum of electronic and thermal Enthalpies=     -6689.584651
Sum of electronic and thermal Free Energies=   -6689.715080

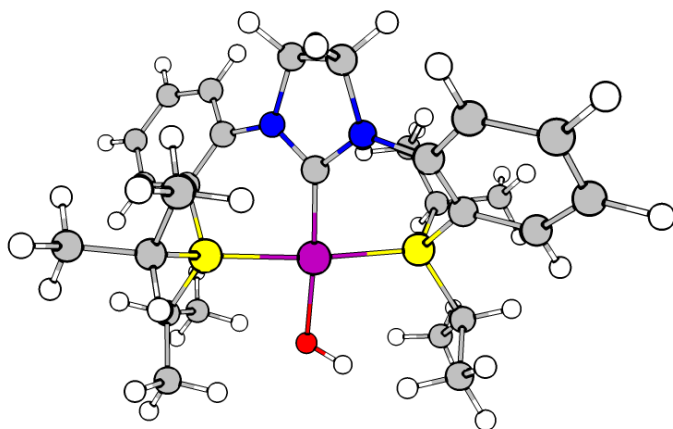
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              1              2              3
              A              A              A
Frequencies --  31.1861      36.6480      50.5908

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C-P-OA-SM-OH (1i)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.577517	-3.362592	-0.496718
2	1	0	1.379549	-4.036175	-0.192725
3	1	0	0.248322	-3.626383	-1.508334
4	6	0	0.005366	-1.119623	-0.005310
5	6	0	-0.580131	-3.361876	0.471914
6	1	0	-1.388651	-4.026109	0.164311
7	1	0	-0.250813	-3.637471	1.480312
8	6	0	-2.273740	-1.626031	0.943278
9	6	0	-3.022031	-0.516583	0.497332

10	6	0	-4.316398	-0.349476	1.000219
11	1	0	-4.911694	0.491248	0.662218
12	6	0	-4.877220	-1.224753	1.924464
13	1	0	-5.884958	-1.059809	2.290701
14	6	0	-4.124037	-2.303527	2.371817
15	1	0	-4.528027	-2.995515	3.103695
16	6	0	-2.838973	-2.501195	1.881425
17	1	0	-2.270164	-3.345796	2.250846
18	6	0	2.289434	-1.634662	-0.931570
19	6	0	3.029197	-0.520347	-0.481888
20	6	0	4.340196	-0.369809	-0.946393
21	1	0	4.935179	0.466362	-0.596695
22	6	0	4.922905	-1.257769	-1.844132
23	1	0	5.943093	-1.104055	-2.179302
24	6	0	4.174569	-2.334488	-2.304521
25	1	0	4.593834	-3.035137	-3.019320
26	6	0	2.875985	-2.520284	-1.847515
27	1	0	2.312646	-3.365192	-2.224259
28	6	0	-2.678709	0.067366	-2.332212
29	1	0	-2.280404	0.837461	-3.001886
30	6	0	-1.939195	-1.236032	-2.649799
31	1	0	-2.271934	-2.050578	-1.997784
32	1	0	-0.859093	-1.117001	-2.535857
33	1	0	-2.144601	-1.532097	-3.683570
34	6	0	-4.181145	-0.081560	-2.584259
35	1	0	-4.354331	-0.445431	-3.602286
36	1	0	-4.715296	0.866119	-2.480472
37	1	0	-4.626852	-0.803461	-1.892700
38	6	0	-3.294499	2.232594	-0.457804
39	1	0	-4.347113	1.967042	-0.605060
40	6	0	-2.899893	3.244236	-1.543052
41	1	0	-3.462363	4.171688	-1.391363
42	1	0	-3.130259	2.883515	-2.550201
43	1	0	-1.831866	3.465009	-1.464392
44	6	0	-3.116044	2.838205	0.940461
45	1	0	-2.074458	3.143042	1.070557
46	1	0	-3.382358	2.134037	1.734060
47	1	0	-3.764468	3.715857	1.039787
48	6	0	3.297573	2.240076	0.424240
49	1	0	4.345371	1.972121	0.590968
50	6	0	3.180587	2.812927	-0.994902
51	1	0	2.145586	3.041781	-1.259306
52	1	0	3.552744	2.111292	-1.745449
53	1	0	3.769362	3.732384	-1.071846
54	6	0	2.919958	3.264811	1.505876
55	1	0	3.397994	4.224669	1.287782
56	1	0	3.262388	2.947643	2.494594
57	1	0	1.840072	3.425042	1.565370
58	6	0	2.645426	0.126873	2.331200
59	1	0	2.253422	0.920318	2.977159

60	6	0	4.142863	-0.041866	2.599694
61	1	0	4.301469	-0.368142	3.632551
62	1	0	4.699467	0.889025	2.463784
63	1	0	4.578152	-0.799438	1.940734
64	6	0	1.881686	-1.156152	2.674358
65	1	0	2.206643	-1.990828	2.044209
66	1	0	0.804757	-1.022607	2.548124
67	1	0	2.074917	-1.430472	3.716302
68	7	0	1.008023	-1.965369	-0.439207
69	7	0	-1.000071	-1.961183	0.427222
70	15	0	2.237438	0.724463	0.609091
71	15	0	-2.253379	0.708481	-0.631041
72	45	0	-0.004255	0.838883	-0.008493
73	8	0	-0.165424	2.925834	-0.010017
74	1	0	0.685578	3.370565	-0.056992

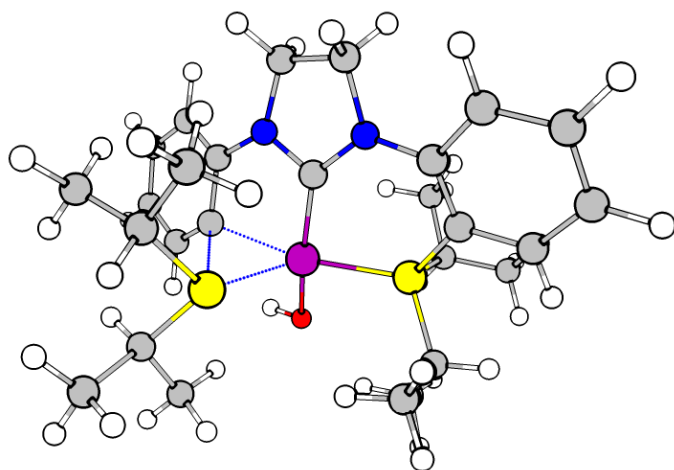
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SCF Done: E(RwB97XD) = -6608.46591427 A.U. after 21 cycles
              Conv g = 0.4115D-08 -V/T = 2.0048
Zero-point correction= 0.642728 (Hartree/Particle)
Thermal correction to Energy= 0.687230
Thermal correction to Enthalpy= 0.688285
Thermal correction to Gibbs Free Energy= 0.565553
Sum of electronic and zero-point Energies= -6607.823186
Sum of electronic and thermal Energies= -6607.778684
Sum of electronic and thermal Enthalpies= -6607.777629
Sum of electronic and thermal Free Energies= -6607.900362

              1              2              3
              A              A              A
Frequencies -- 16.6562      35.1731      54.1953

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C-P-OA-TS-OH (2i)



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

```

1	6	0	-0.565238	3.473627	-0.821200
2	1	0	-1.317829	4.156536	-0.421506
3	1	0	-0.417964	3.689846	-1.885009
4	6	0	0.082134	1.294118	-0.226005
5	6	0	0.745506	3.529120	-0.037000
6	1	0	1.516464	4.103965	-0.551513
7	1	0	0.587363	3.953849	0.958961
8	6	0	2.372093	1.737869	0.623861
9	6	0	2.926756	0.441662	0.507860
10	6	0	4.186528	0.220200	1.078314
11	1	0	4.635021	-0.763717	1.001641
12	6	0	4.901110	1.211438	1.740405
13	1	0	5.874643	0.992668	2.165560
14	6	0	4.344856	2.480020	1.845207
15	1	0	4.872949	3.276147	2.359786
16	6	0	3.097394	2.736297	1.291918
17	1	0	2.685326	3.731190	1.401122
18	6	0	-2.086145	1.458101	-1.150479
19	6	0	-2.266280	0.092182	-0.813660
20	6	0	-3.306677	-0.567315	-1.481537
21	1	0	-3.451277	-1.631785	-1.328744
22	6	0	-4.182846	0.098714	-2.337835
23	1	0	-4.985412	-0.449340	-2.821320
24	6	0	-4.026844	1.462731	-2.570571
25	1	0	-4.713629	1.992449	-3.222821
26	6	0	-2.958835	2.144644	-1.991274
27	1	0	-2.801206	3.195749	-2.212514
28	6	0	2.923805	-1.053093	-1.992611
29	1	0	2.400335	-1.888990	-2.470274
30	6	0	2.635362	0.213151	-2.805982
31	1	0	3.076112	1.096519	-2.330447
32	1	0	1.560011	0.378040	-2.914557
33	1	0	3.070460	0.122017	-3.806029
34	6	0	4.422329	-1.352009	-1.936638
35	1	0	4.811042	-1.489935	-2.950698
36	1	0	4.645131	-2.263262	-1.374559
37	1	0	4.974092	-0.523406	-1.482602
38	6	0	2.556725	-2.457470	0.589638
39	1	0	3.644599	-2.469277	0.711510
40	6	0	2.146220	-3.711615	-0.191940
41	1	0	2.337726	-4.595867	0.425063
42	1	0	2.724004	-3.821382	-1.114388
43	1	0	1.086216	-3.677409	-0.461348
44	6	0	1.906411	-2.426681	1.976090
45	1	0	0.817118	-2.457962	1.888188
46	1	0	2.173567	-1.526024	2.536908
47	1	0	2.233495	-3.296238	2.555233
48	6	0	-3.255314	-1.832926	1.311990
49	1	0	-4.088917	-1.500810	0.686000
50	6	0	-2.746446	-3.194467	0.820552

51	1	0	-2.020147	-3.600019	1.533301
52	1	0	-2.231179	-3.141063	-0.140803
53	1	0	-3.578687	-3.903402	0.747154
54	6	0	-3.782271	-1.985217	2.747560
55	1	0	-4.442942	-2.857099	2.796247
56	1	0	-4.360671	-1.120300	3.081045
57	1	0	-2.967099	-2.150589	3.460738
58	6	0	-2.612158	0.866759	2.138936
59	1	0	-2.821106	0.379401	3.099217
60	6	0	-3.938857	1.422001	1.615761
61	1	0	-4.375062	2.102977	2.355846
62	1	0	-4.667415	0.630683	1.420114
63	1	0	-3.803853	1.980225	0.686927
64	6	0	-1.618499	1.988514	2.468404
65	1	0	-1.564979	2.720265	1.660799
66	1	0	-0.611430	1.601895	2.652180
67	1	0	-1.945329	2.521212	3.367620
68	7	0	-0.942876	2.084245	-0.634865
69	7	0	1.128950	2.111582	0.065917
70	15	0	-1.836729	-0.606991	1.269849
71	15	0	2.065939	-0.938025	-0.353430
72	45	0	-0.222972	-0.608021	-0.503920
73	8	0	-0.427374	-2.457192	-1.449681
74	1	0	-1.252403	-2.416967	-1.950419

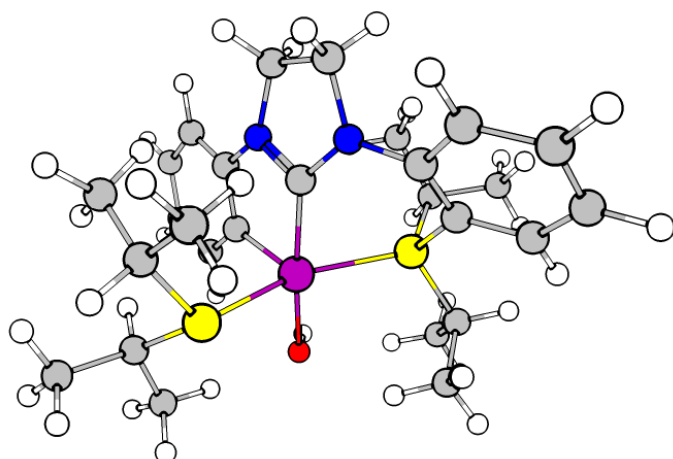
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SCF Done:  E(RwB97XD) = -6608.41200199      A.U. after   1 cycles
              Convrg =   0.2044D-08          -V/T =   2.0048
Zero-point correction=                      0.640841 (Hartree/Particle)
Thermal correction to Energy=                0.685125
Thermal correction to Enthalpy=              0.686180
Thermal correction to Gibbs Free Energy=      0.564009
Sum of electronic and zero-point Energies=    -6607.771161
Sum of electronic and thermal Energies=       -6607.726877
Sum of electronic and thermal Enthalpies=     -6607.725822
Sum of electronic and thermal Free Energies=   -6607.847993

              1              2              3
              A              A              A
Frequencies --  -221.3400          21.3751          33.7451

```

C-P-OA-PR-OH-conf1 (3i)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.053298	2.941234	1.879559
2	1	0	0.787901	3.746718	1.927401
3	1	0	-0.320719	2.742139	2.889370
4	6	0	-0.107582	1.185744	0.328298
5	6	0	-1.073394	3.242506	0.878564
6	1	0	-2.025046	3.468395	1.362647
7	1	0	-0.806226	4.072889	0.218968
8	6	0	-2.332690	1.639544	-0.611378
9	6	0	-2.862270	0.329564	-0.580789
10	6	0	-4.063824	0.111144	-1.263465
11	1	0	-4.508333	-0.877126	-1.265595
12	6	0	-4.730169	1.127093	-1.943334
13	1	0	-5.661906	0.912907	-2.455752
14	6	0	-4.193092	2.409015	-1.958538
15	1	0	-4.693574	3.212431	-2.488571
16	6	0	-2.997994	2.659391	-1.294508
17	1	0	-2.567698	3.655131	-1.316131
18	6	0	1.596630	0.893960	1.895670
19	6	0	1.687769	-0.368864	1.285122
20	6	0	2.612293	-1.268306	1.811621
21	1	0	2.732973	-2.243293	1.348840
22	6	0	3.403349	-0.917043	2.911916
23	1	0	4.119063	-1.632663	3.306085
24	6	0	3.288838	0.342490	3.496809
25	1	0	3.908738	0.611661	4.345974
26	6	0	2.376601	1.267183	2.983664
27	1	0	2.284231	2.255175	3.426248
28	6	0	-2.673521	-0.994451	2.020354
29	1	0	-2.235207	-1.879043	2.495380
30	6	0	-2.158751	0.230473	2.780888
31	1	0	-2.532469	1.158148	2.334492

32	1	0	-1.066397	0.259062	2.799545
33	1	0	-2.512689	0.197700	3.815624
34	6	0	-4.198699	-1.094049	2.091399
35	1	0	-4.520663	-1.101894	3.137495
36	1	0	-4.579101	-2.006284	1.624799
37	1	0	-4.672357	-0.237216	1.603016
38	6	0	-2.694681	-2.592380	-0.451038
39	1	0	-3.787291	-2.525542	-0.441356
40	6	0	-2.294107	-3.813282	0.385792
41	1	0	-2.673172	-4.718296	-0.098396
42	1	0	-2.710990	-3.783472	1.396196
43	1	0	-1.206938	-3.895499	0.443889
44	6	0	-2.202687	-2.739336	-1.896429
45	1	0	-1.118807	-2.884874	-1.902176
46	1	0	-2.447397	-1.866745	-2.509236
47	1	0	-2.676025	-3.613053	-2.355952
48	6	0	3.763434	-0.885279	-1.405038
49	1	0	4.019128	-0.666364	-0.362481
50	6	0	3.688208	-2.407127	-1.576942
51	1	0	3.560114	-2.660991	-2.635886
52	1	0	2.837318	-2.828217	-1.035029
53	1	0	4.621412	-2.868914	-1.231479
54	6	0	4.872972	-0.321419	-2.303274
55	1	0	5.790543	-0.900788	-2.151627
56	1	0	5.110498	0.723693	-2.090490
57	1	0	4.607008	-0.402747	-3.363443
58	6	0	2.534898	1.681819	-1.907970
59	1	0	3.245747	1.660487	-2.743626
60	6	0	3.239608	2.346712	-0.719506
61	1	0	3.725661	3.277310	-1.036436
62	1	0	4.001656	1.705081	-0.269841
63	1	0	2.521506	2.596820	0.063747
64	6	0	1.347767	2.521990	-2.388596
65	1	0	0.573839	2.605982	-1.621473
66	1	0	0.882966	2.086556	-3.277587
67	1	0	1.677387	3.537179	-2.638551
68	7	0	0.631151	1.731600	1.310603
69	7	0	-1.169440	1.991369	0.110948
70	15	0	2.078450	-0.129503	-1.749140
71	15	0	-1.984647	-1.050241	0.293296
72	45	0	0.403569	-0.660413	-0.236936
73	8	0	0.804020	-2.703535	-0.475748
74	1	0	0.790335	-3.080171	0.413202

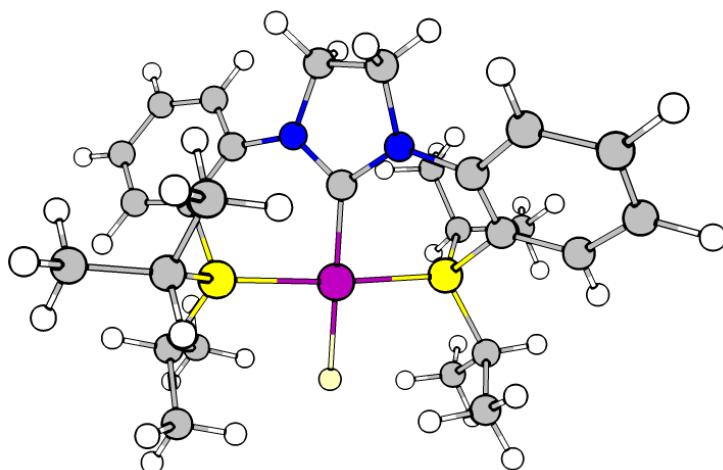
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SCF Done: E(RwB97XD) = -6608.42486874 A.U. after 1 cycles
          Conv = 0.2281D-08 -V/T = 2.0048
Zero-point correction= 0.640414 (Hartree/Particle)
Thermal correction to Energy= 0.685719
Thermal correction to Enthalpy= 0.686774
Thermal correction to Gibbs Free Energy= 0.562084

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Sum of electronic and zero-point Energies=	-6607.784454
Sum of electronic and thermal Energies=	-6607.739150
Sum of electronic and thermal Enthalpies=	-6607.738095
Sum of electronic and thermal Free Energies=	-6607.862785
	1
	A
Frequencies --	27.2471
	2
	A
	31.4439
	3
	A
	38.0714

C-P-OA-SM-F (1j)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.585919	-3.374924	-0.477048
2	1	0	1.388856	-4.039987	-0.157219
3	1	0	0.271721	-3.649864	-1.490152
4	6	0	-0.000025	-1.137129	-0.000023
5	6	0	-0.586145	-3.374959	0.476666
6	1	0	-1.389156	-4.039874	0.156711
7	1	0	-0.271982	-3.650124	1.489718
8	6	0	-2.287048	-1.633202	0.929403
9	6	0	-3.021436	-0.512766	0.485778
10	6	0	-4.318272	-0.335092	0.977299
11	1	0	-4.899413	0.516425	0.640720
12	6	0	-4.896910	-1.212492	1.888610
13	1	0	-5.905776	-1.040064	2.248018
14	6	0	-4.159637	-2.304075	2.331147
15	1	0	-4.578320	-2.998969	3.051846
16	6	0	-2.871526	-2.511435	1.852050
17	1	0	-2.316308	-3.366241	2.218574
18	6	0	2.287023	-1.633232	-0.929412
19	6	0	3.021514	-0.512977	-0.485478
20	6	0	4.318450	-0.335422	-0.976760
21	1	0	4.899725	0.515886	-0.639878
22	6	0	4.897065	-1.212689	-1.888215

23	1	0	5.905998	-1.040317	-2.247463
24	6	0	4.159656	-2.304016	-2.331152
25	1	0	4.578293	-2.998760	-3.052023
26	6	0	2.871464	-2.511307	-1.852235
27	1	0	2.316154	-3.365930	-2.219043
28	6	0	-2.690316	0.101797	-2.335989
29	1	0	-2.268500	0.862264	-3.002222
30	6	0	-1.992618	-1.224006	-2.656392
31	1	0	-2.348123	-2.027705	-2.002823
32	1	0	-0.908783	-1.138699	-2.545835
33	1	0	-2.209708	-1.514097	-3.689290
34	6	0	-4.197513	0.004655	-2.583688
35	1	0	-4.385615	-0.334819	-3.607382
36	1	0	-4.701011	0.966810	-2.460425
37	1	0	-4.663240	-0.715397	-1.903596
38	6	0	-3.211441	2.270587	-0.420034
39	1	0	-4.276102	2.062002	-0.572103
40	6	0	-2.761034	3.286548	-1.479036
41	1	0	-3.282798	4.234771	-1.313518
42	1	0	-2.994729	2.958206	-2.496243
43	1	0	-1.686013	3.463081	-1.390113
44	6	0	-2.998662	2.831487	0.991522
45	1	0	-1.942327	3.074773	1.130765
46	1	0	-3.304463	2.125525	1.768851
47	1	0	-3.591833	3.744085	1.113816
48	6	0	3.211678	2.270394	0.419987
49	1	0	4.276308	2.061711	0.572148
50	6	0	2.999168	2.830909	-0.991770
51	1	0	1.942850	3.074140	-1.131232
52	1	0	3.305150	2.124612	-1.768740
53	1	0	3.592363	3.743465	-1.114247
54	6	0	2.761404	3.286586	1.478813
55	1	0	3.283328	4.234698	1.313172
56	1	0	2.995045	2.958330	2.496065
57	1	0	1.686410	3.463249	1.389883
58	6	0	2.690007	0.101853	2.336221
59	1	0	2.268276	0.862491	3.002309
60	6	0	4.197155	0.004400	2.584123
61	1	0	4.385058	-0.335062	3.607858
62	1	0	4.700870	0.966440	2.460863
63	1	0	4.662820	-0.715804	1.904149
64	6	0	1.991947	-1.223750	2.656642
65	1	0	2.347407	-2.027589	2.003226
66	1	0	0.908152	-1.138211	2.545871
67	1	0	2.208769	-1.513786	3.689612
68	7	0	1.007937	-1.974605	-0.427406
69	7	0	-1.008022	-1.974592	0.427286
70	15	0	2.237394	0.709433	0.632485
71	15	0	-2.237361	0.709498	-0.632363
72	45	0	0.000050	0.803077	-0.000174

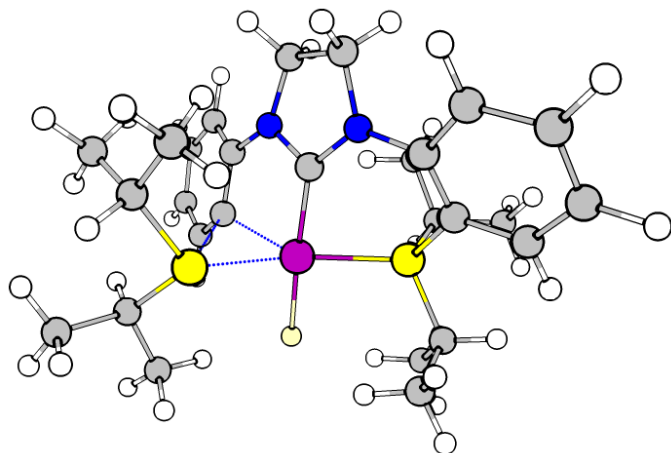
73	9	0	-0.000075	2.893983	0.000005
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SCF Done: E(RwB97XD) = -6632.52358743 A.U. after 1 cycles
 Conv g = 0.3325D-08 -V/T = 2.0048

Zero-point correction= 0.631694 (Hartree/Particle)
 Thermal correction to Energy= 0.675491
 Thermal correction to Enthalpy= 0.676546
 Thermal correction to Gibbs Free Energy= 0.555196
 Sum of electronic and zero-point Energies= -6631.891894
 Sum of electronic and thermal Energies= -6631.848096
 Sum of electronic and thermal Enthalpies= -6631.847041
 Sum of electronic and thermal Free Energies= -6631.968391

	1	2	3
	A	A	A
Frequencies --	26.1312	35.7487	49.8300

C-P-OA-TS-F (2j)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.295722	-3.270621	1.140489
2	1	0	-1.056132	-4.028136	0.940782
3	1	0	-0.008925	-3.323697	2.196642
4	6	0	0.139259	-1.187810	0.146904
5	6	0	0.913116	-3.394863	0.207526
6	1	0	1.783033	-3.835208	0.697087
7	1	0	0.668625	-3.985711	-0.679977
8	6	0	2.393240	-1.615452	-0.778788
9	6	0	2.958383	-0.333635	-0.600419
10	6	0	4.189852	-0.076264	-1.209494
11	1	0	4.650044	0.898306	-1.092550
12	6	0	4.861356	-1.033584	-1.965018
13	1	0	5.815487	-0.793917	-2.421781
14	6	0	4.295385	-2.292602	-2.123529

15	1	0	4.798041	-3.054223	-2.710383
16	6	0	3.070024	-2.578841	-1.532186
17	1	0	2.632496	-3.560268	-1.675254
18	6	0	-1.829168	-1.248089	1.426583
19	6	0	-2.062057	0.052642	0.927802
20	6	0	-2.944242	0.848150	1.662677
21	1	0	-3.086690	1.884643	1.378184
22	6	0	-3.641565	0.342874	2.763156
23	1	0	-4.326961	0.987282	3.304982
24	6	0	-3.459737	-0.976746	3.165540
25	1	0	-4.013292	-1.377166	4.008686
26	6	0	-2.526410	-1.778033	2.505476
27	1	0	-2.335673	-2.790886	2.847912
28	6	0	2.715800	0.696887	2.111241
29	1	0	2.245570	1.510832	2.673301
30	6	0	2.205440	-0.622710	2.697482
31	1	0	2.622375	-1.482629	2.162255
32	1	0	1.114358	-0.679723	2.661705
33	1	0	2.514854	-0.704297	3.743803
34	6	0	4.236614	0.810574	2.237868
35	1	0	4.528969	0.711294	3.287903
36	1	0	4.612830	1.772942	1.881472
37	1	0	4.739758	0.017459	1.676232
38	6	0	2.795723	2.572599	-0.166760
39	1	0	3.888960	2.509456	-0.156868
40	6	0	2.363847	3.678687	0.806010
41	1	0	2.708595	4.643636	0.420700
42	1	0	2.802888	3.547599	1.799294
43	1	0	1.273369	3.702482	0.886658
44	6	0	2.315392	2.877266	-1.590402
45	1	0	1.230725	3.011366	-1.593691
46	1	0	2.571657	2.080272	-2.294607
47	1	0	2.781738	3.802158	-1.944596
48	6	0	-3.669311	1.432430	-1.274973
49	1	0	-4.264688	1.148657	-0.401974
50	6	0	-3.271965	2.910390	-1.162291
51	1	0	-2.819073	3.248056	-2.100698
52	1	0	-2.533601	3.095109	-0.379379
53	1	0	-4.166026	3.517622	-0.980119
54	6	0	-4.542881	1.237897	-2.524036
55	1	0	-5.320629	2.008463	-2.534185
56	1	0	-5.046459	0.268611	-2.548555
57	1	0	-3.961489	1.349626	-3.445695
58	6	0	-2.826829	-1.287048	-1.848812
59	1	0	-3.297494	-0.977676	-2.789763
60	6	0	-3.922856	-1.917460	-0.985159
61	1	0	-4.451146	-2.689116	-1.556772
62	1	0	-4.659668	-1.182724	-0.650214
63	1	0	-3.506999	-2.390096	-0.093465
64	6	0	-1.761430	-2.314168	-2.253024

65	1	0	-1.427653	-2.898529	-1.394077
66	1	0	-0.886486	-1.839644	-2.706341
67	1	0	-2.180217	-3.019087	-2.978905
68	7	0	-0.771240	-1.936510	0.812780
69	7	0	1.180342	-1.997621	-0.163068
70	15	0	-2.122408	0.377072	-1.355479
71	15	0	2.083875	0.955688	0.381170
72	45	0	-0.226633	0.718936	0.003927
73	9	0	-0.546428	2.766382	0.194335

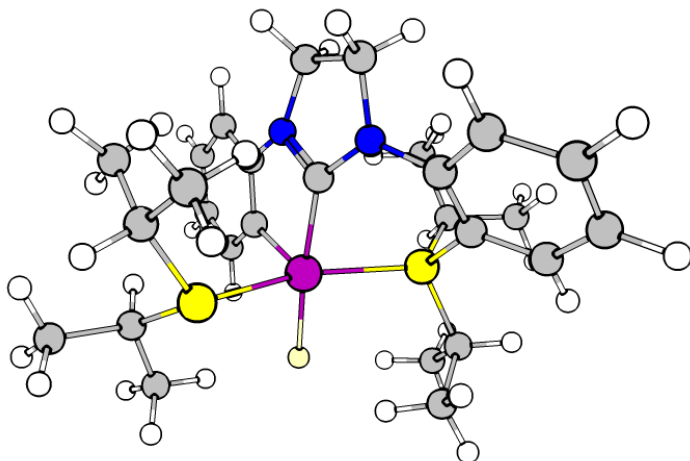
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SCF Done: E(RwB97XD) = -6632.46574701      A.U. after   1 cycles
              Conv =   0.2295D-08              -V/T =   2.0048
Zero-point correction=                      0.629987 (Hartree/Particle)
Thermal correction to Energy=                0.673465
Thermal correction to Enthalpy=              0.674520
Thermal correction to Gibbs Free Energy=      0.554295
Sum of electronic and zero-point Energies=    -6631.835760
Sum of electronic and thermal Energies=       -6631.792282
Sum of electronic and thermal Enthalpies=     -6631.791227
Sum of electronic and thermal Free Energies=   -6631.911452

              1                      2                      3
              A                      A                      A
Frequencies --  -234.3881              25.1026              36.8584

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C-P-OA-PR-F-conf1 (3j)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.051919	2.890934	1.931187
2	1	0	0.785568	3.695510	2.001893
3	1	0	-0.322682	2.663828	2.934730
4	6	0	-0.107275	1.181637	0.332791
5	6	0	-1.074726	3.218673	0.937398
6	1	0	-2.028094	3.422943	1.427385

7	1	0	-0.811387	4.071501	0.305870
8	6	0	-2.348542	1.650339	-0.574275
9	6	0	-2.878597	0.340238	-0.553904
10	6	0	-4.101459	0.131660	-1.200324
11	1	0	-4.542437	-0.858857	-1.204613
12	6	0	-4.787869	1.159778	-1.840825
13	1	0	-5.735206	0.956231	-2.328252
14	6	0	-4.248741	2.441183	-1.850970
15	1	0	-4.764012	3.253509	-2.352445
16	6	0	-3.033626	2.681278	-1.219713
17	1	0	-2.604746	3.677707	-1.237039
18	6	0	1.557279	0.813404	1.913373
19	6	0	1.609943	-0.430069	1.265294
20	6	0	2.450992	-1.405661	1.789402
21	1	0	2.505554	-2.375918	1.306226
22	6	0	3.223420	-1.129381	2.924108
23	1	0	3.879990	-1.896732	3.323644
24	6	0	3.164305	0.119329	3.541333
25	1	0	3.771037	0.325788	4.417095
26	6	0	2.320169	1.110893	3.035306
27	1	0	2.264542	2.087159	3.508778
28	6	0	-2.612081	-1.087114	1.989850
29	1	0	-2.129674	-1.970526	2.421433
30	6	0	-2.126011	0.130699	2.779904
31	1	0	-2.536756	1.059346	2.368856
32	1	0	-1.035279	0.192576	2.786208
33	1	0	-2.462642	0.054280	3.817982
34	6	0	-4.130649	-1.246205	2.090075
35	1	0	-4.427379	-1.299793	3.142137
36	1	0	-4.487050	-2.157299	1.602852
37	1	0	-4.646578	-0.392184	1.640893
38	6	0	-2.627095	-2.592160	-0.541958
39	1	0	-3.720477	-2.593585	-0.482777
40	6	0	-2.095159	-3.809661	0.226799
41	1	0	-2.393600	-4.722340	-0.298060
42	1	0	-2.500342	-3.868858	1.240871
43	1	0	-1.003073	-3.780509	0.269404
44	6	0	-2.195300	-2.648132	-2.012697
45	1	0	-1.107859	-2.740938	-2.076026
46	1	0	-2.509684	-1.764194	-2.575074
47	1	0	-2.645507	-3.524487	-2.489540
48	6	0	3.758595	-0.848083	-1.364804
49	1	0	3.989998	-0.667414	-0.309153
50	6	0	3.635008	-2.360974	-1.579789
51	1	0	3.497402	-2.581928	-2.644525
52	1	0	2.778965	-2.780145	-1.048650
53	1	0	4.554248	-2.859094	-1.248954
54	6	0	4.913445	-0.302242	-2.215766
55	1	0	5.807203	-0.914281	-2.051277
56	1	0	5.177505	0.729333	-1.970683

57	1	0	4.676302	-0.349312	-3.284736
58	6	0	2.633696	1.789158	-1.775206
59	1	0	3.358237	1.796991	-2.599506
60	6	0	3.337065	2.361561	-0.539144
61	1	0	3.858038	3.291904	-0.795455
62	1	0	4.070689	1.672231	-0.113799
63	1	0	2.613924	2.592555	0.245089
64	6	0	1.480110	2.692539	-2.221828
65	1	0	0.703545	2.764913	-1.455830
66	1	0	1.008646	2.318998	-3.135130
67	1	0	1.846363	3.706986	-2.416868
68	7	0	0.632603	1.698785	1.330572
69	7	0	-1.167326	1.993187	0.126967
70	15	0	2.119707	-0.014047	-1.745722
71	15	0	-1.967722	-1.054807	0.247695
72	45	0	0.385891	-0.613462	-0.309448
73	9	0	0.750221	-2.618091	-0.671540

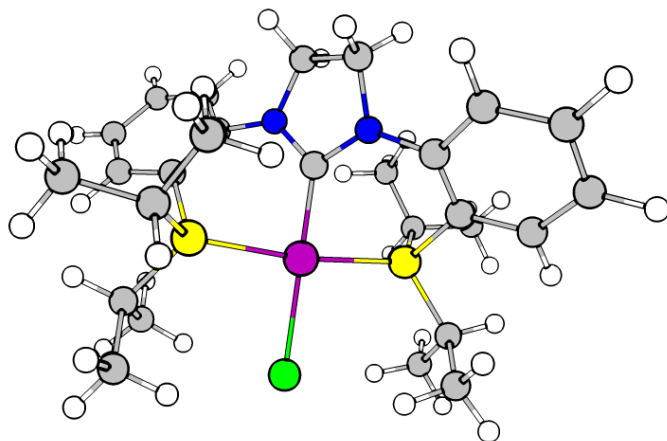
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SCF Done:  E(RwB97XD) = -6632.48093029      A.U. after   1 cycles
                Conv g =   0.2466D-08          -V/T =   2.0048
Zero-point correction=                      0.629872 (Hartree/Particle)
Thermal correction to Energy=                0.674393
Thermal correction to Enthalpy=              0.675448
Thermal correction to Gibbs Free Energy=      0.552655
Sum of electronic and zero-point Energies=    -6631.851058
Sum of electronic and thermal Energies=        -6631.806538
Sum of electronic and thermal Enthalpies=      -6631.805483
Sum of electronic and thermal Free Energies=    -6631.928275

                1                2                3
                A                A                A
Frequencies --   30.2212          33.7824          45.3488

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C-P-OA-SM-Cl (1k)



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

```

1	6	0	-0.559260	-3.413185	0.505362
2	1	0	-1.383393	-4.070861	0.227614
3	1	0	-0.194192	-3.691732	1.499867
4	6	0	0.000433	-1.176788	-0.000156
5	6	0	0.559058	-3.412476	-0.509896
6	1	0	1.382647	-4.071274	-0.233249
7	1	0	0.194005	-3.688693	-1.505055
8	6	0	2.250365	-1.676129	-1.004874
9	6	0	3.019066	-0.601719	-0.516348
10	6	0	4.322857	-0.461057	-1.004426
11	1	0	4.948946	0.342138	-0.634685
12	6	0	4.861339	-1.319859	-1.957245
13	1	0	5.877316	-1.173316	-2.307910
14	6	0	4.078114	-2.353252	-2.456000
15	1	0	4.464856	-3.026459	-3.213942
16	6	0	2.786202	-2.530177	-1.976715
17	1	0	2.189247	-3.341496	-2.375919
18	6	0	-2.248944	-1.676737	1.005137
19	6	0	-3.018592	-0.602771	0.517112
20	6	0	-4.321671	-0.462268	1.007096
21	1	0	-4.948738	0.340418	0.637933
22	6	0	-4.858390	-1.320812	1.961205
23	1	0	-5.873839	-1.174328	2.313439
24	6	0	-4.074199	-2.353798	2.459245
25	1	0	-4.459657	-3.026750	3.218068
26	6	0	-2.782953	-2.530605	1.978013
27	1	0	-2.185147	-3.341769	2.376316
28	6	0	2.625038	-0.074976	2.333016
29	1	0	2.263031	0.709747	3.006259
30	6	0	1.810777	-1.336457	2.635329
31	1	0	2.112219	-2.167231	1.988488
32	1	0	0.740191	-1.160921	2.507853
33	1	0	1.985552	-1.643365	3.671243
34	6	0	4.112616	-0.317654	2.603270
35	1	0	4.244220	-0.728366	3.609380
36	1	0	4.704749	0.598704	2.547016
37	1	0	4.529137	-1.039123	1.893367
38	6	0	3.414951	2.074063	0.533569
39	1	0	4.429920	1.696417	0.692778
40	6	0	3.126751	3.081062	1.655036
41	1	0	3.786048	3.946513	1.534458
42	1	0	3.318999	2.660179	2.645946
43	1	0	2.093901	3.431487	1.611799
44	6	0	3.357275	2.738941	-0.847136
45	1	0	2.376662	3.186238	-1.014277
46	1	0	3.555147	2.031779	-1.656843
47	1	0	4.115276	3.527716	-0.898393
48	6	0	-3.416775	2.072172	-0.533988
49	1	0	-4.431399	1.693250	-0.692309

50	6	0	-3.358958	2.737882	0.846322
51	1	0	-2.378413	3.185546	1.012978
52	1	0	-3.556450	2.031127	1.656476
53	1	0	-4.117142	3.526479	0.897273
54	6	0	-3.130480	3.078898	-1.656198
55	1	0	-3.790568	3.943725	-1.535505
56	1	0	-3.323103	2.657331	-2.646766
57	1	0	-2.097963	3.430357	-1.613971
58	6	0	-2.625456	-0.076399	-2.332913
59	1	0	-2.264670	0.708879	-3.006196
60	6	0	-4.112920	-0.320691	-2.602480
61	1	0	-4.244562	-0.731860	-3.608394
62	1	0	-4.705961	0.595093	-2.546213
63	1	0	-4.528385	-1.042322	-1.892117
64	6	0	-1.809911	-1.336849	-2.635994
65	1	0	-2.110713	-2.168442	-1.989905
66	1	0	-0.739516	-1.160408	-2.508158
67	1	0	-1.984172	-1.643082	-3.672186
68	7	0	-0.976394	-2.009047	0.483379
69	7	0	0.977114	-2.008596	-0.485092
70	15	0	-2.261973	0.617601	-0.634880
71	15	0	2.261378	0.618561	0.634704
72	17	0	-0.001216	3.266736	-0.001436
73	45	0	-0.000167	0.785002	0.000232

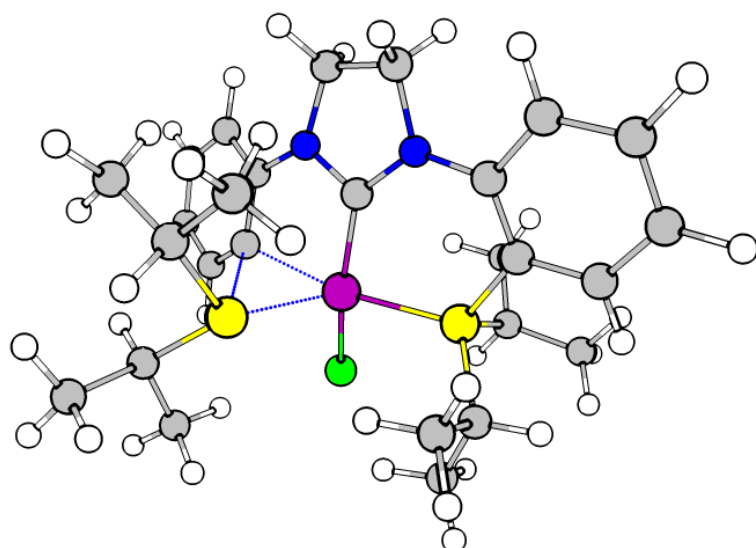
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SCF Done: E(RwB97XD) = -6992.85688437 A.U. after 1 cycles
          Conv = 0.2385D-08 -V/T = 2.0048
Zero-point correction= 0.632604 (Hartree/Particle)
Thermal correction to Energy= 0.676356
Thermal correction to Enthalpy= 0.677411
Thermal correction to Gibbs Free Energy= 0.556145
Sum of electronic and zero-point Energies= -6992.224280
Sum of electronic and thermal Energies= -6992.180528
Sum of electronic and thermal Enthalpies= -6992.179473
Sum of electronic and thermal Free Energies= -6992.300739

          1          2          3
          A          A          A
Frequencies -- 16.4591 39.7175 55.3037

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C-P-OA-TS-Cl (2k)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.534149	3.506323	-1.040668
2	1	0	-1.241351	4.219152	-0.612373
3	1	0	-0.478385	3.666250	-2.122342
4	6	0	0.118013	1.352220	-0.361113
5	6	0	0.839341	3.578671	-0.381667
6	1	0	1.574117	4.080118	-1.012009
7	1	0	0.789336	4.088648	0.584768
8	6	0	2.480627	1.821852	0.294704
9	6	0	2.992549	0.506854	0.320945
10	6	0	4.301093	0.323897	0.788451
11	1	0	4.712923	-0.677618	0.829584
12	6	0	5.103830	1.372199	1.217720
13	1	0	6.111402	1.181369	1.570590
14	6	0	4.585691	2.660814	1.192852
15	1	0	5.179613	3.503745	1.530460
16	6	0	3.292869	2.878827	0.738472
17	1	0	2.920033	3.894040	0.745732
18	6	0	-2.088202	1.511125	-1.205897
19	6	0	-2.267253	0.167339	-0.820444
20	6	0	-3.319574	-0.515070	-1.441483
21	1	0	-3.443886	-1.576584	-1.264924
22	6	0	-4.213415	0.127076	-2.296415
23	1	0	-5.024079	-0.435224	-2.748588
24	6	0	-4.061038	1.483329	-2.573741
25	1	0	-4.762242	1.994246	-3.225772
26	6	0	-2.977359	2.179578	-2.044993
27	1	0	-2.822994	3.222324	-2.303591
28	6	0	2.833111	-1.577706	-1.729679

29	1	0	2.213726	-2.443371	-1.989475
30	6	0	2.646685	-0.525767	-2.828570
31	1	0	3.175683	0.401955	-2.583388
32	1	0	1.588538	-0.295950	-2.978519
33	1	0	3.049734	-0.901081	-3.773893
34	6	0	4.292752	-2.018841	-1.617557
35	1	0	4.602567	-2.483406	-2.558747
36	1	0	4.448321	-2.756414	-0.825158
37	1	0	4.957719	-1.168960	-1.439132
38	6	0	2.424269	-2.183645	1.165606
39	1	0	3.514154	-2.279546	1.206030
40	6	0	1.841947	-3.568425	0.871370
41	1	0	2.151932	-4.259293	1.662010
42	1	0	2.187595	-3.972771	-0.083450
43	1	0	0.751288	-3.538951	0.838186
44	6	0	1.931649	-1.653981	2.516127
45	1	0	0.844263	-1.536128	2.510140
46	1	0	2.381225	-0.689162	2.767700
47	1	0	2.196765	-2.364933	3.304925
48	6	0	-3.451930	-1.394340	1.464234
49	1	0	-4.207623	-0.965024	0.801450
50	6	0	-3.197669	-2.858668	1.081658
51	1	0	-2.550864	-3.333783	1.827052
52	1	0	-2.700955	-2.975074	0.116706
53	1	0	-4.145176	-3.408026	1.056587
54	6	0	-3.999467	-1.345946	2.899288
55	1	0	-4.800226	-2.086008	2.998516
56	1	0	-4.421850	-0.372656	3.160132
57	1	0	-3.229880	-1.600341	3.636744
58	6	0	-2.252173	1.139617	2.221296
59	1	0	-2.558226	0.704143	3.180008
60	6	0	-3.427001	1.980803	1.716933
61	1	0	-3.760028	2.668885	2.502172
62	1	0	-4.280242	1.363431	1.423548
63	1	0	-3.145442	2.580352	0.848837
64	6	0	-1.027896	2.003025	2.549864
65	1	0	-0.803142	2.702089	1.742852
66	1	0	-0.136300	1.396884	2.734609
67	1	0	-1.224261	2.599489	3.446894
68	7	0	-0.916028	2.135960	-0.752522
69	7	0	1.195432	2.161749	-0.187414
70	15	0	-1.824452	-0.459297	1.343778
71	15	0	2.019639	-0.967445	-0.180553
72	45	0	-0.251294	-0.564367	-0.425772
73	17	0	-0.611352	-2.772947	-1.493983

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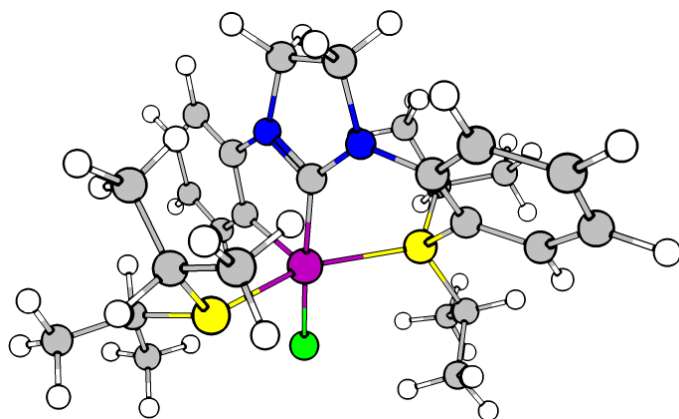
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SCF Done:  E(RwB97XD) = -6992.80295642      A.U. after   1 cycles
              Conv g =   0.2781D-08           -V/T =   2.0048
Zero-point correction=                      0.629102 (Hartree/Particle)
Thermal correction to Energy=                0.673370

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Thermal correction to Enthalpy=	0.674425
Thermal correction to Gibbs Free Energy=	0.550906
Sum of electronic and zero-point Energies=	-6992.173854
Sum of electronic and thermal Energies=	-6992.129587
Sum of electronic and thermal Enthalpies=	-6992.128532
Sum of electronic and thermal Free Energies=	-6992.252050

	1	2	3
	A	A	A
Frequencies --	-217.2890	21.6605	32.7600

C-P-OA-PR-Cl-conf1 (3k)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.265890	2.606099	2.339304
2	1	0	1.033155	3.369893	2.476820
3	1	0	-0.075688	2.263255	3.321632
4	6	0	-0.052422	1.092017	0.580037
5	6	0	-0.882988	3.092173	1.445534
6	1	0	-1.796695	3.306543	2.001556
7	1	0	-0.594012	3.982944	0.880648
8	6	0	-2.288933	1.795879	-0.198010
9	6	0	-2.880561	0.529906	-0.398833
10	6	0	-4.107152	0.499629	-1.071430
11	1	0	-4.601105	-0.448494	-1.245090
12	6	0	-4.736787	1.653611	-1.528569
13	1	0	-5.688872	1.580532	-2.042909
14	6	0	-4.136294	2.889230	-1.321168
15	1	0	-4.605769	3.799760	-1.677772
16	6	0	-2.917213	2.955512	-0.657458
17	1	0	-2.442394	3.918933	-0.507046
18	6	0	1.751337	0.555577	1.954586
19	6	0	1.744900	-0.614222	1.178346
20	6	0	2.608245	-1.638351	1.559983
21	1	0	2.607000	-2.572881	1.011130
22	6	0	3.473463	-1.468428	2.646883

23	1	0	4.144547	-2.276096	2.923526
24	6	0	3.486858	-0.278844	3.372036
25	1	0	4.168993	-0.152127	4.206463
26	6	0	2.607239	0.750553	3.031799
27	1	0	2.589065	1.676339	3.599812
28	6	0	-2.616285	-1.250495	1.917153
29	1	0	-2.223973	-2.239187	2.178103
30	6	0	-1.966469	-0.241757	2.867477
31	1	0	-2.302972	0.778429	2.655092
32	1	0	-0.876073	-0.279927	2.809065
33	1	0	-2.253892	-0.472707	3.897466
34	6	0	-4.138570	-1.255645	2.074697
35	1	0	-4.399175	-1.436744	3.122004
36	1	0	-4.619028	-2.035742	1.479120
37	1	0	-4.568137	-0.291646	1.785529
38	6	0	-2.921184	-2.367296	-0.776176
39	1	0	-3.998935	-2.209974	-0.669963
40	6	0	-2.598910	-3.742007	-0.175151
41	1	0	-3.030430	-4.517526	-0.815198
42	1	0	-3.029893	-3.865625	0.822053
43	1	0	-1.521294	-3.909821	-0.122965
44	6	0	-2.555285	-2.303095	-2.264048
45	1	0	-1.497869	-2.534245	-2.408915
46	1	0	-2.757285	-1.320756	-2.700450
47	1	0	-3.146575	-3.040662	-2.815509
48	6	0	3.808952	-0.191964	-1.355888
49	1	0	3.988727	0.024308	-0.296771
50	6	0	4.054457	-1.685126	-1.596898
51	1	0	3.961659	-1.919785	-2.662715
52	1	0	3.343093	-2.316968	-1.067672
53	1	0	5.068177	-1.951263	-1.276401
54	6	0	4.810223	0.614981	-2.196197
55	1	0	5.816399	0.211051	-2.040770
56	1	0	4.842732	1.674570	-1.933607
57	1	0	4.588847	0.533360	-3.266369
58	6	0	2.134499	2.109827	-1.821725
59	1	0	2.847090	2.229814	-2.647674
60	6	0	2.700825	2.879520	-0.622288
61	1	0	3.059428	3.865355	-0.940333
62	1	0	3.531872	2.359759	-0.139008
63	1	0	1.933091	3.040118	0.136745
64	6	0	0.823245	2.730255	-2.313533
65	1	0	0.031294	2.650509	-1.565424
66	1	0	0.466625	2.242884	-3.224829
67	1	0	0.966197	3.795069	-2.530633
68	7	0	0.769109	1.480103	1.567310
69	7	0	-1.089935	1.955087	0.534043
70	15	0	2.019817	0.238620	-1.747868
71	15	0	-2.044532	-1.025505	0.158869
72	45	0	0.379993	-0.617939	-0.315378

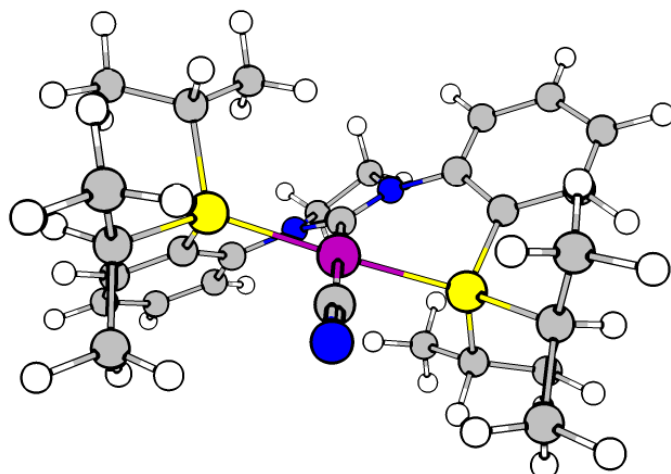
73	17	0	0.807788	-2.956017	-1.024352
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SCF Done: E(RwB97XD) = -6992.81231564 A.U. after 1 cycles
 Conv g = 0.2821D-08 -V/T = 2.0048

Zero-point correction= 0.629109 (Hartree/Particle)
 Thermal correction to Energy= 0.674329
 Thermal correction to Enthalpy= 0.675384
 Thermal correction to Gibbs Free Energy= 0.549842
 Sum of electronic and zero-point Energies= -6992.183207
 Sum of electronic and thermal Energies= -6992.137987
 Sum of electronic and thermal Enthalpies= -6992.136932
 Sum of electronic and thermal Free Energies= -6992.262473

	1	2	3
	A	A	A
Frequencies --	18.5847	32.0054	37.2223

C-P-OA-SM-CN (1I)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.578173	-3.438691	0.485973
2	1	0	-1.396443	-4.088130	0.173823
3	1	0	-0.251669	-3.726784	1.490703
4	6	0	-0.000036	-1.208105	-0.000445
5	6	0	0.577872	-3.438240	-0.489215
6	1	0	1.395976	-4.088185	-0.177716
7	1	0	0.251424	-3.725083	-1.494318
8	6	0	2.260123	-1.676785	-0.974232
9	6	0	3.003127	-0.572584	-0.507375
10	6	0	4.302398	-0.412023	-1.001693
11	1	0	4.908022	0.415189	-0.651861
12	6	0	4.863240	-1.277721	-1.935238
13	1	0	5.874774	-1.112357	-2.290268
14	6	0	4.108193	-2.343416	-2.406906

15	1	0	4.511891	-3.025704	-3.147643
16	6	0	2.820768	-2.540156	-1.923046
17	1	0	2.246666	-3.376664	-2.302682
18	6	0	-2.259751	-1.677333	0.973874
19	6	0	-3.002906	-0.572810	0.508033
20	6	0	-4.301639	-0.411954	1.003670
21	1	0	-4.907357	0.415564	0.654748
22	6	0	-4.861806	-1.277841	1.937458
23	1	0	-5.872939	-1.112326	2.293559
24	6	0	-4.106658	-2.343962	2.407976
25	1	0	-4.509886	-3.026397	3.148835
26	6	0	-2.819728	-2.540924	1.922849
27	1	0	-2.245512	-3.377742	2.301631
28	6	0	2.614915	-0.011445	2.334400
29	1	0	2.254561	0.779014	3.001594
30	6	0	1.804083	-1.271410	2.652131
31	1	0	2.104957	-2.107982	2.012658
32	1	0	0.732626	-1.099612	2.525852
33	1	0	1.982700	-1.567507	3.690525
34	6	0	4.104529	-0.247268	2.598873
35	1	0	4.243246	-0.642030	3.610351
36	1	0	4.694135	0.669489	2.524677
37	1	0	4.517992	-0.978316	1.897142
38	6	0	3.375338	2.131615	0.512151
39	1	0	4.399336	1.776627	0.663664
40	6	0	3.075700	3.139095	1.630010
41	1	0	3.704480	4.023698	1.490024
42	1	0	3.297384	2.733101	2.620883
43	1	0	2.034293	3.464461	1.604421
44	6	0	3.287554	2.792559	-0.868973
45	1	0	2.311131	3.256198	-1.012424
46	1	0	3.453230	2.081604	-1.682786
47	1	0	4.052017	3.572842	-0.943432
48	6	0	-3.375845	2.131199	-0.511308
49	1	0	-4.399867	1.775714	-0.661476
50	6	0	-3.286841	2.792750	0.869425
51	1	0	-2.310439	3.256765	1.011813
52	1	0	-3.451533	2.081991	1.683615
53	1	0	-4.051431	3.572859	0.944394
54	6	0	-3.077901	3.138247	-1.630096
55	1	0	-3.706600	4.022816	-1.489516
56	1	0	-3.301037	2.731862	-2.620476
57	1	0	-2.036498	3.463734	-1.606208
58	6	0	-2.615477	-0.011694	-2.333851
59	1	0	-2.256000	0.779174	-3.001030
60	6	0	-4.105136	-0.248518	-2.597401
61	1	0	-4.244344	-0.643351	-3.608782
62	1	0	-4.695213	0.667892	-2.522702
63	1	0	-4.517712	-0.979865	-1.895452
64	6	0	-1.803950	-1.271042	-2.652218

65	1	0	-2.104321	-2.108120	-2.013193
66	1	0	-0.732587	-1.098662	-2.525850
67	1	0	-1.982387	-1.566668	-3.690768
68	7	0	-0.984984	-2.029516	0.462184
69	7	0	0.984903	-2.029127	-0.463809
70	15	0	-2.242690	0.662830	-0.630855
71	15	0	2.242455	0.662997	0.631307
72	45	0	-0.000020	0.818498	0.000092
73	6	0	-0.000249	2.877062	-0.002008
74	7	0	-0.000363	4.049993	-0.003256

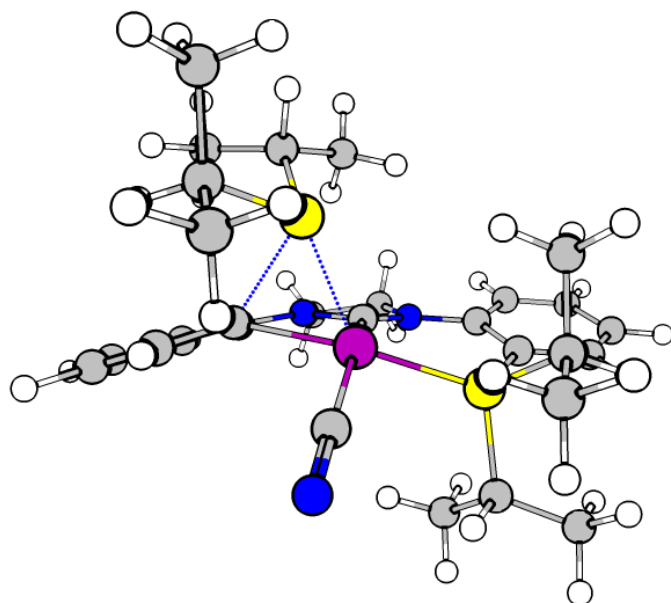
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SCF Done:  E(RwB97XD) = -6625.49884325      A.U. after   1 cycles
              Convg =   0.2082D-08              -V/T =   2.0049
Zero-point correction=                          0.639480 (Hartree/Particle)
Thermal correction to Energy=                     0.684096
Thermal correction to Enthalpy=                   0.685151
Thermal correction to Gibbs Free Energy=           0.562827
Sum of electronic and zero-point Energies=        -6624.859364
Sum of electronic and thermal Energies=           -6624.814747
Sum of electronic and thermal Enthalpies=         -6624.813692
Sum of electronic and thermal Free Energies=       -6624.936016

              1              2              3
              A              A              A
Frequencies --   24.6326          40.9071          57.9792

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C-P-OA-TS-CN (2I)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.499295	3.529454	-0.969412

2	1	0	-1.227251	4.237127	-0.568286
3	1	0	-0.394400	3.698518	-2.046070
4	6	0	0.120147	1.375425	-0.269911
5	6	0	0.843199	3.597568	-0.243697
6	1	0	1.609884	4.103720	-0.830878
7	1	0	0.744857	4.097241	0.723999
8	6	0	2.465538	1.804048	0.425739
9	6	0	2.987198	0.492477	0.351613
10	6	0	4.301329	0.293626	0.797227
11	1	0	4.729992	-0.700463	0.754578
12	6	0	5.093435	1.315379	1.304641
13	1	0	6.105905	1.109301	1.634169
14	6	0	4.559473	2.594642	1.389490
15	1	0	5.143159	3.414166	1.795461
16	6	0	3.263047	2.830882	0.954635
17	1	0	2.871204	3.835540	1.044472
18	6	0	-2.044517	1.526057	-1.213710
19	6	0	-2.230228	0.170775	-0.862963
20	6	0	-3.273030	-0.497003	-1.510940
21	1	0	-3.408352	-1.559450	-1.346704
22	6	0	-4.147044	0.160420	-2.377759
23	1	0	-4.950455	-0.392581	-2.853575
24	6	0	-3.982369	1.517709	-2.633772
25	1	0	-4.665410	2.040265	-3.295675
26	6	0	-2.910599	2.204930	-2.065899
27	1	0	-2.749688	3.251629	-2.303978
28	6	0	2.824345	-1.455186	-1.842217
29	1	0	2.234300	-2.330216	-2.137183
30	6	0	2.573022	-0.350235	-2.874040
31	1	0	3.074480	0.580085	-2.584905
32	1	0	1.504320	-0.149614	-2.987646
33	1	0	2.968171	-0.654192	-3.847794
34	6	0	4.302217	-1.843833	-1.788300
35	1	0	4.607037	-2.244257	-2.759929
36	1	0	4.506249	-2.615142	-1.040197
37	1	0	4.935892	-0.977799	-1.577207
38	6	0	2.494198	-2.270534	1.006181
39	1	0	3.586800	-2.316043	1.046948
40	6	0	1.986507	-3.655715	0.597882
41	1	0	2.339522	-4.390510	1.328356
42	1	0	2.348628	-3.962510	-0.386493
43	1	0	0.896415	-3.688544	0.573449
44	6	0	1.970981	-1.876248	2.390942
45	1	0	0.879588	-1.806854	2.384832
46	1	0	2.372728	-0.915194	2.724820
47	1	0	2.264851	-2.635579	3.122241
48	6	0	-3.424094	-1.561912	1.378855
49	1	0	-4.193170	-1.152964	0.717871
50	6	0	-3.095986	-2.998037	0.956570
51	1	0	-2.373147	-3.441762	1.649420

52	1	0	-2.662300	-3.069625	-0.040269
53	1	0	-4.005381	-3.608168	0.979886
54	6	0	-3.991065	-1.585761	2.808817
55	1	0	-4.753467	-2.368164	2.875886
56	1	0	-4.467260	-0.645182	3.094176
57	1	0	-3.217093	-1.820984	3.547825
58	6	0	-2.456891	1.050143	2.165482
59	1	0	-2.735211	0.597728	3.125395
60	6	0	-3.698218	1.766931	1.629234
61	1	0	-4.079225	2.467291	2.381260
62	1	0	-4.502918	1.070380	1.380460
63	1	0	-3.470931	2.337881	0.726773
64	6	0	-1.332139	2.037260	2.504709
65	1	0	-1.182361	2.762016	1.702686
66	1	0	-0.381056	1.529351	2.690361
67	1	0	-1.594685	2.602950	3.404708
68	7	0	-0.891698	2.153663	-0.711064
69	7	0	1.185466	2.176637	-0.047514
70	15	0	-1.862101	-0.516346	1.324174
71	15	0	2.032123	-0.969818	-0.238138
72	45	0	-0.252737	-0.586511	-0.391855
73	6	0	-0.556598	-2.462967	-1.225038
74	7	0	-0.685595	-3.453976	-1.836631

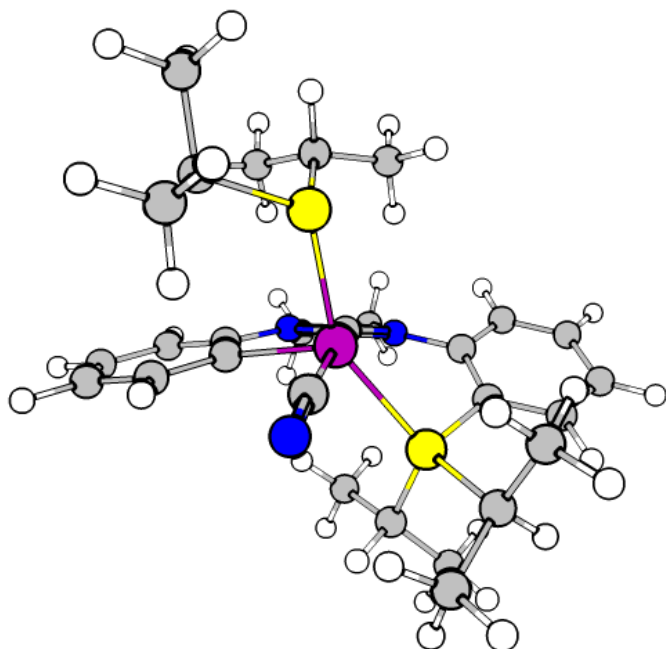
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SCF Done: E(RwB97XD) = -6625.44079600 A.U. after 1 cycles
          Conv = 0.3932D-08 -V/T = 2.0049
Zero-point correction= 0.635672 (Hartree/Particle)
Thermal correction to Energy= 0.680838
Thermal correction to Enthalpy= 0.681893
Thermal correction to Gibbs Free Energy= 0.556607
Sum of electronic and zero-point Energies= -6624.805124
Sum of electronic and thermal Energies= -6624.759958
Sum of electronic and thermal Enthalpies= -6624.758903
Sum of electronic and thermal Free Energies= -6624.884189

          1          2          3
          A          A          A
Frequencies -- -214.6391      21.1036      24.7806

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C-P-OA-PR-CN-conf1 (3l)



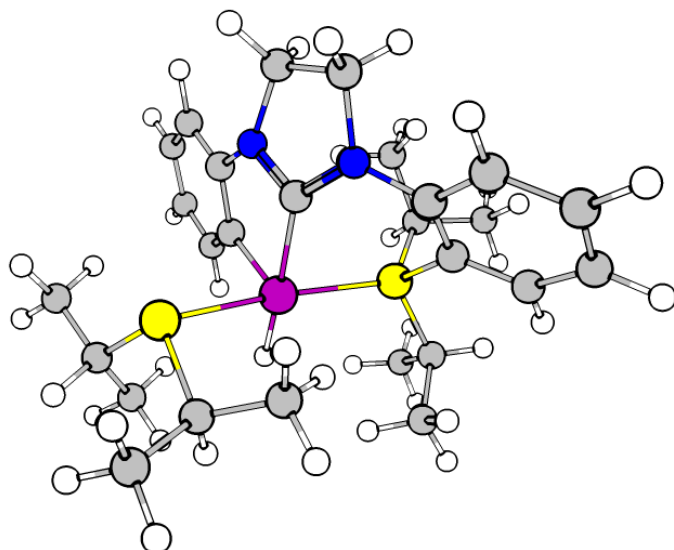
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.117194	-2.875067	2.030946
2	1	0	-0.859098	-3.672839	2.090810
3	1	0	0.216995	-2.624918	3.043189
4	6	0	0.121195	-1.198694	0.412918
5	6	0	1.044351	-3.232525	1.091354
6	1	0	1.974457	-3.445141	1.620658
7	1	0	0.792410	-4.087809	0.458255
8	6	0	2.357726	-1.722299	-0.453193
9	6	0	2.884316	-0.412933	-0.522321
10	6	0	4.095796	-0.250940	-1.203562
11	1	0	4.543666	0.732044	-1.282009
12	6	0	4.771256	-1.317842	-1.790293
13	1	0	5.710102	-1.144033	-2.304778
14	6	0	4.234979	-2.596918	-1.709121
15	1	0	4.741673	-3.440051	-2.166359
16	6	0	3.031464	-2.793413	-1.042558
17	1	0	2.602978	-3.788442	-0.987910
18	6	0	-1.645282	-0.825275	1.896385
19	6	0	-1.704190	0.426299	1.258497
20	6	0	-2.607353	1.356301	1.771123
21	1	0	-2.679342	2.340754	1.322990
22	6	0	-3.423963	1.036671	2.861505
23	1	0	-4.119814	1.779202	3.240398
24	6	0	-3.356533	-0.219834	3.458269
25	1	0	-3.997908	-0.465081	4.298526

26	6	0	-2.453187	-1.167095	2.974793
27	1	0	-2.382852	-2.148189	3.435728
28	6	0	2.590199	1.085106	1.987918
29	1	0	2.164974	2.022111	2.363040
30	6	0	1.997582	-0.047555	2.829206
31	1	0	2.373556	-1.022885	2.502910
32	1	0	0.906101	-0.049767	2.786416
33	1	0	2.291313	0.083665	3.874723
34	6	0	4.114091	1.134552	2.121191
35	1	0	4.387986	1.213082	3.177706
36	1	0	4.552384	1.992754	1.605922
37	1	0	4.573826	0.225185	1.722660
38	6	0	2.794190	2.513442	-0.563909
39	1	0	3.879306	2.384902	-0.509517
40	6	0	2.449721	3.795315	0.205287
41	1	0	2.853105	4.653023	-0.341075
42	1	0	2.895514	3.806804	1.203389
43	1	0	1.371350	3.936455	0.293625
44	6	0	2.378636	2.613347	-2.036287
45	1	0	1.311644	2.829587	-2.122495
46	1	0	2.590455	1.695520	-2.592034
47	1	0	2.927215	3.429883	-2.515278
48	6	0	-3.817507	0.545660	-1.401936
49	1	0	-4.064900	0.264126	-0.372055
50	6	0	-3.935697	2.067207	-1.525998
51	1	0	-3.707562	2.393098	-2.546234
52	1	0	-3.261281	2.598852	-0.858546
53	1	0	-4.961228	2.376217	-1.294848
54	6	0	-4.838168	-0.108329	-2.346547
55	1	0	-5.814953	0.365973	-2.205312
56	1	0	-4.970891	-1.177131	-2.166698
57	1	0	-4.556273	0.030628	-3.396221
58	6	0	-2.341045	-1.874364	-1.903769
59	1	0	-3.029447	-1.900752	-2.757747
60	6	0	-3.021891	-2.614935	-0.746284
61	1	0	-3.421993	-3.574052	-1.095321
62	1	0	-3.846798	-2.047405	-0.308821
63	1	0	-2.309449	-2.824471	0.053736
64	6	0	-1.079788	-2.606416	-2.371289
65	1	0	-0.317007	-2.646973	-1.590800
66	1	0	-0.633299	-2.119420	-3.242623
67	1	0	-1.323813	-3.638677	-2.647080
68	7	0	-0.664253	-1.691273	1.379863
69	7	0	1.182217	-2.016242	0.274508
70	15	0	-2.058314	-0.026937	-1.741858
71	15	0	1.996713	1.035474	0.225369
72	45	0	-0.386292	0.640103	-0.276470
73	6	0	-0.819979	2.642738	-0.552053
74	7	0	-0.992006	3.795841	-0.652099

SCF Done: E(RwB97XD) = -6625.45269604 A.U. after 1 cycles
 Conv = 0.2332D-08 -V/T = 2.0049
 Zero-point correction= 0.637673 (Hartree/Particle)
 Thermal correction to Energy= 0.682942
 Thermal correction to Enthalpy= 0.683997
 Thermal correction to Gibbs Free Energy= 0.560376
 Sum of electronic and zero-point Energies= -6624.815023
 Sum of electronic and thermal Energies= -6624.769754
 Sum of electronic and thermal Enthalpies= -6624.768699
 Sum of electronic and thermal Free Energies= -6624.892320

	1	2	3
	A	A	A
Frequencies --	32.2670	38.2806	42.7906

C-P-OA-PR-conf2 (3a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.159164	2.606523	-2.569771
2	1	0	0.448499	2.856458	-3.440058
3	1	0	-0.434099	3.532382	-2.053468
4	6	0	-0.163680	0.645520	-1.295441
5	6	0	-1.387424	1.755315	-2.946048
6	1	0	-2.328314	2.300913	-2.852003
7	1	0	-1.305852	1.364118	-3.962485
8	6	0	-2.477525	-0.068328	-1.558328
9	6	0	-2.762570	-0.356950	-0.198453
10	6	0	-3.970597	-1.010362	0.071226
11	1	0	-4.232234	-1.243625	1.096888
12	6	0	-4.872550	-1.367629	-0.927164
13	1	0	-5.797136	-1.871325	-0.666093

14	6	0	-4.576544	-1.070767	-2.251929
15	1	0	-5.262580	-1.344137	-3.046642
16	6	0	-3.384526	-0.425185	-2.558756
17	1	0	-3.144437	-0.204140	-3.593537
18	6	0	1.518263	2.136974	-0.700309
19	6	0	1.634717	1.301328	0.433548
20	6	0	2.440349	1.758598	1.474692
21	1	0	2.538619	1.156838	2.371863
22	6	0	3.131208	2.972248	1.376519
23	1	0	3.758791	3.299767	2.200326
24	6	0	3.033271	3.751254	0.226704
25	1	0	3.581055	4.684608	0.145417
26	6	0	2.212299	3.334930	-0.824198
27	1	0	2.111517	3.944242	-1.717989
28	6	0	-2.149205	1.780884	1.700489
29	1	0	-1.505166	2.011292	2.556020
30	6	0	-1.840383	2.811080	0.611527
31	1	0	-2.405303	2.605111	-0.303940
32	1	0	-0.774006	2.836170	0.379238
33	1	0	-2.129271	3.808012	0.957619
34	6	0	-3.613603	1.863510	2.137743
35	1	0	-3.849548	2.888624	2.439824
36	1	0	-3.834320	1.213978	2.988288
37	1	0	-4.286445	1.595293	1.317554
38	6	0	-2.121923	-1.003494	2.613660
39	1	0	-3.195970	-0.892192	2.791211
40	6	0	-1.378314	-0.549318	3.876144
41	1	0	-1.597654	-1.241551	4.694457
42	1	0	-1.677418	0.450293	4.201879
43	1	0	-0.297656	-0.553603	3.706407
44	6	0	-1.810911	-2.474758	2.320599
45	1	0	-0.730779	-2.619653	2.223563
46	1	0	-2.289175	-2.833860	1.405060
47	1	0	-2.163785	-3.097097	3.148783
48	6	0	1.702520	-3.057012	-0.695475
49	1	0	1.903685	-3.365728	0.336251
50	6	0	0.179033	-2.992359	-0.867352
51	1	0	-0.104722	-2.611267	-1.853080
52	1	0	-0.306996	-2.355292	-0.103158
53	1	0	-0.282970	-3.977789	-0.735041
54	6	0	2.314058	-4.083300	-1.650545
55	1	0	1.890443	-5.080625	-1.476967
56	1	0	3.397903	-4.157915	-1.521095
57	1	0	2.121231	-3.810040	-2.693029
58	6	0	4.031757	-1.453965	-0.041319
59	1	0	4.510737	-2.321642	-0.517610
60	6	0	3.993834	-1.710136	1.464437
61	1	0	5.008927	-1.868573	1.850648
62	1	0	3.396938	-2.590353	1.718211
63	1	0	3.553346	-0.858863	1.987390

64	6	0	4.892954	-0.227230	-0.368833
65	1	0	4.449768	0.685835	0.039149
66	1	0	5.001481	-0.092683	-1.448956
67	1	0	5.895028	-0.333821	0.063723
68	7	0	0.557506	1.719113	-1.653395
69	7	0	-1.328409	0.655559	-1.965675
70	15	0	2.391476	-1.321538	-0.946171
71	15	0	-1.601423	0.075046	1.192637
72	45	0	0.581917	-0.400370	0.315539
73	1	0	1.235057	-1.021067	1.682405

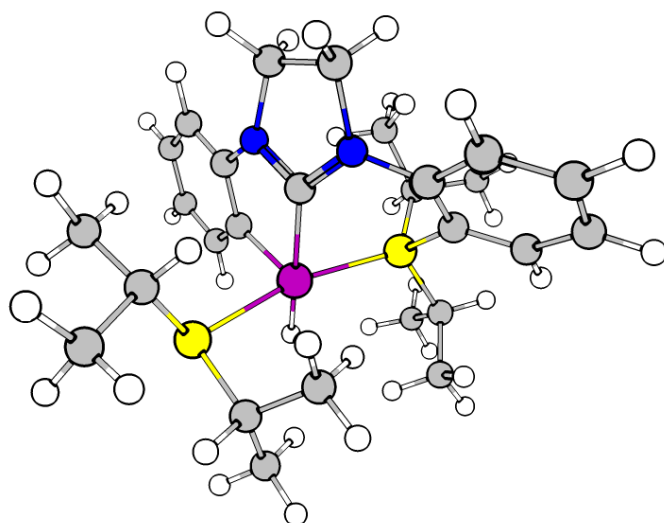
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SCF Done:  E(RwB97XD) = -6533.18852736      A.U. after   1 cycles
              Convg =   0.2290D-08              -V/T =   2.0048
Zero-point correction=                          0.633118 (Hartree/Particle)
Thermal correction to Energy=                    0.676606
Thermal correction to Enthalpy=                  0.677661
Thermal correction to Gibbs Free Energy=          0.556292
Sum of electronic and zero-point Energies=        -6532.555409
Sum of electronic and thermal Energies=           -6532.511922
Sum of electronic and thermal Enthalpies=         -6532.510867
Sum of electronic and thermal Free Energies=       -6532.632236

              1              2              3
              A              A              A
Frequencies --   27.5624          35.7975          42.7740

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C-P-OA-PR-conf3 (3a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.677968	-2.407567	2.511770
2	1	0	1.495292	-2.561426	3.217460
3	1	0	0.330206	-3.383148	2.156722

4	6	0	0.280507	-0.548335	1.139691
5	6	0	-0.457413	-1.560167	3.116480
6	1	0	-1.370598	-2.133038	3.288766
7	1	0	-0.152910	-1.095724	4.056991
8	6	0	-1.936934	0.104908	1.912663
9	6	0	-2.572849	0.217757	0.650085
10	6	0	-3.847156	0.796785	0.630507
11	1	0	-4.372295	0.898957	-0.312174
12	6	0	-4.486189	1.244367	1.783491
13	1	0	-5.474144	1.687113	1.716030
14	6	0	-3.847999	1.118132	3.011471
15	1	0	-4.325760	1.465135	3.921563
16	6	0	-2.580266	0.551113	3.068949
17	1	0	-2.072264	0.460798	4.023567
18	6	0	1.857623	-2.024539	0.272451
19	6	0	1.718229	-1.240023	-0.892847
20	6	0	2.421445	-1.654598	-2.023397
21	1	0	2.354915	-1.064510	-2.930988
22	6	0	3.214493	-2.806987	-1.997360
23	1	0	3.751821	-3.107351	-2.892180
24	6	0	3.329356	-3.563379	-0.832932
25	1	0	3.950762	-4.453009	-0.813983
26	6	0	2.647257	-3.168741	0.319177
27	1	0	2.739481	-3.742261	1.237434
28	6	0	-2.316290	-2.106014	-1.118041
29	1	0	-1.905817	-2.397287	-2.090704
30	6	0	-1.663014	-3.003826	-0.066060
31	1	0	-1.991673	-2.736466	0.943860
32	1	0	-0.574244	-2.949622	-0.119919
33	1	0	-1.953510	-4.044331	-0.239102
34	6	0	-3.834920	-2.293594	-1.136832
35	1	0	-4.071793	-3.354232	-1.266129
36	1	0	-4.314631	-1.751777	-1.955491
37	1	0	-4.285390	-1.963711	-0.195751
38	6	0	-2.696391	0.547228	-2.280918
39	1	0	-3.768306	0.358130	-2.168342
40	6	0	-2.252946	-0.011510	-3.638909
41	1	0	-2.729096	0.562159	-4.439611
42	1	0	-2.534869	-1.058743	-3.774382
43	1	0	-1.168804	0.076467	-3.755711
44	6	0	-2.448224	2.057617	-2.226935
45	1	0	-1.395123	2.274457	-2.424447
46	1	0	-2.712677	2.497027	-1.261336
47	1	0	-3.045750	2.555190	-2.996953
48	6	0	2.999224	1.506262	1.381310
49	1	0	2.112828	1.228064	1.964017
50	6	0	4.039771	0.387498	1.513720
51	1	0	4.977126	0.682120	1.029399
52	1	0	3.712469	-0.543629	1.047197
53	1	0	4.256856	0.182721	2.569443

54	6	0	3.572974	2.801897	1.967140
55	1	0	4.028391	2.608890	2.945953
56	1	0	2.808166	3.570062	2.110085
57	1	0	4.352206	3.217020	1.317196
58	6	0	1.512763	3.260346	-0.399177
59	1	0	2.099144	3.998300	0.158406
60	6	0	0.168889	3.078179	0.320156
61	1	0	-0.410534	4.009732	0.340942
62	1	0	0.295221	2.731135	1.348596
63	1	0	-0.482319	2.354925	-0.202568
64	6	0	1.319548	3.826953	-1.809206
65	1	0	0.769681	3.129251	-2.446809
66	1	0	2.284078	4.020154	-2.286426
67	1	0	0.762334	4.770923	-1.773844
68	7	0	1.098883	-1.584374	1.380060
69	7	0	-0.681130	-0.531704	2.083163
70	15	0	2.527814	1.666922	-0.446525
71	15	0	-1.766187	-0.335592	-0.934471
72	45	0	0.534041	0.363387	-0.697332
73	1	0	0.734279	0.833113	-2.253135

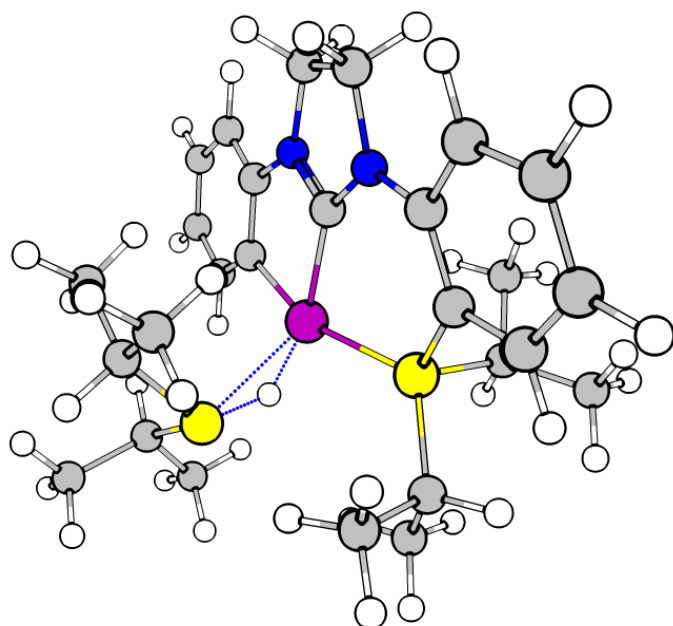
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SCF Done: E(RwB97XD) = -6533.18912376      A.U. after   1 cycles
                Conv g =   0.2260D-08          -V/T =   2.0048
Zero-point correction=                      0.634090 (Hartree/Particle)
Thermal correction to Energy=                0.677314
Thermal correction to Enthalpy=              0.678369
Thermal correction to Gibbs Free Energy=      0.558077
Sum of electronic and zero-point Energies=    -6532.555034
Sum of electronic and thermal Energies=       -6532.511810
Sum of electronic and thermal Enthalpies=     -6532.510755
Sum of electronic and thermal Free Energies=   -6532.631047

                1                2                3
                A                A                A
Frequencies --   30.1830          37.6388          39.6960

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P-H-RE-TS-conf1 (4a)



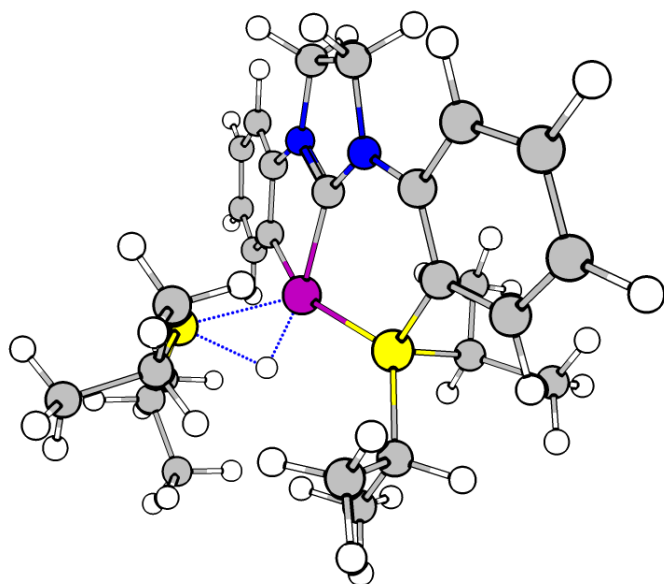
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.013773	3.930845	0.477518
2	1	0	-0.628451	4.368959	1.266627
3	1	0	0.060018	4.647699	-0.345267
4	6	0	0.268831	1.638025	0.041614
5	6	0	1.358093	3.482163	0.991822
6	1	0	2.170232	4.067163	0.557619
7	1	0	1.416417	3.549811	2.080929
8	6	0	2.620925	1.319601	0.797638
9	6	0	2.855883	0.006321	0.313628
10	6	0	4.098278	-0.575179	0.600055
11	1	0	4.308429	-1.571532	0.230060
12	6	0	5.089702	0.058555	1.337941
13	1	0	6.032986	-0.440904	1.530444
14	6	0	4.842457	1.337048	1.817151
15	1	0	5.587304	1.865719	2.403008
16	6	0	3.628442	1.953203	1.545996
17	1	0	3.475072	2.948914	1.938894
18	6	0	-1.893154	2.461661	-0.461813
19	6	0	-2.183992	1.114000	-0.764515
20	6	0	-3.461629	0.882153	-1.278308
21	1	0	-3.746253	-0.129781	-1.559509
22	6	0	-4.402359	1.909573	-1.442279
23	1	0	-5.389175	1.684625	-1.837745
24	6	0	-4.076645	3.217337	-1.098172
25	1	0	-4.803033	4.015566	-1.215868
26	6	0	-2.798991	3.505523	-0.605881

27	1	0	-2.532354	4.528420	-0.352911
28	6	0	2.239450	-0.636718	-2.437219
29	1	0	1.561899	-1.235035	-3.056317
30	6	0	2.023591	0.836650	-2.806357
31	1	0	2.623731	1.494867	-2.168904
32	1	0	0.975576	1.130659	-2.711661
33	1	0	2.331956	1.007142	-3.842722
34	6	0	3.679142	-1.059641	-2.736864
35	1	0	3.904478	-0.865654	-3.790444
36	1	0	3.851559	-2.124069	-2.559067
37	1	0	4.392714	-0.488924	-2.135324
38	6	0	2.120432	-2.745486	-0.404127
39	1	0	3.164403	-2.901181	-0.691970
40	6	0	1.254952	-3.628400	-1.312484
41	1	0	1.477065	-4.682142	-1.117284
42	1	0	1.445706	-3.442194	-2.373156
43	1	0	0.191220	-3.466937	-1.118028
44	6	0	1.955755	-3.146439	1.066016
45	1	0	0.903765	-3.105060	1.355097
46	1	0	2.527526	-2.502932	1.739932
47	1	0	2.307167	-4.174256	1.205432
48	6	0	-3.397985	-2.314371	0.417471
49	1	0	-3.935124	-1.371017	0.276745
50	6	0	-3.507934	-3.128271	-0.875646
51	1	0	-2.983112	-4.085442	-0.782564
52	1	0	-3.083986	-2.595615	-1.732874
53	1	0	-4.557551	-3.342499	-1.103541
54	6	0	-4.052742	-3.074590	1.576684
55	1	0	-5.061409	-3.395254	1.294893
56	1	0	-4.148000	-2.460325	2.475509
57	1	0	-3.478955	-3.971205	1.837396
58	6	0	-1.769887	-0.947644	2.376717
59	1	0	-2.172411	-1.730729	3.035822
60	6	0	-2.728540	0.240235	2.415232
61	1	0	-2.883452	0.558607	3.453274
62	1	0	-3.706752	0.005456	1.987892
63	1	0	-2.322015	1.084320	1.854712
64	6	0	-0.401004	-0.563600	2.945825
65	1	0	0.060408	0.228032	2.349237
66	1	0	0.288209	-1.412643	2.963986
67	1	0	-0.511852	-0.195593	3.972329
68	7	0	-0.579015	2.675982	0.014013
69	7	0	1.446542	2.072229	0.561322
70	15	0	-1.591439	-1.943462	0.781291
71	15	0	1.648183	-0.968578	-0.688113
72	45	0	-0.545624	-0.134401	-0.553499
73	1	0	-1.568509	-1.439189	-0.818083

SCF Done: E(RwB97XD) = -6533.19018243 A.U. after 1 cycles
Convrg = 0.3606D-08 -V/T = 2.0047

Zero-point correction=	0.633369 (Hartree/Particle)		
Thermal correction to Energy=	0.676466		
Thermal correction to Enthalpy=	0.677521		
Thermal correction to Gibbs Free Energy=	0.556133		
Sum of electronic and zero-point Energies=	-6532.556813		
Sum of electronic and thermal Energies=	-6532.513716		
Sum of electronic and thermal Enthalpies=	-6532.512661		
Sum of electronic and thermal Free Energies=	-6532.634050		
	1	2	3
	A	A	A
Frequencies --	-209.3629	18.0042	36.7880

P-H-RE-TS-conf2 (4a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.244434	3.815535	-1.271893
2	1	0	0.817111	4.022039	-2.178298
3	1	0	0.281448	4.698069	-0.626833
4	6	0	-0.124133	1.687475	-0.342623
5	6	0	-1.191167	3.374577	-1.574359
6	1	0	-1.920587	4.086203	-1.184616
7	1	0	-1.358888	3.246084	-2.646104
8	6	0	-2.559094	1.421043	-0.795546
9	6	0	-2.816946	0.238130	-0.054735
10	6	0	-4.143912	-0.213860	-0.002931
11	1	0	-4.372078	-1.101012	0.575990
12	6	0	-5.194848	0.407181	-0.662994
13	1	0	-6.200612	0.008469	-0.587519
14	6	0	-4.919914	1.533273	-1.426883
15	1	0	-5.707229	2.037688	-1.977561

16	6	0	-3.625306	2.027490	-1.486035
17	1	0	-3.454175	2.906995	-2.090912
18	6	0	2.066058	2.515768	-0.034367
19	6	0	2.307677	1.273179	0.586763
20	6	0	3.529748	1.164759	1.251783
21	1	0	3.767295	0.249093	1.783186
22	6	0	4.475710	2.199634	1.248661
23	1	0	5.420429	2.068982	1.769330
24	6	0	4.217059	3.385282	0.569084
25	1	0	4.954672	4.181468	0.547077
26	6	0	2.988832	3.554982	-0.076468
27	1	0	2.766563	4.488555	-0.586505
28	6	0	-1.815307	-0.292123	2.623520
29	1	0	-1.149214	-0.968619	3.170280
30	6	0	-1.326288	1.141925	2.870691
31	1	0	-1.881962	1.858415	2.256454
32	1	0	-0.260759	1.262357	2.654066
33	1	0	-1.485127	1.409324	3.920287
34	6	0	-3.234827	-0.462554	3.169366
35	1	0	-3.236491	-0.242397	4.241617
36	1	0	-3.622177	-1.477267	3.049449
37	1	0	-3.930764	0.231268	2.689631
38	6	0	-2.218088	-2.508553	0.765442
39	1	0	-3.139269	-2.537120	1.354423
40	6	0	-1.209439	-3.441773	1.443182
41	1	0	-1.599705	-4.464257	1.449679
42	1	0	-1.008662	-3.157307	2.479664
43	1	0	-0.257563	-3.440706	0.908022
44	6	0	-2.553662	-3.004029	-0.645244
45	1	0	-1.662400	-3.078121	-1.268919
46	1	0	-3.267042	-2.359907	-1.162700
47	1	0	-2.992800	-4.004439	-0.578112
48	6	0	0.813100	-2.220523	-2.046005
49	1	0	0.244520	-2.868274	-1.372320
50	6	0	-0.153551	-1.264737	-2.753162
51	1	0	0.395907	-0.580225	-3.409219
52	1	0	-0.725131	-0.660525	-2.045947
53	1	0	-0.865027	-1.824951	-3.370965
54	6	0	1.514360	-3.097536	-3.093684
55	1	0	0.771444	-3.541655	-3.765350
56	1	0	2.082433	-3.917255	-2.648776
57	1	0	2.200898	-2.503986	-3.707490
58	6	0	3.147500	-2.672727	-0.431763
59	1	0	3.633604	-3.003836	-1.358867
60	6	0	2.457770	-3.875056	0.213008
61	1	0	3.184617	-4.671454	0.412814
62	1	0	1.667596	-4.298845	-0.413126
63	1	0	2.011511	-3.585013	1.170295
64	6	0	4.250638	-2.154985	0.491976
65	1	0	3.829005	-1.871269	1.461719

66	1	0	4.760424	-1.283564	0.072639
67	1	0	4.996233	-2.937512	0.672259
68	7	0	0.770970	2.653392	-0.578597
69	7	0	-1.310467	2.075537	-0.879858
70	15	0	2.063369	-1.249928	-1.038285
71	15	0	-1.541374	-0.768634	0.825702
72	45	0	0.694243	-0.020747	0.482525
73	1	0	1.459160	-1.456629	0.816860

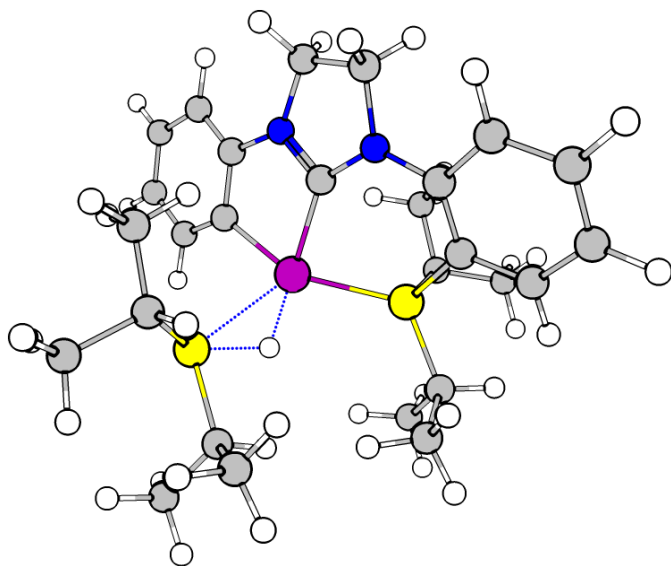
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SCF Done:  E(RwB97XD) = -6533.18281942      A.U. after   1 cycles
              Convg =   0.3228D-08              -V/T =   2.0048
Zero-point correction=                        0.633783 (Hartree/Particle)
Thermal correction to Energy=                  0.676658
Thermal correction to Enthalpy=                0.677713
Thermal correction to Gibbs Free Energy=       0.557856
Sum of electronic and zero-point Energies=    -6532.549036
Sum of electronic and thermal Energies=       -6532.506161
Sum of electronic and thermal Enthalpies=     -6532.505106
Sum of electronic and thermal Free Energies=   -6532.624963

              1              2              3
              A              A              A
Frequencies --  -296.6449          27.2135          36.3039

```

P-H-RE-TS-conf3 (4a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.011257	-3.849872	0.991094
2	1	0	0.691513	-4.300572	1.715672
3	1	0	-0.224668	-4.591010	0.221169
4	6	0	-0.207588	-1.589616	0.394062

5	6	0	-1.242350	-3.269641	1.653176
6	1	0	-2.138716	-3.850433	1.430835
7	1	0	-1.120882	-3.203840	2.737563
8	6	0	-2.486329	-1.118476	1.282789
9	6	0	-2.818604	0.024972	0.512078
10	6	0	-4.032414	0.663725	0.790745
11	1	0	-4.323087	1.527914	0.205257
12	6	0	-4.902054	0.240451	1.790013
13	1	0	-5.831246	0.771387	1.966187
14	6	0	-4.556051	-0.868208	2.549537
15	1	0	-5.205943	-1.221999	3.343148
16	6	0	-3.365949	-1.537133	2.292370
17	1	0	-3.123527	-2.396262	2.904269
18	6	0	1.811734	-2.568570	-0.316777
19	6	0	2.098371	-1.272816	-0.796810
20	6	0	3.265005	-1.158439	-1.555193
21	1	0	3.544267	-0.188275	-1.956656
22	6	0	4.110593	-2.253180	-1.787309
23	1	0	5.017940	-2.118914	-2.369819
24	6	0	3.804228	-3.504361	-1.262793
25	1	0	4.463306	-4.350448	-1.431143
26	6	0	2.630964	-3.671830	-0.519818
27	1	0	2.371784	-4.648942	-0.120561
28	6	0	-2.330924	-0.224305	-2.337940
29	1	0	-1.710425	0.179145	-3.145213
30	6	0	-2.052534	-1.729763	-2.259761
31	1	0	-2.595402	-2.192229	-1.428798
32	1	0	-0.987679	-1.941287	-2.141773
33	1	0	-2.391799	-2.209763	-3.182907
34	6	0	-3.804096	0.027774	-2.672041
35	1	0	-4.073743	-0.526452	-3.576559
36	1	0	-4.019766	1.081467	-2.863705
37	1	0	-4.458712	-0.316486	-1.865566
38	6	0	-2.318142	2.420894	-1.128646
39	1	0	-3.392842	2.406351	-1.329320
40	6	0	-1.613027	2.964797	-2.376994
41	1	0	-1.853515	4.024639	-2.502818
42	1	0	-1.919129	2.445628	-3.288738
43	1	0	-0.525901	2.873376	-2.282954
44	6	0	-2.053359	3.329278	0.072107
45	1	0	-0.981797	3.471682	0.204719
46	1	0	-2.457400	2.929190	1.005516
47	1	0	-2.504967	4.311483	-0.099012
48	6	0	1.845212	3.387894	0.258210
49	1	0	1.118518	3.505166	-0.551850
50	6	0	1.125508	3.755069	1.560357
51	1	0	1.814891	3.813290	2.407208
52	1	0	0.344812	3.034880	1.818110
53	1	0	0.654073	4.740165	1.462887
54	6	0	2.982478	4.376632	-0.036520

55	1	0	2.602216	5.405202	-0.033478
56	1	0	3.431054	4.183885	-1.014495
57	1	0	3.781630	4.318268	0.708173
58	7	0	0.593048	-2.662721	0.388471
59	7	0	-1.340508	-1.918368	1.067731
60	15	0	2.456767	1.588353	0.066094
61	15	0	-1.720417	0.689729	-0.813352
62	45	0	0.555534	0.076902	-0.515770
63	1	0	1.183642	1.494620	-1.121998
64	6	0	2.619115	1.094924	1.897026
65	1	0	1.725612	1.406893	2.443911
66	6	0	2.831219	-0.397693	2.145964
67	1	0	1.927282	-0.969753	1.940642
68	1	0	3.635241	-0.801098	1.523318
69	1	0	3.103747	-0.554976	3.196626
70	6	0	3.838622	1.856479	2.445957
71	1	0	3.766033	2.938801	2.329552
72	1	0	3.952703	1.651864	3.516616
73	1	0	4.753505	1.529308	1.941794

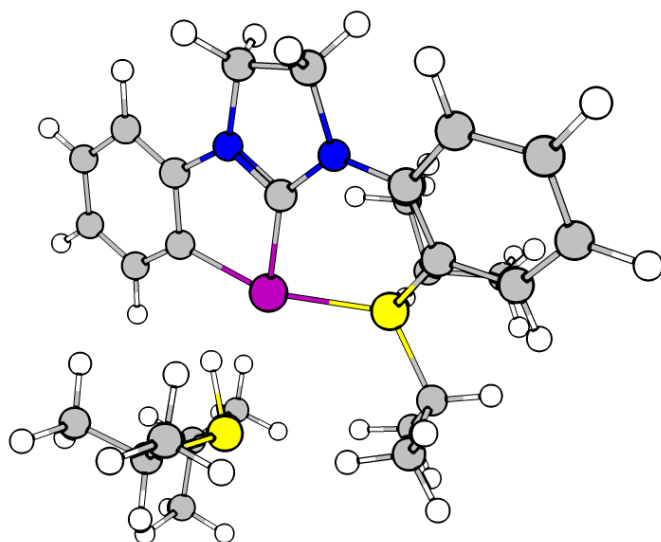
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SCF Done: E(RwB97XD) = -6533.17142285 A.U. after 1 cycles
              Conv = 0.2441D-08 -V/T = 2.0048
Zero-point correction= 0.634920 (Hartree/Particle)
Thermal correction to Energy= 0.677492
Thermal correction to Enthalpy= 0.678547
Thermal correction to Gibbs Free Energy= 0.559156
Sum of electronic and zero-point Energies= -6532.536503
Sum of electronic and thermal Energies= -6532.493931
Sum of electronic and thermal Enthalpies= -6532.492876
Sum of electronic and thermal Free Energies= -6532.612267

              1              2              3
              A              A              A
Frequencies -- -152.4741      23.9713      32.3952

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P-H-RE-PR-conf1 (5a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.432344	3.944606	0.147320
2	1	0	1.115825	4.709923	0.858662
3	1	0	1.628368	4.423090	-0.817556
4	6	0	0.895307	1.649565	0.113495
5	6	0	2.626228	3.140599	0.659951
6	1	0	3.545106	3.370909	0.118765
7	1	0	2.788422	3.318064	1.726752
8	6	0	3.129264	0.697489	0.724921
9	6	0	2.923166	-0.658112	0.370020
10	6	0	3.925189	-1.577466	0.702421
11	1	0	3.795246	-2.620253	0.440069
12	6	0	5.097063	-1.221545	1.359654
13	1	0	5.840862	-1.974193	1.597841
14	6	0	5.291756	0.110685	1.695583
15	1	0	6.194240	0.428681	2.207491
16	6	0	4.321856	1.052487	1.378631
17	1	0	4.508250	2.079436	1.661330
18	6	0	-0.938477	3.089795	-0.272555
19	6	0	-1.660982	1.879210	-0.318537
20	6	0	-3.018640	2.019883	-0.625781
21	1	0	-3.649613	1.135215	-0.694762
22	6	0	-3.617540	3.269091	-0.849551
23	1	0	-4.678276	3.328807	-1.078272
24	6	0	-2.858641	4.432064	-0.775729
25	1	0	-3.316500	5.401924	-0.944521
26	6	0	-1.491996	4.346497	-0.487394
27	1	0	-0.887600	5.248913	-0.442543
28	6	0	1.946617	-1.083651	-2.312595
29	1	0	1.074373	-1.444983	-2.869342

30	6	0	2.174568	0.377130	-2.717312
31	1	0	3.018504	0.812109	-2.171367
32	1	0	1.289075	0.987825	-2.528845
33	1	0	2.409364	0.430098	-3.785321
34	6	0	3.161898	-1.936905	-2.685636
35	1	0	3.386128	-1.809677	-3.749577
36	1	0	3.000156	-3.003833	-2.513526
37	1	0	4.048293	-1.629843	-2.122212
38	6	0	1.371329	-3.059091	-0.239739
39	1	0	2.349705	-3.489019	-0.471904
40	6	0	0.355931	-3.704248	-1.190675
41	1	0	0.266818	-4.771043	-0.961701
42	1	0	0.656155	-3.615565	-2.238247
43	1	0	-0.633331	-3.256722	-1.072563
44	6	0	1.033957	-3.363573	1.223357
45	1	0	0.033322	-2.998476	1.463827
46	1	0	1.743293	-2.902283	1.916225
47	1	0	1.051430	-4.445325	1.392222
48	6	0	-3.991949	-1.829079	-0.510874
49	1	0	-4.565185	-0.906790	-0.375087
50	6	0	-3.554250	-1.908100	-1.976675
51	1	0	-2.992106	-2.827531	-2.171538
52	1	0	-2.921266	-1.058447	-2.253326
53	1	0	-4.427936	-1.904435	-2.636576
54	6	0	-4.875624	-3.015043	-0.116573
55	1	0	-5.754856	-3.068099	-0.767016
56	1	0	-5.231693	-2.929980	0.914639
57	1	0	-4.331352	-3.960751	-0.210163
58	6	0	-3.057012	-1.239707	2.241644
59	1	0	-3.560498	-2.121486	2.657809
60	6	0	-4.028225	-0.058981	2.256807
61	1	0	-4.315643	0.175857	3.287786
62	1	0	-4.946720	-0.268431	1.701520
63	1	0	-3.561446	0.831273	1.825119
64	6	0	-1.826396	-0.944443	3.109506
65	1	0	-1.256520	-0.103881	2.696981
66	1	0	-1.154348	-1.804905	3.171322
67	1	0	-2.135296	-0.682109	4.126938
68	7	0	0.428380	2.909800	0.006285
69	7	0	2.225305	1.740913	0.431765
70	15	0	-2.461072	-1.781582	0.556395
71	15	0	1.410450	-1.220008	-0.519250
72	45	0	-0.415252	0.207856	-0.134501
73	1	0	-2.153349	-0.423662	0.117597

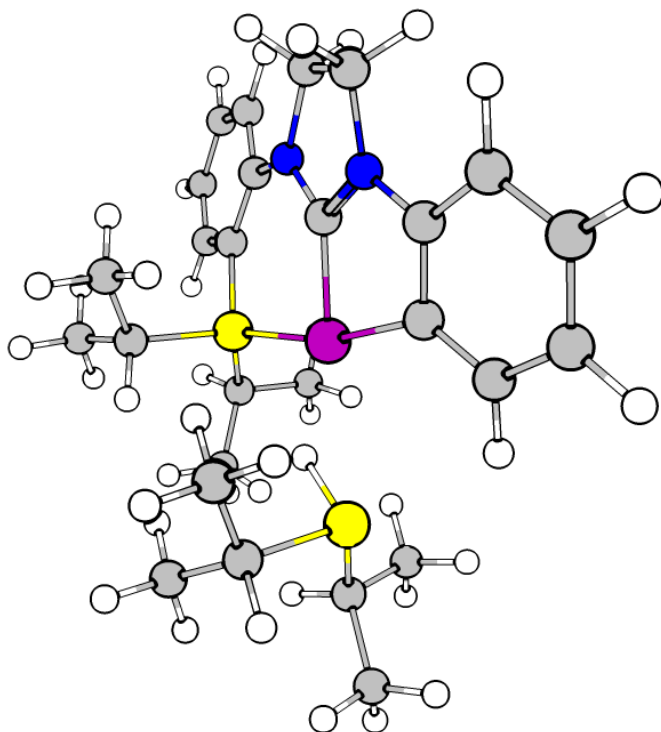
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SCF Done:  E(RwB97XD) = -6533.20194071      A.U. after   1 cycles
              Conv g =   0.3093D-08          -V/T =   2.0047
Zero-point correction=                      0.634999 (Hartree/Particle)
Thermal correction to Energy=                0.679137
Thermal correction to Enthalpy=              0.680192

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Thermal correction to Gibbs Free Energy=	0.554900		
Sum of electronic and zero-point Energies=	-6532.566941		
Sum of electronic and thermal Energies=	-6532.522804		
Sum of electronic and thermal Enthalpies=	-6532.521749		
Sum of electronic and thermal Free Energies=	-6532.647040		
	1	2	3
	A	A	A
Frequencies --	19.5149	30.2823	33.5545

P-H-RE-PR-conf2 (5a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.029081	3.763487	0.387160
2	1	0	-2.059570	4.649175	-0.250656
3	1	0	-1.984096	4.086616	1.431876
4	6	0	-1.181901	1.622863	-0.124780
5	6	0	-3.193910	2.818558	0.109775
6	1	0	-3.921939	2.805079	0.922101
7	1	0	-3.702824	3.090831	-0.818833
8	6	0	-3.346741	0.370339	-0.290573
9	6	0	-2.861464	-0.957928	-0.306841
10	6	0	-3.780678	-1.984428	-0.559502
11	1	0	-3.438621	-3.011522	-0.573874
12	6	0	-5.131246	-1.758597	-0.790930
13	1	0	-5.800508	-2.589961	-0.984241

14	6	0	-5.599072	-0.452069	-0.759762
15	1	0	-6.648141	-0.233682	-0.931082
16	6	0	-4.718970	0.591330	-0.510503
17	1	0	-5.124994	1.592951	-0.498371
18	6	0	0.439925	3.345573	-0.088324
19	6	0	1.324912	2.302733	-0.431844
20	6	0	2.630958	2.728870	-0.700716
21	1	0	3.377598	1.999153	-0.996777
22	6	0	3.031211	4.070206	-0.591324
23	1	0	4.060527	4.343855	-0.809094
24	6	0	2.123810	5.046170	-0.196777
25	1	0	2.431343	6.082397	-0.091971
26	6	0	0.797610	4.682142	0.055480
27	1	0	0.073172	5.435703	0.352917
28	6	0	-1.201637	-1.829617	1.870342
29	1	0	-0.165350	-2.079162	2.126010
30	6	0	-1.594584	-0.600165	2.698111
31	1	0	-2.630311	-0.307769	2.495392
32	1	0	-0.948547	0.254160	2.480086
33	1	0	-1.516290	-0.829155	3.765506
34	6	0	-2.093619	-3.023982	2.213797
35	1	0	-2.021239	-3.239589	3.284740
36	1	0	-1.807746	-3.932763	1.677459
37	1	0	-3.143277	-2.810889	1.991417
38	6	0	-0.863326	-2.991413	-0.822019
39	1	0	-1.687502	-3.669300	-0.587353
40	6	0	0.419341	-3.681018	-0.357099
41	1	0	0.557123	-4.616331	-0.908448
42	1	0	0.400086	-3.925113	0.708699
43	1	0	1.292203	-3.056109	-0.543447
44	6	0	-0.848130	-2.740251	-2.333126
45	1	0	-0.062383	-2.027018	-2.599909
46	1	0	-1.797654	-2.329967	-2.686820
47	1	0	-0.661446	-3.675883	-2.869560
48	6	0	3.750889	-2.141156	-0.926509
49	1	0	3.314967	-3.023529	-0.449368
50	6	0	3.348167	-2.132472	-2.403923
51	1	0	3.792621	-1.279567	-2.926110
52	1	0	2.263133	-2.067464	-2.529697
53	1	0	3.689324	-3.048176	-2.897764
54	6	0	5.273468	-2.216796	-0.766137
55	1	0	5.663539	-3.103798	-1.275678
56	1	0	5.570656	-2.281768	0.284900
57	1	0	5.760397	-1.338231	-1.201644
58	6	0	3.373774	-0.861739	1.702348
59	1	0	4.446456	-0.699855	1.865652
60	6	0	3.010964	-2.257269	2.209860
61	1	0	3.162681	-2.319752	3.293055
62	1	0	3.617139	-3.040893	1.747706
63	1	0	1.959535	-2.483506	2.006903

64	6	0	2.616282	0.224409	2.475482
65	1	0	1.533991	0.105611	2.347301
66	1	0	2.872943	1.228126	2.127315
67	1	0	2.843645	0.155565	3.544676
68	7	0	-0.894109	2.923546	0.067123
69	7	0	-2.547960	1.501595	-0.032260
70	15	0	3.134961	-0.571307	-0.127477
71	15	0	-1.105126	-1.370257	0.060325
72	45	0	0.359575	0.415322	-0.326509
73	1	0	1.723720	-0.977169	-0.136867

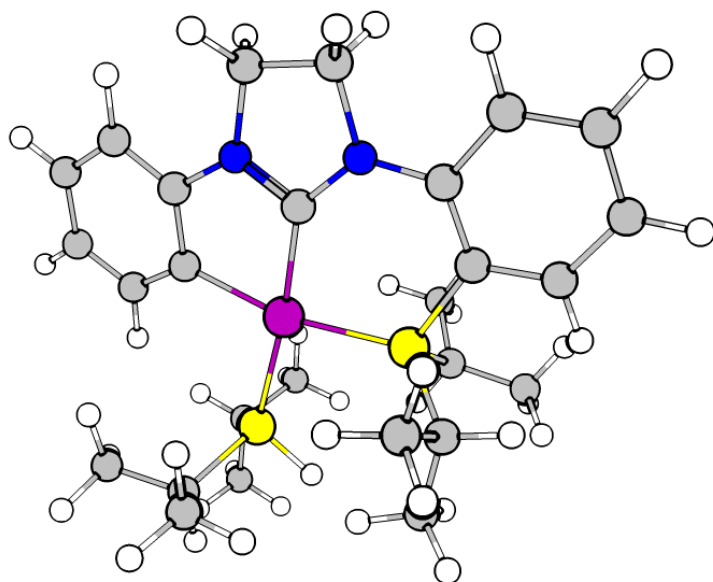
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SCF Done:  E(RwB97XD) = -6533.20055458      A.U. after   1 cycles
              Convg =   0.2172D-08              -V/T =   2.0047
Zero-point correction=                        0.635719 (Hartree/Particle)
Thermal correction to Energy=                  0.679402
Thermal correction to Enthalpy=                0.680457
Thermal correction to Gibbs Free Energy=       0.557248
Sum of electronic and zero-point Energies=    -6532.564836
Sum of electronic and thermal Energies=      -6532.521153
Sum of electronic and thermal Enthalpies=    -6532.520098
Sum of electronic and thermal Free Energies=  -6532.643307

              1              2              3
              A              A              A
Frequencies --  21.2672      24.4699      38.8240

```

P-H-RE-PR-conf1/2 (6a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.925156	4.164205	0.069477

2	1	0	0.720497	4.829236	0.911743
3	1	0	0.768150	4.721666	-0.858665
4	6	0	0.716412	1.814045	0.093198
5	6	0	2.317263	3.540457	0.145051
6	1	0	2.938699	3.844081	-0.699307
7	1	0	2.830262	3.804226	1.072958
8	6	0	3.137947	1.188834	0.075819
9	6	0	3.023180	-0.220951	0.010889
10	6	0	4.212552	-0.965044	-0.021057
11	1	0	4.154546	-2.045153	-0.058302
12	6	0	5.478364	-0.397423	0.003340
13	1	0	6.362517	-1.025123	-0.026557
14	6	0	5.577726	0.985188	0.080376
15	1	0	6.546455	1.473050	0.116497
16	6	0	4.427061	1.757703	0.119151
17	1	0	4.553444	2.828327	0.191445
18	6	0	-1.331668	3.004881	-0.022217
19	6	0	-1.923974	1.723128	-0.097214
20	6	0	-3.308951	1.765047	-0.304735
21	1	0	-3.865979	0.839450	-0.401477
22	6	0	-4.047116	2.954461	-0.400463
23	1	0	-5.121504	2.911739	-0.560124
24	6	0	-3.407954	4.182235	-0.288576
25	1	0	-3.966733	5.111002	-0.353375
26	6	0	-2.022908	4.210211	-0.100924
27	1	0	-1.507566	5.163931	-0.024348
28	6	0	1.473825	-2.131455	-1.580554
29	1	0	0.512355	-2.658552	-1.544165
30	6	0	1.423297	-1.153502	-2.760313
31	1	0	2.363366	-0.596751	-2.838456
32	1	0	0.609986	-0.431860	-2.648309
33	1	0	1.277941	-1.699618	-3.698129
34	6	0	2.572725	-3.175955	-1.800271
35	1	0	2.299530	-3.811440	-2.649145
36	1	0	2.724950	-3.831468	-0.938169
37	1	0	3.526744	-2.703835	-2.047499
38	6	0	1.801756	-2.388357	1.365573
39	1	0	2.819915	-2.759970	1.221705
40	6	0	0.873515	-3.604351	1.358592
41	1	0	1.204316	-4.319022	2.119166
42	1	0	0.863924	-4.124576	0.397004
43	1	0	-0.152408	-3.325797	1.597310
44	6	0	1.750137	-1.659285	2.712386
45	1	0	0.756803	-1.234286	2.883211
46	1	0	2.477017	-0.843035	2.754994
47	1	0	1.975810	-2.354778	3.527429
48	6	0	-3.120947	-1.860727	1.566639
49	1	0	-3.510483	-2.881600	1.492864
50	6	0	-2.270862	-1.750387	2.837149
51	1	0	-1.793084	-0.767432	2.896145

52	1	0	-1.487576	-2.510002	2.883884
53	1	0	-2.904507	-1.879008	3.721111
54	6	0	-4.303964	-0.893924	1.651515
55	1	0	-4.919502	-1.149820	2.520097
56	1	0	-4.948645	-0.936546	0.768843
57	1	0	-3.959360	0.135531	1.774973
58	6	0	-3.195157	-1.741005	-1.400611
59	1	0	-3.864723	-0.877356	-1.377011
60	6	0	-4.039530	-3.017006	-1.380325
61	1	0	-4.673464	-3.064086	-2.271901
62	1	0	-4.695896	-3.064933	-0.507301
63	1	0	-3.403876	-3.908947	-1.375837
64	6	0	-2.356179	-1.636445	-2.678706
65	1	0	-1.628873	-2.453802	-2.745019
66	1	0	-1.808824	-0.690939	-2.710580
67	1	0	-3.001303	-1.693784	-3.561278
68	7	0	0.071908	2.993047	0.108398
69	7	0	2.054984	2.089385	0.100745
70	15	0	-2.054189	-1.579632	0.058303
71	15	0	1.426451	-1.155094	0.014418
72	45	0	-0.473590	0.181042	0.066848
73	1	0	-1.523803	-2.889207	-0.038520

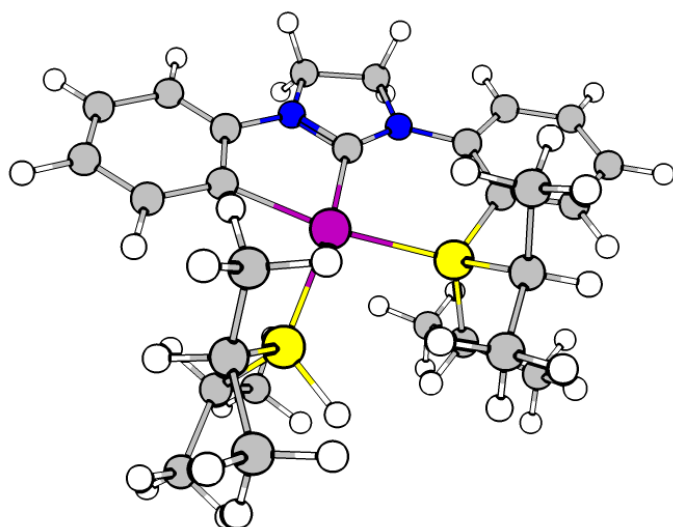
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SCF Done: E(RwB97XD) = -6533.23627132 A.U. after 1 cycles
          Conv = 0.5420D-08 -V/T = 2.0047
Zero-point correction= 0.637359 (Hartree/Particle)
Thermal correction to Energy= 0.680572
Thermal correction to Enthalpy= 0.681627
Thermal correction to Gibbs Free Energy= 0.559981
Sum of electronic and zero-point Energies= -6532.598913
Sum of electronic and thermal Energies= -6532.555700
Sum of electronic and thermal Enthalpies= -6532.554645
Sum of electronic and thermal Free Energies= -6532.676291

          1          2          3
          A          A          A
Frequencies -- 21.9535 23.1771 42.9774

```

P-H-RE-PR-conf1/2-X (6a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.087042	4.103694	0.227948
2	1	0	-0.985157	4.866264	-0.547909
3	1	0	-0.870807	4.564367	1.196388
4	6	0	-0.796455	1.782810	-0.075571
5	6	0	-2.458222	3.427232	0.193363
6	1	0	-3.029692	3.619495	1.103323
7	1	0	-3.043913	3.758681	-0.667557
8	6	0	-3.183381	1.049078	-0.017450
9	6	0	-3.007427	-0.352714	-0.128787
10	6	0	-4.158190	-1.144079	-0.256367
11	1	0	-4.047442	-2.215531	-0.371114
12	6	0	-5.447821	-0.630373	-0.248324
13	1	0	-6.302601	-1.290683	-0.348241
14	6	0	-5.609594	0.741026	-0.103249
15	1	0	-6.599417	1.185547	-0.082009
16	6	0	-4.495974	1.560755	0.005492
17	1	0	-4.667998	2.623082	0.105817
18	6	0	1.208778	3.051428	-0.106235
19	6	0	1.846060	1.795041	-0.226006
20	6	0	3.236956	1.878348	-0.372003
21	1	0	3.821708	0.968175	-0.494944
22	6	0	3.942138	3.091330	-0.373694
23	1	0	5.022901	3.090562	-0.490076
24	6	0	3.260579	4.292967	-0.223085
25	1	0	3.795043	5.238131	-0.214259
26	6	0	1.868424	4.276404	-0.090528
27	1	0	1.325002	5.211534	0.017367
28	6	0	-1.469901	-2.189968	1.512058
29	1	0	-0.468487	-2.633427	1.573331

30	6	0	-1.617649	-1.213825	2.684940
31	1	0	-2.609307	-0.749121	2.678916
32	1	0	-0.869105	-0.419006	2.637462
33	1	0	-1.499958	-1.743036	3.635989
34	6	0	-2.495685	-3.320877	1.616470
35	1	0	-2.300320	-3.903550	2.522883
36	1	0	-2.457295	-4.011717	0.769278
37	1	0	-3.512938	-2.929478	1.698824
38	6	0	-1.546849	-2.448456	-1.447898
39	1	0	-2.482272	-3.001566	-1.321490
40	6	0	-0.401013	-3.462171	-1.432367
41	1	0	-0.566615	-4.220653	-2.204172
42	1	0	-0.304437	-3.978199	-0.472708
43	1	0	0.550690	-2.971915	-1.649776
44	6	0	-1.596865	-1.705473	-2.787189
45	1	0	-0.684917	-1.117322	-2.931971
46	1	0	-2.449263	-1.022932	-2.840804
47	1	0	-1.682374	-2.420948	-3.611562
48	6	0	3.370374	-1.747471	-1.155704
49	1	0	4.285507	-1.217858	-0.865266
50	6	0	3.698547	-3.238278	-1.293358
51	1	0	2.812001	-3.804538	-1.596567
52	1	0	4.066180	-3.669917	-0.359676
53	1	0	4.465051	-3.388347	-2.060966
54	6	0	2.890336	-1.163936	-2.490401
55	1	0	3.656515	-1.306731	-3.260104
56	1	0	2.671774	-0.097231	-2.407869
57	1	0	1.976247	-1.660190	-2.831378
58	6	0	3.142666	-1.060913	1.727863
59	1	0	3.605716	-0.083935	1.556203
60	6	0	4.234109	-2.095790	2.004786
61	1	0	4.771812	-1.836972	2.923042
62	1	0	4.971014	-2.148905	1.199257
63	1	0	3.804746	-3.094127	2.141864
64	6	0	2.187024	-0.924661	2.917914
65	1	0	1.642798	-1.859431	3.097649
66	1	0	1.454952	-0.132209	2.742940
67	1	0	2.746485	-0.685903	3.828169
68	7	0	-0.197394	2.985332	-0.014941
69	7	0	-2.139412	1.992313	0.072708
70	15	0	2.132567	-1.396778	0.204902
71	15	0	-1.370973	-1.203914	-0.072922
72	45	0	0.446027	0.206199	-0.157440
73	1	0	1.767116	-2.729307	0.526746

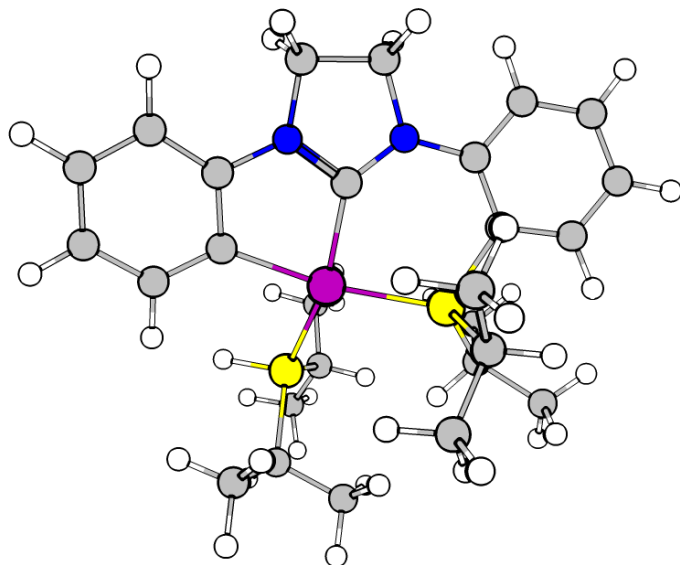
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SCF Done:  E(RwB97XD) = -6533.24104113      A.U. after   1 cycles
              Conv g =   0.4344D-08          -V/T =   2.0047
Zero-point correction=                      0.636782 (Hartree/Particle)
Thermal correction to Energy=                0.680083
Thermal correction to Enthalpy=              0.681138

```

Thermal correction to Gibbs Free Energy=	0.559320
Sum of electronic and zero-point Energies=	-6532.604259
Sum of electronic and thermal Energies=	-6532.560958
Sum of electronic and thermal Enthalpies=	-6532.559903
Sum of electronic and thermal Free Energies=	-6532.681721
	1
	A
Frequencies --	22.0322
	2
	A
	27.2027
	3
	A
	38.1500

P-H-RE-PR-conf3 (6a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.846944	4.186645	-0.464844
2	1	0	0.878521	4.903259	0.360528
3	1	0	0.483476	4.703129	-1.356959
4	6	0	0.609754	1.865190	-0.104720
5	6	0	2.196128	3.503876	-0.696735
6	1	0	2.533890	3.625103	-1.728548
7	1	0	2.967558	3.889460	-0.027005
8	6	0	2.978769	1.148697	-0.449646
9	6	0	2.865711	-0.212207	-0.075881
10	6	0	4.033987	-0.983772	-0.065781
11	1	0	3.971062	-2.011111	0.268719
12	6	0	5.275976	-0.501031	-0.455968
13	1	0	6.148145	-1.145709	-0.436570
14	6	0	5.366410	0.821343	-0.870543
15	1	0	6.313945	1.238815	-1.195676
16	6	0	4.238390	1.629572	-0.857476
17	1	0	4.358347	2.657156	-1.171373
18	6	0	-1.401642	3.106381	0.044762

19	6	0	-2.009489	1.836698	0.165283
20	6	0	-3.386840	1.885142	0.409801
21	1	0	-3.944703	0.959370	0.534703
22	6	0	-4.108685	3.085089	0.499626
23	1	0	-5.178905	3.060732	0.688350
24	6	0	-3.459622	4.304022	0.341085
25	1	0	-4.009761	5.238397	0.399451
26	6	0	-2.079738	4.319123	0.114186
27	1	0	-1.558723	5.266700	0.003685
28	6	0	1.363557	-2.749331	-0.269753
29	1	0	0.317069	-3.039921	-0.133832
30	6	0	1.620958	-2.667380	-1.778569
31	1	0	2.675155	-2.461952	-1.985673
32	1	0	1.030942	-1.876239	-2.248591
33	1	0	1.363502	-3.617177	-2.258919
34	6	0	2.205498	-3.860059	0.373559
35	1	0	1.834453	-4.829285	0.024199
36	1	0	2.148117	-3.864296	1.464122
37	1	0	3.258963	-3.809779	0.089516
38	6	0	1.674669	-1.224232	2.273189
39	1	0	2.614216	-1.784468	2.355628
40	6	0	0.565256	-1.991195	2.994015
41	1	0	0.796729	-2.076403	4.060709
42	1	0	0.437198	-3.004754	2.605410
43	1	0	-0.388307	-1.464444	2.894102
44	6	0	1.875306	0.151546	2.919642
45	1	0	0.963679	0.750627	2.838291
46	1	0	2.693588	0.706520	2.452984
47	1	0	2.114515	0.029649	3.981076
48	6	0	-1.988128	-2.186547	-2.082729
49	1	0	-1.132522	-2.843230	-1.891799
50	6	0	-3.169621	-3.042273	-2.545708
51	1	0	-4.069569	-2.431556	-2.673355
52	1	0	-3.403592	-3.846104	-1.843164
53	1	0	-2.943070	-3.505581	-3.511694
54	6	0	-1.583267	-1.176515	-3.162994
55	1	0	-1.273011	-1.698865	-4.073947
56	1	0	-0.762570	-0.535796	-2.827734
57	1	0	-2.425132	-0.524182	-3.417949
58	6	0	-3.108006	-2.499143	0.629024
59	1	0	-4.008134	-2.860917	0.121511
60	6	0	-3.536001	-1.790126	1.917733
61	1	0	-3.993903	-2.504093	2.610260
62	1	0	-4.266449	-1.000583	1.721628
63	1	0	-2.678352	-1.329828	2.417353
64	6	0	-2.203037	-3.694445	0.927033
65	1	0	-1.300984	-3.376463	1.454382
66	1	0	-1.898656	-4.224049	0.018844
67	1	0	-2.724341	-4.411638	1.569272
68	7	0	-0.006039	3.060340	-0.141359

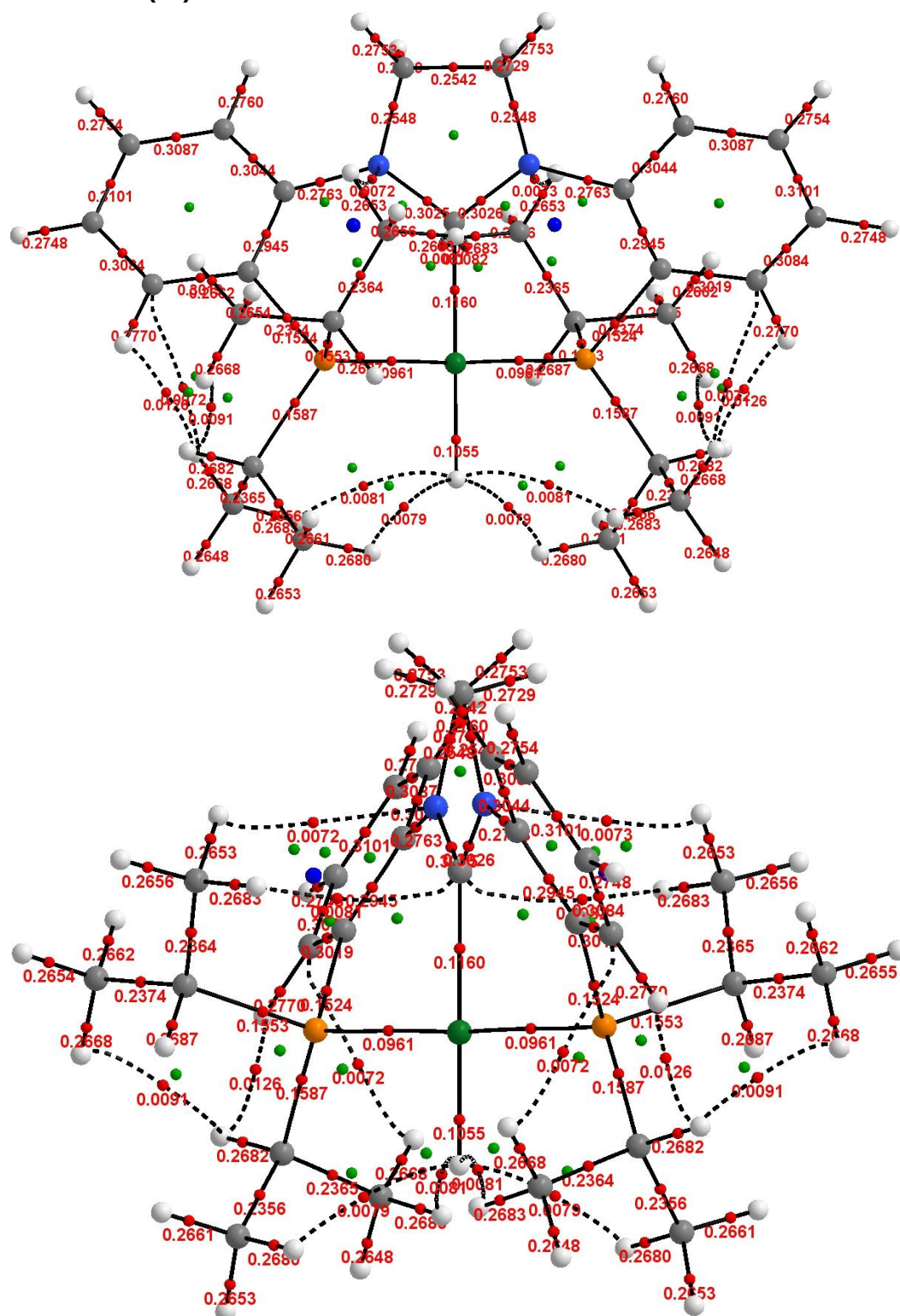
69	7	0	1.926654	2.083683	-0.404897
70	15	0	-2.293683	-1.261388	-0.499240
71	15	0	1.295874	-1.018881	0.457359
72	45	0	-0.601025	0.272259	0.107621
73	1	0	-3.472835	-0.596712	-0.908443

SCF Done: E(RwB97XD) = -6533.23482058 A.U. after 1 cycles
 Conv = 0.1751D-08 -V/T = 2.0047

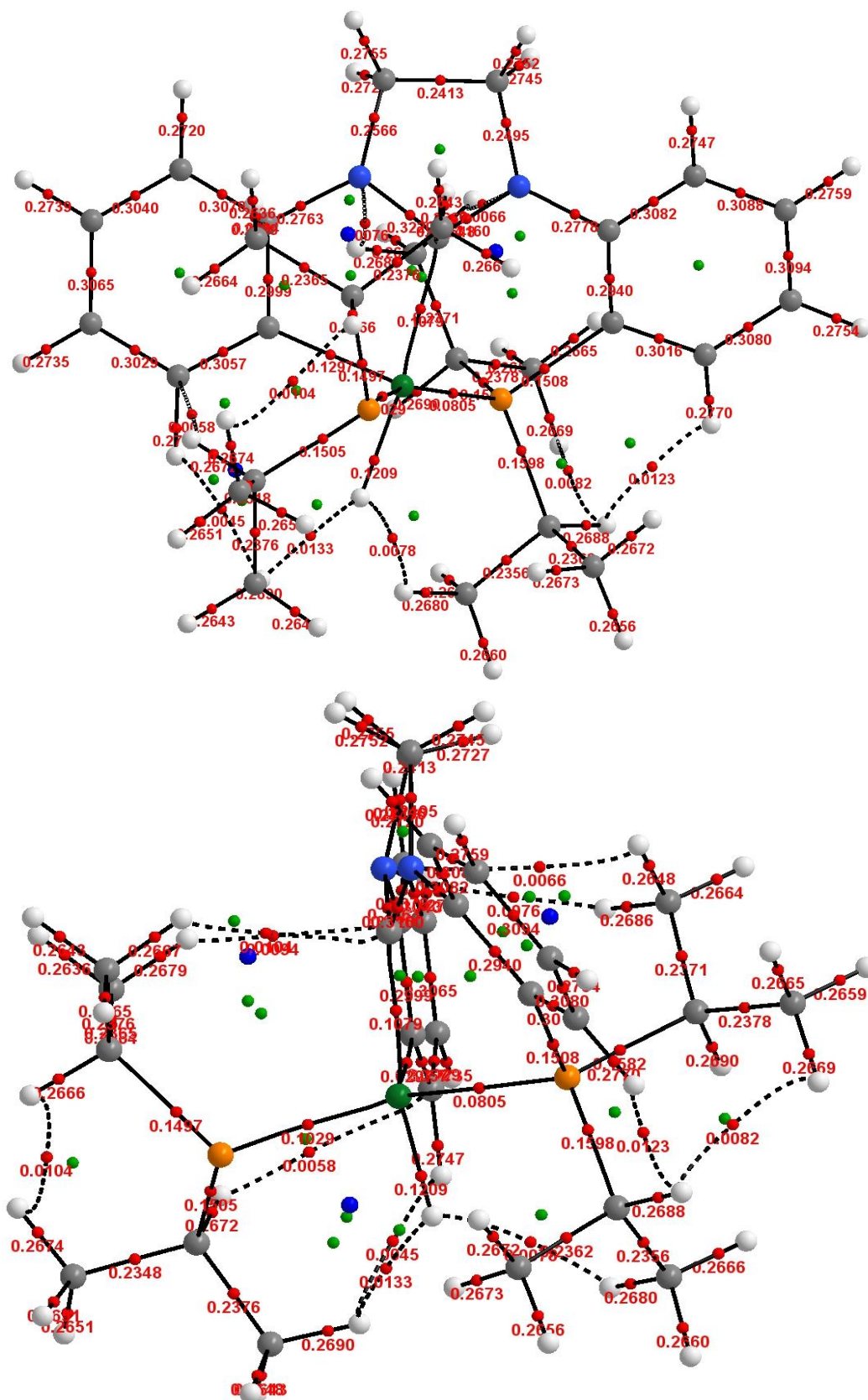
Zero-point correction= 0.636559 (Hartree/Particle)
 Thermal correction to Energy= 0.680100
 Thermal correction to Enthalpy= 0.681155
 Thermal correction to Gibbs Free Energy= 0.558164
 Sum of electronic and zero-point Energies= -6532.598261
 Sum of electronic and thermal Energies= -6532.554721
 Sum of electronic and thermal Enthalpies= -6532.553666
 Sum of electronic and thermal Free Energies= -6532.676657

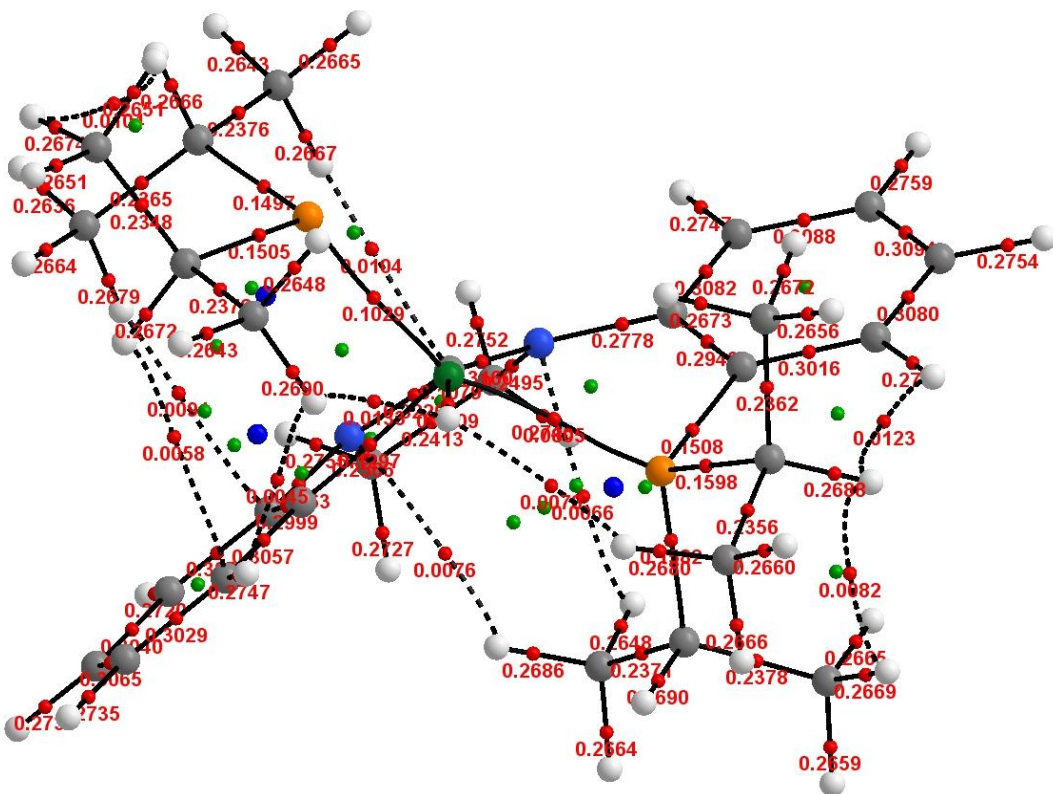
	1	2	3
	A	A	A
Frequencies --	12.3343	21.4544	41.2183

C-P-OA-SM (1a)

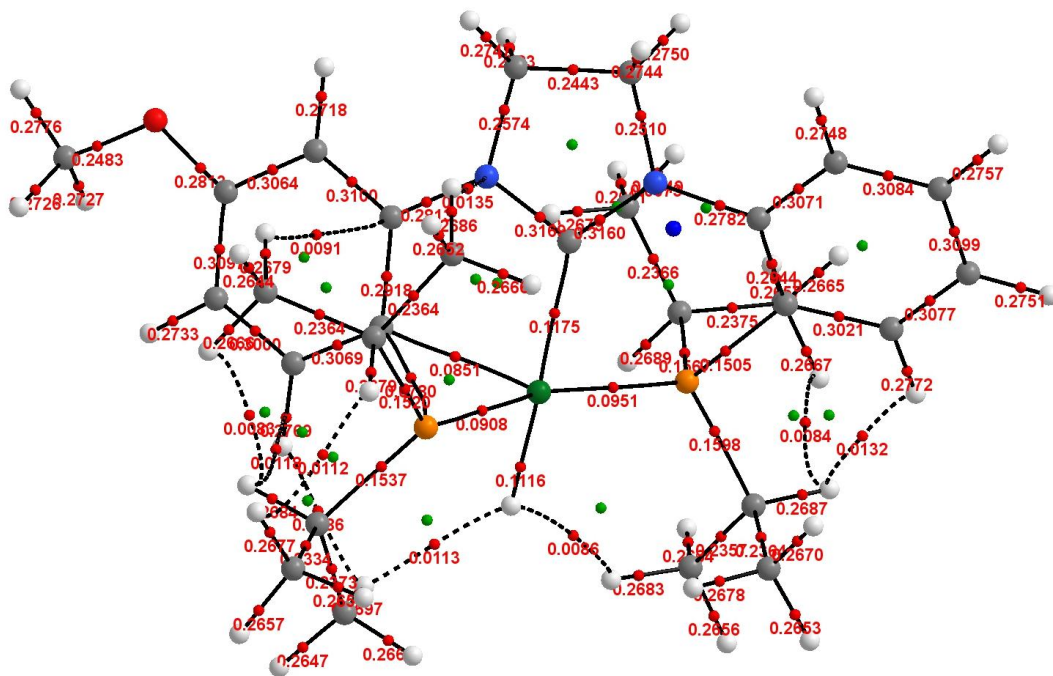


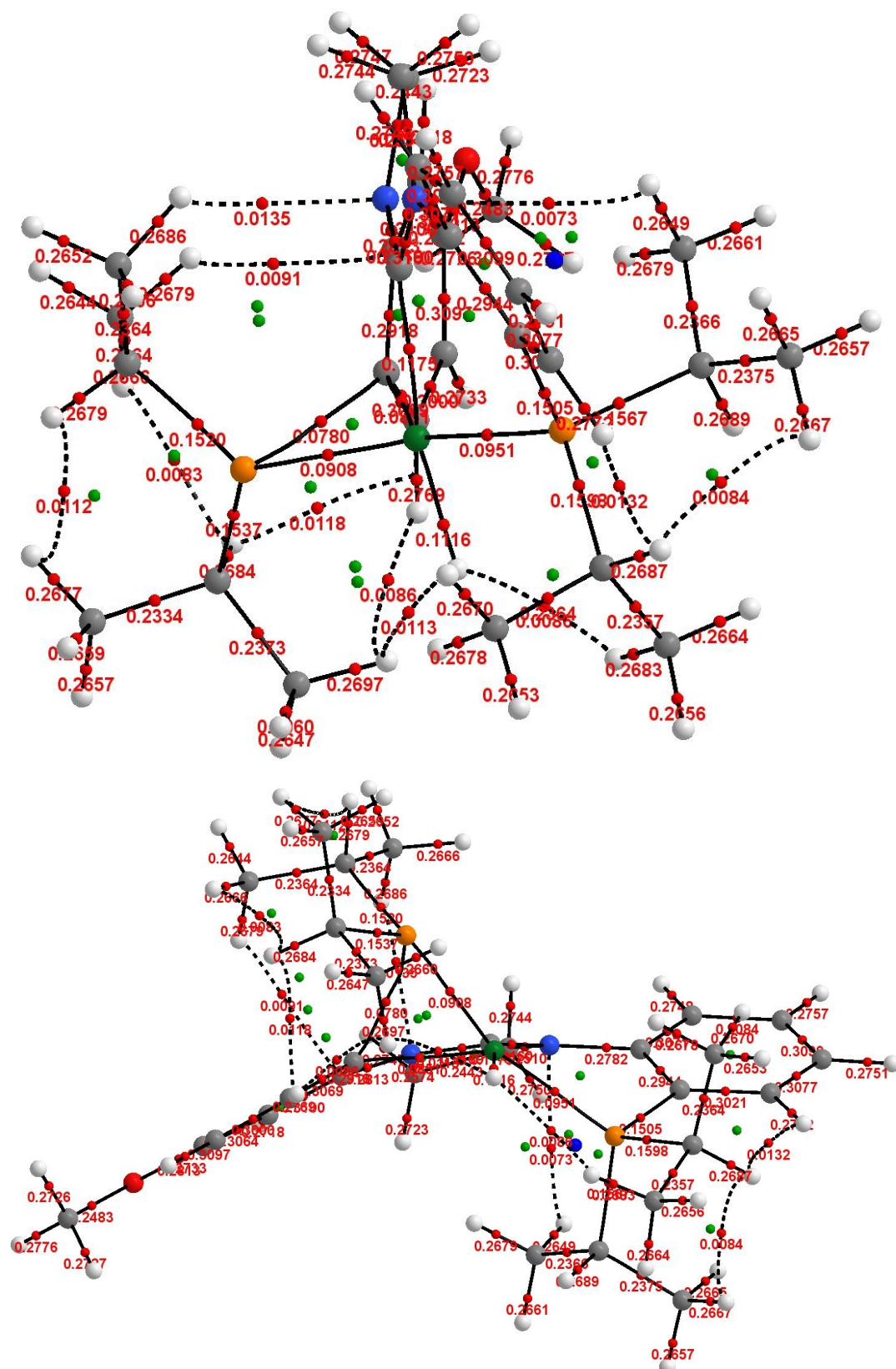
C-P-OA-PR (3a)

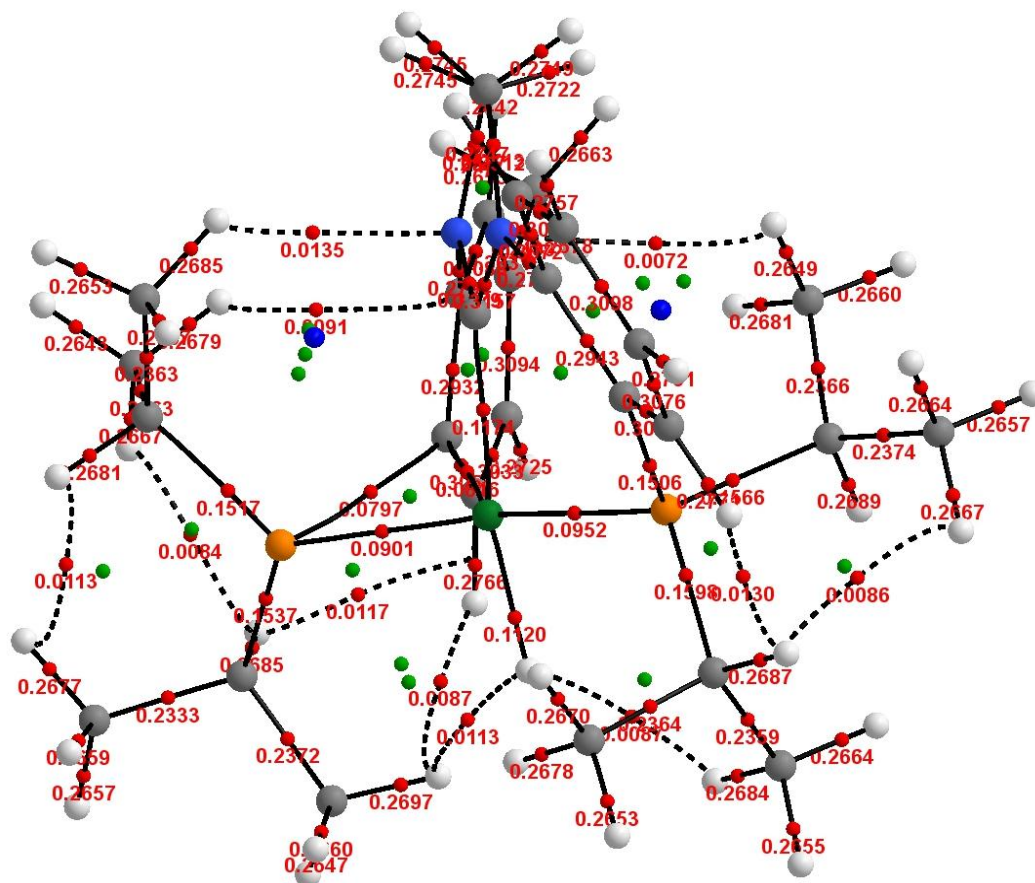


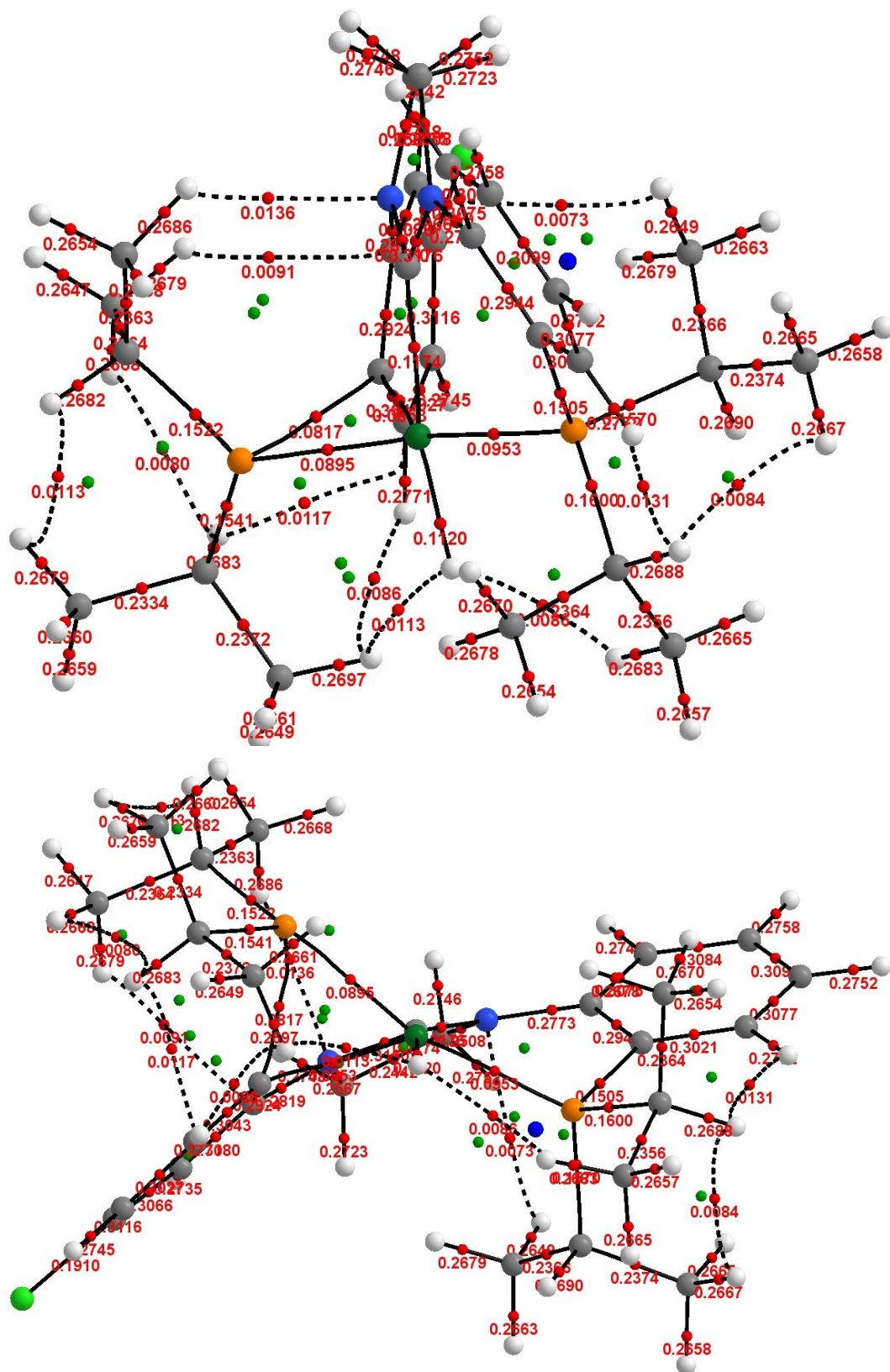


C-P-OA-TS-*p*-MeO (2b)

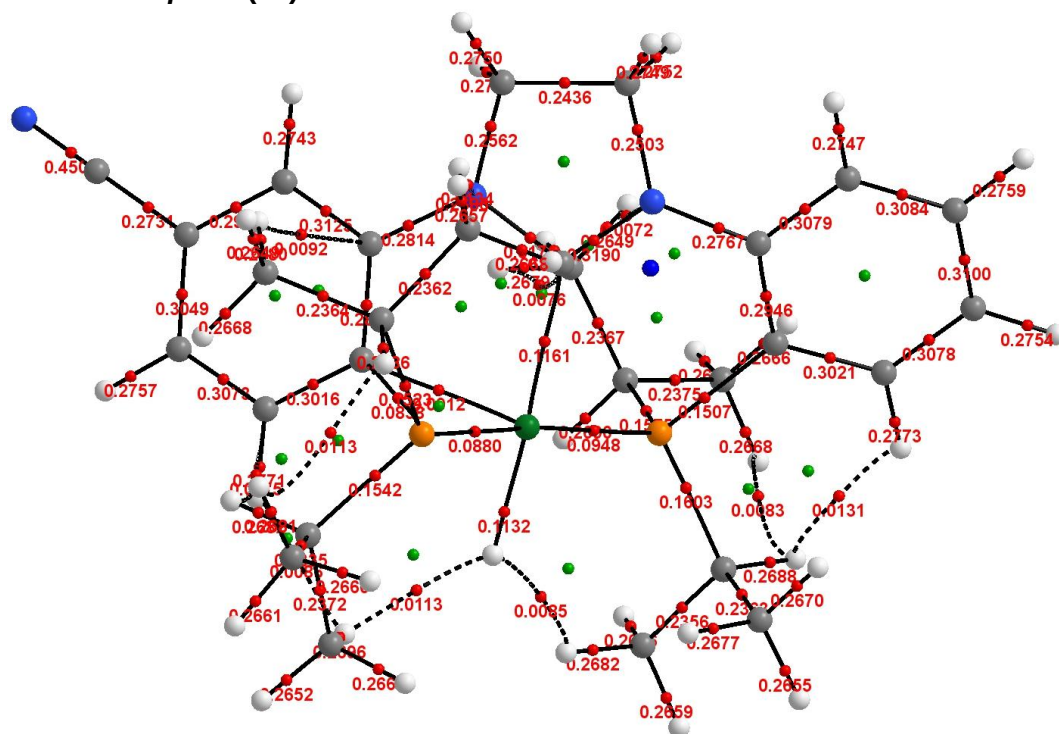


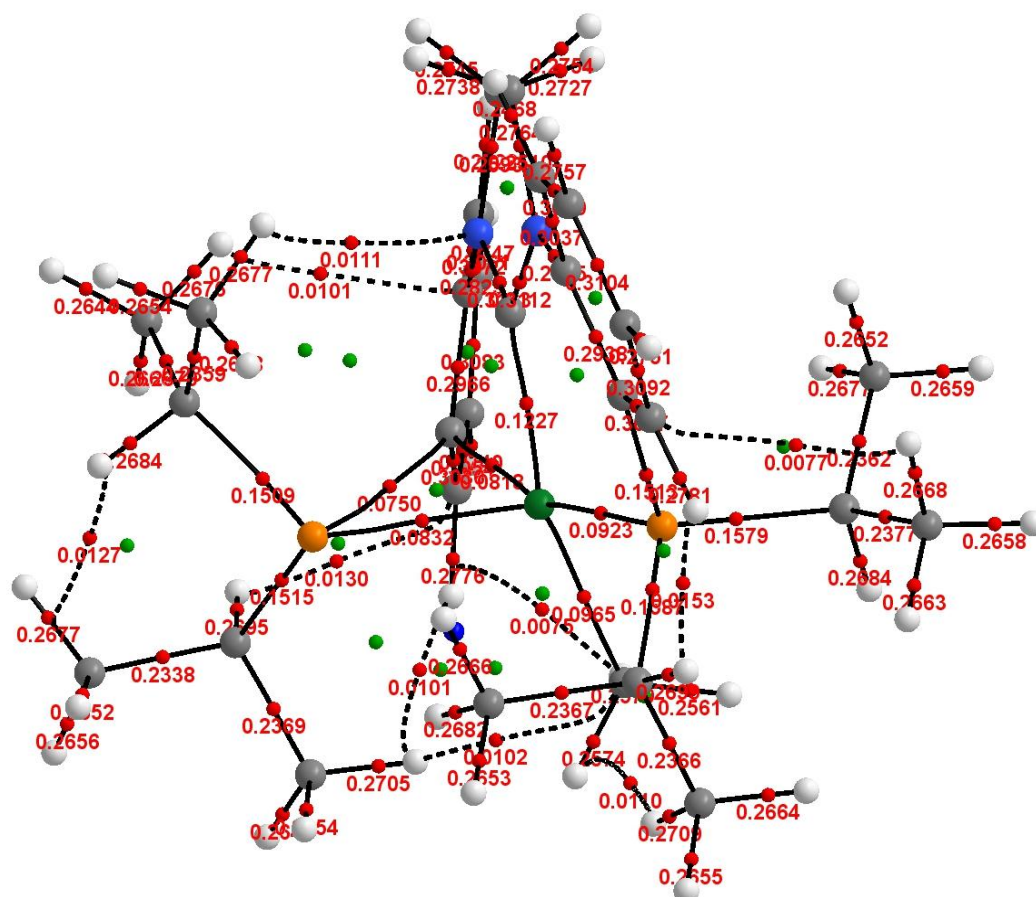


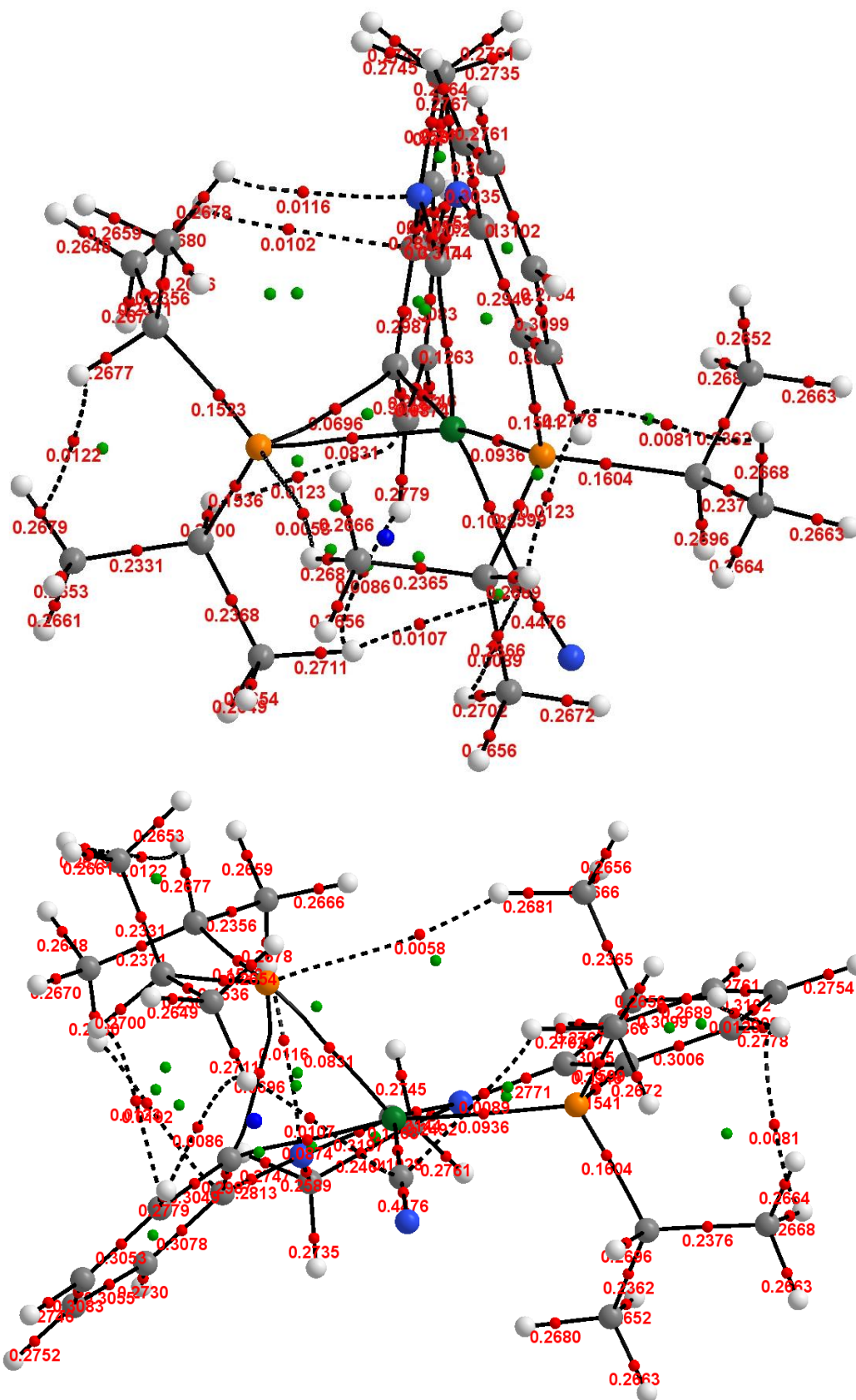




C-P-OA-TS-*p*-CN (2e)

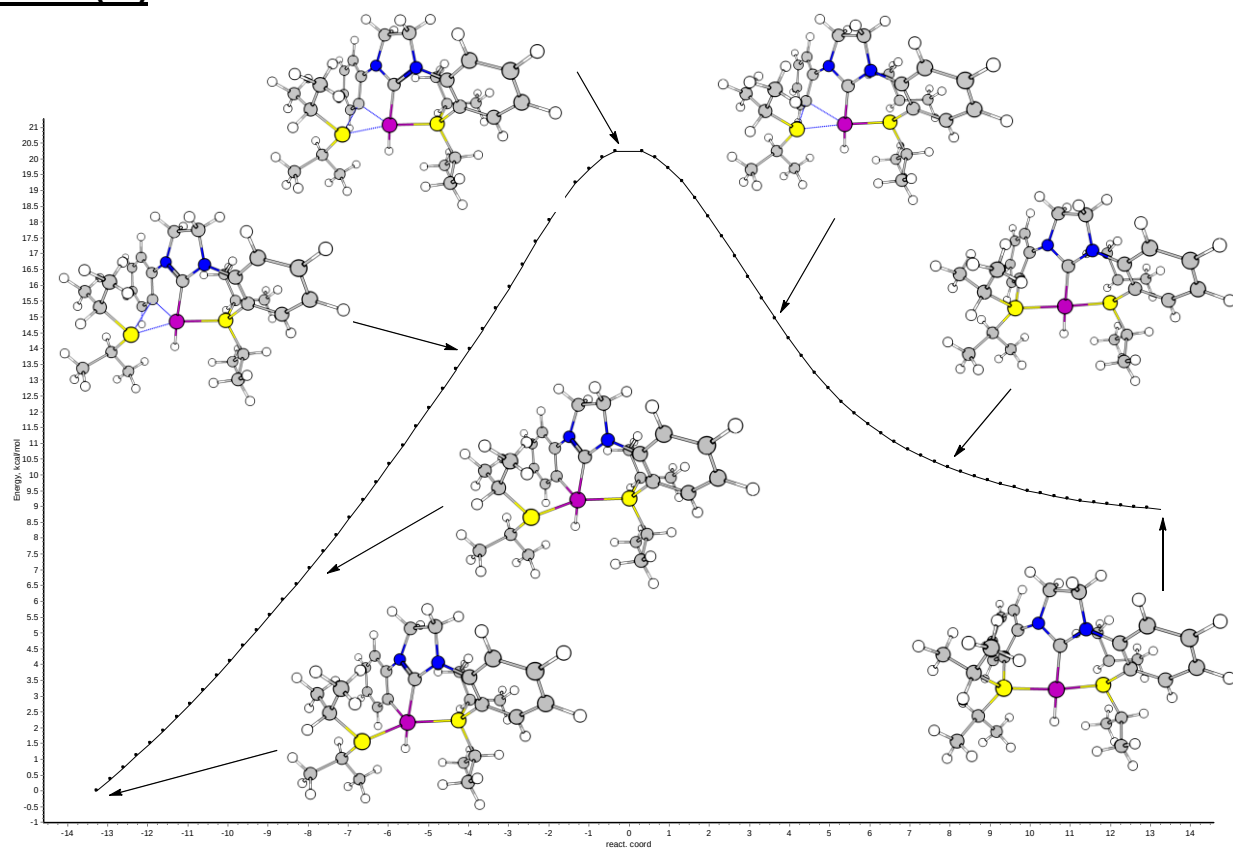




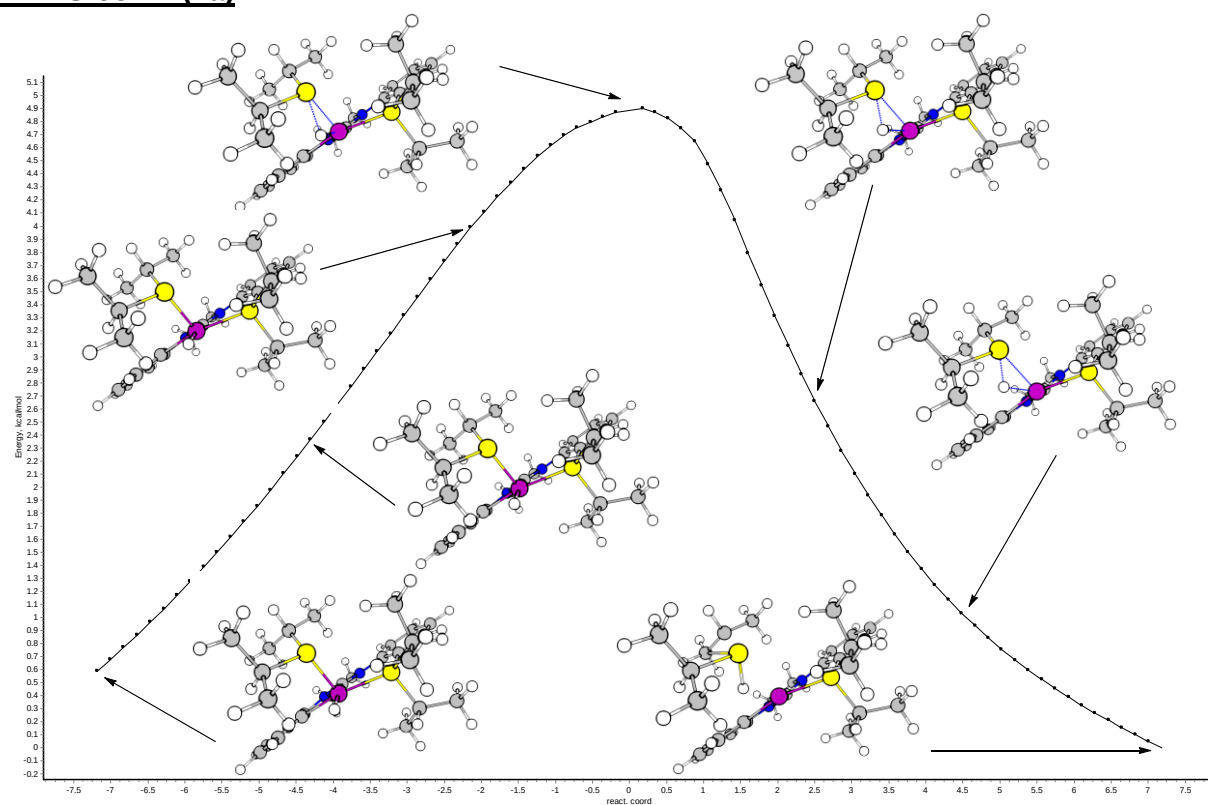


3. IRC plots

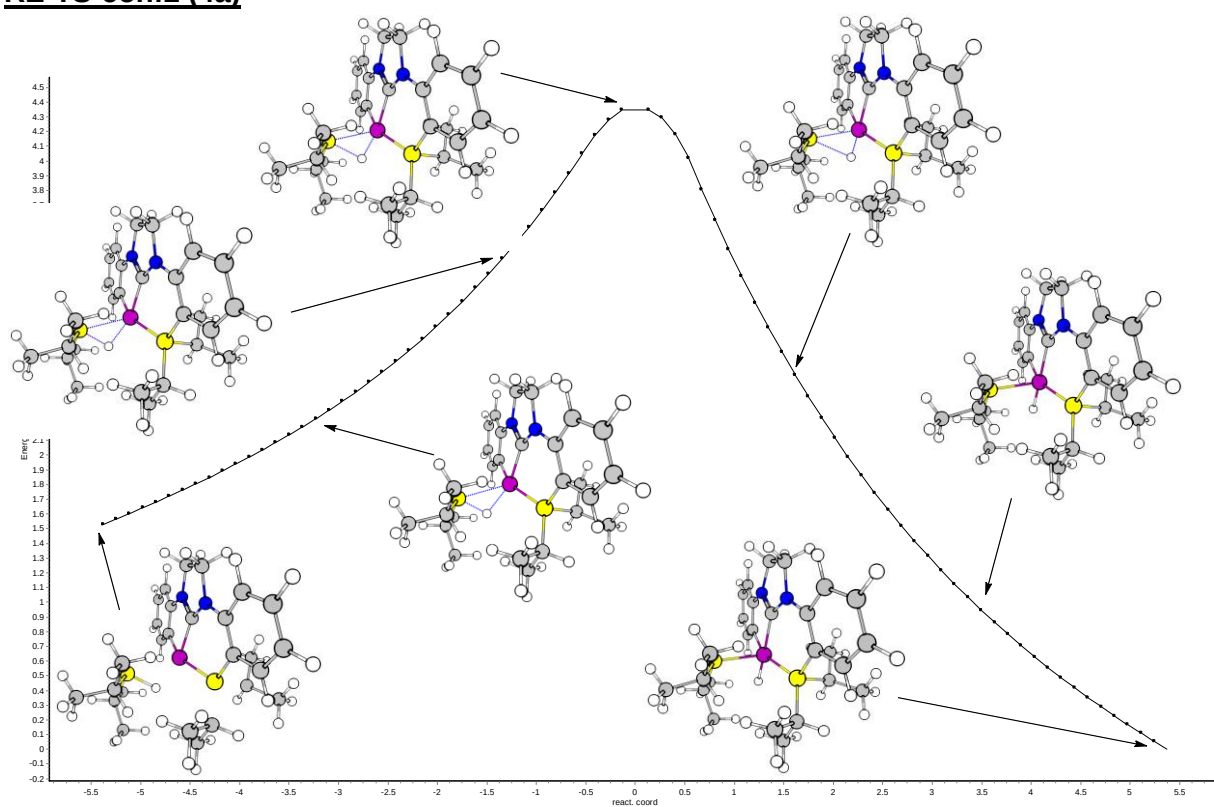
OA-TS (2a)



RE-TS-conf1 (4a)



RE-TS-conf2 (4a)



RE-TS-conf3 (4a)

