Supporting Information

Part II: Computational Details

Addition of C-C and C-H Bonds by Pincer-Iridium Complexes: a Combined Experimental and Computational Study

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Contents

2. Optimized geometries and absolute energies of tBu4 species

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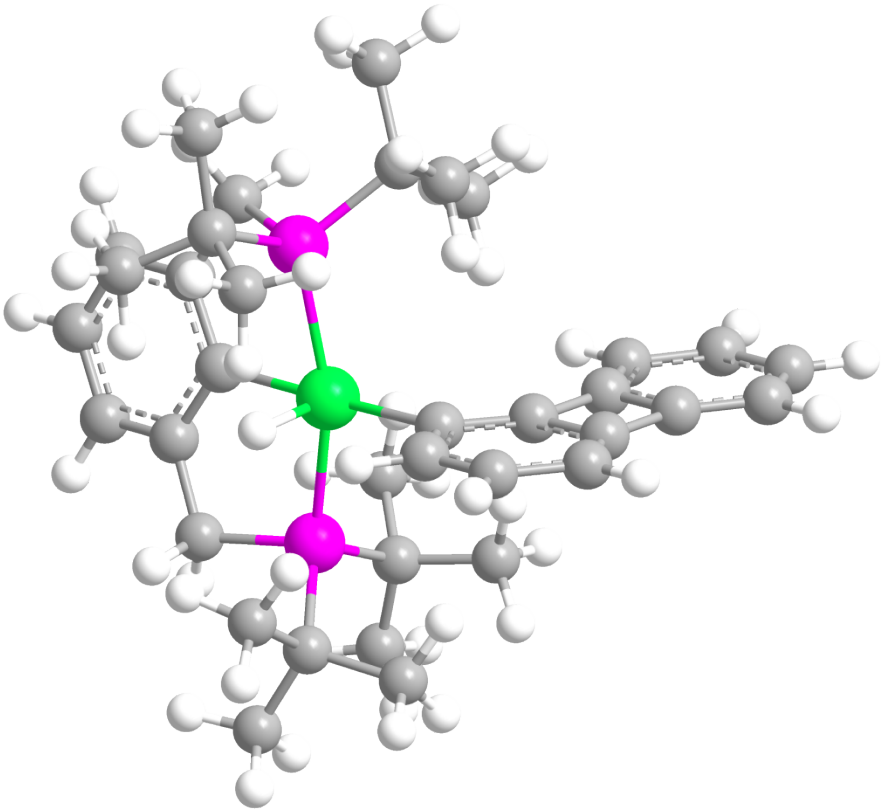
1-C1-anti



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P 0	0.466787	2.393280	0.210516
C 0	2.471217	-2.024323	-1.416970
C 0	2.157070	-2.847074	1.395791
C 0	-0.025847	-3.413831	-0.772144
C 0	2.248350	2.805959	-0.069530
C 0	-0.432568	3.155372	-1.269931
C 0	0.058058	3.307142	1.812268
C 0	3.063133	-0.639347	-1.415870
C 0	4.282615	-0.401962	-2.051170
C 0	4.824143	0.877750	-2.078074
C 0	2.937065	1.686580	-0.803355
C 0	4.148595	1.920614	-1.453706
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C 0	0.613381	-4.621876	-1.459849
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C 0	-0.818515	-2.619965	-1.815912
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C 0	0.650091	2.467656	2.949588
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C 0	1.326382	-2.680275	2.669323
C 0	-1.426071	-0.311891	1.079492
C 0	-2.662998	-0.424013	0.450851
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C 0	-4.616882	-0.669359	-0.199366
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H 0	5.770076	1.060883	-2.577930
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H 0	1.676650	-4.979530	1.263295
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H 0	0.312906	5.373502	1.092732
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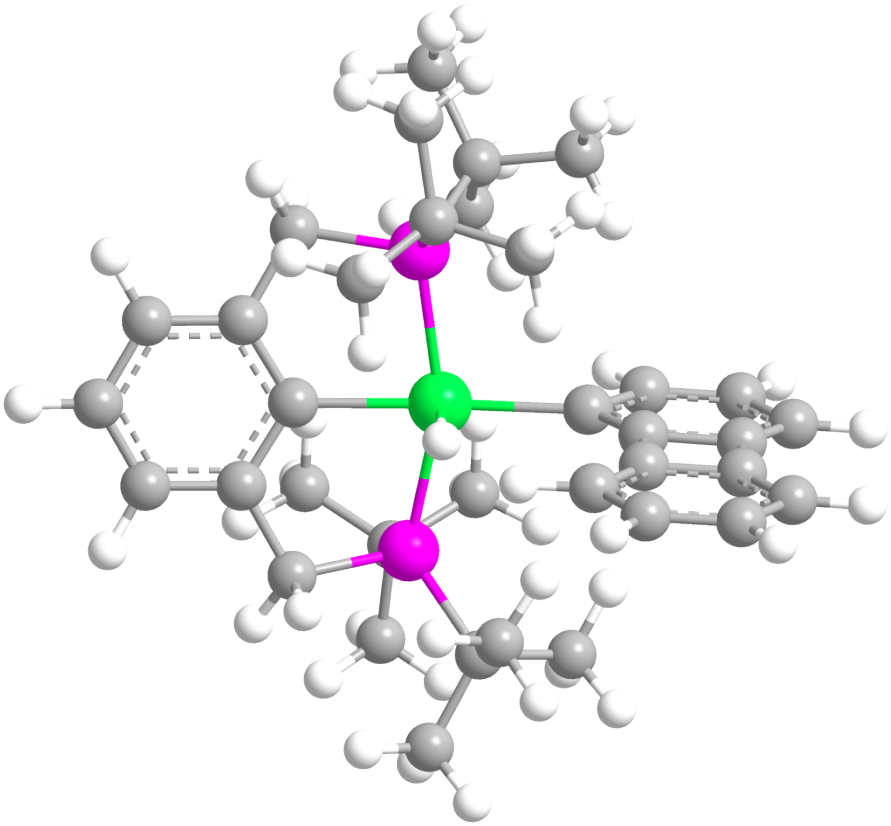
1-C1-syn



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C 0	2.389402	2.663461	-0.230745
C 0	-0.346946	3.365259	-1.069439
C 0	0.475878	3.083733	1.941271
C 0	2.201424	-2.182356	-1.533249
C 0	2.093929	-2.764205	1.371546
C 0	-0.231198	-3.529610	-0.567880
C 0	2.938841	1.499528	-1.010744
C 0	4.101751	1.653542	-1.766561
C 0	4.656593	0.567105	-2.432467
C 0	2.871430	-0.834044	-1.601046
C 0	4.042732	-0.677147	-2.341406
C 0	-0.164222	4.874086	-0.920490
C 0	1.195076	4.418459	2.143294
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C 0	2.413453	-4.257359	1.385273

C	0	1.141698	2.025584	2.832169
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C	0	-1.135868	-2.871127	-1.613957
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C	0	-1.090731	-3.886864	0.646068
C	0	1.352937	-2.370921	2.651462
C	0	-0.992916	3.219149	2.342208
C	0	-1.828561	3.006230	-0.977174
C	0	-1.454098	-0.233243	1.091258
C	0	-2.677337	-0.268781	0.434157
C	0	-1.645403	-0.441742	2.499037
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H	0	4.474520	-1.530804	-2.859890
H	0	-0.652359	5.258918	-0.021827
H	0	0.887545	5.175339	-0.896969
H	0	-0.625392	5.379661	-1.776440
H	0	1.120242	4.707152	3.198082
H	0	2.259793	4.365176	1.903102
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H	0	0.994774	-5.360378	-0.486621
H	0	-0.424005	-5.447554	-1.520828
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H	0	4.035712	-2.250979	0.472873
H	0	3.270143	-0.910006	1.319973
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H	0	-1.524630	-2.995545	1.109747
H	0	-1.920135	-4.527120	0.325853
H	0	1.925506	-2.694513	3.528303
H	0	1.242043	-1.282739	2.717216
H	0	0.351994	-2.802097	2.722841
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H	0	-1.476071	4.055547	1.830284
H	0	-1.562004	2.308193	2.134922
H	0	-2.289393	3.341606	-0.046343
H	0	-2.373853	3.475861	-1.803509
H	0	-1.979176	1.929534	-1.049048
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H	0	-5.036017	-0.846959	2.887061
H	0	-2.291129	0.107710	-2.768599
H	0	-4.411104	0.018104	-4.085586
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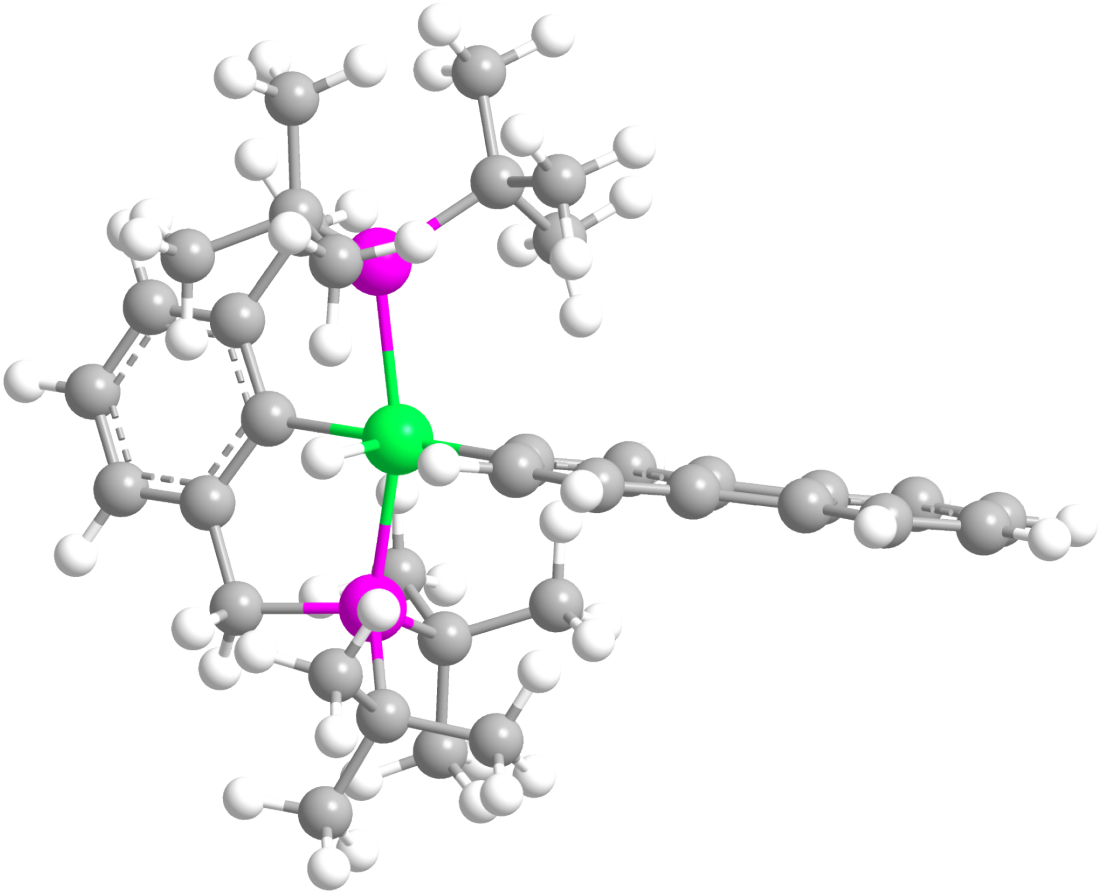
1-C2-anti



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P	0	-0.899908	-2.335330	0.154498
C	0	-2.871474	2.171087	-1.044122
C	0	-1.670219	3.169002	1.452855
C	0	-0.158164	3.260358	-1.288953
C	0	-2.684763	-2.575835	0.565582
C	0	-0.706745	-3.117794	-1.563318
C	0	0.021407	-3.325786	1.470011
C	0	-3.572190	0.877439	-0.720960
C	0	-4.950502	0.757616	-0.901718
C	0	-5.592549	-0.444988	-0.629055
C	0	-3.477812	-1.411271	0.029071
C	0	-4.853568	-1.528421	-0.165701
C	0	-1.939052	4.656316	1.232293

C	0	-0.842849	4.480551	-1.908314
C	0	-0.601164	-4.693893	1.760934
C	0	-0.678420	-4.644603	-1.554252
C	0	0.217269	2.289726	-2.417059
C	0	-2.930899	2.518900	2.035267
C	0	-0.051407	-2.484475	2.750113
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C	0	1.492740	-3.473626	1.078441
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C	0	2.372569	-0.003277	-0.566777
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C	0	5.577496	0.357937	0.562553
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C	0	6.911877	0.470185	0.859886
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H	0	-2.630112	2.213551	-2.114067
H	0	-3.062910	-3.545095	0.216807
H	0	-2.744490	-2.604939	1.661804
H	0	-5.526712	1.607032	-1.263037
H	0	-6.664370	-0.536986	-0.773733
H	0	-5.355438	-2.468380	0.054876
H	0	-1.035685	5.204295	0.954823
H	0	-2.700119	4.836588	0.467146
H	0	-2.308761	5.096874	2.165128
H	0	-0.166994	4.932047	-2.643611
H	0	-1.762294	4.219727	-2.439175
H	0	-1.082402	5.253059	-1.177920
H	0	-0.534376	-5.387661	0.923560
H	0	-0.070045	-5.153129	2.602272
H	0	-1.651915	-4.615073	2.053391
H	0	-0.664735	-5.007642	-2.588401
H	0	0.207528	-5.048524	-1.060565
H	0	-1.564577	-5.072006	-1.075996
H	0	-0.659103	1.911003	-2.954254

H	0	0.849313	2.802678	-3.150259
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H	0	-3.818342	2.699320	1.423342
H	0	-2.821094	1.436948	2.146423
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H	0	0.465749	-1.531662	2.627392
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H	0	0.431966	-3.032317	3.566493
H	0	-1.722238	-3.022173	-3.455859
H	0	-2.841975	-3.073287	-2.092535
H	0	-1.987247	-1.578641	-2.465140
H	0	1.634000	-4.134843	0.219707
H	0	1.948981	-2.505311	0.850688
H	0	2.048874	-3.910275	1.915367
H	0	0.736876	-3.032979	-3.172032
H	0	0.493963	-1.488712	-2.352426
H	0	1.466060	-2.742799	-1.584852
H	0	1.826997	4.107100	-1.280634
H	0	0.926322	4.450059	0.193049
H	0	1.610625	2.833627	-0.075351
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H	0	-0.759053	3.544288	3.371223
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H	0	1.207371	0.574839	2.575515
H	0	3.593150	0.779374	3.100267
H	0	5.647019	-0.319058	-2.813976
H	0	8.085334	-0.119103	-2.299291
H	0	7.284384	0.684876	1.856154
H	0	8.873308	0.365649	-0.043915

Sum of electronic and zero-point Energies=	-2189.095772
Sum of electronic and thermal Energies=	-2189.052652
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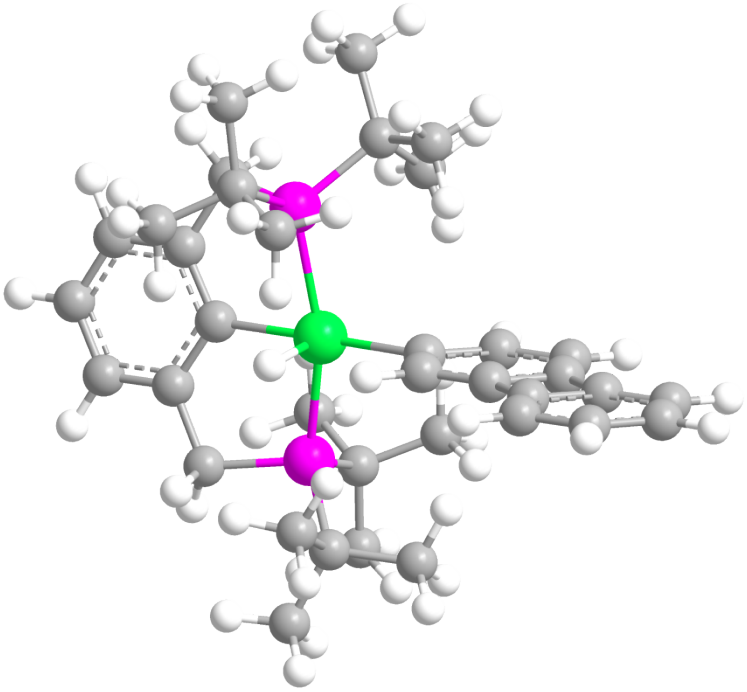
1-C2-syn



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P 0	1.219602	-2.252827	-0.153192
C 0	2.750772	2.537608	0.421533
C 0	0.605454	3.274678	-1.454439
C 0	0.164777	3.184374	1.646267
C 0	2.757708	-2.217546	-1.175402
C 0	1.770258	-3.013409	1.495241
C 0	0.060252	-3.408702	-1.092621
C 0	3.486550	1.364603	-0.171779
C 0	4.840541	1.469678	-0.491688
C 0	5.525739	0.378051	-1.012967
C 0	3.495066	-0.928092	-0.916243
C 0	4.851236	-0.820268	-1.222074
C 0	0.695971	4.790482	-1.288478
C 0	0.822601	4.512289	2.027397
C 0	0.748076	-4.664616	-1.634316
C 0	1.985150	-4.524313	1.443279
C 0	0.371314	2.190793	2.798040
C 0	1.666276	2.823503	-2.465515
C 0	-0.460363	-2.595966	-2.284043

C 0	3.092263	-2.356380	1.908984
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C 0	0.721657	-2.664142	2.552820
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C 0	-0.770825	2.891899	-1.998682
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C 0	-3.706782	-0.080651	-0.301690
C 0	-1.408945	-0.158560	0.444410
C 0	-4.178959	-0.360579	1.003318
C 0	-5.118133	-0.024396	-0.797288
C 0	-1.927553	-0.442301	1.722148
C 0	-3.302760	-0.548201	2.041216
C 0	-5.970045	0.163186	-1.854360
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C 0	-7.351754	0.060289	-1.562982
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C 0	-7.808812	-0.213967	-0.284949
H 0	0.451543	0.057813	-1.465994
H 0	3.113114	3.502194	0.045063
H 0	2.900402	2.567270	1.508555
H 0	3.382361	-3.105035	-1.013194
H 0	2.429766	-2.266130	-2.222404
H 0	5.366040	2.408331	-0.327853
H 0	6.579874	0.461168	-1.258074
H 0	5.384306	-1.673860	-1.635920
H 0	-0.127025	5.192995	-0.693465
H 0	1.638426	5.107089	-0.831742
H 0	0.640833	5.263667	-2.275381
H 0	0.388029	4.866351	2.969260
H 0	1.899126	4.414226	2.190781
H 0	0.663590	5.296457	1.287524
H 0	1.095825	-5.339316	-0.852692
H 0	0.032550	-5.223986	-2.247431
H 0	1.598503	-4.424091	-2.278240
H 0	2.395131	-4.860172	2.402745
H 0	1.058936	-5.078180	1.278683
H 0	2.702072	-4.813667	0.669359
H 0	1.428684	1.962159	2.970954
H 0	-0.023383	2.616427	3.727251
H 0	-0.164164	1.256322	2.612317
H 0	2.671595	3.159445	-2.198863
H 0	1.698373	1.735739	-2.569408
H 0	1.424931	3.250857	-3.444983
H 0	-1.043771	-1.736329	-1.951499

H	0	0.346331	-2.235739	-2.930490
H	0	-1.109644	-3.231786	-2.895788
H	0	3.359682	-2.710826	2.910864
H	0	3.918036	-2.609426	1.239609
H	0	3.022252	-1.266073	1.944550
H	0	-0.855215	-4.442225	0.613942
H	0	-1.625207	-2.897035	0.199493
H	0	-1.874261	-4.320347	-0.816024
H	0	0.992606	-3.123204	3.510437
H	0	0.677574	-1.581250	2.710762
H	0	-0.285795	-2.995436	2.291669
H	0	-1.800580	3.704909	2.369207
H	0	-1.548214	4.148724	0.684220
H	0	-1.828299	2.451019	1.125573
H	0	-1.582621	3.084439	-1.294067
H	0	-0.974889	3.465230	-2.909964
H	0	-0.804658	1.831586	-2.255873
H	0	-2.044191	0.238541	-1.614970
H	0	-1.234671	-0.599794	2.547126
H	0	-3.619170	-0.768891	3.057348
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H	0	-8.878468	-0.282806	-0.112518

Sum of electronic and zero-point Energies=	-2189.096197
Sum of electronic and thermal Energies=	-2189.052966
Sum of electronic and thermal Enthalpies=	-2189.052022
Sum of electronic and thermal Free Energies=	-2189.167821

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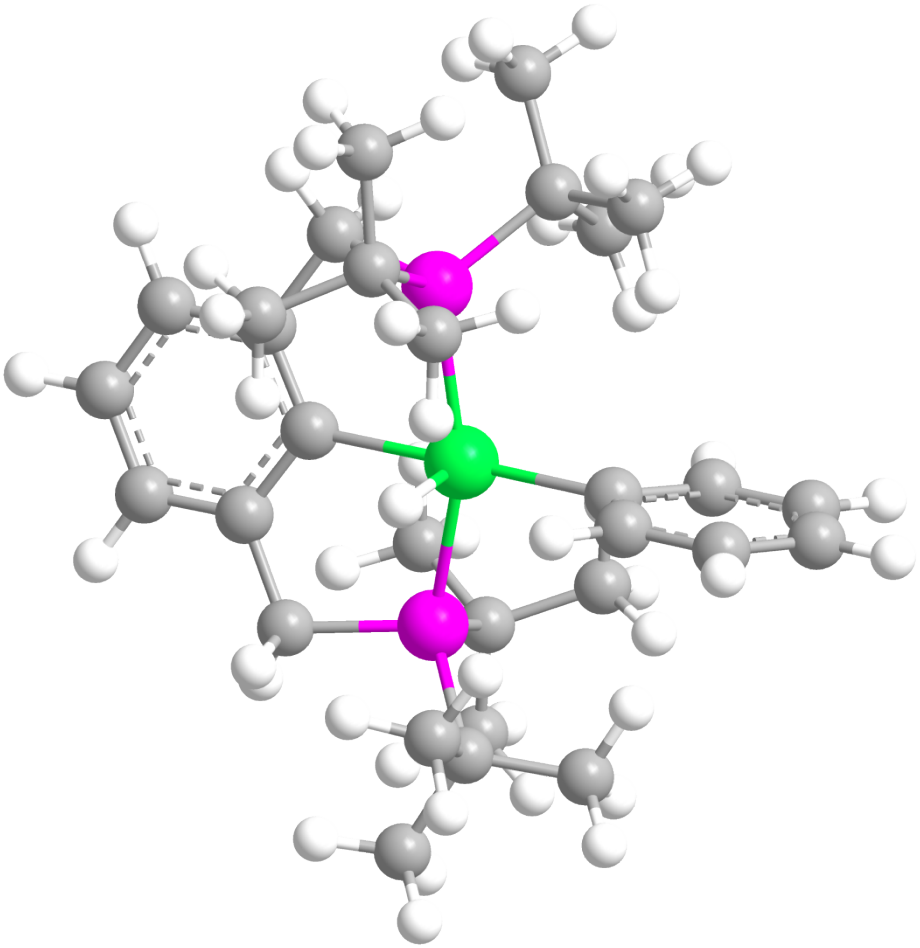
benzene addition product



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P 0	2.291751	-0.351103	0.124288
P 0	-2.300248	-0.313793	-0.109630
C 0	2.372541	-2.059255	0.824898
C 0	3.063370	-0.517184	-1.600781
C 0	3.385983	0.673559	1.270978
C 0	-2.399029	-2.060800	-0.720523
C 0	-3.235394	-0.353668	1.529762
C 0	-3.231175	0.659360	-1.433463
C 0	1.130442	-2.816907	0.430151
C 0	1.116227	-4.210993	0.466778
C 0	-0.039937	-4.910759	0.136436
C 0	-1.170811	-2.817318	-0.286187
C 0	-1.182974	-4.211630	-0.234768
C 0	4.584927	-0.645061	-1.594630
C 0	4.688454	-0.026511	1.667306

C 0	-4.518739	-0.005207	-1.924881
C 0	-4.745036	-0.512365	1.360519
C 0	2.558249	0.900878	2.541905
C 0	2.480591	-1.769083	-2.267082
C 0	-2.246653	0.742149	-2.608174
C 0	-2.698579	-1.550776	2.323494
C 0	-3.522317	2.076703	-0.939247
C 0	-2.930527	0.921622	2.315976
C 0	3.676455	2.036721	0.640626
C 0	2.636571	0.695802	-2.429361
C 0	0.026098	2.196028	0.035044
C 0	-0.179980	2.951934	1.208134
C 0	0.248548	2.974548	-1.121194
C 0	-0.172999	4.344478	1.233366
C 0	0.256554	4.368663	-1.117050
C 0	0.044287	5.068556	0.065369
H 0	-0.053369	-0.002304	1.559710
H 0	3.296610	-2.579457	0.542453
H 0	2.414592	-1.939994	1.915886
H 0	-3.331579	-2.550129	-0.413220
H 0	-2.439772	-2.004453	-1.815958
H 0	2.009598	-4.755901	0.764374
H 0	-0.050219	-5.995446	0.171664
H 0	-2.088852	-4.756907	-0.492203
H 0	5.084303	0.263088	-1.251644
H 0	4.926639	-1.480606	-0.976723
H 0	4.932013	-0.837698	-2.616380
H 0	5.211906	0.590022	2.406691
H 0	4.508231	-0.998859	2.134158
H 0	5.372321	-0.174284	0.832055
H 0	-5.299583	-0.038546	-1.165162
H 0	-4.916097	0.570350	-2.768848
H 0	-4.353230	-1.024168	-2.284634
H 0	-5.202883	-0.666831	2.344024
H 0	-5.209254	0.376041	0.926586
H 0	-5.009871	-1.375773	0.742916
H 0	2.254367	-0.037334	3.017455
H 0	3.163291	1.453962	3.268999
H 0	1.661704	1.485863	2.331913
H 0	2.794470	-2.694092	-1.777358
H 0	1.387612	-1.761847	-2.282058
H 0	2.833012	-1.809134	-3.304057
H 0	-1.345998	1.294828	-2.328794
H 0	-1.951504	-0.245398	-2.979234

H	0	-2.713360	1.275196	-3.443935
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H	0	-2.974062	-2.509240	1.876176
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H	0	-4.291077	2.090284	-0.161925
H	0	-2.624100	2.565698	-0.550361
H	0	-3.895237	2.684348	-1.771401
H	0	-3.485932	0.908877	3.260644
H	0	-1.866842	0.988442	2.552026
H	0	-3.202926	1.833382	1.780259
H	0	4.176550	2.676398	1.376421
H	0	4.339499	1.965850	-0.225539
H	0	2.756689	2.544376	0.334459
H	0	2.908519	1.650747	-1.974572
H	0	3.098052	0.648709	-3.422317
H	0	1.551090	0.702492	-2.573319
H	0	-0.355635	2.435601	2.150269
H	0	0.428756	2.485777	-2.077884
H	0	-0.339774	4.867146	2.172613
H	0	0.432276	4.909599	-2.043638
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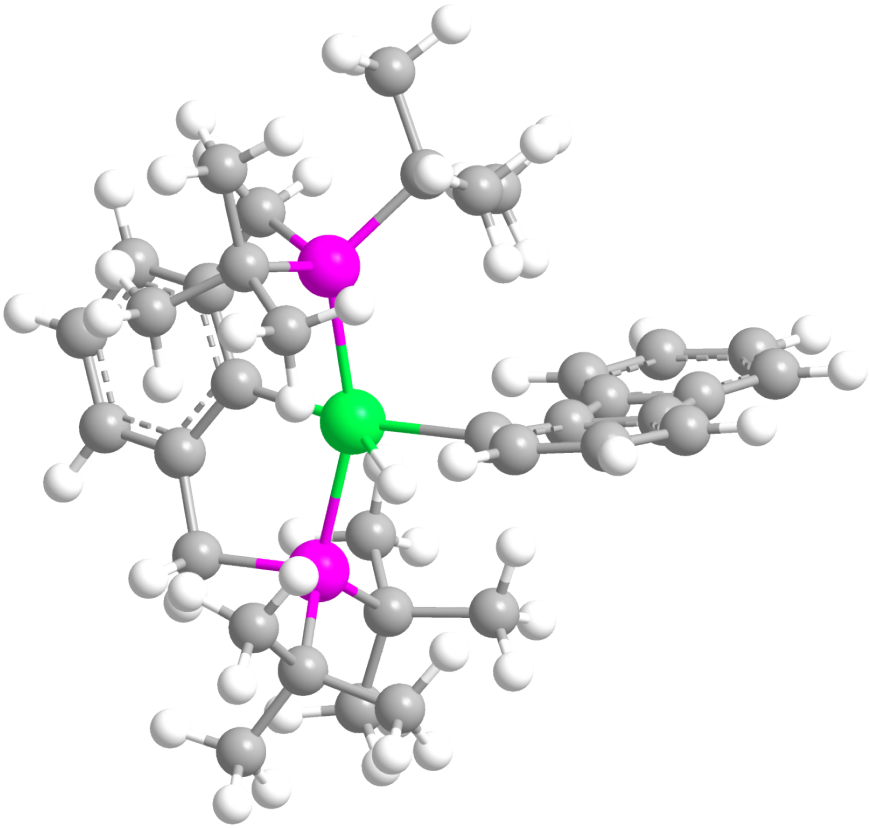
Sum of electronic and zero-point Energies=	-1959.344187
Sum of electronic and thermal Energies=	-1959.304925
Sum of electronic and thermal Enthalpies=	-1959.303981
Sum of electronic and thermal Free Energies=	-1959.410445

TS-1-C1-anti



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P 0	0.574613	-2.322205	0.091131
P 0	-1.976134	1.483375	-0.315528
C 0	-0.171330	-2.883069	1.684104
C 0	-0.127336	-3.503567	-1.220096
C 0	2.415153	-2.684613	0.393404
C 0	-3.464440	0.678406	0.417261
C 0	-1.732390	3.017601	0.769236
C 0	-2.564880	1.960615	-2.053561
C 0	-1.471587	-2.166045	1.907086
C 0	-2.385799	-2.677904	2.829406
C 0	-3.614175	-2.060583	3.022733
C 0	-3.038734	-0.436349	1.328275
C 0	-3.943137	-0.947993	2.257811
C 0	0.401002	-4.933179	-1.124297
C 0	2.673753	-4.022490	1.094680
C 0	-3.971354	2.566997	-2.077761
C 0	-2.852200	4.052743	0.694247

C	0	2.910987	-1.567695	1.316308
C	0	-1.650041	-3.535909	-1.046763
C	0	-2.599297	0.669796	-2.882918
C	0	-1.654981	2.473971	2.202209
C	0	-1.572909	2.930050	-2.696354
C	0	-0.401892	3.681559	0.416532
C	0	3.210685	-2.624316	-0.910084
C	0	0.175642	-2.928224	-2.606175
C	0	1.401247	0.607567	-1.266062
C	0	2.267102	1.363105	-0.491768
C	0	1.906417	0.394101	-2.589111
C	0	3.534474	1.825343	-0.938428
C	0	2.573422	1.882537	0.879097
C	0	3.134819	0.857210	-3.036089
C	0	4.007182	1.590991	-2.204034
C	0	2.187751	1.978289	2.191944
C	0	3.825110	2.362056	0.423736
C	0	3.099420	2.624397	3.057967
C	0	4.720536	2.979747	1.258844
C	0	4.316581	3.111814	2.607836
H	0	-0.005783	0.360545	-1.658701
H	0	-0.288753	-3.973695	1.722816
H	0	0.552444	-2.629924	2.468404
H	0	-4.130549	1.401349	0.903070
H	0	-4.036001	0.258218	-0.419918
H	0	-2.133091	-3.569877	3.398489
H	0	-4.319105	-2.455667	3.747508
H	0	-4.920355	-0.483569	2.370524
H	0	1.460130	-5.008219	-1.379620
H	0	0.254064	-5.366999	-0.130722
H	0	-0.145377	-5.564953	-1.834059
H	0	3.747224	-4.104853	1.300745
H	0	2.161901	-4.095177	2.057358
H	0	2.395763	-4.889815	0.497469
H	0	-4.040824	3.514651	-1.545687
H	0	-4.257502	2.759589	-3.117970
H	0	-4.722943	1.890803	-1.662591
H	0	-2.703065	4.799053	1.483331
H	0	-2.851831	4.592561	-0.255715
H	0	-3.845708	3.620218	0.845844
H	0	2.350209	-1.513345	2.254557
H	0	3.960488	-1.748034	1.575083
H	0	2.846652	-0.593831	0.835781
H	0	-1.957424	-3.967566	-0.090177

H	0	-2.081726	-2.533857	-1.115203
H	0	-2.080884	-4.154973	-1.842186
H	0	-1.601393	0.255272	-3.039908
H	0	-3.206048	-0.113129	-2.417172
H	0	-3.035747	0.886321	-3.864743
H	0	-1.338694	3.276992	2.877117
H	0	-2.619668	2.101176	2.557919
H	0	-0.938310	1.652187	2.285002
H	0	-1.634265	3.929248	-2.258071
H	0	-0.538096	2.582284	-2.608600
H	0	-1.796497	3.032283	-3.764132
H	0	-0.144143	4.423706	1.180713
H	0	0.408953	2.954636	0.377916
H	0	-0.433872	4.199719	-0.543572
H	0	4.281554	-2.682510	-0.683798
H	0	2.979100	-3.457421	-1.578869
H	0	3.041231	-1.689640	-1.450710
H	0	1.245497	-2.825113	-2.802490
H	0	-0.240923	-3.588626	-3.375572
H	0	-0.285163	-1.942385	-2.717251
H	0	1.294881	-0.171175	-3.290283
H	0	3.432159	0.640841	-4.058193
H	0	4.975563	1.928166	-2.557667
H	0	1.246378	1.578691	2.556642
H	0	2.842350	2.738413	4.106449
H	0	5.688091	3.345021	0.930464
H	0	4.982098	3.599496	3.313083

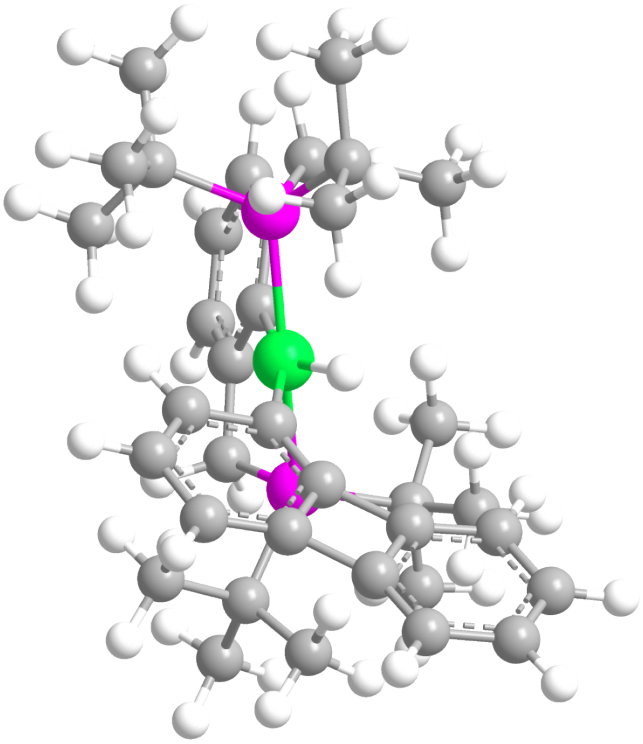
Sum of electronic and zero-point Energies= -2189.082174
Sum of electronic and thermal Energies= -2189.039117
Sum of electronic and thermal Enthalpies= -2189.038173
Sum of electronic and thermal Free Energies= -2189.153363

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
65.6853659 42.9858395 24.4800202
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-629.1496	19.4381	31.5694

Red. masses	--	1.0900	4.6005	3.6446
Frc consts	--	0.2542	0.0010	0.0021
IR Inten	--	536.7956	0.0529	0.0091

TS-1-C1-syn



Charge = 0 Multiplicity = 1

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P 0	2.156659	-1.461351	-0.365110
C 0	0.750998	3.220132	0.889021
C 0	-1.057413	2.941957	-1.437109
C 0	-1.994757	2.491016	1.503240
C 0	3.328159	-0.412920	-1.337739
C 0	3.210181	-1.992199	1.140143
C 0	1.809689	-2.939426	-1.497390
C 0	2.057252	2.703641	0.359135
C 0	3.185327	3.526412	0.322312
C 0	4.379074	3.060097	-0.213563
C 0	3.316768	0.950933	-0.711759
C 0	4.439848	1.774331	-0.743562
C 0	-1.727802	4.310586	-1.335829
C 0	-2.056736	3.951972	1.962678
C 0	3.051316	-3.782785	-1.786695
C 0	4.691845	-2.166113	0.795983
C 0	-1.662795	1.628196	2.726786
C 0	0.237336	3.097928	-2.242058

C	0	1.284409	-2.366440	-2.821359
C	0	3.101486	-0.877921	2.189793
C	0	0.701105	-3.814496	-0.904786
C	0	2.681291	-3.289912	1.754304
C	0	-3.359834	2.065018	0.963231
C	0	-1.961741	1.968387	-2.192573
C	0	-1.164715	-1.178008	0.732703
C	0	-2.487420	-1.407201	0.398786
C	0	-0.809555	-1.797427	1.979896
C	0	-3.419948	-2.078673	1.238049
C	0	-3.546724	-1.277514	-0.654206
C	0	-1.711569	-2.453992	2.797804
C	0	-3.074194	-2.613255	2.448261
C	0	-3.882187	-0.910587	-1.934868
C	0	-4.478350	-1.916277	0.204285
C	0	-5.218393	-1.162165	-2.324288
C	0	-5.774230	-2.165954	-0.166509
C	0	-6.133372	-1.757632	-1.471366
H	0	-0.586574	-0.987462	-0.612947
H	0	0.596925	4.282304	0.659652
H	0	0.710107	3.135478	1.982373
H	0	4.329715	-0.840625	-1.441156
H	0	2.902061	-0.348669	-2.344607
H	0	3.127738	4.540189	0.712512
H	0	5.255146	3.700768	-0.234701
H	0	5.362766	1.416076	-1.194411
H	0	-2.722168	4.263377	-0.887432
H	0	-1.127148	5.027648	-0.768233
H	0	-1.850033	4.723855	-2.343697
H	0	-2.861346	4.052763	2.700184
H	0	-1.135089	4.270852	2.455251
H	0	-2.269588	4.654661	1.157722
H	0	3.411016	-4.317616	-0.904995
H	0	2.812161	-4.537854	-2.544525
H	0	3.876156	-3.180880	-2.180425
H	0	5.220812	-2.539370	1.680425
H	0	4.868354	-2.879364	-0.011683
H	0	5.158906	-1.216261	0.524261
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H	0	-2.349346	1.882117	3.542495
H	0	-1.767923	0.564257	2.516787
H	0	0.930726	3.815253	-1.795155
H	0	0.762950	2.145655	-2.348478
H	0	-0.017916	3.464963	-3.242882

H	0	0.496029	-1.623457	-2.659843
H	0	2.072618	-1.902818	-3.418801
H	0	0.862411	-3.180368	-3.420446
H	0	3.668084	-1.172739	3.081301
H	0	3.509822	0.068379	1.828110
H	0	2.065777	-0.688630	2.485592
H	0	0.975136	-4.276804	0.043449
H	0	-0.219632	-3.248684	-0.743627
H	0	0.470433	-4.623312	-1.607134
H	0	3.196568	-3.468767	2.704860
H	0	1.610407	-3.248503	1.967300
H	0	2.867259	-4.160759	1.121497
H	0	-4.095592	2.088062	1.775251
H	0	-3.726858	2.731377	0.178725
H	0	-3.346040	1.047308	0.567025
H	0	-2.914283	1.790976	-1.688949
H	0	-2.183310	2.367097	-3.189599
H	0	-1.457699	1.004374	-2.313561
H	0	0.210300	-1.691571	2.334972
H	0	-1.356054	-2.854599	3.743256
H	0	-3.765642	-3.141305	3.095851
H	0	-3.181169	-0.463117	-2.629956
H	0	-5.535898	-0.882662	-3.324006
H	0	-6.493784	-2.656128	0.481041
H	0	-7.147437	-1.926482	-1.819275

Sum of electronic and zero-point Energies=	-2189.082922
Sum of electronic and thermal Energies=	-2189.040151
Sum of electronic and thermal Enthalpies=	-2189.039207
Sum of electronic and thermal Free Energies=	-2189.153625

****** 1 imaginary frequencies (negative Signs) ******

Diagonal vibrational polarizability:

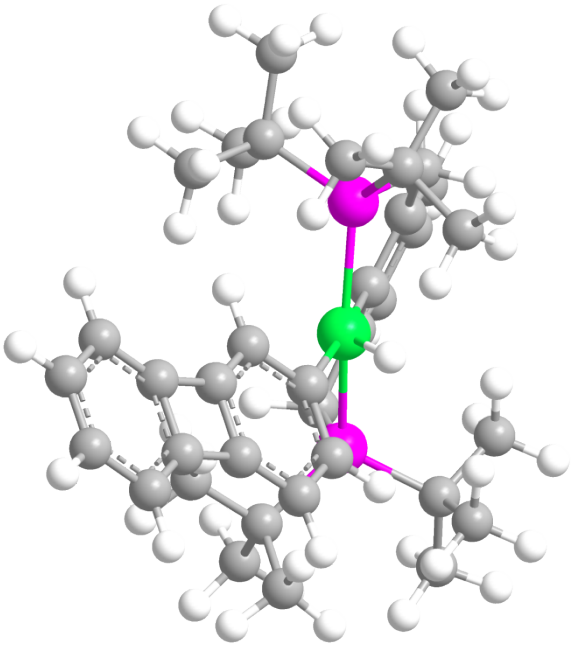
67.8972598 47.5680423 31.5939905

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-648.4543	19.4752	24.6596
Red. masses --	1.1018	4.2788	4.9475

Frc consts	--	0.2730	0.0010	0.0018
IR Inten	--	667.2228	0.2884	0.1839

TS-1-C2-anti



Charge = 0 Multiplicity = 1

Ir	0	0.653627	0.042750	0.157922
C	0	2.641062	0.463892	-0.388776
P	0	1.453758	-2.151178	-0.171469
P	0	0.617669	2.377826	0.239488
C	0	2.851623	-1.822925	-1.347576
C	0	2.309903	-2.946464	1.324458
C	0	0.463488	-3.457584	-1.147064
C	0	2.390763	2.722420	0.643095
C	0	0.391044	3.288460	-1.426568
C	0	-0.304522	3.312706	1.618178
C	0	3.461583	-0.493813	-1.020875
C	0	4.800646	-0.230015	-1.308781
C	0	5.363258	0.992520	-0.960552
C	0	3.242328	1.695109	-0.043888
C	0	4.584221	1.951187	-0.321283
C	0	2.927566	-4.312880	1.030926
C	0	1.364903	-4.374093	-1.983881
C	0	0.397379	4.610981	2.032295
C	0	0.478633	4.809639	-1.303424
C	0	-0.438465	-2.663661	-2.099636
C	0	3.426513	-1.997445	1.774460
C	0	-0.324811	2.381186	2.835965
C	0	1.500113	2.827517	-2.379353

C 0	-1.751185	3.614756	1.226077
C 0	-0.941525	2.903235	-2.069072
C 0	-0.417144	-4.332334	-0.254713
C 0	1.306391	-3.062644	2.472987
C 0	-2.418506	0.275954	-0.148618
C 0	-3.716422	-0.157389	-0.095183
C 0	-1.423182	-0.495738	0.531994
C 0	-4.119967	-1.298067	0.642646
C 0	-5.133848	0.066643	-0.517319
C 0	-1.867649	-1.591798	1.290137
C 0	-3.209851	-2.029608	1.359513
C 0	-6.027201	0.831432	-1.221799
C 0	-5.532949	-1.074190	0.225936
C 0	-7.377343	0.413233	-1.165197
C 0	-6.841191	-1.483998	0.287113
C 0	-7.767676	-0.700583	-0.438960
H 0	-0.208651	-0.058289	1.492651
H 0	3.585917	-2.637391	-1.359372
H 0	2.400334	-1.801800	-2.347581
H 0	2.689661	3.751063	0.406845
H 0	2.472303	2.616782	1.732803
H 0	5.409638	-0.986068	-1.799587
H 0	6.406674	1.195705	-1.180762
H 0	5.024696	2.904388	-0.036976
H 0	2.182149	-5.079285	0.809865
H 0	3.639717	-4.277423	0.201392
H 0	3.483756	-4.650839	1.912988
H 0	0.734776	-5.111088	-2.494582
H 0	1.910546	-3.833453	-2.759472
H 0	2.089056	-4.929494	-1.386149
H 0	0.491700	5.333138	1.221760
H 0	-0.187853	5.090082	2.825416
H 0	1.394351	4.428881	2.439919
H 0	0.456593	5.248121	-2.307812
H 0	-0.356396	5.241600	-0.748623
H 0	1.410314	5.137534	-0.834025
H 0	0.131764	-1.966974	-2.723959
H 0	-0.957240	-3.356595	-2.772021
H 0	-1.188649	-2.083818	-1.558248
H 0	4.237962	-1.929036	1.045880
H 0	3.051630	-0.985807	1.951370
H 0	3.852615	-2.377275	2.710119
H 0	-0.981851	1.523853	2.677927
H 0	0.669612	1.999118	3.087753

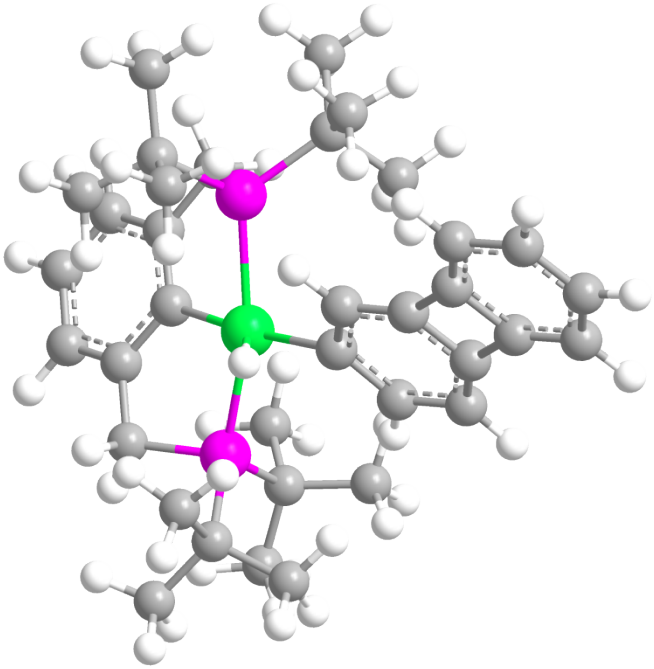
H	0	-0.699139	2.933110	3.705576
H	0	1.314051	3.270774	-3.364414
H	0	2.494973	3.143810	-2.058651
H	0	1.519022	1.741158	-2.494143
H	0	-1.827164	4.358826	0.430049
H	0	-2.287071	2.715251	0.912215
H	0	-2.282158	4.019940	2.094923
H	0	-1.043910	3.427642	-3.026067
H	0	-0.979124	1.830313	-2.276609
H	0	-1.808387	3.168957	-1.459900
H	0	-1.039323	-4.972406	-0.890810
H	0	0.164560	-4.994671	0.390580
H	0	-1.092063	-3.743721	0.366546
H	0	0.469971	-3.727018	2.243495
H	0	1.811456	-3.466430	3.357845
H	0	0.905251	-2.079916	2.738164
H	0	-2.134256	1.148957	-0.719563
H	0	-1.130487	-2.144056	1.864112
H	0	-3.475390	-2.896905	1.957472
H	0	-5.739956	1.706745	-1.795350
H	0	-8.129369	0.979640	-1.705204
H	0	-7.168456	-2.351674	0.850230
H	0	-8.816706	-0.979238	-0.427845

Sum of electronic and zero-point Energies= -2189.077348
Sum of electronic and thermal Energies= -2189.034781
Sum of electronic and thermal Enthalpies= -2189.033837
Sum of electronic and thermal Free Energies= -2189.148431

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
92.5568321 30.6353874 42.0165092
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-553.2375	15.1809	24.1060
Red. masses --	1.0922	4.8396	4.3270
Frc consts --	0.1970	0.0007	0.0015
IR Inten --	665.2783	0.0290	0.3090

TS-1-C2-syn



Charge = 0 Multiplicity = 1

Ir	0	-0.664437	0.028990	0.069390
C	0	-2.552588	0.944287	-0.105186
P	0	-0.003845	2.291326	-0.154385
P	0	-2.045917	-1.847045	0.204334
C	0	-1.472639	2.971546	-1.061930
C	0	0.025639	3.290786	1.459043
C	0	1.412144	2.854322	-1.309185
C	0	-3.575463	-1.088800	0.917337
C	0	-2.674380	-2.565228	-1.452106
C	0	-1.682937	-3.259796	1.427765
C	0	-2.705987	2.253231	-0.607338
C	0	-3.954145	2.874184	-0.656771
C	0	-5.084074	2.211208	-0.192236
C	0	-3.718560	0.298570	0.363845
C	0	-4.962924	0.925841	0.325031
C	0	0.297093	4.781243	1.258395
C	0	1.106825	4.191798	-1.997007
C	0	-2.955090	-3.905382	1.988795
C	0	-3.647558	-3.731013	-1.277254
C	0	1.517081	1.769327	-2.387502
C	0	-1.345036	3.135153	2.127366
C	0	-0.917719	-2.636046	2.600819
C	0	-3.404445	-1.449729	-2.209192

C 0	-0.795485	-4.334874	0.799663
C 0	-1.499104	-3.006152	-2.324434
C 0	2.764108	2.983260	-0.605670
C 0	1.072872	2.690425	2.398677
C 0	2.481093	-0.212172	0.619663
C 0	3.719446	-0.699813	0.298913
C 0	1.335406	-0.817917	0.015750
C 0	3.906492	-1.796767	-0.574659
C 0	5.200397	-0.579351	0.464530
C 0	1.553819	-1.951509	-0.784577
C 0	2.832092	-2.451614	-1.121887
C 0	6.251827	0.084941	1.039821
C 0	5.384684	-1.680345	-0.411598
C 0	7.541132	-0.395608	0.708016
C 0	6.631093	-2.152674	-0.735577
C 0	7.721883	-1.471941	-0.144980
H 0	0.281476	-0.553695	1.210912
H 0	-1.554048	4.060561	-0.963301
H 0	-1.283722	2.772653	-2.124370
H 0	-4.469511	-1.704881	0.761223
H 0	-3.408714	-1.049919	2.001771
H 0	-4.042971	3.883578	-1.052480
H 0	-6.054681	2.696193	-0.227041
H 0	-5.843170	0.408551	0.700523
H 0	1.302796	4.986560	0.886658
H 0	-0.421783	5.245805	0.577283
H 0	0.199798	5.295307	2.221630
H 0	1.969052	4.470350	-2.613341
H 0	0.246300	4.135292	-2.665857
H 0	0.936293	5.009454	-1.294896
H 0	-3.591387	-4.351373	1.224987
H 0	-2.667769	-4.707113	2.678537
H 0	-3.559422	-3.197244	2.560355
H 0	-4.050379	-4.006451	-2.258774
H 0	-3.173101	-4.623762	-0.865506
H 0	-4.501242	-3.471556	-0.644789
H 0	0.557097	1.587055	-2.882980
H 0	2.228734	2.088515	-3.157561
H 0	1.860106	0.817896	-1.976616
H 0	-2.145764	3.615520	1.559954
H 0	-1.614314	2.083756	2.258587
H 0	-1.308036	3.609079	3.115006
H 0	0.091394	-2.338078	2.310516
H 0	-1.422501	-1.755094	3.009839

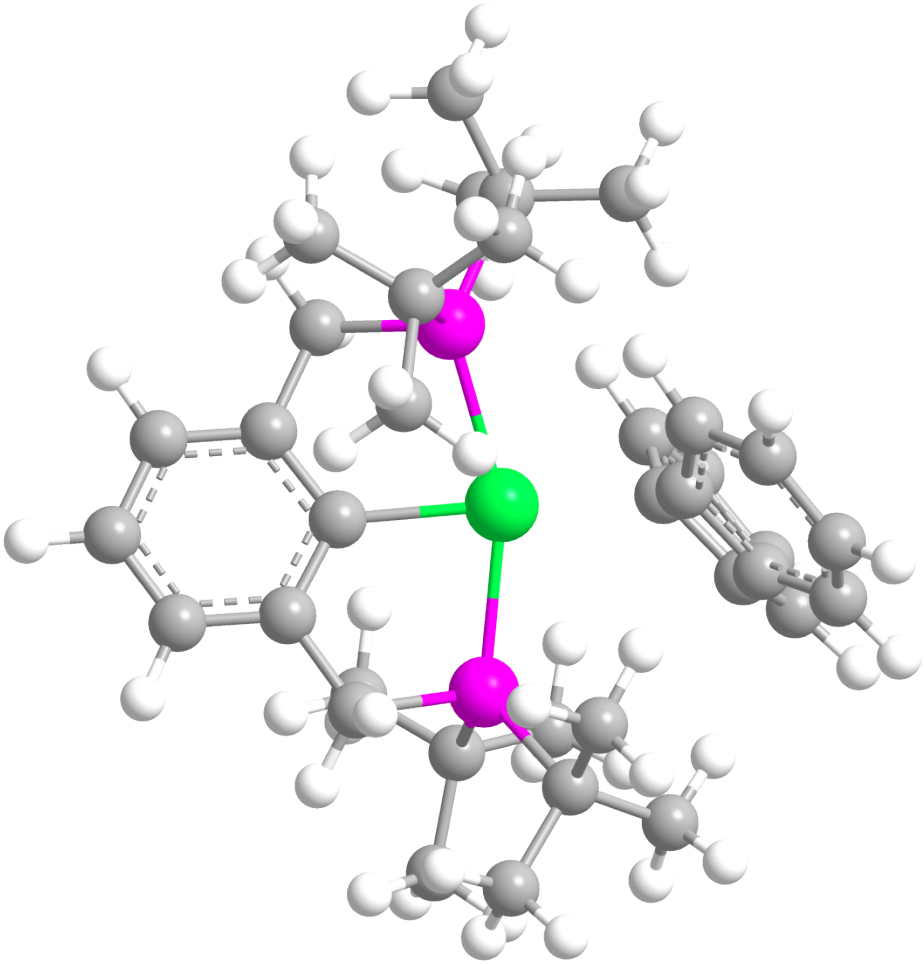
H	0	-0.829842	-3.373583	3.406589
H	0	-3.681376	-1.829646	-3.199313
H	0	-4.321540	-1.127449	-1.711402
H	0	-2.775414	-0.567272	-2.348076
H	0	-1.307169	-4.904048	0.020270
H	0	0.119778	-3.911969	0.377313
H	0	-0.494572	-5.050203	1.573554
H	0	-1.883555	-3.397859	-3.273194
H	0	-0.845817	-2.160873	-2.557071
H	0	-0.895268	-3.794731	-1.869736
H	0	3.532590	3.196585	-1.357470
H	0	2.786829	3.805383	0.113327
H	0	3.062845	2.067413	-0.097420
H	0	2.089821	2.763916	2.006234
H	0	1.052753	3.224670	3.355336
H	0	0.854471	1.637576	2.601341
H	0	2.349099	0.615283	1.308628
H	0	0.695727	-2.452204	-1.211902
H	0	2.927451	-3.309278	-1.781849
H	0	6.128350	0.928284	1.711693
H	0	8.412717	0.091609	1.133319
H	0	6.796032	-2.993009	-1.401656
H	0	8.731709	-1.802342	-0.367117

Sum of electronic and zero-point Energies= -2189.076561
Sum of electronic and thermal Energies= -2189.034049
Sum of electronic and thermal Enthalpies= -2189.033105
Sum of electronic and thermal Free Energies= -2189.147360

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
76.1622075 34.6921320 38.6233659
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-574.0129	18.3264	23.9073
Red. masses --	1.0819	5.0842	4.1970
Frc consts --	0.2100	0.0010	0.0014
IR Inten --	608.4047	0.0986	0.3675

TS-3-PtBu2



Charge = 0 Multiplicity = 1

Ir	0	0.103111	-0.057814	0.104650
C	0	0.706284	-2.041300	0.191000
P	0	-1.962957	-1.139246	-0.209518
P	0	2.475205	0.157160	0.182602
C	0	-1.425382	-2.775705	-0.860900
C	0	-2.885226	-1.602335	1.391835
C	0	-3.221345	-0.670109	-1.571631
C	0	2.858199	-1.321038	1.208878
C	0	3.318044	-0.247284	-1.517855
C	0	3.531458	1.481958	1.075788
C	0	-0.089248	-3.105163	-0.288833
C	0	0.346267	-4.429849	-0.258771
C	0	1.599097	-4.756082	0.241957
C	0	1.975739	-2.412165	0.702484
C	0	2.411320	-3.735739	0.720461

C 0	-4.153095	-2.427446	1.180304
C 0	-4.024086	-1.867348	-2.100585
C 0	5.044534	1.334205	0.887359
C 0	4.513355	-1.187933	-1.334370
C 0	-2.387548	-0.139054	-2.744888
C 0	-1.911482	-2.421658	2.246747
C 0	3.291889	1.328385	2.587691
C 0	2.299247	-0.955592	-2.421461
C 0	3.078509	2.871322	0.623877
C 0	3.784273	1.000248	-2.280312
C 0	-4.222644	0.382892	-1.094284
C 0	-3.225022	-0.329648	2.163961
H 0	-2.170112	-3.560188	-0.682017
H 0	-1.348268	-2.662701	-1.949520
H 0	3.919410	-1.590471	1.223838
H 0	2.573158	-1.054848	2.231085
H 0	-0.306755	-5.211452	-0.641041
H 0	1.937506	-5.786965	0.258767
H 0	3.398303	-3.964180	1.117401
H 0	-4.950798	-1.858642	0.697730
H 0	-3.974398	-3.334850	0.596267
H 0	-4.535489	-2.747700	2.156651
H 0	-4.705768	-1.504873	-2.879121
H 0	-3.393061	-2.626813	-2.565401
H 0	-4.636188	-2.351897	-1.340747
H 0	5.390306	1.517759	-0.128904
H 0	5.550013	2.062869	1.532783
H 0	5.395387	0.344773	1.193284
H 0	4.959413	-1.386256	-2.315700
H 0	5.300185	-0.773742	-0.701246
H 0	4.208248	-2.153234	-0.923210
H 0	-1.731856	-0.916360	-3.150568
H 0	-3.056219	0.179000	-3.553670
H 0	-1.755662	0.704440	-2.474744
H 0	-1.679071	-3.394916	1.806762
H 0	-0.968374	-1.890014	2.400602
H 0	-2.370548	-2.601260	3.225900
H 0	2.266197	1.068214	2.849249
H 0	3.931805	0.550788	3.011459
H 0	3.540040	2.267223	3.094252
H 0	2.760431	-1.115943	-3.404124
H 0	2.001058	-1.928148	-2.026637
H 0	1.390018	-0.361181	-2.555151
H 0	3.276298	3.047487	-0.436636

H	0	2.008579	3.027506	0.791862
H	0	3.618180	3.642393	1.185734
H	0	4.299122	0.670214	-3.189745
H	0	2.953758	1.624284	-2.613004
H	0	4.483954	1.630735	-1.733825
H	0	-4.776567	0.777685	-1.954300
H	0	-4.957341	-0.046022	-0.407333
H	0	-3.753503	1.226940	-0.591919
H	0	-3.913810	0.325696	1.626714
H	0	-3.700001	-0.597656	3.115205
H	0	-2.322515	0.241959	2.392586
C	0	-0.234608	2.143763	2.236160
C	0	-0.735836	1.956846	0.952196
C	0	-1.113779	2.617605	3.228439
C	0	-2.023315	2.497109	0.653859
C	0	-0.436940	2.094041	-0.682297
C	0	-2.406423	3.025724	2.934341
C	0	-2.859571	3.033362	1.601130
C	0	0.481325	2.417355	-1.670963
C	0	-1.753683	2.622692	-0.781195
C	0	0.004273	3.042685	-2.838775
C	0	-2.209639	3.307614	-1.880840
C	0	-1.313282	3.458888	-2.957311
H	0	0.781791	1.895166	2.494488
H	0	-0.760080	2.669424	4.253740
H	0	-3.046285	3.398419	3.727332
H	0	-3.805008	3.495878	1.332740
H	0	1.525694	2.167433	-1.576046
H	0	0.694879	3.212970	-3.659643
H	0	-3.199835	3.752415	-1.909637
H	0	-1.639414	3.954126	-3.866027

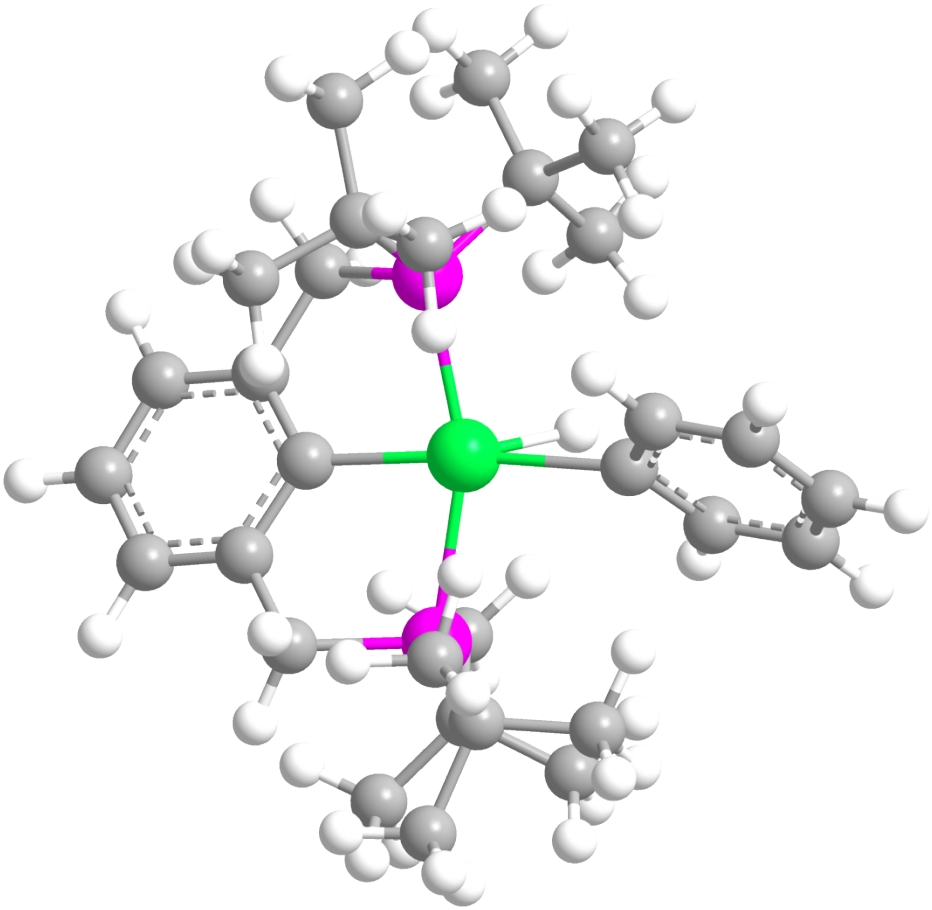
Sum of electronic and zero-point Energies= -2189.069778
Sum of electronic and thermal Energies= -2189.027428
Sum of electronic and thermal Enthalpies= -2189.026484
Sum of electronic and thermal Free Energies= -2189.138222

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
36.9844555 65.0189832 29.8576581
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized

incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-219.3248	22.7021	45.4746
Red. masses --	7.5527	4.0560	3.9114
Frc consts --	0.2141	0.0012	0.0048
IR Inten --	70.4053	0.2388	0.1421

TS-benzene addition



Charge = 0 Multiplicity = 1

Ir 0	−0.072831	0.081359	−0.101293
C 0	−0.267770	−2.001800	0.032845
P 0	−2.369903	−0.106565	−0.118319
P 0	2.208087	−0.496561	0.164012
C 0	−2.613019	−1.800770	−0.818452
C 0	−1.441615	−2.651718	−0.412921
C 0	−1.515309	−4.042723	−0.487049
C 0	−0.427580	−4.826547	−0.118401
C 0	0.733430	−4.216322	0.345166
C 0	0.808469	−2.826893	0.432536
C 0	2.021948	−2.147291	0.992639
C 0	−3.148883	−0.218697	1.617217
C 0	−3.436113	0.981343	−1.250476
C 0	3.181532	−0.922596	−1.422688
C 0	3.287529	0.438276	1.419309
C 0	4.600286	−0.294321	1.698635

C 0	3.581022	1.881671	1.001700
C 0	2.458504	0.523623	2.710153
C 0	4.079537	-2.151443	-1.264015
C 0	4.031868	0.259572	-1.887486
C 0	2.136327	-1.228200	-2.502157
C 0	-2.628561	1.209743	-2.535083
C 0	-4.763665	0.327515	-1.647747
C 0	-3.688555	2.341830	-0.600176
C 0	-2.719334	0.992995	2.445448
C 0	-2.589744	-1.467018	2.309703
C 0	-4.672895	-0.326858	1.605718
C 0	0.345823	2.239530	-0.244357
C 0	-0.166687	3.069311	0.769790
C 0	0.209924	4.405092	0.885942
C 0	1.074177	4.982367	-0.040142
C 0	1.550339	4.203695	-1.088941
C 0	1.187159	2.864333	-1.184902
H 0	-0.213357	1.164929	-1.249967
H 0	-3.577335	-2.244077	-0.538602
H 0	-2.637119	-1.674851	-1.908720
H 0	-2.426927	-4.517841	-0.843212
H 0	-0.486320	-5.908346	-0.186250
H 0	1.581370	-4.825640	0.650910
H 0	2.925023	-2.760607	0.936810
H 0	1.860058	-1.935211	2.054556
H 0	5.273581	-0.277565	0.837413
H 0	5.125845	0.198724	2.524776
H 0	4.446817	-1.337388	1.990267
H 0	2.668865	2.475458	0.943547
H 0	4.221340	2.338112	1.765574
H 0	4.102912	1.969546	0.049547
H 0	1.456744	0.921928	2.512557
H 0	2.354303	-0.435907	3.220996
H 0	2.956098	1.205580	3.408090
H 0	4.661783	-2.286569	-2.182654
H 0	4.790974	-2.062153	-0.439402
H 0	3.497513	-3.064861	-1.118740
H 0	4.889969	0.438944	-1.235005
H 0	4.425780	0.043789	-2.887201
H 0	3.455787	1.185689	-1.955762
H 0	1.474289	-2.048103	-2.210665
H 0	1.503250	-0.360620	-2.707328
H 0	2.649391	-1.514306	-3.428413
H 0	-1.771230	1.863645	-2.366206

H	0	-2.258567	0.277507	-2.973063
H	0	-3.270546	1.692978	-3.280172
H	0	-5.420179	0.124958	-0.802732
H	0	-5.303842	1.002017	-2.321860
H	0	-4.612692	-0.609293	-2.190199
H	0	-2.755839	2.810717	-0.270782
H	0	-4.152794	3.015212	-1.329602
H	0	-4.365013	2.279878	0.255608
H	0	-3.036766	1.944699	2.013526
H	0	-3.157264	0.923310	3.447958
H	0	-1.631206	1.014375	2.556058
H	0	-2.888984	-2.396356	1.818850
H	0	-1.498237	-1.453973	2.357289
H	0	-2.975728	-1.496243	3.335170
H	0	-5.025573	-0.500041	2.629020
H	0	-5.160614	0.582893	1.249853
H	0	-5.025679	-1.166838	1.000133
H	0	-0.845572	2.656067	1.508020
H	0	-0.180611	5.000778	1.707110
H	0	1.359317	6.025794	0.047722
H	0	2.210233	4.638500	-1.834919
H	0	1.573134	2.276830	-2.016608

Sum of electronic and zero-point Energies= -1959.321234
Sum of electronic and thermal Energies= -1959.282291
Sum of electronic and thermal Enthalpies= -1959.281347
Sum of electronic and thermal Free Energies= -1959.388443

****** 1 imaginary frequencies (negative Signs) ******
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-703.3077	22.0711	25.6347
Red. masses --	1.0606	4.1074	4.0876
Frc consts --	0.3091	0.0012	0.0016
IR Inten --	546.4811	0.3218	0.0585

3. Optimized geometries and absolute energies of tMe4 species

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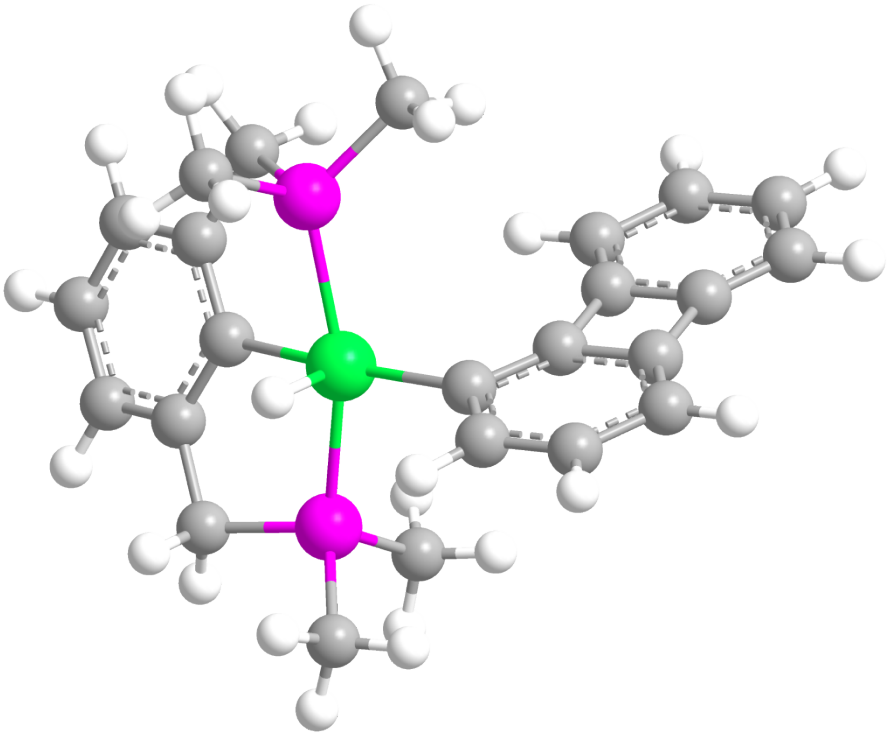
1-C1-anti



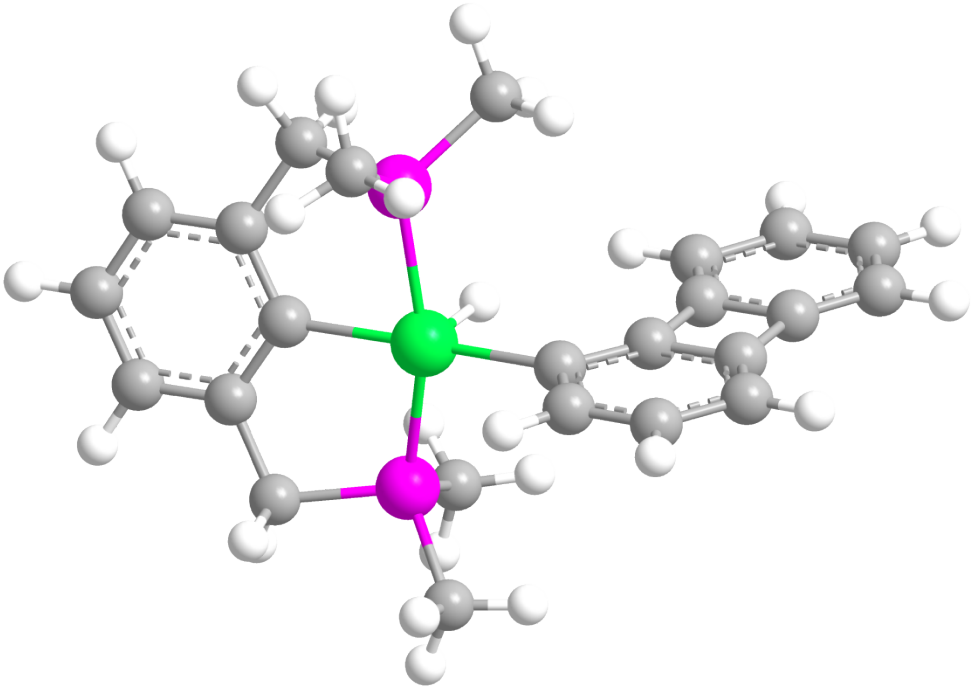
Charge = 0 Multiplicity = 1

Ir 0	0.506915	-0.313526	-0.426197
C 0	2.363574	0.400838	0.302874
P 0	0.549414	1.762043	-1.441005
P 0	1.169447	-2.169407	0.742049
C 0	1.695930	2.729176	-0.361670
C 0	1.362515	1.797691	-3.073801
C 0	-0.910669	2.829837	-1.673213
C 0	2.991662	-1.947802	0.919577
C 0	0.546846	-2.241846	2.458155
C 0	0.928376	-3.867980	0.131328
C 0	2.694515	1.776901	0.251908
C 0	3.898286	2.247926	0.776355
C 0	4.790753	1.370259	1.382358
C 0	3.299339	-0.470446	0.913051
C 0	4.488622	0.013765	1.454947
C 0	-1.456432	-0.917688	-0.902730
C 0	-2.484958	-0.341351	-0.176730
C 0	-1.960358	-1.884358	-1.825701
C 0	-3.865196	-0.635759	-0.303500

C	0	-2.795199	0.652585	0.895514
C	0	-3.309308	-2.191302	-1.970761
C	0	-4.320143	-1.565901	-1.203641
C	0	-2.321901	1.566066	1.803559
C	0	-4.180405	0.365648	0.763960
C	0	-3.298062	2.219195	2.597720
C	0	-5.128725	0.992347	1.528349
C	0	-4.647191	1.943930	2.463037
H	0	0.998156	-0.968954	-1.739442
H	0	2.171868	3.551740	-0.909383
H	0	1.074982	3.198482	0.413741
H	0	0.777233	1.224324	-3.794484
H	0	1.477222	2.821655	-3.439380
H	0	2.347230	1.335360	-2.986486
H	0	-1.599686	2.350202	-2.371377
H	0	-0.635139	3.814384	-2.061645
H	0	-1.436378	2.951426	-0.724019
H	0	3.383684	-2.465397	1.803044
H	0	3.446629	-2.435462	0.046653
H	0	-0.541588	-2.331309	2.451428
H	0	0.809822	-1.316176	2.974479
H	0	0.972994	-3.085749	3.007651
H	0	-0.141013	-4.083046	0.085560
H	0	1.330752	-3.952794	-0.879612
H	0	1.415708	-4.606352	0.773906
H	0	4.137808	3.307769	0.723509
H	0	5.722174	1.742443	1.797300
H	0	5.192686	-0.669968	1.924169
H	0	-1.254058	-2.416901	-2.461800
H	0	-3.598913	-2.940137	-2.703854
H	0	-5.366480	-1.820277	-1.337965
H	0	-1.263685	1.787246	1.931311
H	0	-2.979951	2.951787	3.333065
H	0	-6.191474	0.788822	1.444849
H	0	-5.357196	2.468490	3.094661

Sum of electronic and zero-point Energies=	-1717.634807
Sum of electronic and thermal Energies=	-1717.606465
Sum of electronic and thermal Enthalpies=	-1717.605521
Sum of electronic and thermal Free Energies=	-1717.694478

1-C1-syn



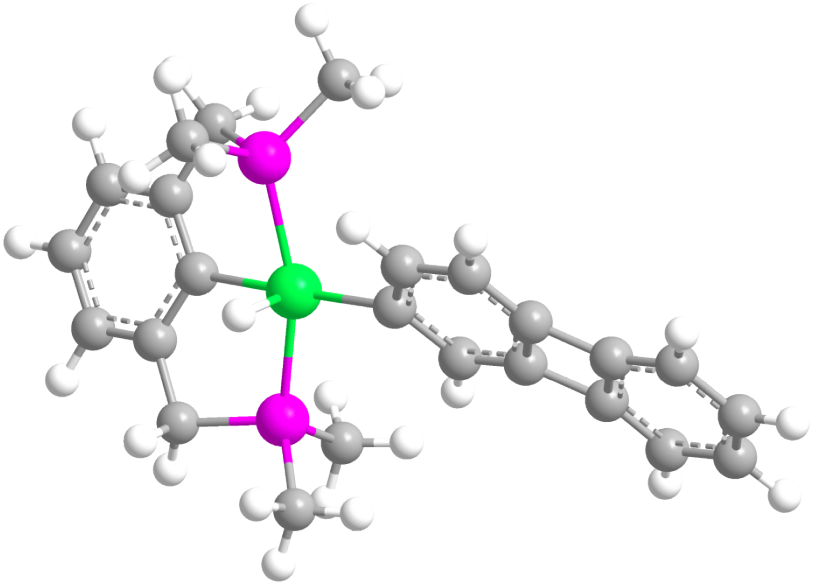
Charge = 0 Multiplicity = 1

Ir 0	0.563103	-0.034903	-0.352855
C 0	2.563405	0.072414	0.330581
P 0	0.960646	-2.278355	0.002158
P 0	0.779867	2.246927	-0.304407
C 0	2.804198	-2.400611	-0.045373
C 0	0.504960	-2.859010	1.669683
C 0	0.358510	-3.615399	-1.083115
C 0	2.241190	2.521149	0.788808
C 0	1.229809	3.054023	-1.880849
C 0	-0.549683	3.303231	0.350394
C 0	3.388349	-1.076888	0.389510
C 0	4.712759	-0.991425	0.818723
C 0	5.253903	0.236459	1.184367
C 0	3.132740	1.303438	0.739316
C 0	4.464597	1.381648	1.143851
C 0	-1.398596	-0.129194	-1.137666
C 0	-2.575758	-0.075333	-0.414891
C 0	-1.662468	-0.242583	-2.540073
C 0	-3.884145	-0.118056	-0.959992
C 0	-3.155991	0.034331	0.960132
C 0	-2.935130	-0.286174	-3.098510
C 0	-4.106820	-0.223353	-2.309345

C	0	-2.938255	0.139325	2.311130
C	0	-4.466121	-0.006928	0.412783
C	0	-4.094839	0.207092	3.126929
C	0	-5.589046	0.058594	1.195098
C	0	-5.370044	0.168918	2.590698
H	0	-0.057283	0.040607	1.060708
H	0	3.170589	-3.244032	0.552476
H	0	3.075647	-2.624671	-1.086027
H	0	0.808411	-3.896549	1.833005
H	0	-0.575389	-2.773919	1.804339
H	0	0.992471	-2.221879	2.409819
H	0	0.636279	-3.407760	-2.118086
H	0	-0.731631	-3.651451	-1.033502
H	0	0.762985	-4.589518	-0.794233
H	0	2.767608	3.450398	0.540798
H	0	1.843014	2.655346	1.803847
H	0	1.407868	4.124494	-1.746929
H	0	0.427286	2.915011	-2.608169
H	0	2.137642	2.593754	-2.276153
H	0	-1.413146	3.241133	-0.315219
H	0	-0.239359	4.347593	0.442532
H	0	-0.861126	2.930769	1.327973
H	0	5.330948	-1.885663	0.860143
H	0	6.287978	0.300209	1.508134
H	0	4.887116	2.337104	1.447268
H	0	-0.818160	-0.298665	-3.230936
H	0	-3.031898	-0.371964	-4.177965
H	0	-5.092605	-0.258031	-2.761756
H	0	-1.946274	0.168367	2.754070
H	0	-3.978717	0.291002	4.203282
H	0	-6.597041	0.029069	0.793637
H	0	-6.224936	0.224169	3.257390

Sum of electronic and zero-point Energies=	-1717.633149
Sum of electronic and thermal Energies=	-1717.605019
Sum of electronic and thermal Enthalpies=	-1717.604075
Sum of electronic and thermal Free Energies=	-1717.692204

1-C2-anti



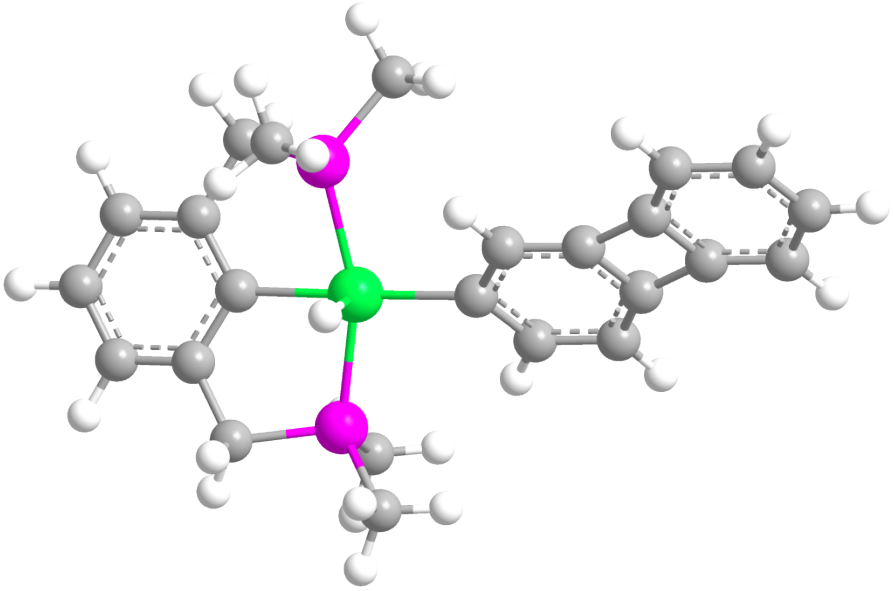
Charge = 0 Multiplicity = 1

Ir 0	0.859889	-0.080225	0.098291
C 0	2.934053	0.290637	-0.187614
P 0	1.630511	-2.243446	-0.133681
P 0	0.877019	2.207042	0.346614
C 0	3.196580	-2.031345	-1.089289
C 0	2.175890	-3.040318	1.415069
C 0	0.736934	-3.580770	-0.996594
C 0	2.625465	2.565306	0.808440
C 0	0.642541	3.195054	-1.175966
C 0	-0.145562	3.082526	1.573988
C 0	3.795771	-0.696215	-0.722484
C 0	5.152656	-0.441282	-0.920188
C 0	5.684835	0.804752	-0.606221
C 0	3.511563	1.538496	0.149555
C 0	4.863777	1.793535	-0.072746
C 0	-2.173893	0.468655	-0.274279
C 0	-3.508799	0.167573	-0.187519
C 0	-1.219195	-0.446764	0.279478
C 0	-3.983895	-1.001968	0.452802
C 0	-4.918581	0.571481	-0.488975
C 0	-1.742958	-1.595101	0.907007
C 0	-3.116715	-1.903478	1.017940
C 0	-5.768778	1.487371	-1.051550
C 0	-5.388909	-0.602904	0.154990
C 0	-7.150319	1.193251	-0.952965

C	0	-6.725805	-0.893853	0.254775
C	0	-7.609174	0.047843	-0.324537
H	0	0.977436	-0.233531	1.634263
H	0	3.885849	-2.869296	-0.928868
H	0	2.920314	-2.059965	-2.152135
H	0	1.323141	-3.192962	2.079162
H	0	2.885411	-2.380340	1.917308
H	0	2.655714	-4.003561	1.222022
H	0	-0.172388	-3.827701	-0.445601
H	0	0.438409	-3.242731	-1.990396
H	0	1.353042	-4.478988	-1.095418
H	0	2.907581	3.597986	0.571229
H	0	2.679841	2.469881	1.901434
H	0	0.811888	4.258563	-0.985924
H	0	-0.367695	3.064744	-1.568162
H	0	1.351986	2.856413	-1.933727
H	0	-1.199368	2.978520	1.308092
H	0	0.107476	4.144689	1.632863
H	0	-0.004651	2.625046	2.554575
H	0	5.798221	-1.214821	-1.330586
H	0	6.739282	1.003194	-0.770334
H	0	5.285937	2.761901	0.187142
H	0	-1.835838	1.380599	-0.766928
H	0	-1.042057	-2.298217	1.357440
H	0	-3.445203	-2.807196	1.524317
H	0	-5.428277	2.390148	-1.548501
H	0	-7.869957	1.883752	-1.381385
H	0	-7.106864	-1.785099	0.742439
H	0	-8.678545	-0.132547	-0.275469

Sum of electronic and zero-point Energies=	-1717.627903
Sum of electronic and thermal Energies=	-1717.599690
Sum of electronic and thermal Enthalpies=	-1717.598746
Sum of electronic and thermal Free Energies=	-1717.686683

1-C2-syn



Charge = 0 Multiplicity = 1

Ir 0	0.860164	-0.086266	0.002032
C 0	2.949365	0.311277	0.010158
P 0	0.836205	2.218359	0.137469
P 0	1.658244	-2.228898	-0.249250
C 0	2.480309	2.611314	0.881194
C 0	0.871202	3.091269	-1.465111
C 0	-0.359036	3.192457	1.114738
C 0	3.345885	-1.967889	-0.943534
C 0	1.984422	-3.163962	1.289423
C 0	0.862248	-3.462387	-1.327209
C 0	3.464286	1.559298	0.433127
C 0	4.836896	1.806145	0.452771
C 0	5.733010	0.814850	0.067171
C 0	3.884928	-0.667122	-0.403595
C 0	5.256294	-0.420963	-0.359359
C 0	-2.203979	0.397150	-0.417403
C 0	-3.527068	0.122599	-0.195253
C 0	-1.213513	-0.483138	0.131787
C 0	-3.957224	-0.995784	0.562326
C 0	-4.954013	0.521337	-0.407612
C 0	-1.691730	-1.597241	0.849784
C 0	-3.055408	-1.877242	1.100632
C 0	-5.841556	1.406400	-0.962803
C 0	-5.378119	-0.599523	0.352889

C	0	-7.211686	1.137403	-0.731474
C	0	-6.704746	-0.866717	0.580401
C	0	-7.625609	0.043757	0.011084
H	0	0.761205	0.035815	-1.539036
H	0	2.801633	3.631202	0.637128
H	0	2.344523	2.584231	1.970976
H	0	-0.054247	2.907464	-2.013954
H	0	1.701818	2.702840	-2.057126
H	0	0.998843	4.168778	-1.330817
H	0	-0.401701	2.807163	2.134950
H	0	-1.356349	3.091732	0.682677
H	0	-0.086702	4.251277	1.144767
H	0	4.004271	-2.823312	-0.751110
H	0	3.223519	-1.906541	-2.033490
H	0	1.051530	-3.379402	1.813480
H	0	2.616396	-2.561958	1.945437
H	0	2.495468	-4.107148	1.076966
H	0	0.711695	-3.032581	-2.318809
H	0	1.459385	-4.374031	-1.416601
H	0	-0.120046	-3.713327	-0.921932
H	0	5.211904	2.773593	0.779840
H	0	6.801043	1.006761	0.092529
H	0	5.958643	-1.189399	-0.675186
H	0	-1.895530	1.260000	-1.007109
H	0	-0.965075	-2.299114	1.261141
H	0	-3.347225	-2.749471	1.679396
H	0	-5.536696	2.267398	-1.548982
H	0	-7.959411	1.805516	-1.147130
H	0	-7.050642	-1.717756	1.157837
H	0	-8.688615	-0.118861	0.159636

Sum of electronic and zero-point Energies=	-1717.628295
Sum of electronic and thermal Energies=	-1717.600098
Sum of electronic and thermal Enthalpies=	-1717.599154
Sum of electronic and thermal Free Energies=	-1717.687102

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3

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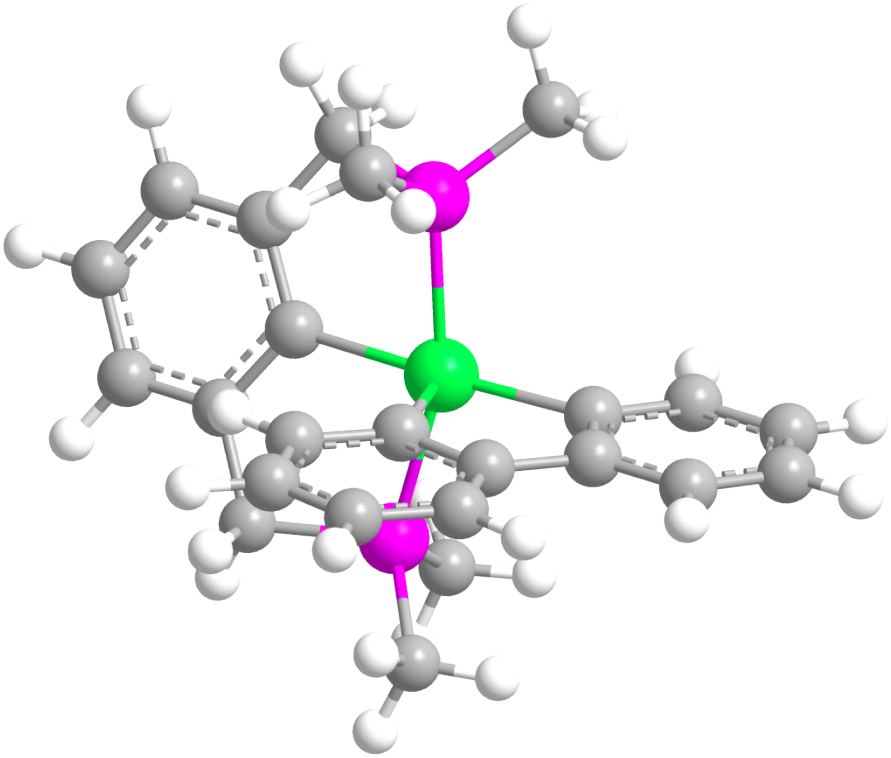

Charge = 0 Multiplicity = 1

Ir 0	−0.065324	0.128255	−0.454577
C 0	−2.169289	0.036550	−0.152547
P 0	−0.461357	2.319757	0.175210
P 0	−0.397022	−2.108707	−0.893752
C 0	−2.259046	2.547724	−0.191059
C 0	−0.318396	2.650082	1.960950
C 0	0.376252	3.748728	−0.587875
C 0	−2.006153	−2.462166	−0.062662
C 0	−0.675555	−2.553612	−2.642490
C 0	0.760865	−3.375212	−0.290491
C 0	−2.953019	1.211872	−0.064418
C 0	−4.334893	1.142232	0.114857
C 0	−4.970496	−0.092591	0.189186
C 0	−2.842227	−1.206366	−0.056811
C 0	−4.226023	−1.265308	0.100943
C 0	−0.005712	−0.746974	2.425722
C 0	0.762325	−0.384062	1.320225
C 0	0.614743	−1.118552	3.619819
C 0	2.175542	−0.392003	1.403079
C 0	1.991830	0.280962	−0.894069

C	0	2.003482	-1.126241	3.712119
C	0	2.772777	-0.765046	2.612571
C	0	2.570142	0.649034	-2.113270
C	0	2.869739	-0.014909	0.177001
C	0	3.954197	0.718902	-2.275174
C	0	4.256899	0.057051	0.018261
C	0	4.799823	0.423258	-1.207528
H	0	-2.704725	3.320948	0.446483
H	0	-2.326009	2.925768	-1.220141
H	0	0.708652	2.477844	2.289873
H	0	-0.611579	3.676487	2.196217
H	0	-0.960921	1.954991	2.504112
H	0	1.438630	3.713555	-0.338396
H	0	-0.042675	4.698641	-0.244415
H	0	0.290019	3.692583	-1.674467
H	0	-2.519952	-3.323187	-0.505999
H	0	-1.748945	-2.749430	0.966840
H	0	0.226535	-2.352321	-3.223497
H	0	-1.488095	-1.945518	-3.044959
H	0	-0.939740	-3.609302	-2.748186
H	0	1.721850	-3.252177	-0.794164
H	0	0.923507	-3.230158	0.779738
H	0	0.386404	-4.386807	-0.468003
H	0	-4.922574	2.054788	0.187275
H	0	-6.046953	-0.141875	0.320264
H	0	-4.727725	-2.227882	0.172004
H	0	-1.091000	-0.732263	2.358897
H	0	0.007237	-1.398909	4.475458
H	0	2.485915	-1.414340	4.640723
H	0	3.857267	-0.775823	2.688546
H	0	1.931467	0.889638	-2.965086
H	0	4.376385	1.005848	-3.235071
H	0	4.918992	-0.172157	0.850703
H	0	5.876785	0.479544	-1.332212

Sum of electronic and zero-point Energies=	-1717.706188
Sum of electronic and thermal Energies=	-1717.678369
Sum of electronic and thermal Enthalpies=	-1717.677424
Sum of electronic and thermal Free Energies=	-1717.763678

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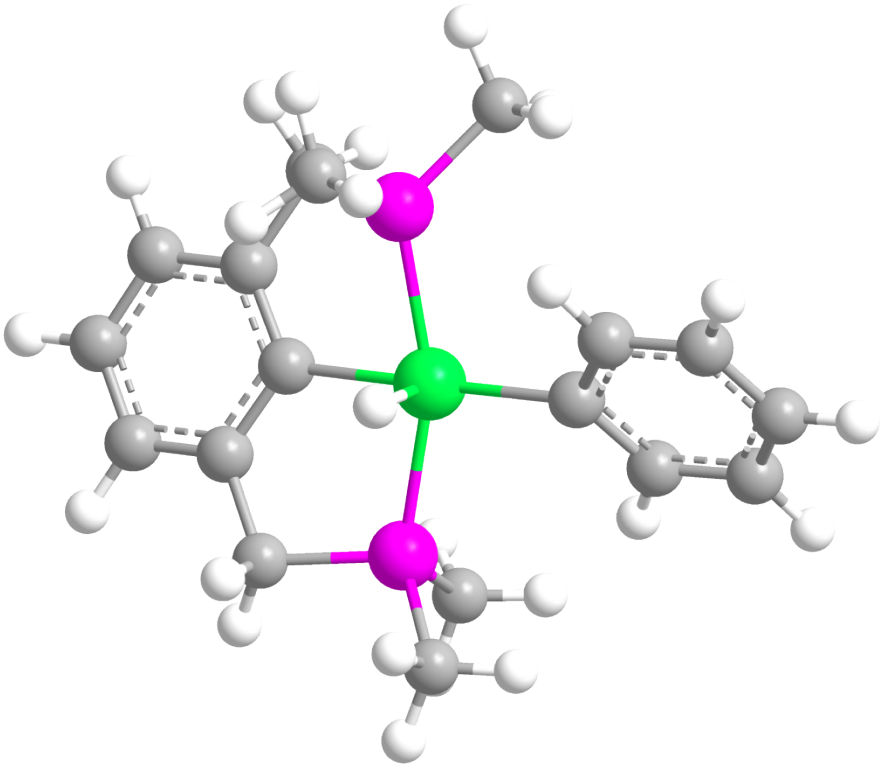
benzene addition product



Charge = 0 Multiplicity = 1

Ir 0	-0.161331	-0.002904	-0.020106
C 0	1.964196	0.007461	0.058959
P 0	0.232619	-2.264914	-0.128718
P 0	0.231770	2.270265	-0.009648
C 0	1.966632	-2.361733	-0.748359
C 0	0.314403	-3.155160	1.468229
C 0	-0.733745	-3.391605	-1.184553
C 0	1.899662	2.407475	0.773002
C 0	0.467132	3.021407	-1.656585
C 0	-0.792395	3.503697	0.863670
C 0	2.717033	-1.149191	-0.257081
C 0	4.108089	-1.153950	-0.166914
C 0	4.789947	-0.000304	0.208250
C 0	2.686327	1.166114	0.431040
C 0	4.079612	1.160355	0.495968
C 0	-2.280771	-0.014247	0.013999
C 0	-3.080114	0.973264	-0.601830
C 0	-3.006390	-1.001407	0.714938
C 0	-4.468895	0.988111	-0.518766
C 0	-4.395282	-0.993309	0.823933

C 0	-5.138856	0.004146	0.202980
H 0	-0.225044	0.049804	-1.565601
H 0	2.446567	-3.308937	-0.474698
H 0	1.901709	-2.350226	-1.844902
H 0	-0.663066	-3.162100	1.953926
H 0	0.646440	-4.187668	1.328277
H 0	1.021588	-2.644884	2.125296
H 0	-1.760741	-3.436622	-0.816669
H 0	-0.311578	-4.400181	-1.201116
H 0	-0.763276	-2.997526	-2.201665
H 0	2.409903	3.332773	0.478723
H 0	1.731565	2.480945	1.856150
H 0	-0.462901	2.974529	-2.226060
H 0	1.226501	2.452451	-2.195920
H 0	0.786908	4.064076	-1.579134
H 0	-1.781871	3.547643	0.404910
H 0	-0.924952	3.202478	1.904217
H 0	-0.338247	4.498291	0.835342
H 0	4.667165	-2.055842	-0.407003
H 0	5.873682	-0.004478	0.269501
H 0	4.615649	2.062851	0.782034
H 0	-2.596599	1.759969	-1.182814
H 0	-2.466419	-1.810346	1.210686
H 0	-5.034103	1.771757	-1.017938
H 0	-4.899688	-1.774356	1.387976
H 0	-6.222055	0.012177	0.274896

Sum of electronic and zero-point Energies=	-1487.875508
Sum of electronic and thermal Energies=	-1487.851341
Sum of electronic and thermal Enthalpies=	-1487.850397
Sum of electronic and thermal Free Energies=	-1487.928803

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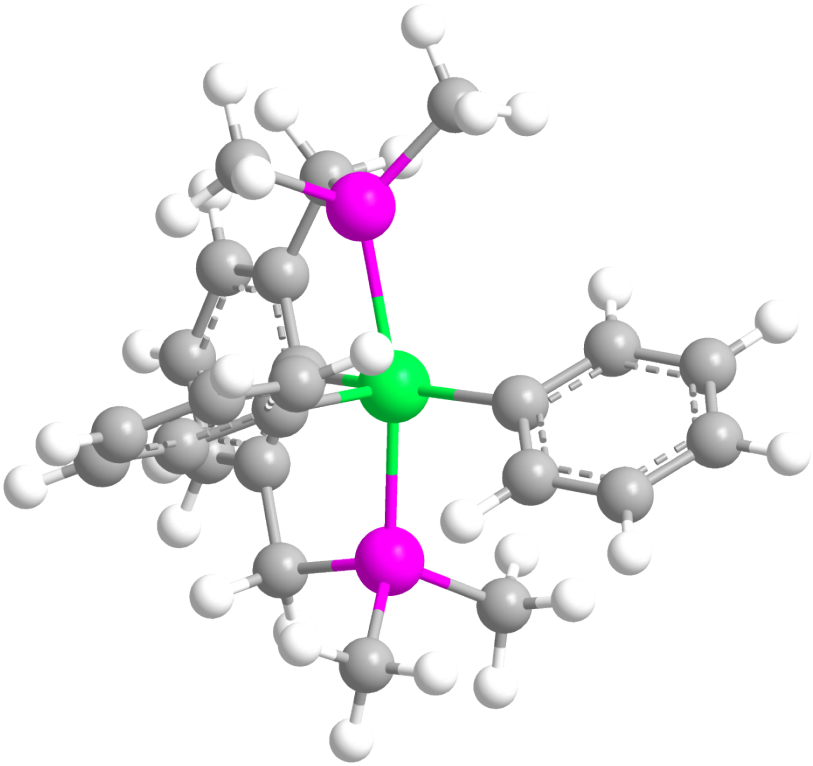
biphenyl addition product



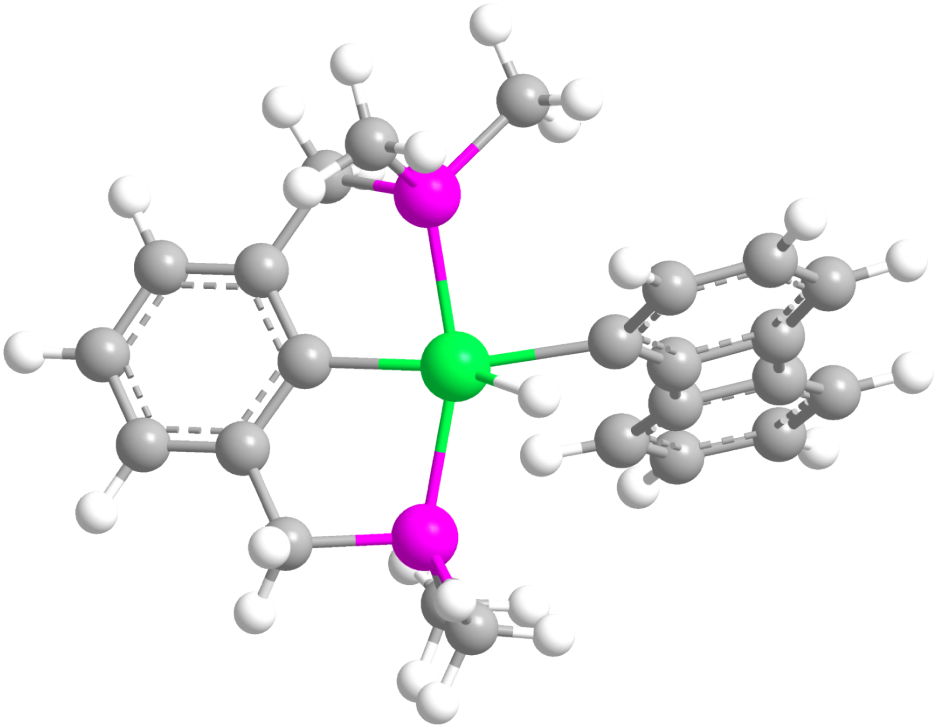
Charge = 0 Multiplicity = 1

Ir 0	0.118039	0.043396	-0.315449
C 0	-1.982952	-0.185702	-0.574773
P 0	0.001787	-2.256807	-0.248520
P 0	-0.509629	2.285678	-0.402836
C 0	-1.784673	-2.620600	0.031767
C 0	0.408832	-3.075273	-1.828115
C 0	0.898843	-3.241791	0.990797
C 0	-2.129644	2.221309	-1.287236
C 0	-0.941170	3.044044	1.198765
C 0	0.418284	3.615390	-1.244009
C 0	-2.611286	-1.450150	-0.441923
C 0	-3.968648	-1.614892	-0.715649
C 0	-4.741442	-0.530192	-1.117054
C 0	-2.787929	0.889129	-1.023416
C 0	-4.149969	0.718046	-1.272795
C 0	0.201543	0.145759	1.711825
C 0	1.269728	0.777949	2.366233
C 0	-0.840177	-0.361899	2.501542
C 0	1.297365	0.877589	3.755288
C 0	-0.804414	-0.260806	3.891241

C 0	0.265701	0.356052	4.528463
C 0	2.219170	0.112727	-0.603387
C 0	2.653918	0.678454	-1.818065
C 0	3.212932	-0.552343	0.139953
C 0	3.967843	0.573406	-2.273570
C 0	4.531309	-0.656108	-0.294976
C 0	4.917678	-0.095717	-1.510021
H 0	-2.076079	-3.564118	-0.444552
H 0	-1.905973	-2.777709	1.112486
H 0	1.453257	-2.875514	-2.077996
H 0	-0.218767	-2.666208	-2.622567
H 0	0.250536	-4.155701	-1.774360
H 0	1.967112	-3.214551	0.768874
H 0	0.741406	-2.806915	1.980286
H 0	0.560415	-4.281427	0.993456
H 0	-2.765225	3.073254	-1.016188
H 0	-1.910814	2.334291	-2.357767
H 0	-0.052500	3.161872	1.820282
H 0	-1.410183	4.019315	1.044733
H 0	-1.632333	2.386557	1.729949
H 0	1.378047	3.761725	-0.744388
H 0	-0.136599	4.557750	-1.234687
H 0	0.621660	3.336485	-2.279210
H 0	-4.430502	-2.593916	-0.607375
H 0	-5.800177	-0.660519	-1.317627
H 0	-4.751546	1.561166	-1.605662
H 0	2.082592	1.198961	1.785080
H 0	-1.710947	-0.801892	2.027351
H 0	2.139662	1.371244	4.232544
H 0	-1.631600	-0.658168	4.473169
H 0	0.291658	0.436578	5.610181
H 0	1.940973	1.220485	-2.443783
H 0	2.948746	-0.995898	1.099971
H 0	4.252286	1.026452	-3.220242
H 0	5.263566	-1.180265	0.314926
H 0	5.944906	-0.174185	-1.852309

Sum of electronic and zero-point Energies=	-1718.866243
Sum of electronic and thermal Energies=	-1718.837196
Sum of electronic and thermal Enthalpies=	-1718.836252
Sum of electronic and thermal Free Energies=	-1718.925867

TS-1-C1-anti



Charge = 0 Multiplicity = 1

Ir 0	0.584641	0.220043	0.131109
C 0	2.460724	-0.721741	-0.083440
P 0	-0.084036	-1.934418	-0.405147
P 0	1.982542	1.976519	0.605802
C 0	1.357020	-2.529531	-1.399076
C 0	-0.125864	-3.164741	0.946803
C 0	-1.522767	-2.390370	-1.434090
C 0	3.487301	1.127384	1.249654
C 0	2.657402	2.920544	-0.810457
C 0	1.600755	3.288545	1.815426
C 0	2.597719	-1.936697	-0.792366
C 0	3.840732	-2.554719	-0.927511
C 0	4.975664	-1.970557	-0.376107
C 0	3.631396	-0.152582	0.471053
C 0	4.871909	-0.770133	0.319040
C 0	-1.251433	1.169124	-0.325330
C 0	-2.548960	0.708113	-0.177881
C 0	-1.195242	2.371589	-1.103907
C 0	-3.682609	1.277173	-0.813927
C 0	-3.434727	-0.272245	0.516166
C 0	-2.297069	2.933988	-1.727818

C	0	-3.598222	2.391549	-1.605359
C	0	-3.552651	-1.284634	1.435457
C	0	-4.564476	0.273584	-0.146919
C	0	-4.860752	-1.780057	1.651777
C	0	-5.834483	-0.197586	0.059760
C	0	-5.958263	-1.262620	0.984373
H	0	-0.582789	0.833111	1.075204
H	0	1.387639	-3.624503	-1.457396
H	0	1.205531	-2.162446	-2.422023
H	0	-0.932812	-2.944343	1.645815
H	0	-0.262792	-4.176487	0.554027
H	0	0.819056	-3.115152	1.490787
H	0	-1.599556	-1.703000	-2.278774
H	0	-2.445809	-2.319363	-0.856772
H	0	-1.419777	-3.412065	-1.811037
H	0	4.379085	1.763572	1.199458
H	0	3.301704	0.918266	2.310648
H	0	1.874873	3.506995	-1.294611
H	0	3.455914	3.596126	-0.489911
H	0	3.057104	2.217163	-1.543054
H	0	0.764111	3.887026	1.447863
H	0	2.456862	3.946710	1.988185
H	0	1.299148	2.837309	2.761948
H	0	3.925949	-3.491344	-1.473465
H	0	5.942735	-2.451070	-0.487806
H	0	5.760929	-0.319350	0.753847
H	0	-0.230752	2.849137	-1.252667
H	0	-2.152404	3.827349	-2.329093
H	0	-4.450114	2.856712	-2.089255
H	0	-2.707941	-1.683872	1.987946
H	0	-5.009523	-2.585085	2.364645
H	0	-6.708892	0.210556	-0.436458
H	0	-6.941049	-1.677084	1.184850

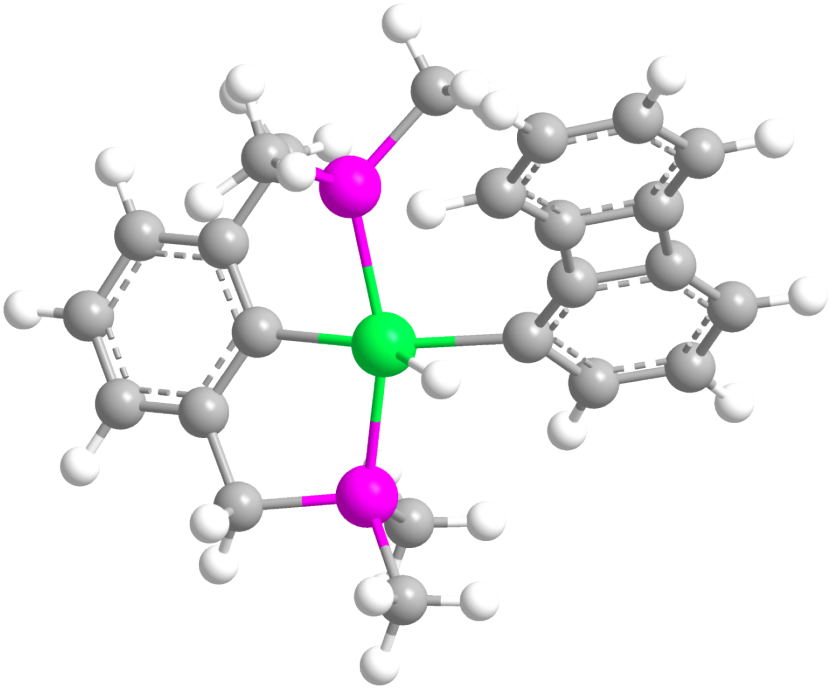
Sum of electronic and zero-point Energies= -1717.621148
Sum of electronic and thermal Energies= -1717.593525
Sum of electronic and thermal Enthalpies= -1717.592581
Sum of electronic and thermal Free Energies= -1717.679237

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
84.1594412 26.8129531 34.5905746
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering

activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-604.0990	16.9965	26.1343
Red. masses --	1.0832	5.5429	4.6173
Frc consts --	0.2329	0.0009	0.0019
IR Inten --	523.7734	0.0949	0.2576

TS-1-C1-syn



Charge = 0 Multiplicity = 1

Ir 0	0.584641	0.220043	0.131109
C 0	2.460724	-0.721741	-0.083440
P 0	-0.084036	-1.934418	-0.405147
P 0	1.982542	1.976519	0.605802
C 0	1.357020	-2.529531	-1.399076
C 0	-0.125864	-3.164741	0.946803
C 0	-1.522767	-2.390370	-1.434090
C 0	3.487301	1.127384	1.249654
C 0	2.657402	2.920544	-0.810457
C 0	1.600755	3.288545	1.815426
C 0	2.597719	-1.936697	-0.792366
C 0	3.840732	-2.554719	-0.927511
C 0	4.975664	-1.970557	-0.376107
C 0	3.631396	-0.152582	0.471053
C 0	4.871909	-0.770133	0.319040
C 0	-1.251433	1.169124	-0.325330
C 0	-2.548960	0.708113	-0.177881
C 0	-1.195242	2.371589	-1.103907
C 0	-3.682609	1.277173	-0.813927
C 0	-3.434727	-0.272245	0.516166
C 0	-2.297069	2.933988	-1.727818
C 0	-3.598222	2.391549	-1.605359

C	0	-3.552651	-1.284634	1.435457
C	0	-4.564476	0.273584	-0.146919
C	0	-4.860752	-1.780057	1.651777
C	0	-5.834483	-0.197586	0.059760
C	0	-5.958263	-1.262620	0.984373
H	0	-0.582789	0.833111	1.075204
H	0	1.387639	-3.624503	-1.457396
H	0	1.205531	-2.162446	-2.422023
H	0	-0.932812	-2.944343	1.645815
H	0	-0.262792	-4.176487	0.554027
H	0	0.819056	-3.115152	1.490787
H	0	-1.599556	-1.703000	-2.278774
H	0	-2.445809	-2.319363	-0.856772
H	0	-1.419777	-3.412065	-1.811037
H	0	4.379085	1.763572	1.199458
H	0	3.301704	0.918266	2.310648
H	0	1.874873	3.506995	-1.294611
H	0	3.455914	3.596126	-0.489911
H	0	3.057104	2.217163	-1.543054
H	0	0.764111	3.887026	1.447863
H	0	2.456862	3.946710	1.988185
H	0	1.299148	2.837309	2.761948
H	0	3.925949	-3.491344	-1.473465
H	0	5.942735	-2.451070	-0.487806
H	0	5.760929	-0.319350	0.753847
H	0	-0.230752	2.849137	-1.252667
H	0	-2.152404	3.827349	-2.329093
H	0	-4.450114	2.856712	-2.089255
H	0	-2.707941	-1.683872	1.987946
H	0	-5.009523	-2.585085	2.364645
H	0	-6.708892	0.210556	-0.436458
H	0	-6.941049	-1.677084	1.184850

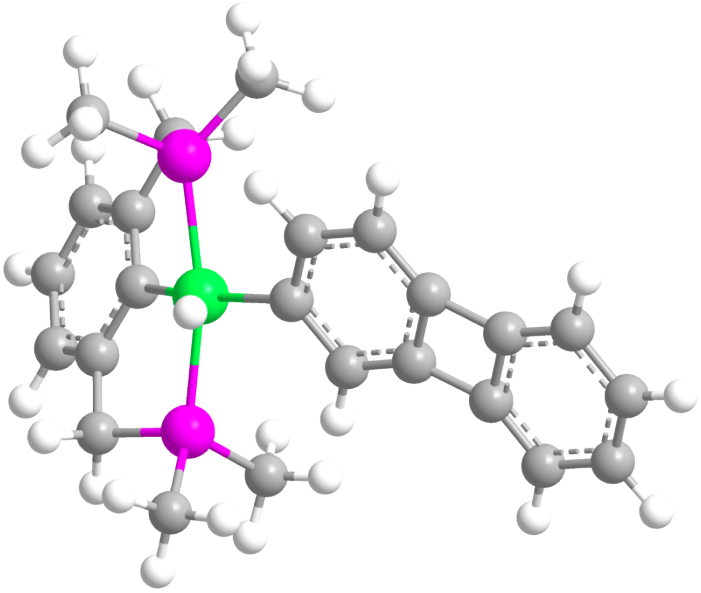
Sum of electronic and zero-point Energies= -1717.626858
Sum of electronic and thermal Energies= -1717.599121
Sum of electronic and thermal Enthalpies= -1717.598176
Sum of electronic and thermal Free Energies= -1717.684654

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
68.6658525 28.0710247 35.9988046
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized

incident light, reduced masses (AMU), force constants (mDyne/A),
and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-583.0802	23.9706	31.1820
Red. masses --	1.0907	4.6453	4.9066
Frc consts --	0.2185	0.0016	0.0028
IR Inten --	487.5883	0.1040	0.1440

TS-1-C2-anti



Charge = 0 Multiplicity = 1

Ir 0	0.866246	-0.078683	0.333635
C 0	2.829996	0.294574	-0.371516
P 0	1.613599	-2.245856	0.011950
P 0	0.913693	2.212167	0.462673
C 0	2.914828	-2.030166	-1.280870
C 0	2.538305	-2.980276	1.407340
C 0	0.660267	-3.676698	-0.620103
C 0	2.710309	2.585117	0.628461
C 0	0.473209	3.136849	-1.055375
C 0	0.103073	3.180846	1.780738
C 0	3.570787	-0.696298	-1.056464
C 0	4.866167	-0.446151	-1.508903
C 0	5.450269	0.798579	-1.303674
C 0	3.459110	1.545187	-0.160375
C 0	4.748066	1.792440	-0.630066
C 0	-2.128497	0.546242	0.077645
C 0	-3.446542	0.205417	-0.064226
C 0	-1.211010	-0.478126	0.479738
C 0	-3.941043	-1.091432	0.220204
C 0	-4.827715	0.648122	-0.430497
C 0	-1.747034	-1.736171	0.809537
C 0	-3.107925	-2.082185	0.673847
C 0	-5.645754	1.660536	-0.859643
C 0	-5.317414	-0.652049	-0.141717

C	0	-7.014987	1.331710	-0.999324
C	0	-6.644133	-0.977190	-0.272905
C	0	-7.493754	0.062797	-0.716505
H	0	-0.036235	-0.232945	1.651188
H	0	3.628204	-2.863517	-1.283309
H	0	2.397918	-2.057506	-2.248869
H	0	3.001701	-3.930780	1.127262
H	0	1.866227	-3.145140	2.251675
H	0	3.312804	-2.280132	1.724500
H	0	1.336700	-4.444605	-1.006888
H	0	-0.010259	-3.353478	-1.418092
H	0	0.051795	-4.119251	0.169507
H	0	2.950569	3.611366	0.325773
H	0	2.951629	2.503312	1.695914
H	0	-0.579293	2.995163	-1.306074
H	0	1.070374	2.750668	-1.883616
H	0	0.671104	4.206544	-0.940550
H	0	0.395839	2.785228	2.754619
H	0	-0.981588	3.087825	1.694923
H	0	0.371839	4.239656	1.728740
H	0	5.419758	-1.223111	-2.030934
H	0	6.455790	0.993152	-1.663776
H	0	5.213716	2.759993	-0.457806
H	0	-1.774954	1.548988	-0.142154
H	0	-1.071702	-2.489175	1.205440
H	0	-3.451057	-3.080046	0.931112
H	0	-5.289197	2.660219	-1.085645
H	0	-7.709941	2.093753	-1.337401
H	0	-7.040245	-1.963865	-0.056996
H	0	-8.553275	-0.138471	-0.839847

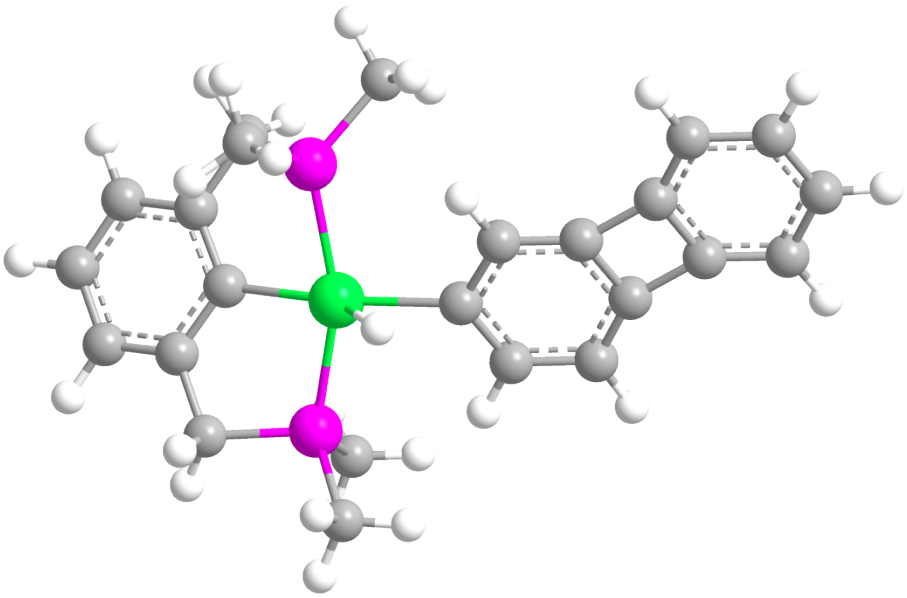
Sum of electronic and zero-point Energies= -1717.623135
Sum of electronic and thermal Energies= -1717.595323
Sum of electronic and thermal Enthalpies= -1717.594379
Sum of electronic and thermal Free Energies= -1717.681805

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
96.3911789 23.7370337 44.0839566
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A),

and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-579.9232	17.7241	20.1740
Red. masses --	1.0631	4.2608	5.3905
Frc consts --	0.2107	0.0008	0.0013
IR Inten --	515.2883	0.4502	0.0133

TS-1-C2-syn



Charge = 0 Multiplicity = 1

Ir 0	0.863276	-0.105448	-0.259428
C 0	2.864081	0.377523	0.252535
P 0	0.738312	2.206851	-0.185184
P 0	1.793557	-2.203100	-0.235883
C 0	2.101330	2.639369	0.983238
C 0	1.231325	3.067261	-1.721069
C 0	-0.639843	3.254300	0.418106
C 0	3.575537	-1.876373	-0.568048
C 0	1.854994	-3.063333	1.378936
C 0	1.330560	-3.536926	-1.392845
C 0	3.207087	1.640673	0.787419
C 0	4.525433	1.950986	1.120345
C 0	5.531716	1.008431	0.942763
C 0	3.913809	-0.553816	0.064583
C 0	5.226411	-0.241729	0.415103
C 0	-2.222865	0.398078	-0.487702
C 0	-3.514113	0.098401	-0.149448
C 0	-1.204841	-0.561369	-0.182697
C 0	-3.883253	-1.131488	0.447687
C 0	-4.945192	0.533962	-0.130185
C 0	-1.617872	-1.801013	0.340288
C 0	-2.950257	-2.107134	0.691722
C 0	-5.866330	1.504041	-0.427422
C 0	-5.308937	-0.699511	0.469711

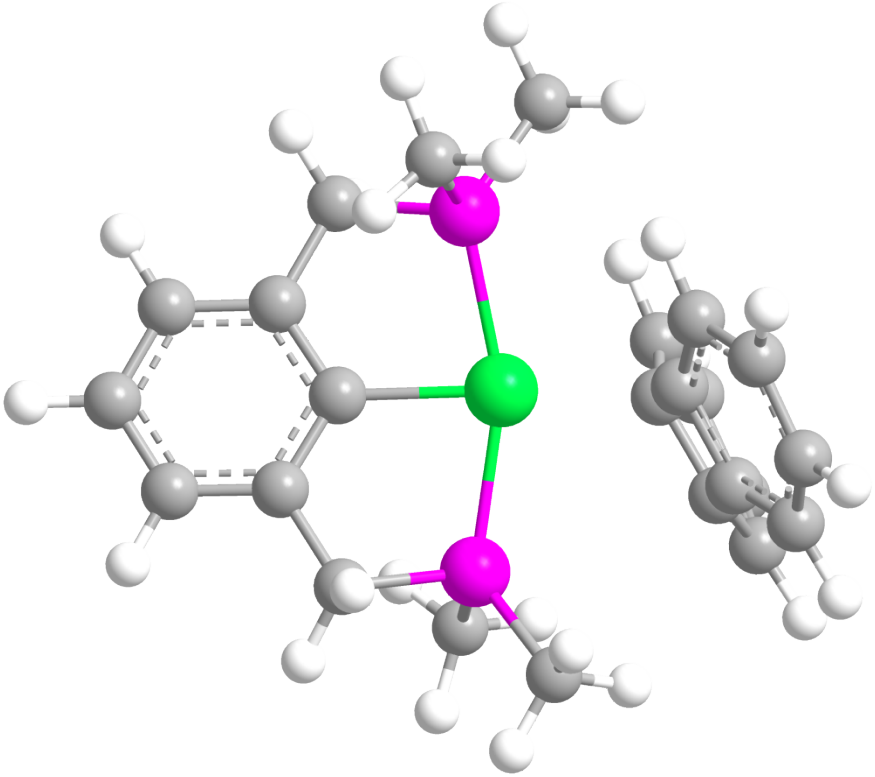
C	0	-7.209163	1.203396	-0.096722
C	0	-6.609108	-0.998842	0.790309
C	0	-7.564793	-0.000544	0.488887
H	0	-0.133805	-0.460635	-1.467839
H	0	2.432970	3.676984	0.853830
H	0	1.679103	2.568552	1.993952
H	0	0.497598	2.875601	-2.506255
H	0	2.192213	2.671311	-2.053482
H	0	1.317722	4.146850	-1.567106
H	0	-1.101572	2.797399	1.295021
H	0	-1.409609	3.366495	-0.346683
H	0	-0.271574	4.249708	0.683352
H	0	4.218768	-2.695571	-0.225109
H	0	3.686693	-1.818947	-1.658321
H	0	0.849219	-3.306965	1.725199
H	0	2.444897	-3.982533	1.318466
H	0	2.309860	-2.395156	2.112661
H	0	0.302779	-3.852253	-1.201277
H	0	1.990254	-4.403778	-1.296035
H	0	1.379314	-3.162876	-2.416734
H	0	4.767710	2.929765	1.527687
H	0	6.555831	1.249725	1.210258
H	0	6.018141	-0.971585	0.263072
H	0	-1.957834	1.326772	-0.982791
H	0	-0.869592	-2.567125	0.519945
H	0	-3.195577	-3.073417	1.122695
H	0	-5.606850	2.451586	-0.888395
H	0	-7.982221	1.935391	-0.307724
H	0	-6.910032	-1.935517	1.247596
H	0	-8.608990	-0.182628	0.722997

Sum of electronic and zero-point Energies= -1717.622682
Sum of electronic and thermal Energies= -1717.594942
Sum of electronic and thermal Enthalpies= -1717.593998
Sum of electronic and thermal Free Energies= -1717.681050

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
87.7767376 26.6218985 42.9211786
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-546.6058	16.0975	28.8706
Red. masses --	1.0721	4.8034	4.9377
Frc consts --	0.1887	0.0007	0.0024
IR Inten --	470.6682	0.2584	0.1040

TS-3-PMe2



Charge = 0 Multiplicity = 1

Ir 0	-0.189039	-0.140335	-0.060412
C 0	-2.155252	0.465715	-0.088069
P 0	0.094769	2.122563	-0.384405
P 0	-1.223819	-2.171913	0.194671
C 0	-1.483574	2.617590	-1.178672
C 0	0.124472	3.117900	1.150009
C 0	1.379748	2.950777	-1.391965
C 0	-2.801993	-1.697407	1.003835
C 0	-1.796995	-2.969132	-1.352375
C 0	-0.629310	-3.615936	1.157578
C 0	-2.549079	1.723183	-0.611893
C 0	-3.885011	2.118864	-0.614030
C 0	-4.875637	1.279272	-0.117937
C 0	-3.186357	-0.365510	0.422144
C 0	-4.520394	0.036764	0.393186
H 0	-1.703513	3.683338	-1.043441
H 0	-1.362429	2.448040	-2.256489
H 0	0.117473	4.192115	0.941010
H 0	1.016289	2.868085	1.729088
H 0	-0.750622	2.860542	1.749559

H	0	1.492120	2.443624	-2.351616
H	0	2.340443	2.917413	-0.874129
H	0	1.114792	3.998250	-1.565019
H	0	-3.585618	-2.455707	0.888382
H	0	-2.589224	-1.609877	2.077445
H	0	-2.352529	-2.230917	-1.933471
H	0	-0.948328	-3.296942	-1.955664
H	0	-2.442811	-3.828670	-1.148503
H	0	-0.517013	-3.343678	2.208568
H	0	0.345462	-3.946934	0.790643
H	0	-1.329167	-4.453865	1.090713
H	0	-4.153292	3.091846	-1.019537
H	0	-5.915141	1.590790	-0.129492
H	0	-5.287258	-0.626780	0.786678
C	0	1.599962	-0.875241	2.304120
C	0	1.774544	-0.413522	0.999168
C	0	2.243461	-0.160987	3.330613
C	0	2.797708	0.560593	0.742493
C	0	1.962227	-0.869630	-0.553443
C	0	3.128548	0.876797	3.070041
C	0	3.473418	1.212064	1.740639
C	0	1.922853	-1.912889	-1.463539
C	0	2.949712	0.146397	-0.667141
C	0	2.769802	-1.815903	-2.587800
C	0	3.806141	0.222196	-1.735332
C	0	3.663306	-0.768255	-2.734504
H	0	0.941585	-1.702745	2.540169
H	0	2.037462	-0.431289	4.361891
H	0	3.605554	1.392782	3.896456
H	0	4.280525	1.908955	1.533780
H	0	1.256612	-2.760882	-1.350620
H	0	2.717295	-2.581123	-3.355648
H	0	4.589714	0.970545	-1.802727
H	0	4.299547	-0.733091	-3.613062

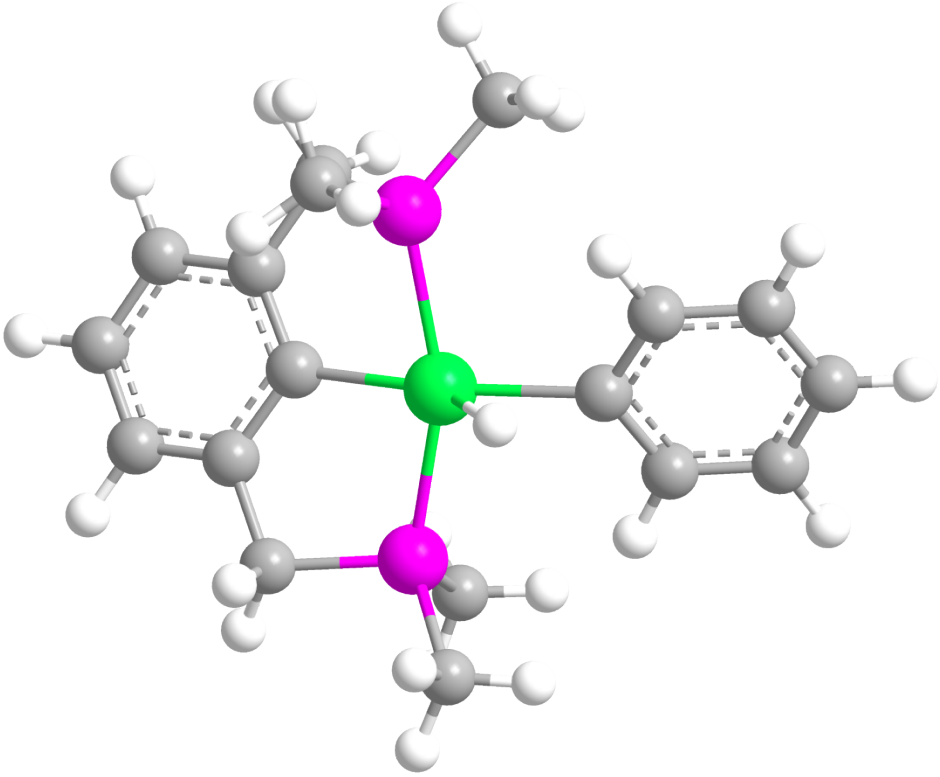
Sum of electronic and zero-point Energies= -1717.627672
Sum of electronic and thermal Energies= -1717.600036
Sum of electronic and thermal Enthalpies= -1717.599092
Sum of electronic and thermal Free Energies= -1717.684556

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
142.1958975 29.2751434 67.2633954

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-176.1334	22.3295	40.1673
Red. masses --	6.9531	5.2518	4.8953
Frc consts --	0.1271	0.0015	0.0047
IR Inten --	52.1545	1.4675	0.0360

TS-benzene addition



Charge = 0 Multiplicity = 1

Ir 0	0.174905	-0.024993	0.222926
C 0	-1.907033	0.050020	-0.179094
P 0	-0.316714	-2.264717	0.211084
P 0	-0.170805	2.264230	0.185862
C 0	-2.108642	-2.305643	0.638225
C 0	-2.738133	-1.073053	0.047737
C 0	-4.103718	-1.027431	-0.228993
C 0	-4.679705	0.139480	-0.719945
C 0	-3.892283	1.264798	-0.935002
C 0	-2.522466	1.222196	-0.675554
C 0	-1.649259	2.422838	-0.910566
C 0	-0.292084	-3.108933	-1.413437
C 0	0.461934	-3.488984	1.319354
C 0	-0.758346	2.989097	1.758200
C 0	0.935931	3.577895	-0.453112
C 0	2.286126	-0.062318	0.019182
C 0	2.915064	-1.194215	-0.538355
C 0	4.246718	-1.178995	-0.939158
C 0	5.028560	-0.043866	-0.751491

C	0	4.457493	1.066931	-0.139676
C	0	3.123530	1.046631	0.250709
H	0	1.292121	-0.170401	1.367049
H	0	-2.591858	-3.234505	0.312147
H	0	-2.171986	-2.281345	1.733557
H	0	-4.725149	-1.901381	-0.048023
H	0	-5.744353	0.172911	-0.929940
H	0	-4.346347	2.177522	-1.313806
H	0	-2.174592	3.372465	-0.749955
H	0	-1.272736	2.442406	-1.941430
H	0	0.721623	-3.142001	-1.815931
H	0	-0.911469	-2.540762	-2.110089
H	0	-0.681166	-4.128617	-1.339054
H	0	1.519499	-3.594616	1.068757
H	0	0.396781	-3.138220	2.350560
H	0	-0.019010	-4.468238	1.242694
H	0	0.033204	2.942145	2.508307
H	0	-1.602978	2.401638	2.121646
H	0	-1.069242	4.030054	1.629613
H	0	1.704247	3.828829	0.279589
H	0	0.363346	4.483246	-0.675313
H	0	1.436009	3.236949	-1.361152
H	0	2.344704	-2.105713	-0.694904
H	0	4.677722	-2.066133	-1.395582
H	0	6.069642	-0.033394	-1.057077
H	0	5.057369	1.954048	0.045414
H	0	2.717644	1.916186	0.759253

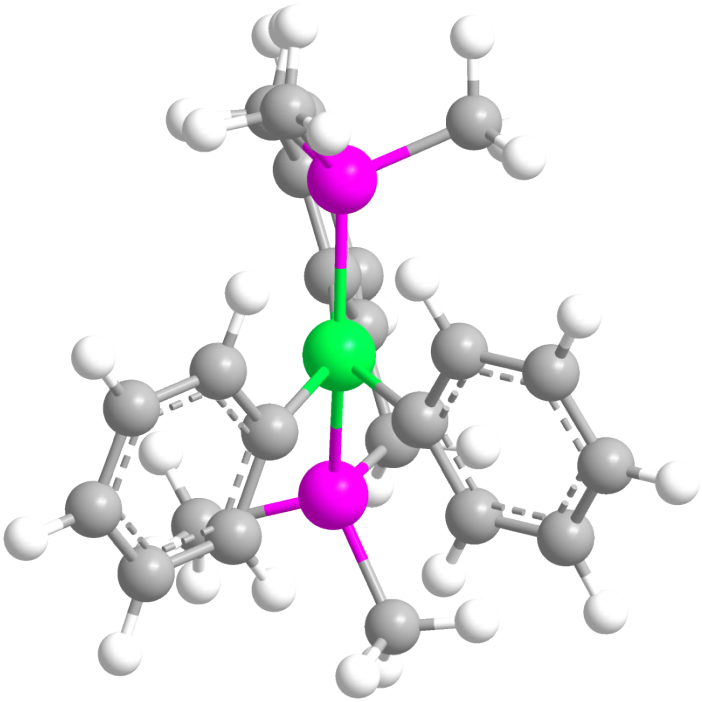
Sum of electronic and zero-point Energies= -1487.870674
Sum of electronic and thermal Energies= -1487.846985
Sum of electronic and thermal Enthalpies= -1487.846041
Sum of electronic and thermal Free Energies= -1487.923794

****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:
82.7601785 23.8557235 44.9491827
Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

1	2	3
A	A	A

Frequencies --	-507.8620	18.2219	37.4587
Red. masses --	1.0885	4.1670	4.7014
Frc consts --	0.1654	0.0008	0.0039
IR Inten --	360.4914	0.5443	0.0873

TS-biphenyl addition



Charge = 0 Multiplicity = 1

Ir 0	0.109074	-0.000007	-0.000017
C 0	2.232720	0.000000	-0.000029
P 0	0.585105	2.267489	-0.183428
P 0	0.585141	-2.267499	0.183403
C 0	2.222108	2.282878	-1.011904
C 0	-0.274521	3.637109	-1.055415
C 0	0.938266	3.041055	1.435970
C 0	2.222152	-2.282880	1.011855
C 0	-0.274487	-3.637109	1.055430
C 0	0.938291	-3.041104	-1.435984
C 0	2.978323	1.099890	-0.487723
C 0	4.372557	1.099351	-0.479642
C 0	5.073004	0.000043	0.000013
C 0	2.978340	-1.099870	0.487683
C 0	4.372576	-1.099286	0.479645
C 0	-1.802441	-0.168418	-0.943932
C 0	-2.277681	0.900253	-1.732032
C 0	-2.283833	-1.449331	-1.294659
C 0	-3.070562	0.693945	-2.851578
C 0	-3.074946	-1.658765	-2.414350
C 0	-3.465529	-0.589803	-3.215743
C 0	-1.802413	0.168407	0.943954

C	0	-2.283779	1.449327	1.294694
C	0	-2.277637	-0.900254	1.732075
C	0	-3.074839	1.658777	2.414419
C	0	-3.070467	-0.693931	2.851654
C	0	-3.465398	0.589823	3.215835
H	0	2.034685	2.188705	-2.089162
H	0	2.751646	3.230906	-0.859067
H	0	0.345968	4.537563	-1.019138
H	0	-1.237064	3.870969	-0.595855
H	0	-0.445701	3.371677	-2.099983
H	0	0.026508	3.066781	2.036460
H	0	1.669550	2.427256	1.964499
H	0	1.329952	4.056443	1.324652
H	0	2.034752	-2.188742	2.089120
H	0	2.751702	-3.230896	0.858981
H	0	-1.237050	-3.870948	0.595899
H	0	-0.445628	-3.371666	2.100001
H	0	0.345983	-4.537576	1.019137
H	0	0.026565	-3.066715	-2.036528
H	0	1.669682	-2.427394	-1.964468
H	0	1.329846	-4.056541	-1.324648
H	0	4.912981	1.963132	-0.859396
H	0	6.158464	0.000060	0.000030
H	0	4.913015	-1.963051	0.859416
H	0	-2.021817	1.915467	-1.460044
H	0	-2.035533	-2.302820	-0.672515
H	0	-3.389019	1.548905	-3.441359
H	0	-3.397541	-2.667618	-2.656157
H	0	-4.089828	-0.750942	-4.087838
H	0	-2.035502	2.302807	0.672527
H	0	-2.021804	-1.915473	1.460078
H	0	-3.397411	2.667635	2.656234
H	0	-3.388911	-1.548885	3.441451
H	0	-4.089654	0.750974	4.087958

Sum of electronic and zero-point Energies= -1718.845087
Sum of electronic and thermal Energies= -1718.817282
Sum of electronic and thermal Enthalpies= -1718.816338
Sum of electronic and thermal Free Energies= -1718.901324

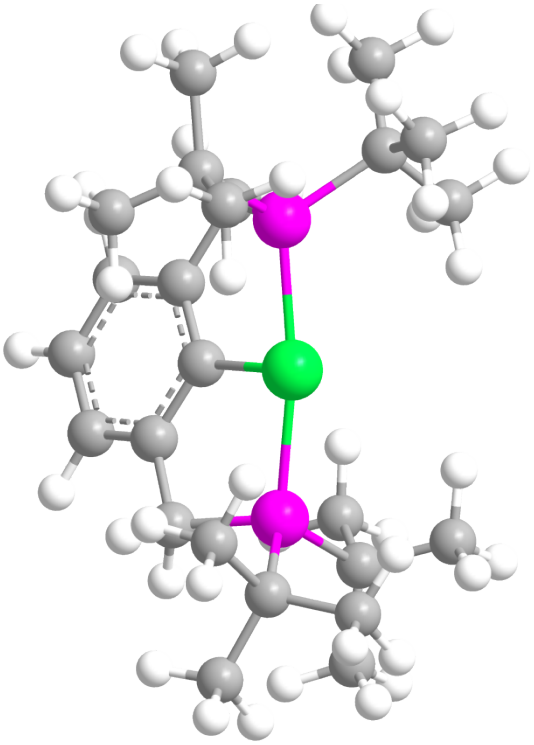
****** 1 imaginary frequencies (negative Signs) ******
Diagonal vibrational polarizability:

66.5384721 21.7998475 27.3270947

Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates:

	1	2	3
	A	A	A
Frequencies --	-244.4818	27.0843	33.5053
Red. masses --	7.9405	4.0086	5.4491
Frc consts --	0.2796	0.0017	0.0036
IR Inten --	82.2768	0.0382	0.1812

(^{tBu}PCP)Ir



Charge = 0 Multiplicity = 1

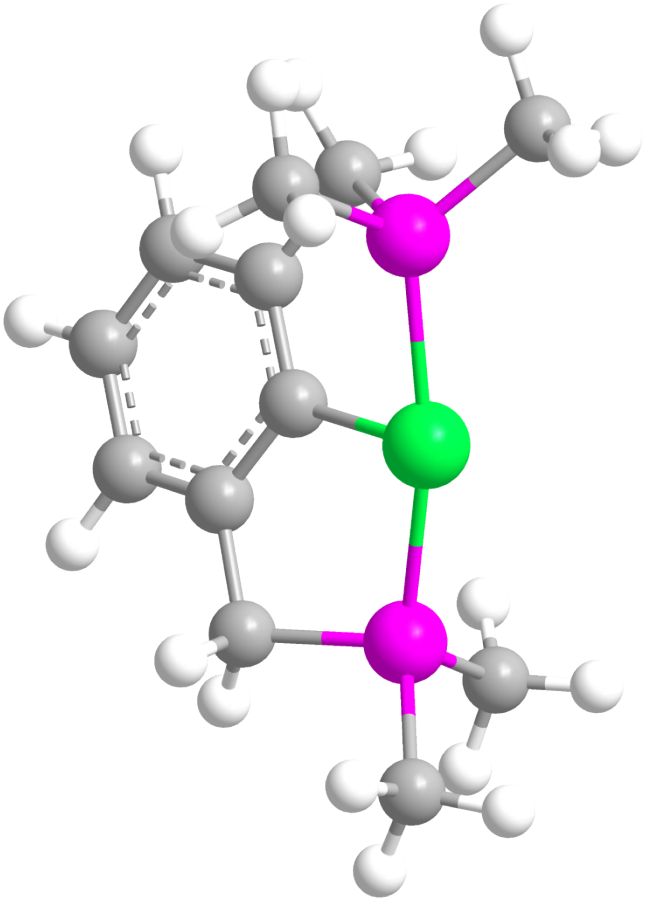
Ir 0	−0.000002	0.444332	−0.000025
C 0	−0.000012	−1.536173	−0.000026
P 0	−2.284347	0.196467	−0.098092
P 0	2.284339	0.196452	0.098103
C 0	−2.420717	−1.536976	−0.710521
C 0	−3.142204	0.177811	1.591836
C 0	−3.290733	1.191660	−1.357837
C 0	2.420691	−1.537011	0.710482
C 0	3.142247	0.177861	−1.591799
C 0	3.290710	1.191602	1.357891
C 0	−1.167716	−2.275391	−0.326605
C 0	−1.156464	−3.668344	−0.311930
C 0	−0.000025	−4.373506	−0.000047
C 0	1.167685	−2.275406	0.326544
C 0	1.156420	−3.668359	0.311848
C 0	−4.658706	0.015399	1.540076
C 0	−4.603148	0.525886	−1.775752
C 0	4.603113	0.525802	1.775804
C 0	4.658752	0.015499	−1.539981
C 0	−2.392247	1.312165	−2.594766
C 0	−2.537931	−1.003868	2.359288

C	0	2.392205	1.312088	2.594809
C	0	2.538041	-1.003816	-2.359309
C	0	3.567343	2.594645	0.819142
C	0	2.772920	1.459748	-2.343422
C	0	-3.567340	2.594696	-0.819054
C	0	-2.772887	1.459687	2.343485
H	0	-3.329497	-2.045617	-0.365431
H	0	-2.500470	-1.470844	-1.802828
H	0	3.329470	-2.045651	0.365388
H	0	2.500435	-1.470905	1.802791
H	0	-2.069784	-4.206339	-0.557853
H	0	-0.000030	-5.458438	-0.000054
H	0	2.069734	-4.206367	0.557767
H	0	-5.159637	0.892381	1.122349
H	0	-4.963616	-0.861477	0.960437
H	0	-5.046733	-0.120537	2.556450
H	0	-5.077336	1.123472	-2.563202
H	0	-4.445020	-0.474158	-2.187589
H	0	-5.320114	0.443165	-0.958907
H	0	5.320081	0.443081	0.958960
H	0	5.077306	1.123370	2.563265
H	0	4.444966	-0.474245	2.187626
H	0	5.046826	-0.120393	-2.556343
H	0	5.159636	0.892485	-1.122204
H	0	4.963666	-0.861385	-0.960355
H	0	-2.128174	0.335165	-3.010597
H	0	-2.916509	1.874771	-3.376213
H	0	-1.453854	1.823969	-2.364145
H	0	-2.806755	-1.970375	1.924637
H	0	-1.445765	-0.942411	2.387715
H	0	-2.911452	-0.989149	3.389538
H	0	1.453820	1.823908	2.364185
H	0	2.128114	0.335082	3.010614
H	0	2.916460	1.874670	3.376278
H	0	2.911606	-0.989055	-3.389542
H	0	2.806878	-1.970327	-1.924675
H	0	1.445875	-0.942393	-2.387780
H	0	4.294298	2.590985	0.002915
H	0	2.654338	3.079840	0.458505
H	0	3.979028	3.223781	1.616477
H	0	3.175327	1.417963	-3.362347
H	0	1.684980	1.563302	-2.411641
H	0	3.171818	2.360657	-1.871867
H	0	-3.979026	3.223854	-1.616371

H	0	-4.294284	2.591029	-0.002819
H	0	-2.654323	3.079871	-0.458419
H	0	-3.171826	2.360598	1.871972
H	0	-3.175256	1.417859	3.362423
H	0	-1.684947	1.563269	2.411668

Sum of electronic and zero-point Energies=	-1727.157663
Sum of electronic and thermal Energies=	-1727.123995
Sum of electronic and thermal Enthalpies=	-1727.123051
Sum of electronic and thermal Free Energies=	-1727.218653

(^{Me}PCP)Ir



Charge = 0 Multiplicity = 1

Ir 0	0.000005	0.880235	-0.000027
C 0	-0.000005	-1.102045	-0.000025
P 0	-2.266756	0.588194	0.042584
P 0	2.266766	0.588175	-0.042544
C 0	-2.403210	-1.077945	-0.726708
C 0	-3.077136	0.352427	1.668937
C 0	-3.505241	1.600854	-0.848876
C 0	2.403179	-1.077973	0.726734
C 0	3.077206	0.352420	-1.668869
C 0	3.505225	1.600817	0.848976
C 0	-1.166614	-1.838213	-0.336700
C 0	-1.156315	-3.230691	-0.318762
C 0	-0.000026	-3.933920	-0.000005
C 0	1.166586	-1.838226	0.336685
C 0	1.156269	-3.230703	0.318757
H 0	-3.326245	-1.600600	-0.449018
H 0	-2.437174	-0.916285	-1.811514

H	0	-2.522816	-0.404588	2.226662
H	0	-4.116711	0.028732	1.559351
H	0	-3.051881	1.278776	2.245240
H	0	-4.492873	1.130387	-0.828307
H	0	-3.195556	1.731101	-1.886932
H	0	-3.583710	2.589675	-0.392536
H	0	3.326216	-1.600636	0.449068
H	0	2.437114	-0.916319	1.811542
H	0	4.116773	0.028714	-1.559245
H	0	2.522900	-0.404584	-2.226625
H	0	3.051982	1.278775	-2.245160
H	0	3.195501	1.731057	1.887020
H	0	4.492854	1.130342	0.828441
H	0	3.583720	2.589642	0.392648
H	0	-2.066729	-3.769875	-0.571426
H	0	-0.000035	-5.018857	0.000003
H	0	2.066672	-3.769898	0.571440

Sum of electronic and zero-point Energies=	-1255.691862
Sum of electronic and thermal Energies=	-1255.673699
Sum of electronic and thermal Enthalpies=	-1255.672755
Sum of electronic and thermal Free Energies=	-1255.737705

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benzene

Charge = 0 Multiplicity = 1

C	0	-0.063720	-1.389810	0.000001
C	0	1.171869	-0.750059	-0.000021
C	0	1.235567	0.639734	0.000017
C	0	0.063668	1.389813	-0.000004
C	0	-1.171841	0.750101	-0.000014
C	0	-1.235543	-0.639779	0.000015
H	0	-0.113193	-2.474031	-0.000003
H	0	2.086022	-1.335136	-0.000002
H	0	2.199239	1.139045	0.000020
H	0	0.113284	2.474027	0.000012
H	0	-2.086070	1.335061	-0.000021
H	0	-2.199279	-1.138966	0.000027

Sum of electronic and zero-point Energies=	-232.168399
Sum of electronic and thermal Energies=	-232.163991
Sum of electronic and thermal Enthalpies=	-232.163046
Sum of electronic and thermal Free Energies=	-232.195863

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biphenyl

Charge = 0 Multiplicity = 1

C	0	2.847441	-1.149080	-0.350378
C	0	1.458970	-1.148812	-0.349813
C	0	0.737815	-0.000009	0.000001
C	0	1.458963	1.148809	0.349817
C	0	2.847425	1.149088	0.350380
C	0	3.548710	0.000003	-0.000001
C	0	-0.737815	-0.000009	-0.000002
C	0	-1.458964	1.148809	-0.349818
C	0	-1.458970	-1.148811	0.349815
C	0	-2.847426	1.149087	-0.350379
C	0	-2.847441	-1.149080	0.350377
C	0	-3.548710	0.000003	0.000000
H	0	3.384698	-2.048347	-0.634276
H	0	0.921443	-2.043044	-0.650454
H	0	0.921415	2.043030	0.650455
H	0	3.384691	2.048350	0.634275
H	0	4.633650	0.000019	0.000001
H	0	-0.921416	2.043030	-0.650455
H	0	-0.921441	-2.043043	0.650454
H	0	-3.384692	2.048350	-0.634273
H	0	-3.384697	-2.048348	0.634276
H	0	-4.633650	0.000018	-0.000001

Sum of electronic and zero-point Energies=	-463.167449
Sum of electronic and thermal Energies=	-463.158574
Sum of electronic and thermal Enthalpies=	-463.157630
Sum of electronic and thermal Free Energies=	-463.201926

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biphenylene

Charge = 0 Multiplicity = 1

C	0	-3.105608	0.693207	-0.000136
C	0	-3.105638	-0.693144	-0.000112
C	0	-1.906277	-1.440913	-0.000066
C	0	-0.747076	-0.708397	-0.000061
C	0	-0.747064	0.708344	-0.000087
C	0	-1.906214	1.440890	-0.000113
C	0	0.747076	-0.708397	0.000023
C	0	1.906278	-1.440913	0.000107
C	0	3.105638	-0.693144	0.000184
C	0	3.105608	0.693207	0.000156
C	0	1.906213	1.440890	0.000072
C	0	0.747064	0.708344	0.000000
H	0	-4.055163	1.218321	-0.000163
H	0	-4.055209	-1.218233	-0.000130
H	0	-1.925887	-2.525414	-0.000039
H	0	-1.925681	2.525399	-0.000128
H	0	1.925887	-2.525414	0.000134
H	0	4.055210	-1.218233	0.000253
H	0	4.055163	1.218322	0.000213
H	0	1.925681	2.525399	0.000056

Sum of electronic and zero-point Energies=	-461.919062
Sum of electronic and thermal Energies=	-461.910909
Sum of electronic and thermal Enthalpies=	-461.909965
Sum of electronic and thermal Free Energies=	-461.952294