

Exploring the mechanism of the Pd-catalyzed spirocyclization reaction: a combined DFT and experimental study

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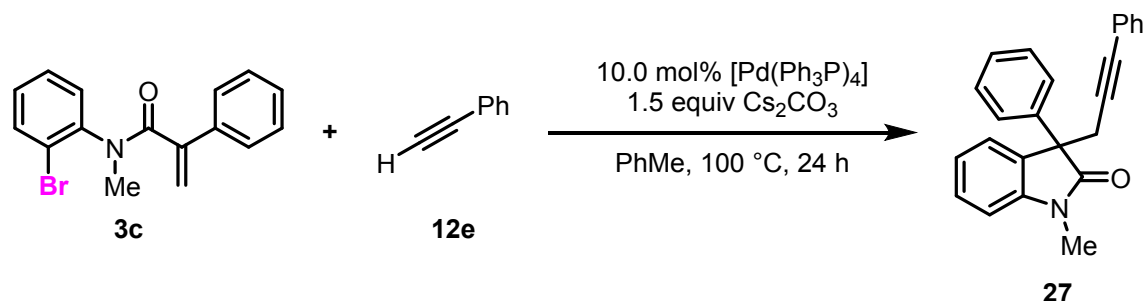
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1 – Additional Experimental Data

Synthesis of the Sonogashira-type product 27

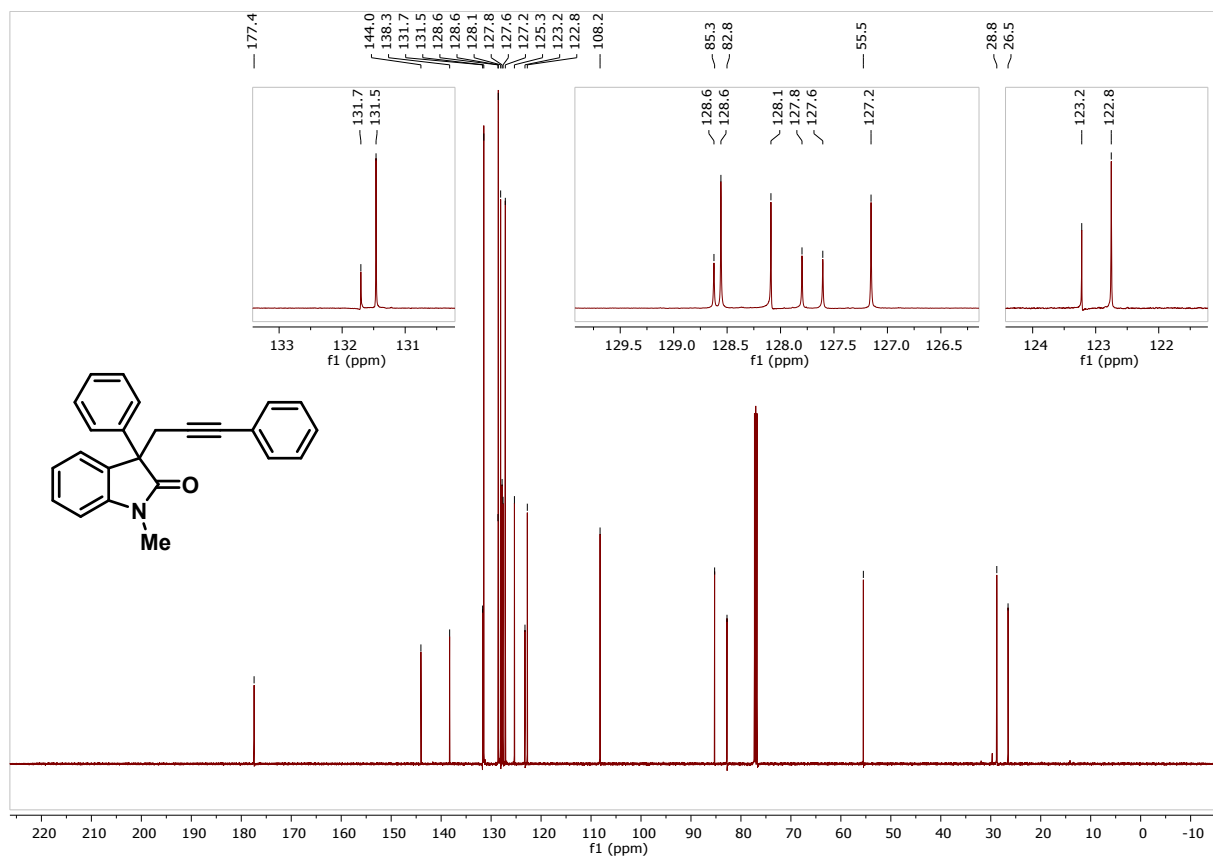
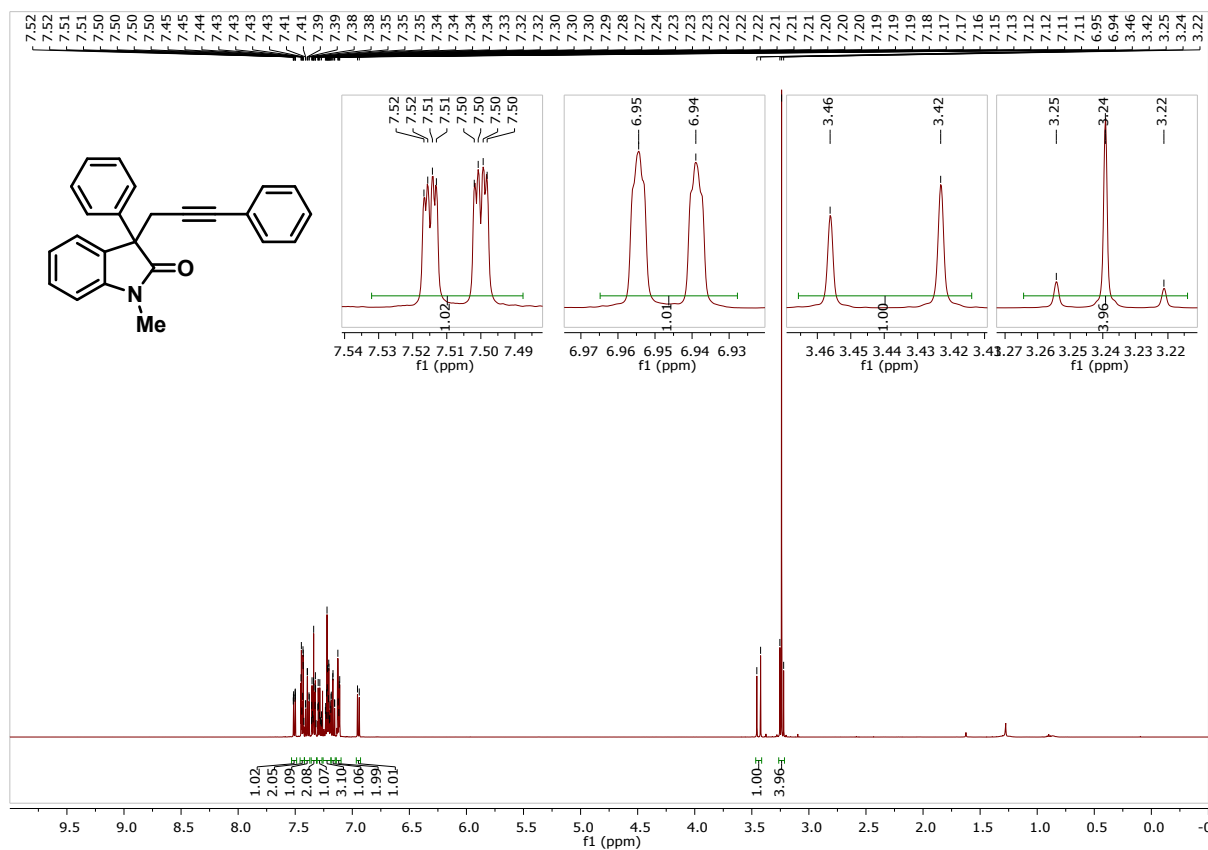


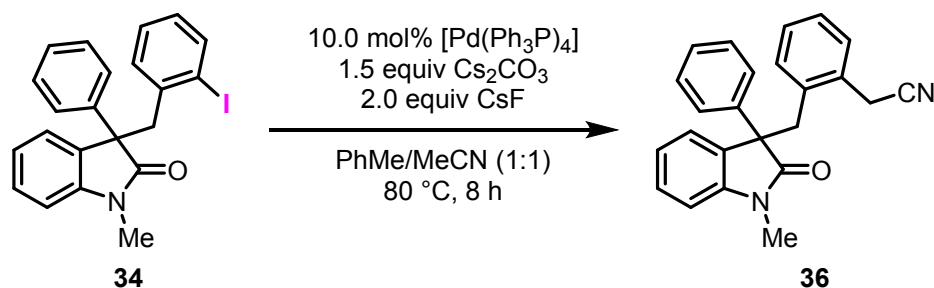
To a flame dried two dram vial under argon atmosphere, *N*-(2-bromophenyl)-*N*-methyl-2-phenylacrylamide **3c** (63.2 mg, 0.2 mmol, 1.0 equiv), $[\text{Pd}(\text{Ph}_3\text{P})_4]$ (23.1 mg, 0.02 mmol, 0.10 equiv), and Cs_2CO_3 (97.7 mg, 0.3 mmol, 1.5 equiv) were added. PhMe (0.1 M) and phenylacetylene **12e** (44 μL , 0.4 mmol, 2.0 equiv) were added in sequence. A Teflon line screw cap was fitted, the vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The pure oxindole **27** was purified by flash column chromatography (hexanes/EtOAc 4:1) and was obtained as a pale orange oil (65 mg, 0.193 mmol, 96% yield).

Spectroscopic data are in agreement with the previously reported: M.-B. Zhou, X.-C. Huang, Y.-Y. Liu, R.-J. Song, and J.-H. Li, *Chem. Eur. J.*, 2014, **20**, 1843.

1-methyl-3-phenyl-3-(3-phenylprop-2-yn-1-yl)indolin-2-one (**27**)

^1H NMR (500 MHz, CDCl_3) δ 7.51 (ddd, J = 7.5, 1.5, 0.5 Hz, 1H), 7.46 – 7.42 (m, 2H), 7.39 (td, J = 7.5, 1.0 Hz, 1H), 7.37 – 7.31 (m, 2H), 7.31 – 7.26 (m, 1H), 7.25 – 7.19 (m, 3H), 7.17 (td, J = 7.5, 1.0 Hz, 1H), 7.14 – 7.10 (m, 2H), 6.98 – 6.92 (m, 1H), 3.44 (d, J = 16.5 Hz, 1H), 3.24 (s, 3H), 3.24 (d, J = 16.5 Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 177.4, 144.0, 138.3, 131.7, 131.5, 128.6, 128.6, 128.1, 127.8, 127.6, 127.2, 125.3, 123.2, 122.8, 108.2, 85.3, 82.8, 55.5, 28.8, 26.5.

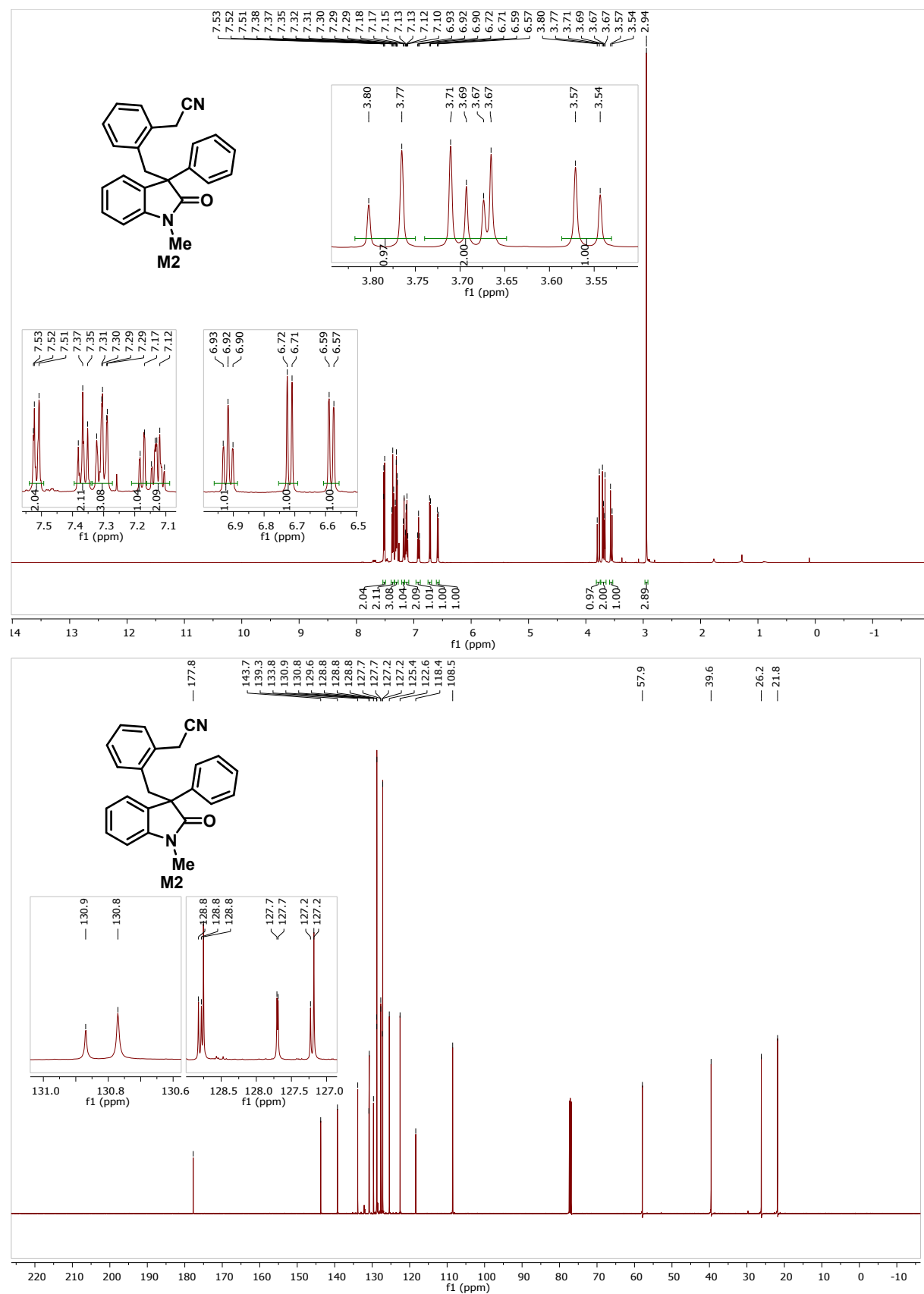


Synthesis of product 36

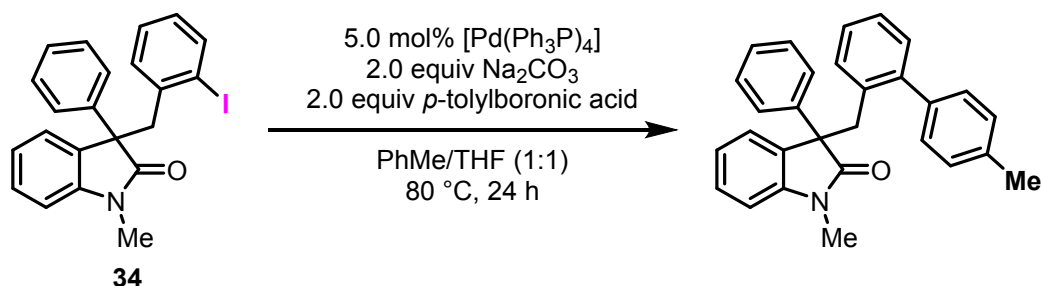
To a flame dried 2 dram vial cooled under argon, 3-(2-iodobenzyl)-1-methyl-3-phenylindolin-2-one **34** (87.9 mg, 0.2 mmol, 1.0 equiv), $[\text{Pd}(\text{Ph}_3\text{P})_4]$ (23.1 mg, 0.02 mmol, 0.1 equiv), CsF (60.8 mg, 0.4 mmol, 2.0 equiv), and Cs_2CO_3 (97.7 mg, 0.3 mmol, 1.5 equiv) were added and allowed to purge for 10 minutes. PhMe/MeCN (1:1) (0.1 M) was added. A Teflon line screw cap was fitted on the two dram vial, sealed with Teflon tape and place in a preheated oil bath at 80°C for 6 hours. The reaction mixture was cooled to room temperature. Once cooled, the reaction was passed through a plug of silica gel using EtOAc . The product was purified by flash column chromatography (hexanes/ EtOAc 4:1) and was obtained as a white foam (36.6 mg, 0.102 mmol, 52% yield).

2-(2-((1-methyl-2-oxo-3-phenylindolin-3-yl)methyl)phenyl)acetonitrile (36)

^1H NMR (500 MHz, CDCl_3) δ 7.56 – 7.48 (m, 2H), 7.37 (m, 2H), 7.33 – 7.27 (m, 3H), 7.18 (m, 1H), 7.16 – 7.09 (m, 2H), 6.92 (m, 1H), 6.72 (d, $J = 8.0$ Hz, 1H), 6.58 (d, $J = 8.0$ Hz, 1H), 3.78 (d, $J = 18.5$ Hz, 1H), 3.71– 3.67 (m, 2H), 3.56 (d, $J = 14.0$ Hz, 1H), 2.94 (s, 3H). **^{13}C NMR** (126 MHz, CDCl_3) δ 177.8, 143.7, 139.3, 133.9, 130.9, 130.8, 129.7, 128.8, 128.8, 127.7, 127.7, 127.2, 127.2, 125.4, 122.6, 118.4, 108.5, 57.9, 39.6, 26.2, 21.8. **IR** (neat film, cm^{-1}) 3057, 3024, 2934, 2247, 1701, 1611, 1493, 1373, 1352, 1258, 1130, 1080, 756. **HRMS** (DART) calculated 353.1648 m/z (found 353.1646 m/z for $\text{C}_{24}\text{H}_{21}\text{N}_2\text{O}$).



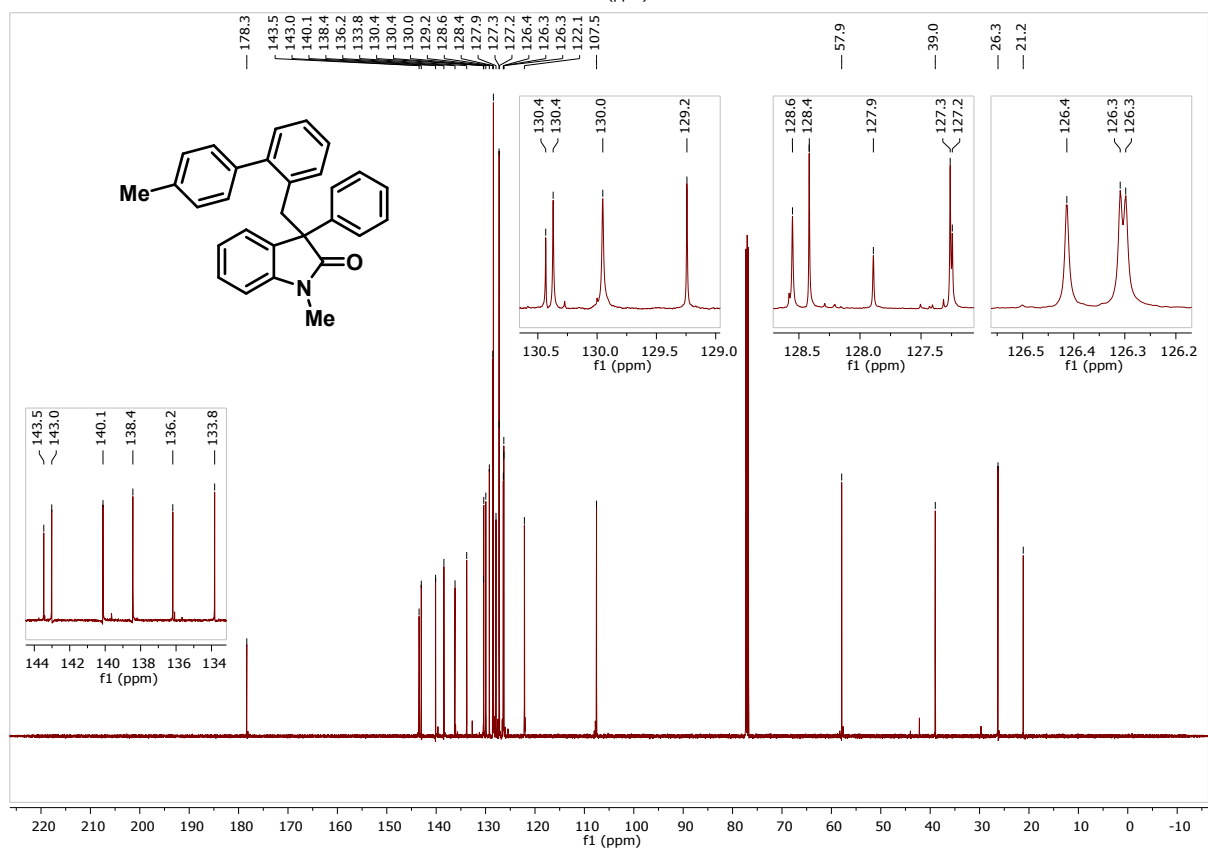
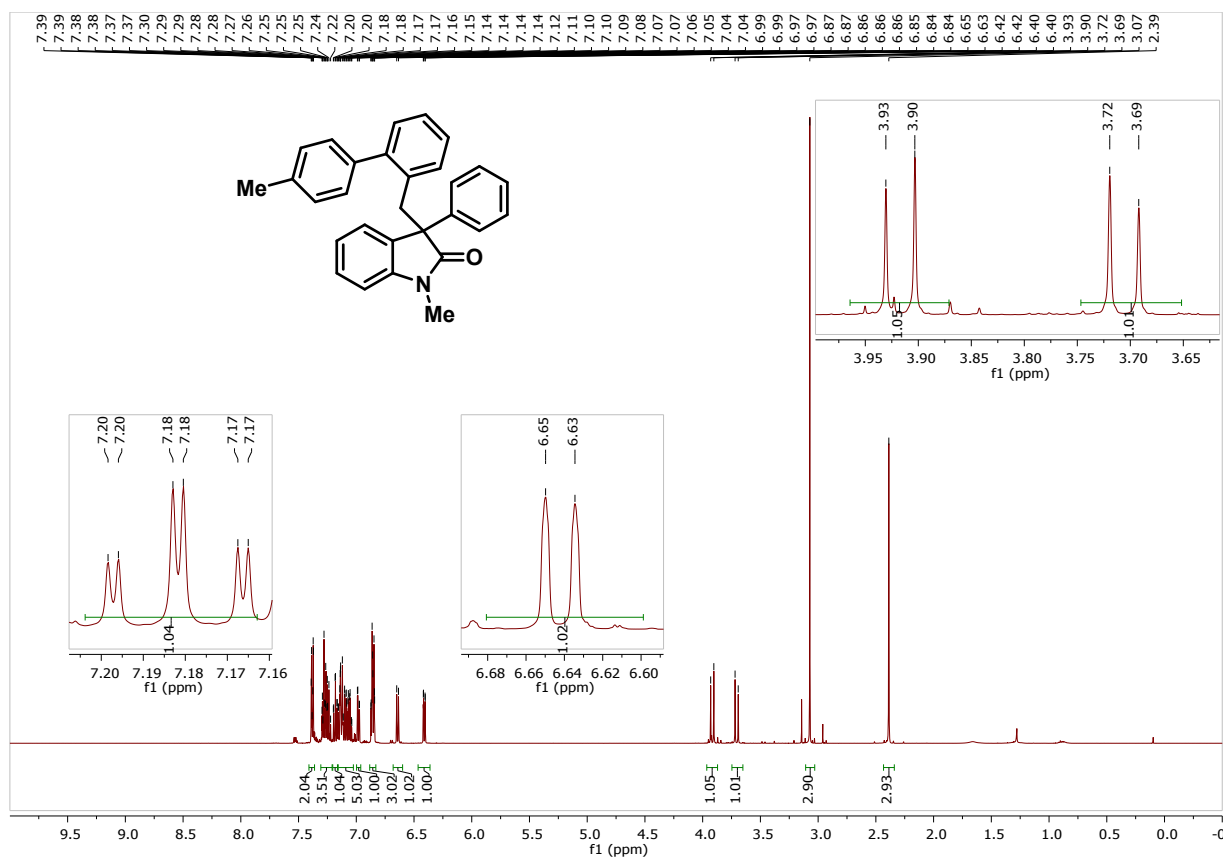
Synthesis of the Suzuki-Miyaura product



To a flame dried 2 dram vial cooled under argon, 3-(2-iodobenzyl)-1-methyl-3-phenylindolin-2-one (87.9 mg, 0.2 mmol, 1.0 equiv), $[\text{Pd}(\text{Ph}_3\text{P})_4]$ (11.6 mg, 0.01 mmol, 0.05 equiv), and *p*-tolylboronic acid (54.4 mg, 0.4 mmol, 2.0 equiv) were added and allowed to purge for 10 minutes. PhMe/THF (1:1) (0.1 M) and Na_2CO_3 (aq.) (0.2 mL (2 M), 0.4 mmol, 2.0 equiv) were added. A Teflon line screw cap was fitted on the two dram vial, sealed with Teflon tape and place in a preheated oil bath at 80°C for 24 hours. The reaction mixture was cooled to room temperature. Once cooled, the reaction was passed through a plug of silica gel using EtOAc. The product was purified by flash column chromatography (hexanes/ CH_2Cl_2 /EtOAc 12:8:1) and was obtained as an off white powder (70.2 mg, 0.174 mmol, 87% yield).

1-methyl-3-((4'-methyl-[1,1'-biphenyl]-2-yl)methyl)-3-phenylindolin-2-one

^1H NMR (500 MHz, CDCl_3) δ 7.41 – 7.35 (m, 2H), 7.31 – 7.21 (m, 3H), 7.18 (td, $J = 7.5$, 1.0 Hz, 1H), 7.16 – 7.02 (m, 5H), 7.01 – 6.96 (m, 1H), 6.90 – 6.82 (m, 3H), 6.64 (d, $J = 7.5$ Hz, 1H), 6.44 – 6.38 (m, 1H), 3.92 (d, $J = 13.5$ Hz, 1H), 3.71 (d, $J = 13.5$ Hz, 1H), 3.07 (s, 3H), 2.39 (s, 3H). **^{13}C NMR** (126 MHz, CDCl_3) δ 178.3, 143.5, 143.0, 140.1, 138.4, 136.2, 133.8, 130.4, 130.4, 130.0, 129.2, 128.6, 128.4, 127.9, 127.3, 127.2, 126.4, 126.3, 126.3, 122.1, 107.5, 57.9, 39.0, 26.3, 21.2. **IR** (neat film, cm^{-1}) 3055, 3022, 2922, 1708, 1613, 1495, 1472, 1447, 1374, 1348, 1258, 1130. **HRMS** (ESI+) calculated 404.20144 m/z (found 404.20087 m/z for $\text{C}_{29}\text{H}_{26}\text{NO}$). **MP** 143–145 $^\circ\text{C}$.



2 – ICM Comparisons between selected Computed and Single-Crystal X-Ray Structures

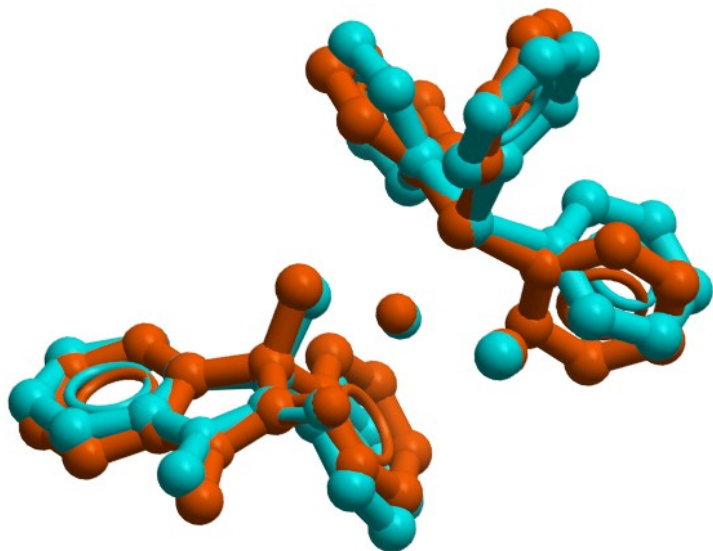


Figure S1. Superimposition of computed **7b** (cyano) and the X-ray structure (orange) from reference 20 in the main text.

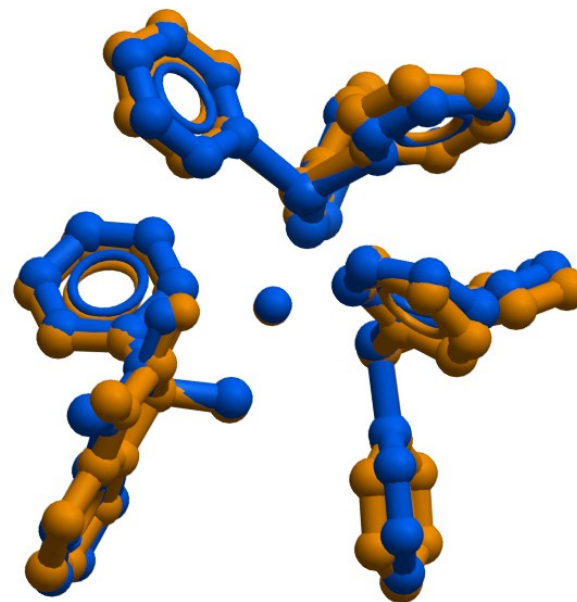


Figure S2. Superimposition of computed palladacycle **11** (yellow) and the X-ray structure (blue) from reference 14 in the main text.

3 – Additional Potential Energy Profiles

The potential energy profiles reported in this section connect transition states to the corresponding IRC/QRC intermediates. Furthermore, the various steps are connected by structural similarities between intermediates.

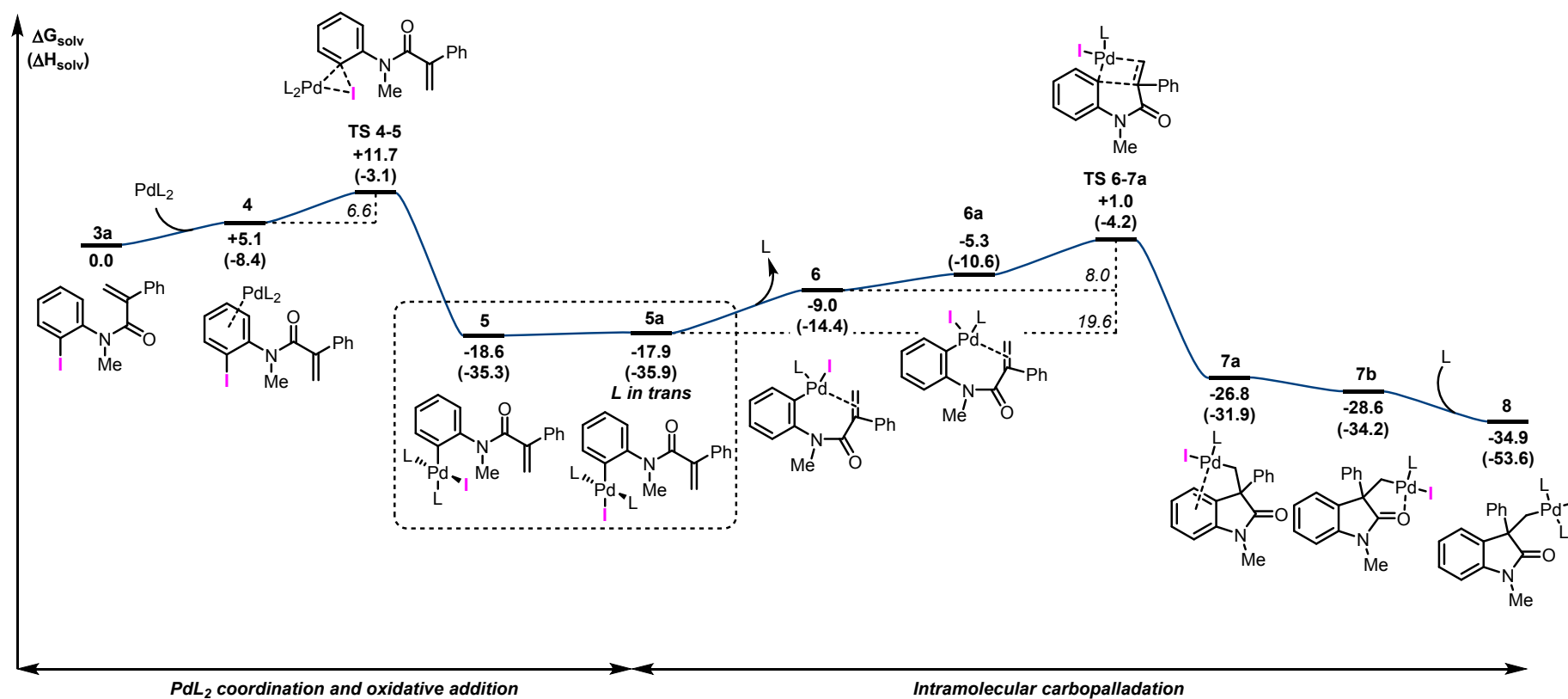


Figure S3. Detailed potential energy surface for the oxidative addition and intramolecular carbopalladation steps ($\text{L} = \text{Ph}_3\text{P}$).

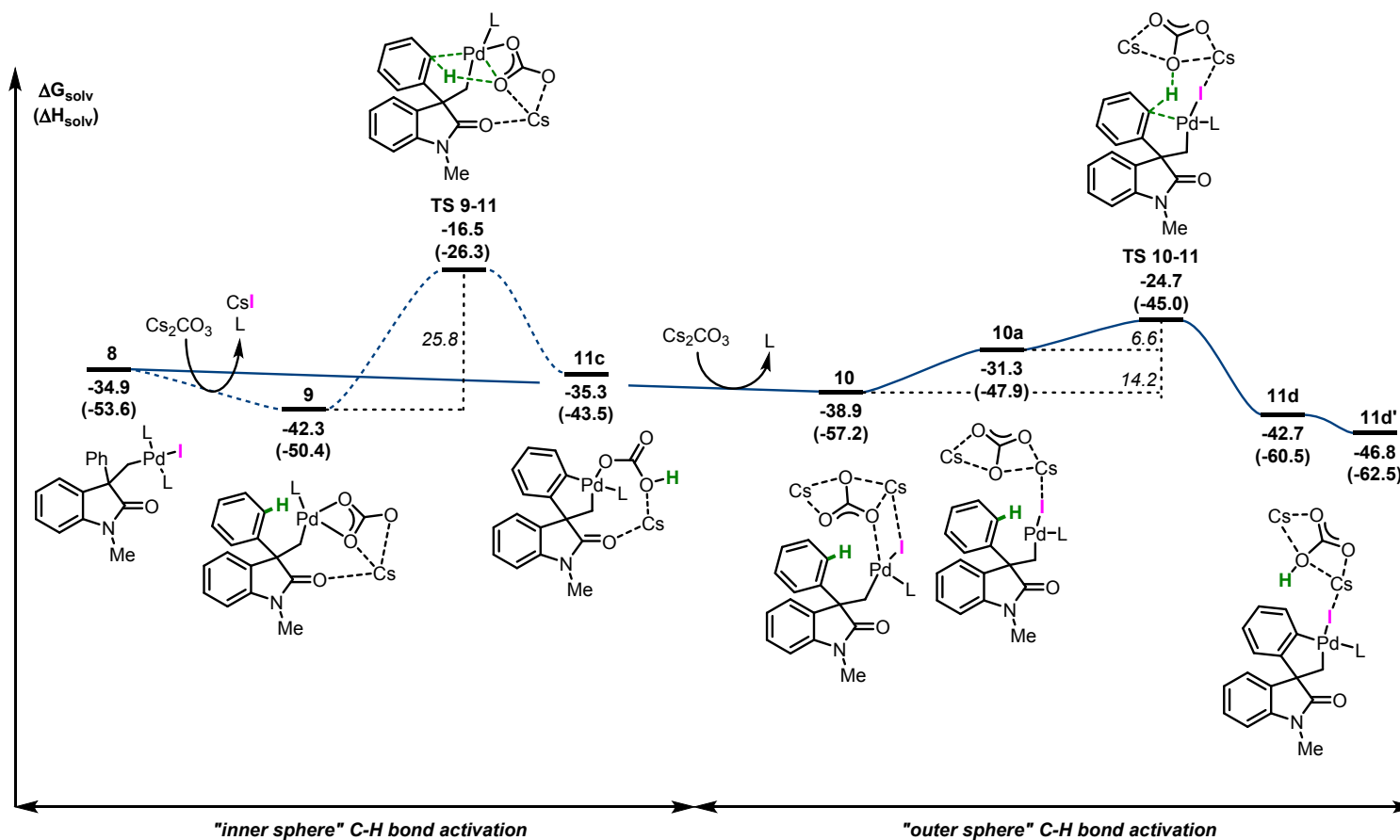


Figure S4. Detailed potential energy surface for the oxidative two possible pathways for the C-H bond activation step (L = Ph₃P).

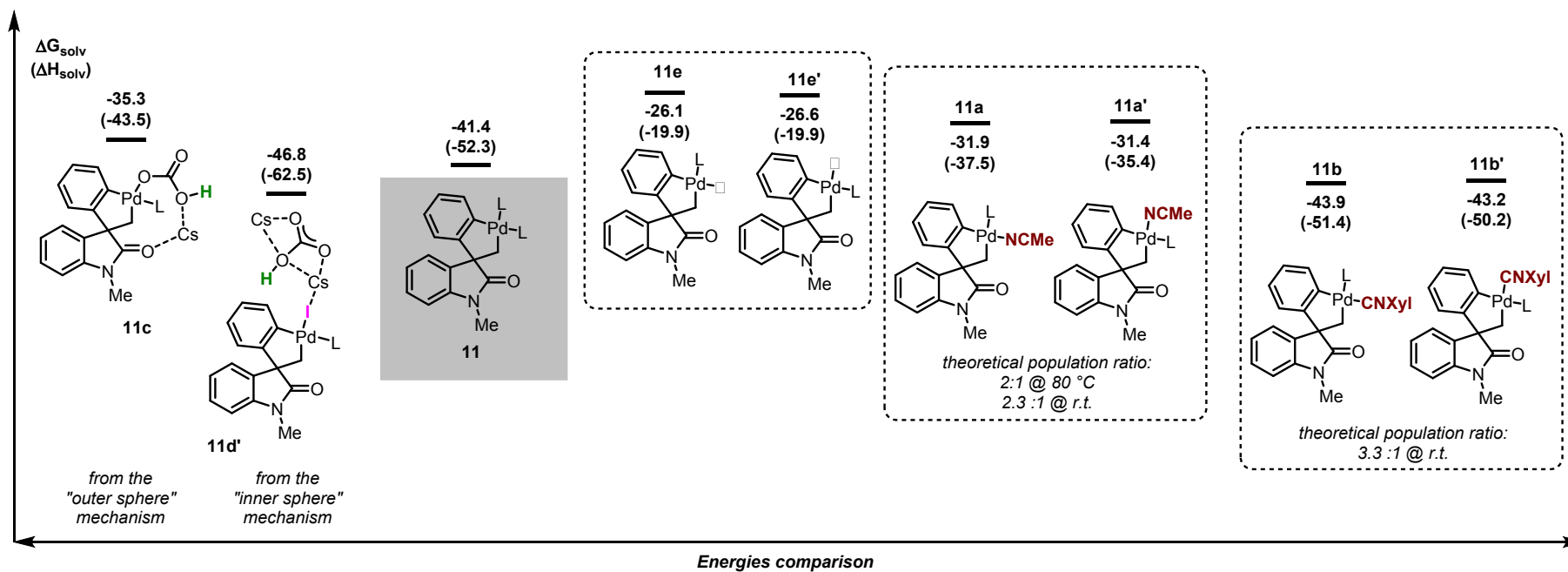


Figure S5. Relative energies of different analogues of **11** (L = Ph₃P).

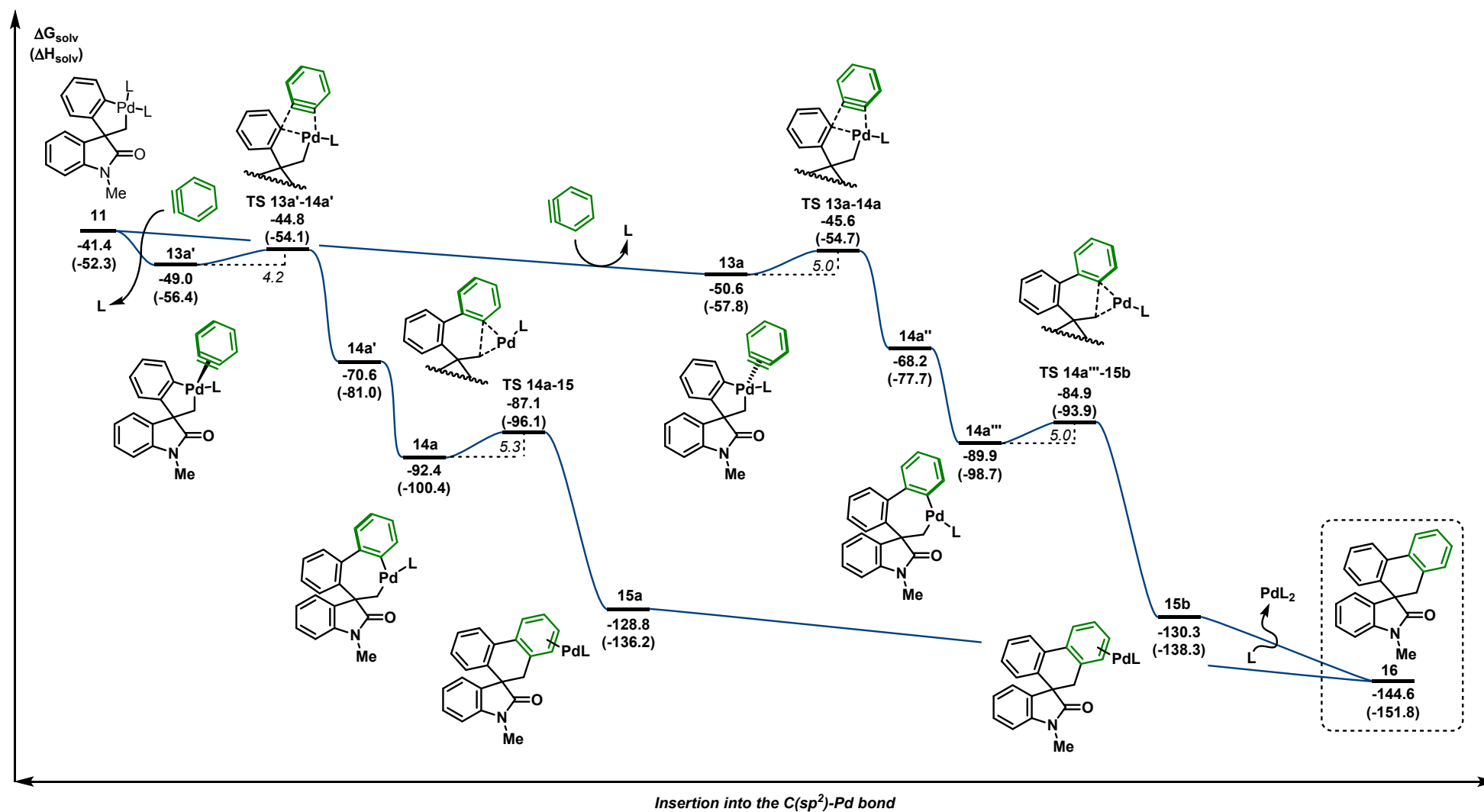


Figure S6. Detailed potential energy surface for the migratory insertion of **12a** into the Pd–C(sp²) bond (L = Ph₃P).

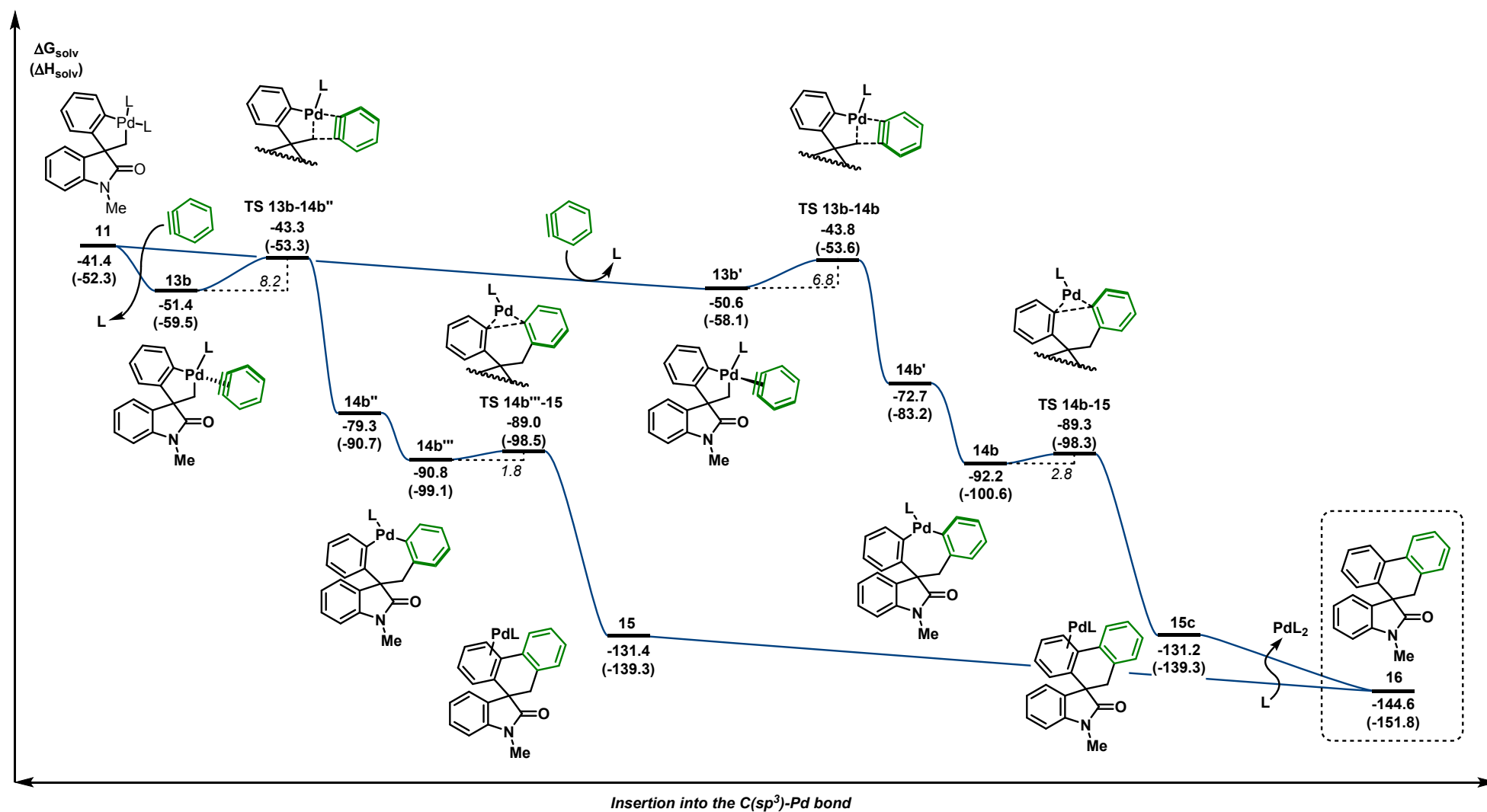


Figure S7. Detailed potential energy surface for the migratory insertion of **12a** into the Pd-C(sp³)-Pd bond (L = Ph₃P).

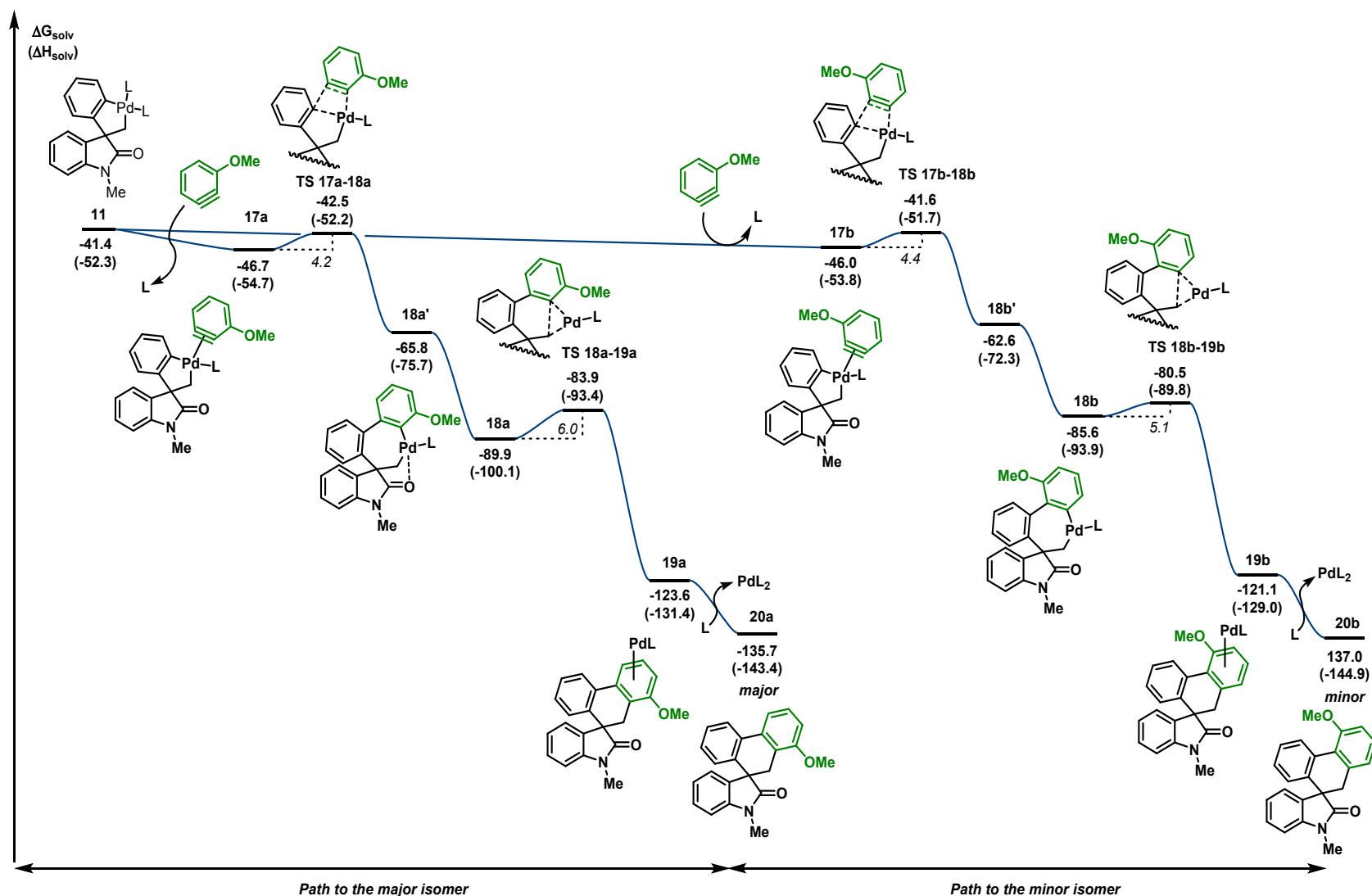


Figure S8. Detailed potential energy surface for the migratory insertion of **12b** into the Pd-C(sp²) bond (L = Ph₃P).

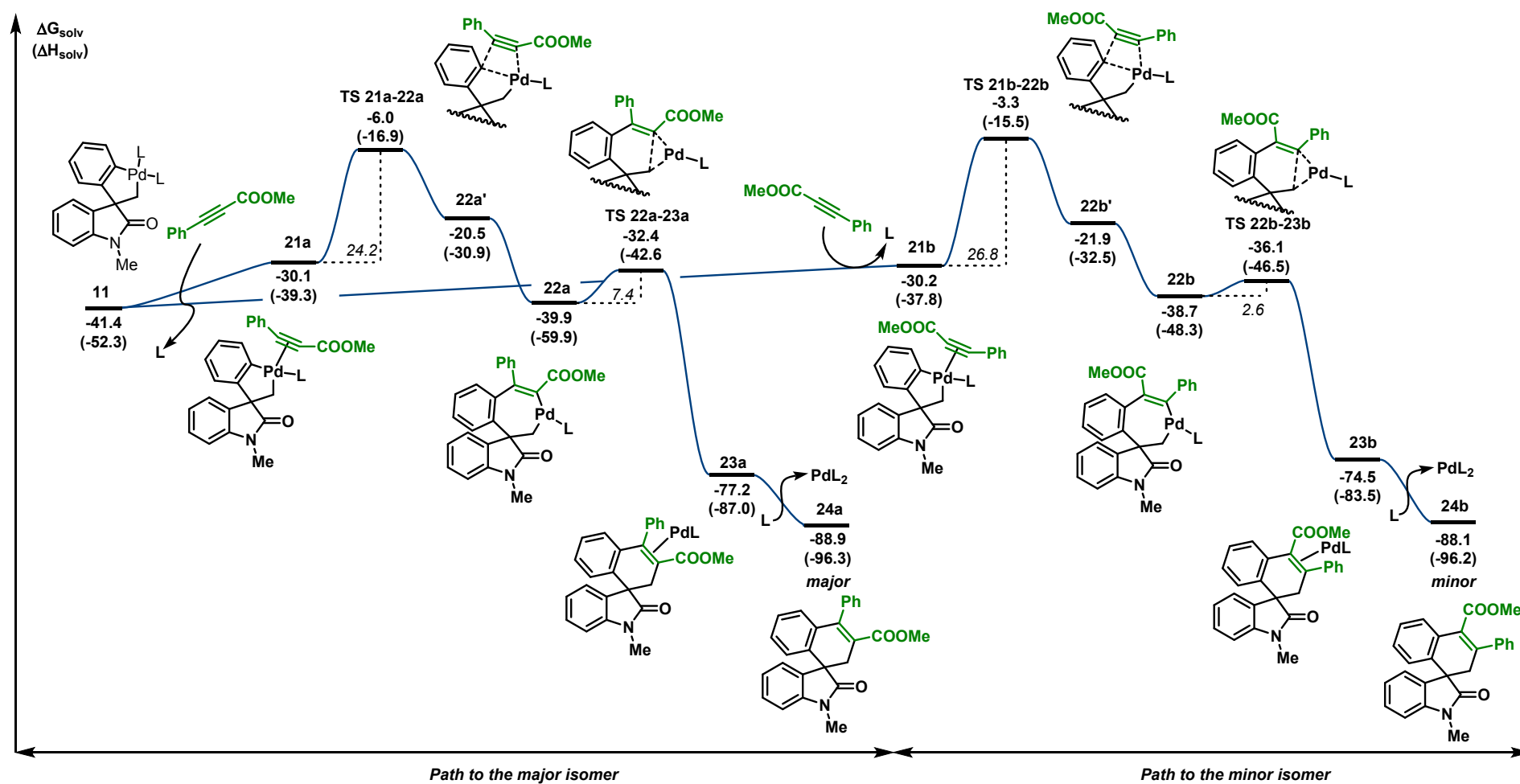


Figure S9. Detailed potential energy surface for the migratory insertion of **12c** into the Pd-C(sp²) bond (L = Ph₃P).

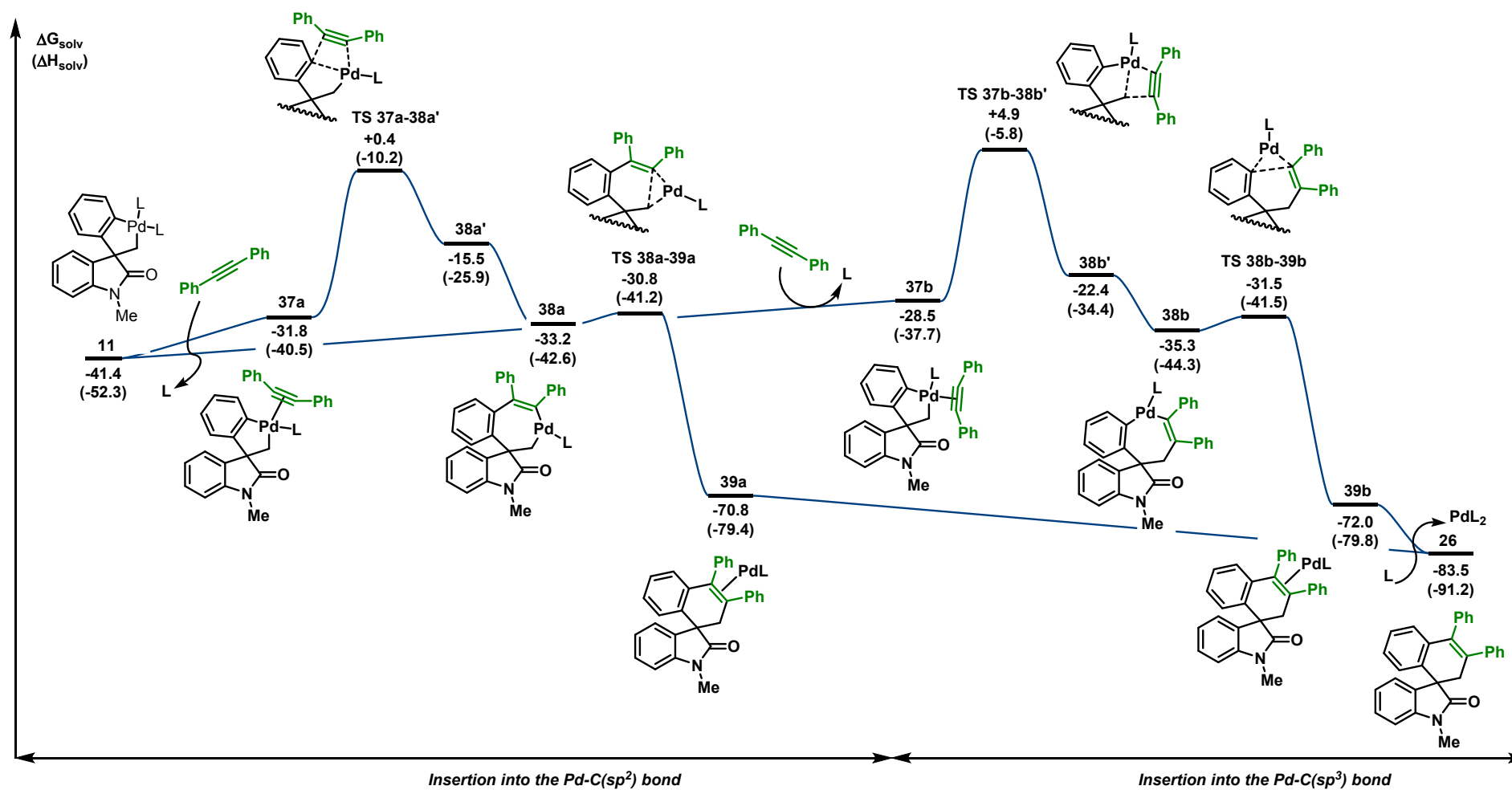


Figure S10. Potential energy surface for the migratory insertion of **12d** into the Pd-C(sp²) and Pd-C(sp³) bonds (L = Ph₃P).

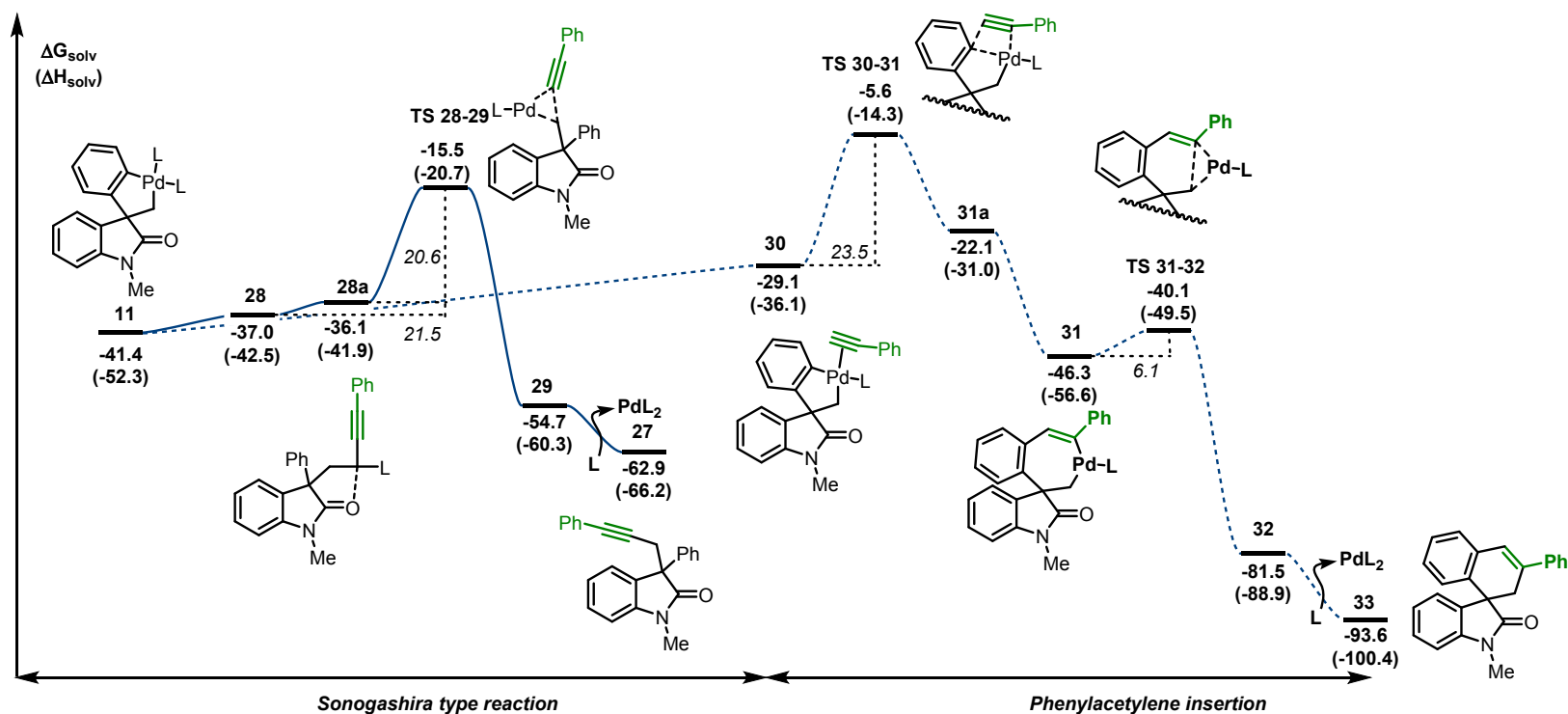


Figure S11. Detailed potential energy surface for comparing between the Sonogashira type reaction and the migratory insertion of alkyne **12e** (L = Ph₃P).

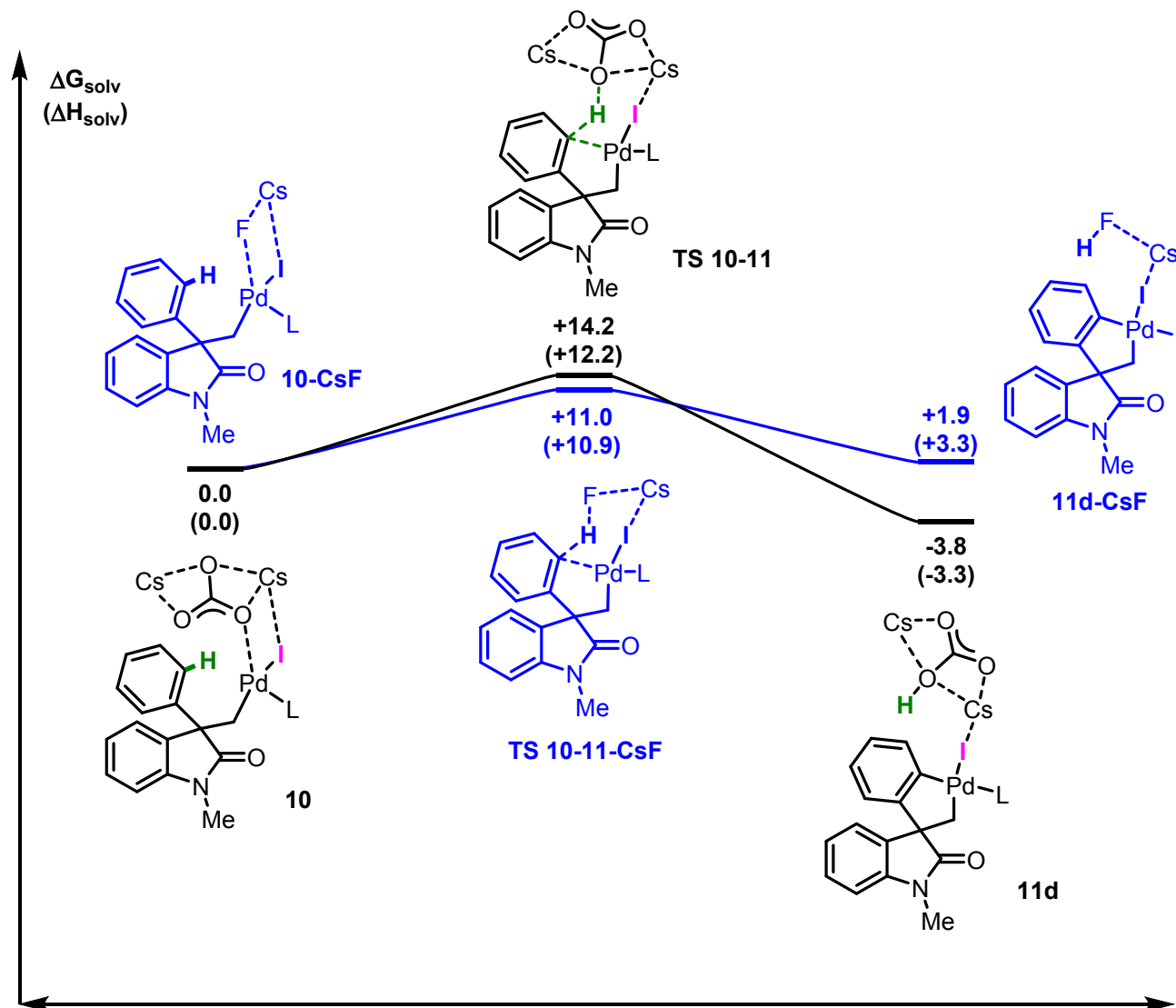


Figure S12. Comparison between the *outer-sphere* type mechanism for the C–H bond activation step with Cs_2CO_3 and CsF ($\text{L} = \text{Ph}_3\text{P}$).

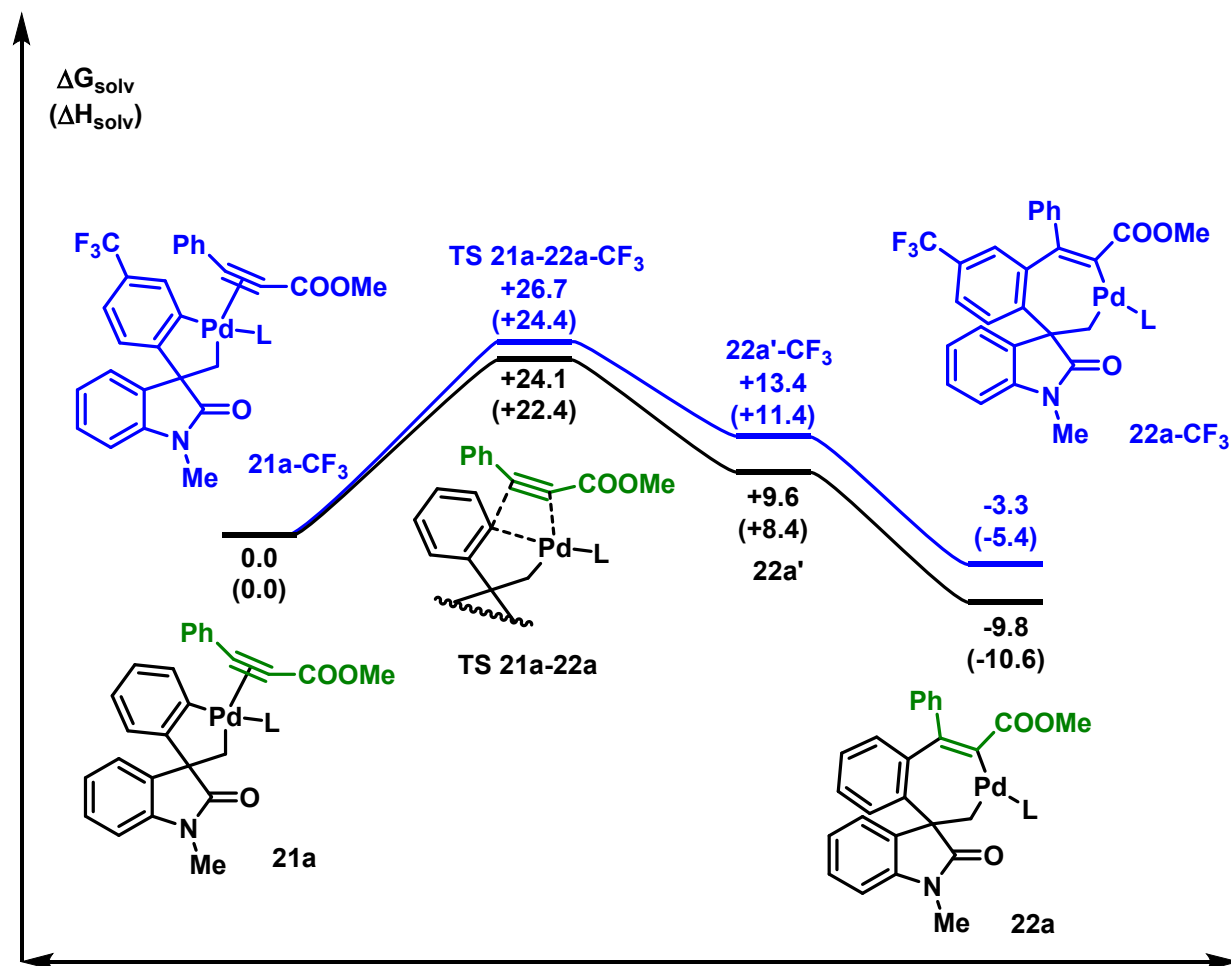


Figure S13. Comparison between the migratory insertion of alkyne **12c** in the presence and in the absence of a trifluoromethyl group in the tethered aromatic ring (L = Ph₃P).

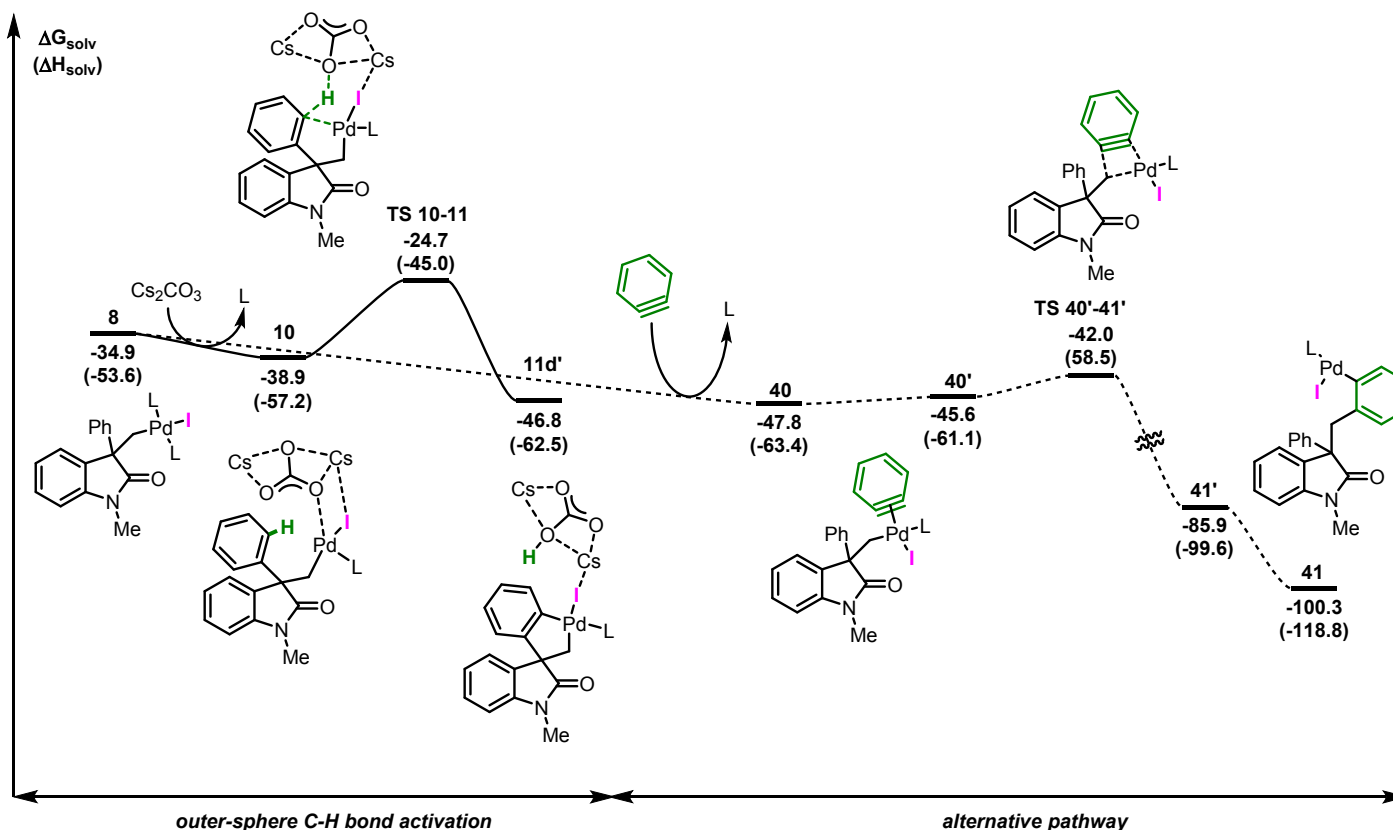


Figure S14. Comparison between C–H bond activation and benzyne migratory insertion in intermediate **8** (L = Ph₃P).

Comment: Comparison between the potential energy profiles for the C–H bond activation and the benzyne migratory insertion in intermediate **8** shows that the latter process would be kinetically and thermodynamically favored. This situation strongly contrast with the experimental data that support the C–H bond activation mechanism (see main text). Evaluation of the energetic for the benzyne coordination to **8** and the geometrical features of intermediate **40** suggests that the DFT calculation may fail in a correct (or even approximate) estimation of the relative energy of this coordination process.

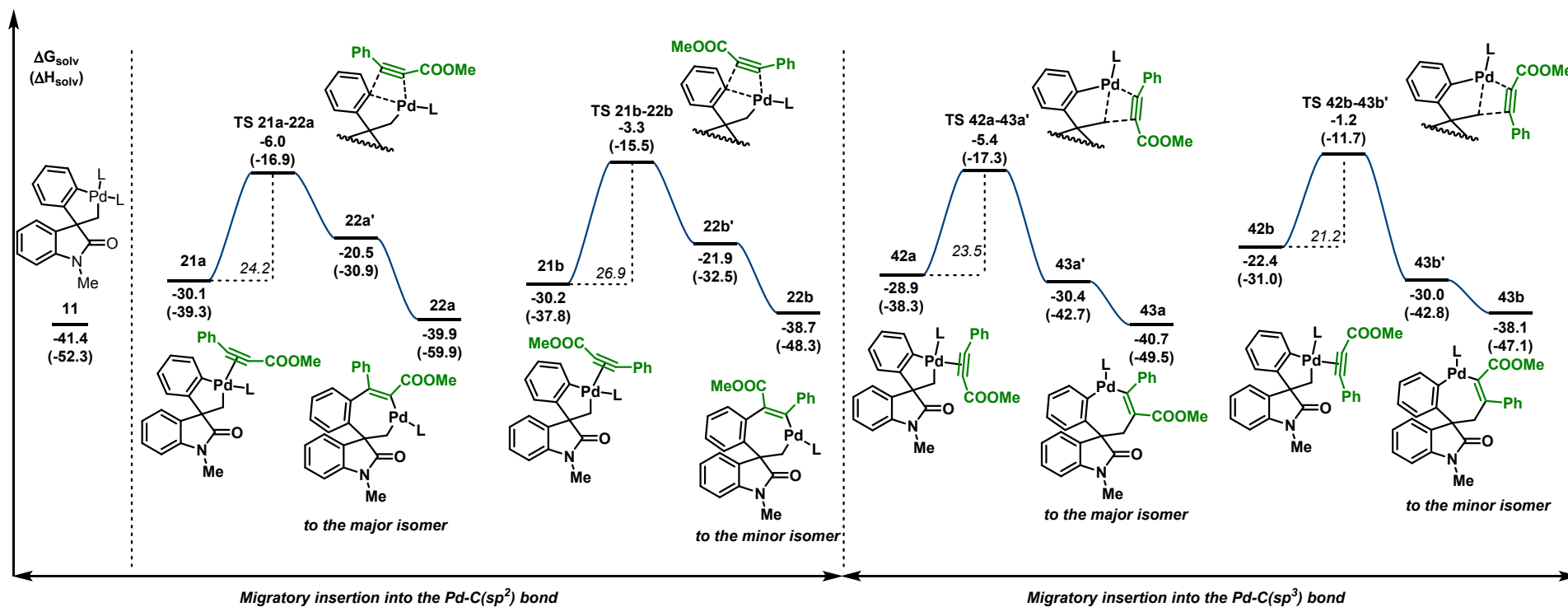


Figure S15. Comparison between the migratory insertion of alkyne **12c** into the Pd-C(sp²) and the Pd-C(sp³) bonds (L = Ph₃P).

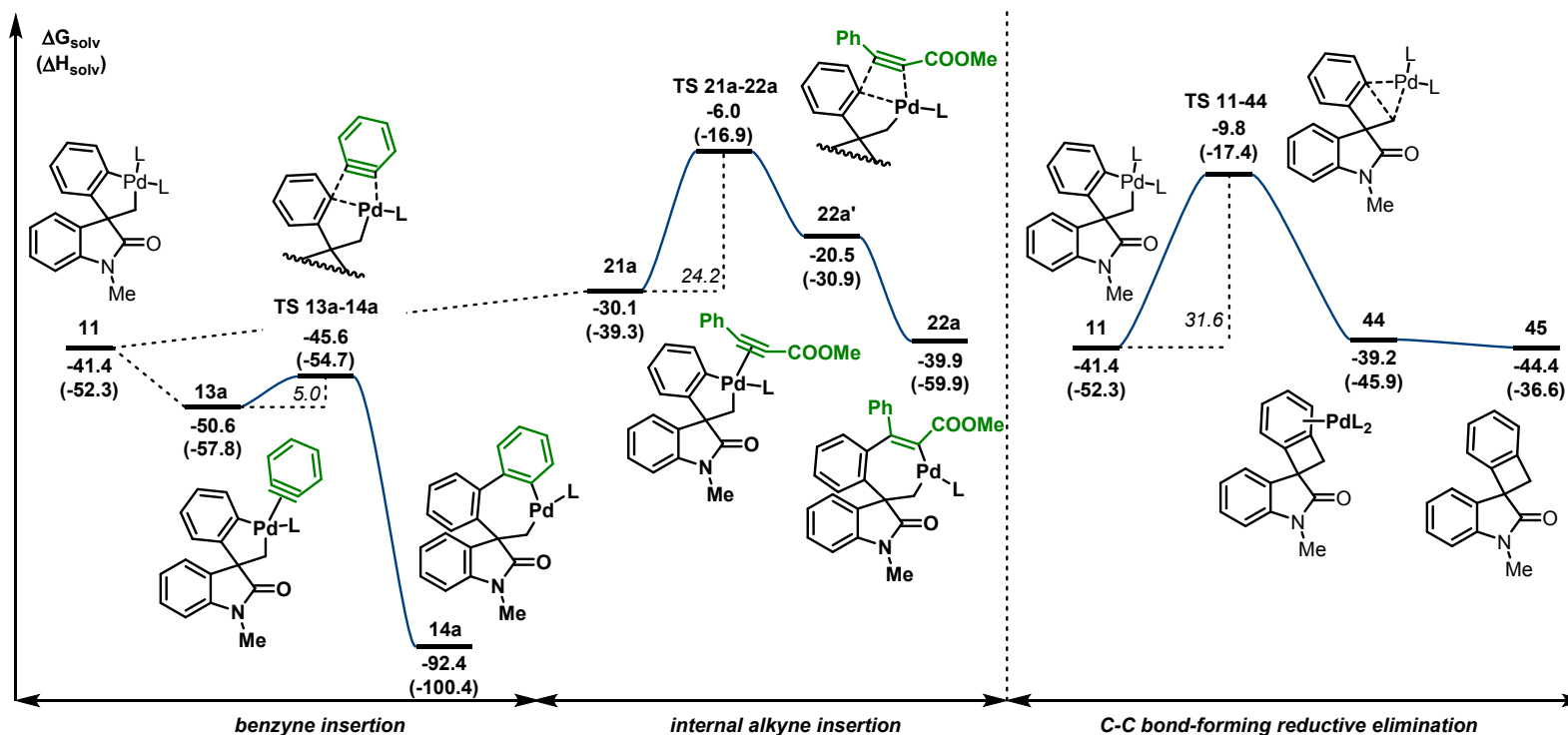
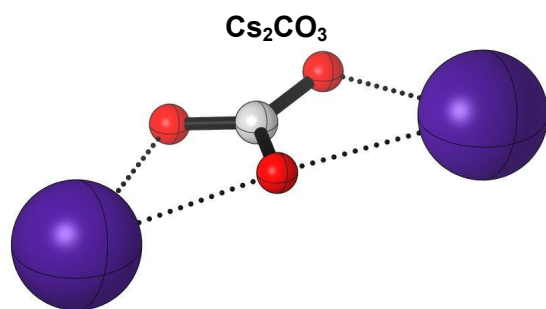


Figure S16. Evaluation of the possible C–C bond-forming reductive elimination process in intermediate **11** and comparison with benzyne and alkyne migratory insertions (L = Ph₃P).

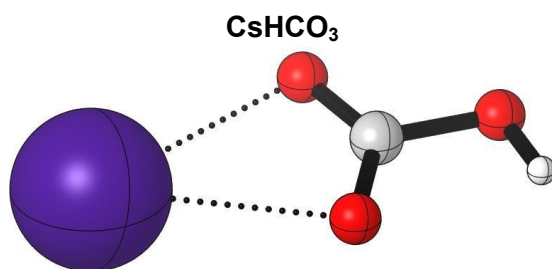
Comment: A potential C–C bond-forming reductive process was evaluate in the case of palladacycle **11**. The results show a pronounced activation energy ($\Delta G^\ddagger = 31.6$ kcal mol⁻¹). Although this process highly unfavored with respect to the insertion of benzyne ($\Delta\Delta G = 35.8$ kcal mol⁻¹), it is slightly favored with respect to the insertion of alkynes ($\Delta\Delta G = -3.8$ kcal mol⁻¹). Experimental data show lack of formation of the Spirocyclobutane product **45** has never been observed in any catalytic reaction suggesting a non-precise estimation of the relative energies between these processes possessing different molecularities.

4 – Energies and Cartesian coordinates for all the intermediates and transition states



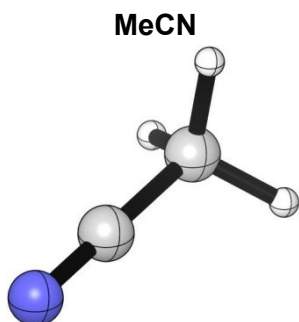
Zero-point correction= 0.013976 (Hartree/Particle)
 Thermal correction to Energy= 0.021531
 Thermal correction to Enthalpy= 0.022476
 Thermal correction to Gibbs Free Energy= -0.024014
 Sum of electronic and zero-point Energies= -303.666289
 Sum of electronic and thermal Energies= -303.658734
 Sum of electronic and thermal Enthalpies= -303.657790
 Sum of electronic and thermal Free Energies= -303.704280
 E(RM06L) = -304.336334552

C	0.00014	1.19037	0.00013
O	1.1256	1.85041	0.02856
O	0.00009	-0.14206	0.0001
O	-1.12542	1.85035	-0.02868
Cs	2.90745	-0.32362	-0.00125
Cs	-2.90751	-0.32359	0.00117



Zero-point correction= 0.026733 (Hartree/Particle)
 Thermal correction to Energy= 0.032313
 Thermal correction to Enthalpy= 0.033257
 Thermal correction to Gibbs Free Energy= -0.005275
 Sum of electronic and zero-point Energies= -284.342741
 Sum of electronic and thermal Energies= -284.337162
 Sum of electronic and thermal Enthalpies= -284.336218
 Sum of electronic and thermal Free Energies= -284.374750
 E(RM06L) = -284.732917610

C	-2.01569	0.04334	0.0002
O	-1.4908	-1.12273	0.00041
O	-1.44537	1.17092	0.00036
O	-3.42036	0.07562	-0.00048
H	-3.64742	-0.8761	-0.00054
Cs	1.2108	-0.00681	-0.00005

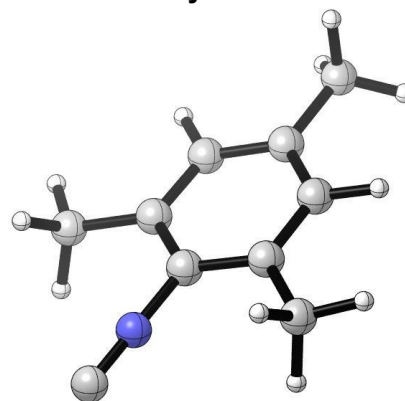


Zero-point correction= 0.044081 (Hartree/Particle)
 Thermal correction to Energy= 0.047725
 Thermal correction to Enthalpy= 0.048669
 Thermal correction to Gibbs Free Energy= 0.021057
 Sum of electronic and zero-point Energies= -132.710534
 Sum of electronic and thermal Energies= -132.706890
 Sum of electronic and thermal Enthalpies= -132.705946

Sum of electronic and thermal Free Energies= -132.733558
 E(RM06L) = -132.792584299

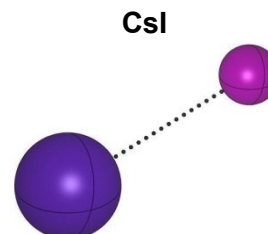
C	0.	0.	-1.18503
H	0.	1.03326	-1.56888
H	-0.89483	-0.51663	-1.56888
H	0.89483	-0.51663	-1.56888
C	0.	0.	0.27709
N	0.	0.	1.45062

XyINC



Zero-point correction= 0.175889 (Hartree/Particle)
 Thermal correction to Energy= 0.187770
 Thermal correction to Enthalpy= 0.188714
 Thermal correction to Gibbs Free Energy= 0.137706
 Sum of electronic and zero-point Energies= -442.237824
 Sum of electronic and thermal Energies= -442.225943
 Sum of electronic and thermal Enthalpies= -442.224999
 Sum of electronic and thermal Free Energies= -442.276007
 E(RM06L) = -442.512906725

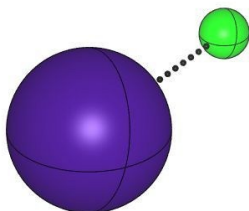
C	-0.1813	-1.24123	-0.00233
C	-0.86634	-0.00001	0.00269
C	-0.1813	1.24123	-0.0023
C	1.22196	1.20909	-0.01026
C	1.94321	0.	-0.01091
C	1.22197	-1.20908	-0.01028
H	1.76793	2.15992	-0.01761
H	1.76794	-2.15991	-0.01766
C	-0.94771	-2.54159	-0.00364
H	-1.59988	-2.62445	0.88346
H	-1.60828	-2.61819	-0.88505
H	-0.26152	-3.40243	-0.0098
C	-0.94773	2.54158	-0.00365
H	-1.60796	2.61835	-0.88531
H	-1.60025	2.62426	0.8832
H	-0.26155	3.40243	-0.0094
C	3.4562	0.00001	0.0155
H	3.83574	-0.00001	1.05407
H	3.8696	-0.89262	-0.48203
H	3.8696	0.89265	-0.482
C	-3.45034	0.	0.01157
N	-2.25473	-0.00001	0.00711



Zero-point correction= 0.000227 (Hartree/Particle)
 Thermal correction to Energy= 0.003323
 Thermal correction to Enthalpy= 0.004267
 Thermal correction to Gibbs Free Energy= -0.027277
 Sum of electronic and zero-point Energies= -31.409059
 Sum of electronic and thermal Energies= -31.405962
 Sum of electronic and thermal Enthalpies= -31.405018
 Sum of electronic and thermal Free Energies= -31.436563

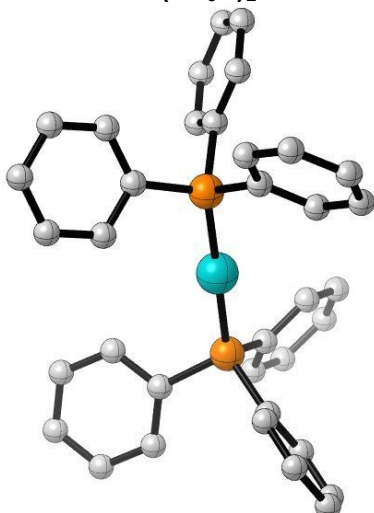
E(RM06L) = -318.140125234

Cs	0.	0.	1.76926
I	0.	0.	-1.83603

CsF

Zero-point correction= 0.000664 (Hartree/Particle)
 Thermal correction to Energy= 0.003455
 Thermal correction to Enthalpy= 0.004400
 Thermal correction to Gibbs Free Energy= -0.023534
 Sum of electronic and zero-point Energies= -119.733986
 Sum of electronic and thermal Energies= -119.731195
 Sum of electronic and thermal Enthalpies= -119.730250
 Sum of electronic and thermal Free Energies= -119.758184
 E(RM06L) = -120.096110519

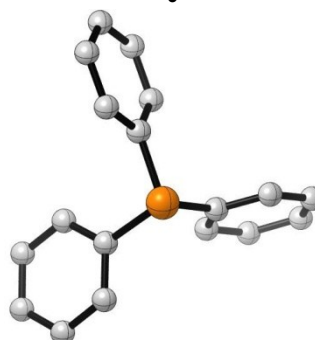
F	0.	0.	-2.23656
Cs	0.	0.	0.36598

Pd(Ph₃P)₂

Zero-point correction= 0.533519 (Hartree/Particle)
 Thermal correction to Energy= 0.570400
 Thermal correction to Enthalpy= 0.571344
 Thermal correction to Gibbs Free Energy= 0.455359
 Sum of electronic and zero-point Energies= -2198.966152
 Sum of electronic and thermal Energies= -2198.929272
 Sum of electronic and thermal Enthalpies= -2198.928328
 Sum of electronic and thermal Free Energies= -2199.044313
 E(RM06L) = -2200.99044489

Pd	0.00327	-0.00932	0.00537
P	-2.29606	-0.00648	-0.00668
P	2.30415	0.00217	0.00065
C	3.09972	-1.06979	-1.28805
C	4.34459	-1.71037	-1.11349
C	2.39948	-1.24926	-2.50147
C	4.88331	-2.50404	-2.14006
H	4.88831	-1.59778	-0.16966
C	2.94389	-2.03465	-3.52818
H	1.41531	-0.7791	-2.61803
C	4.18742	-2.66431	-3.34899
H	5.84792	-3.00153	-1.99145
H	2.39073	-2.16581	-4.46444
H	4.60774	-3.28706	-4.14597
C	3.0903	-0.57702	1.57907
C	4.32084	-0.09238	2.07091

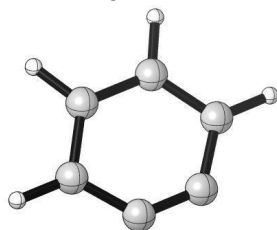
C	2.39551	-1.5598	2.31778
C	4.85161	-0.59506	3.27076
H	4.8598	0.68718	1.5222
C	2.93131	-2.06558	3.51124
H	1.42218	-1.90674	1.94884
C	4.16159	-1.58405	3.99004
H	5.80547	-0.20818	3.64571
H	2.38189	-2.8278	4.07412
H	4.57609	-1.97069	4.92724
C	3.0775	1.6634	-0.28701
C	4.3073	1.85321	-0.95205
C	2.37331	2.79095	0.19011
C	4.82751	3.14712	-1.12278
H	4.85248	0.99026	-1.349
C	2.9001	4.08071	0.02733
H	1.40003	2.63891	0.67309
C	4.1288	4.26113	-0.63022
H	5.78017	3.28383	-1.64609
H	2.34426	4.94693	0.40189
H	4.53599	5.26858	-0.76775
C	-3.09087	-0.02382	1.67129
C	-2.40372	0.63254	2.71611
C	-4.3236	-0.65077	1.94953
C	-2.95016	0.68205	4.00701
H	-1.429	1.0886	2.50246
C	-4.86509	-0.60663	3.24521
H	-4.85486	-1.18454	1.15458
C	-4.18294	0.06253	4.27398
H	-2.4071	1.19476	4.80822
H	-5.82067	-1.1013	3.45084
H	-4.60556	0.09199	5.284
C	-3.08097	1.46286	-0.82597
C	-2.37992	2.05888	-1.89752
C	-4.32132	2.00689	-0.4308
C	-2.91927	3.16322	-2.57389
H	-1.39984	1.6535	-2.17778
C	-4.85516	3.118	-1.1046
H	-4.86384	1.56837	0.41326
C	-4.15831	3.69507	-2.17823
H	-2.36582	3.61679	-3.40311
H	-5.81588	3.53633	-0.78525
H	-4.5747	4.56403	-2.69903
C	-3.08265	-1.45111	-0.86602
C	-4.30916	-1.38005	-1.56051
C	-2.39561	-2.68377	-0.81022
C	-4.84294	-2.52587	-2.17378
H	-4.84065	-0.42534	-1.63351
C	-2.93618	-3.82834	-1.41447
H	-1.42548	-2.72477	-0.29961
C	-4.16142	-3.75136	-2.09791
H	-5.79299	-2.45856	-2.71506
H	-2.3936	-4.77841	-1.36322
H	-4.57923	-4.64214	-2.57919

Ph₃P

Zero-point correction= 0.265537 (Hartree/Particle)
 Thermal correction to Energy= 0.281911
 Thermal correction to Enthalpy= 0.282855
 Thermal correction to Gibbs Free Energy= 0.219485
 Sum of electronic and zero-point Energies= -1036.053209
 Sum of electronic and thermal Energies= -1036.036835
 Sum of electronic and thermal Enthalpies= -1036.035891
 Sum of electronic and thermal Free Energies= -1036.099260
 E(RM06L) = -1036.45087228

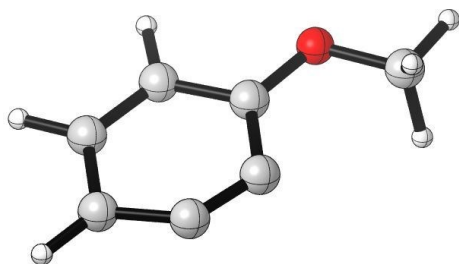
P	-0.0037	-0.00178	-1.22427
C	0.60543	1.55735	-0.41205
C	1.7367	2.178	-0.99592

C	-0.00592	2.16756	0.7052
C	2.25173	3.368	-0.46194
H	2.2098	1.72761	-1.8745
C	0.50272	3.36581	1.22873
H	-0.88788	1.70621	1.16188
C	1.63771	3.96816	0.65155
H	3.13296	3.83551	-0.92347
H	0.01449	3.83075	2.09266
H	2.03215	4.9029	1.06022
C	-1.65454	-0.25668	-0.40886
C	-1.85708	-1.01989	0.76064
C	-2.77528	0.33663	-1.03936
C	-3.1483	-1.18051	1.28964
H	-1.00285	-1.49059	1.25404
C	-4.05939	0.18489	-0.49959
H	-2.63375	0.91258	-1.96049
C	-4.25168	-0.57456	0.66597
H	-3.29191	-1.77659	2.19607
H	-4.91667	0.6538	-0.99763
H	-5.25727	-0.70311	1.08051
C	1.04608	-1.30181	-0.40658
C	1.08189	-2.57227	-1.02538
C	1.81823	-1.09008	0.75389
C	1.85478	-3.61089	-0.48619
H	0.50223	-2.74479	-1.93862
C	2.60215	-2.12731	1.28543
H	1.80862	-0.10772	1.23967
C	2.62139	-3.39022	0.67349
H	1.86963	-4.59167	-0.97329
H	3.19992	-1.9468	2.1872
H	3.2363	-4.19436	1.08779

Benzene – 12a

Zero-point correction= 0.072967 (Hartree/Particle)
 Thermal correction to Energy= 0.077579
 Thermal correction to Enthalpy= 0.078524
 Thermal correction to Gibbs Free Energy= 0.045521
 Sum of electronic and zero-point Energies= -230.841772
 Sum of electronic and thermal Energies= -230.837159
 Sum of electronic and thermal Enthalpies= -230.836215
 Sum of electronic and thermal Free Energies= -230.869218
 E(RM06L) = -230.961584887

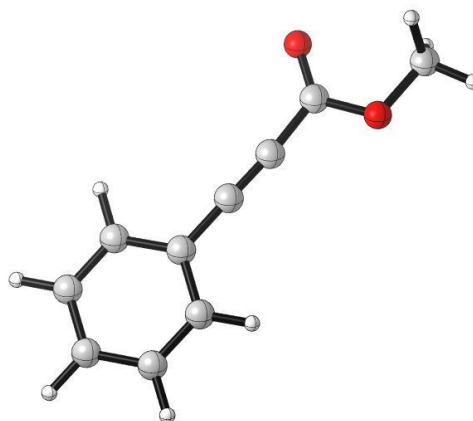
C	1.47178	-0.13557	-0.00001
C	0.63222	-1.24339	0.00001
C	-0.63234	-1.2434	0.00001
C	-1.47178	-0.13547	-0.00001
C	-0.70562	1.06394	0.
C	0.7057	1.06389	0.
H	2.56545	-0.13318	0.
H	-2.56545	-0.13299	0.
H	-1.23665	2.02313	0.00001
H	1.23679	2.02305	0.00002

3-methoxybenzene – 12b

Zero-point correction= 0.104494 (Hartree/Particle)
 Thermal correction to Energy= 0.111814

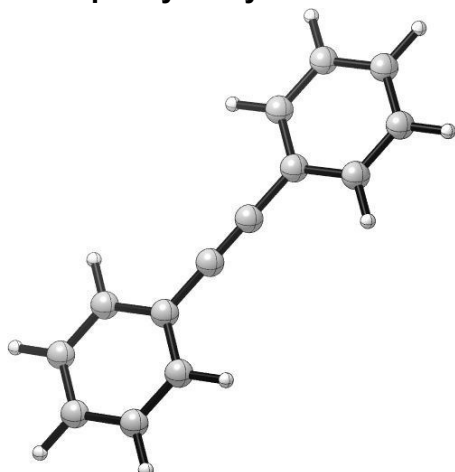
Thermal correction to Enthalpy= 0.112759
 Thermal correction to Gibbs Free Energy= 0.072851
 Sum of electronic and zero-point Energies= -345.343469
 Sum of electronic and thermal Energies= -345.336149
 Sum of electronic and thermal Enthalpies= -345.335205
 Sum of electronic and thermal Free Energies= -345.375112
 E(RM06L) = -345.522727065

C	-2.35162	-0.53513	0.00001
C	-1.21805	-1.31971	0.00004
C	0.03	-1.09753	-0.00013
C	0.47895	0.23384	-0.00003
C	-0.56927	1.20266	0.
C	-1.92273	0.82767	0.00004
H	-3.39869	-0.84021	0.0001
H	-2.69024	1.61103	0.00011
H	-0.29239	2.26164	0.00002
O	1.76931	0.66327	-0.00009
C	2.75182	-0.38214	0.0001
H	3.72998	0.119	0.00012
H	2.65102	-1.01767	0.89866
H	2.65117	-1.01785	-0.89835

Methyl 3-phenylpropionate – 12c

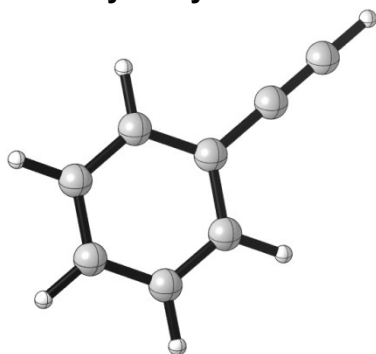
Zero-point correction= 0.148489 (Hartree/Particle)
 Thermal correction to Energy= 0.159872
 Thermal correction to Enthalpy= 0.160816
 Thermal correction to Gibbs Free Energy= 0.109152
 Sum of electronic and zero-point Energies= -536.129046
 Sum of electronic and thermal Energies= -536.117663
 Sum of electronic and thermal Enthalpies= -536.116719
 Sum of electronic and thermal Free Energies= -536.168383
 E(RM06L) = -536.404742888

C	1.21837	0.17482	0.00067
C	-0.00803	0.1093	0.00056
C	-1.42984	0.02121	0.00035
C	-2.07225	-1.24378	0.00031
C	-2.21991	1.19966	-0.00003
C	-3.46911	-1.32138	-0.00005
H	-1.46082	-2.15063	0.00057
C	-3.61597	1.10881	-0.00044
H	-1.72182	2.17332	0.00007
C	-4.24361	-0.14863	-0.00044
H	-3.95737	-2.30104	-0.00005
H	-4.21835	2.02272	-0.00075
H	-5.33631	-0.21473	-0.00079
C	2.64709	0.37164	0.0003
O	3.3049	-0.82802	0.00004
C	4.74727	-0.70201	-0.00072
H	5.09106	-0.15904	0.89426
H	5.12722	-1.73233	-0.0007
H	5.09014	-0.15944	-0.8963
O	3.20287	1.46593	0.00004

Diphenylacetylene – 12d

Zero-point correction= 0.185746 (Hartree/Particle)
 Thermal correction to Energy= 0.197246
 Thermal correction to Enthalpy= 0.198190
 Thermal correction to Gibbs Free Energy= 0.146707
 Sum of electronic and zero-point Energies= -539.274581
 Sum of electronic and thermal Energies= -539.263081
 Sum of electronic and thermal Enthalpies= -539.262137
 Sum of electronic and thermal Free Energies= -539.313620
 E(RM06L) = -539.576061597

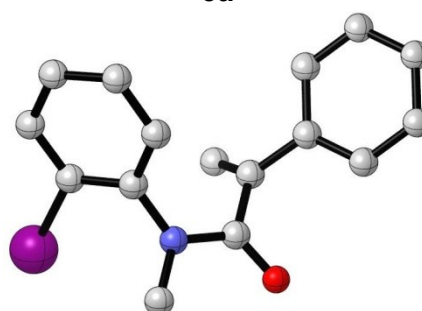
C	-0.08193	-0.60966	-0.00001
C	0.08193	0.60966	-0.00001
C	-0.27195	-2.02113	-0.00001
C	-1.57917	-2.57505	-0.00006
C	0.84219	-2.90116	0.00005
C	-1.75967	-3.96253	-0.00005
H	-2.44084	-1.90112	-0.0001
C	0.64932	-4.28696	0.00006
H	1.8514	-2.47906	0.00009
C	-0.64932	-4.82384	0.00001
H	-2.77373	-4.37551	-0.00009
H	1.51805	-4.95343	0.00011
H	-0.79546	-5.90871	0.00002
C	0.27195	2.02113	-0.00001
C	1.57917	2.57505	-0.00006
C	-0.84219	2.90116	0.00005
C	1.75967	3.96253	-0.00005
H	2.44084	1.90112	-0.0001
C	-0.64932	4.28696	0.00006
H	-1.8514	2.47906	0.00009
C	0.64932	4.82384	0.00001
H	2.77373	4.37551	-0.00009
H	-1.51805	4.95343	0.00011
H	0.79546	5.90871	0.00002

Phenylacetylene – 12e

Zero-point correction= 0.106028 (Hartree/Particle)
 Thermal correction to Energy= 0.112762
 Thermal correction to Enthalpy= 0.113706
 Thermal correction to Gibbs Free Energy= 0.075402
 Sum of electronic and zero-point Energies= -308.285024
 Sum of electronic and thermal Energies= -308.278290
 Sum of electronic and thermal Enthalpies= -308.277346

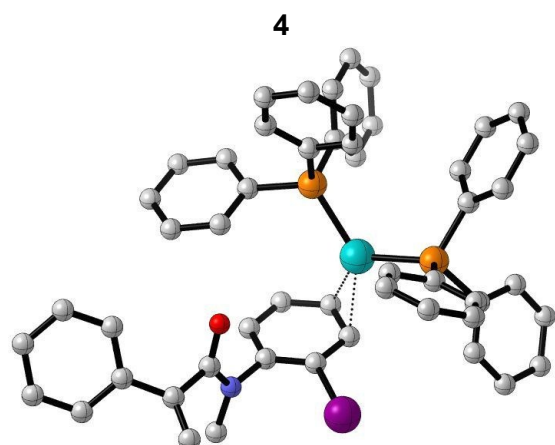
Sum of electronic and thermal Free Energies= -308.315650
 E(RM06L) = -308.461832106

C	3.25226	-0.00001	0.00001
H	4.32555	-0.00003	0.00004
C	2.02947	0.00003	-0.00002
C	0.5995	0.00001	-0.00001
C	-0.12021	1.22114	0.
C	-0.12018	-1.22112	-0.00001
C	-1.52007	1.21535	0.
H	0.43346	2.16454	-0.00001
C	-1.52005	-1.21537	0.
H	0.43351	-2.16451	-0.00001
C	-2.22468	-0.00002	0.00001
H	-2.0647	2.16512	0.
H	-2.06463	-2.16517	0.00001
H	-3.3194	-0.00003	0.00001

3a

Zero-point correction= 0.251053 (Hartree/Particle)
 Thermal correction to Energy= 0.269013
 Thermal correction to Enthalpy= 0.269957
 Thermal correction to Gibbs Free Energy= 0.201879
 Sum of electronic and zero-point Energies= -759.251768
 Sum of electronic and thermal Energies= -759.233808
 Sum of electronic and thermal Enthalpies= -759.232864
 Sum of electronic and thermal Free Energies= -759.300942
 E(RM06L) = -1046.14363480

C	0.03808	2.84548	1.21001
C	0.32717	1.47924	1.31121
C	-0.57089	0.50154	0.82858
C	-1.78245	0.94422	0.25369
C	-2.09044	2.30942	0.16576
C	-1.17577	3.2614	0.64327
H	0.75634	3.58159	1.58387
H	1.26274	1.13962	1.76654
H	-3.0342	2.62773	-0.28433
H	-1.41855	4.3259	0.56596
I	-3.18909	-0.46277	-0.57214
C	0.91066	-1.45344	0.46415
C	1.57633	-0.73336	-0.68962
C	0.88277	-0.56103	-1.83858
H	-0.17314	-0.83775	-1.91501
H	1.36465	-0.16781	-2.73968
C	3.00408	-0.33587	-0.53664
C	3.91146	-1.08517	0.24934
C	3.47551	0.83313	-1.18087
C	5.24954	-0.68221	0.36779
H	3.55376	-1.99279	0.7425
C	4.81461	1.22861	-1.06259
H	2.77379	1.44624	-1.75598
C	5.70897	0.47167	-0.28738
H	5.93938	-1.27986	0.97338
H	5.15737	2.13897	-1.56613
H	6.75431	0.78322	-0.19007
O	1.34829	-2.53033	0.89272
N	-0.25283	-0.88521	0.98516
C	-0.90345	-1.59874	2.09857
H	-0.46956	-1.2957	3.06917
H	-1.98081	-1.37767	2.09713
H	-0.73777	-2.67527	1.95807

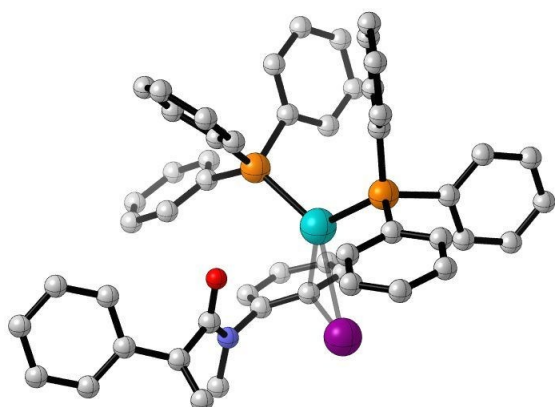


Zero-point correction= 0.784960 (Hartree/Particle)
 Thermal correction to Energy= 0.841570
 Thermal correction to Enthalpy= 0.842514
 Thermal correction to Gibbs Free Energy= 0.682896
 Sum of electronic and zero-point Energies= -2958.214356
 Sum of electronic and thermal Energies= -2958.157747
 Sum of electronic and thermal Enthalpies= -2958.156802
 Sum of electronic and thermal Free Energies= -2958.316420
 E(RM06L) = -3247.14867755

C	-1.10897	0.55706	-3.08586
C	-2.35324	0.24868	-2.54303
C	-2.52419	-0.91178	-1.74552
C	-1.43386	-1.76581	-1.5446
C	-0.14718	-1.49015	-2.08491
C	0.00664	-0.285	-2.84692
H	-0.98516	1.45944	-3.69193
H	-3.21319	0.90663	-2.69584
H	0.60803	-2.27893	-2.13276
H	0.92842	-0.14094	-3.42234
C	-4.19626	-0.66769	-0.01397
C	-5.55045	-1.03242	0.56593
C	-5.81292	-2.32116	0.88797
H	-5.11387	-3.12583	0.6409
H	-6.71405	-2.59276	1.44775
C	-6.50172	0.07412	0.87212
C	-7.89012	-0.13372	0.69608
C	-6.0618	1.33518	1.33924
C	-8.81209	0.8805	0.98956
H	-8.24108	-1.0941	0.30321
C	-6.98834	2.34743	1.62906
H	-4.99053	1.49063	1.49162
C	-8.36482	2.12693	1.45743
H	-9.88214	0.70013	0.84049
H	-6.63034	3.3138	2.00026
H	-9.08409	2.92131	1.68305
O	-3.43278	0.07771	0.62267
N	-3.83671	-1.21395	-1.23474
C	-4.73618	-1.91759	-2.15842
H	-4.75311	-1.39537	-3.13115
H	-4.39194	-2.95461	-2.3212
H	-5.75114	-1.94047	-1.74168
Pd	1.03008	0.0806	-0.75325
I	-1.72065	-3.60545	-0.45541
P	0.95224	2.39446	-0.26127
P	2.57814	-1.34726	0.32927
C	1.97908	-2.14196	1.89268
C	2.51851	-3.33479	2.42412
C	0.92422	-1.50116	2.5779
C	2.01748	-3.8664	3.623
H	3.31859	-3.85674	1.88869
C	0.42883	-2.0323	3.77893
H	0.4883	-0.59018	2.1509
C	0.97483	-3.21496	4.30332
H	2.44029	-4.79397	4.02434
H	-0.3937	-1.52728	4.29582
H	0.5828	-3.63503	5.23584
C	3.2237	-2.78984	-0.65177
C	2.38077	-3.9055	-0.87149
C	4.4816	-2.75942	-1.29333
C	2.79005	-4.96079	-1.7007
H	1.40319	-3.95533	-0.37926
C	4.88423	-3.81452	-2.12801
H	5.15379	-1.91051	-1.13433
C	4.04267	-4.91889	-2.33538

H	2.1245	-5.81787	-1.8504
H	5.86617	-3.77376	-2.61225
H	4.36011	-5.74093	-2.98549
C	4.16782	-0.51927	0.83527
C	4.62746	0.54703	0.03166
C	4.93108	-0.90398	1.9583
C	5.83326	1.20135	0.32889
H	4.01597	0.87528	-0.81672
C	6.12866	-0.23736	2.26413
H	4.5836	-1.71766	2.60297
C	6.5855	0.81144	1.44874
H	6.17026	2.02807	-0.30493
H	6.70675	-0.53987	3.14421
H	7.51972	1.32891	1.6918
C	2.32244	3.3821	-1.04119
C	2.90741	4.5136	-0.43398
C	2.79914	2.9653	-2.30387
C	3.9422	5.2118	-1.07845
H	2.55588	4.84528	0.54831
C	3.82677	3.66826	-2.95136
H	2.36419	2.07085	-2.76537
C	4.40292	4.79344	-2.33754
H	4.39003	6.08582	-0.59302
H	4.18416	3.33198	-3.9307
H	5.21086	5.33913	-2.83658
C	1.08689	2.87696	1.53216
C	0.30589	3.898	2.11569
C	2.01811	2.18644	2.3388
C	0.45329	4.21647	3.47616
H	-0.4235	4.44036	1.50672
C	2.17199	2.51528	3.69365
H	2.62553	1.38984	1.89766
C	1.38635	3.52846	4.26775
H	-0.16525	5.00612	3.91663
H	2.90092	1.97005	4.30242
H	1.49787	3.7776	5.32853
C	-0.56272	3.3341	-0.77798
C	-0.52594	4.5657	-1.46696
C	-1.81628	2.76118	-0.46332
C	-1.71877	5.21794	-1.82211
H	0.43639	5.02099	-1.72132
C	-3.00427	3.42731	-0.80262
H	-1.87677	1.78792	0.03802
C	-2.96032	4.65547	-1.48409
H	-1.67444	6.17321	-2.35694
H	-3.96501	2.9722	-0.53908
H	-3.88901	5.16921	-1.75555

TS 4-5

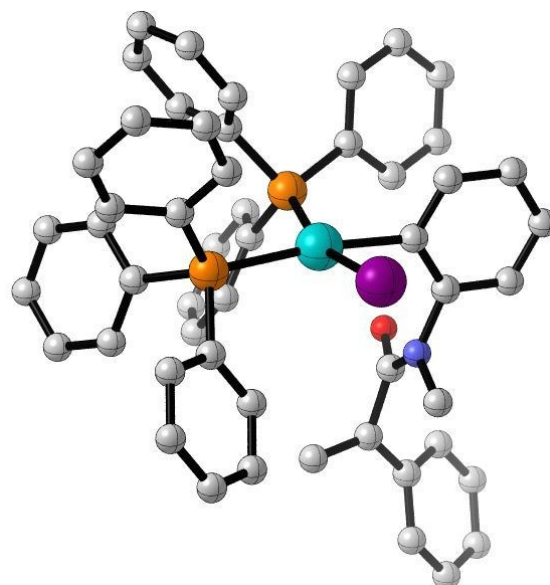


Zero-point correction= 0.784278 (Hartree/Particle)
 Thermal correction to Energy= 0.840405
 Thermal correction to Enthalpy= 0.841349
 Thermal correction to Gibbs Free Energy= 0.683953
 Sum of electronic and zero-point Energies= -2958.197276
 Sum of electronic and thermal Energies= -2958.141149
 Sum of electronic and thermal Enthalpies= -2958.140205
 Sum of electronic and thermal Free Energies= -2958.297601
 E(RM06L) = -3247.13910666
 Imaginary frequency = -86.56 cm⁻¹

C	-1.52566	0.81983	-4.1659
C	-2.44927	0.24796	-3.276
C	-2.05682	-0.70735	-2.32341
C	-0.6725	-1.02489	-2.21541
C	0.24794	-0.51575	-3.17067
C	-0.1808	0.42238	-4.12494
H	-1.86631	1.55678	-4.89871
H	-3.49972	0.5544	-3.30578
H	1.28087	-0.87367	-3.16939
H	0.53947	0.82301	-4.84631
C	-3.11208	-1.3875	-0.19946
C	-4.11353	-2.2815	0.51315
C	-3.95499	-3.62545	0.48118
H	-3.18677	-4.09447	-0.14134
H	-4.56338	-4.28193	1.11215
C	-5.17266	-1.62236	1.33003
C	-6.46657	-2.1928	1.38132
C	-4.92847	-0.43726	2.06335
C	-7.48179	-1.60543	2.14905
H	-6.67719	-3.09286	0.79356
C	-5.94834	0.14808	2.82757
H	-3.92444	-0.00555	2.04699
C	-7.2272	-0.43054	2.8753
H	-8.47786	-2.06063	2.1698
H	-5.73709	1.06004	3.39614
H	-8.02104	0.03177	3.47146
O	-2.35676	-0.67146	0.4805
N	-3.07791	-1.40652	-1.58307
C	-4.01139	-2.18736	-2.41247
H	-4.43216	-1.54977	-3.20584
H	-3.4896	-3.03889	-2.88583
H	-4.82841	-2.5705	-1.78961
Pd	0.55507	-0.20505	-0.48851
I	-0.13925	-3.04032	-1.30695
P	-0.3336	2.04021	-0.15343
P	2.65651	-0.73212	0.52236
C	2.597	-2.28707	1.53535
C	3.7008	-3.15472	1.67912
C	1.39034	-2.5978	2.19983
C	3.60062	-4.30454	2.47895
H	4.64024	-2.92997	1.16338
C	1.29674	-3.74103	3.00893
H	0.51993	-1.94602	2.06175
C	2.40125	-4.59738	3.14911
H	4.46347	-4.97195	2.57972
H	0.35431	-3.96846	3.51841
H	2.32562	-5.49451	3.77294
C	4.07189	-1.07314	-0.64093
C	3.81879	-1.89614	-1.76207
C	5.37055	-0.55134	-0.46319
C	4.83875	-2.19252	-2.67741
H	2.81515	-2.31206	-1.90754
C	6.38783	-0.83897	-1.38963

H	5.58812	0.08457	0.40007
C	6.12678	-1.65931	-2.4975
H	4.62516	-2.83769	-3.53658
H	7.38924	-0.42113	-1.23868
H	6.92113	-1.88266	-3.21765
C	3.41631	0.47418	1.7174
C	3.62961	1.80427	1.28803
C	3.75539	0.12703	3.04291
C	4.18306	2.75494	2.15791
H	3.35943	2.09949	0.26913
C	4.29345	1.08698	3.91641
H	3.60195	-0.89729	3.395
C	4.51281	2.40117	3.47719
H	4.34026	3.77851	1.80279
H	4.54634	0.8005	4.94319
H	4.93391	3.14757	4.15918
C	0.97611	3.2737	-0.64406
C	1.28974	4.43436	0.09321
C	1.70072	3.00698	-1.82824
C	2.30216	5.30567	-0.34376
H	0.75049	4.65443	1.01976
C	2.7034	3.88425	-2.27083
H	1.47604	2.09587	-2.39372
C	3.01045	5.0356	-1.52602
H	2.53613	6.20047	0.24377
H	3.25302	3.66175	-3.19194
H	3.79943	5.7162	-1.86357
C	-0.66271	2.45407	1.62927
C	-1.41394	3.58226	2.03022
C	-0.13383	1.6031	2.62103
C	-1.61907	3.85402	3.39218
H	-1.84998	4.24145	1.27263
C	-0.33762	1.87634	3.98255
H	0.43106	0.71885	2.3061
C	-1.08002	3.00274	4.37123
H	-2.20452	4.73154	3.6882
H	0.08035	1.20414	4.73923
H	-1.24411	3.2142	5.43347
C	-1.8368	2.80736	-0.95428
C	-1.75443	3.80412	-1.95024
C	-3.11448	2.32435	-0.58657
C	-2.91657	4.30439	-2.56077
H	-0.77818	4.1975	-2.24919
C	-4.27387	2.834	-1.18985
H	-3.195	1.54284	0.17456
C	-4.18073	3.82471	-2.18269
H	-2.83086	5.08283	-3.32733
H	-5.25395	2.45398	-0.88052
H	-5.08613	4.22226	-2.654

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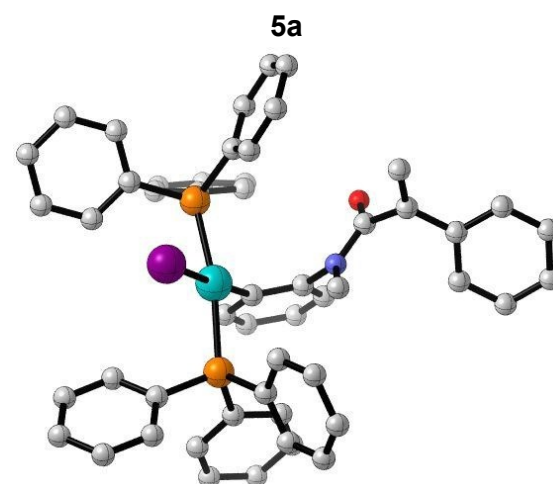


Zero-point correction= 0.786847 (Hartree/Particle)
 Thermal correction to Energy= 0.842777
 Thermal correction to Enthalpy= 0.843721
 Thermal correction to Gibbs Free Energy= 0.689195
 Sum of electronic and zero-point Energies= -2958.241992
 Sum of electronic and thermal Energies= -2958.186063

Sum of electronic and thermal Enthalpies= -2958.185118
 Sum of electronic and thermal Free Energies= -2958.339644
 E(RM06L) = -3247.19273552

C	-3.08537	1.6824	-3.87575
C	-3.39906	0.75548	-2.87546
C	-2.39706	0.25399	-2.01741
C	-1.06434	0.69482	-2.13998
C	-0.76249	1.62152	-3.1591
C	-1.75521	2.10732	-4.02353
H	-3.86999	2.06282	-4.53793
H	-4.42781	0.40031	-2.74516
H	0.2696	1.96296	-3.28761
H	-1.48658	2.82042	-4.81058
C	-3.40081	-0.42542	0.09394
C	-3.97039	-1.5151	0.99023
C	-3.14845	-2.28794	1.73733
H	-2.06077	-2.23179	1.63695
H	-3.54417	-2.97436	2.4932
C	-5.45528	-1.60191	1.0847
C	-6.0775	-2.85517	1.29628
C	-6.27449	-0.4553	0.95925
C	-7.47114	-2.95713	1.40116
H	-5.45903	-3.75732	1.35257
C	-7.6687	-0.56254	1.0628
H	-5.79598	0.51597	0.80609
C	-8.27384	-1.81008	1.28583
H	-7.93261	-3.93793	1.55889
H	-8.28635	0.33756	0.97237
H	-9.36338	-1.89017	1.36175
O	-3.50751	0.75951	0.4645
N	-2.79249	-0.79152	-1.08423
C	-2.88705	-2.1396	-1.67158
H	-3.62592	-2.14844	-2.49387
H	-1.90472	-2.42813	-2.07993
H	-3.19587	-2.85802	-0.90129
Pd	0.43839	0.01101	-0.92144
I	0.83486	-1.78789	-2.97179
P	0.18882	2.0068	0.32212
P	2.20962	-1.18489	0.3996
C	1.87546	-3.01083	0.38807
C	2.89964	-3.97332	0.48238
C	0.53158	-3.43807	0.34927
C	2.58225	-5.33996	0.54163
H	3.94758	-3.65855	0.49735
C	0.21601	-4.8028	0.42686
H	-0.26477	-2.69551	0.22585
C	1.24208	-5.75704	0.52047
H	3.38743	-6.07991	0.60135
H	-0.83139	-5.12011	0.39419
H	0.99784	-6.82355	0.56663
C	3.95554	-1.02181	-0.21596
C	4.17905	-0.64329	-1.55714
C	5.06848	-1.28536	0.61461
C	5.48671	-0.53588	2.05638
H	3.32261	-0.46029	-2.21493
C	6.37451	-1.17568	0.11111
H	4.91537	-1.56373	1.66179
C	6.58688	-0.8004	-1.22515
H	5.64191	-0.24831	-3.10165
H	7.2264	-1.38364	0.76737
H	7.60628	-0.71503	-1.61649
C	2.41727	-0.88886	2.22989
C	3.10984	0.2546	2.68953
C	1.84676	-1.76194	3.1822
C	3.22842	0.51229	4.06349
H	3.57376	0.93925	1.97417
C	1.96412	-1.49716	4.55626
H	1.31763	-2.6602	2.85099
C	2.6547	-0.36012	5.0022
H	3.77339	1.40138	4.39742
H	1.52109	-2.19103	5.27877
H	2.74884	-0.15645	6.074
C	1.8746	2.70313	0.66137
C	2.16987	3.47579	1.80388
C	2.88481	2.48562	-0.30021
C	3.45321	4.01728	1.97858
H	1.40162	3.64264	2.56466
C	4.16792	3.02843	-0.12358
H	2.66255	1.87352	-1.18209
C	4.45453	3.79474	1.01785
H	3.67188	4.61278	2.87149
H	4.94348	2.83723	-0.87188
H	5.45598	4.21409	1.16088
C	-0.64265	1.92386	1.96747
C	-1.13641	3.08345	2.60667

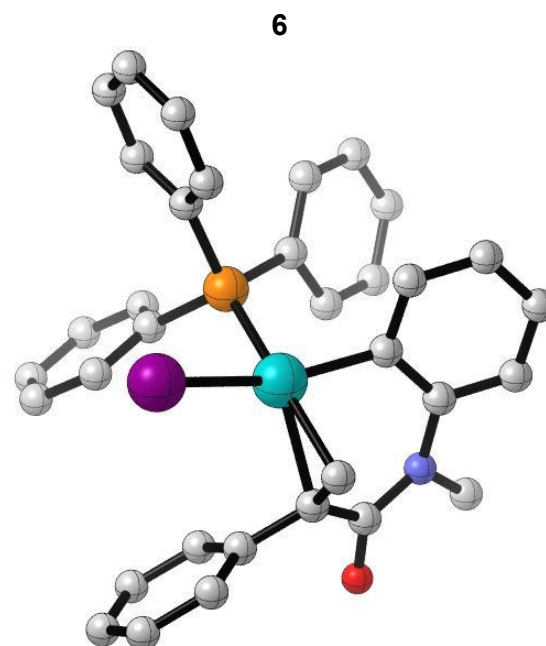
C	-0.78097	0.67642	2.60399
C	-1.73673	2.98951	3.87105
H	-1.07235	4.05392	2.10483
C	-1.38131	0.58565	3.86821
H	-0.42295	-0.22332	2.09514
C	-1.85807	1.74175	4.50453
H	-2.12097	3.893	4.35623
H	-1.48637	-0.39182	4.34863
H	-2.33538	1.67042	5.48754
C	-0.65179	3.45211	-0.47985
C	0.08314	4.53294	-1.01041
C	-2.06262	3.45717	-0.57152
C	-0.58282	5.6092	-1.61971
H	1.17491	4.54506	-0.94574
C	-2.7165	4.53935	-1.17769
H	-2.64425	2.61108	-0.18683
C	-1.98297	5.61658	-1.70266
H	-0.0009	6.44397	-2.02499
H	-3.8094	4.53361	-1.24494
H	-2.50108	6.45723	-2.17671



Zero-point correction= 0.786311 (Hartree/Particle)
 Thermal correction to Energy= 0.841497
 Thermal correction to Enthalpy= 0.842442
 Thermal correction to Gibbs Free Energy= 0.690070
 Sum of electronic and zero-point Energies= -2958.245281
 Sum of electronic and thermal Energies= -2958.190095
 Sum of electronic and thermal Enthalpies= -2958.189151
 Sum of electronic and thermal Free Energies= -2958.341523
 E(RM06L) = -3247.19248373

C	-1.98645	-0.44226	3.94425
C	-2.60589	-0.40547	2.69168
C	-1.85171	-0.2345	1.50633
C	-0.43875	-0.13541	1.57548
C	0.16206	-0.17756	2.85339
C	-0.5909	-0.32016	4.0278
H	-2.59238	-0.56437	4.8481
H	-3.69449	-0.48041	2.61365
H	1.25062	-0.09115	2.93551
H	-0.08672	-0.33931	4.99993
C	-3.67479	0.68531	0.15009
C	-4.59811	0.52145	-1.05327
C	-4.4207	1.31049	-2.13728
H	-3.5883	2.01685	-2.19821
H	-5.09688	1.26396	-2.9973
C	-5.73804	-0.42402	-0.89688
C	-5.63697	-1.55385	-0.05125
C	-6.95774	-0.21718	-1.58487
C	-6.70234	-2.45653	0.0794
H	-4.71006	-1.72948	0.5039
C	-8.02008	-1.1199	-1.45569
C	-7.07999	0.67784	-2.20298
C	-7.8975	-2.2476	-0.62553
H	-6.59671	-3.32602	0.73697
H	-8.95583	-0.93424	-1.99386
H	-8.7317	-2.94895	-0.52038
O	-3.94151	1.5538	0.99423
N	-2.59771	-0.18544	0.26522
C	-2.19276	-1.07592	-0.82519
H	-1.17097	-0.81748	-1.16581

H	-2.192	-2.13049	-0.49863
H	-2.88508	-0.95906	-1.66899
Pd	0.8108	0.06628	-0.03391
I	2.35866	0.31489	-2.36138
P	1.36846	-2.28595	0.07094
P	0.59762	2.44501	0.18201
C	0.08481	3.09837	1.84043
C	1.04055	3.65613	2.71706
C	-1.26047	2.99763	2.26319
C	0.65918	4.10668	3.99105
H	2.08447	3.74852	2.40441
C	-1.63352	3.45829	3.53458
H	-2.033	2.55736	1.62358
C	-0.67849	4.01133	4.40296
H	1.41314	4.53961	4.65733
H	-2.6805	3.3718	3.84191
H	-0.97541	4.36576	5.39594
C	2.2102	3.32055	-0.08533
C	3.4116	2.67578	0.27317
C	2.25535	4.64438	-0.56689
C	4.63739	3.34942	0.16619
H	3.38098	1.63557	0.61242
C	3.48532	5.31052	-0.68684
H	1.33178	5.15415	-0.85767
C	4.67692	4.66716	-0.31749
H	5.56438	2.8365	0.44247
H	3.5095	6.33499	-1.07304
H	5.6353	5.18815	-0.41397
C	-0.5537	3.26961	-1.01313
C	-0.64406	2.76128	-2.32722
C	-1.27568	4.43495	-0.67272
C	-1.43117	3.41892	-3.2855
H	-0.07323	1.86642	-2.6005
C	-2.07007	5.08104	-1.63366
H	-1.22475	4.83358	0.34445
C	-2.1465	4.5785	-2.94221
H	-1.48369	3.01977	-4.30392
H	-2.62997	5.97977	-1.35469
H	-2.76343	5.08706	-3.69069
C	3.19156	-2.54461	-0.10819
C	3.73101	-3.64623	-0.80028
C	4.06269	-1.62826	0.51845
C	5.12251	-3.82584	-0.86345
H	3.0677	-4.35984	-1.29819
C	5.45041	-1.82024	0.4679
H	3.64475	-0.75781	1.03601
C	5.9835	-2.91827	-0.2279
H	5.5322	-4.67878	-1.41465
H	6.11681	-1.10324	0.95854
H	7.06791	-3.06087	-0.2801
C	0.60369	-3.4053	-1.19721
C	0.35089	-4.76751	-0.91622
C	0.29485	-2.89959	-2.47883
C	-0.20466	-5.60302	-1.89826
H	0.58199	-5.17507	0.07221
C	-0.26038	-3.74078	-3.45554
H	0.51458	-1.85141	-2.71222
C	-0.51454	-5.09147	-3.16837
H	-0.39645	-6.65598	-1.66599
H	-0.49376	-3.33437	-4.44518
H	-0.95215	-5.7439	-3.93142
C	1.00277	-3.17925	1.65905
C	2.02909	-3.60733	2.52613
C	-0.34093	-3.41914	2.02483
C	1.7173	-4.2607	3.7306
H	3.07585	-3.43689	2.26038
C	-0.64823	-4.07783	3.22225
H	-1.15377	-3.07788	1.37778
C	0.38091	-4.50002	4.08092
H	2.52736	-4.58746	4.39129
H	-1.69553	-4.2515	3.48923
H	0.13993	-5.01041	5.01933

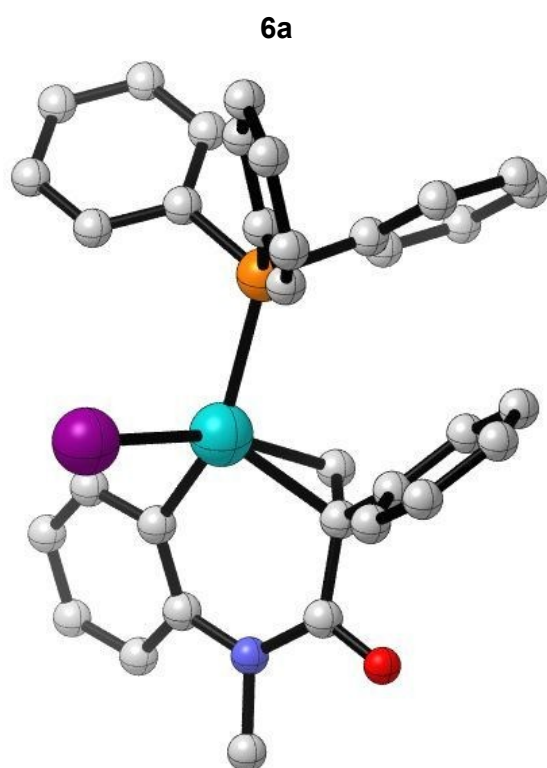


Zero-point correction= 0.519799 (Hartree/Particle)
 Thermal correction to Energy= 0.557197
 Thermal correction to Enthalpy= 0.558141
 Thermal correction to Gibbs Free Energy= 0.446070
 Sum of electronic and zero-point Energies= -1922.195446
 Sum of electronic and thermal Energies= -1922.158048
 Sum of electronic and thermal Enthalpies= -1922.157104
 Sum of electronic and thermal Free Energies= -1922.269175
 E(RM06L) = -2210.70587558

C	1.84028	4.41112	-2.02148
C	0.78554	4.51681	-1.10648
C	0.1297	3.3653	-0.60306
C	0.54413	2.09236	-1.05517
C	1.59547	2.00363	-1.98396
C	2.25457	3.14907	-2.46509
H	2.32849	5.31959	-2.3885
H	0.44734	5.50884	-0.79408
H	1.92528	1.01916	-2.33403
H	3.0851	3.04547	-3.1709
C	-2.04982	2.77719	0.53886
C	-2.36553	1.55424	-0.31384
C	-2.1931	1.52394	-1.71124
H	-1.76249	2.37684	-2.2424
H	-2.7381	0.79124	-2.31291
C	-3.28801	0.59099	0.36333
C	-3.06124	0.19212	1.70135
C	-4.41772	0.07923	-0.3111
C	-3.92241	-0.71158	2.33258
H	-2.19664	0.58699	2.24179
C	-5.28706	-0.81528	0.32621
H	-4.6292	0.3988	-1.33537
C	-5.03972	-1.21931	1.64747
H	-3.72247	-1.01741	3.36444
H	-6.16117	-1.19555	-0.21193
H	-5.7189	-1.91986	2.14462
O	-2.89238	3.10125	1.39191
N	-0.90536	3.55065	0.36173
C	-0.83162	4.74411	1.22229
H	0.22225	4.94456	1.46548
H	-1.26947	5.63358	0.73331
H	-1.41248	4.53989	2.13094
Pd	-0.4861	0.36442	-0.83904
I	-1.51508	-2.04291	-1.83679
P	1.30462	-0.64342	0.37573
C	0.74573	-1.5143	1.91525
C	1.49697	-1.44272	3.11049
C	-0.4221	-2.30618	1.87957
C	1.08653	-2.15713	4.24723
H	2.3995	-0.82645	3.15684
C	-0.8218	-3.0205	3.0193
H	-1.01299	-2.36633	0.95836
C	-0.07246	-2.94804	4.20452
H	1.67676	-2.09199	5.16747
H	-1.72892	-3.63179	2.97554

H	-0.39134	-3.50344	5.09294
C	2.56692	0.55067	1.019
C	3.93957	0.44524	0.72063
C	2.12145	1.61394	1.83676
C	4.85192	1.38082	1.23947
H	4.30084	-0.36912	0.08624
C	3.03591	2.53505	2.36408
H	1.05402	1.72053	2.05893
C	4.40512	2.42225	2.06471
H	5.91561	1.28868	0.99604
H	2.67871	3.3475	3.00556
H	5.11786	3.14738	2.47108
C	2.30669	-1.90759	-0.52619
C	3.14363	-2.80419	0.17375
C	2.25786	-1.96083	-1.93373
C	3.93521	-3.72392	-0.53042
H	3.16879	-2.79011	1.26831
C	3.05587	-2.87918	-2.63414
H	1.56171	-1.3129	-2.47537
C	3.89634	-3.75875	-1.93457
H	4.57759	-4.41928	0.01998
H	3.00326	-2.91768	-3.72683
H	4.51153	-4.48115	-2.48125

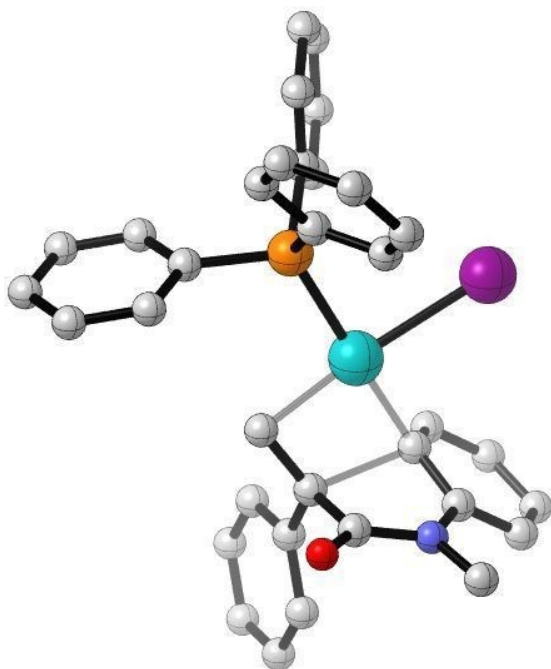
H	0.22616	1.12484	-2.45192
C	0.66988	2.70398	-0.2083
C	0.88456	3.07615	1.14253
C	-0.40752	3.29121	-0.90631
C	0.04694	4.00454	1.76921
H	1.70746	2.61931	1.69895
C	-1.24572	4.22317	-0.27517
H	-0.5757	3.04447	-1.95855
C	-1.02162	4.5853	1.06145
H	0.23075	4.27972	2.81279
H	-2.06908	4.67347	-0.83856
H	-1.6708	5.31986	1.54927
O	3.3331	3.28095	-0.46683
N	4.06694	1.11826	-0.54653
C	5.41767	1.64702	-0.29388
H	5.96775	0.93502	0.33889
H	5.97663	1.81463	-1.23251
H	5.30828	2.61393	0.21338
Pd	0.90723	-0.23945	-0.16788
I	1.09806	-1.18999	2.38869
P	-1.62724	-0.39076	-0.28856
C	-2.67392	0.03088	1.17448
C	-3.9072	-0.60938	1.42185
C	-2.22358	1.03758	2.05245
C	-4.68239	-0.23818	2.53062
H	-4.25504	-1.4034	0.75338
C	-3.00773	1.41049	3.15549
H	-1.25736	1.52022	1.8775
C	-4.23468	0.77313	3.39734
H	-5.6352	-0.74373	2.72024
H	-2.6488	2.19141	3.83355
H	-4.83915	1.05728	4.26531
C	-2.05648	-2.16891	-0.63539
C	-3.06906	-2.54247	-1.5469
C	-1.36498	-3.17987	0.06935
C	-3.37225	-3.8978	-1.75687
H	-3.62129	-1.77621	-2.09854
C	-1.67638	-4.5318	-0.14105
H	-0.59042	-2.90432	0.79509
C	-2.67589	-4.89584	-1.05766
H	-4.15807	-4.17057	-2.46943
H	-1.13147	-5.30149	0.41556
H	-2.91261	-5.95187	-1.22504
C	-2.45791	0.49602	-1.68932
C	-3.43712	1.48831	-1.4747
C	-2.05198	0.21734	-3.01652
C	-3.99711	2.18347	-2.55969
H	-3.76483	1.71525	-0.45614
C	-2.6162	0.91099	-4.09809
H	-1.30396	-0.56102	-3.20595
C	-3.58913	1.89967	-3.87223
H	-4.76065	2.94664	-2.37482
H	-2.29605	0.67617	-5.11871
H	-4.02811	2.44206	-4.71593



Zero-point correction= 0.519661 (Hartree/Particle)
 Thermal correction to Energy= 0.557137
 Thermal correction to Enthalpy= 0.558081
 Thermal correction to Gibbs Free Energy= 0.445928
 Sum of electronic and zero-point Energies= -1922.191874
 Sum of electronic and thermal Energies= -1922.154398
 Sum of electronic and thermal Enthalpies= -1922.153453
 Sum of electronic and thermal Free Energies= -1922.265607
 E(RM06L) = -2210.69980739

C	4.99435	-2.36978	-1.51603
C	5.04909	-0.98906	-1.28953
C	3.93	-0.28196	-0.78206
C	2.74168	-0.99589	-0.52723
C	2.69382	-2.37971	-0.76151
C	3.81373	-3.07531	-1.25254
H	5.8787	-2.88711	-1.90164
H	5.96658	-0.44516	-1.52989
H	1.77858	-2.93441	-0.53054
H	3.75891	-4.15813	-1.40436
C	3.06636	2.07431	-0.59971
C	1.60329	1.73997	-0.87294
C	1.20735	0.9684	-1.99488
H	1.9649	0.49725	-2.62768

TS 6-7a

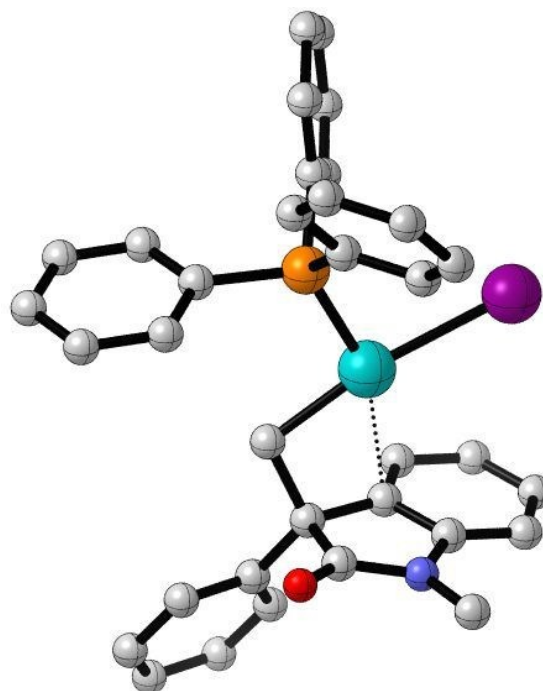


Zero-point correction= 0.518582 (Hartree/Particle)
 Thermal correction to Energy= 0.555656
 Thermal correction to Enthalpy= 0.556601
 Thermal correction to Gibbs Free Energy= 0.444167
 Sum of electronic and zero-point Energies= -1922.184704
 Sum of electronic and thermal Energies= -1922.147630
 Sum of electronic and thermal Enthalpies= -1922.146686
 Sum of electronic and thermal Free Energies= -1922.259119
 E(RM06L) = -2210.68805922
 Imaginary frequency = 192.14 cm⁻¹

C	-4.40614	-2.6901	-0.87133
C	-4.21662	-2.27721	0.45379
C	-3.22893	-1.31289	0.73753
C	-2.38309	-0.82457	-0.28182
C	-2.66774	-1.15714	-1.61831
C	-3.65686	-2.10949	-1.91067
H	-5.1688	-3.44178	-1.09851
H	-4.85364	-2.66703	1.25377
H	-2.06519	-0.73886	-2.43077
H	-3.81968	-2.4208	-2.94753
C	-2.58841	0.58352	2.03215
C	-2.24602	1.15721	0.65048
C	-0.93179	1.72413	0.57446
H	-0.41568	1.85798	1.53193
H	-0.72824	2.49928	-0.17161
C	-3.35916	1.74118	-0.17054
C	-4.65157	1.86983	0.38051
C	-3.12359	2.2414	-1.47089
C	-5.6799	2.48751	-0.34807
H	-4.85097	1.50695	1.39339
C	-4.1521	2.85216	-2.19688
H	-2.13188	2.12919	-1.92175
C	-5.43661	2.97913	-1.63843
H	-6.67398	2.58504	0.10037
H	-3.95253	3.22673	-3.20632
H	-6.24005	3.45722	-2.20797
O	-2.39694	1.22853	3.06993
N	-3.11605	-0.69541	2.00091
C	-3.56303	-1.32751	3.23821
H	-4.66533	-1.39113	3.28317
H	-3.13874	-2.3412	3.31809
H	-3.20624	-0.69848	4.06639
Pd	-0.32275	-0.21433	-0.03528
I	0.38428	-2.84758	-0.47784
P	1.95281	0.43427	0.02705
C	2.92971	-0.16183	-1.42424
C	4.31276	-0.42149	-1.35251
C	2.26068	-0.31132	-2.65747
C	5.01587	-0.81391	-2.50242
H	4.84009	-0.33528	-0.39774
C	2.97003	-0.68747	-3.80758

H	1.17696	-0.15871	-2.70134
C	4.34922	-0.94081	-3.73129
H	6.08804	-1.02594	-2.43404
H	2.43949	-0.80418	-4.75816
H	4.90097	-1.24907	-4.62552
C	2.89192	-0.06594	1.53895
C	4.07868	0.60291	1.91967
C	2.42111	-1.13793	2.3258
C	4.78413	0.19717	3.06262
H	4.4427	1.45219	1.33289
C	3.13028	-1.53605	3.47038
H	1.51208	-1.66832	2.02292
C	4.31048	-0.87252	3.8402
H	5.70183	0.72229	3.34789
H	2.75484	-2.36961	4.07273
H	4.85952	-1.18471	4.73488
C	2.22817	2.27257	-0.02795
C	2.50765	2.93141	-1.24401
C	2.06504	3.04701	1.14389
C	2.62326	4.33032	-1.2861
H	2.64745	2.34866	-2.15983
C	2.18394	4.44433	1.09785
H	1.86226	2.55588	2.10151
C	2.4618	5.09088	-0.1175
H	2.84777	4.82439	-2.23738
H	2.05932	5.02729	2.01638
H	2.55406	6.18132	-0.15221

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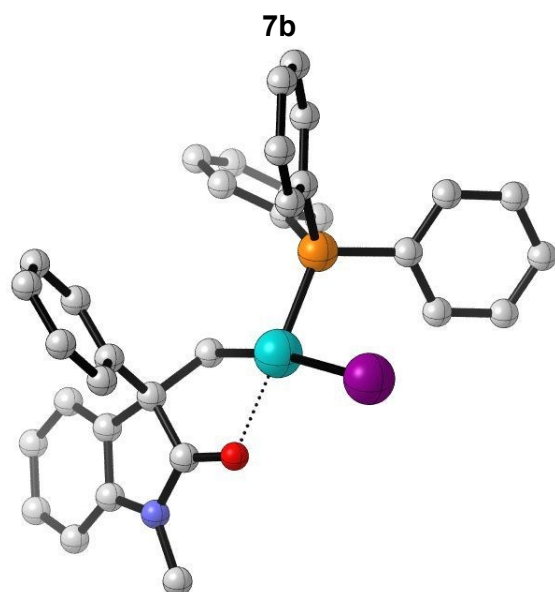
Zero-point correction= 0.520859 (Hartree/Particle)
 Thermal correction to Energy= 0.558099
 Thermal correction to Enthalpy= 0.559044
 Thermal correction to Gibbs Free Energy= 0.446489
 Sum of electronic and zero-point Energies= -1922.229207
 Sum of electronic and thermal Energies= -1922.191966
 Sum of electronic and thermal Enthalpies= -1922.191022
 Sum of electronic and thermal Free Energies= -1922.303577
 E(RM06L) = -2210.73466094

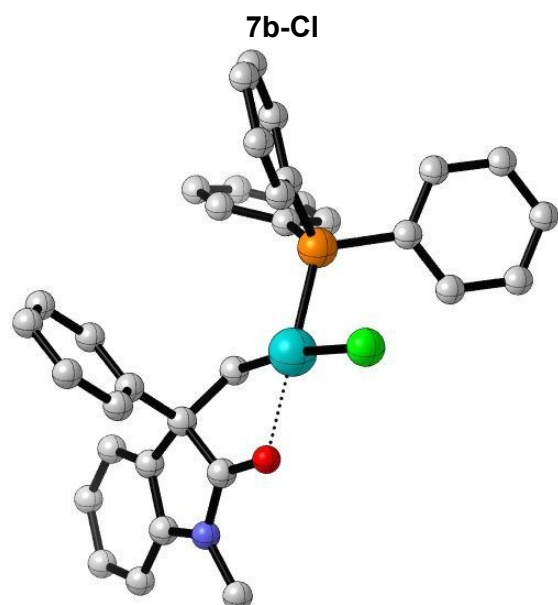
C	-2.64826	-3.77138	-0.63483
C	-2.84903	-3.24542	0.6572
C	-2.8005	-1.85731	0.80709
C	-2.55914	-0.99271	-0.30063
C	-2.36959	-1.54377	-1.5859
C	-2.41608	-2.94299	-1.74346
H	-2.66535	-4.85699	-0.77109
H	-3.02598	-3.90632	1.51006
H	-2.22206	-0.88681	-2.44885
H	-2.24664	-3.38496	-2.72872
C	-2.86779	0.27563	1.70193

C	-2.70714	0.46117	0.15956
C	-1.37566	1.16492	-0.1446
H	-1.08306	1.88822	0.62906
H	-1.36961	1.63781	-1.14111
C	-3.9364	1.21796	-0.37539
C	-4.14519	2.54761	0.05325
C	-4.85397	0.64085	-1.27311
C	-5.24383	3.28136	-0.41441
H	-3.45325	2.99004	0.77548
C	-5.954	1.37948	-1.74118
H	-4.71331	-0.39079	-1.61033
C	-6.15182	2.70166	-1.31676
H	-5.39297	4.31034	-0.06985
H	-6.65748	0.91489	-2.44056
H	-7.00796	3.27701	-1.68448
O	-2.87515	1.15552	2.55883
N	-3.00138	-1.09369	1.96285
C	-3.13924	-1.62545	3.30892
H	-4.05388	-2.23673	3.39773
H	-2.26356	-2.24139	3.5791
H	-3.20518	-0.76187	3.98711
Pd	-0.14141	-0.50415	-0.22931
I	1.11885	-2.97294	-0.32538
P	1.75114	0.74331	0.00406
C	2.99348	0.37673	-1.31501
C	4.36566	0.64981	-1.13775
C	2.54128	-0.14093	-2.54623
C	5.2696	0.41443	-2.18493
H	4.73293	1.02892	-0.1792
C	3.44737	-0.36134	-3.59462
H	1.48246	-0.39593	-2.66267
C	4.81218	-0.08512	-3.41512
H	6.33521	0.61745	-2.03545
H	3.08725	-0.76835	-4.54496
H	5.52105	-0.26988	-4.22908
C	2.62215	0.55221	1.62387
C	3.50271	1.54932	2.10518
C	2.42425	-0.61964	2.38286
C	4.17967	1.36631	3.32077
H	3.6479	2.47517	1.53999
C	3.10398	-0.79434	3.59857
H	1.75402	-1.39869	2.00217
C	3.98149	0.19463	4.06944
H	4.8591	2.14461	3.68391
H	2.94381	-1.71007	4.17689
H	4.5082	0.05616	5.01958
C	1.52397	2.57645	-0.13742
C	1.76815	3.24502	-1.35526
C	1.02325	3.31339	0.96065
C	1.5299	4.62421	-1.4679
H	2.15574	2.68837	-2.21394
C	0.79213	4.69233	0.84462
H	0.82795	2.81149	1.91421
C	1.04458	5.35137	-0.36981
H	1.73115	5.13077	-2.41766
H	0.41133	5.25038	1.70629
H	0.8626	6.42732	-0.45937

Zero-point correction= 0.521511 (Hartree/Particle)
 Thermal correction to Energy= 0.558434
 Thermal correction to Enthalpy= 0.559378
 Thermal correction to Gibbs Free Energy= 0.447599
 Sum of electronic and zero-point Energies= -1922.231094
 Sum of electronic and thermal Energies= -1922.194172
 Sum of electronic and thermal Enthalpies= -1922.193228
 Sum of electronic and thermal Free Energies= -1922.305006
 E(RM06L) = -2210.73867609

C	-6.60183	0.79516	-1.86321
C	-6.05976	-0.48628	-1.64092
C	-4.78404	-0.55403	-1.07578
C	-4.04185	0.59774	-0.71948
C	-4.59502	1.85758	-0.95395
C	-5.8789	1.95169	-1.53125
H	-7.59897	0.88442	-2.30577
H	-6.61808	-1.38911	-1.90556
H	-4.03988	2.76705	-0.70468
H	-6.31367	2.93761	-1.72278
C	-2.781	-1.3609	-0.34267
C	-2.7129	0.14407	-0.10057
C	-1.39483	0.59323	-0.78995
H	-1.15189	1.63585	-0.54403
H	-1.46336	0.48412	-1.88831
C	-2.67519	0.46886	1.41216
C	-2.72123	-0.52624	2.40793
C	-2.60801	1.81964	1.81454
C	-2.70617	-0.17864	3.76923
H	-2.74041	-1.58401	2.13014
C	-2.59431	2.16661	3.17279
H	-2.56101	2.61115	1.0597
C	-2.64628	1.16694	4.15808
H	-2.73626	-0.97002	4.52537
H	-2.54383	3.22199	3.46163
H	-2.63526	1.43653	5.21917
O	-1.80376	-2.13795	-0.20922
N	-4.0164	-1.71829	-0.80969
C	-4.37953	-3.07575	-1.19311
H	-5.26457	-3.41293	-0.62778
H	-4.59928	-3.12641	-2.2735
H	-3.52379	-3.72646	-0.96265
Pd	0.02115	-0.82805	-0.18017
I	1.5584	-3.03274	0.48943
P	1.74925	0.6128	-0.27555
C	3.09753	0.02847	-1.39833
C	4.42107	0.50042	-1.28073
C	2.77198	-0.87544	-2.43088
C	5.40214	0.07732	-2.19048
H	4.69324	1.18124	-0.46861
C	3.75361	-1.28447	-3.34628
H	1.75415	-1.27597	-2.48983
C	5.06958	-0.80997	-3.22701
H	6.43055	0.43812	-2.08358
H	3.49174	-1.99129	-4.14024
H	5.83846	-1.1404	-3.93338
C	2.54184	1.00344	1.35119
C	3.3129	2.17758	1.52262
C	2.39647	0.10965	2.43188
C	3.93773	2.43998	2.75124
H	3.41336	2.89556	0.70269
C	3.02214	0.38084	3.65911
H	1.80874	-0.80478	2.2967
C	3.79339	1.54193	3.82161
H	4.53393	3.35074	2.87173
H	2.90206	-0.32251	4.48943
H	4.2786	1.75073	4.78107
C	1.37237	2.30227	-0.94732
C	1.64528	2.63102	-2.29093
C	0.7362	3.26016	-0.12415
C	1.3014	3.89531	-2.79757
H	2.13651	1.90102	-2.94149
C	0.40066	4.5239	-0.63248
H	0.51102	3.0171	0.91987
C	0.68268	4.84552	-1.97114
H	1.52617	4.13744	-3.84168
H	-0.08053	5.26	0.02042
H	0.42127	5.83256	-2.36664

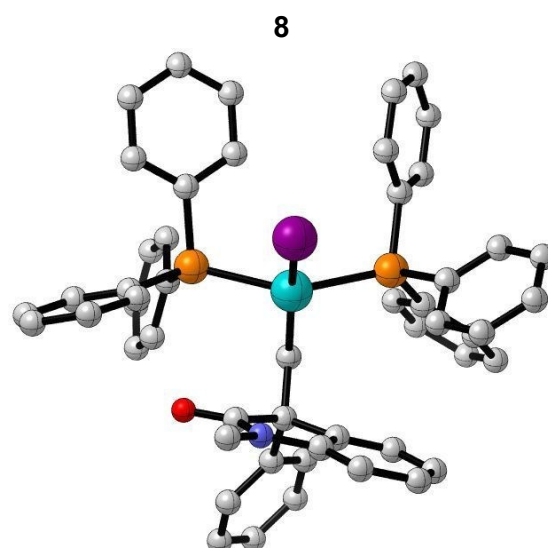




Zero-point correction= 0.522026 (Hartree/Particle)
 Thermal correction to Energy= 0.558544
 Thermal correction to Enthalpy= 0.559488
 Thermal correction to Gibbs Free Energy= 0.449957
 Sum of electronic and zero-point Energies= -1925.782951
 Sum of electronic and thermal Energies= -1925.746433
 Sum of electronic and thermal Enthalpies= -1925.745489
 Sum of electronic and thermal Free Energies= -1925.855020
 E(RM06L) = -2373.06686928

C	6.36174	-0.96126	1.89343
C	5.92897	-1.53249	0.68024
C	4.66976	-1.15577	0.20694
C	3.83957	-0.23391	0.88895
C	4.28618	0.31754	2.09076
C	5.55137	-0.05319	2.59286
H	7.34296	-1.23565	2.2935
H	6.55655	-2.24466	0.13627
H	3.66237	1.02412	2.64662
H	5.90277	0.3718	3.5382
C	2.75196	-1.0828	-1.02603
C	2.55912	-0.03645	0.06791
C	1.20127	-0.41546	0.7259
H	0.87234	0.35837	1.43305
H	1.27917	-1.38183	1.25861
C	2.49871	1.39204	-0.52217
C	2.66679	1.65667	-1.89521
C	2.28285	2.47983	0.35032
C	2.62408	2.97388	-2.38177
H	2.80308	0.83299	-2.60204
C	2.24186	3.79459	-0.13477
H	2.13859	2.29859	1.42049
C	2.41469	4.04805	-1.5055
H	2.74976	3.15422	-3.45445
H	2.07407	4.62372	0.56109
H	2.38071	5.07412	-1.88585
O	1.84659	-1.44567	-1.81559
N	4.0053	-1.62821	-0.95505
C	4.47423	-2.7017	-1.82015
H	5.39573	-2.39981	-2.34582
H	4.67556	-3.6131	-1.2311
H	3.68094	-2.90703	-2.55322
Pd	-0.07957	-0.75766	-0.88059
P	-1.93706	-0.111	0.20911
C	-3.22253	-1.43864	0.24482
C	-4.5478	-1.15546	0.63967
C	-2.86584	-2.75718	-0.10139
C	-5.49957	-2.18405	0.69691
H	-4.84118	-0.13062	0.8888
C	-3.82125	-3.78382	-0.03602
H	-1.84892	-2.95926	-0.45233
C	-5.13654	-3.49979	0.36284
H	-6.5277	-1.95554	0.99695
H	-3.5378	-4.80404	-0.3143
H	-5.88273	-4.30043	0.40414
C	-2.77563	1.38004	-0.50025
C	-3.55829	2.23744	0.30704

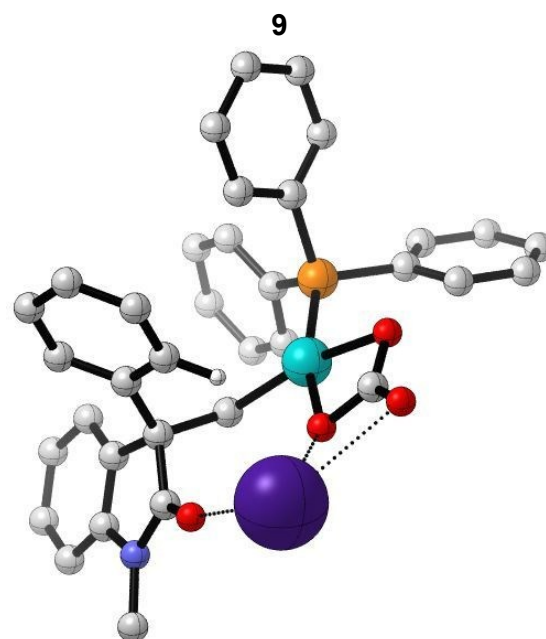
C	-2.66959	1.63528	-1.88451
C	-4.22288	3.33377	-0.26435
H	-3.64066	2.05979	1.38372
C	-3.33899	2.73406	-2.44582
H	-2.08524	0.9521	-2.5133
C	-4.11271	3.58542	-1.64129
H	-4.8248	3.99245	0.37085
H	-3.2512	2.92216	-3.52095
H	-4.62924	4.44354	-2.08467
C	-1.73114	0.32605	1.99805
C	-2.07813	-0.58454	3.01718
C	-1.13966	1.56005	2.35642
C	-1.8555	-0.2616	4.36615
H	-2.53177	-1.5456	2.75687
C	-0.92703	1.88194	3.70522
H	-0.85109	2.27292	1.57639
C	-1.28533	0.97213	4.71455
H	-2.13578	-0.97784	5.14569
H	-0.48084	2.8471	3.96794
H	-1.11888	1.22458	5.76695
Cl	-1.3417	-1.37299	-2.91113



Zero-point correction= 0.789331 (Hartree/Particle)
 Thermal correction to Energy= 0.844331
 Thermal correction to Enthalpy= 0.845275
 Thermal correction to Gibbs Free Energy= 0.693960
 Sum of electronic and zero-point Energies= -2958.279095
 Sum of electronic and thermal Energies= -2958.224095
 Sum of electronic and thermal Enthalpies= -2958.223151
 Sum of electronic and thermal Free Energies= -2958.374466
 E(RM06L) = -3247.22347588

C	-3.09697	3.15887	3.04163
C	-1.78622	2.80977	3.42249
C	-0.83066	2.68126	2.40707
C	-1.14536	2.8741	1.04197
C	-2.44799	3.22491	0.6855
C	-3.42705	3.36374	1.69259
H	-3.86481	3.27599	3.81337
H	-1.52365	2.6579	4.47348
H	-2.70974	3.40358	-0.3615
H	-4.44992	3.63965	1.41833
C	1.19032	2.45391	1.31626
C	0.1291	2.72007	0.20912
C	0.10788	1.53441	-0.80448
H	1.00763	1.57952	-1.43365
H	-0.77909	1.63114	-1.44278
C	0.4386	4.0348	-0.55069
C	1.40799	4.95316	-0.09639
C	-0.29242	4.36052	-1.71535
C	1.6316	6.16069	-0.77796
H	2.01037	4.71999	0.78535
C	-0.06851	5.56681	-2.39491
H	-1.04049	3.6636	-2.10627
C	0.89436	6.4758	-1.92858
H	2.3902	6.85634	-0.40296
H	-0.65015	5.79451	-3.29487
H	1.06982	7.41756	-2.45917
O	2.41088	2.3207	1.17292

N	0.54033	2.40596	2.5422
C	1.21617	2.08335	3.7875
H	1.08625	2.89484	4.525
H	0.82311	1.13904	4.20264
H	2.28356	1.96202	3.55208
Pd	0.0359	-0.35216	0.13261
I	-0.10308	-2.19434	2.26905
P	2.3983	-0.72446	-0.25587
C	2.59656	-2.52174	-0.67412
C	3.8061	-3.2086	-0.44205
C	1.52785	-3.20014	-1.29486
C	3.94078	-4.55107	-0.82939
H	4.63969	-2.6965	0.04752
C	1.66918	-4.53877	-1.69049
H	0.57875	-2.67674	-1.45466
C	2.87603	-5.21752	-1.45656
H	4.88188	-5.07702	-0.63625
H	0.82605	-5.0503	-2.16558
H	2.98438	-6.26572	-1.75527
C	3.72811	-0.44793	1.00886
C	5.04088	-0.08137	0.64106
C	3.43326	-0.67553	2.36931
C	6.03728	0.06161	1.62022
H	5.28724	0.09934	-0.40903
C	4.43564	-0.53892	3.34156
H	2.4198	-0.97451	2.65963
C	5.73824	-0.1659	2.9723
H	7.0502	0.35153	1.32066
H	4.19382	-0.72597	4.39343
H	6.51736	-0.05471	3.73413
C	3.077	0.09408	-1.78227
C	3.20761	-0.61534	-2.99593
C	3.40949	1.47013	-1.754
C	3.6675	0.03318	-4.15352
H	2.96029	-1.67993	-3.03727
C	3.87377	2.10904	-2.91474
H	3.29637	2.03349	-0.82072
C	4.00369	1.39547	-4.11708
H	3.76898	-0.53479	-5.08467
H	4.12769	3.17353	-2.8753
H	4.36406	1.89839	-5.02091
P	-2.23433	-0.75451	-0.52949
C	-2.35069	-2.39493	-1.4179
C	-2.01552	-3.56794	-0.70401
C	-2.81234	-2.51699	-2.74687
C	-2.13975	-4.82773	-1.30846
H	-1.65082	-3.49191	0.32666
C	-2.92264	-3.78105	-3.35054
H	-3.1013	-1.62946	-3.31538
C	-2.58848	-4.94046	-2.63515
H	-1.88074	-5.72344	-0.73413
H	-3.28189	-3.8538	-4.38268
H	-2.68204	-5.92516	-3.10551
C	-3.55341	-0.9261	0.75402
C	-4.71972	-1.68472	0.50921
C	-3.39496	-0.27507	1.99259
C	-5.71583	-1.78186	1.49204
H	-4.84387	-2.2047	-0.44612
C	-4.39638	-0.37409	2.97143
H	-2.48225	0.29279	2.19394
C	-5.55451	-1.12693	2.72493
H	-6.61489	-2.37601	1.29679
H	-4.25977	0.13098	3.9327
H	-6.32906	-1.21104	3.49481
C	-2.98381	0.40625	-1.77011
C	-4.22336	1.04252	-1.55346
C	-2.2776	0.68391	-2.96534
C	-4.75016	1.92413	-2.51253
H	-4.78118	0.84443	-0.63407
C	-2.8108	1.55784	-3.92603
H	-1.30857	0.20534	-3.14757
C	-4.04919	2.18256	-3.70074
H	-5.71642	2.4059	-2.32888
H	-2.25385	1.75223	-4.84857
H	-4.46367	2.86761	-4.44762

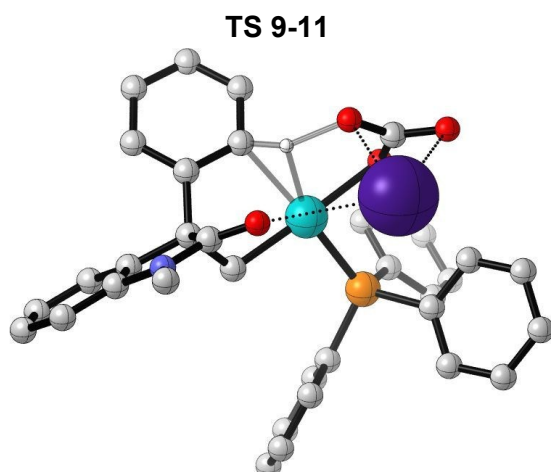


Zero-point correction= 0.536769 (Hartree/Particle)
 Thermal correction to Energy= 0.578056
 Thermal correction to Enthalpy= 0.579000
 Thermal correction to Gibbs Free Energy= 0.456288
 Sum of electronic and zero-point Energies= -2194.549833
 Sum of electronic and thermal Energies= -2194.508545
 Sum of electronic and thermal Enthalpies= -2194.507601
 Sum of electronic and thermal Free Energies= -2194.630314
 E(RM06L) = -2196.96204173

C	-1.88164	5.84545	-1.11262
C	-2.82399	4.87685	-1.50982
C	-2.64889	3.57173	-1.03567
C	-1.57737	3.2044	-0.19369
C	-0.63931	4.17539	0.17011
C	-0.80204	5.50137	-0.28282
H	-1.99385	6.87696	-1.46243
H	-3.66046	5.13961	-2.1647
H	0.21689	3.9088	0.79851
H	-0.07594	6.26581	0.01122
C	-2.97123	1.31578	-0.62123
C	-1.61791	1.69814	0.06873
C	-0.36594	1.11544	-0.71715
H	0.45838	1.80761	-0.48855
H	-0.57267	1.21216	-1.80178
C	-1.69716	1.2951	1.55059
C	-1.74314	-0.07633	1.89315
C	-1.78287	2.24602	2.58661
C	-1.84334	-0.4746	3.23613
H	-1.68717	-0.82291	1.09195
C	-1.88021	1.8454	3.93098
H	-1.77254	3.31268	2.34438
C	-1.90776	0.48335	4.26337
H	-1.85494	-1.54313	3.48218
H	-1.93415	2.60595	4.7178
H	-1.97926	0.16976	5.31075
O	-3.58458	0.24243	-0.59619
N	-3.44927	2.44391	-1.28683
C	-4.67704	2.45133	-2.05845
H	-5.40963	3.15978	-1.63121
H	-4.48341	2.73021	-3.10949
H	-5.08727	1.43158	-2.0188
Pd	0.32778	-0.84995	-0.50875
P	2.50301	-0.2768	-0.15614
C	3.6759	-1.23366	-1.22744
C	4.93033	-0.71466	-1.61854
C	3.29761	-2.53095	-1.64188
C	5.79786	-1.4844	-2.41028
H	5.22557	0.29419	-1.31262
C	4.17499	-3.29285	-2.43019
H	2.31867	-2.93345	-1.34818
C	5.42183	-2.77494	-2.81672
H	6.76708	-1.07178	-2.71134
H	3.87431	-4.29684	-2.74842
H	6.09863	-3.37291	-3.43691
C	3.04786	-0.65645	1.57232

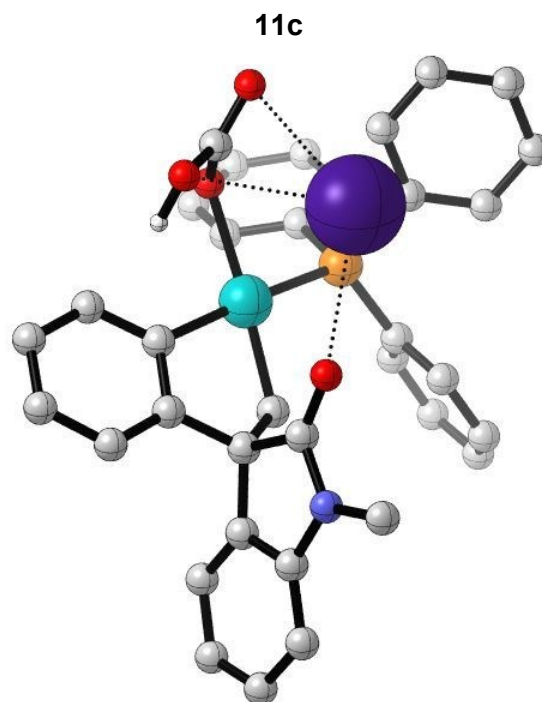
C	4.36976	-1.03546	1.88869
C	2.09098	-0.55424	2.60454
C	4.72861	-1.29864	3.22011
H	5.11385	-1.13661	1.09179
C	2.45678	-0.81036	3.93508
H	1.05726	-0.28927	2.35442
C	3.77461	-1.18374	4.24493
H	5.75502	-1.59994	3.45591
H	1.70413	-0.72809	4.72612
H	4.05703	-1.39406	5.28223
C	3.05857	1.47202	-0.41645
C	2.83493	2.05596	-1.68466
C	3.65649	2.24903	0.59675
C	3.22184	3.37923	-1.93834
H	2.35303	1.46693	-2.47323
C	4.03627	3.57807	0.34149
H	3.83177	1.81336	1.58516
C	3.82462	4.14429	-0.9249
H	3.04479	3.81653	-2.9266
H	4.50372	4.16892	1.13676
H	4.12337	5.17941	-1.1218
C	-0.83889	-3.11305	-0.64082
O	0.45755	-3.01359	-0.41316
O	-1.43999	-1.91612	-0.83781
O	-1.50191	-4.17481	-0.65353
Cs	-4.1841	-2.74095	-0.30557

H	-0.61853	-1.22107	4.0469
H	-4.60123	0.41202	4.59565
H	-2.49258	-0.51112	5.58969
O	-2.14312	-1.88148	-0.78551
N	-4.04656	-0.76256	-1.48809
C	-4.47437	-1.74305	-2.46756
H	-5.49244	-2.10698	-2.24235
H	-4.4668	-1.31679	-3.48712
H	-3.7658	-2.58269	-2.4144
Pd	0.11012	0.11263	0.91782
P	1.8071	1.14794	-0.19684
C	2.90766	0.05827	-1.22495
C	3.27289	0.35933	-2.55573
C	3.41763	-1.11084	-0.60967
C	4.12122	-0.50402	-3.27053
H	2.90516	1.26978	-3.03777
C	4.26815	-1.96231	-1.33452
H	3.1486	-1.36674	0.42718
C	4.61955	-1.66837	-2.66397
H	4.39963	-0.25575	-4.30073
H	4.66	-2.85632	-0.8367
H	5.28875	-2.33416	-3.22078
C	2.97514	1.91765	1.00537
C	4.25709	2.35038	0.60283
C	2.57314	2.07754	2.34634
C	5.11844	2.9534	1.53118
H	4.58372	2.20647	-0.43263
C	3.43933	2.68168	3.27101
H	1.59349	1.69716	2.65508
C	4.70915	3.12178	2.86515
H	6.11317	3.28467	1.21452
H	3.12484	2.79411	4.3137
H	5.38603	3.58682	3.5899
C	1.33824	2.53124	-1.3334
C	0.61389	2.24914	-2.51545
C	1.61149	3.8777	-1.01284
C	0.19835	3.28468	-3.36555
H	0.38264	1.21054	-2.7763
C	1.18416	4.91326	-1.85993
H	2.16597	4.1163	-0.10047
C	0.48156	4.62116	-3.03892
H	-0.35472	3.04698	-4.28049
H	1.40671	5.95254	-1.59586
H	0.15147	5.43008	-3.69895
C	1.36441	-2.28952	1.76112
O	1.63249	-0.96999	1.94007
O	0.11129	-2.67346	1.75083
O	2.32908	-3.08209	1.52914
Cs	0.44714	-3.74157	-0.92198



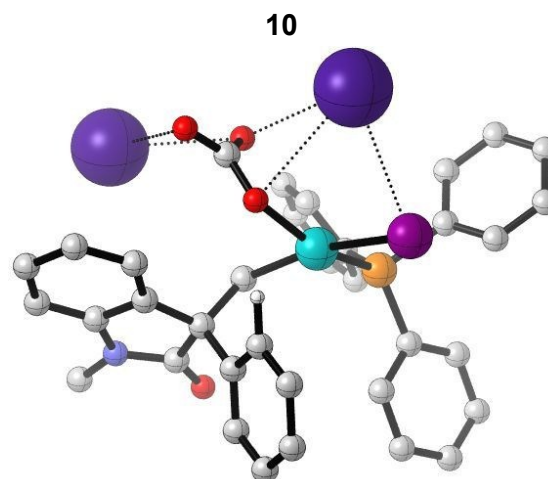
Zero-point correction= 0.533112 (Hartree/Particle)
 Thermal correction to Energy= 0.573636
 Thermal correction to Enthalpy= 0.574581
 Thermal correction to Gibbs Free Energy= 0.454541
 Sum of electronic and zero-point Energies= -2194.516323
 Sum of electronic and thermal Energies= -2194.475799
 Sum of electronic and thermal Enthalpies= -2194.474854
 Sum of electronic and thermal Free Energies= -2194.594894
 E(RM06L) = -2196.91923456
 Imaginary frequency = 153-73 cm⁻¹

C	-6.23287	2.28622	-1.51019
C	-5.8055	1.00126	-1.89983
C	-4.67687	0.47552	-1.26104
C	-3.97509	1.17969	-0.25934
C	-4.40854	2.45574	0.10784
C	-5.5447	3.00752	-0.52099
H	-7.11336	2.72513	-1.99082
H	-6.33824	0.4406	-2.67404
H	-3.8727	3.01898	0.87902
H	-5.89103	4.0058	-0.23555
C	-2.90466	-0.90999	-0.70143
C	-2.78616	0.35298	0.2125
C	-1.43911	1.09049	-0.05493
H	-1.50297	2.09713	0.39865
H	-1.2724	1.21474	-1.13816
C	-2.8062	-0.01478	1.70552
C	-1.62993	-0.59438	2.25709
C	-3.87055	0.32554	2.55844
C	-1.52872	-0.75443	3.6573
H	-0.90164	-1.40126	1.74438
C	-3.76036	0.13863	3.94821
H	-4.78403	0.76302	2.14377
C	-2.58097	-0.38243	4.50533



Zero-point correction= 0.536319 (Hartree/Particle)
 Thermal correction to Energy= 0.577809
 Thermal correction to Enthalpy= 0.578754
 Thermal correction to Gibbs Free Energy= 0.456117
 Sum of electronic and zero-point Energies= -2194.554779
 Sum of electronic and thermal Energies= -2194.513289
 Sum of electronic and thermal Enthalpies= -2194.512345
 Sum of electronic and thermal Free Energies= -2194.634981
 E(RM06L) = -2196.95078055

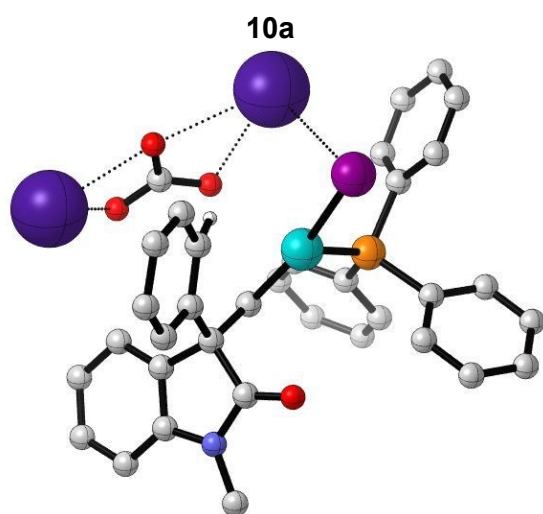
C	-6.33839	2.70251	-0.56537
C	-5.8637	1.72367	-1.46143
C	-4.72744	1.00134	-1.08092
C	-4.06171	1.22387	0.14271
C	-4.5489	2.19341	1.02069
C	-5.69296	2.936	0.66017
H	-7.22567	3.28583	-0.83276
H	-6.36853	1.53994	-2.41492
H	-4.04985	2.36852	1.9797
H	-6.08209	3.69846	1.34236
C	-2.95106	-0.48589	-1.09296
C	-2.85802	0.29855	0.25041
C	-1.50316	1.08018	0.32365
H	-1.6161	1.88176	1.07705
H	-1.26514	1.55852	-0.64162
C	-2.87443	-0.63168	1.45939
C	-1.59268	-0.90465	2.00791
C	-4.04216	-1.14915	2.04691
C	-1.52969	-1.65419	3.20534
H	-0.38077	-2.87816	1.86088
C	-3.95335	-1.9277	3.21431
H	-5.02356	-0.92362	1.61207
C	-2.70056	-2.16663	3.80059
H	-0.55687	-1.83001	3.68171
H	-4.86366	-2.32623	3.67561
H	-2.63106	-2.74587	4.72891
O	-2.19354	-1.36216	-1.53578
N	-4.06211	-0.0196	-1.79069
C	-4.46017	-0.52066	-3.09259
H	-5.47958	-0.9445	-3.05759
H	-4.43616	0.28193	-3.85163
H	-3.74453	-1.30916	-3.36842
Pd	0.00588	-0.12505	1.03052
P	1.86355	1.08127	0.04736
C	2.98275	0.22212	-1.17096
C	3.28964	0.72108	-2.45607
C	3.52534	-1.02198	-0.76834
C	4.11406	-0.01391	-3.32667
H	2.89232	1.6883	-2.7788
C	4.35232	-1.74677	-1.64213
H	3.29042	-1.44866	0.21574
C	4.64801	-1.24909	-2.924
H	4.34777	0.39026	-4.318
H	4.76283	-2.70493	-1.30539
H	5.29762	-1.81464	-3.6013
C	3.04355	1.58473	1.37784
C	4.36416	1.9986	1.09909
C	2.59455	1.55125	2.71434
C	5.2175	2.38415	2.14371
H	4.72551	2.01098	0.06524
C	3.45171	1.93877	3.75652
H	1.57747	1.20093	2.92611
C	4.76162	2.35601	3.47301
H	6.24188	2.70104	1.92033
H	3.09728	1.90213	4.7919
H	5.43181	2.65146	4.2874
C	1.45215	2.67213	-0.8091
C	0.64414	2.63095	-1.97
C	1.84999	3.92974	-0.30991
C	0.26681	3.81208	-2.62614
H	0.3106	1.66447	-2.36513
C	1.45921	5.11224	-0.96005
H	2.46996	3.98495	0.5897
C	0.67246	5.05836	-2.12057
H	-0.35424	3.75887	-3.52677
H	1.77646	6.07963	-0.55623
H	0.37093	5.98167	-2.62605
C	1.49974	-2.7861	1.40254
O	1.50607	-1.57424	1.85874
O	0.27358	-3.47258	1.42301
O	2.44773	-3.40655	0.88131
Cs	0.44504	-2.88635	-1.64435



Zero-point correction= 0.537257 (Hartree/Particle)
 Thermal correction to Energy= 0.583325
 Thermal correction to Enthalpy= 0.584270
 Thermal correction to Gibbs Free Energy= 0.449174
 Sum of electronic and zero-point Energies= -2225.965109
 Sum of electronic and thermal Energies= -2225.919041
 Sum of electronic and thermal Enthalpies= -2225.918096
 Sum of electronic and thermal Free Energies= -2226.053192
 E(RM06L) = -2515.11397313

C	-6.00399	0.15335	-1.27263
C	-5.7944	1.21064	-0.35986
C	-4.47604	1.6496	-0.16789
C	-3.36686	1.0596	-0.83023
C	-3.59497	0.00532	-1.72098
C	-4.91966	-0.44106	-1.93969
H	-7.02581	-0.1937	-1.46538
H	-6.63426	1.69221	0.15168
H	-2.75317	-0.51681	-2.18737
H	-5.09019	-1.26696	-2.63762
C	-2.64763	2.83161	0.61001
C	-2.08057	1.77695	-0.39536
C	-1.10066	0.8982	0.46484
H	-1.61247	0.02692	0.90443
H	-0.71001	1.54102	1.26652
C	-1.40547	2.48451	-1.59475
C	-1.34493	3.88849	-1.71176
C	-0.8428	1.69729	-2.62605
C	-0.73366	4.49058	-2.82649
H	-1.74839	4.52276	-0.91827
C	-0.22573	2.30212	-3.73208
H	-0.88568	0.60455	-2.56995
C	-0.16988	3.70076	-3.83955
H	-0.70124	5.58392	-2.896
H	0.22709	1.66553	-4.49865
H	0.31274	4.17014	-4.70369
O	-2.02282	3.65528	1.27937
N	-4.03688	2.67785	0.67603
C	-4.8768	3.50402	1.52182
H	-5.60779	4.07489	0.92192
H	-5.42647	2.89364	2.26239
H	-4.20573	4.20051	2.04719
Pd	0.52887	-0.01083	-0.51391
I	2.49142	-0.74439	-2.53593
P	2.02952	0.85112	0.98484
C	2.71278	2.55756	0.80013
C	3.87714	2.99709	1.47075
C	2.02797	3.44684	-0.05302
C	4.33634	4.31194	1.29935
H	4.43297	2.30495	2.11217
C	2.49046	4.76199	-0.21873
H	1.1397	3.10294	-0.5933
C	3.64144	5.19652	0.45658
H	5.2415	4.64388	1.81953
H	1.95	5.439	-0.88771
H	4.00486	6.2209	0.32036
C	3.55956	-0.19163	1.18302
C	3.64899	-1.20258	2.16506
C	4.63181	-0.0271	0.27685
C	4.78286	-2.03104	2.23797
H	2.83906	-1.33057	2.89055
C	5.76736	-0.84654	0.36201
H	4.5738	0.73734	-0.50241

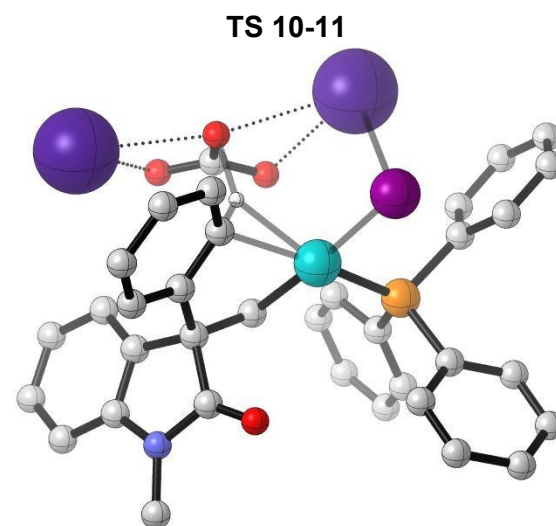
C	5.84643	-1.85434	1.33727
H	4.84287	-2.79861	3.01837
H	6.58833	-0.7017	-0.34793
H	6.73496	-2.49209	1.40065
C	1.32651	0.7841	2.70842
C	1.63796	1.72011	3.7148
C	0.46303	-0.2962	3.01223
C	1.11704	1.57068	5.01087
H	2.28123	2.57554	3.48646
C	-0.03499	-0.45009	4.3166
H	0.15512	-0.9901	2.21339
C	0.28996	0.47933	5.31916
H	1.36129	2.31054	5.78082
H	-0.68931	-1.29918	4.54788
H	-0.10771	0.36041	6.33317
C	-1.49167	-2.20851	-0.55023
O	-0.87856	-1.3331	-1.37332
O	-1.10667	-2.31982	0.6913
O	-2.43357	-2.91049	-1.05863
Cs	-4.11699	-2.02734	1.22609
Cs	1.33893	-3.69917	-0.5281



Zero-point correction= 0.535798 (Hartree/Particle)
 Thermal correction to Energy= 0.582385
 Thermal correction to Enthalpy= 0.583329
 Thermal correction to Gibbs Free Energy= 0.445552
 Sum of electronic and zero-point Energies= -2225.951124
 Sum of electronic and thermal Energies= -2225.904537
 Sum of electronic and thermal Enthalpies= -2225.903593
 Sum of electronic and thermal Free Energies= -2226.041370
 E(RM06L) = -2515.09823251

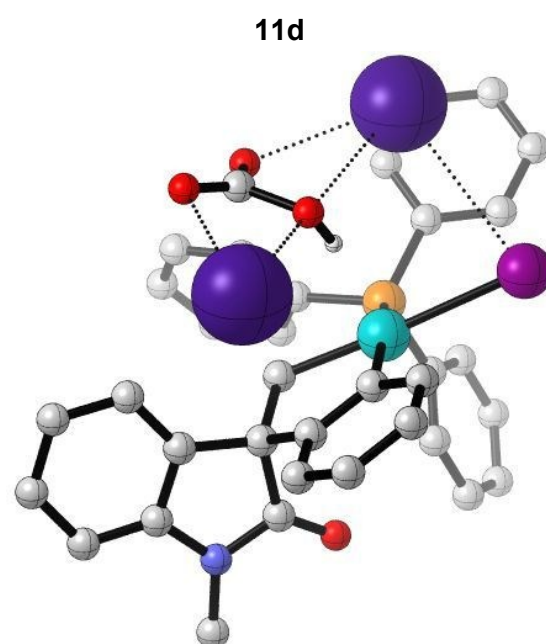
C	-4.93133	3.75899	1.77225
C	-4.2258	4.39376	0.72891
C	-3.23901	3.64832	0.07381
C	-2.96525	2.30467	0.41912
C	-3.6393	1.69258	1.48095
C	-4.63601	2.43834	2.15106
H	-5.70532	4.31962	2.30789
H	-4.43457	5.43298	0.45647
H	-3.35016	0.68221	1.83452
H	-5.16505	1.98738	2.99789
C	-1.47101	3.04599	-1.30265
C	-1.83902	1.7803	-0.47094
C	-0.63117	1.36037	0.39297
H	-0.91031	0.64884	1.19363
H	-0.14981	2.24931	0.82537
C	-2.31468	0.67981	-1.43307
C	-3.23903	0.98635	-2.45827
C	-1.82376	-0.64143	-1.34151
C	-3.64455	0.01337	-3.38143
H	-3.63168	2.00592	-2.54126
C	-2.21599	-1.61422	-2.28884
H	-1.25744	-0.99397	-0.45695
C	-3.11916	-1.29414	-3.30845
H	-4.35022	0.27933	-4.1762
H	-1.79405	-2.62094	-2.21326
H	-3.40536	-2.04561	-4.05251
O	-0.55765	3.17184	-2.11928

N	-2.36836	4.0606	-0.9556
C	-2.27802	5.40643	-1.49308
H	-3.22136	5.7	-1.98664
H	-2.05048	6.13716	-0.69627
H	-1.46168	5.40123	-2.23089
Pd	0.64953	0.18175	-0.74756
I	1.77397	-1.5922	-2.63044
P	2.43504	0.89905	0.47635
C	3.47611	2.05602	-0.51296
C	4.8548	2.23566	-0.26097
C	2.85326	2.78901	-1.54596
C	5.59804	3.14327	-1.03134
H	5.34701	1.66007	0.52981
C	3.60324	3.69912	-2.30757
H	1.78701	2.63743	-1.75592
C	4.97285	3.87633	-2.05406
H	6.66753	3.27397	-0.83436
H	3.11342	4.25963	-3.11032
H	5.55674	4.57943	-2.65779
C	3.59559	-0.46814	0.95639
C	3.66697	-0.94995	2.2835
C	4.3763	-1.09685	-0.04311
C	4.49263	-2.04255	2.60109
H	3.08144	-0.46712	3.07145
C	5.20778	-2.17909	0.28282
H	4.31487	-0.75302	-1.07957
C	5.26533	-2.66149	1.6031
H	4.54293	-2.39622	3.63698
H	5.80777	-2.65027	-0.50293
H	5.91724	-3.5055	1.85392
C	2.1178	1.75332	2.08824
C	2.8112	2.93135	2.44108
C	1.17149	1.19926	2.98612
C	2.57793	3.54305	3.68285
H	3.53291	3.37231	1.74689
C	0.9571	1.81853	4.22919
H	0.57213	0.30815	2.72467
C	1.65452	2.98535	4.58153
H	3.1201	4.45818	3.94484
H	0.21966	1.38552	4.91332
H	1.47149	3.46597	5.54889
C	-1.79347	-1.7219	1.93102
O	-1.91843	-2.71317	1.06932
O	-0.59275	-1.26186	2.1883
O	-2.84426	-1.18758	2.47562
Cs	-4.72109	-1.96698	0.38524
Cs	1.04501	-3.3419	0.82259



Zero-point correction= 0.534275 (Hartree/Particle)
 Thermal correction to Energy= 0.579570
 Thermal correction to Enthalpy= 0.580514
 Thermal correction to Gibbs Free Energy= 0.448632
 Sum of electronic and zero-point Energies= -2225.951260
 Sum of electronic and thermal Energies= -2225.905964
 Sum of electronic and thermal Enthalpies= -2225.905020
 Sum of electronic and thermal Free Energies= -2226.036903
 E(RM06L) = -2515.09079178
 Imaginary frequency = 116.13 cm⁻¹

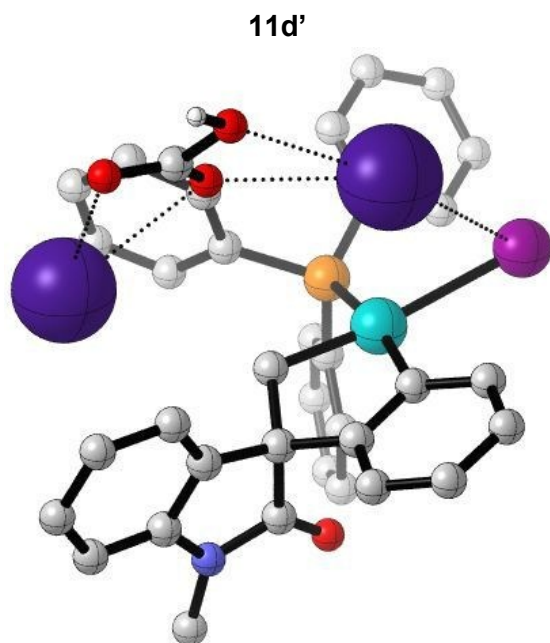
C	-5.42842	3.14799	1.85116
C	-4.82357	3.8529	0.78983
C	-3.7392	3.24314	0.14838
C	-3.27285	1.96216	0.52323
C	-3.84981	1.28647	1.60337
C	-4.94357	1.89431	2.26138
H	-6.27501	3.60306	2.37692
H	-5.18077	4.84464	0.49555
H	-3.41544	0.33511	1.9696
H	-5.40039	1.39229	3.12138
C	-1.88946	2.88119	-1.20467
C	-2.09133	1.57995	-0.36301
C	-0.81642	1.2879	0.45931
H	-1.02743	0.64764	1.33181
H	-0.35441	2.22643	0.79713
C	-2.40592	0.44749	-1.34774
C	-3.45401	0.58718	-2.28477
C	-1.57335	-0.70474	-1.38703
C	-3.67029	-0.3862	-3.27081
H	-4.08893	1.48061	-2.25561
C	-1.78855	-1.6601	-2.41691
H	-1.14343	-1.20809	-0.40134
C	-2.81983	-1.51048	-3.34905
H	-4.48028	-0.25526	-3.99747
H	-1.12582	-2.52963	-2.4623
H	-2.96052	-2.25274	-4.14279
O	-0.99216	3.1317	-2.00848
N	-2.93507	3.75575	-0.88916
C	-3.03874	5.0904	-1.45161
H	-4.00981	5.23194	-1.95822
H	-2.93035	5.86071	-0.66697
H	-2.22282	5.19323	-2.1826
Pd	0.47441	0.12353	-0.67542
I	1.91405	-1.4992	-2.5358
P	2.28884	1.0716	0.39298
C	3.16863	2.28398	-0.68248
C	4.52453	2.62882	-0.48574
C	2.43516	2.90065	-1.71894
C	5.13727	3.57851	-1.31751
H	5.10198	2.14976	0.31166
C	3.05445	3.85425	-2.54258
H	1.38335	2.63318	-1.8789
C	4.4029	4.19207	-2.34642
H	6.19042	3.83678	-1.16272
H	2.47868	4.32398	-3.34654
H	4.88511	4.92925	-2.99751
C	3.61709	-0.13135	0.89675
C	3.75811	-0.55893	2.23621
C	4.47493	-0.67649	-0.08777
C	4.72541	-1.51937	2.58106
H	3.11647	-0.13607	3.01465
C	5.44617	-1.62749	0.26415
H	4.37314	-0.36653	-1.13126
C	5.57196	-2.05798	1.59667
H	4.82674	-1.8297	3.62705
H	6.10537	-2.03286	-0.51077
H	6.33446	-2.79635	1.8683
C	1.95161	1.97315	1.97723
C	2.49465	3.25127	2.22767
C	1.13178	1.35367	2.95346
C	2.24101	3.89943	3.44711
H	3.1134	3.74317	1.47118
C	0.8958	2.01165	4.17255
H	0.64683	0.37647	2.76878
C	1.44672	3.27873	4.42427
H	2.66554	4.89267	3.62979
H	0.25727	1.52669	4.91855
H	1.24877	3.78703	5.37445
C	-1.45058	-1.7402	1.92533
O	-1.44585	-2.43076	0.75902
O	-0.30863	-1.35984	2.40936
O	-2.58586	-1.47217	2.48188
Cs	-4.37678	-2.24329	0.29264
Cs	1.48513	-3.22056	0.94714



Zero-point correction= 0.536335 (Hartree/Particle)
 Thermal correction to Energy= 0.582690
 Thermal correction to Enthalpy= 0.583635
 Thermal correction to Gibbs Free Energy= 0.447843
 Sum of electronic and zero-point Energies= -2225.993924
 Sum of electronic and thermal Energies= -2225.947569
 Sum of electronic and thermal Enthalpies= -2225.946624
 Sum of electronic and thermal Free Energies= -2226.082416
 E(RM06L) = -2515.11865168

C	-5.77427	2.34633	2.37489
C	-5.36591	3.21675	1.34418
C	-4.2658	2.83143	0.56711
C	-3.58681	1.60934	0.7821
C	-3.98504	0.7717	1.82693
C	-5.09002	1.14512	2.62454
H	-6.62764	2.62609	3.00186
H	-5.88381	4.16505	1.17052
H	-3.41879	-0.13903	2.06433
H	-5.40003	0.50366	3.45608
C	-2.51072	2.85527	-0.95033
C	-2.45965	1.47142	-0.23257
C	-1.07646	1.21507	0.41666
H	-1.19649	0.54547	1.2868
H	-0.64113	2.15778	0.785
C	-2.70219	0.40122	-1.29235
C	-3.96861	0.19311	-1.88069
C	-1.55138	-0.32616	-1.71086
C	-4.12602	-0.76257	-2.89909
H	-4.82828	0.78917	-1.5477
C	-1.74425	-1.29105	-2.73093
H	-0.39663	-1.74355	0.28811
C	-3.00602	-1.50697	-3.31871
H	-5.10325	-0.90626	-3.3759
H	-0.88283	-1.86532	-3.08862
H	-3.10874	-2.24181	-4.12744
O	-1.74103	3.30676	-1.79589
N	-3.64123	3.53804	-0.47439
C	-4.00333	4.86842	-0.92689
H	-5.02435	4.88052	-1.34829
H	-3.95005	5.59926	-0.09968
H	-3.2792	5.14573	-1.70776
Pd	0.2296	0.18645	-0.81869
I	1.87849	-1.46966	-2.48288
P	2.11268	1.29156	0.25268
C	2.61717	2.72272	-0.80422
C	3.90573	3.29893	-0.74589
C	1.65487	3.26106	-1.68676
C	4.22763	4.39478	-1.56148
H	4.66008	2.88508	-0.06879
C	1.98328	4.36113	-2.49536
H	0.64851	2.8272	-1.7402
C	3.2669	4.92651	-2.43811
H	5.23111	4.83151	-1.51283
H	1.22837	4.76777	-3.17585

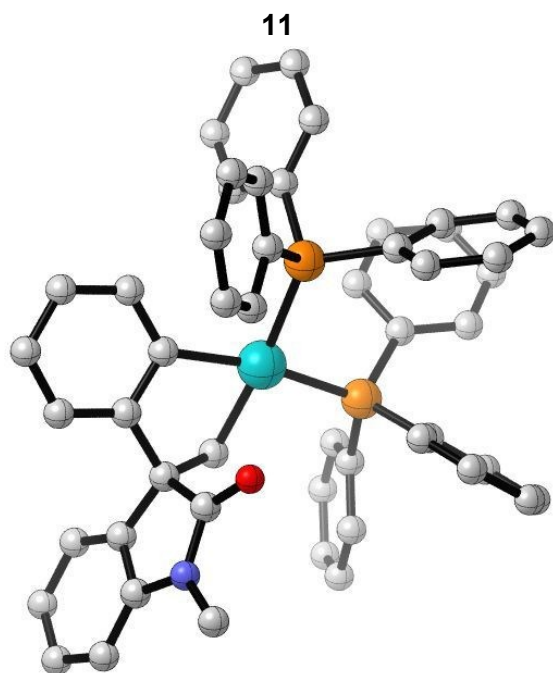
H	3.52166	5.7789	-3.07734
C	3.7354	0.43503	0.59121
C	4.16174	0.12385	1.90294
C	4.52824	0.00104	-0.4994
C	5.33917	-0.61507	2.12026
H	3.57489	0.46847	2.76033
C	5.70757	-0.72893	-0.27764
H	4.21302	0.22184	-1.52292
C	6.11514	-1.04684	1.03017
H	5.65945	-0.83112	3.14594
H	6.30727	-1.05226	-1.1352
H	7.03887	-1.6114	1.19881
C	1.74639	2.04052	1.91169
C	2.08838	3.36927	2.23933
C	1.10662	1.23043	2.87938
C	1.80431	3.8792	3.51669
H	2.57184	4.00868	1.49402
C	0.8396	1.74437	4.15885
H	0.79553	0.20187	2.64428
C	1.18478	3.06743	4.48052
H	2.06867	4.91495	3.7565
H	0.34242	1.10454	4.89547
H	0.96316	3.46813	5.47571
C	-0.96819	-2.2861	2.13764
O	-0.8647	-2.52995	0.68953
O	0.08089	-1.84024	2.67765
O	-2.08745	-2.59896	2.6093
Cs	-3.78283	-2.78497	0.0963
Cs	2.37415	-2.96654	1.04406



Zero-point correction= 0.536325 (Hartree/Particle)
 Thermal correction to Energy= 0.583170
 Thermal correction to Enthalpy= 0.584114
 Thermal correction to Gibbs Free Energy= 0.444954
 Sum of electronic and zero-point Energies= -2225.999715
 Sum of electronic and thermal Energies= -2225.952870
 Sum of electronic and thermal Enthalpies= -2225.951926
 Sum of electronic and thermal Free Energies= -2226.091086
 E(RM06L) = -2515.12236642

C	-5.95056	1.2707	-1.26534
C	-5.07604	2.00028	-2.09892
C	-3.77196	1.51066	-2.26529
C	-3.3158	0.34463	-1.59931
C	-4.20468	-0.37872	-0.8006
C	-5.52986	0.08782	-0.63116
H	-6.98014	1.62135	-1.13491
H	-5.41629	2.90282	-2.61614
H	-3.87795	-1.30588	-0.3165
H	-6.23453	-0.48718	-0.02094
C	-1.59275	1.20887	-3.0002
C	-1.84958	0.10802	-1.92791
C	-0.91664	0.39047	-0.7015

H	-1.32972	-0.12923	0.18494
H	-0.86217	1.47505	-0.48498
C	-1.50123	-1.27672	-2.44381
C	-2.37622	-2.02379	-3.25717
C	-0.21089	-1.76066	-2.08844
C	-1.98847	-3.28258	-3.73894
H	-3.36465	-1.62056	-3.51035
C	0.15723	-3.02812	-2.60214
H	-3.43522	-3.51801	3.40901
C	-0.71654	-3.77963	-3.41072
H	-2.6694	-3.8648	-4.3699
H	1.15726	-3.42197	-2.38665
H	-0.39189	-4.7537	-3.79759
O	-0.58527	1.41339	-3.67032
N	-2.74764	2.01569	-3.0726
C	-2.85729	3.14842	-3.97338
H	-3.6737	2.99913	-4.70258
H	-3.04009	4.0862	-3.41839
H	-1.89761	3.21963	-4.50715
Pd	0.9452	-0.51272	-0.9153
I	3.2297	-2.1951	-0.88198
P	2.09709	1.25957	0.26885
C	2.54768	2.62902	-0.89569
C	3.44244	3.66528	-0.54007
C	1.9857	2.61443	-2.18875
C	3.74952	4.68013	-1.45884
H	3.91196	3.6656	0.4494
C	2.29925	3.63234	-3.10524
H	1.31173	1.80109	-2.48329
C	3.1761	4.66612	-2.7427
H	4.44593	5.4769	-1.17545
H	1.85865	3.60215	-4.10693
H	3.42485	5.45499	-3.46112
C	3.70054	1.03421	1.1912
C	3.81118	1.12551	2.59359
C	4.85567	0.73078	0.43437
C	5.04988	0.92307	3.22646
H	2.93466	1.36673	3.20173
C	6.09107	0.54134	1.06909
H	4.78766	0.63617	-0.65282
C	6.19288	0.63391	2.46689
H	5.11737	1.0021	4.31709
H	6.97452	0.30722	0.46617
H	7.15843	0.47979	2.96048
C	1.06577	2.10002	1.57803
C	0.91426	3.49888	1.68604
C	0.44602	1.27694	2.54593
C	0.19605	4.06232	2.75543
H	1.3724	4.1525	0.9372
C	-0.23986	1.84003	3.6356
H	0.48207	0.18762	2.44794
C	-0.36356	3.23717	3.74716
H	0.09747	5.15126	2.82696
H	-0.67715	1.17493	4.38896
H	-0.88224	3.68084	4.60517
C	-2.73263	-1.80053	2.9836
O	-2.57134	-3.21869	3.06171
O	-1.7058	-1.1935	2.55589
O	-3.85981	-1.35391	3.32655
Cs	-3.37282	1.39085	2.07975
Cs	0.02153	-3.34326	1.15698

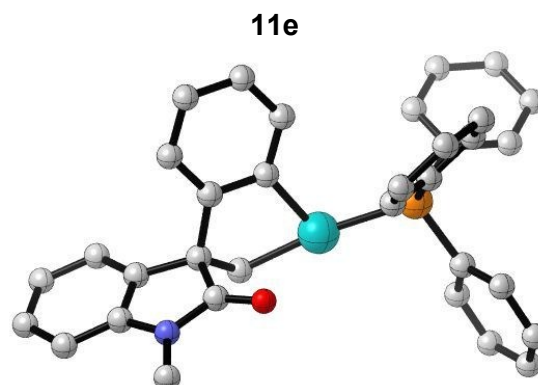


Zero-point correction= 0.776422 (Hartree/Particle)
 Thermal correction to Energy= 0.828561
 Thermal correction to Enthalpy= 0.829505
 Thermal correction to Gibbs Free Energy= 0.686415
 Sum of electronic and zero-point Energies= -2946.220168
 Sum of electronic and thermal Energies= -2946.168029
 Sum of electronic and thermal Enthalpies= -2946.167085
 Sum of electronic and thermal Free Energies= -2946.310175
 E(RM06L) = -2948.68397460

Pd	0.25847	-0.2668	-0.47792
P	-0.33345	2.0511	-0.15487
P	-1.88526	-1.28603	0.07728
O	2.24223	-0.86719	2.05946
N	4.50554	-0.53435	1.67663
C	1.15347	-2.09793	-0.96053
C	0.54853	-3.27466	-1.45194
H	-0.53039	-3.31287	-1.63278
C	1.29736	-4.43661	-1.71794
H	0.79159	-5.3295	-2.10453
C	2.67996	-4.45749	-1.48248
H	3.26477	-5.36223	-1.68271
C	3.31236	-3.3017	-0.99914
H	4.39591	-3.29386	-0.83193
C	2.56023	-2.13741	-0.76024
C	3.17035	-0.827	-0.28761
C	2.24807	0.28484	-0.85048
H	2.35552	0.31935	-1.94915
H	2.51413	1.27424	-0.44493
C	4.63801	-0.60993	-0.62018
C	5.29917	-0.55261	-1.84773
H	4.74209	-0.69913	-2.77929
C	6.68984	-0.31343	-1.87267
H	7.21647	-0.2684	-2.83133
C	7.40263	-0.13505	-0.67573
H	8.48168	0.04958	-0.70785
C	6.75254	-0.19209	0.57366
H	7.30993	-0.05642	1.50568
C	5.37306	-0.431	0.57357
C	3.18749	-0.76077	1.27248
C	4.89659	-0.40982	3.06804
H	3.98304	-0.53478	3.66846
H	5.33753	0.58315	3.26933
H	5.63081	-1.18743	3.3453
C	0.82968	3.31168	-0.88395
C	1.94646	3.75663	-0.14089
H	2.08816	3.41336	0.88886
C	2.87076	4.64939	-0.70538
H	3.7279	4.98572	-0.11242
C	2.69952	5.10707	-2.02128
H	3.42086	5.80387	-2.46073
C	1.59791	4.66397	-2.76996
H	1.45298	5.01651	-3.79678
C	0.67113	3.77183	-2.20806

H	-0.18752	3.44299	-2.80171
C	-0.4359	2.61537	1.60416
C	-0.56511	3.97411	1.97685
H	-0.59577	4.75295	1.20785
C	-0.61575	4.3359	3.33104
H	-0.71773	5.39059	3.60843
C	-0.52043	3.34948	4.32813
H	-0.55327	3.63518	5.38504
C	-0.36371	2.00297	3.96703
H	-0.2647	1.23312	4.73904
C	-0.31939	1.63582	2.6119
H	-0.15815	0.59138	2.32388
C	-1.92942	2.53205	-0.97295
C	-2.81907	3.51348	-0.4904
H	-2.61333	4.02443	0.45422
C	-3.98886	3.82156	-1.20317
H	-4.67435	4.58216	-0.81396
C	-4.28423	3.15734	-2.40557
H	-5.19906	3.39955	-2.95677
C	-3.40656	2.17497	-2.89214
H	-3.63502	1.6379	-3.81836
C	-2.2396	1.86132	-2.17672
H	-1.56689	1.07329	-2.53409
C	-3.11006	-0.4582	1.21321
C	-3.08803	-0.72069	2.60101
H	-2.37982	-1.45039	3.00515
C	-3.98218	-0.07233	3.46662
H	-3.95332	-0.29638	4.53838
C	-4.916	0.84631	2.96262
H	-5.61902	1.34582	3.63763
C	-4.94288	1.11805	1.58577
H	-5.6653	1.83296	1.1781
C	-4.04519	0.47783	0.71713
H	-4.08591	0.70011	-0.35324
C	-2.94	-1.71145	-1.39243
C	-4.31017	-2.04474	-1.29834
H	-4.81139	-2.02784	-0.32535
C	-5.04459	-2.37068	-2.44955
H	-6.10585	-2.62681	-2.36059
C	-4.42408	-2.36566	-3.70974
H	-4.99983	-2.62021	-4.606
C	-3.06581	-2.02621	-3.81608
H	-2.57535	-2.01462	-4.79526
C	-2.33022	-1.69664	-2.66625
H	-1.27033	-1.42405	-2.74222
C	-1.6318	-2.8905	0.98115
C	-0.48149	-3.00307	1.79241
H	0.26801	-2.20187	1.79578
C	-0.27596	-4.15953	2.56246
H	0.62064	-4.23671	3.18629
C	-1.19727	-5.21745	2.51345
H	-1.02702	-6.12379	3.10462
C	-2.33264	-5.11639	1.69284
H	-3.04902	-5.9434	1.63949
C	-2.55391	-3.95611	0.93463
H	-3.43802	-3.8917	0.29292

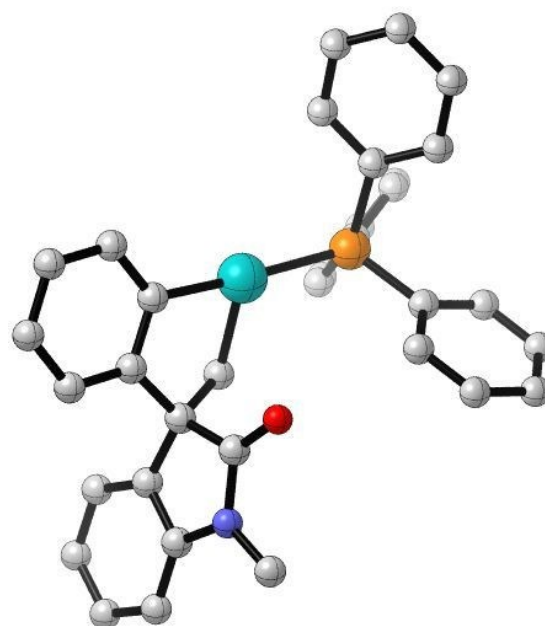
3



Zero-point correction= 0.507822 (Hartree/Particle)
 Thermal correction to Energy= 0.542530
 Thermal correction to Enthalpy= 0.543474
 Thermal correction to Gibbs Free Energy= 0.436477
 Sum of electronic and zero-point Energies= -1910.157173
 Sum of electronic and thermal Energies= -1910.122465
 Sum of electronic and thermal Enthalpies= -1910.121521
 Sum of electronic and thermal Free Energies= -1910.228518
 E(RM06L) = -1912.17832368

Pd	-0.08735	-0.10561	-0.90655
P	2.1886	-0.09237	-0.14432
O	-2.02755	-1.47249	1.39273
N	-4.29422	-1.51724	0.88591
C	-0.98672	1.44065	-0.01607
C	-0.3077	2.57874	0.44962
H	0.77605	2.67356	0.32781
C	-1.02412	3.60574	1.09498
H	-0.48704	4.48887	1.4594
C	-2.41236	3.49982	1.27606
H	-2.9642	4.30363	1.77511
C	-3.09485	2.36291	0.81367
H	-4.18049	2.27695	0.93894
C	-2.39019	1.33504	0.16344
C	-2.99419	0.04907	-0.37107
C	-2.04227	-0.38741	-1.52196
H	-2.21621	0.25575	-2.40281
H	-2.17659	-1.4484	-1.81024
C	-4.46337	0.09272	-0.75342
C	-5.14344	0.86968	-1.69227
H	-4.60428	1.61815	-2.28324
C	-6.53148	0.68346	-1.86737
H	-7.07275	1.28929	-2.60096
C	-7.22162	-0.27356	-1.10581
H	-8.29839	-0.4102	-1.25124
C	-6.55208	-1.06522	-0.15104
H	-7.09241	-1.8089	0.44263
C	-5.17596	-0.86246	0.00725
C	-2.98493	-1.04912	0.74447
C	-4.66137	-2.56204	1.82399
H	-3.74024	-2.8582	2.3479
H	-5.08436	-3.43658	1.29789
H	-5.40186	-2.19476	2.55693
C	2.86543	-1.79214	-0.43962
C	3.43642	-2.58859	0.57368
H	3.52203	-2.19425	1.59095
C	3.88982	-3.88574	0.28145
H	4.3316	-4.49607	1.07637
C	3.77777	-4.39985	-1.01987
H	4.13002	-5.41236	-1.24281
C	3.2064	-3.61359	-2.035
H	3.11225	-4.00975	-3.05155
C	2.74858	-2.32019	-1.74654
H	2.30436	-1.70956	-2.54281
C	3.4566	0.99523	-0.94067
C	4.83774	0.69797	-0.9245
H	5.19262	-0.2175	-0.43891
C	5.75441	1.55971	-1.54644
H	6.82302	1.32015	-1.52959
C	5.30279	2.72129	-2.19571
H	6.02004	3.38978	-2.68349
C	3.93039	3.01511	-2.23081
H	3.57211	3.91054	-2.74937
C	3.01026	2.15382	-1.61198
H	1.93592	2.36525	-1.65992
C	2.36774	0.16766	1.67521
C	1.28343	-0.23967	2.48628
H	0.37915	-0.65458	2.02387
C	1.35696	-0.09027	3.87965
H	0.51245	-0.40808	4.49975
C	2.49536	0.4801	4.47276
H	2.54416	0.60519	5.5598
C	3.5666	0.90212	3.6687
H	4.45172	1.35778	4.12547
C	3.50643	0.74624	2.27454
H	4.34164	1.08512	1.65341

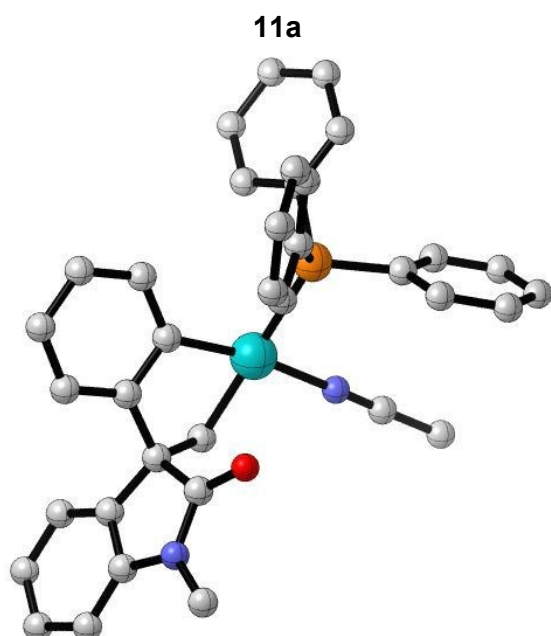
11e'



Zero-point correction= 0.507844 (Hartree/Particle)
 Thermal correction to Energy= 0.542646
 Thermal correction to Enthalpy= 0.543590
 Thermal correction to Gibbs Free Energy= 0.435769
 Sum of electronic and zero-point Energies= -1910.158455
 Sum of electronic and thermal Energies= -1910.123653
 Sum of electronic and thermal Enthalpies= -1910.122709
 Sum of electronic and thermal Free Energies= -1910.230530
 E(RM06L) = -1912.17838994

Pd	-0.08496	1.12299	0.16143
P	-2.1054	-0.166	0.11957
O	1.96073	-0.28576	-2.24618
N	3.8347	-1.35099	-1.37977
C	1.54129	2.31201	0.04622
C	1.48236	3.71581	-0.04717
H	0.51592	4.23604	-0.01748
C	2.66458	4.46903	-0.1815
H	2.60936	5.56142	-0.25706
C	3.91426	3.82646	-0.21061
H	4.83216	4.41674	-0.30669
C	3.98963	2.42727	-0.1088
H	4.96407	1.9246	-0.11881
C	2.80749	1.67823	0.01999
C	2.73176	0.16162	0.11243
C	1.38137	-0.16112	0.81012
H	1.45559	0.04812	1.89087
H	1.04602	-1.19772	0.63963
C	3.91565	-0.52937	0.77083
C	4.43982	-0.41345	2.05883
H	3.98506	0.27527	2.77903
C	5.56691	-1.18397	2.41572
H	5.98594	-1.10059	3.42338
C	6.15646	-2.05305	1.48324
H	7.03185	-2.64489	1.77075
C	5.64478	-2.17694	0.17582
H	6.11037	-2.85114	-0.5494
C	4.52438	-1.40594	-0.15628
C	2.74651	-0.47425	-1.31814
C	4.16301	-2.11734	-2.56772
H	3.42436	-1.84417	-3.33606
H	4.10598	-3.20266	-2.36906
H	5.17812	-1.87327	-2.92828
C	-2.83841	-0.82222	1.68771
C	-1.95869	-1.33116	2.66762
H	-0.87799	-1.29843	2.49248
C	-2.46038	-1.86393	3.86444
H	-1.76813	-2.25583	4.61702
C	-3.84481	-1.88163	4.102
H	-4.23555	-2.29009	5.03988
C	-4.72606	-1.36448	3.13873
H	-5.80562	-1.36809	3.32352
C	-4.22776	-0.8372	1.93632
H	-4.91788	-0.4253	1.19244

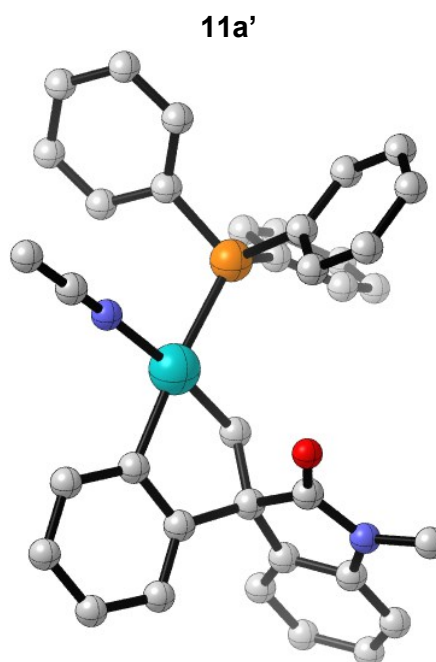
C	-2.12723	-1.61106	-1.03059
C	-3.08436	-2.64595	-0.94517
H	-3.84182	-2.62796	-0.15439
C	-3.05997	-3.70568	-1.86463
H	-3.80421	-4.50596	-1.79139
C	-2.08093	-3.74239	-2.87239
H	-2.06283	-4.57235	-3.58697
C	-1.12101	-2.72111	-2.95443
H	-0.34732	-2.74976	-3.72849
C	-1.13577	-1.65888	-2.03558
H	-0.3669	-0.8774	-2.08582
C	-3.41631	0.97355	-0.52278
C	-4.24401	0.66979	-1.6229
H	-4.15439	-0.30209	-2.11798
C	-5.17843	1.61126	-2.08544
H	-5.81573	1.36524	-2.94148
C	-5.29565	2.86138	-1.45766
H	-6.02323	3.59346	-1.8232
C	-4.47225	3.17361	-0.36253
H	-4.55597	4.14829	0.12952
C	-3.53432	2.23898	0.09934
H	-2.89043	2.48665	0.95257



Zero-point correction= 0.554306 (Hartree/Particle)
 Thermal correction to Energy= 0.593627
 Thermal correction to Enthalpy= 0.594571
 Thermal correction to Gibbs Free Energy= 0.478850
 Sum of electronic and zero-point Energies= -2042.886915
 Sum of electronic and thermal Energies= -2042.847594
 Sum of electronic and thermal Enthalpies= -2042.846650
 Sum of electronic and thermal Free Energies= -2042.962371
 E(RM06L) = -2045.00138812

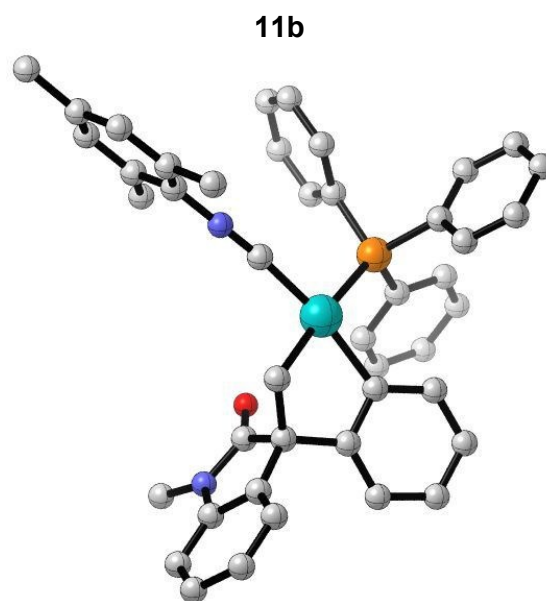
Pd	0.12253	0.40595	-0.77195
P	-2.10176	-0.14362	0.00653
O	2.06907	0.85197	1.86068
N	4.33584	1.0236	1.39375
C	0.97787	-1.41036	-0.45181
C	0.33692	-2.66678	-0.40541
H	-0.74548	-2.74319	-0.55534
C	1.0591	-3.85059	-0.16376
H	0.53116	-4.81124	-0.13783
C	2.44531	-3.80416	0.04857
H	3.0084	-4.72485	0.23782
C	3.10946	-2.56794	0.00926
H	4.19458	-2.51891	0.15834
C	2.38665	-1.38977	-0.24758
C	3.01553	-0.00608	-0.31766
C	2.10374	0.8136	-1.27023
H	2.25267	0.46086	-2.30605
H	2.30999	1.89743	-1.22311
C	4.48793	0.05566	-0.68947
C	5.16125	-0.37146	-1.83479

H	4.61281	-0.87144	-2.64048
C	6.5529	-0.15953	-1.93842
H	7.08864	-0.49345	-2.83282
C	7.25446	0.4749	-0.90034
H	8.33413	0.6345	-0.99193
C	6.59235	0.91038	0.26537
H	7.14108	1.40201	1.07471
C	5.21232	0.68829	0.34676
C	3.01857	0.65411	1.10019
C	4.71467	1.67382	2.63377
H	3.79508	1.78407	3.22815
C	5.15344	2.67001	2.44323
H	5.44657	1.06491	3.19446
C	-3.12392	1.33881	0.46756
C	-3.12556	1.84142	1.78616
H	-2.59168	1.29995	2.57357
C	-3.81127	3.02645	2.09817
H	-3.80769	3.39622	3.12917
C	-4.5074	3.72804	1.10068
H	-5.05274	4.64485	1.349
C	-4.50879	3.23777	-0.21705
H	-5.06149	3.76776	-1.00113
C	-3.81737	2.05711	-0.53315
H	-3.82988	1.68259	-1.5621
C	-3.21511	-1.03723	-1.17363
C	-4.61578	-1.12926	-1.00288
H	-5.09616	-0.63218	-0.15356
C	-5.39958	-1.83001	-1.9323
H	-6.48348	-1.89592	-1.78888
C	-4.7973	-2.43976	-3.04612
H	-5.41152	-2.98488	-3.77072
C	-3.41019	-2.33691	-3.23467
H	-2.93746	-2.79724	-4.10856
C	-2.62271	-1.63569	-2.30688
H	-1.54092	-1.53689	-2.45513
C	-2.09451	-1.13227	1.57214
C	-0.97794	-0.9658	2.42308
H	-0.13855	-0.33164	2.10971
C	-0.92899	-1.63996	3.65427
H	-0.0596	-1.50448	4.30591
C	-1.97209	-2.4991	4.03457
H	-1.92415	-3.03367	4.98945
C	-3.07121	-2.68502	3.17987
H	-3.88058	-3.36617	3.46431
C	-3.13606	-2.00262	1.95534
H	-3.99169	-2.16419	1.2926
N	-0.4418	2.40728	-1.13219
C	-0.7398	3.53585	-1.23039
C	-1.13772	4.93484	-1.32638
H	-0.45891	5.56645	-0.72988
H	-1.10736	5.27452	-2.37486
H	-2.16461	5.04858	-0.93983



Zero-point correction= 0.553886 (Hartree/Particle)
 Thermal correction to Energy= 0.593537
 Thermal correction to Enthalpy= 0.594481
 Thermal correction to Gibbs Free Energy= 0.476153
 Sum of electronic and zero-point Energies= -2042.885326
 Sum of electronic and thermal Energies= -2042.845675
 Sum of electronic and thermal Enthalpies= -2042.844731
 Sum of electronic and thermal Free Energies= -2042.963059
 E(RM06L) = -2044.99794270

Pd	0.13718	1.10275	-0.28031
P	1.87146	-0.57093	-0.13927
O	-1.86723	0.20737	2.23349
N	-3.74729	-0.99847	1.59929
C	-1.46703	2.3747	-0.41085
C	-1.41679	3.77379	-0.56773
H	-0.44963	4.28115	-0.66503
C	-2.59784	4.53912	-0.61122
H	-2.53929	5.62692	-0.74065
C	-3.85037	3.91485	-0.49333
H	-4.76955	4.51038	-0.5287
C	-3.923	2.5205	-0.33997
H	-4.89737	2.02341	-0.26295
C	-2.74097	1.75982	-0.30787
C	-2.69039	0.24593	-0.15204
C	-1.35851	-0.20323	-0.82128
H	-1.4627	-0.10521	-1.91694
H	-1.11982	-1.25579	-0.5914
C	-3.90479	-0.52193	-0.64752
C	-4.47299	-0.6129	-1.91866
H	-4.04242	-0.05073	-2.75437
C	-5.60863	-1.42871	-2.1115
H	-6.06091	-1.50503	-3.10552
C	-6.16294	-2.14058	-1.03533
H	-7.04461	-2.7701	-1.19656
C	-5.60496	-2.05851	0.25656
H	-6.04054	-2.61207	1.09423
C	-4.47882	-1.24346	0.42434
C	-2.66759	-0.13817	1.36369
C	-4.03671	-1.56097	2.90425
H	-3.27464	-1.16892	3.59462
H	-3.98354	-2.66462	2.88337
H	-5.04118	-1.26055	3.2532
C	1.69711	-2.14965	-1.09801
C	0.84568	-3.15889	-0.59261
H	0.37288	-3.03338	0.38713
C	0.61494	-4.33089	-1.32816
H	-0.04568	-5.10356	-0.92087
C	1.22596	-4.51203	-2.57958
H	1.04463	-5.42656	-3.1538
C	2.07127	-3.51412	-3.0891
H	2.55705	-3.64888	-4.06152
C	2.30537	-2.33966	-2.35621
H	2.97195	-1.57312	-2.76333
C	2.16367	-1.1869	1.5786
C	3.03791	-2.25902	1.87309
H	3.55698	-2.77939	1.06087
C	3.22242	-2.67575	3.19979
H	3.90278	-3.50541	3.42032
C	2.52563	-2.03801	4.24156
H	2.66687	-2.36964	5.27598
C	1.63405	-0.99351	3.95246
H	1.06603	-0.51453	4.75668
C	1.44847	-0.56816	2.62602
H	0.71673	0.21336	2.38818
C	3.49492	0.11194	-0.72317
C	4.72845	-0.08165	-0.06848
H	4.77361	-0.67375	0.85044
C	5.90304	0.49392	-0.58104
H	6.85352	0.3378	-0.05919
C	5.86316	1.26196	-1.75561
H	6.78201	1.70438	-2.15497
C	4.63745	1.46886	-2.41016
H	4.594	2.07714	-3.31998
C	3.45965	0.91014	-1.8905
H	2.49638	1.10484	-2.37708
N	1.4741	2.62771	0.35559
C	2.11775	3.49334	0.81257
C	2.90875	4.57294	1.3918
H	3.24585	5.26603	0.60341
H	2.30367	5.13539	2.12214
H	3.79486	4.16386	1.90439



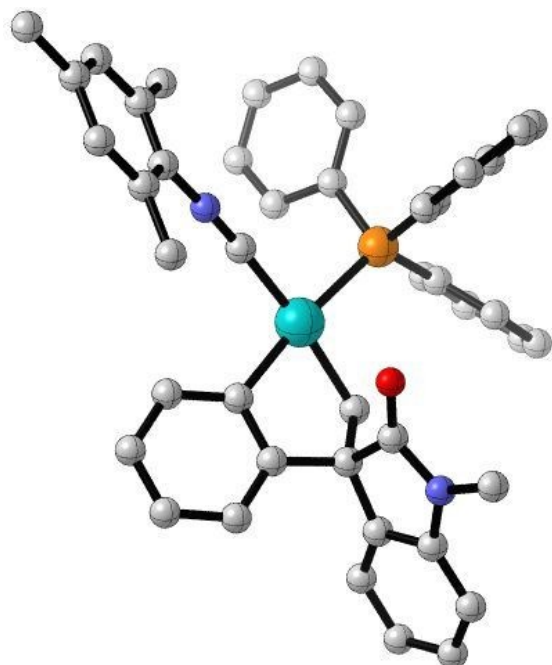
Zero-point correction= 0.686780 (Hartree/Particle)
 Thermal correction to Energy= 0.734354
 Thermal correction to Enthalpy= 0.735298
 Thermal correction to Gibbs Free Energy= 0.599186
 Sum of electronic and zero-point Energies= -2352.433206
 Sum of electronic and thermal Energies= -2352.385632
 Sum of electronic and thermal Enthalpies= -2352.384688
 Sum of electronic and thermal Free Energies= -2352.520801
 E(RM06L) = -2354.74453906

Pd	-0.37657	0.11032	-0.54956
P	0.89546	2.0806	0.0184
O	-2.05477	-0.78422	2.05804
N	-3.72196	-2.36551	1.72742
C	-2.19964	1.08571	-0.7623
C	-2.44423	2.44196	-1.06949
H	-1.6091	3.13268	-1.23376
C	-3.75199	2.95221	-1.17175
H	-3.9054	4.00938	-1.41935
C	-4.85594	2.11463	-0.95201
H	-5.87542	2.50927	-1.0279
C	-4.64668	0.76189	-0.64033
H	-5.50134	0.09436	-0.47927
C	-3.33692	0.25588	-0.56001
C	-3.01324	-1.19758	-0.23829
C	-1.66967	-1.50221	-0.94996
H	-1.82625	-1.50149	-2.04262
H	-1.25458	-2.47765	-0.64542
C	-4.09926	-2.21757	-0.53962
C	-4.71967	-2.56691	-1.73982
H	-4.45092	-2.05038	-2.66758
C	-5.69948	-3.58287	-1.74129
H	-6.192	-3.86201	-2.67826
C	-6.04779	-4.23588	-0.54771
H	-6.80926	-5.02295	-0.56094
C	-5.43504	-3.89407	0.67485
H	-5.71062	-4.40215	1.60419
C	-4.46678	-2.88301	0.65248
C	-2.83255	-1.37332	1.30463
C	-3.82518	-2.79788	3.10839
H	-3.10478	-2.19795	3.68456
H	-3.57671	-3.86986	3.20887
H	-4.84392	-2.63054	3.50173
C	2.50673	1.76927	0.88833
C	2.65641	1.96715	2.27643
H	1.823	2.36776	2.86117
C	3.87101	1.65864	2.91223
H	3.97198	1.82211	3.99054
C	4.95109	1.1536	2.17171
H	5.89915	0.92073	2.66786
C	4.80885	0.94885	0.78793
H	5.64556	0.55509	0.20108
C	3.59505	1.24749	0.15229
H	3.49465	1.0845	-0.92601
C	1.4286	3.11634	-1.42138
C	2.47489	4.06327	-1.34132
H	3.02571	4.19015	-0.40353
C	2.83039	4.82307	-2.46639

H	3.6422	5.55471	-2.39322
C	2.15296	4.64081	-3.684
H	2.43447	5.23309	-4.56117
C	1.12481	3.68944	-3.77693
H	0.60304	3.53327	-4.72691
C	0.76644	2.92656	-2.65373
H	-0.02531	2.17122	-2.72126
C	0.01936	3.21454	1.18785
C	-0.89882	2.62286	2.08436
H	-1.11899	1.55027	2.01461
C	-1.55215	3.41596	3.04134
H	-2.26306	2.94937	3.73105
C	-1.31545	4.79883	3.09749
H	-1.83686	5.41627	3.83689
C	-0.41911	5.39254	2.1936
H	-0.24135	6.47296	2.224
C	0.25079	4.60465	1.24458
H	0.94183	5.07718	0.53943
C	2.95468	-2.97891	-0.28801
C	3.52125	-3.27614	0.97924
C	3.34195	-3.66221	-1.47023
C	4.49998	-4.28125	1.03039
C	4.32678	-4.65554	-1.35343
C	4.92106	-4.97916	-0.11824
H	4.94491	-4.52773	2.00189
H	4.63576	-5.19531	-2.25658
C	2.70364	-3.32547	-2.79618
H	1.61011	-3.47641	-2.76625
H	2.86608	-2.26664	-3.06555
H	3.11642	-3.9523	-3.60173
C	3.07616	-2.53236	2.21444
H	3.31003	-1.4555	2.1396
H	1.98453	-2.6091	2.36099
H	3.57448	-2.93102	3.11183
C	6.00354	-6.03314	-0.03054
H	7.00696	-5.58519	-0.15561
H	5.99452	-6.5416	0.94772
H	5.88862	-6.79827	-0.81592
C	1.14798	-1.15014	-0.42735
N	1.98361	-1.99782	-0.37219

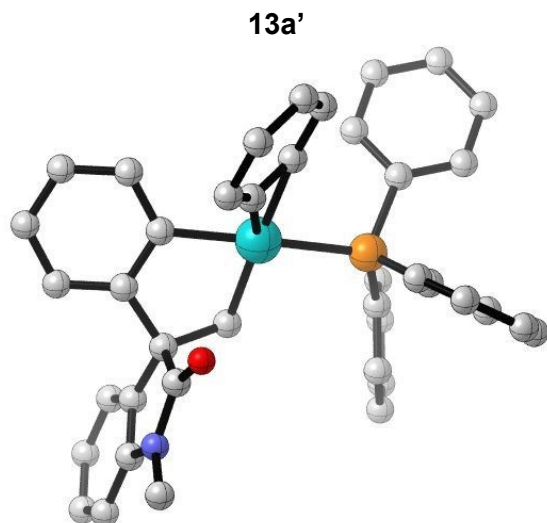
Pd	0.1664	-0.23472	-0.64515
P	-0.07265	2.08712	-0.04871
O	1.65305	-1.45791	1.97799
N	3.95093	-1.76222	1.83274
C	0.62278	-2.17341	-1.20525
C	-0.23493	-3.0989	-1.83495
H	-1.25499	-2.80482	-2.10844
C	0.2027	-4.40266	-2.13961
H	-0.4774	-5.10336	-2.63888
C	1.50654	-4.80434	-1.8086
H	1.84884	-5.81851	-2.04299
C	2.37934	-3.89536	-1.18853
H	3.4064	-4.19479	-0.94845
C	1.94483	-2.58882	-0.9013
C	2.81385	-1.51449	-0.25991
C	2.25642	-0.15733	-0.77372
H	2.49701	-0.05824	-1.84775
H	2.70723	0.69702	-0.24042
C	4.31433	-1.67873	-0.43965
C	5.10142	-1.70228	-1.59173
H	4.63458	-1.60829	-2.57817
C	6.49955	-1.85462	-1.47149
H	7.12374	-1.87426	-2.37062
C	7.09389	-1.9831	-0.20566
H	8.17972	-2.10117	-0.12423
C	6.31528	-1.96521	0.96919
H	6.78032	-2.06892	1.95449
C	4.93091	-1.81257	0.82565
C	2.6727	-1.57172	1.29627
C	4.20207	-1.86002	3.25786
H	3.22722	-1.76528	3.7596
H	4.87393	-1.05215	3.60026
H	4.6572	-2.83334	3.51562
C	1.3165	3.26709	-0.38795
C	2.43131	3.27462	0.48159
H	2.42946	2.64355	1.37663
C	3.53533	4.09815	0.21568
H	4.38973	4.09455	0.90069
C	3.54677	4.91994	-0.92329
H	4.40991	5.56097	-1.13068
C	2.44622	4.91384	-1.79403
H	2.44435	5.5542	-2.68259
C	1.3376	4.09327	-1.53062
H	0.48288	4.10386	-2.21403
C	-0.40709	2.37539	1.74566
C	-0.43562	3.6667	2.32207
H	-0.22674	4.54684	1.70447
C	-0.70497	3.82381	3.68977
H	-0.72846	4.82749	4.12767
C	-0.93223	2.69572	4.49739
H	-1.1372	2.8212	5.566
C	-0.87558	1.41008	3.9376
H	-1.02417	0.52743	4.56813
C	-0.61126	1.24684	2.56754
H	-0.52312	0.24535	2.13185
C	-1.49703	2.83278	-0.97262
C	-2.41614	3.74902	-0.4214
H	-2.32406	4.05582	0.62484
C	-3.46349	4.26099	-1.20552
H	-4.17432	4.96744	-0.76342
C	-3.59906	3.87388	-2.54854
H	-4.41337	4.28004	-3.15784
C	-2.69217	2.95589	-3.10418
H	-2.79689	2.63983	-4.14751
C	-1.65596	2.42829	-2.31822
H	-0.96895	1.68267	-2.73608
N	-2.87454	-1.04731	-0.23603
C	-1.76924	-0.65575	-0.44874
C	-4.09927	-1.62062	0.05726
C	-5.28574	-0.92811	-0.29627
C	-4.1211	-2.88872	0.69805
C	-6.51082	-1.54325	0.00572
C	-5.37808	-3.45087	0.97129
C	-6.58169	-2.79935	0.63854
H	-7.4383	-1.02472	-0.26531
H	-5.41582	-4.43191	1.45981
C	-2.83717	-3.58894	1.06949
H	-2.17158	-3.72043	0.1982
H	-2.25974	-3.0034	1.80711
H	-3.04315	-4.57924	1.50433
C	-5.2168	0.41712	-0.97719
H	-4.6843	1.1594	-0.35695
H	-4.66593	0.36051	-1.9323
H	-6.2268	0.8035	-1.18489
C	-7.91836	-3.42274	0.97791

11b'



Zero-point correction= 0.686343 (Hartree/Particle)
 Thermal correction to Energy= 0.734025
 Thermal correction to Enthalpy= 0.734969
 Thermal correction to Gibbs Free Energy= 0.598024
 Sum of electronic and zero-point Energies= -2352.432757
 Sum of electronic and thermal Energies= -2352.385075
 Sum of electronic and thermal Enthalpies= -2352.384131
 Sum of electronic and thermal Free Energies= -2352.521076
 E(RM06L) = -2354.74228417

H	-8.23575	-3.1519	2.00214
H	-8.71012	-3.08228	0.29049
H	-7.87424	-4.52355	0.93247

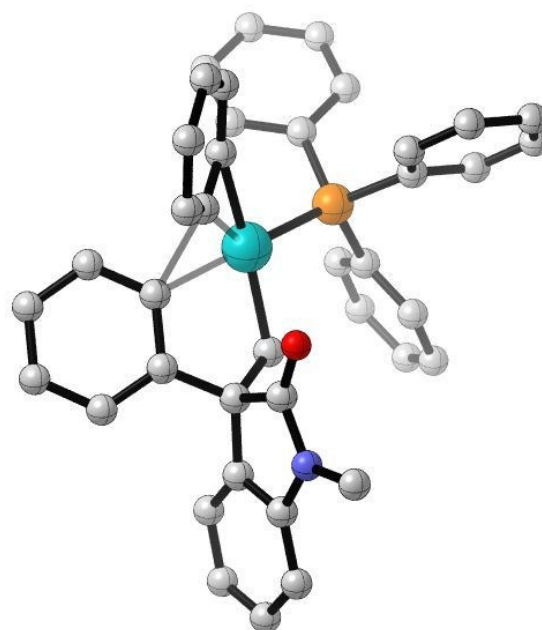


Zero-point correction= 0.583842 (Hartree/Particle)
 Thermal correction to Energy= 0.624095
 Thermal correction to Enthalpy= 0.625040
 Thermal correction to Gibbs Free Energy= 0.506759
 Sum of electronic and zero-point Energies= -2141.047232
 Sum of electronic and thermal Energies= -2141.006979
 Sum of electronic and thermal Enthalpies= -2141.006035
 Sum of electronic and thermal Free Energies= -2141.124316
 E(RM06L) = -2143.20108369

Pd	-0.09652	-0.88547	-0.34186
P	-1.9039	0.77336	-0.07828
O	2.24199	-1.00684	2.14782
N	4.02109	0.46184	1.87168
C	1.52463	-1.94784	-1.04259
C	1.40864	-3.15167	-1.75908
H	0.42975	-3.62476	-1.887
C	2.55473	-3.75164	-2.31578
H	2.45634	-4.68368	-2.88415
C	3.81806	-3.16601	-2.13769
H	4.70877	-3.63821	-2.56633
C	3.94137	-1.96651	-1.41669
H	4.92186	-1.49187	-1.2951
C	2.79843	-1.35241	-0.87555
C	2.78457	-0.03883	-0.11792
C	1.39429	0.5925	-0.40342
H	1.3752	0.98039	-1.43825
H	1.1637	1.42133	0.28583
C	3.93925	0.91286	-0.38593
C	4.36884	1.51978	-1.56683
H	3.85606	1.30991	-2.51178
C	5.47263	2.39855	-1.5298
H	5.81741	2.87764	-2.45161
C	6.13192	2.65939	-0.31761
H	6.98732	3.34305	-0.30062
C	5.71421	2.05322	0.88432
H	6.23222	2.25597	1.82665
C	4.61832	1.18381	0.82436
C	2.93327	-0.29516	1.42181
C	4.44988	0.47435	3.25791
H	3.77707	-0.20345	3.8046
H	4.37913	1.48979	3.68763
H	5.49134	0.11872	3.35419
C	-1.50734	2.51446	-0.57069
C	-0.75594	3.33411	0.30301
H	-0.48784	2.96829	1.29988
C	-0.36946	4.62482	-0.08806
H	0.20704	5.24902	0.60268
C	-0.71718	5.11243	-1.35841
H	-0.41291	6.11903	-1.66335
C	-1.45581	4.30223	-2.23477
H	-1.734	4.67551	-3.22607
C	-1.84882	3.01149	-1.84626
H	-2.43056	2.3914	-2.53529

C	-2.59444	0.96281	1.62623
C	-3.31622	2.1117	2.0239
H	-3.44525	2.94584	1.3266
C	-3.84856	2.19946	3.31928
H	-4.40601	3.09396	3.61703
C	-3.66061	1.14784	4.23169
H	-4.07294	1.22049	5.24365
C	-2.934	0.01019	3.84707
H	-2.77262	-0.80705	4.55745
C	-2.39954	-0.08423	2.5522
H	-1.82582	-0.96745	2.25583
C	-3.34598	0.35168	-1.16074
C	-4.65763	0.80139	-0.90378
H	-4.86846	1.39405	-0.00807
C	-5.70111	0.47455	-1.78384
H	-6.71809	0.82059	-1.57083
C	-5.44403	-0.29539	-2.9303
H	-6.26045	-0.54889	-3.61478
C	-4.14051	-0.7478	-3.19161
H	-3.93556	-1.3568	-4.07823
C	-3.09678	-0.43298	-2.30706
H	-2.0829	-0.8098	-2.4865
C	-0.03634	-3.70856	1.49008
C	-0.4222	-2.68175	0.64245
C	-1.58207	-2.49785	0.03727
C	-2.65425	-3.37422	0.24423
C	-2.36838	-4.4559	1.11716
C	-1.10457	-4.61479	1.72422
H	0.9486	-3.81063	1.95042
H	-3.63925	-3.26487	-0.22279
H	-3.15283	-5.19306	1.32651
H	-0.93929	-5.46163	2.40042

TS 13a'-14a'

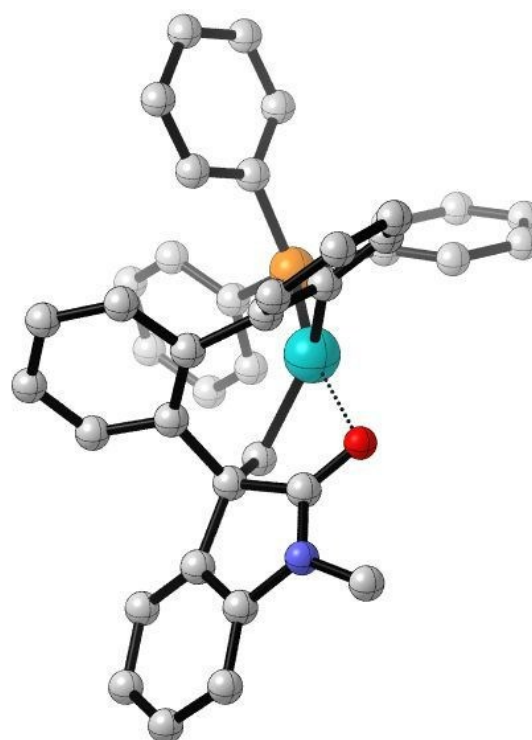


Zero-point correction= 0.583418 (Hartree/Particle)
 Thermal correction to Energy= 0.622787
 Thermal correction to Enthalpy= 0.623731
 Thermal correction to Gibbs Free Energy= 0.508400
 Sum of electronic and zero-point Energies= -2141.042965
 Sum of electronic and thermal Energies= -2141.003596
 Sum of electronic and thermal Enthalpies= -2141.002652
 Sum of electronic and thermal Free Energies= -2141.117983
 E(RM06L) = -2143.19611812
 Imaginary frequency = -186.86 cm⁻¹

Pd	-0.1448	-0.80636	-0.30447
P	-1.97335	0.67781	-0.07468
O	2.17777	-0.9198	2.15579
N	3.90387	0.61143	1.89878
C	1.49939	-1.89963	-1.06513
C	1.40806	-2.95138	-1.99836

H	0.45492	-3.47188	-2.1312
C	2.53794	-3.35507	-2.73098
H	2.4526	-4.17484	-3.45269
C	3.77168	-2.72229	-2.51864
H	4.66132	-3.04771	-3.06854
C	3.86228	-1.64456	-1.62106
H	4.80787	-1.10268	-1.51054
C	2.73319	-1.20629	-0.90638
C	2.69305	0.0837	-0.09945
C	1.2968	0.72293	-0.38592
H	1.29682	1.12693	-1.41396
H	1.08453	1.5511	0.31112
C	3.82636	1.06714	-0.35598
C	4.23684	1.70535	-1.52789
H	3.73724	1.48659	-2.4778
C	5.30305	2.62857	-1.47571
H	5.63261	3.13034	-2.391
C	5.94252	2.90684	-0.25677
H	6.76793	3.62598	-0.22773
C	5.54049	2.27471	0.9369
H	6.04	2.49346	1.88565
C	4.48297	1.35994	0.86136
C	2.84638	-0.1805	1.43625
C	4.31243	0.63929	3.29083
H	3.65943	-0.0652	3.82773
H	4.19538	1.65075	3.71983
H	5.36581	0.32543	3.40116
C	-1.68511	2.44041	-0.56028
C	-0.98963	3.30408	0.31666
H	-0.69802	2.95225	1.31188
C	-0.6871	4.61801	-0.07088
H	-0.15381	5.27711	0.62215
C	-1.06345	5.08439	-1.34103
H	-0.82476	6.10935	-1.64333
C	-1.74541	4.22982	-2.22133
H	-2.04349	4.58613	-3.21308
C	-2.05489	2.91566	-1.83606
H	-2.59198	2.25898	-2.52739
C	-2.66301	0.80574	1.63704
C	-3.41577	1.92145	2.0684
H	-3.56493	2.77472	1.39901
C	-3.95265	1.95322	3.36471
H	-4.53305	2.82328	3.68982
C	-3.74026	0.87764	4.24289
H	-4.15631	0.90693	5.25554
C	-2.98532	-0.22892	3.82296
H	-2.80602	-1.06549	4.50608
C	-2.44487	-0.26636	2.52794
H	-1.85098	-1.12532	2.19907
C	-3.40129	0.17269	-1.14144
C	-4.70617	0.67169	-0.94207
H	-4.91315	1.35149	-0.10953
C	-5.74857	0.28411	-1.79715
H	-6.75981	0.66951	-1.62914
C	-5.49762	-0.5982	-2.86176
H	-6.31351	-0.89966	-3.52725
C	-4.20223	-1.09937	-3.06461
H	-4.00263	-1.79414	-3.88713
C	-3.15835	-0.72141	-2.20473
H	-2.14985	-1.13058	-2.33517
C	0.84449	-3.75911	1.15916
C	0.19592	-2.77912	0.41803
C	-1.12054	-2.66377	0.16565
C	-2.00537	-3.62942	0.67152
C	-1.42743	-4.68717	1.41331
C	-0.03997	-4.74382	1.65943
H	1.91893	-3.77903	1.35282
H	-3.09044	-3.58329	0.51977
H	-2.07253	-5.47586	1.81886
H	0.36887	-5.56684	2.25657

14a'

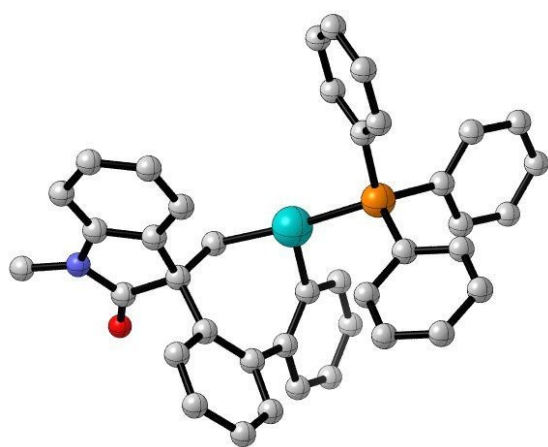


Zero-point correction= 0.585862 (Hartree/Particle)
 Thermal correction to Energy= 0.624852
 Thermal correction to Enthalpy= 0.625796
 Thermal correction to Gibbs Free Energy= 0.512271
 Sum of electronic and zero-point Energies= -2141.082116
 Sum of electronic and thermal Energies= -2141.043127
 Sum of electronic and thermal Enthalpies= -2141.042183
 Sum of electronic and thermal Free Energies= -2141.155708
 E(RM06L) = -2143.24109874

Pd	0.00191	-0.24775	0.78275
P	-2.01411	0.44106	0.1446
O	1.85402	-0.97037	1.88843
N	4.0947	-0.45367	1.51863
C	1.59068	-1.42078	-1.43631
C	1.45286	-1.85116	-2.78684
H	1.03265	-2.84917	-2.9456
C	1.7814	-1.0677	-3.89761
H	1.64117	-1.46199	-4.90972
C	2.26788	0.2249	-3.68402
H	2.51842	0.88372	-4.52199
C	2.4485	0.67031	-2.36998
H	2.85929	1.67022	-2.22707
C	2.15087	-0.10469	-1.22565
C	2.47518	0.63503	0.13786
C	1.2478	1.48805	0.62257
H	0.97104	2.22675	-0.14734
H	1.49728	2.00917	1.56508
C	3.83773	1.35181	0.09171
C	4.26081	2.55394	-0.48321
H	3.55508	3.18901	-1.02882
C	5.59903	2.97189	-0.32622
H	5.92807	3.91051	-0.783
C	6.50597	2.20266	0.41909
H	7.54271	2.53606	0.53032
C	6.09099	1.01617	1.05476
H	6.78251	0.43498	1.6722
C	4.75961	0.62611	0.88578
C	2.75177	-0.37328	1.25348
C	4.66547	-1.29801	2.55738
H	3.86838	-1.96038	2.92378
H	5.04781	-0.68688	3.39433
H	5.49001	-1.90485	2.14756
C	-2.17083	2.16989	-0.51191
C	-1.64034	3.22411	0.26477
H	-1.14565	2.9938	1.2146
C	-1.73526	4.54972	-0.17995
H	-1.32563	5.35892	0.434

C	-2.34465	4.83871	-1.41401
H	-2.41043	5.87401	-1.76509
C	-2.86335	3.79563	-2.19546
H	-3.33683	4.01291	-3.15895
C	-2.78232	2.46585	-1.74674
H	-3.19492	1.65824	-2.35872
C	-3.13376	0.46806	1.62075
C	-4.26979	1.30426	1.68158
H	-4.49383	1.98164	0.85107
C	-5.10416	1.28102	2.81086
H	-5.98206	1.93476	2.85012
C	-4.80973	0.43022	3.88872
H	-5.45937	0.4181	4.77037
C	-3.67486	-0.39616	3.83841
H	-3.43397	-1.05214	4.68152
C	-2.83866	-0.37682	2.71182
H	-1.93657	-0.99914	2.66722
C	-2.91026	-0.57103	-1.12161
C	-4.29775	-0.81633	-1.05606
H	-4.88467	-0.42897	-0.21751
C	-4.93013	-1.571	-2.05783
H	-6.00612	-1.76461	-1.99126
C	-4.1875	-2.07762	-3.13579
H	-4.68274	-2.6666	-3.91512
C	-2.80534	-1.8363	-3.20512
H	-2.21668	-2.23732	-4.03674
C	-2.16625	-1.09609	-2.19959
H	-1.08325	-0.93948	-2.24088
C	1.57818	-3.77977	-0.58545
C	1.04745	-2.47211	-0.47235
C	-0.08232	-2.25768	0.38311
C	-0.6684	-3.36149	1.02222
C	-0.13917	-4.65941	0.88431
C	1.00177	-4.86376	0.0957
H	2.45307	-3.9445	-1.22684
H	-1.54891	-3.21373	1.65942
H	-0.60939	-5.50256	1.40476
H	1.43755	-5.86399	-0.00409

14a

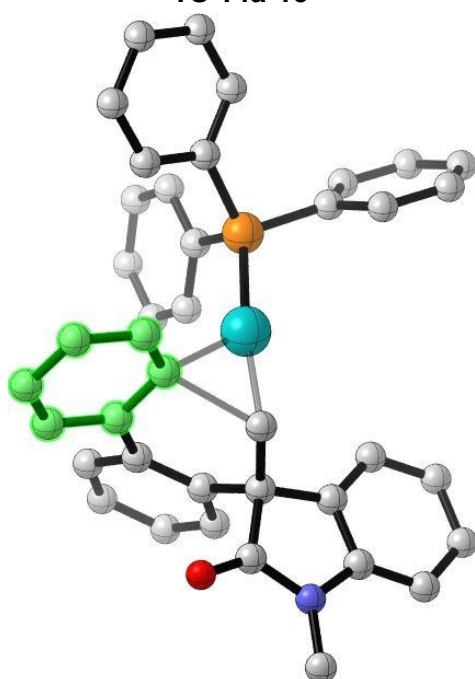


Zero-point correction= 0.586241 (Hartree/Particle)
 Thermal correction to Energy= 0.625719
 Thermal correction to Enthalpy= 0.626663
 Thermal correction to Gibbs Free Energy= 0.509353
 Sum of electronic and zero-point Energies= -2141.116745
 Sum of electronic and thermal Energies= -2141.077267
 Sum of electronic and thermal Enthalpies= -2141.076323
 Sum of electronic and thermal Free Energies= -2141.193634
 E(RM06L) = -2143.27289846

Pd	0.01893	-0.11404	-0.91783
P	2.20475	0.38222	-0.04712
O	-4.77742	-1.51027	-1.35613
N	-5.07864	0.77289	-1.00052
C	-1.87866	-2.1332	0.93549
C	-1.79764	-2.7966	2.189
H	-1.15721	-3.68194	2.25662
C	-2.47679	-2.35201	3.32747
H	-2.37984	-2.89752	4.27233
C	-3.27499	-1.20313	3.23757
H	-3.8258	-0.83098	4.10784
C	-3.35766	-0.5259	2.01631
H	-3.976	0.37548	1.95362
C	-2.66959	-0.94957	0.8546

C	-2.91894	-0.09891	-0.41299
C	-1.93515	-0.28804	-1.59257
H	-2.00966	0.56932	-2.29156
H	-2.16837	-1.20931	-2.14528
C	-3.04813	1.38862	-0.09986
C	-2.12688	2.28914	0.43356
H	-1.14229	1.93263	0.76324
C	-2.48321	3.64897	0.56275
H	-1.76704	4.36189	0.98295
C	-3.75485	4.08801	0.15907
H	-4.02294	5.14469	0.26373
C	-4.69949	3.19115	-0.37899
H	-5.68967	3.53675	-0.6914
C	-4.32468	1.84631	-0.49927
C	-4.35301	-0.4261	-0.96888
C	-6.43291	0.85587	-1.51572
H	-6.71191	-0.15925	-1.83651
H	-6.4879	1.54416	-2.37826
H	-7.13582	1.20275	-0.73718
C	2.41274	2.21966	-0.15072
C	2.03035	2.84332	-1.36202
H	1.65463	2.23072	-2.19135
C	2.12943	4.23467	-1.50947
H	1.83204	4.70376	-2.45308
C	2.59676	5.02267	-0.44413
H	2.66606	6.10981	-0.55511
C	2.96669	4.41324	0.76551
H	3.32647	5.02414	1.60029
C	2.87745	3.01933	0.91403
H	3.16526	2.55156	1.86064
C	3.72624	-0.28781	-0.86036
C	4.78283	0.53098	-1.31025
H	4.72597	1.61613	-1.1798
C	5.90783	-0.04153	-1.92709
H	6.72187	0.60413	-2.27363
C	5.9905	-1.4323	-2.09624
H	6.8683	-1.87593	-2.57767
C	4.94096	-2.25328	-1.64964
H	4.99723	-3.33885	-1.78214
C	3.8118	-1.68752	-1.04026
H	2.99002	-2.33229	-0.71086
C	2.45898	-0.02924	1.73488
C	3.73832	-0.07127	2.33204
H	4.63012	0.12238	1.72643
C	3.86888	-0.3748	3.69587
H	4.86389	-0.40775	4.15244
C	2.72785	-0.64409	4.47133
H	2.83438	-0.88691	5.53397
C	1.4546	-0.61522	3.88054
H	0.56248	-0.84231	4.47265
C	1.31903	-0.31311	2.51627
H	0.3297	-0.31579	2.04346
C	-1.22145	-4.18731	-0.33362
C	-1.11014	-2.78208	-0.17673
C	-0.2149	-2.09283	-1.02681
C	0.51414	-2.78328	-2.0137
C	0.39348	-4.17935	-2.14047
C	-0.48342	-4.88197	-1.30079
H	-1.93006	-4.72995	0.30163
H	1.18098	-2.23513	-2.68655
H	0.9722	-4.70624	-2.90764
H	-0.60738	-5.96462	-1.40834

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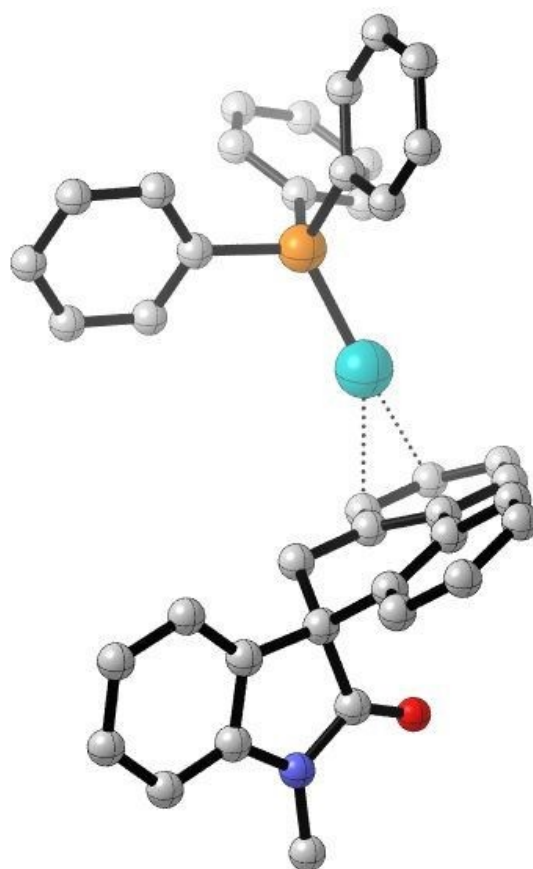


Zero-point correction= 0.585607 (Hartree/Particle)
 Thermal correction to Energy= 0.624564
 Thermal correction to Enthalpy= 0.625509
 Thermal correction to Gibbs Free Energy= 0.509721
 Sum of electronic and zero-point Energies= -2141.111811
 Sum of electronic and thermal Energies= -2141.072853
 Sum of electronic and thermal Enthalpies= -2141.071909
 Sum of electronic and thermal Free Energies= -2141.187697
 E(RM06L) = -2143.26476066
 Imaginary frequency = -239.13 cm⁻¹

Pd	0.09763	-0.13937	-0.84372
P	2.25509	0.35596	-0.08262
O	-4.6653	-1.68217	-0.99289
N	-5.19329	0.58031	-0.822
C	-1.89273	-1.87061	1.1726
C	-1.71149	-2.39619	2.47486
H	-1.14938	-3.32926	2.58355
C	-2.19634	-1.74486	3.61476
H	-2.03391	-2.18201	4.60579
C	-2.87998	-0.5291	3.47151
H	-3.27164	-0.00034	4.34691
C	-3.06122	0.01239	2.19122
H	-3.59547	0.96121	2.08508
C	-2.57371	-0.62797	1.03166
C	-2.91348	-0.00085	-0.34216
C	-1.93413	-0.32354	-1.50582
H	-1.71166	0.5851	-2.10872
H	-2.363	-1.06796	-2.18734
C	-3.1552	1.5029	-0.26042
C	-2.28112	2.55307	0.02105
H	-1.23113	2.34135	0.25737
C	-2.76503	3.87844	-0.00177
H	-2.08631	4.70851	0.21769
C	-4.11263	4.13613	-0.30288
H	-4.47804	5.16835	-0.31805
C	-5.00892	3.08739	-0.58941
H	-6.05745	3.29159	-0.82616
C	-4.50815	1.77937	-0.56233
C	-4.33923	-0.52408	-0.75097
C	-6.5908	0.46703	-1.19865
H	-6.79142	-0.60353	-1.35524
H	-6.79705	1.02049	-2.13237
H	-7.24875	0.85429	-0.40065
C	2.73396	2.12847	-0.35155
C	2.35078	2.72227	-1.57603
H	1.79384	2.12702	-2.31011
C	2.66836	4.06016	-1.8504
H	2.3666	4.50584	-2.80412
C	3.35904	4.82884	-0.89791
H	3.59824	5.87692	-1.10651

C	3.73334	4.25113	0.32535
H	4.26602	4.84737	1.07401
C	3.42568	2.90768	0.59921
H	3.71782	2.4667	1.55757
C	3.63115	-0.5914	-0.88126
C	4.87678	-0.01198	-1.20282
H	5.05366	1.0492	-0.99917
C	5.88683	-0.79035	-1.79213
H	6.8491	-0.33076	-2.04228
C	5.66392	-2.15012	-2.06114
H	6.45242	-2.75446	-2.52207
C	4.4238	-2.73107	-1.74651
H	4.24116	-3.7889	-1.96309
C	3.40804	-1.9566	-1.16673
H	2.43139	-2.40213	-0.9468
C	2.53233	0.07745	1.72495
C	3.81368	-0.12971	2.28092
H	4.69371	-0.15632	1.62929
C	3.96038	-0.3173	3.6643
H	4.95728	-0.48073	4.08763
C	2.83221	-0.30452	4.50202
H	2.94989	-0.45728	5.5802
C	1.55415	-0.11093	3.95364
H	0.66755	-0.11992	4.59548
C	1.40311	0.07428	2.57057
H	0.4059	0.19722	2.13197
C	-1.43036	-4.05833	0.01422
C	-1.34966	-2.64516	0.02427
C	-0.71182	-1.99921	-1.06144
C	-0.23218	-2.75468	-2.15551
C	-0.30614	-4.15647	-2.13303
C	-0.90846	-4.81128	-1.04496
H	-1.94589	-4.56392	0.83788
H	0.21122	-2.2451	-3.01677
H	0.09282	-4.73347	-2.97494
H	-0.99823	-5.90241	-1.03616

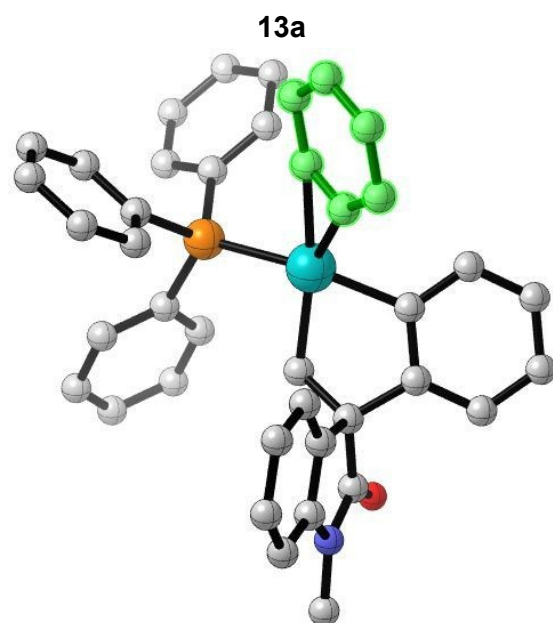
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Zero-point correction= 0.588336 (Hartree/Particle)
 Thermal correction to Energy= 0.627543
 Thermal correction to Enthalpy= 0.628487
 Thermal correction to Gibbs Free Energy= 0.510229
 Sum of electronic and zero-point Energies= -2141.177373
 Sum of electronic and thermal Energies= -2141.138166

Sum of electronic and thermal Enthalpies= -2141.137222
 Sum of electronic and thermal Free Energies= -2141.255480
 E(RM06L) = -2143.33176105

Pd	1.40782	-0.69097	-1.23041
P	3.10602	0.21184	-0.0259
O	-4.61561	-1.2806	-2.12642
N	-5.83029	0.60079	-1.46929
C	-2.81791	-2.09382	0.69025
C	-2.74953	-3.17354	1.60551
H	-1.93928	-3.89752	1.51409
C	-3.6849	-3.31972	2.63555
H	-3.60197	-4.16438	3.32608
C	-4.71584	-2.38134	2.785
H	-5.45573	-2.48284	3.58444
C	-4.78598	-1.28888	1.90408
H	-5.57801	-0.54487	2.02738
C	-3.84632	-1.12617	0.86763
C	-3.9394	0.05781	-0.09933
C	-2.50553	0.46874	-0.55277
H	-2.01005	0.9203	0.32351
H	-2.56862	1.25826	-1.32226
C	-4.69616	1.27246	0.42137
C	-4.45413	2.0922	1.52213
H	-3.6172	1.88179	2.2008
C	-5.3031	3.19769	1.75644
H	-5.1215	3.84829	2.61678
C	-6.37766	3.45816	0.89467
H	-7.03287	4.31795	1.08563
C	-6.63565	2.63659	-0.22214
H	-7.47772	2.84753	-0.89368
C	-5.78104	1.54995	-0.4371
C	-4.79295	-0.33722	-1.35577
C	-6.8165	0.54755	-2.53029
H	-6.56628	-0.32551	-3.15512
H	-6.78977	1.46386	-3.14668
H	-7.83709	0.42119	-2.11795
C	2.84482	1.95999	0.53993
C	2.12253	2.81912	-0.31857
H	1.72871	2.41441	-1.26371
C	1.90152	4.1583	0.03236
H	1.33861	4.81108	-0.64506
C	2.37799	4.6531	1.25583
H	2.18993	5.69984	1.5359
C	3.08015	3.80323	2.1216
H	3.44933	4.18273	3.08549
C	3.31932	2.46416	1.76615
H	3.86686	1.80966	2.45443
C	4.71822	0.308	-0.94668
C	5.64787	1.35794	-0.78631
H	5.42549	2.18303	-0.10099
C	6.84824	1.36073	-1.51442
H	7.55911	2.1849	-1.38527
C	7.13511	0.31048	-2.40489
H	8.07312	0.31507	-2.97162
C	6.21324	-0.73762	-2.57287
H	6.42949	-1.55278	-3.27283
C	5.01003	-0.7317	-1.8552
H	4.27277	-1.53169	-1.99644
C	3.57388	-0.6711	1.542
C	4.88527	-0.69854	2.06004
H	5.69092	-0.19285	1.51835
C	5.16165	-1.38011	3.25833
H	6.18046	-1.40141	3.64986
C	4.12785	-2.03746	3.95191
H	4.35005	-2.56885	4.88212
C	2.82073	-2.01991	3.43435
H	2.01378	-2.5428	3.96619
C	2.54445	-1.34845	2.23272
H	1.53288	-1.35129	1.81312
C	-1.0694	-3.05575	-0.87908
C	-1.84782	-1.96183	-0.42104
C	-1.6965	-0.70744	-1.05272
C	-0.79559	-0.55129	-2.13385
C	-0.03078	-1.66167	-2.60421
C	-0.16328	-2.9136	-1.93334
H	-1.19628	-4.04246	-0.42612
H	-0.79252	0.38995	-2.69634
H	0.50982	-1.60074	-3.55542
H	0.39927	-3.77807	-2.29436

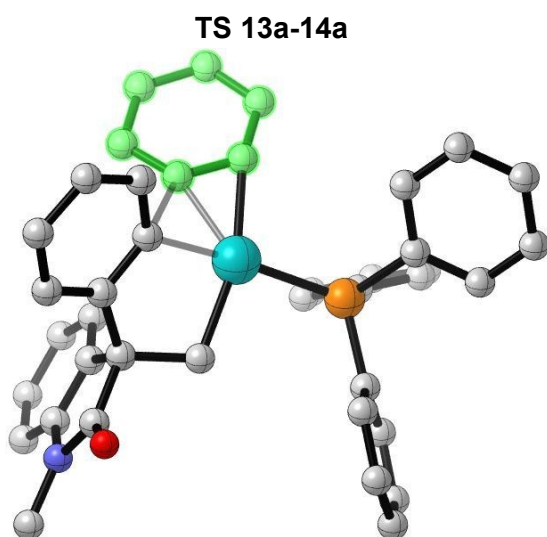


Zero-point correction= 0.583851 (Hartree/Particle)
 Thermal correction to Energy= 0.624152
 Thermal correction to Enthalpy= 0.625096
 Thermal correction to Gibbs Free Energy= 0.506438
 Sum of electronic and zero-point Energies= -2141.046514
 Sum of electronic and thermal Energies= -2141.006213
 Sum of electronic and thermal Enthalpies= -2141.005269
 Sum of electronic and thermal Free Energies= -2141.123927
 E(RM06L) = -2143.2033766

Pd	0.0145	-0.88454	-0.4126
P	1.91903	0.62458	-0.07706
O	-3.61351	1.95501	-2.28144
N	-4.46631	1.96692	-0.11377
C	-1.65293	-1.69979	-1.35059
C	-1.60332	-2.8918	-2.09487
H	-0.68719	-3.48949	-2.1236
C	-2.73717	-3.32122	-2.81169
H	-2.68789	-4.24678	-3.39659
C	-3.92456	-2.57477	-2.77227
H	-4.80584	-2.91174	-3.32855
C	-3.97814	-1.38186	-2.03333
H	-4.89247	-0.77814	-2.03436
C	-2.84601	-0.93749	-1.32844
C	-2.74964	0.35932	-0.55049
C	-1.26151	0.7817	-0.64694
H	-0.99738	1.54473	0.10361
H	-1.06655	1.17719	-1.6586
C	-3.26343	0.26978	0.88403
C	-2.90168	-0.56441	1.94156
H	-2.12907	-1.32672	1.7957
C	-3.54169	-0.41065	3.19086
H	-3.26546	-1.06274	4.02582
C	-4.53246	0.56846	3.36758
H	-5.02287	0.67734	4.34081
C	-4.91167	1.41779	2.30899
H	-5.68474	2.17998	2.44705
C	-4.26475	1.24911	1.07855
C	-3.6354	1.50135	-1.13844
C	-5.3992	3.06306	-0.2937
H	-5.29873	3.39678	-1.33772
H	-5.16353	3.9008	0.3871
H	-6.43818	2.73609	-0.10865
C	3.35485	0.30397	-1.19852
C	4.32269	1.30279	-1.45218
H	4.21356	2.29411	-1.00078
C	5.40998	1.03557	-2.29793
H	6.15426	1.81629	-2.48721
C	5.53725	-0.2238	-2.90741
H	6.38272	-0.42734	-3.57296
C	4.57216	-1.21533	-2.67077
H	4.65868	-2.19416	-3.15383
C	3.48439	-0.95493	-1.82219
H	2.72446	-1.72204	-1.63882
C	1.61902	2.4329	-0.33033
C	1.27616	2.87971	-1.62739

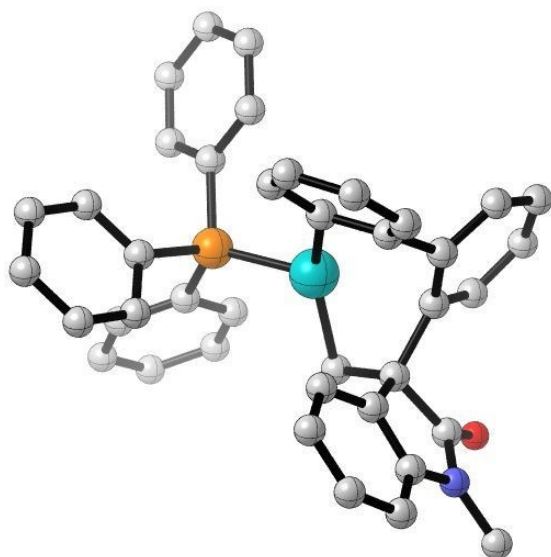
H	1.2347	2.16734	-2.4586
C	0.99468	4.23289	-1.85989
H	0.73094	4.56503	-2.86918
C	1.03948	5.15542	-0.80059
H	0.81396	6.21126	-0.9828
C	1.36833	4.71763	0.49117
H	1.40459	5.43076	1.32151
C	1.65638	3.36298	0.7286
H	1.91599	3.03006	1.73803
C	2.57523	0.52334	1.64734
C	3.93191	0.73501	1.96966
H	4.65847	0.94314	1.17777
C	4.35771	0.66283	3.30551
H	5.41453	0.81973	3.54608
C	3.43535	0.38762	4.32816
H	3.7716	0.33126	5.36879
C	2.08333	0.1746	4.01291
H	1.36131	-0.05038	4.80455
C	1.65517	0.23229	2.67815
H	0.60649	0.03851	2.42564
C	-0.55723	-3.9037	1.02327
C	0.01876	-2.76803	0.46696
C	1.30789	-2.51564	0.30448
C	2.29567	-3.39787	0.75692
C	1.79753	-4.56911	1.38121
C	0.41464	-4.81414	1.51257
H	-1.63099	-4.09638	1.09738
H	3.3725	-3.23154	0.6416
H	2.50725	-5.31074	1.76647
H	0.0783	-5.73393	2.00473

H	-0.9197	1.72286	-0.00309
H	-1.01421	1.26482	-1.73834
C	-3.15576	0.46827	0.88836
C	-2.79668	-0.30299	1.99518
H	-2.04836	-1.0948	1.89688
C	-3.41224	-0.05733	3.24231
H	-3.13567	-0.66532	4.1098
C	-4.37511	0.95478	3.37621
H	-4.84582	1.13573	4.3484
C	-4.74845	1.74663	2.27283
H	-5.49775	2.53772	2.374
C	-4.12819	1.48506	1.0449
C	-3.54762	1.59132	-1.19369
C	-5.24112	3.25291	-0.40131
H	-5.15743	3.52249	-1.46509
H	-4.96301	4.12058	0.22357
H	-6.28429	2.96971	-0.17282
C	3.46047	-0.06182	-1.05272
C	4.51193	0.81748	-1.39692
H	4.45987	1.87228	-1.10832
C	5.6173	0.34668	-2.12259
H	6.42611	1.03646	-2.38604
C	5.68154	-1.00013	-2.51599
H	6.54188	-1.36347	-3.08795
C	4.6353	-1.87576	-2.18393
H	4.67514	-2.92401	-2.49826
C	3.52712	-1.4116	-1.45816
H	2.69773	-2.08252	-1.20437
C	1.90697	2.31236	-0.48817
C	1.56842	2.66843	-1.81368
H	1.39229	1.88651	-2.56058
C	1.4557	4.01697	-2.17827
H	1.19216	4.27935	-3.20798
C	1.6664	5.02611	-1.22277
H	1.57065	6.07923	-1.5069
C	1.99341	4.67965	0.09683
H	2.15694	5.46105	0.84653
C	2.11485	3.32906	0.46573
H	2.37254	3.06679	1.49632
C	2.55004	0.48432	1.69432
C	3.90735	0.5519	2.07155
H	4.68649	0.60362	1.30447
C	4.26174	0.53816	3.4299
H	5.31834	0.58241	3.71456
C	3.26769	0.46328	4.4191
H	3.54815	0.45002	5.4776
C	1.91443	0.39613	4.04883
H	1.13566	0.32963	4.81545
C	1.55527	0.39887	2.69255
H	0.50227	0.32271	2.39856
C	-1.43844	-3.55267	0.99566
C	-0.59142	-2.65836	0.34758
C	0.75459	-2.67975	0.31004
C	1.44751	-3.68611	1.00059
C	0.66187	-4.6424	1.68622
C	-0.74583	-4.57425	1.68871
H	-2.53019	-3.49504	0.97925
H	2.54231	-3.74816	1.02464
H	1.15667	-5.45458	2.23197
H	-1.32353	-5.32894	2.23408



Zero-point correction= 0.583602 (Hartree/Particle)
 Thermal correction to Energy= 0.622994
 Thermal correction to Enthalpy= 0.623938
 Thermal correction to Gibbs Free Energy= 0.508396
 Sum of electronic and zero-point Energies= -2141.042396
 Sum of electronic and thermal Energies= -2141.003004
 Sum of electronic and thermal Enthalpies= -2141.002060
 Sum of electronic and thermal Free Energies= -2141.117603
 E(RM06L) = -2143.19729784
 Imaginary frequency = -174.88 cm⁻¹

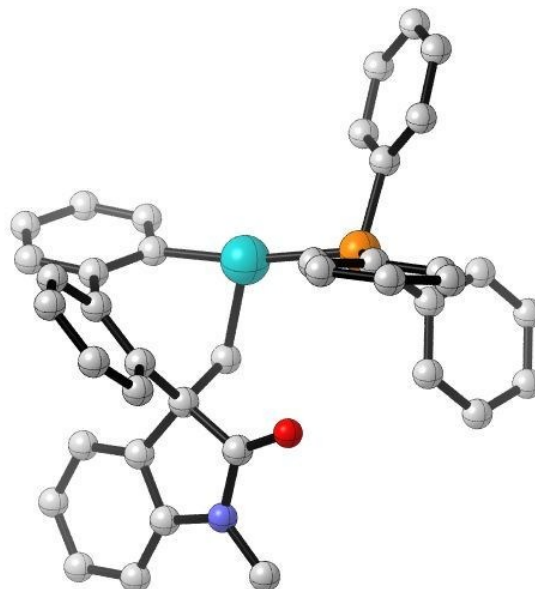
Pd	0.05075	-0.7803	-0.41334
P	2.00233	0.51395	-0.06998
O	-3.54947	1.97428	-2.36303
N	-4.33728	2.13992	-0.17999
C	-1.63615	-1.69382	-1.31215
C	-1.57931	-2.79961	-2.18209
H	-0.69032	-3.43681	-2.19191
C	-2.6706	-3.10338	-3.01481
H	-2.61617	-3.96677	-3.68677
C	-3.8269	-2.31196	-2.9674
H	-4.6862	-2.55155	-3.60264
C	-3.87204	-1.18292	-2.13227
H	-4.74317	-0.52084	-2.17
C	-2.78163	-0.84789	-1.30922
C	-2.6624	0.4708	-0.55907
C	-1.17204	0.91029	-0.7051

14a''

Zero-point correction= 0.585495 (Hartree/Particle)
 Thermal correction to Energy= 0.624864
 Thermal correction to Enthalpy= 0.625808
 Thermal correction to Gibbs Free Energy= 0.510805
 Sum of electronic and zero-point Energies= -2141.077881
 Sum of electronic and thermal Energies= -2141.038512
 Sum of electronic and thermal Enthalpies= -2141.037568
 Sum of electronic and thermal Free Energies= -2141.152572
 E(RM06L) = -2143.23573796

Pd	-0.08792	-0.0487	-0.48111
P	2.04603	0.32254	0.09177
O	-3.58725	2.9795	-1.2707
N	-4.51471	1.86859	0.53388
C	-2.2865	-1.30491	-1.69325
C	-2.56887	-1.82712	-2.97985
H	-2.58992	-2.91753	-3.08142
C	-2.71467	-1.01891	-4.11034
H	-2.92784	-1.46973	-5.08554
C	-2.50594	0.36335	-3.98682
H	-2.54372	1.01646	-4.86473
C	-2.27895	0.91595	-2.72432
H	-2.21108	2.00115	-2.62966
C	-2.25899	0.13179	-1.53213
C	-2.3829	1.02183	-0.19584
C	-1.03257	1.7774	-0.0405
H	-0.83589	2.12706	0.98429
H	-0.95799	2.60873	-0.75811
C	-2.88011	0.32476	1.07343
C	-2.29952	-0.62559	1.92025
H	-1.32396	-1.05622	1.67865
C	-2.98364	-1.04553	3.08083
H	-2.52625	-1.80044	3.72769
C	-4.24079	-0.51466	3.40308
H	-4.76523	-0.85321	4.30287
C	-4.8352	0.46272	2.58362
H	-5.80528	0.89995	2.83805
C	-4.13564	0.86607	1.44068
C	-3.54112	2.08082	-0.42974
C	-5.69485	2.70753	0.65515
H	-5.65772	3.43574	-0.16811
H	-5.70025	3.24219	1.62198
H	-6.61541	2.10346	0.57494
C	3.21772	-0.29446	-1.20306
C	4.47394	0.31442	-1.41633
H	4.76751	1.18675	-0.82373
C	5.34388	-0.18969	-2.39622
H	6.31419	0.29165	-2.55859
C	4.96847	-1.30068	-3.16908
H	5.64673	-1.68835	-3.93669
C	3.71881	-1.90746	-2.96112
H	3.41819	-2.76925	-3.56625
C	2.84219	-1.40708	-1.98629
H	1.85457	-1.85709	-1.82656
C	2.57662	2.07974	0.34554
C	2.12948	3.04527	-0.58255
H	1.46138	2.73706	-1.39401
C	2.52135	4.38509	-0.45519

H	2.16976	5.12529	-1.18152
C	3.34972	4.77903	0.61009
H	3.64574	5.828	0.71609
C	3.78942	3.82656	1.54223
H	4.43097	4.12914	2.37675
C	3.4092	2.48002	1.41135
H	3.75783	1.74128	2.1396
C	2.56848	-0.51763	1.65432
C	3.80346	-1.18758	1.7787
H	4.48665	-1.23766	0.92493
C	4.15676	-1.79602	2.99498
H	5.11511	-2.31926	3.07993
C	3.28639	-1.73624	4.09438
H	3.56389	-2.21252	5.04059
C	2.05347	-1.07204	3.97523
H	1.36643	-1.02985	4.82677
C	1.69147	-0.47312	2.76027
H	0.71935	0.02138	2.6575
C	-2.41119	-3.48673	-0.37096
C	-1.71686	-2.31586	-0.73551
C	-0.34121	-2.12643	-0.39043
C	0.29942	-3.174	0.30297
C	-0.39376	-4.34213	0.67681
C	-1.75193	-4.4948	0.35035
H	-3.46426	-3.60685	-0.6543
H	1.35786	-3.07953	0.57704
H	0.12651	-5.13342	1.23038
H	-2.29301	-5.40048	0.64564

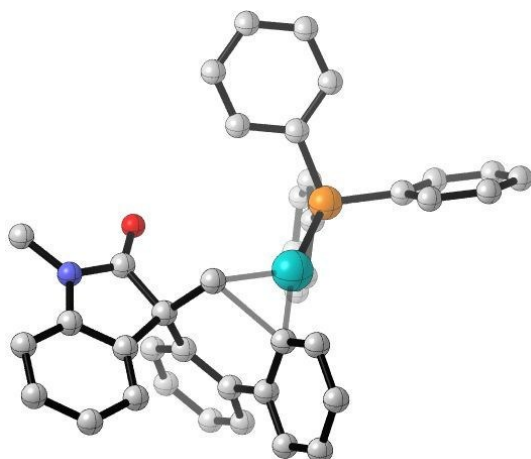
14a'''

Zero-point correction= 0.586783 (Hartree/Particle)
 Thermal correction to Energy= 0.626172
 Thermal correction to Enthalpy= 0.627116
 Thermal correction to Gibbs Free Energy= 0.510890
 Sum of electronic and zero-point Energies= -2141.116392
 Sum of electronic and thermal Energies= -2141.077003
 Sum of electronic and thermal Enthalpies= -2141.076059
 Sum of electronic and thermal Free Energies= -2141.192285
 E(RM06L) = -2143.27049667

Pd	-0.24575	-1.15284	-0.38376
P	-2.28828	0.11716	-0.09995
O	0.70286	2.51915	0.56635
N	2.81286	2.93732	-0.30861
C	2.44506	-1.5259	1.41324
C	2.66037	-2.07618	2.69938
H	2.7254	-3.166	2.78561
C	2.7565	-1.28248	3.84872
H	2.91414	-1.74859	4.82712
C	2.63391	0.10679	3.72646
H	2.70105	0.75516	4.6065
C	2.42581	0.67296	2.46066
H	2.33213	1.75977	2.3894
C	2.32378	-0.10904	1.28924
C	2.22771	0.62761	-0.07146
C	1.23565	0.06358	-1.14165

H	1.7822	-0.45642	-1.93881
H	0.62497	0.86902	-1.58288
C	3.6278	0.81168	-0.67185
C	4.57977	-0.11826	-1.094
H	4.3801	-1.1912	-1.01128
C	5.80111	0.34365	-1.62878
H	6.55181	-0.37957	-1.96265
C	6.06106	1.71908	-1.73601
H	7.01333	2.06302	-2.15302
C	5.11167	2.67073	-1.31425
H	5.31276	3.7432	-1.39703
C	3.90704	2.19164	-0.78771
C	1.78597	2.11075	0.13607
C	2.7131	4.38555	-0.31461
H	1.7299	4.63972	0.10885
H	2.78909	4.78335	-1.34227
H	3.50961	4.83778	0.30226
C	-2.58865	0.96296	1.51157
C	-3.60673	1.92489	1.691
H	-4.23391	2.21991	0.8429
C	-3.80498	2.51519	2.94863
H	-4.59528	3.2621	3.08013
C	-2.98816	2.15398	4.03356
H	-3.14255	2.61921	5.01302
C	-1.96602	1.20763	3.85751
H	-1.31485	0.93677	4.6949
C	-1.76175	0.61795	2.60049
H	-0.94546	-0.09747	2.44879
C	-2.75032	1.39628	-1.35545
C	-1.95785	2.56602	-1.42317
H	-1.13204	2.70918	-0.71564
C	-2.23402	3.54419	-2.38996
H	-1.61913	4.44976	-2.43222
C	-3.28804	3.3665	-3.30239
H	-3.49617	4.13063	-4.05885
C	-4.07278	2.20477	-3.24046
H	-4.89841	2.05979	-3.94555
C	-3.80862	1.22289	-2.27088
H	-4.42806	0.3216	-2.22644
C	-3.63537	-1.152	-0.22424
C	-4.7726	-1.18073	0.60953
H	-4.90873	-0.40736	1.37196
C	-5.7253	-2.20308	0.47164
H	-6.60205	-2.21772	1.12792
C	-5.55704	-3.20383	-0.49929
H	-6.30144	-4.00052	-0.60099
C	-4.4268	-3.18548	-1.333
H	-4.28503	-3.96689	-2.08698
C	-3.46813	-2.17067	-1.19146
H	-2.57466	-2.16008	-1.82932
C	3.31191	-3.52762	0.16365
C	2.34443	-2.49924	0.28142
C	1.2498	-2.47245	-0.61862
C	1.1758	-3.442	-1.64228
C	2.13735	-4.46296	-1.7448
C	3.21152	-4.50147	-0.84102
H	4.15927	-3.5461	0.85927
H	0.35236	-3.40912	-2.36539
H	2.05458	-5.21706	-2.53596
H	3.97727	-5.28033	-0.9245

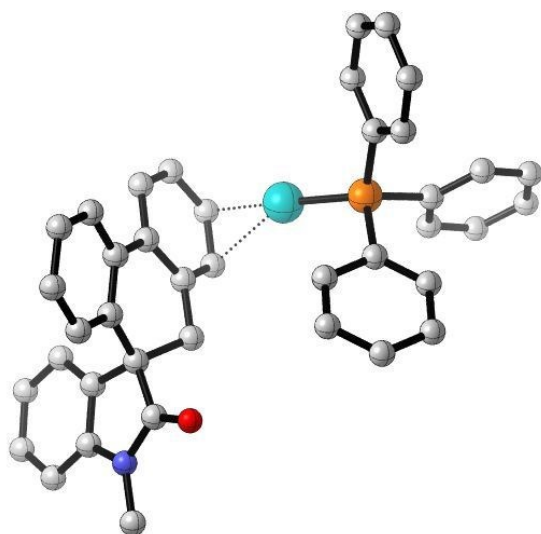
TS 14a'''-15b



Zero-point correction= 0.585809 (Hartree/Particle)
 Thermal correction to Energy= 0.624803
 Thermal correction to Enthalpy= 0.625747
 Thermal correction to Gibbs Free Energy= 0.509931
 Sum of electronic and zero-point Energies= -2141.111404
 Sum of electronic and thermal Energies= -2141.072409
 Sum of electronic and thermal Enthalpies= -2141.071465
 Sum of electronic and thermal Free Energies= -2141.187282
 E(RM06L) = -2143.26157371
 Imaginary frequency = -226.73 cm⁻¹

Pd	-0.28666	-0.80089	-0.63712
P	-2.42236	0.11986	-0.17403
O	1.37889	2.78708	0.00227
N	3.64028	2.6683	-0.50504
C	2.05989	-1.37162	1.49136
C	1.91921	-1.83664	2.81809
H	1.73684	-2.90437	2.98023
C	1.97588	-0.96397	3.91328
H	1.85904	-1.35275	4.93049
C	2.17177	0.40526	3.69026
H	2.21147	1.10663	4.53008
C	2.31542	0.883	2.37824
H	2.45826	1.95565	2.22171
C	2.2629	0.02045	1.26666
C	2.54856	0.5653	-0.15151
C	1.60507	0.03998	-1.27633
H	2.17905	-0.36215	-2.11967
H	0.95496	0.85407	-1.65305
C	4.03202	0.39373	-0.50593
C	4.8249	-0.74522	-0.664
H	4.39822	-1.74202	-0.52062
C	6.18447	-0.59619	-1.01163
H	6.80878	-1.4863	-1.13808
C	6.74143	0.67884	-1.19527
H	7.7983	0.77929	-1.46346
C	5.95748	1.83866	-1.04119
H	6.38767	2.83426	-1.18603
C	4.61139	1.66876	-0.69882
C	2.40193	2.1235	-0.183
C	3.85431	4.0945	-0.67425
H	2.88958	4.58772	-0.48367
H	4.19135	4.32264	-1.70104
H	4.60876	4.46828	0.04029
C	-2.71604	0.55454	1.60039
C	-3.6631	1.51915	2.00762
H	-4.23943	2.0686	1.25541
C	-3.85431	1.78978	3.37186
H	-4.58899	2.54214	3.67854
C	-3.10016	1.1053	4.33949
H	-3.24719	1.32265	5.40288
C	-2.14636	0.15496	3.94015
H	-1.53923	-0.36575	4.68764
C	-1.94995	-0.11572	2.57734
H	-1.18353	-0.83299	2.25904
C	-2.86883	1.6786	-1.06947
C	-1.89944	2.70731	-1.10193
H	-0.92513	2.5649	-0.61772
C	-2.18084	3.91414	-1.75892
H	-1.42472	4.7062	-1.77447
C	-3.41616	4.10231	-2.40266
H	-3.62758	5.0424	-2.9235
C	-4.37593	3.0786	-2.38221
H	-5.3389	3.21656	-2.88591
C	-4.10725	1.87071	-1.71607
H	-4.86036	1.07627	-1.70362
C	-3.79955	-1.05091	-0.58569
C	-5.0145	-1.10966	0.12903
H	-5.17482	-0.44704	0.98564
C	-6.01203	-2.02505	-0.2443
H	-6.94894	-2.06659	0.3216
C	-5.80904	-2.88753	-1.33386
H	-6.58748	-3.60289	-1.61969
C	-4.60069	-2.83814	-2.04864
H	-4.43215	-3.51518	-2.89279
C	-3.59939	-1.93031	-1.67282
H	-2.64415	-1.90048	-2.21165
C	2.62962	-3.61589	0.47797
C	2.00075	-2.35196	0.37275
C	1.29095	-2.04081	-0.81389
C	1.291	-2.947	-1.89687
C	1.91256	-4.20023	-1.7709
C	2.58038	-4.53533	-0.57993
H	3.18586	-3.8606	1.39
H	0.78691	-2.6781	-2.83131

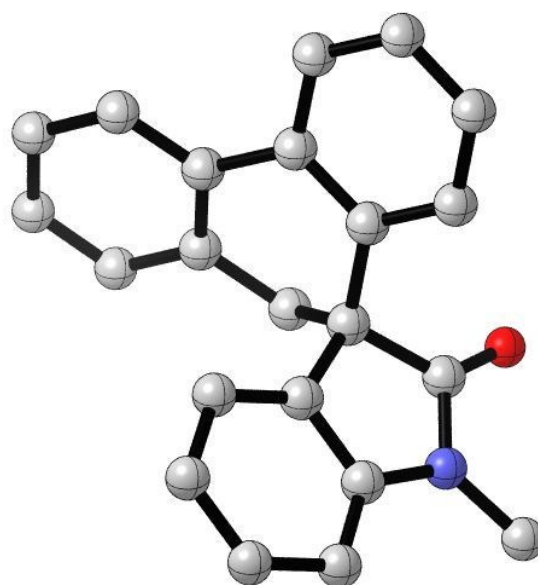
H	1.88305	-4.91042	-2.60473
H	3.08331	-5.50338	-0.48393

15b

Zero-point correction= 0.588701 (Hartree/Particle)
 Thermal correction to Energy= 0.627902
 Thermal correction to Enthalpy= 0.628846
 Thermal correction to Gibbs Free Energy= 0.511508
 Sum of electronic and zero-point Energies= -2141.179165
 Sum of electronic and thermal Energies= -2141.139964
 Sum of electronic and thermal Enthalpies= -2141.139020
 Sum of electronic and thermal Free Energies= -2141.256357
 E(RM06L) = -2143.33541679

Pd	1.40739	0.48113	-1.56392
P	3.00838	-0.16792	-0.08231
O	-3.35674	-1.69492	2.37837
N	-5.14256	-2.01186	0.9159
C	-2.63917	2.07742	0.41129
C	-2.58327	3.35291	1.02244
H	-1.87571	4.09806	0.64669
C	-3.38786	3.67371	2.12137
H	-3.31696	4.66747	2.57567
C	-4.27076	2.716	2.64368
H	-4.90406	2.95378	3.5044
C	-4.3243	1.43981	2.06585
H	-4.99729	0.68647	2.48792
C	-3.51596	1.10298	0.96658
C	-3.60405	-0.2858	0.32507
C	-2.21704	-0.69081	-0.25128
H	-2.31272	-1.62931	-0.82528
H	-1.56072	-0.9141	0.61279
C	-4.74023	-0.39982	-0.68814
C	-5.02061	0.31864	-1.85126
H	-4.3672	1.13815	-2.16553
C	-6.15856	-0.02362	-2.6125
H	-6.38485	0.53248	-3.52755
C	-7.00242	-1.06831	-2.20331
H	-7.88271	-1.32268	-2.80276
C	-6.73964	-1.79718	-1.02653
H	-7.40137	-2.6074	-0.70574
C	-5.60598	-1.4432	-0.28628
C	-3.98025	-1.38497	1.36314
C	-5.7566	-3.12647	1.61523
H	-5.14307	-3.3211	2.50765
H	-5.77873	-4.02848	0.97832
H	-6.78873	-2.88091	1.92186
C	3.94856	1.17474	0.7892
C	4.37253	1.07986	2.13155
H	4.13266	0.18519	2.71577
C	5.08617	2.1339	2.72623
H	5.40455	2.05168	3.77116
C	5.386	3.28969	1.98778
H	5.93943	4.11144	2.45463
C	4.96273	3.39417	0.65181
H	5.18419	4.29797	0.07402
C	4.24154	2.34727	0.05936
H	3.88582	2.43308	-0.97463
C	2.32265	-1.18162	1.31394

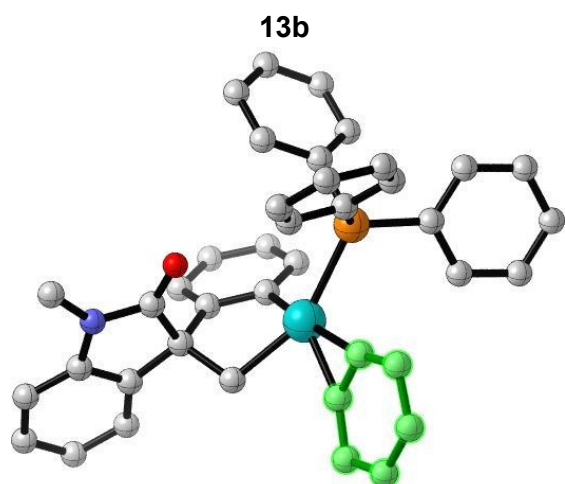
C	1.04695	-0.82215	1.80354
H	0.52914	0.03179	1.35041
C	0.44031	-1.55519	2.83422
H	-0.56332	-1.28336	3.17779
C	1.10606	-2.66317	3.3874
H	0.62987	-3.24699	4.18224
C	2.37466	-3.028	2.90979
H	2.89345	-3.89422	3.33503
C	2.98295	-2.29389	1.87664
H	3.96546	-2.59641	1.49934
C	4.35952	-1.23576	-0.77582
C	5.66709	-1.28054	-0.24663
H	5.93083	-0.64833	0.60786
C	6.63576	-2.12103	-0.81992
H	7.64896	-2.14375	-0.40413
C	6.30968	-2.92553	-1.92374
H	7.06785	-3.57747	-2.37066
C	5.01201	-2.88226	-2.46057
H	4.75517	-3.49928	-3.32837
C	4.04571	-2.03727	-1.89489
H	3.03627	-1.97506	-2.32004
C	-1.18594	2.75121	-1.5623
C	-1.80533	1.74776	-0.7691
C	-1.59688	0.38806	-1.10534
C	-0.78655	0.04259	-2.21984
C	-0.17103	1.05836	-3.01423
C	-0.37171	2.42139	-2.64823
H	-1.36292	3.80673	-1.33578
H	-0.76055	-1.00192	-2.54923
H	0.28875	0.80769	-3.97734
H	0.07422	3.21437	-3.2571

16

Zero-point correction= 0.321605 (Hartree/Particle)
 Thermal correction to Energy= 0.340327
 Thermal correction to Enthalpy= 0.341271
 Thermal correction to Gibbs Free Energy= 0.275289
 Sum of electronic and zero-point Energies= -978.290721
 Sum of electronic and thermal Energies= -978.271999
 Sum of electronic and thermal Enthalpies= -978.271054
 Sum of electronic and thermal Free Energies= -978.337037
 E(RM06L) = -978.818295702

O	1.75944	1.60637	-2.25124
N	2.88284	0.18149	-0.78852
C	-1.71669	1.1571	0.28826
C	-2.46446	2.19347	0.89239
H	-3.54665	2.07727	1.00656
C	-1.85607	3.3794	1.31797
H	-2.46105	4.16747	1.77786
C	-0.47589	3.55773	1.13944
H	0.01099	4.48279	1.46409
C	0.27814	2.54983	0.52315
H	1.34999	2.70115	0.36192
C	-0.32239	1.35656	0.08727
C	0.50734	0.24667	-0.56712
C	-0.36383	-0.47215	-1.63883

H	0.19494	-1.32196	-2.06769
H	-0.52045	0.26086	-2.45531
C	1.14297	-0.70233	0.44626
C	0.58772	-1.49321	1.45292
H	-0.49287	-1.49475	1.62232
C	1.43768	-2.28914	2.24948
H	1.00964	-2.91478	3.03863
C	2.82527	-2.28175	2.03942
H	3.47361	-2.90318	2.66562
C	3.40386	-1.48126	1.03531
H	4.48621	-1.47024	0.87665
C	2.54414	-0.70001	0.25536
C	1.75308	0.80334	-1.32027
C	4.2235	0.42566	-1.28941
H	4.1291	1.15029	-2.11189
H	4.67934	-0.50624	-1.66774
H	4.87154	0.84497	-0.49965
C	-2.27396	-2.1431	-1.49359
C	-1.68772	-0.93609	-1.08035
C	-2.3541	-0.11641	-0.13144
C	-3.59036	-0.55543	0.39271
C	-4.16971	-1.75829	-0.03172
C	-3.51394	-2.55541	-0.98289
H	-1.74769	-2.76689	-2.22529
H	-4.09452	0.03915	1.16094
H	-5.12774	-2.07849	0.39059
H	-3.95726	-3.5	-1.31405

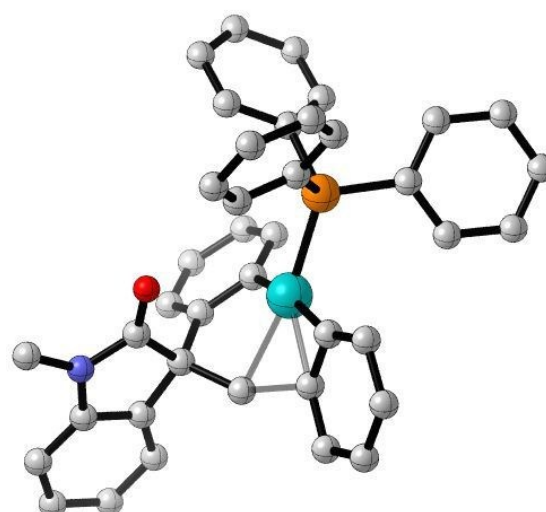


Zero-point correction= 0.584353 (Hartree/Particle)
 Thermal correction to Energy= 0.624463
 Thermal correction to Enthalpy= 0.625407
 Thermal correction to Gibbs Free Energy= 0.508245
 Sum of electronic and zero-point Energies= -2141.046538
 Sum of electronic and thermal Energies= -2141.006428
 Sum of electronic and thermal Enthalpies= -2141.005484
 Sum of electronic and thermal Free Energies= -2141.122645
 E(RM06L) = -2143.20553867

Pd	-0.01452	-0.76586	-0.6699
P	1.96929	0.41532	0.15946
O	-1.72601	0.32509	1.93549
N	-4.02904	0.0733	1.82301
C	-0.91174	0.96443	-1.35288
C	-0.27145	1.93325	-2.14609
H	0.77686	1.80431	-2.4389
C	-0.96844	3.07677	-2.58057
H	-0.45711	3.82021	-3.20289
C	-2.31043	3.2695	-2.21602
H	-2.84925	4.16314	-2.54937
C	-2.96951	2.30241	-1.43926
H	-4.02733	2.42757	-1.18049
C	-2.27649	1.15051	-1.0291
C	-2.88887	-0.01891	-0.2768
C	-2.08783	-1.26422	-0.74836
H	-2.34424	-1.48629	-1.79581
H	-2.27582	-2.15085	-0.12275
C	-4.389	-0.20854	-0.43407
C	-5.16944	-0.42126	-1.57131
H	-4.70279	-0.4524	-2.56168
C	-6.56352	-0.58586	-1.42853
H	-7.1847	-0.75264	-2.3141
C	-7.15866	-0.5347	-0.15735

H	-8.24162	-0.66389	-0.05927
C	-6.38638	-0.31569	1.00128
H	-6.85342	-0.27245	1.98984
C	-5.00584	-0.15563	0.836
C	-2.751	0.15619	1.26987
C	-4.28403	0.18371	3.24793
H	-3.31138	0.34702	3.7352
H	-4.74309	-0.74101	3.64072
H	-4.95397	1.0347	3.46444
C	1.81045	2.22988	0.5153
C	2.40761	3.21541	-0.29912
H	3.03107	2.92376	-1.14886
C	2.21	4.57907	-0.02731
H	2.68606	5.33058	-0.66627
C	1.40611	4.9758	1.05101
H	1.25321	6.03931	1.26257
C	0.78762	3.9999	1.84991
H	0.14448	4.29861	2.68434
C	0.98058	2.63739	1.58321
H	0.46558	1.89257	2.19624
C	3.47556	0.27987	-0.89904
C	4.67823	0.97126	-0.61852
H	4.73569	1.64248	0.24442
C	5.79568	0.81762	-1.45317
H	6.72132	1.35652	-1.22473
C	5.72595	-0.02001	-2.57935
H	6.59897	-0.13568	-3.23029
C	4.53451	-0.70179	-2.87074
H	4.47179	-1.35093	-3.75015
C	3.41455	-0.55258	-2.03677
H	2.48306	-1.08476	-2.25792
C	2.42585	-0.30848	1.80573
C	3.75417	-0.56202	2.20351
H	4.5852	-0.34638	1.52608
C	4.02067	-1.11316	3.46814
H	5.05688	-1.31099	3.76301
C	2.96764	-1.41156	4.34655
H	3.17877	-1.84043	5.33195
C	1.6422	-1.1696	3.95018
H	0.81315	-1.41218	4.62333
C	1.36637	-0.63258	2.68345
H	0.32784	-0.47544	2.36863
C	-0.30039	-4.03479	-1.59707
C	0.09752	-2.80818	-1.07715
C	1.12751	-2.58417	-0.28015
C	2.01019	-3.5905	0.1201
C	1.69767	-4.87138	-0.40179
C	0.58032	-5.08722	-1.23602
H	-1.17728	-4.20467	-2.22972
H	2.86447	-3.43563	0.78726
H	2.33851	-5.72277	-0.14345
H	0.38542	-6.09646	-1.61701

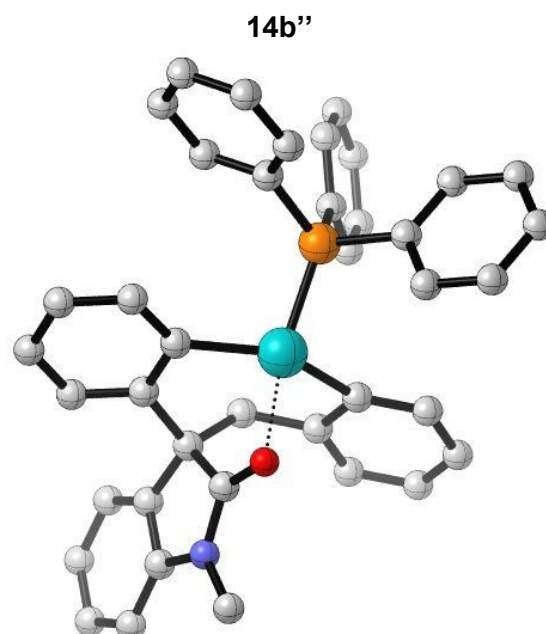
TS 13b-14b''



Zero-point correction= 0.584391 (Hartree/Particle)
 Thermal correction to Energy= 0.623619
 Thermal correction to Enthalpy= 0.624564
 Thermal correction to Gibbs Free Energy= 0.510479
 Sum of electronic and zero-point Energies= -2141.037208

Sum of electronic and thermal Energies= -2140.997979
 Sum of electronic and thermal Enthalpies= -2140.997035
 Sum of electronic and thermal Free Energies= -2141.111119
 E(RM06L) = -2143.19569372
 Imaginary frequency = -190.52 cm⁻¹

Pd	-0.02225	-0.47381	-0.60997
P	2.06587	0.26892	0.09588
O	-1.68383	0.06348	1.94117
N	-3.99797	-0.05046	1.82975
C	-0.84642	1.35643	-1.1061
C	-0.23627	2.47344	-1.70783
H	0.82311	2.43895	-1.98284
C	-0.95902	3.65121	-1.97291
H	-0.45821	4.50267	-2.44875
C	-2.31551	3.73839	-1.6248
H	-2.88007	4.65758	-1.81613
C	-2.95471	2.63073	-1.04643
H	-4.02149	2.68057	-0.80017
C	-2.23081	1.44583	-0.81203
C	-2.87914	0.17525	-0.27532
C	-2.23703	-1.06241	-0.98586
H	-2.32285	-0.94488	-2.07547
H	-2.79522	-1.94948	-0.66172
C	-4.3923	0.09343	-0.43492
C	-5.19371	0.12141	-1.57759
H	-4.73997	0.24664	-2.56638
C	-6.59295	0.0013	-1.44034
H	-7.23021	0.02419	-2.32982
C	-7.17199	-0.14245	-0.16896
H	-8.25918	-0.23322	-0.07469
C	-6.37843	-0.16889	0.99535
H	-6.83318	-0.27771	1.98454
C	-4.99276	-0.0505	0.83619
C	-2.72123	0.0614	1.27718
C	-4.23477	-0.16568	3.25749
H	-3.25115	-0.13014	3.74876
H	-4.73365	-1.12078	3.50037
H	-4.86042	0.6681	3.62233
C	2.32578	2.05704	0.51669
C	2.8892	2.96532	-0.40579
H	3.23987	2.61198	-1.38032
C	3.01625	4.32472	-0.07899
H	3.46132	5.01479	-0.80367
C	2.57298	4.79676	1.16567
H	2.67132	5.85752	1.41892
C	1.99887	3.90179	2.08312
H	1.64621	4.26121	3.05547
C	1.87393	2.54241	1.76257
H	1.4248	1.85533	2.486
C	3.43066	-0.11803	-1.09009
C	4.73851	0.40063	-0.94088
H	4.96361	1.09264	-0.12311
C	5.74781	0.05322	-1.85188
H	6.75599	0.46188	-1.72562
C	5.46419	-0.80916	-2.92412
H	6.25252	-1.07593	-3.63595
C	4.16683	-1.31974	-3.08527
H	3.93701	-1.98505	-3.92393
C	3.15419	-0.97497	-2.176
H	2.13845	-1.36645	-2.29613
C	2.51406	-0.57976	1.68564
C	3.83736	-0.92926	2.0237
H	4.65519	-0.7439	1.32129
C	4.11343	-1.54032	3.25775
H	5.14384	-1.81771	3.50481
C	3.07553	-1.79804	4.16707
H	3.29407	-2.27367	5.12916
C	1.75571	-1.45444	3.83251
H	0.93849	-1.66224	4.53123
C	1.46869	-0.85875	2.59409
H	0.43369	-0.61934	2.32379
C	-1.27825	-3.71547	-1.42653
C	-0.69244	-2.56063	-0.91511
C	0.51429	-2.47718	-0.33465
C	1.30733	-3.61962	-0.15976
C	0.768	-4.83543	-0.63779
C	-0.49152	-4.8808	-1.26711
H	-2.26287	-3.75153	-1.90576
H	2.29419	-3.59043	0.31576
H	1.34105	-5.76293	-0.52224
H	-0.88033	-5.83685	-1.63496

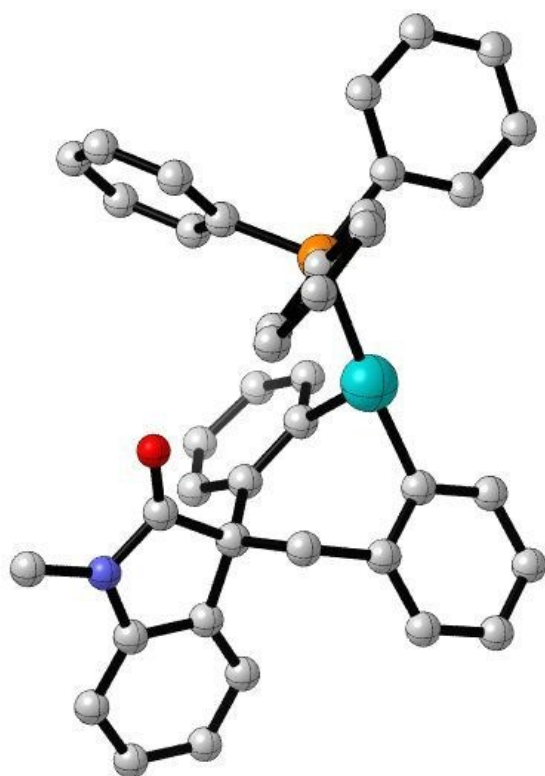


Zero-point correction= 0.587428 (Hartree/Particle)
 Thermal correction to Energy= 0.626099
 Thermal correction to Enthalpy= 0.627043
 Thermal correction to Gibbs Free Energy= 0.515095
 Sum of electronic and zero-point Energies= -2141.097007
 Sum of electronic and thermal Energies= -2141.058336
 Sum of electronic and thermal Enthalpies= -2141.057392
 Sum of electronic and thermal Free Energies= -2141.169340
 E(RM06L) = -2143.25778622

Pd	-0.01876	-0.09386	-0.69808
P	-2.12943	0.08269	0.04557
O	1.8068	-0.45643	-1.89171
N	4.09818	-0.42845	-1.52337
C	0.73192	1.85044	-0.54525
C	0.22425	3.12697	-0.84455
H	-0.76455	3.21535	-1.30788
C	0.95301	4.30142	-0.57605
H	0.53164	5.28064	-0.83392
C	2.21892	4.2119	0.01653
H	2.79629	5.11562	0.2409
C	2.76225	2.94961	0.30863
H	3.76402	2.88752	0.74625
C	2.0378	1.77124	0.03551
C	2.72542	0.37005	0.26085
C	1.93392	-0.60278	1.26341
H	1.07124	-0.03229	1.6505
H	2.60805	-0.78224	2.1192
C	4.2053	0.42267	0.6168
C	4.86193	0.79994	1.79069
H	4.29151	1.16829	2.65011
C	6.26862	0.71018	1.85537
H	6.78919	1.01121	2.76973
C	7.00463	0.23923	0.75604
H	8.09562	0.17457	0.81928
C	6.36024	-0.16182	-0.43067
H	6.93206	-0.54113	-1.28269
C	4.96593	-0.06302	-0.47038
C	2.79226	-0.22545	-1.15369
C	4.50807	-0.95361	-2.81664
H	3.5981	-1.13115	-3.4069
H	5.05585	-1.90366	-2.693
H	5.15261	-0.22845	-3.34264
C	-2.95526	1.72913	-0.16385
C	-2.61225	2.79083	0.70399
H	-1.88507	2.62709	1.50528
C	-3.19886	4.05491	0.54684
H	-2.92882	4.86469	1.23264
C	-4.11437	4.28537	-0.49383
H	-4.56606	5.27496	-0.61981
C	-4.44168	3.24305	-1.37474
H	-5.15091	3.41455	-2.19144
C	-3.86935	1.97083	-1.21052
H	-4.14138	1.16224	-1.89561
C	-2.50396	-0.33092	1.81561
C	-3.59285	0.25475	2.50086

H	-4.21157	1.0079	2.00411
C	-3.8779	-0.11246	3.82558
H	-4.72224	0.35261	4.34562
C	-3.08338	-1.06651	4.48107
H	-3.30509	-1.34827	5.51595
C	-2.00254	-1.6544	3.80487
H	-1.37702	-2.39916	4.30802
C	-1.71142	-1.28995	2.48108
H	-0.87263	-1.75199	1.95085
C	-3.21867	-1.05497	-0.93359
C	-4.46306	-1.51075	-0.45076
H	-4.80379	-1.2212	0.54852
C	-5.26302	-2.34897	-1.2434
H	-6.22411	-2.70426	-0.85659
C	-4.83247	-2.73459	-2.5235
H	-5.45828	-3.39055	-3.1379
C	-3.59354	-2.28526	-3.00937
H	-3.24815	-2.58866	-4.00325
C	-2.78616	-1.45506	-2.21571
H	-1.80261	-1.1204	-2.56953
C	2.09952	-3.13919	1.17714
C	1.44351	-1.96871	0.74202
C	0.31252	-2.07493	-0.12807
C	-0.12722	-3.35242	-0.50983
C	0.53789	-4.51558	-0.07066
C	1.65383	-4.40925	0.77206
H	2.96325	-3.05413	1.85029
H	-1.00172	-3.45212	-1.16438
H	0.18112	-5.50331	-0.38725
H	2.17321	-5.30837	1.12173

14b'''

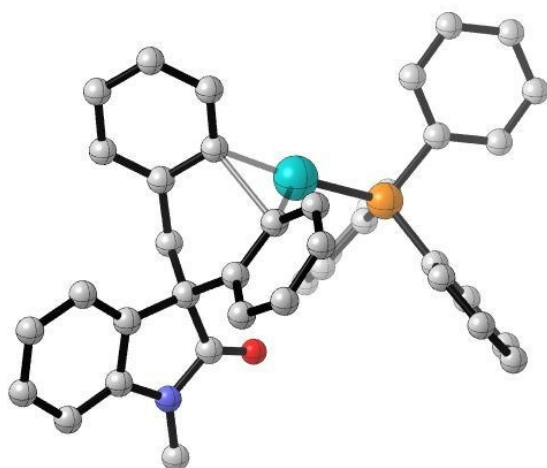


Zero-point correction= 0.586833 (Hartree/Particle)
 Thermal correction to Energy= 0.626347
 Thermal correction to Enthalpy= 0.627291
 Thermal correction to Gibbs Free Energy= 0.510417
 Sum of electronic and zero-point Energies= -2141.118955
 Sum of electronic and thermal Energies= -2141.079441
 Sum of electronic and thermal Enthalpies= -2141.078497
 Sum of electronic and thermal Free Energies= -2141.195371
 E(RM06L) = -2143.27135568

Pd	0.45091	1.29317	0.02172
P	2.42044	-0.12833	-0.05208
O	-1.25324	-2.23355	-0.87351
N	-3.5638	-2.46264	-0.74803
C	-0.84604	0.69133	1.43215
C	-0.39952	0.93748	2.75108

H	0.49704	1.54447	2.91185
C	-1.07268	0.39917	3.85869
H	-0.70043	0.59438	4.87073
C	-2.22091	-0.38013	3.65312
H	-2.76057	-0.81551	4.50066
C	-2.69329	-0.57683	2.35141
H	-3.61148	-1.15492	2.20163
C	-2.04456	-0.02887	1.21501
C	-2.70118	-0.30784	-0.15799
C	-2.25104	0.6155	-1.34681
H	-2.93984	0.42448	-2.18922
H	-1.24429	0.27581	-1.65148
C	-4.22292	-0.35748	-0.07282
C	-5.15591	0.61935	0.28071
C	-4.82023	1.61466	0.58662
C	-6.53054	0.30218	0.24175
H	-7.26937	1.06199	0.51538
C	-6.95695	-0.98045	-0.13918
H	-8.02661	-1.21368	-0.1622
C	-6.02855	-1.98087	-0.48979
H	-6.3609	-2.98188	-0.78107
C	-4.67015	-1.64491	-0.44827
C	-2.36327	-1.76515	-0.61727
C	-3.62937	-3.84729	-1.17988
H	-2.59387	-4.17877	-1.34858
H	-4.20565	-3.94193	-2.11744
H	-4.09896	-4.48107	-0.40684
C	2.495	-1.76685	0.8007
C	1.89271	-1.89445	2.07029
H	1.34542	-1.05063	2.50266
C	1.96979	-3.1095	2.76802
H	1.49374	-3.19938	3.75001
C	2.63816	-4.20818	2.20412
H	2.69109	-5.15735	2.74798
C	3.22841	-4.09093	0.93524
H	3.74225	-4.94754	0.4859
C	3.15727	-2.87717	0.23381
H	3.60624	-2.79427	-0.76124
C	3.98733	0.70982	0.47092
C	5.1646	0.01047	0.81268
H	5.17203	-1.08426	0.79248
C	6.31969	0.7127	1.19081
H	7.22673	0.16068	1.4594
C	6.31305	2.1172	1.2296
H	7.21515	2.66147	1.52841
C	5.14529	2.82133	0.89387
H	5.13164	3.91569	0.93044
C	3.98721	2.12044	0.52337
H	3.06406	2.66386	0.28304
C	2.70031	-0.55686	-1.83187
C	3.87421	-0.22066	-2.53652
H	4.69691	0.28371	-2.01994
C	3.99139	-0.5326	-3.90177
H	4.90623	-0.26497	-4.44141
C	2.94395	-1.18518	-4.56979
H	3.03797	-1.42699	-5.63382
C	1.77276	-1.52449	-3.87007
H	0.95222	-2.03426	-4.38613
C	1.64146	-1.20728	-2.51022
H	0.7238	-1.47183	-1.96957
C	-3.17939	2.99826	-1.45454
C	-2.19217	2.09187	-1.02173
C	-1.08985	2.56527	-0.27141
C	-1.02588	3.92397	0.09433
C	-2.01351	4.82449	-0.34976
C	-3.08817	4.36208	-1.12544
H	-4.02258	2.63314	-2.05369
H	-0.20026	4.29201	0.71421
H	-1.94383	5.88549	-0.08339
H	-3.85988	5.05979	-1.46851

TS 14b'''-15

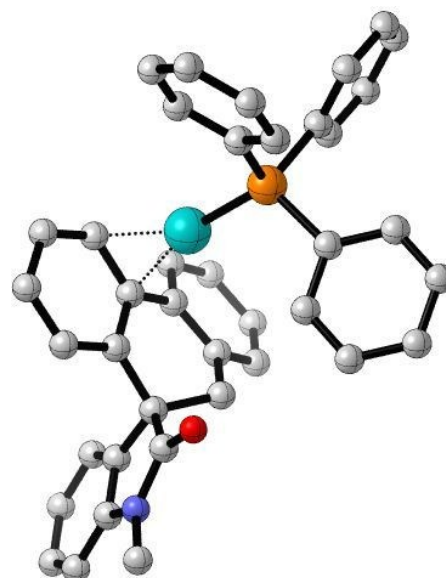


Zero-point correction= 0.586351 (Hartree/Particle)
 Thermal correction to Energy= 0.625224
 Thermal correction to Enthalpy= 0.626168
 Thermal correction to Gibbs Free Energy= 0.511131
 Sum of electronic and zero-point Energies= -2141.118948
 Sum of electronic and thermal Energies= -2141.080075
 Sum of electronic and thermal Enthalpies= -2141.079131
 Sum of electronic and thermal Free Energies= -2141.194168
 E(RM06L) = -2143.26928802
 Imaginary frequency = -110.19 cm⁻¹

Pd	0.46001	1.17923	-0.02826
P	2.46892	-0.13502	-0.0754
O	-1.32726	-2.33496	-0.64271
N	-3.64516	-2.51341	-0.59441
C	-1.01271	0.89606	1.34495
C	-0.63972	1.32036	2.64331
H	0.20699	2.00359	2.76287
C	-1.32267	0.86274	3.77966
H	-1.00199	1.18807	4.77578
C	-2.41663	-0.00361	3.62687
H	-2.96245	-0.37391	4.50085
C	-2.83168	-0.36486	2.34051
H	-3.71617	-1.00078	2.22385
C	-2.16538	0.09036	1.17656
C	-2.76458	-0.32587	-0.1844
C	-2.23582	0.4839	-1.42253
H	-2.89465	0.26081	-2.27998
H	-1.22862	0.09054	-1.65466
C	-4.28929	-0.34164	-0.15946
C	-5.21456	0.68094	0.05741
H	-4.87103	1.69631	0.27692
C	-6.59275	0.38397	-0.00593
H	-7.32629	1.17907	0.16068
C	-7.02958	-0.9234	-0.27441
H	-8.10205	-1.14035	-0.3175
C	-6.10893	-1.9692	-0.48549
H	-6.4505	-2.98867	-0.68879
C	-4.74658	-1.65297	-0.42302
C	-2.43689	-1.82523	-0.48369
C	-3.72064	-3.93421	-0.88353
H	-2.68598	-4.29876	-0.96822
H	-4.25565	-4.1173	-1.8324
H	-4.23804	-4.47554	-0.07175
C	2.63674	-1.53338	1.12328
C	2.02224	-1.40997	2.387
H	1.4221	-0.52234	2.61387
C	2.15317	-2.43381	3.33769
H	1.66707	-2.33121	4.31349
C	2.88795	-3.59118	3.03309
H	2.98225	-4.39254	3.77368
C	3.4903	-3.7257	1.77142
H	4.05455	-4.63154	1.52484
C	3.36503	-2.70319	0.8177
H	3.82166	-2.81787	-0.17087
C	4.00962	0.86247	0.17786
C	5.21313	0.32228	0.67844
H	5.26134	-0.736	0.95482
C	6.34429	1.13914	0.83595
H	7.27154	0.71092	1.23155
C	6.2879	2.49982	0.49211

H	7.17117	3.13468	0.61901
C	5.09355	3.04651	-0.00561
H	5.04056	4.10837	-0.26794
C	3.95946	2.23385	-0.1543
H	3.0173	2.66183	-0.5203
C	2.72368	-0.94918	-1.72013
C	3.90019	-0.8017	-2.48299
H	4.72984	-0.19948	-2.09932
C	4.01117	-1.42362	-3.7384
H	4.92787	-1.29909	-4.32493
C	2.95447	-2.20042	-4.23728
H	3.04284	-2.68407	-5.21601
C	1.78077	-2.35174	-3.47861
H	0.95168	-2.95554	-3.86271
C	1.6557	-1.72517	-2.22995
H	0.73223	-1.84292	-1.64908
C	-3.02624	2.90082	-1.75457
C	-2.14108	1.972	-1.17666
C	-1.11705	2.43188	-0.31494
C	-1.0342	3.79795	0.01644
C	-1.91755	4.71938	-0.57698
C	-2.90959	4.272	-1.46431
H	-3.80978	2.54722	-2.43576
H	-0.2763	4.14927	0.7251
H	-1.83221	5.78594	-0.33987
H	-3.60124	4.98746	-1.92197

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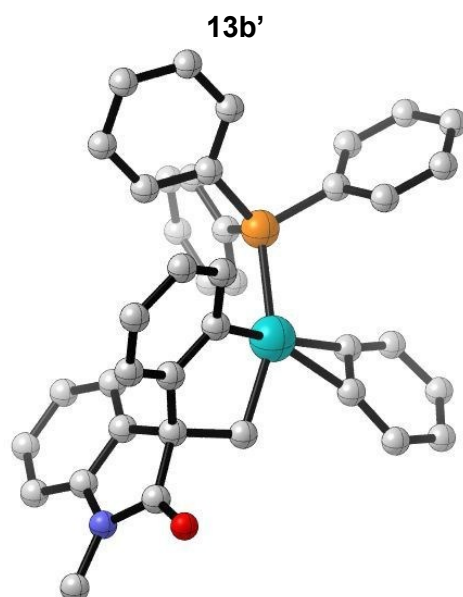
Zero-point correction= 0.588402 (Hartree/Particle)
 Thermal correction to Energy= 0.627732
 Thermal correction to Enthalpy= 0.628677
 Thermal correction to Gibbs Free Energy= 0.511173
 Sum of electronic and zero-point Energies= -2141.178863
 Sum of electronic and thermal Energies= -2141.139532
 Sum of electronic and thermal Enthalpies= -2141.138588
 Sum of electronic and thermal Free Energies= -2141.256091
 E(RM06L) = -2143.33690364

Pd	0.59	0.46923	0.91636
P	2.57057	-0.14807	-0.02728
O	-1.95827	-2.55577	-0.96074
N	-4.26646	-2.35861	-0.74651
C	-1.55126	1.0726	1.30017
C	-0.83239	1.24661	2.53333
H	-0.38027	2.21592	2.76611
C	-0.86327	0.24483	3.53616
H	-0.32404	0.41325	4.47376
C	-1.60048	-0.92775	3.33958
H	-1.64064	-1.69335	4.12063
C	-2.2673	-1.13705	2.11778
H	-2.81956	-2.0693	1.95855
C	-2.22714	-0.18406	1.08889
C	-3.00418	-0.40404	-0.2122
C	-2.37787	0.44291	-1.35944
H	-2.99339	0.35025	-2.27102
H	-1.38655	-0.00264	-1.57685
C	-4.5048	-0.17314	-0.04052

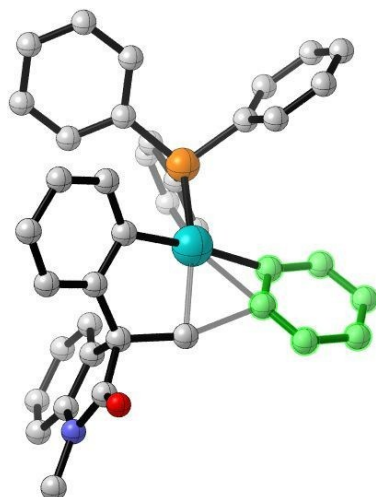
C	-5.22949	0.94687	0.37108
H	-4.7124	1.87147	0.64433
C	-6.63736	0.87015	0.42894
H	-7.2137	1.74431	0.74745
C	-7.30279	-0.31677	0.08353
H	-8.39562	-0.36234	0.13419
C	-6.58639	-1.45876	-0.32592
H	-7.10515	-2.38498	-0.5907
C	-5.19135	-1.36204	-0.37797
C	-2.95497	-1.89382	-0.6697
C	-4.60296	-3.70119	-1.18631
H	-3.65431	-4.21485	-1.40239
H	-5.22473	-3.67364	-2.09868
H	-5.14912	-4.24947	-0.39862
C	3.6199	-1.29818	0.98454
C	3.60235	-1.13306	2.38674
H	2.95402	-0.36245	2.82073
C	4.38301	-1.95619	3.21117
H	4.36045	-1.81686	4.29743
C	5.17792	-2.96816	2.64639
H	5.77841	-3.61939	3.29053
C	5.1896	-3.15002	1.25445
H	5.79895	-3.94411	0.80931
C	4.41736	-2.31892	0.42541
H	4.42478	-2.47274	-0.65873
C	3.73322	1.24134	-0.43041
C	5.13837	1.12062	-0.388
H	5.59538	0.17217	-0.08674
C	5.9542	2.21638	-0.7165
H	7.04399	2.11319	-0.67404
C	5.37712	3.43957	-1.09325
H	6.01554	4.29296	-1.34586
C	3.97833	3.56885	-1.13344
H	3.52198	4.52355	-1.41632
C	3.16156	2.47978	-0.79584
H	2.06911	2.5783	-0.7961
C	2.38599	-1.0376	-1.64358
C	3.33619	-0.96568	-2.68506
H	4.23324	-0.34867	-2.5656
C	3.12595	-1.66914	-3.88281
H	3.86664	-1.60333	-4.68738
C	1.96878	-2.4475	-4.05195
H	1.80647	-2.99005	-4.98976
C	1.01628	-2.51709	-3.02169
H	0.10206	-3.10682	-3.14253
C	1.21934	-1.81241	-1.82535
H	0.4578	-1.85003	-1.03706
C	-2.4687	2.93223	-1.87838
C	-2.21674	1.89211	-0.97023
C	-1.76995	2.19565	0.34413
C	-1.60925	3.55067	0.71102
C	-1.85237	4.58002	-0.20869
C	-2.27997	4.27412	-1.51064
H	-2.81591	2.68357	-2.88805
H	-1.30737	3.80526	1.73173
H	-1.72036	5.62297	0.09802
H	-2.47993	5.07424	-2.23073

Zero-point correction= 0.583964 (Hartree/Particle)
 Thermal correction to Energy= 0.624226
 Thermal correction to Enthalpy= 0.625170
 Thermal correction to Gibbs Free Energy= 0.506966
 Sum of electronic and zero-point Energies= -2141.043528
 Sum of electronic and thermal Energies= -2141.003266
 Sum of electronic and thermal Enthalpies= -2141.002322
 Sum of electronic and thermal Free Energies= -2141.120526
 E(RM06L) = -2143.20389990

Pd	-0.10443	0.92969	-0.56729
P	1.84334	-0.43182	0.10178
O	-4.88956	1.15888	-1.96613
N	-5.33667	0.31089	0.15704
C	-1.02527	-0.55631	-1.67062
C	-0.36393	-1.34045	-2.63383
H	0.71171	-1.2229	-2.8046
C	-1.07315	-2.29369	-3.38919
H	-0.54509	-2.89251	-4.13989
C	-2.44771	-2.48236	-3.17819
H	-2.99787	-3.22706	-3.76354
C	-3.12502	-1.69556	-2.23243
H	-4.20598	-1.81277	-2.09627
C	-2.42138	-0.72515	-1.49895
C	-2.16053	1.53023	-0.61374
H	-2.33138	2.22303	0.22452
H	-2.35282	2.03302	-1.57359
C	-3.22966	-0.28392	0.88788
C	-2.31279	-0.76939	1.81952
H	-1.2447	-0.79179	1.5761
C	-2.7718	-1.21011	3.07965
H	-2.055	-1.58867	3.81505
C	-4.13912	-1.16149	3.39396
H	-4.48524	-1.5075	4.3737
C	-5.07995	-0.66786	2.46831
H	-6.14476	-0.62341	2.71663
C	-4.60204	-0.23343	1.22596
C	-4.5067	0.64482	-0.91706
C	-6.76791	0.55033	0.1492
H	-7.00982	0.99834	-0.82654
H	-7.05863	1.24537	0.95732
H	-7.32907	-0.39322	0.27185
C	1.99619	-0.55205	1.94653
C	2.64511	-1.64889	2.55847
H	3.04527	-2.45998	1.94204
C	2.76778	-1.71094	3.95528
H	3.27383	-2.56587	4.41618
C	2.23792	-0.6874	4.75782
H	2.32942	-0.74135	5.84778
C	1.58257	0.39951	4.15781
H	1.15708	1.19634	4.77668
C	1.45906	0.46829	2.76112
H	0.94487	1.31307	2.29112
C	1.95931	-2.20968	-0.40285
C	0.86015	-3.05323	-0.12381
H	-0.03878	-2.64219	0.34683
C	0.90648	-4.41202	-0.46274
H	0.04801	-5.05391	-0.24054
C	2.04011	-4.94241	-1.10223
H	2.07084	-6.00262	-1.37464
C	3.12792	-4.10752	-1.39894
H	4.01224	-4.51287	-1.90205
C	3.09124	-2.74646	-1.05053
H	3.94678	-2.10386	-1.27908
C	3.45011	0.28152	-0.47112
C	4.64088	0.18319	0.27843
H	4.63223	-0.30598	1.2578
C	5.83684	0.72202	-0.22305
H	6.75486	0.64691	0.36945
C	5.85589	1.35654	-1.47559
H	6.78977	1.77674	-1.86339
C	4.67212	1.46164	-2.22461
H	4.67748	1.96665	-3.19603
C	3.47302	0.93502	-1.72207
H	2.54265	1.04504	-2.29038
C	-0.31823	4.27902	-1.01793
C	0.04559	2.99856	-0.62085
C	1.02956	2.65605	0.19393
C	1.90384	3.60419	0.73804
C	1.62892	4.94116	0.35627
C	0.55393	5.26898	-0.49676
H	-1.15926	4.52873	-1.67155
H	2.73293	3.36483	1.41281
H	2.26798	5.74627	0.73759
H	0.38865	6.31753	-0.76993
C	-3.0429	0.26109	-0.52492



TS 13b-14b

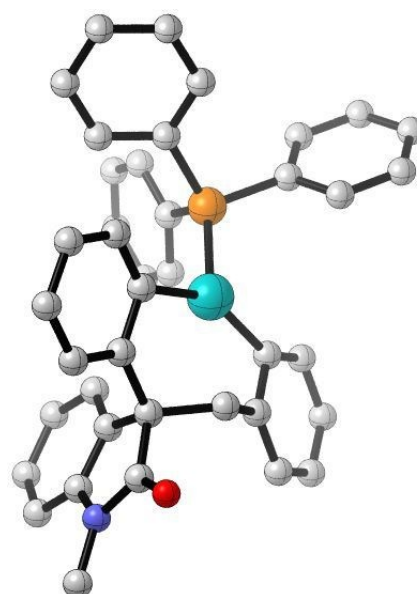


Zero-point correction= 0.584233 (Hartree/Particle)
 Thermal correction to Energy= 0.623502
 Thermal correction to Enthalpy= 0.624446
 Thermal correction to Gibbs Free Energy= 0.510022
 Sum of electronic and zero-point Energies= -2141.035730
 Sum of electronic and thermal Energies= -2140.996461
 Sum of electronic and thermal Enthalpies= -2140.995517
 Sum of electronic and thermal Free Energies= -2141.109941
 E(RM06L) = -2143.19605951
 Imaginary frequency = -191.21 cm⁻¹

Pd	-0.09378	0.66994	-0.58629
P	1.89763	-0.30763	0.11092
O	-4.91335	0.57448	-2.0689
N	-5.26315	0.05216	0.17318
C	-0.9213	-0.96694	-1.53632
C	-0.28038	-1.90423	-2.36978
H	0.80195	-1.84947	-2.53051
C	-1.00564	-2.92535	-3.01124
H	-0.48488	-3.63603	-3.66353
C	-2.39039	-3.03419	-2.81473
H	-2.95924	-3.83085	-3.30639
C	-3.05308	-2.10033	-2.00293
H	-4.14042	-2.16267	-1.88353
C	-2.3282	-1.06513	-1.38317
C	-2.97962	0.0353	-0.55735
C	-2.28446	1.40177	-0.87309
H	-2.76346	2.16787	-0.2485
H	-2.43864	1.62275	-1.93808
C	-3.10807	-0.28455	0.93083
C	-2.14873	-0.56912	1.90214
H	-1.08653	-0.56403	1.63173
C	-2.55869	-0.84272	3.22452
H	-1.80739	-1.06228	3.98954
C	-3.92113	-0.83133	3.56274
H	-4.22918	-1.04636	4.59144
C	-4.90547	-0.54245	2.59705
H	-5.96732	-0.52925	2.86093
C	-4.47513	-0.2716	1.29266
C	-4.4794	0.25715	-0.963
C	-6.70806	0.19105	0.16691
H	-6.99676	0.46548	-0.85893
H	-7.03313	0.98144	0.86695
H	-7.1987	-0.75773	0.44814
C	2.17032	-0.18269	1.94334
C	3.01472	-1.09694	2.61443
H	3.49207	-1.90983	2.05836
C	3.23171	-0.97802	3.99594
H	3.88766	-1.69285	4.504
C	2.60378	0.0455	4.7243
H	2.76858	0.13147	5.80357
C	1.75694	0.95095	4.06555
H	1.25602	1.74582	4.62796
C	1.53776	0.83842	2.68338
H	0.87306	1.53731	2.16364
C	2.21286	-2.10592	-0.18853
C	1.26206	-3.03503	0.29019
H	0.35334	-2.67952	0.78641
C	1.46822	-4.40977	0.11601
H	0.72456	-5.12023	0.49103

C	2.61386	-4.87308	-0.55411
H	2.7687	-5.94768	-0.69699
C	3.55329	-3.95531	-1.04712
H	4.44479	-4.30938	-1.57547
C	3.35718	-2.57532	-0.86479
H	4.0974	-1.86559	-1.246
C	3.34926	0.53829	-0.65986
C	4.59892	0.65111	-0.01497
H	4.73297	0.25168	0.9955
C	5.67013	1.28905	-0.66103
H	6.63441	1.37908	-0.14972
C	5.50503	1.8142	-1.95305
H	6.34179	2.31365	-2.45259
C	4.26208	1.70752	-2.59839
H	4.12388	2.12493	-3.60107
C	3.18623	1.07953	-1.95326
H	2.20534	1.02093	-2.43902
C	-1.18065	3.97358	-1.17088
C	-0.67604	2.77411	-0.67591
C	0.46922	2.60924	0.00983
C	1.27542	3.71772	0.31305
C	0.81661	4.97578	-0.13686
C	-0.37998	5.09958	-0.87067
H	-2.11451	4.06566	-1.73515
H	2.22122	3.63189	0.86048
H	1.40694	5.87419	0.07781
H	-0.70314	6.08698	-1.21846

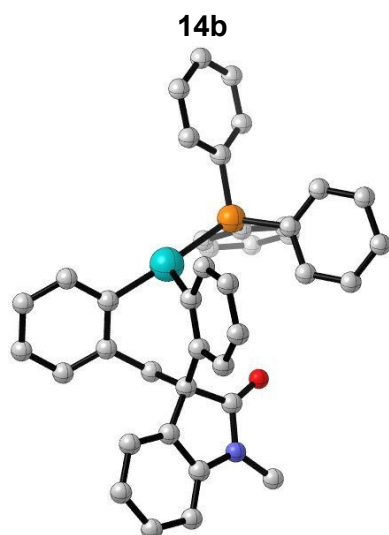
14b'



Zero-point correction= 0.586156 (Hartree/Particle)
 Thermal correction to Energy= 0.625188
 Thermal correction to Enthalpy= 0.626132
 Thermal correction to Gibbs Free Energy= 0.512719
 Sum of electronic and zero-point Energies= -2141.079579
 Sum of electronic and thermal Energies= -2141.040547
 Sum of electronic and thermal Enthalpies= -2141.039603
 Sum of electronic and thermal Free Energies= -2141.153016
 E(RM06L) = -2143.24481101

Pd	0.01178	-0.00284	-0.81161
P	2.07588	-0.07002	0.04973
O	-4.80894	-0.87496	-2.21914
N	-5.18977	-0.2289	-0.01746
C	-0.75469	-1.94109	-0.71146
C	-0.1728	-3.2195	-0.75649
H	0.91648	-3.31441	-0.81791
C	-0.95081	-4.39207	-0.72964
H	-0.46507	-5.37408	-0.77271
C	-2.34615	-4.29674	-0.65288
H	-2.96685	-5.1991	-0.63174
C	-2.95535	-3.03231	-0.63026
H	-4.04905	-2.97054	-0.60781
C	-2.1833	-1.85429	-0.67752
C	-2.89388	-0.46402	-0.65879
C	-2.21242	0.52135	-1.70985
H	-2.91691	0.61036	-2.55919

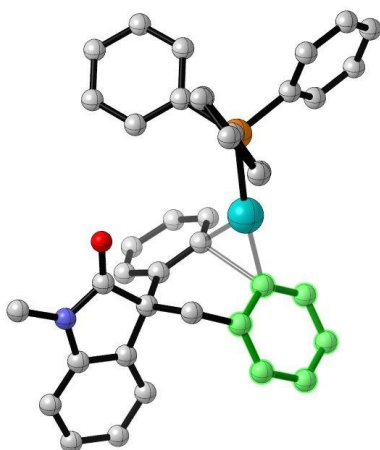
H	-1.39335	-0.05443	-2.24339
C	-3.03916	0.04528	0.77671
C	-2.09448	0.33425	1.76122
H	-1.02543	0.23351	1.5389
C	-2.5242	0.74673	3.03998
H	-1.78083	0.98162	3.80821
C	-3.89306	0.85181	3.33093
H	-4.21649	1.17143	4.32718
C	-4.86428	0.54204	2.35887
H	-5.93232	0.60964	2.58691
C	-4.41353	0.14021	1.09647
C	-4.38855	-0.57972	-1.10005
C	-6.63941	-0.19969	-0.08636
H	-6.9164	-0.49449	-1.10966
H	-7.0238	0.81417	0.1242
H	-7.08499	-0.90655	0.63594
C	2.23724	0.67737	1.73971
C	3.24221	0.25241	2.63863
H	3.91281	-0.56731	2.36406
C	3.37533	0.86557	3.89439
H	4.15572	0.52371	4.58245
C	2.51021	1.90624	4.26814
H	2.61337	2.37999	5.25003
C	1.51042	2.33329	3.37967
H	0.83017	3.1433	3.66251
C	1.37069	1.72341	2.12288
H	0.59119	2.05924	1.43136
C	2.86677	-1.7275	0.25755
C	2.38844	-2.59566	1.26563
H	1.56966	-2.27644	1.91846
C	2.9541	-3.86774	1.43113
H	2.57878	-4.52757	2.22004
C	3.98418	-4.29958	0.57814
H	4.41988	-5.29615	0.70427
C	4.44625	-3.45244	-0.44092
H	5.24432	-3.78422	-1.11326
C	3.89386	-2.17095	-0.60116
H	4.26844	-1.51287	-1.39088
C	3.2807	0.86269	-1.00137
C	4.49914	1.34676	-0.4789
H	4.736	1.20801	0.58088
C	5.40427	2.02014	-1.31349
H	6.34382	2.40031	-0.89885
C	5.10413	2.2109	-2.67258
H	5.81136	2.73942	-3.3204
C	3.89221	1.73282	-3.19664
H	3.64913	1.88769	-4.25284
C	2.97961	1.06682	-2.36372
H	2.0173	0.71513	-2.75303
C	-2.5186	3.06509	-1.41346
C	-1.6995	1.92661	-1.32756
C	-0.32449	2.04295	-0.99249
C	0.21898	3.32287	-0.7983
C	-0.60337	4.46609	-0.88029
C	-1.97036	4.33744	-1.17439
H	-3.57415	2.9602	-1.69627
H	1.28586	3.44759	-0.57514
H	-0.17232	5.46074	-0.7144
H	-2.60474	5.22771	-1.2435



Zero-point correction= 0.586863 (Hartree/Particle)
 Thermal correction to Energy= 0.626324
 Thermal correction to Enthalpy= 0.627268
 Thermal correction to Gibbs Free Energy= 0.510565
 Sum of electronic and zero-point Energies= -2141.119805
 Sum of electronic and thermal Energies= -2141.080343
 Sum of electronic and thermal Enthalpies= -2141.079399
 Sum of electronic and thermal Free Energies= -2141.196103
 E(RM06L) = -2143.27370908

Pd	-0.45433	1.2679	0.07498
P	-2.46418	-0.09826	0.12228
O	1.51327	-2.38508	0.97021
N	3.83672	-2.36425	0.87519
C	0.76527	0.50286	-1.33687
C	0.21457	0.6061	-2.6348
H	-0.7186	1.1574	-2.78473
C	0.82813	-0.00306	-3.73872
H	0.37117	0.08226	-4.73084
C	2.02192	-0.7161	-3.55591
H	2.51785	-1.20351	-4.40184
C	2.58794	-0.78663	-2.27999
H	3.53518	-1.3211	-2.14599
C	1.99684	-0.16755	-1.14817
C	2.75292	-0.34461	0.18606
C	2.28981	0.57159	1.37421
H	2.98209	0.39375	2.21686
H	1.28735	0.21862	1.67879
C	4.26792	-0.26216	0.02852
C	5.0894	0.76423	-0.4415
H	4.64899	1.6942	-0.81229
C	6.48877	0.57989	-0.43744
H	7.14092	1.37917	-0.80336
C	7.04958	-0.62071	0.02703
H	8.13692	-0.75049	0.0235
C	6.23452	-1.67144	0.49347
H	6.67167	-2.61047	0.84643
C	4.84953	-1.46864	0.48166
C	2.56928	-1.80849	0.70366
C	4.04694	-3.70931	1.37942
H	3.05215	-4.13229	1.58471
H	4.64072	-3.69361	2.31054
H	4.56878	-4.33555	0.63395
C	-3.9799	0.83477	-0.39211
C	-5.2842	0.48128	0.01671
H	-5.43312	-0.37699	0.68041
C	-6.38836	1.23435	-0.4121
H	-7.39597	0.95418	-0.08691
C	-6.20272	2.3473	-1.24962
H	-7.0661	2.93502	-1.57893
C	-4.90826	2.7113	-1.65399
H	-4.7575	3.58431	-2.29766
C	-3.80234	1.96171	-1.2236
H	-2.78485	2.24997	-1.51583
C	-2.46467	-1.62395	-0.91729
C	-3.5145	-1.9538	-1.799
H	-4.38484	-1.29613	-1.88683
C	-3.44549	-3.12633	-2.56945
H	-4.26407	-3.37314	-3.2542
C	-2.33365	-3.97623	-2.46187
H	-2.28127	-4.8896	-3.06419
C	-1.28495	-3.64751	-1.58628
H	-0.41005	-4.30028	-1.50228
C	-1.33858	-2.47327	-0.82111
H	-0.50218	-2.22108	-0.15778
C	-2.89749	-0.71882	1.81207
C	-3.53661	-1.95634	2.0362
H	-3.77156	-2.60753	1.18791
C	-3.85409	-2.36151	3.34284
H	-4.34645	-3.32602	3.50682
C	-3.53586	-1.53879	4.43533
H	-3.7804	-1.85971	5.45335
C	-2.89175	-0.30883	4.22108
H	-2.62993	0.33126	5.07005
C	-2.56893	0.09559	2.91739
H	-2.04936	1.04815	2.75406
C	3.22135	2.95295	1.4378
C	2.22344	2.04443	1.03376
C	1.1141	2.51229	0.29045
C	1.05328	3.86507	-0.0986
C	2.05353	4.76665	0.31414
C	3.1346	4.31105	1.08502
H	4.07102	2.59294	2.03055
H	0.21956	4.22819	-0.71051
H	1.98735	5.82303	0.02911
H	3.91527	5.00956	1.40548

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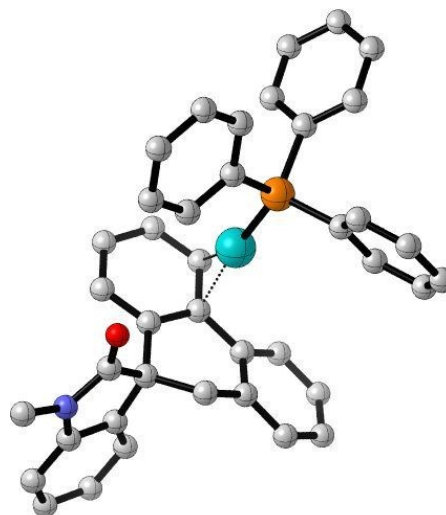


Zero-point correction= 0.586239 (Hartree/Particle)
 Thermal correction to Energy= 0.625180
 Thermal correction to Enthalpy= 0.626124
 Thermal correction to Gibbs Free Energy= 0.510300
 Sum of electronic and zero-point Energies= -2141.119009
 Sum of electronic and thermal Energies= -2141.080068
 Sum of electronic and thermal Enthalpies= -2141.079123
 Sum of electronic and thermal Free Energies= -2141.194948
 E(RM06L) = -2143.26887212
 Imaginary frequency = -121.19 cm⁻¹

Pd	-0.4736	1.15242	0.01422
P	-2.50548	-0.12045	0.10863
O	1.45768	-2.4523	0.50813
N	3.78113	-2.48898	0.59556
C	1.0078	0.84747	-1.35769
C	0.6075	1.25094	-2.65426
H	-0.25296	1.91692	-2.7696
C	1.27705	0.79193	-3.79704
H	0.93002	1.09758	-4.79037
C	2.389	-0.05309	-3.65595
H	2.92608	-0.42148	-4.53614
C	2.82871	-0.398	-2.37395
H	3.72449	-1.0197	-2.2634
C	2.17131	0.05418	-1.20407
C	2.79403	-0.35714	0.14393
C	2.22241	0.40536	1.393
H	2.86012	0.16503	2.26162
H	1.21289	-0.00478	1.58316
C	4.31778	-0.29312	0.13609
C	5.19269	0.77215	-0.08514
H	4.80189	1.76301	-0.33468
C	6.58303	0.55005	0.01278
H	7.27697	1.37903	-0.15834
C	7.0823	-0.72539	0.32209
H	8.16351	-0.88379	0.39305
C	6.21368	-1.81388	0.53768
H	6.60381	-2.80924	0.77096
C	4.83846	-1.57249	0.4377
C	2.54163	-1.87467	0.41685
C	3.9254	-3.90234	0.89479
H	2.91007	-4.32296	0.94749
H	4.43711	-4.05121	1.86214
H	4.4995	-4.4179	0.10439
C	-4.04366	0.86094	-0.21656
C	-5.28884	0.57227	0.38148
H	-5.37312	-0.25944	1.08868
C	-6.41561	1.35553	0.08327
H	-7.37627	1.12613	0.55671
C	-6.31201	2.43084	-0.81424
H	-7.19204	3.04147	-1.04229
C	-5.07491	2.72839	-1.4094
H	-4.98607	3.57237	-2.10159
C	-3.94567	1.95289	-1.10655
H	-2.97137	2.1929	-1.54865
C	-2.61279	-1.54705	-1.06089
C	-3.76396	-1.8267	-1.82649
H	-4.64758	-1.18611	-1.74209
C	-3.77699	-2.92475	-2.70272
H	-4.67311	-3.13208	-3.29763
C	-2.64744	-3.75028	-2.81615
H	-2.65951	-4.60458	-3.50159
C	-1.49998	-3.47343	-2.0537

H	-0.61293	-4.10943	-2.14029
C	-1.47238	-2.37279	-1.18457
H	-0.56565	-2.15999	-0.60531
C	-2.8207	-0.88007	1.7672
C	-3.47887	-2.11648	1.93517
H	-3.80567	-2.68217	1.05646
C	-3.69955	-2.6306	3.22345
H	-4.20678	-3.59392	3.34334
C	-3.26666	-1.91745	4.35298
H	-3.43636	-2.32293	5.35602
C	-2.60389	-0.68898	4.19342
H	-2.25305	-0.13441	5.07007
C	-2.3759	-0.17679	2.9077
H	-1.8386	0.77147	2.78093
C	3.00586	2.81616	1.78242
C	2.12788	1.89824	1.17634
C	1.12314	2.37527	0.30109
C	1.05318	3.74515	-0.01665
C	1.93062	4.65427	0.60375
C	2.902	4.1912	1.50592
H	3.77615	2.45006	2.47191
H	0.30921	4.10885	-0.7335
H	1.85537	5.72392	0.37754
H	3.58844	4.89748	1.98515

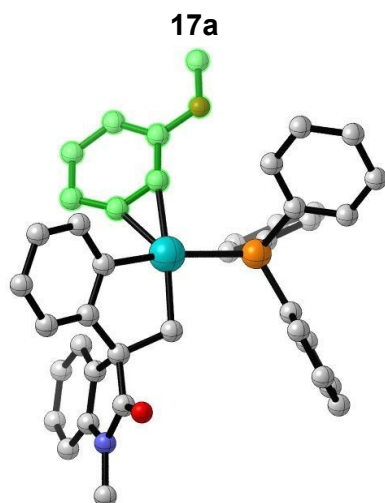
15c



Zero-point correction= 0.588408 (Hartree/Particle)
 Thermal correction to Energy= 0.627726
 Thermal correction to Enthalpy= 0.628671
 Thermal correction to Gibbs Free Energy= 0.511443
 Sum of electronic and zero-point Energies= -2141.178883
 Sum of electronic and thermal Energies= -2141.139565
 Sum of electronic and thermal Enthalpies= -2141.138620
 Sum of electronic and thermal Free Energies= -2141.255848
 E(RM06L) = -2143.33675574

Pd	-0.53496	0.48806	-0.80901
P	-2.54799	-0.15	0.04333
O	1.8892	-2.52587	0.96405
N	4.20285	-2.38722	0.7571
C	1.55979	1.10069	-1.29029
C	0.82892	1.28124	-2.51517
H	0.36491	2.24889	-2.72978
C	0.85703	0.29178	-3.52821
H	0.31421	0.46929	-4.46214
C	1.59216	-0.88453	-3.34448
H	1.63071	-1.64195	-4.13359
C	2.25373	-1.11117	-2.12297
H	2.79673	-2.04996	-1.96998
C	2.22162	-0.16564	-1.08628
C	2.99118	-0.40296	0.21572
C	2.37888	0.4569	1.36112
H	2.98256	0.34585	2.27842
H	1.3733	0.0348	1.56181
C	4.4971	-0.20872	0.05032
C	5.24987	0.89366	-0.35811
H	4.75565	1.82978	-0.63455
C	6.65584	0.78391	-0.40843

H	7.25436	1.64395	-0.72446
C	7.2911	-0.41813	-0.0585
H	8.38281	-0.48949	-0.10315
C	6.54589	-1.5427	0.34785
H	7.04157	-2.48048	0.61614
C	5.15321	-1.41341	0.3924
C	2.90308	-1.89072	0.67409
C	4.50519	-3.73514	1.20513
H	3.54386	-4.22308	1.42463
H	5.12695	-3.71752	2.11774
H	5.03747	-4.30238	0.42132
C	-4.02281	0.22322	-1.02249
C	-5.27429	0.62028	-0.50656
H	-5.4056	0.73744	0.5742
C	-6.34996	0.87717	-1.37364
H	-7.31519	1.19121	-0.96157
C	-6.18939	0.73514	-2.76086
H	-7.02858	0.93817	-3.43474
C	-4.94475	0.34236	-3.28246
H	-4.81064	0.23849	-4.36468
C	-3.86646	0.09688	-2.42023
H	-2.88444	-0.18302	-2.82011
C	-2.72879	-1.96404	0.38603
C	-3.97028	-2.63548	0.35279
H	-4.88108	-2.0853	0.09343
C	-4.03952	-4.00966	0.63418
H	-5.00688	-4.52283	0.6005
C	-2.87243	-4.7243	0.95133
H	-2.92875	-5.79692	1.1669
C	-1.63349	-4.063	0.97805
H	-0.71507	-4.61148	1.21094
C	-1.5574	-2.69161	0.6892
H	-0.58208	-2.19002	0.68374
C	-2.98456	0.65203	1.66007
C	-3.70398	0.00316	2.68567
H	-4.02458	-1.03551	2.55386
C	-3.99817	0.67882	3.88214
H	-4.55141	0.16232	4.67412
C	-3.58169	2.00688	4.06541
H	-3.80966	2.5298	5.00043
C	-2.86115	2.65883	3.05012
H	-2.5233	3.69114	3.19083
C	-2.5571	1.98341	1.85913
H	-1.97025	2.4748	1.07364
C	2.53495	2.94547	1.87828
C	2.25285	1.91003	0.97412
C	1.80354	2.22133	-0.33749
C	1.66492	3.57826	-0.70523
C	1.93605	4.60362	0.21151
C	2.37046	4.29054	1.50938
H	2.8847	2.6913	2.88567
H	1.36054	3.83656	-1.72433
H	1.82122	5.64872	-0.09479
H	2.59345	5.08752	2.22622

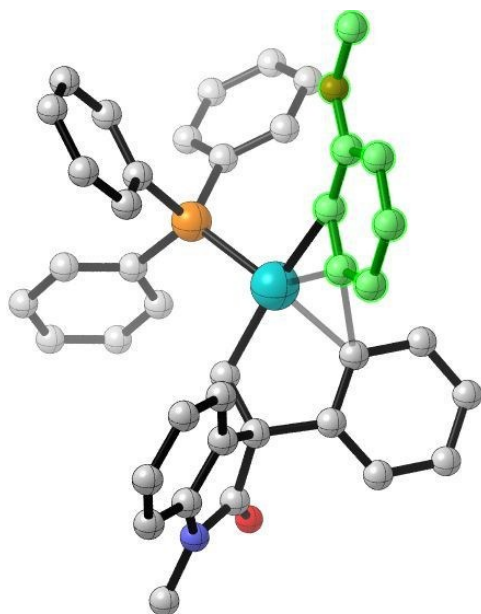


Zero-point correction= 0.615537 (Hartree/Particle)
 Thermal correction to Energy= 0.658460
 Thermal correction to Enthalpy= 0.659404
 Thermal correction to Gibbs Free Energy= 0.535066
 Sum of electronic and zero-point Energies= -2255.541541

Sum of electronic and thermal Energies= -2255.498618
 Sum of electronic and thermal Enthalpies= -2255.497674
 Sum of electronic and thermal Free Energies= -2255.622012
 E(RM06L) = -2257.75962841

Pd	-0.03962	-0.68198	-0.46428
P	1.63391	1.09287	-0.05604
O	-4.04505	1.6854	-2.1128
N	-4.95664	1.35172	0.00431
C	-1.56244	-1.6828	-1.44128
C	-1.32411	-2.79431	-2.26847
H	-0.3239	-3.23383	-2.32988
C	-2.37753	-3.34475	-3.02351
H	-2.18441	-4.20551	-3.67379
C	-3.66863	-2.8015	-2.93787
H	-4.48737	-3.23293	-3.52373
C	-3.91011	-1.69196	-2.11176
H	-4.91049	-1.24659	-2.07255
C	-2.86155	-1.12505	-1.36604
C	-2.97468	0.10435	-0.48658
C	-1.57024	0.76052	-0.50978
H	-1.42327	1.46446	0.3256
H	-1.44606	1.29524	-1.46775
C	-3.49663	-0.18356	0.91918
C	-3.01733	-1.01867	1.92811
H	-2.11425	-1.61517	1.76355
C	-3.70722	-1.07999	3.1585
H	-3.33791	-1.73395	3.95511
C	-4.86392	-0.31186	3.36591
H	-5.3916	-0.36983	4.32386
C	-5.3617	0.53769	2.35795
H	-6.26246	1.13746	2.52024
C	-4.66231	0.58475	1.14574
C	-4.02446	1.1319	-1.01459
C	-6.06014	2.28421	-0.12755
H	-5.98962	2.71766	-1.1368
H	-5.9926	3.08895	0.62652
H	-7.03146	1.77045	-0.01298
C	2.99145	1.14675	-1.31094
C	3.6808	2.34447	-1.60894
H	3.39767	3.27701	-1.11064
C	4.71378	2.34848	-2.55892
H	5.23985	3.28254	-2.78302
C	5.06469	1.16244	-3.22442
H	5.86608	1.16932	-3.97087
C	4.38018	-0.02879	-2.9358
H	4.64489	-0.95544	-3.45552
C	3.34728	-0.04044	-1.98556
H	2.81657	-0.96898	-1.75357
C	0.99895	2.83039	-0.06586
C	0.49418	3.35699	-1.2776
H	0.53521	2.75809	-2.19398
C	-0.05244	4.64712	-1.3182
H	-0.4376	5.04163	-2.26401
C	-0.11589	5.42411	-0.14896
H	-0.54773	6.42979	-0.18091
C	0.37114	4.90405	1.05977
H	0.32403	5.50309	1.97537
C	0.92596	3.61403	1.10438
H	1.30808	3.21869	2.05039
C	2.47029	0.94218	1.58496
C	3.75496	1.46959	1.83137
H	4.30991	1.95658	1.02318
C	4.32906	1.35773	3.10697
H	5.32984	1.76375	3.28878
C	3.6256	0.725	4.14559
H	4.07685	0.6393	5.13978
C	2.34785	0.19491	3.90499
H	1.79911	-0.30809	4.70789
C	1.77411	0.29524	2.62783
H	0.78832	-0.13905	2.42797
C	-0.27289	-3.75653	0.91132
C	0.20653	-2.58281	0.33749
C	1.45053	-2.23043	0.05626
C	2.5095	-3.07931	0.40758
C	2.14038	-4.29781	1.04225
C	0.78696	-4.61606	1.28438
H	-1.32352	-4.00409	1.07631
H	2.90683	-5.01616	1.34792
H	0.55245	-5.56549	1.77997
O	3.79758	-2.70793	0.10897
C	4.83981	-3.61697	0.46581
H	5.77747	-3.14401	0.13954
H	4.87845	-3.7859	1.55909
H	4.72446	-4.59243	-0.04511

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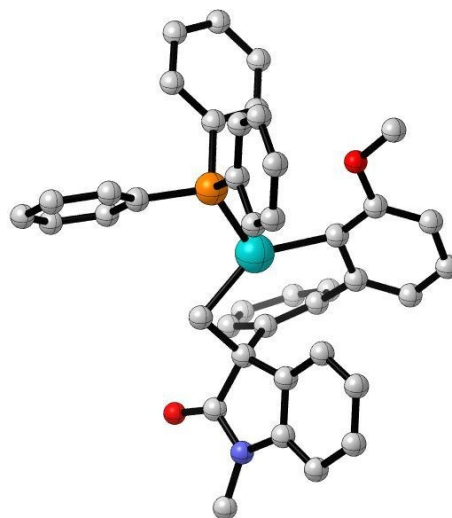


Zero-point correction= 0.615310 (Hartree/Particle)
 Thermal correction to Energy= 0.657337
 Thermal correction to Enthalpy= 0.658281
 Thermal correction to Gibbs Free Energy= 0.536689
 Sum of electronic and zero-point Energies= -2255.538016
 Sum of electronic and thermal Energies= -2255.495989
 Sum of electronic and thermal Enthalpies= -2255.495045
 Sum of electronic and thermal Free Energies= -2255.616637
 E(RM06L) = -2257.75453864
 Imaginary frequency = -153.25 cm⁻¹

Pd	0.00691	-0.55225	-0.54783
P	1.72966	1.01301	-0.0742
O	-4.02853	1.85299	-2.03098
N	-4.78026	1.57243	0.1529
C	-1.55028	-1.57535	-1.54605
C	-1.35522	-2.52797	-2.56444
H	-0.37823	-3.00635	-2.6791
C	-2.419	-2.88661	-3.41075
H	-2.25783	-3.62951	-4.1995
C	-3.6829	-2.30696	-3.2293
H	-4.51924	-2.59339	-3.87575
C	-3.87138	-1.3265	-2.24078
H	-4.83762	-0.81724	-2.16505
C	-2.81354	-0.93606	-1.39991
C	-2.87181	0.26521	-0.46775
C	-1.4718	0.94564	-0.56276
H	-1.31825	1.67119	0.25357
H	-1.40565	1.47131	-1.53053
C	-3.31607	-0.01654	0.9684
C	-2.80311	-0.86027	1.95526
H	-1.94023	-1.49846	1.74342
C	-3.41262	-0.8898	3.22896
H	-3.01536	-1.55575	4.00187
C	-4.52188	-0.07724	3.50906
H	-4.98633	-0.10951	4.5004
C	-5.05102	0.78503	2.52904
H	-5.91444	1.42184	2.74462
C	-4.43389	0.79727	1.27212
C	-3.93777	1.31102	-0.93015
C	-5.85682	2.54336	0.09635
H	-5.84691	2.96904	-0.91853
H	-5.70485	3.34867	0.83736
H	-6.83416	2.06473	0.28678
C	3.24929	0.8405	-1.11617
C	4.05941	1.9552	-1.43031
H	3.77887	2.95291	-1.07837
C	5.21786	1.79015	-2.20558
H	5.83661	2.66109	-2.44673
C	5.57737	0.51604	-2.67427
H	6.47816	0.39063	-3.28457
C	4.77504	-0.59375	-2.36404
H	5.04738	-1.58928	-2.72988
C	3.61351	-0.43668	-1.5922
H	2.98595	-1.30023	-1.3492

C	1.2958	2.79984	-0.27609
C	0.84633	3.23551	-1.54375
H	0.77795	2.52315	-2.37341
C	0.48721	4.57504	-1.74641
H	0.14076	4.89942	-2.73301
C	0.55854	5.49315	-0.68451
H	0.27009	6.53763	-0.84219
C	0.99381	5.06552	0.57879
H	1.04941	5.77518	1.41108
C	1.3622	3.72504	0.78498
H	1.70454	3.39886	1.77164
C	2.31416	0.88115	1.67336
C	3.63237	1.20524	2.05726
H	4.35877	1.52354	1.30252
C	4.01785	1.10646	3.4034
H	5.04499	1.35333	3.69245
C	3.09278	0.6893	4.37463
H	3.39728	0.61193	5.42376
C	1.77974	0.36352	3.99718
H	1.05673	0.03004	4.74872
C	1.39199	0.45148	2.65152
H	0.37525	0.17668	2.34852
C	-1.03718	-3.65911	0.50315
C	-0.32359	-2.59266	-0.04565
C	1.00542	-2.41978	-0.12624
C	1.83965	-3.40697	0.42362
C	1.21485	-4.54117	1.00447
C	-0.19125	-4.65089	1.04255
H	-2.12604	-3.74031	0.51574
H	1.81351	-5.34928	1.43501
H	-0.63884	-5.53922	1.50272
O	3.20202	-3.21609	0.36188
C	4.0321	-4.22305	0.93997
H	5.06739	-3.87937	0.79915
H	3.83342	-4.34548	2.02224
H	3.90111	-5.2016	0.43825

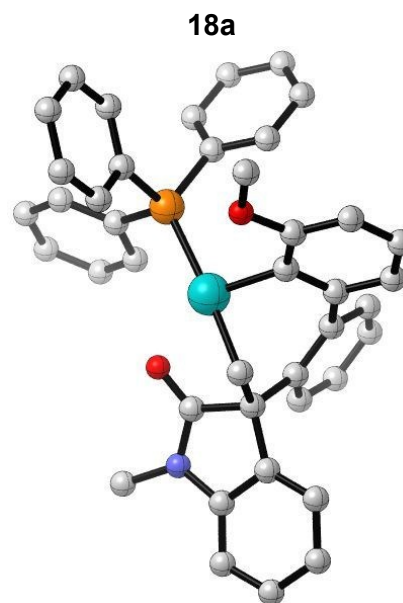
18a'



Zero-point correction= 0.616974 (Hartree/Particle)
 Thermal correction to Energy= 0.659072
 Thermal correction to Enthalpy= 0.660017
 Thermal correction to Gibbs Free Energy= 0.538816
 Sum of electronic and zero-point Energies= -2255.572051
 Sum of electronic and thermal Energies= -2255.529953
 Sum of electronic and thermal Enthalpies= -2255.529009
 Sum of electronic and thermal Free Energies= -2255.650209
 E(RM06L) = -2257.79370952

Pd	-0.14325	0.05472	-0.49677
P	1.95161	0.53907	0.12194
O	-3.67131	3.19894	-0.61188
N	-4.61422	1.70176	0.87778
C	-2.30545	-0.93294	-1.94939
C	-2.52393	-1.2101	-3.32413
H	-2.47141	-2.25973	-3.63198
C	-2.71935	-0.2115	-4.27931
H	-2.88207	-0.47658	-5.3295
C	-2.64	1.13097	-3.87781

H	-2.73135	1.94103	-4.60897
C	-2.47029	1.43833	-2.52679
H	-2.48766	2.4858	-2.21848
C	-2.38278	0.44053	-1.51167
C	-2.48271	1.03571	-0.02265
C	-1.12551	1.7365	0.26536
H	-0.93443	1.90561	1.33634
H	-1.0345	2.67652	-0.29941
C	-2.96952	0.089	1.08095
C	-2.37704	-1.00645	1.71838
H	-1.3967	-1.36774	1.39598
C	-3.05419	-1.66048	2.76949
H	-2.58615	-2.5247	3.25067
C	-4.31733	-1.22162	3.19081
H	-4.8372	-1.74246	4.00187
C	-4.92326	-0.10421	2.58736
H	-5.89734	0.26226	2.9247
C	-4.22892	0.53208	1.55223
C	-3.63363	2.1272	-0.00525
C	-5.79242	2.49558	1.18247
H	-5.75324	3.38862	0.54181
H	-5.79689	2.80251	2.24384
H	-6.71427	1.92638	0.97067
C	3.21821	0.12138	-1.1626
C	4.44355	0.82178	-1.23475
H	4.64915	1.64079	-0.53783
C	5.39431	0.48114	-2.20974
H	6.34063	1.03037	-2.25914
C	5.12725	-0.55069	-3.12436
H	5.86703	-0.80928	-3.8896
C	3.90588	-1.24116	-3.06225
H	3.68873	-2.03932	-3.78
C	2.95144	-0.90943	-2.0881
H	1.99273	-1.43609	-2.03368
C	2.29774	2.33164	0.45157
C	1.856	3.27219	-0.50531
H	1.30462	2.92227	-1.38518
C	2.10454	4.63922	-0.32417
H	1.75839	5.3583	-1.07397
C	2.78247	5.08656	0.82377
H	2.96662	6.156	0.97056
C	3.21415	4.15959	1.78413
H	3.73819	4.50238	2.68276
C	2.97735	2.78597	1.60025
H	3.32142	2.06883	2.35187
C	2.50634	-0.2952	1.67591
C	3.82669	-0.75601	1.85673
H	4.55552	-0.65733	1.04611
C	4.20762	-1.34677	3.07314
H	5.23458	-1.70505	3.20283
C	3.27846	-1.47714	4.11776
H	3.57819	-1.93792	5.06496
C	1.96181	-1.01903	3.9424
H	1.23041	-1.12228	4.75081
C	1.57511	-0.43643	2.72639
H	0.5432	-0.09959	2.57967
C	-2.4741	-3.30933	-1.03344
C	-1.74337	-2.11008	-1.18935
C	-0.37493	-2.00333	-0.81812
C	0.24256	-3.16666	-0.30441
C	-0.4725	-4.37118	-0.13337
C	-1.83243	-4.42929	-0.49342
H	-3.52749	-3.35543	-1.33189
H	0.00844	-5.26287	0.27995
H	-2.38356	-5.36593	-0.35495
O	1.58086	-3.03504	0.02626
C	2.24927	-4.17793	0.55156
H	3.28105	-3.85574	0.7546
H	1.78938	-4.52842	1.49642
H	2.26173	-5.01834	-0.17068



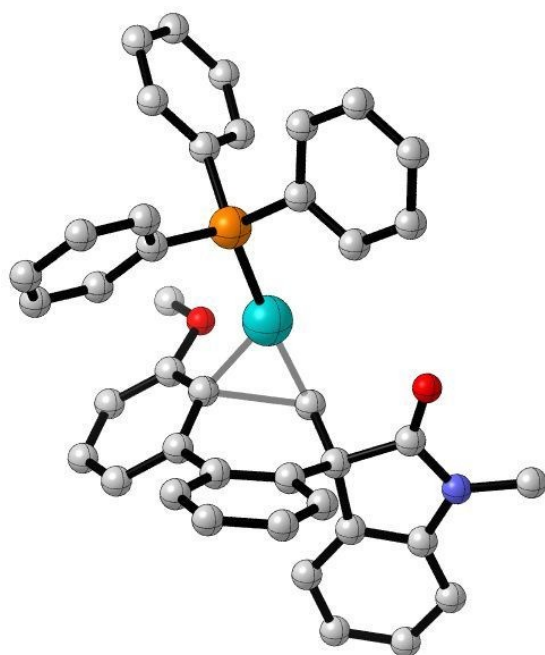
Zero-point correction= 0.618331 (Hartree/Particle)
 Thermal correction to Energy= 0.660095
 Thermal correction to Enthalpy= 0.661039
 Thermal correction to Gibbs Free Energy= 0.540204
 Sum of electronic and zero-point Energies= -2255.616586
 Sum of electronic and thermal Energies= -2255.574822
 Sum of electronic and thermal Enthalpies= -2255.573878
 Sum of electronic and thermal Free Energies= -2255.694713
 E(RM06L) = -2257.83356453

Pd	0.11762	-0.11157	-0.66323
P	-2.06254	0.60525	0.04294
O	1.37958	1.9746	-0.50439
N	3.68508	2.22849	-0.71871
C	1.82732	-1.60465	1.51781
C	1.75405	-1.8956	2.90664
H	1.1223	-2.73495	3.21372
C	2.41401	-1.14323	3.88308
H	2.30711	-1.40515	4.94108
C	3.19863	-0.05145	3.48866
H	3.72921	0.55839	4.22741
C	3.298	0.25154	2.12687
H	3.93293	1.09043	1.82006
C	2.62772	-0.48609	1.12356
C	2.89135	0.00569	-0.32866
C	1.99411	-0.6451	-1.39807
H	2.22087	-1.71021	-1.53646
H	2.09197	-0.12595	-2.3698
C	4.38862	0.02491	-0.63991
C	5.32617	-1.00416	-0.73124
H	5.02515	-2.04223	-0.55508
C	6.66237	-0.68796	-1.05397
H	7.40465	-1.48844	-1.13386
C	7.04964	0.64465	-1.27172
H	8.09089	0.87492	-1.5195
C	6.11773	1.69778	-1.17402
H	6.42096	2.73601	-1.34038
C	4.79852	1.36002	-0.85698
C	2.53683	1.50559	-0.47539
C	3.69045	3.65062	-1.0249
H	2.65425	4.00865	-0.93999
H	4.05757	3.82584	-2.05154
H	4.33244	4.20155	-0.31619
C	-3.30196	0.52659	-1.33243
C	-4.69441	0.45027	-1.11923
H	-5.08794	0.4099	-0.09807
C	-5.57684	0.41509	-2.21152
H	-6.65622	0.35225	-2.03574
C	-5.07815	0.45842	-3.52378
H	-5.76843	0.4308	-4.37383
C	-3.69179	0.52759	-3.74365
H	-3.29726	0.55185	-4.76518
C	-2.80767	0.55381	-2.65423
H	-1.72281	0.57093	-2.81378
C	-2.93735	-0.20798	1.46159
C	-2.76601	-1.59656	1.6505
H	-2.09675	-2.15352	0.98744

C	-3.43215	-2.25532	2.69539
H	-3.28818	-3.33228	2.83289
C	-4.26761	-1.53793	3.5671
H	-4.78131	-2.05353	4.38563
C	-4.43426	-0.15472	3.39179
H	-5.07777	0.41294	4.07271
C	-3.77285	0.50891	2.34587
H	-3.89884	1.58911	2.21992
C	-2.07926	2.3919	0.54401
C	-3.02079	3.32906	0.07044
H	-3.79452	3.01467	-0.63694
C	-2.9705	4.66516	0.503
H	-3.70557	5.38453	0.12593
C	-1.98618	5.07597	1.41515
H	-1.95033	6.1173	1.75286
C	-1.04152	4.14843	1.88703
H	-0.26501	4.46449	2.59184
C	-1.07956	2.81782	1.44715
H	-0.32449	2.10278	1.78999
C	1.15637	-3.9374	0.87894
C	1.03587	-2.54231	0.64052
C	0.12251	-2.08191	-0.33698
C	-0.63522	-3.01865	-1.07676
C	-0.51949	-4.40097	-0.8244
C	0.38886	-4.85075	0.15012
H	1.87754	-4.29645	1.62083
H	-1.11224	-5.12734	-1.38756
H	0.49808	-5.92575	0.3291
O	-1.48217	-2.48659	-2.03
C	-2.31262	-3.3926	-2.75234
H	-2.9314	-2.76638	-3.41158
H	-1.71899	-4.09805	-3.36681
H	-2.97255	-3.9742	-2.07903

H	0.98634	-1.34354	3.78091
C	1.77576	0.65649	4.01698
H	1.53675	0.70693	5.08444
C	2.36613	1.74816	3.36514
H	2.60661	2.66377	3.91543
C	2.64526	1.66464	1.99416
H	3.11284	2.52181	1.49919
C	2.34205	0.51197	1.24097
C	2.7865	0.46254	-0.2388
C	1.89932	-0.38643	-1.19876
H	2.4335	-1.26579	-1.57528
H	1.58445	0.20074	-2.09458
C	4.26097	0.07184	-0.34568
C	4.92999	-1.09211	0.03322
H	4.38362	-1.91207	0.51154
C	6.31701	-1.19316	-0.20695
H	6.85279	-2.10151	0.08601
C	7.01431	-0.13733	-0.81605
H	8.09045	-0.22905	-0.9964
C	6.35259	1.04604	-1.2009
H	6.89742	1.86854	-1.67428
C	4.97755	1.12653	-0.95362
C	2.79703	1.9016	-0.84221
C	4.4656	3.42912	-1.90641
H	3.54735	4.02911	-1.99229
H	4.87299	3.22997	-2.91356
H	5.2183	3.98646	-1.32117
C	-3.68238	-0.37134	-1.21273
C	-4.9648	-0.72046	-0.73909
H	-5.20944	-0.58726	0.3201
C	-5.9237	-1.25166	-1.61764
H	-6.91503	-1.52321	-1.23884
C	-5.61286	-1.43822	-2.97418
H	-6.3616	-1.85465	-3.6565
C	-4.33491	-1.1007	-3.45101
H	-4.08328	-1.25495	-4.50584
C	-3.37239	-0.57899	-2.5742
H	-2.36315	-0.3414	-2.9315
C	-2.88001	-0.13656	1.56686
C	-2.42624	-1.38685	2.04229
H	-1.75867	-1.99012	1.41715
C	-2.80915	-1.84177	3.31265
H	-2.45383	-2.81446	3.66918
C	-3.63116	-1.04742	4.12996
H	-3.92127	-1.39984	5.1256
C	-4.06961	0.20472	3.67129
H	-4.701	0.83364	4.30826
C	-3.69861	0.65964	2.39491
H	-4.0389	1.64001	2.04595
C	-2.70748	2.1842	-0.22357
C	-4.00004	2.71756	-0.42218
H	-4.85519	2.04479	-0.54746
C	-4.19127	4.10703	-0.48016
H	-5.1974	4.51081	-0.63719
C	-3.09523	4.9759	-0.34686
H	-3.24626	6.05959	-0.39826
C	-1.80549	4.4519	-0.16404
H	-0.9439	5.12202	-0.07842
C	-1.60777	3.06316	-0.10687
H	-0.59323	2.65989	0.00393
C	1.65268	-3.11738	1.82366
C	1.41413	-1.86637	1.19681
C	0.83694	-1.8296	-0.0913
C	0.58914	-3.04933	-0.77756
C	0.81159	-4.28323	-0.14102
C	1.34424	-4.30865	1.16257
H	2.10641	-3.14001	2.81982
H	0.58321	-5.2237	-0.64956
H	1.53529	-5.27217	1.64637
O	0.13174	-2.923	-2.0719
C	-0.12806	-4.12617	-2.79502
H	-0.45924	-3.80948	-3.79462
H	0.78003	-4.75268	-2.89219
H	-0.9288	-4.7247	-2.3194

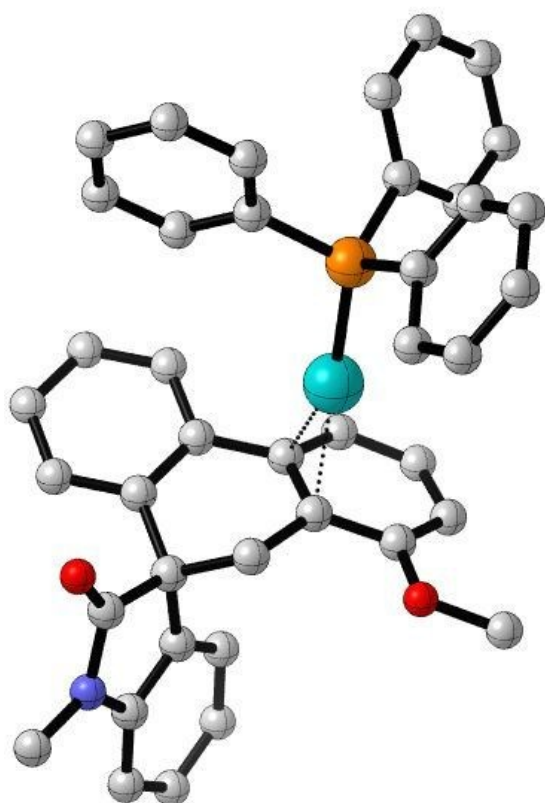
TS 18a-19a



Zero-point correction= 0.617106 (Hartree/Particle)
 Thermal correction to Energy= 0.658752
 Thermal correction to Enthalpy= 0.659696
 Thermal correction to Gibbs Free Energy= 0.537786
 Sum of electronic and zero-point Energies= -2255.606879
 Sum of electronic and thermal Energies= -2255.565232
 Sum of electronic and thermal Enthalpies= -2255.564288
 Sum of electronic and thermal Free Energies= -2255.686199
 E(RM06L) = -2257.82158812
 Imaginary frequency = -246.18 cm⁻¹

Pd	-0.15855	-0.15101	-0.70875
P	-2.36138	0.36497	-0.13984
O	1.83376	2.65657	-0.99186
N	4.10051	2.19134	-1.24051
C	1.75006	-0.59896	1.90192
C	1.47707	-0.49927	3.28621

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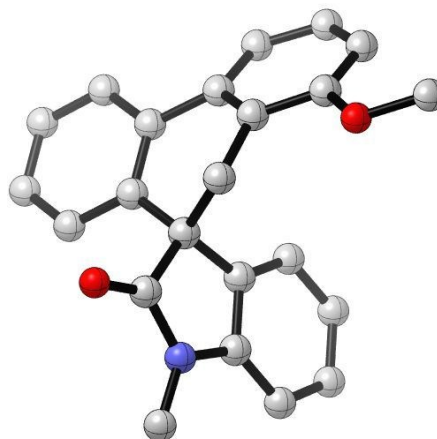


Zero-point correction= 0.619844 (Hartree/Particle)
 Thermal correction to Energy= 0.662037
 Thermal correction to Enthalpy= 0.662981
 Thermal correction to Gibbs Free Energy= 0.538466
 Sum of electronic and zero-point Energies= -2255.665116
 Sum of electronic and thermal Energies= -2255.622923
 Sum of electronic and thermal Enthalpies= -2255.621979
 Sum of electronic and thermal Free Energies= -2255.746494
 E(RM06L) = -2257.88544491

Pd	0.62512	-0.57733	-0.18286
P	2.76189	0.07811	0.17508
O	-3.11769	2.22942	2.24552
N	-5.13974	1.19899	1.71808
C	-1.67165	0.82852	-1.61072
C	-1.09842	1.59331	-2.65289
H	-0.33252	1.13659	-3.28786
C	-1.46636	2.92833	-2.85644
H	-1.00556	3.5028	-3.66691
C	-2.41695	3.52695	-2.01304
H	-2.70916	4.57177	-2.1603
C	-2.9875	2.78217	-0.97077
H	-3.71532	3.25699	-0.30536
C	-2.62644	1.44074	-0.75378
C	-3.27677	0.60295	0.35141
C	-2.22469	-0.38092	0.95203
H	-2.70953	-1.05036	1.68046
H	-1.48916	0.23312	1.50395
C	-4.55689	-0.0968	-0.10139
C	-4.81151	-0.98196	-1.15051
H	-4.01241	-1.27365	-1.83906
C	-6.11656	-1.49273	-1.31816
H	-6.32318	-2.18923	-2.13679
C	-7.14974	-1.1114	-0.44794
H	-8.15796	-1.51431	-0.59037
C	-6.9138	-0.20898	0.60807
H	-7.72105	0.09454	1.28148
C	-5.61316	0.28573	0.75852
C	-3.78176	1.47098	1.54116
C	-5.93007	1.79958	2.77717
H	-5.2575	2.46628	3.33768
H	-6.33486	1.02775	3.45567
H	-6.76956	2.38451	2.36117
C	3.60149	-0.67309	1.65305
C	4.96696	-1.02703	1.67925

H	5.58645	-0.8772	0.78887
C	5.5339	-1.5823	2.83905
H	6.59412	-1.85808	2.8454
C	4.74684	-1.78574	3.9834
H	5.19088	-2.22039	4.88535
C	3.38484	-1.43959	3.96395
H	2.76277	-1.60377	4.85041
C	2.81399	-0.89575	2.80429
H	1.74628	-0.64712	2.77403
C	3.93343	-0.3118	-1.21262
C	3.69415	-1.49611	-1.94377
H	2.82224	-2.10905	-1.68424
C	4.54329	-1.86788	-2.99618
H	4.34716	-2.78991	-3.55412
C	5.63252	-1.05097	-3.34452
H	6.28919	-1.33406	-4.17416
C	5.86932	0.13603	-2.63313
H	6.71104	0.78162	-2.90667
C	5.02713	0.50469	-1.57026
H	5.2142	1.43587	-1.02504
C	2.99559	1.89815	0.45092
C	4.05412	2.43589	1.21442
H	4.7757	1.76581	1.69387
C	4.17537	3.82556	1.378
H	4.99708	4.23176	1.9779
C	3.24281	4.69065	0.78271
H	3.3359	5.77369	0.917
C	2.1824	4.16229	0.02801
H	1.44203	4.82971	-0.42521
C	2.05461	2.77421	-0.13179
H	1.21255	2.35356	-0.69472
C	-1.00225	-1.44875	-2.54021
C	-1.32676	-0.6103	-1.42864
C	-1.56012	-1.2083	-0.13897
C	-1.4327	-2.63347	-0.01044
C	-1.12832	-3.43563	-1.12397
C	-0.92731	-2.83298	-2.38304
H	-0.87356	-0.99998	-3.52895
H	-1.05876	-4.52109	-1.02635
H	-0.70213	-3.46614	-3.24744
O	-1.6983	-3.126	1.24245
C	-1.57888	-4.53598	1.43828
H	-1.8099	-4.71096	2.49889
H	-2.29623	-5.09817	0.81029
H	-0.55222	-4.88755	1.22312

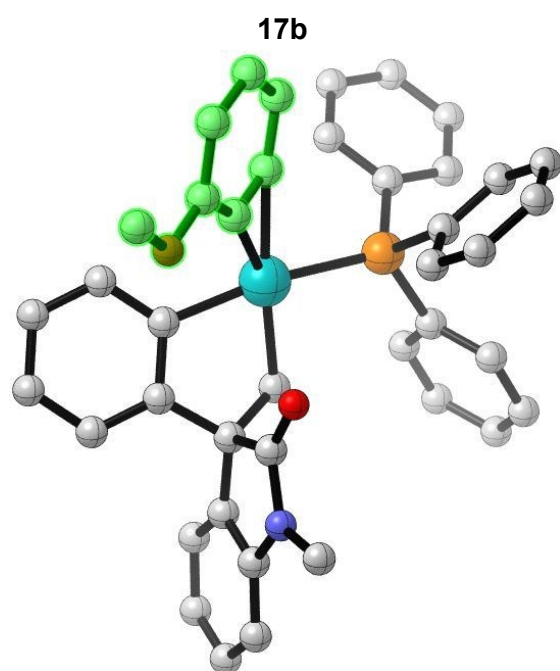
20a



Zero-point correction= 0.353027 (Hartree/Particle)
 Thermal correction to Energy= 0.374516
 Thermal correction to Enthalpy= 0.375460
 Thermal correction to Gibbs Free Energy= 0.303228
 Sum of electronic and zero-point Energies= -1092.785271
 Sum of electronic and thermal Energies= -1092.763782
 Sum of electronic and thermal Enthalpies= -1092.762838
 Sum of electronic and thermal Free Energies= -1092.835070
 E(RM06L) = -1093.36594537

O	2.3709	0.36823	-2.48831
N	2.83292	-1.05982	-0.7062
C	-0.68071	2.15508	0.04528
C	-0.83241	3.51752	0.39219
H	-1.83911	3.91551	0.5551
C	0.27626	4.3662	0.49063

H	0.13432	5.41911	0.75603
C	1.56393	3.86487	0.23791
H	2.43792	4.52059	0.30779
C	1.72779	2.51751	-0.11471
H	2.73087	2.13464	-0.32723
C	0.62312	1.6539	-0.21862
C	0.79338	0.1697	-0.55687
C	-0.40591	-0.30986	-1.43285
H	-0.33803	-1.39676	-1.5998
H	-0.30272	0.18412	-2.41671
C	1.01823	-0.70414	0.67569
C	0.26498	-0.88524	1.83708
H	-0.66478	-0.32853	1.98997
C	0.72072	-1.79185	2.81814
H	0.13415	-1.94109	3.73008
C	1.91987	-2.49813	2.63555
H	2.26242	-3.19744	3.40546
C	2.69941	-2.31797	1.47578
H	3.63831	-2.86249	1.33716
C	2.2304	-1.4155	0.5142
C	2.07592	-0.10957	-1.39421
C	4.07956	-1.59511	-1.22231
H	4.26323	-1.10031	-2.18794
H	4.00912	-2.68686	-1.37414
H	4.9162	-1.38418	-0.53276
C	-2.97282	1.40415	0.87009
C	-1.85248	1.23473	-0.0017
C	-1.7364	0.02376	-0.77332
C	-2.77123	-0.96589	-0.65664
C	-3.85371	-0.78028	0.22075
C	-3.93632	0.40176	0.98548
H	-3.03547	2.30112	1.49224
H	-4.62385	-1.54742	0.3255
H	-4.77658	0.53315	1.67504
O	-2.57153	-2.1004	-1.4022
C	-3.57086	-3.11914	-1.33764
H	-3.22991	-3.91548	-2.01477
H	-3.6723	-3.52808	-0.31417
H	-4.55347	-2.74245	-1.67898

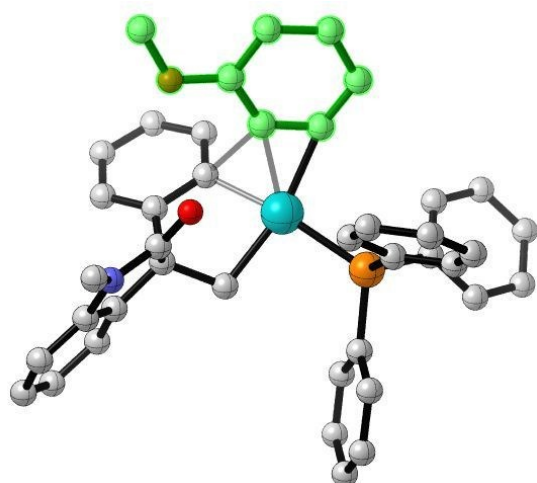


Zero-point correction= 0.615469 (Hartree/Particle)
 Thermal correction to Energy= 0.658400
 Thermal correction to Enthalpy= 0.659344
 Thermal correction to Gibbs Free Energy= 0.534826
 Sum of electronic and zero-point Energies= -2255.539529
 Sum of electronic and thermal Energies= -2255.496598
 Sum of electronic and thermal Enthalpies= -2255.495654
 Sum of electronic and thermal Free Energies= -2255.620172
 E(RM06L) = -2257.75821246

Pd	-0.13738	-0.65982	-0.66805
P	-1.94021	0.87915	-0.08414

O	1.93128	-0.57208	1.96401
N	3.75972	0.85004	1.80434
C	1.58794	-1.57534	-1.37195
C	1.60339	-2.72353	-2.18341
H	0.66689	-3.22577	-2.4457
C	2.8246	-3.23554	-2.6616
H	2.82548	-4.12501	-3.30242
C	4.03595	-2.61846	-2.31274
H	4.98635	-3.02334	-2.67762
C	4.02916	-1.46604	-1.50984
H	4.96906	-0.95795	-1.2654
C	2.80984	-0.93692	-1.05106
C	2.66163	0.35639	-0.26644
C	1.26906	0.91281	-0.65968
H	1.30465	1.28201	-1.70043
H	0.95075	1.73443	0.00132
C	3.79543	1.35531	-0.44188
C	4.27453	2.00218	-1.58164
H	3.81832	1.80631	-2.55806
C	5.35418	2.90321	-1.46191
C	5.73579	3.41598	-2.35054
C	5.94355	3.14245	-0.20982
H	6.78174	3.84265	-0.12878
C	5.47666	2.49387	0.95112
H	5.93951	2.68041	1.92499
C	4.40329	1.60596	0.80921
C	2.69446	0.10956	1.28027
C	4.08037	0.87328	3.21922
H	3.37072	0.19543	3.71698
C	3.97212	1.89128	3.63518
H	5.11296	0.52379	3.39787
C	-1.52819	2.67993	0.06687
C	-1.49885	3.35141	1.3059
H	-1.7598	2.81453	2.22294
C	-1.14044	4.70894	1.36741
H	-1.12567	5.21995	2.33599
C	-0.80705	5.40722	0.19726
H	-0.52793	6.46481	0.24783
C	-0.82644	4.74191	-1.04081
H	-0.56145	5.27841	-1.95795
C	-1.1785	3.38701	-1.10642
H	-1.18672	2.87374	-2.07445
C	-2.58894	0.43828	1.58799
C	-3.93638	0.60364	1.96851
H	-4.66877	0.98028	1.24783
C	-4.34686	0.26903	3.26867
H	-5.39719	0.39238	3.55371
C	-3.41686	-0.22527	4.19756
H	-3.74065	-0.48591	5.21091
C	-2.07471	-0.39642	3.82087
H	-1.34708	-0.7945	4.53559
C	-1.65829	-0.07663	2.51908
H	-0.61516	-0.24045	2.22002
C	-3.38707	0.93203	-1.23588
C	-4.34759	1.96735	-1.16892
H	-4.2367	2.76844	-0.43076
C	-5.43133	1.9871	-2.05972
H	-6.17112	2.79217	-1.9965
C	-5.5603	0.98534	-3.03647
H	-6.40307	1.00673	-3.73547
C	-4.59957	-0.03449	-3.12243
H	-4.68589	-0.80908	-3.89161
C	-3.51678	-0.06203	-2.22832
H	-2.75901	-0.85076	-2.29248
C	-0.16557	-3.84306	0.56903
C	-0.48193	-2.60762	0.00191
C	-1.66669	-2.24878	-0.43952
C	-2.81937	-3.03693	-0.3521
C	-2.57978	-4.29809	0.24247
C	-1.30261	-4.69375	0.69371
H	-3.81142	-2.74172	-0.70625
H	-3.41335	-5.0015	0.35921
H	-1.19172	-5.67932	1.15541
O	1.10432	-4.1456	0.95981
C	1.31713	-5.43259	1.54134
H	2.39101	-5.48264	1.77061
H	0.73679	-5.55938	2.47557
H	1.05401	-6.24696	0.83913

TS 17b-18b

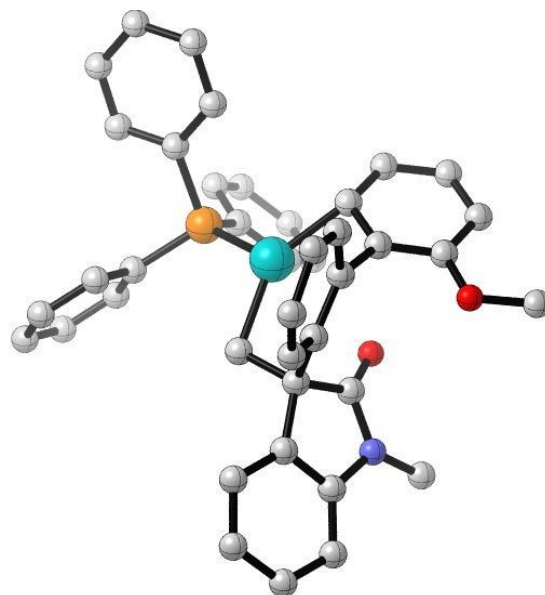


Zero-point correction= 0.615138 (Hartree/Particle)
 Thermal correction to Energy= 0.657134
 Thermal correction to Enthalpy= 0.658078
 Thermal correction to Gibbs Free Energy= 0.537128
 Sum of electronic and zero-point Energies= -2255.536102
 Sum of electronic and thermal Energies= -2255.494105
 Sum of electronic and thermal Enthalpies= -2255.493161
 Sum of electronic and thermal Free Energies= -2255.614111
 E(RM06L) = -2257.75351673
 Imaginary frequency = -161.00 cm⁻¹

Pd	-0.18614	-0.59587	-0.60963
P	-2.16864	0.56596	-0.06475
O	1.89364	-0.47324	1.9177
N	3.55306	1.14566	1.83071
C	1.60673	-1.3448	-1.4419
C	1.70071	-2.31292	-2.45985
H	0.8371	-2.94539	-2.68617
C	2.9052	-2.48871	-3.16401
H	2.96545	-3.24167	-3.9577
C	4.02716	-1.71417	-2.83502
H	4.97456	-1.86208	-3.36478
C	3.93033	-0.72061	-1.84536
H	4.78694	-0.06995	-1.63868
C	2.72306	-0.50955	-1.15702
C	2.45917	0.68904	-0.25178
C	1.00322	1.14418	-0.57478
H	0.98642	1.58887	-1.58565
H	0.64673	1.89972	0.14581
C	3.47454	1.81765	-0.36894
C	3.83811	2.61157	-1.45808
H	3.37983	2.44388	-2.43865
C	4.80324	3.6262	-1.28302
H	5.09324	4.25291	-2.13234
C	5.39321	3.83609	-0.02599
H	6.14081	4.62661	0.09845
C	5.03899	3.04495	1.08506
H	5.49819	3.21122	2.0643
C	4.07909	2.04473	0.88797
C	2.56164	0.33291	1.27055
C	3.89165	1.11192	3.24122
H	3.27132	0.32642	3.6983
H	3.67504	2.08139	3.72536
H	4.96002	0.87222	3.38692
C	-2.12361	2.41305	-0.16807
C	-2.3625	3.24979	0.94062
H	-2.60718	2.81019	1.91245
C	-2.29011	4.64666	0.80142
H	-2.47722	5.28666	1.67029
C	-1.98234	5.21887	-0.44186
H	-1.92684	6.30737	-0.54757
C	-1.73768	4.38978	-1.55054
H	-1.48981	4.82966	-2.52227
C	-1.79989	2.99647	-1.41413
H	-1.59368	2.3534	-2.27719
C	-2.6682	0.21642	1.67985
C	-4.00737	0.29645	2.11739
H	-4.80222	0.54788	1.40769
C	-4.3269	0.0372	3.45926
H	-5.36972	0.09376	3.78936

C	-3.31429	-0.30088	4.37238
H	-3.56683	-0.50726	5.41801
C	-1.98099	-0.38497	3.94001
H	-1.18907	-0.66001	4.64427
C	-1.65374	-0.13461	2.59783
H	-0.61476	-0.22634	2.25754
C	-3.64344	0.15119	-1.1052
C	-4.733	1.04129	-1.23668
H	-4.70562	2.01654	-0.73947
C	-5.84435	0.68761	-2.01755
H	-6.68333	1.38502	-2.11408
C	-5.87638	-0.55095	-2.67937
H	-6.74199	-0.82202	-3.29315
C	-4.79148	-1.43458	-2.56106
H	-4.80594	-2.39629	-3.08474
C	-3.67742	-1.0866	-1.78104
H	-2.81725	-1.7608	-1.69131
C	1.18675	-3.54182	0.53954
C	0.40591	-2.55859	-0.0764
C	-0.91959	-2.59636	-0.25664
C	-1.69093	-3.68272	0.18455
C	-0.96633	-4.72451	0.80183
C	0.43119	-4.66119	0.98172
H	-2.77964	-3.73798	0.07696
H	-1.49764	-5.61266	1.16549
H	0.93868	-5.49301	1.47852
O	2.53686	-3.39514	0.66385
C	3.25096	-4.45429	1.30105
H	4.3067	-4.14732	1.29782
H	2.91545	-4.60173	2.34549
H	3.14659	-5.40862	0.7495

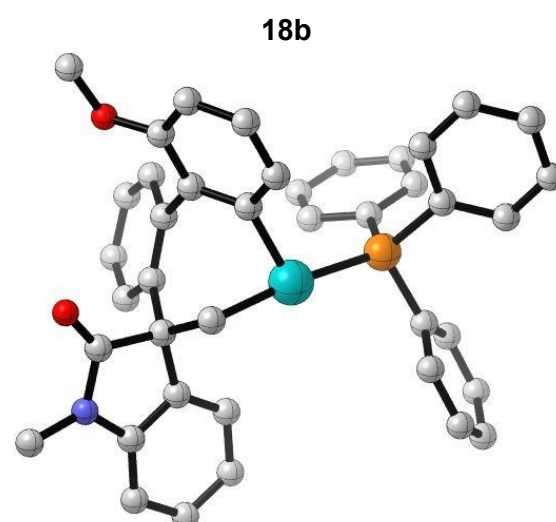
18b'



Zero-point correction= 0.616891 (Hartree/Particle)
 Thermal correction to Energy= 0.658995
 Thermal correction to Enthalpy= 0.659939
 Thermal correction to Gibbs Free Energy= 0.538352
 Sum of electronic and zero-point Energies= -2255.568832
 Sum of electronic and thermal Energies= -2255.526729
 Sum of electronic and thermal Enthalpies= -2255.525785
 Sum of electronic and thermal Free Energies= -2255.647372
 E(RM06L) = -2257.78815556

Pd	-0.24399	-0.34737	-0.42018
P	-2.30007	0.36939	0.04015
O	1.84965	-0.59275	1.83563
N	3.76646	0.70227	1.72359
C	1.76841	-1.34159	-1.49732
C	1.69009	-1.92055	-2.79638
H	1.16529	-2.87733	-2.87975
C	2.29328	-1.3571	-3.92242
H	2.21854	-1.85295	-4.89574
C	3.01891	-0.1697	-3.76802
H	3.54107	0.28318	-4.61787
C	3.05996	0.45985	-2.51797

H	3.60271	1.40265	-2.43203
C	2.42645	-0.06094	-1.36742
C	2.27322	0.91476	-0.14124
C	0.81138	1.46267	-0.1979
H	0.70313	2.11213	-1.08415
H	0.55872	2.03611	0.70969
C	3.32329	2.0299	-0.10439
C	3.48289	3.17955	-0.88307
H	2.78571	3.39404	-1.70003
C	4.53763	4.07432	-0.6008
H	4.6668	4.97068	-1.21544
C	5.41392	3.82478	0.46661
H	6.23096	4.52309	0.67604
C	5.24483	2.69572	1.29213
H	5.90658	2.51716	2.14505
C	4.18982	1.82492	0.99432
C	2.55434	0.21329	1.22814
C	4.3084	0.28714	3.0047
H	3.66796	-0.5271	3.37484
H	4.29704	1.12072	3.73066
H	5.3452	-0.07527	2.89384
C	-2.58718	2.19689	-0.02519
C	-3.05632	2.94336	1.07468
H	-3.29262	2.43893	2.01649
C	-3.22353	4.335	0.96606
H	-3.58603	4.90453	1.82853
C	-2.92968	4.99127	-0.2383
H	-3.06075	6.07542	-0.32004
C	-2.45832	4.25304	-1.33837
H	-2.22108	4.75994	-2.27976
C	-2.27901	2.86755	-1.23079
H	-1.89088	2.29717	-2.08217
C	-2.8118	-0.12563	1.74734
C	-4.16709	-0.21895	2.13126
H	-4.95873	-0.01901	1.40156
C	-4.50396	-0.58513	3.44369
H	-5.55774	-0.6612	3.73253
C	-3.49316	-0.86051	4.37988
H	-3.75867	-1.15044	5.40222
C	-2.14397	-0.77655	3.99956
H	-1.35283	-1.00454	4.72136
C	-1.79933	-0.41685	2.68703
H	-0.74782	-0.38057	2.37612
C	-3.61859	-0.29772	-1.07834
C	-4.82765	0.39743	-1.30244
H	-4.99139	1.37672	-0.84058
C	-5.8161	-0.15578	-2.13218
H	-6.74889	0.39221	-2.30352
C	-5.60642	-1.40173	-2.74531
H	-6.37689	-1.82857	-3.3963
C	-4.40206	-2.09218	-2.53117
H	-4.22886	-3.05855	-3.01665
C	-3.40823	-1.54319	-1.70645
H	-2.45077	-2.05673	-1.54985
C	2.08367	-3.25103	0.17675
C	1.21826	-2.31036	-0.43827
C	-0.18361	-2.3907	-0.23448
C	-0.72418	-3.45318	0.50923
C	0.13748	-4.40769	1.07564
C	1.53291	-4.3095	0.92488
H	-1.80417	-3.52435	0.68379
H	-0.27267	-5.23423	1.66912
H	2.17939	-5.06184	1.38395
O	3.42992	-3.07896	-0.0551
C	4.31493	-4.07471	0.45414
H	5.32408	-3.77235	0.13722
H	4.28055	-4.12844	1.55964
H	4.08667	-5.07645	0.04094

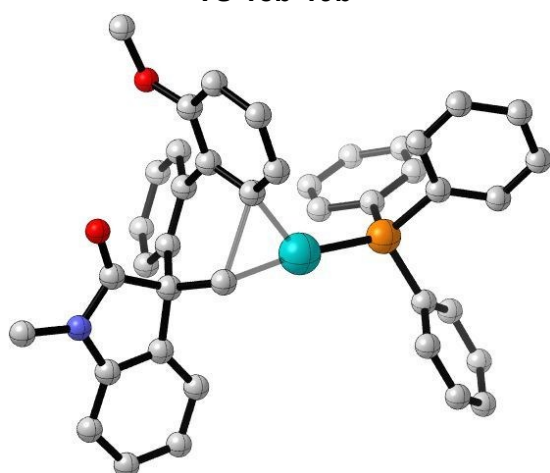


Zero-point correction= 0.617465 (Hartree/Particle)
 Thermal correction to Energy= 0.659719
 Thermal correction to Enthalpy= 0.660663
 Thermal correction to Gibbs Free Energy= 0.536831
 Sum of electronic and zero-point Energies= -2255.605526
 Sum of electronic and thermal Energies= -2255.563272
 Sum of electronic and thermal Enthalpies= -2255.562328
 Sum of electronic and thermal Free Energies= -2255.686160
 E(RM06L) = -2257.82330073

Pd	0.13787	0.12312	-0.91245
P	2.38011	0.26255	-0.06001
O	-4.77248	-0.67034	-1.23984
N	-4.84647	1.63691	-0.9249
C	-1.95261	-1.55644	0.95744
C	-1.84188	-2.18195	2.226
H	-1.36223	-3.16336	2.27168
C	-2.3203	-1.59546	3.40113
H	-2.21252	-2.11811	4.35785
C	-2.94309	-0.34094	3.33248
H	-3.34189	0.13948	4.23238
C	-3.04793	0.30076	2.0938
H	-3.52326	1.28547	2.04698
C	-2.54955	-0.26402	0.89538
C	-2.75962	0.57633	-0.3883
C	-1.82382	0.26241	-1.58405
H	-1.77252	1.13226	-2.2691
H	-2.1936	-0.60572	-2.1475
C	-2.73215	2.07799	-0.12079
C	-1.70567	2.902	0.33965
H	-0.74501	2.46424	0.64016
C	-1.92292	4.29359	0.43323
H	-1.123	4.9462	0.7967
C	-3.1628	4.84172	0.06578
H	-3.32307	5.92241	0.14221
C	-4.2114	4.02433	-0.40154
H	-5.17574	4.45518	-0.68771
C	-3.97382	2.64601	-0.48728
C	-4.23436	0.37603	-0.89142
C	-6.20441	1.83617	-1.39589
H	-6.59074	0.84412	-1.67501
H	-6.22583	2.50186	-2.27762
H	-6.84115	2.2713	-0.60485
C	2.89915	2.03439	-0.21734
C	2.58738	2.68915	-1.43233
H	2.08306	2.13232	-2.23233
C	2.91796	4.03923	-1.61992
H	2.67194	4.53263	-2.56593
C	3.55179	4.75675	-0.59146
H	3.80293	5.81307	-0.7334
C	3.85514	4.11784	0.62155
H	4.34454	4.67479	1.4277
C	3.53252	2.76386	0.8104
H	3.76865	2.2732	1.75989
C	3.75406	-0.67806	-0.86733
C	4.97022	-0.07986	-1.2589
H	5.12993	0.9906	-1.09483
C	5.97639	-0.85293	-1.86192
H	6.91625	-0.37817	-2.16351
C	5.77996	-2.2262	-2.0758
H	6.56564	-2.82639	-2.54668

C	4.56954	-2.82681	-1.69026
H	4.40698	-3.89613	-1.8616
C	3.55795	-2.05923	-1.09469
H	2.60696	-2.52809	-0.81972
C	2.58895	-0.13653	1.73118
C	3.85272	-0.37565	2.31489
H	4.75359	-0.35608	1.69209
C	3.95369	-0.65235	3.68688
H	4.93661	-0.83795	4.13306
C	2.79668	-0.7004	4.48385
H	2.87859	-0.92312	5.55311
C	1.53673	-0.47803	3.90599
H	0.62792	-0.53436	4.51331
C	1.43067	-0.20048	2.53385
H	0.44678	-0.0534	2.07331
C	-1.78465	-3.68526	-0.41207
C	-1.38538	-2.32807	-0.19824
C	-0.40881	-1.79444	-1.06187
C	0.15759	-2.55059	-2.10717
C	-0.23746	-3.8857	-2.2768
C	-1.21075	-4.45465	-1.44199
H	0.8964	-2.10442	-2.77844
H	0.20458	-4.48836	-3.07856
H	-1.52627	-5.48747	-1.60439
O	-2.76803	-4.16682	0.42026
C	-3.28449	-5.47033	0.15792
H	-4.08463	-5.62674	0.8962
H	-3.70836	-5.54441	-0.86169
H	-2.51306	-6.25493	0.28582

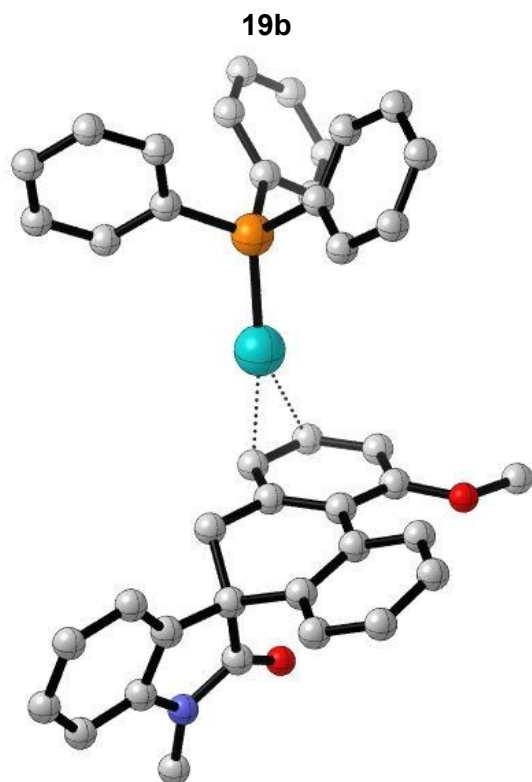
TS 18b-19b



Zero-point correction= 0.616711 (Hartree/Particle)
 Thermal correction to Energy= 0.658468
 Thermal correction to Enthalpy= 0.659413
 Thermal correction to Gibbs Free Energy= 0.537227
 Sum of electronic and zero-point Energies= -2255.601159
 Sum of electronic and thermal Energies= -2255.559402
 Sum of electronic and thermal Enthalpies= -2255.558457
 Sum of electronic and thermal Free Energies= -2255.680643
 E(RM06L) = -2257.81557250
 Imaginary frequency = -237.06 cm⁻¹

Pd	0.25464	0.21993	-0.7918
P	2.48668	0.33105	-0.09232
O	-4.45078	-1.15785	-1.01435
N	-5.11186	1.06203	-0.80556
C	-1.86303	-1.33861	1.10607
C	-1.6048	-1.89576	2.37965
H	-1.16246	-2.89337	2.43009
C	-1.89982	-1.20605	3.56214
H	-1.68712	-1.67007	4.53139
C	-2.46658	0.07399	3.49206
H	-2.71398	0.62806	4.40395
C	-2.72444	0.64649	2.2376
H	-3.17012	1.64371	2.18684
C	-2.42234	-0.02972	1.03801
C	-2.80415	0.61603	-0.31514
C	-1.7688	0.40402	-1.46014
H	-1.39817	1.38303	-1.84529
H	-2.20531	-0.13448	-2.30999

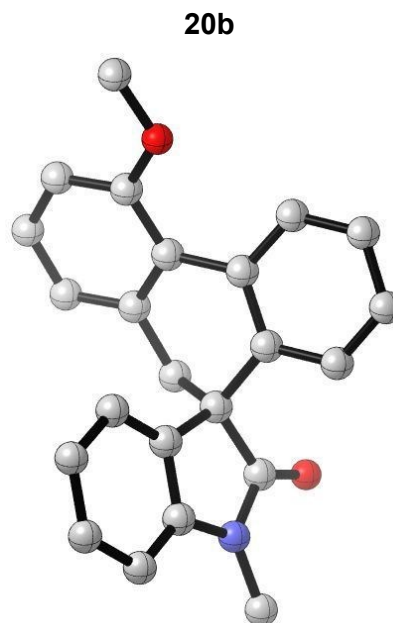
C	-3.14371	2.0995	-0.20704
C	-2.34036	3.20069	0.09473
H	-1.28082	3.05768	0.33571
C	-2.9082	4.4926	0.09055
H	-2.28511	5.36046	0.3281
C	-4.26754	4.66876	-0.21595
H	-4.69829	5.67556	-0.21734
C	-5.0919	3.5695	-0.52648
H	-6.14954	3.70977	-0.76922
C	-4.50874	2.29584	-0.51598
C	-4.18891	0.0116	-0.75014
C	-6.49699	0.86653	-1.1925
H	-6.62647	-0.2114	-1.3721
H	-6.73519	1.42494	-2.11573
H	-7.18239	1.19292	-0.39031
C	3.24323	2.0129	-0.30416
C	2.8954	2.73856	-1.46608
H	2.19414	2.29601	-2.18428
C	3.4325	4.01305	-1.69783
H	3.15595	4.56298	-2.60365
C	4.31226	4.58671	-0.76402
H	4.72452	5.58592	-0.93974
C	4.65283	3.87885	0.39936
H	5.33184	4.32432	1.13438
C	4.12368	2.59781	0.62977
H	4.39001	2.05395	1.54172
C	3.66205	-0.78322	-0.9912
C	4.99213	-0.41769	-1.28939
H	5.36102	0.57561	-1.0127
C	5.84183	-1.31961	-1.95094
H	6.87134	-1.02489	-2.1814
C	5.37364	-2.5914	-2.31804
H	6.03772	-3.29234	-2.83493
C	4.048	-2.95738	-2.03065
H	3.67287	-3.94314	-2.32544
C	3.19227	-2.05754	-1.37775
H	2.14917	-2.3298	-1.18185
C	2.77991	-0.07489	1.68925
C	4.01755	-0.5467	2.17815
H	4.84878	-0.71767	1.48579
C	4.18072	-0.81375	3.54676
H	5.14321	-1.18298	3.91703
C	3.11163	-0.61596	4.43678
H	3.24054	-0.82963	5.50328
C	1.87418	-0.16015	3.95437
H	1.02885	-0.02463	4.63636
C	1.70522	0.1025	2.5861
H	0.7315	0.42592	2.1998
C	-1.82573	-3.49522	-0.25911
C	-1.50029	-2.11193	-0.11548
C	-0.80363	-1.48433	-1.16914
C	-0.47303	-2.18027	-2.35454
C	-0.77987	-3.54191	-2.45468
C	-1.45763	-4.20409	-1.41669
H	0.02803	-1.66166	-3.17689
H	-0.5013	-4.09966	-3.3561
H	-1.7141	-5.25986	-1.52688
O	-2.52916	-4.06498	0.77662
C	-2.99788	-5.4014	0.60651
H	-3.57719	-5.63114	1.51295
H	-3.65332	-5.49347	-0.28023
H	-2.16378	-6.12456	0.51601



Zero-point correction= 0.620191 (Hartree/Particle)
 Thermal correction to Energy= 0.662144
 Thermal correction to Enthalpy= 0.663088
 Thermal correction to Gibbs Free Energy= 0.538683
 Sum of electronic and zero-point Energies= -2255.666088
 Sum of electronic and thermal Energies= -2255.624136
 Sum of electronic and thermal Enthalpies= -2255.623192
 Sum of electronic and thermal Free Energies= -2255.747597
 E(RM06L) = -2257.88177928

Pd	1.20213	-0.10999	-1.01167
P	3.1691	0.42354	-0.02991
O	-4.54051	-1.1852	-1.98159
N	-5.78443	0.7346	-1.55557
C	-2.83239	-1.72573	0.94678
C	-2.74407	-2.66885	2.00017
H	-1.93397	-3.39777	1.98843
C	-3.67166	-2.68774	3.04964
H	-3.56983	-3.43328	3.84565
C	-4.72107	-1.75964	3.07861
H	-5.45974	-1.77407	3.88683
C	-4.80811	-0.79356	2.06536
H	-5.60596	-0.04509	2.09363
C	-3.8725	-0.74956	1.01836
C	-3.95891	0.33604	-0.06027
C	-2.50849	0.72134	-0.47137
H	-2.04632	1.21682	0.40379
H	-2.52694	1.46852	-1.28343
C	-4.74404	1.58181	0.31823
C	-4.55453	2.50873	1.34433
H	-3.75197	2.36745	2.0763
C	-5.41777	3.62147	1.43739
H	-5.27842	4.351	2.24111
C	-6.45378	3.79545	0.50565
H	-7.11767	4.66239	0.58757
C	-6.65761	2.87172	-0.53833
H	-7.46469	3.01099	-1.26378
C	-5.79048	1.77462	-0.61292
C	-4.75309	-0.1807	-1.30915
C	-6.72559	0.57721	-2.64933
H	-6.44267	-0.34393	-3.18089
H	-6.67482	1.43482	-3.34366
H	-7.75945	0.4832	-2.27197
C	3.39434	2.22718	0.3567
C	2.81002	3.15614	-0.53246
H	2.23556	2.77865	-1.38752
C	2.94797	4.53486	-0.31584
H	2.49079	5.24405	-1.01429
C	3.65744	5.00423	0.80277

H	3.75591	6.08068	0.9793
C	4.23007	4.08852	1.69981
H	4.77639	4.44884	2.57832
C	4.10257	2.70667	1.47879
H	4.54577	1.99868	2.1868
C	4.68264	0.02266	-1.03103
C	5.84315	0.8248	-1.04534
H	5.8751	1.74774	-0.45692
C	6.95406	0.45283	-1.82136
H	7.84674	1.08779	-1.82926
C	6.92055	-0.7239	-2.58588
H	7.78662	-1.01038	-3.19201
C	5.76696	-1.52672	-2.57974
H	5.73079	-2.44106	-3.18197
C	4.65297	-1.15137	-1.81508
H	3.73757	-1.75525	-1.82592
C	3.5238	-0.40374	1.59568
C	4.8233	-0.72791	2.04074
H	5.68806	-0.50557	1.40669
C	5.01221	-1.34805	3.2871
H	6.02513	-1.60037	3.61954
C	3.90877	-1.64786	4.10221
H	4.05893	-2.13405	5.07213
C	2.61123	-1.3332	3.66424
H	1.7453	-1.57426	4.29008
C	2.41961	-0.72338	2.41547
H	1.40916	-0.50241	2.05042
C	-1.14334	-2.84505	-0.65637
C	-1.87048	-1.69854	-0.18697
C	-1.68922	-0.4815	-0.88269
C	-0.80187	-0.37432	-1.99086
C	-0.04843	-1.51196	-2.39483
C	-0.23863	-2.74396	-1.72399
H	-0.84111	0.52116	-2.6222
H	0.53859	-1.48838	-3.31826
H	0.3102	-3.62192	-2.0698
O	-1.39818	-4.03964	-0.02719
C	-0.76731	-5.21672	-0.53322
H	-1.14798	-6.04423	0.08298
H	-1.0328	-5.39561	-1.59216
H	0.334	-5.16629	-0.43688



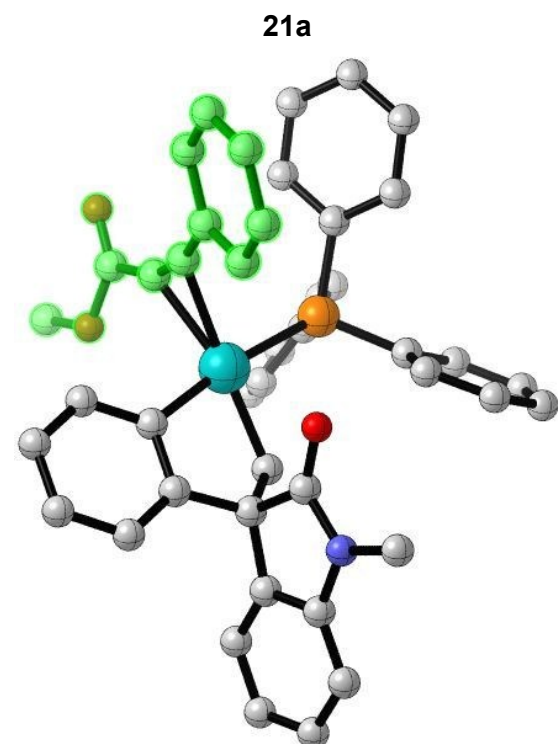
Zero-point correction= 0.353264 (Hartree/Particle)
 Thermal correction to Energy= 0.374619
 Thermal correction to Enthalpy= 0.375564
 Thermal correction to Gibbs Free Energy= 0.303778
 Sum of electronic and zero-point Energies= -1092.781135
 Sum of electronic and thermal Energies= -1092.759779
 Sum of electronic and thermal Enthalpies= -1092.758835
 Sum of electronic and thermal Free Energies= -1092.830620
 E(RM06L) = -1093.36848452

O	-2.53599	1.66645	2.01154
N	-3.40756	0.1358	0.48681

C	1.27451	1.2264	-0.01128
C	2.05869	2.30068	-0.49897
H	3.14458	2.21443	-0.47618
C	1.47125	3.46742	-1.00183
H	2.11019	4.27836	-1.36699
C	0.07625	3.59614	-1.03341
H	-0.39309	4.50135	-1.43187
C	-0.71814	2.55905	-0.52721
H	-1.8066	2.67173	-0.51595
C	-0.1432	1.38971	-0.00316
C	-1.02683	0.28116	0.57619
C	-0.28063	-0.3399	1.78937
H	-0.86937	-1.17214	2.21177
H	-0.2315	0.45236	2.56271
C	-1.49206	-0.73975	-0.46001
C	-0.78475	-1.55885	-1.34117
H	0.30799	-1.52657	-1.36801
C	-1.49672	-2.42595	-2.19645
H	-0.94887	-3.0741	-2.88737
C	-2.89929	-2.4613	-2.17014
H	-3.43913	-3.13843	-2.8401
C	-3.63029	-1.63295	-1.29668
H	-4.72397	-1.6554	-1.28159
C	-2.90575	-0.78123	-0.45534
C	-2.37852	0.82373	1.13016
C	-4.81009	0.35515	0.78971
H	-4.85013	1.12388	1.57583
H	-5.28537	-0.57236	1.15481
H	-5.35683	0.70896	-0.10215
C	3.15942	-0.53455	0.14772
C	1.8712	-0.03309	0.51478
C	1.10217	-0.8165	1.41635
C	1.60246	-2.01116	1.95953
C	2.88045	-2.4602	1.61361
C	3.6551	-1.73017	0.70262
H	3.27615	-3.38855	2.03791
H	4.64403	-2.09859	0.42232
C	5.12369	-0.33497	-1.2293
H	5.48685	0.37608	-1.98522
H	5.86069	-0.4002	-0.40654
H	5.00684	-1.33311	-1.69182
O	3.87188	0.188	-0.78174
H	0.97966	-2.58724	2.6518

Sum of electronic and zero-point Energies= -2446.298604
 Sum of electronic and thermal Energies= -2446.251302
 Sum of electronic and thermal Enthalpies= -2446.250357
 Sum of electronic and thermal Free Energies= -2446.384398
 E(RM06L) = -2448.61650203

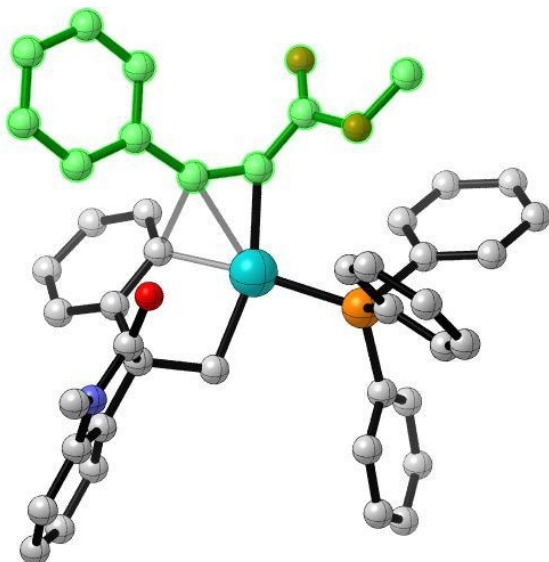
Pd	-0.01179	0.52792	-0.58285
P	1.48426	-1.27454	0.17533
O	-2.22145	0.77097	2.04318
N	-4.2729	-0.25359	1.69354
C	-1.4542	1.86271	-1.17426
C	-1.21638	3.11264	-1.77953
H	-0.19106	3.43578	-1.98797
C	-2.28469	3.96023	-2.12577
H	-2.07972	4.92794	-2.59899
C	-3.60969	3.57186	-1.86822
H	-4.4413	4.23186	-2.13891
C	-3.86741	2.32913	-1.26907
H	-4.89951	2.01129	-1.07955
C	-2.79798	1.47904	-0.93166
C	-2.96521	0.1153	-0.27533
C	-1.69672	-0.7074	-0.63975
H	-1.77648	-1.00883	-1.70037
H	-1.60701	-1.61625	-0.02218
C	-4.27076	-0.60226	-0.58174
C	-4.80265	-1.05694	-1.78892
H	-4.25486	-0.90201	-2.72476
C	-6.05458	-1.70809	-1.78977
H	-6.47924	-2.06869	-2.73201
C	-6.76046	-1.89333	-0.5898
H	-7.73145	-2.39953	-0.60296
C	-6.24184	-1.43524	0.63807
H	-6.79517	-1.57802	1.57134
C	-4.9979	-0.79405	0.61401
C	-3.05463	0.2795	1.27438
C	-4.6999	-0.26284	3.08041
H	-3.90844	0.23268	3.66226
H	-4.83767	-1.29608	3.44669
H	-5.64912	0.28808	3.20483
C	2.10196	-2.32293	-1.22103
C	1.34153	-2.3649	-2.40965
H	0.43565	-1.75401	-2.48736
C	1.75154	-3.1659	-3.48738
H	1.15222	-3.19089	-4.40365
C	2.92901	-3.92487	-3.39388
H	3.25116	-4.54579	-4.23656
C	3.69947	-3.87863	-2.21985
H	4.62379	-4.46148	-2.1457
C	3.29101	-3.08207	-1.13881
H	3.90364	-3.0358	-0.23263
C	0.71575	-2.47485	1.35791
C	1.0133	-3.85352	1.36203
H	1.69746	-4.26841	0.61528
C	0.42932	-4.70024	2.31728
H	0.66283	-5.77028	2.30755
C	-0.44885	-4.17882	3.28123
H	-0.90091	-4.8414	4.02703
C	-0.75384	-2.80814	3.27833
H	-1.44625	-2.39549	4.01947
C	-0.18592	-1.95827	2.31553
H	-0.46031	-0.89699	2.29263
C	3.05131	-0.79224	1.04684
C	3.23103	-1.00451	2.43007
H	2.45464	-1.5121	3.0099
C	4.40422	-0.5729	3.0701
H	4.52853	-0.74964	4.14382
C	5.41206	0.07508	2.34015
H	6.32688	0.40936	2.84083
C	5.23982	0.29419	0.96333
H	6.01728	0.80133	0.38244
C	4.06799	-0.13003	0.31988
H	3.95559	0.05675	-0.7521
C	1.73622	1.76812	-1.23429
C	1.50283	2.17025	-0.06366
C	2.4259	1.68251	-2.50875
C	1.52523	2.86289	1.18792
C	0.44095	2.78817	2.09844
C	2.66411	3.65155	1.50582
C	0.50423	3.50029	3.30299
H	-0.43164	2.17226	1.85187
C	2.70742	4.35731	2.71186
H	3.49712	3.69536	0.79818
C	1.62903	4.28361	3.61262
H	-0.33465	3.44208	4.00387
H	3.58511	4.96607	2.95258
H	1.66841	4.83755	4.55667



Zero-point correction= 0.658532 (Hartree/Particle)
 Thermal correction to Energy= 0.705834
 Thermal correction to Enthalpy= 0.706778
 Thermal correction to Gibbs Free Energy= 0.572738

O	3.61969	1.94606	-2.65245
O	1.60508	1.2758	-3.51533
C	2.2529	1.18865	-4.80689
H	3.04803	0.42601	-4.7892
H	1.45774	0.90512	-5.50886
H	2.69387	2.15834	-5.08755

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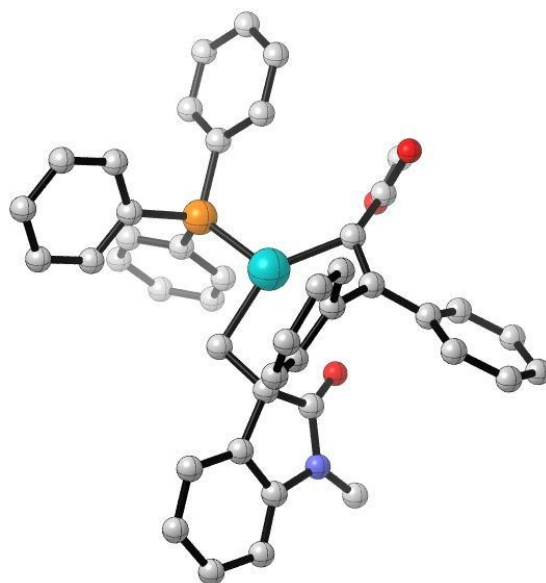


Zero-point correction= 0.657689 (Hartree/Particle)
 Thermal correction to Energy= 0.703974
 Thermal correction to Enthalpy= 0.704918
 Thermal correction to Gibbs Free Energy= 0.573513
 Sum of electronic and zero-point Energies= -2446.265278
 Sum of electronic and thermal Energies= -2446.218993
 Sum of electronic and thermal Enthalpies= -2446.218049
 Sum of electronic and thermal Free Energies= -2446.349455
 E(RM06L) = -2448.57883250
 Imaginary frequency = -222.59 cm⁻¹

Pd	0.12439	0.27428	-0.46663
P	2.07398	-0.89944	-0.01213
O	-2.08104	0.2424	1.95655
N	-3.61848	-1.49213	1.84765
C	-1.62775	1.13334	-1.3631
C	-1.64663	1.97569	-2.49882
H	-0.7822	2.61629	-2.69793
C	-2.77689	2.05553	-3.32822
H	-2.77231	2.72874	-4.19196
C	-3.9116	1.29133	-3.02552
H	-4.81396	1.37119	-3.64115
C	-3.87616	0.37686	-1.95752
H	-4.72523	-0.29497	-1.79407
C	-2.73963	0.25228	-1.13987
C	-2.53312	-0.9508	-0.21589
C	-1.0733	-1.45136	-0.48058
H	-1.03138	-1.90189	-1.48775
H	-0.78554	-2.2211	0.25579
C	-3.53667	-2.08683	-0.37397
C	-3.87751	-2.86351	-1.48387
H	-3.42819	-2.65573	-2.46077
C	-4.80907	-3.91271	-1.33468
H	-5.08377	-4.52178	-2.20166
C	-5.38331	-4.1813	-0.08153
H	-6.10415	-4.99905	0.02231
C	-5.04502	-3.41541	1.05176
H	-5.48894	-3.62881	2.02888
C	-4.12123	-2.37764	0.87955
C	-2.68047	-0.6127	1.30205
C	-3.9724	-1.49063	3.25542
H	-3.3982	-0.67962	3.72779
H	-3.71165	-2.45308	3.73102
H	-5.05303	-1.30712	3.39084
C	3.57637	-0.16387	-0.81443
C	3.38943	0.65278	-1.94895
H	2.36885	0.87679	-2.28076
C	4.49497	1.19352	-2.62552

H	4.33595	1.82796	-3.50361
C	5.7964	0.93321	-2.16716
H	6.65877	1.36096	-2.6894
C	5.98913	0.12947	-1.03094
H	7.00165	-0.06907	-0.66345
C	4.88645	-0.42024	-0.35917
H	5.04839	-1.03585	0.53085
C	2.12921	-2.65574	-0.60188
C	2.66951	-2.96925	-1.86756
H	3.13204	-2.18329	-2.47296
C	2.62637	-4.28489	-2.35376
H	3.05487	-4.51194	-3.33574
C	2.04391	-5.30548	-1.58542
H	2.01344	-6.33194	-1.96546
C	1.50126	-5.00275	-0.32646
H	1.04501	-5.79168	0.28075
C	1.53879	-3.68757	0.16216
H	1.12161	-3.46641	1.14974
C	2.46205	-1.03022	1.79039
C	3.35561	-1.99242	2.31375
H	3.81985	-2.72889	1.64961
C	3.62971	-2.02835	3.6897
H	4.32236	-2.77869	4.08572
C	3.01088	-1.11125	4.55564
H	3.22243	-1.14436	5.62978
C	2.11145	-0.16257	4.04363
H	1.61413	0.5446	4.71541
C	1.8335	-0.122	2.66816
H	1.11995	0.60415	2.26543
C	0.66559	2.30173	-0.25436
C	-0.63969	2.41463	-0.16325
C	1.81794	3.16683	-0.05263
C	-1.6144	3.4122	0.29166
C	-2.87863	3.10724	0.83944
C	-1.22496	4.77243	0.17187
C	-3.72774	4.1352	1.27012
H	-3.17238	2.06304	0.94731
C	-2.0828	5.79116	0.60568
H	-0.25055	5.01111	-0.26682
C	-3.3379	5.4796	1.15489
H	-4.70295	3.88211	1.70001
H	-1.76957	6.83599	0.50461
H	-4.00891	6.27909	1.48673
O	2.00308	4.24649	-0.62151
O	2.72264	2.62245	0.82031
C	3.90869	3.42206	1.02076
H	3.64565	4.44754	1.32629
H	4.47351	2.91121	1.81236
H	4.50266	3.46771	0.09332

22a'

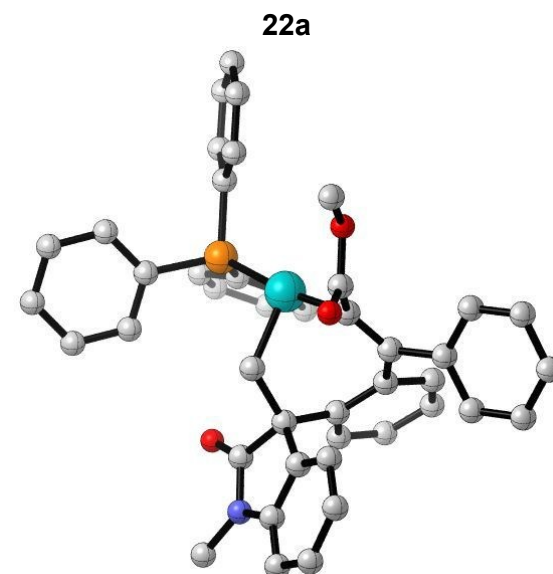


Zero-point correction= 0.659370 (Hartree/Particle)
 Thermal correction to Energy= 0.705841
 Thermal correction to Enthalpy= 0.706785
 Thermal correction to Gibbs Free Energy= 0.574546
 Sum of electronic and zero-point Energies= -2446.285998
 Sum of electronic and thermal Energies= -2446.239527

Sum of electronic and thermal Enthalpies= -2446.238583
 Sum of electronic and thermal Free Energies= -2446.370822
 E(RM06L) = -2448.60308727

C	1.82628	4.51702	1.54894
H	1.31074	5.46986	1.34494
H	2.00837	4.39902	2.62647
H	2.77854	4.5057	0.99379

Pd	0.2749	0.1425	-0.37076
P	2.36493	-0.52832	0.08694
O	-2.03494	0.52789	1.68295
N	-3.81476	-0.95677	1.63531
C	-1.68605	0.71212	-1.71861
C	-1.51841	1.07039	-3.08792
H	-1.06092	2.0438	-3.29033
C	-1.96666	0.27167	-4.14268
H	-1.8336	0.60048	-5.17841
C	-2.61898	-0.93156	-3.84419
H	-3.02118	-1.56349	-4.64324
C	-2.73613	-1.34687	-2.51081
H	-3.20646	-2.31084	-2.30792
C	-2.26072	-0.58382	-1.42255
C	-2.13126	-1.31141	-0.03417
C	-0.62891	-1.69318	0.12461
H	-0.36639	-2.47106	-0.6118
H	-0.40239	-2.03806	1.14751
C	-3.0623	-2.51781	0.11733
C	-3.03438	-3.78998	-0.46086
H	-2.24414	-4.05865	-1.17011
C	-4.02466	-4.73473	-0.11518
H	-4.00809	-5.72912	-0.572
C	-5.02424	-4.40734	0.81397
H	-5.79032	-5.14577	1.07239
C	-5.04715	-3.14514	1.43924
H	-5.80757	-2.89972	2.18646
C	-4.05211	-2.22606	1.08534
C	-2.60714	-0.4302	1.16782
C	-4.52371	-0.3895	2.76926
H	-4.02117	0.55561	3.02153
H	-4.48801	-1.06837	3.64096
H	-5.57793	-0.19132	2.51078
C	3.69233	0.72431	-0.24938
C	3.42625	1.76938	-1.15671
H	2.42996	1.84662	-1.60579
C	4.418	2.71969	-1.4517
H	4.1919	3.53311	-2.14809
C	5.67854	2.63504	-0.83999
H	6.44908	3.38066	-1.06348
C	5.9473	1.5979	0.06985
H	6.9265	1.53263	0.5562
C	4.96125	0.64507	0.36507
H	5.1761	-0.1512	1.08435
C	2.929	-2.01225	-0.86259
C	3.73978	-1.8711	-2.00883
H	4.10409	-0.881	-2.29997
C	4.08544	-2.9947	-2.77601
H	4.71678	-2.86994	-3.66211
C	3.63092	-4.27075	-2.40813
H	3.90483	-5.14625	-3.00604
C	2.82305	-4.41963	-1.26831
H	2.46679	-5.41209	-0.97226
C	2.46805	-3.29934	-0.50266
H	1.83946	-3.42544	0.38437
C	2.58446	-0.99521	1.86115
C	3.57686	-1.90016	2.2986
H	4.22297	-2.4006	1.56982
C	3.72374	-2.17949	3.66678
H	4.49367	-2.88521	3.99652
C	2.88347	-1.56127	4.60711
H	2.99854	-1.78321	5.67337
C	1.88882	-0.66791	4.17657
H	1.22286	-0.19265	4.90426
C	1.73363	-0.38795	2.81014
H	0.94463	0.29029	2.46479
C	-0.05654	2.17151	-0.56441
C	-1.37983	1.90815	-0.79047
C	0.63905	3.38708	-0.15974
C	-2.54167	2.72675	-0.34579
C	-3.78105	2.66397	-1.02507
C	-2.42717	3.60813	0.75671
C	-4.8586	3.4728	-0.63382
H	-3.89642	1.98683	-1.87715
C	-3.50259	4.41735	1.14089
H	-1.49347	3.62827	1.3253
C	-4.72477	4.35718	0.44773
H	-5.8055	3.41348	-1.18187
H	-3.39156	5.09077	1.99806
H	-5.5657	4.98888	0.75345
O	0.98269	4.27876	-0.93989
O	1.00376	3.39039	1.17192



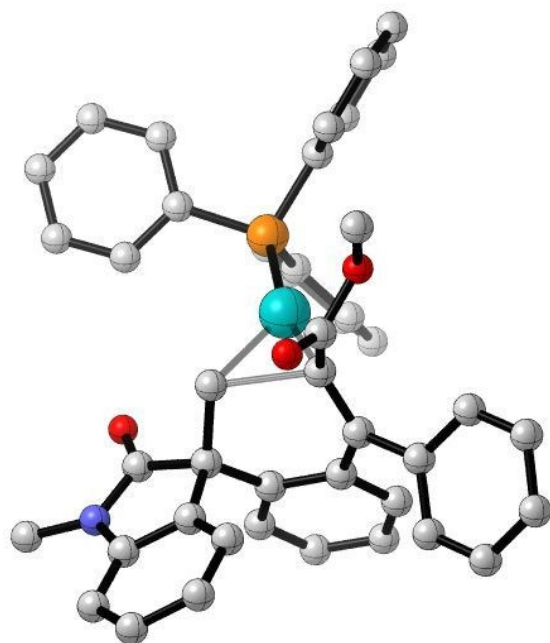
Zero-point correction= 0.660844 (Hartree/Particle)
 Thermal correction to Energy= 0.707207
 Thermal correction to Enthalpy= 0.708151
 Thermal correction to Gibbs Free Energy= 0.575398
 Sum of electronic and zero-point Energies= -2446.323171
 Sum of electronic and thermal Energies= -2446.276808
 Sum of electronic and thermal Enthalpies= -2446.275863
 Sum of electronic and thermal Free Energies= -2446.408616
 E(RM06L) = -2448.63474108

Pd	0.42751	0.8263	-0.26114
P	2.73763	0.20581	-0.00613
O	0.2696	-3.46751	-0.0364
N	-1.89386	-3.961	-0.70912
C	-2.13512	0.07884	1.5569
C	-2.37841	0.34754	2.92496
H	-2.78121	1.33013	3.19087
C	-2.10307	-0.58565	3.9312
H	-2.29545	-0.33634	4.98013
C	-1.5751	-1.83104	3.57198
H	-1.34542	-2.58368	4.33369
C	-1.34681	-2.12577	2.21894
H	-0.92142	-3.10044	1.9727
C	-1.6213	-1.20222	1.18682
C	-1.44391	-1.64228	-0.30415
C	-0.47526	-0.78975	-1.17219
H	-0.98281	-0.401	-2.06647
H	0.41593	-1.3716	-1.454
C	-2.81714	-1.85781	-0.96368
C	-3.78033	-0.96386	-1.44106
H	-3.60671	0.11486	-1.41924
C	-4.96832	-1.47171	-2.0108
H	-5.7216	-0.77131	-2.38444
C	-5.18604	-2.85359	-2.11258
H	-6.11533	-3.2307	-2.55233
C	-4.20767	-3.76927	-1.67874
H	-4.35497	-4.84814	-1.78703
H	-3.03545	-3.24617	-1.12382
C	-0.87758	-3.10421	-0.3169
C	-1.70637	-5.39418	-0.85089
H	-0.68156	-5.61863	-0.52014
H	-1.83228	-5.70548	-1.90337
H	-2.42868	-5.94793	-0.22617
C	3.74737	1.75937	-0.02585
C	3.30099	2.81268	-0.85602
H	2.38537	2.68084	-1.44647
C	4.01379	4.02032	-0.91772
H	3.65828	4.82874	-1.56506
C	5.17059	4.19426	-0.14102
H	5.72213	5.13943	-0.18177
C	5.61287	3.15719	0.69704
H	6.50937	3.29249	1.31139

C	4.9075	1.9451	0.75552
H	5.25197	1.14533	1.4188
C	3.5372	-0.88637	-1.26517
C	4.53652	-0.42193	-2.14499
H	4.89962	0.60744	-2.06485
C	5.07044	-1.27844	-3.12187
H	5.84812	-0.90849	-3.79867
C	4.61386	-2.60147	-3.22782
H	5.03194	-3.26719	-3.99034
C	3.61718	-3.06721	-2.35371
H	3.25357	-4.09726	-2.4311
C	3.07381	-2.21831	-1.37762
H	2.28966	-2.59494	-0.7093
C	3.15151	-0.60657	1.598
C	4.34319	-1.33721	1.79903
H	5.04751	-1.46842	0.97076
C	4.61431	-1.91141	3.0505
H	5.539	-2.47916	3.19929
C	3.69834	-1.7664	4.10637
H	3.91041	-2.22073	5.0801
C	2.50528	-1.05306	3.90813
H	1.77764	-0.95559	4.72
C	2.22955	-0.47854	2.65777
H	1.28613	0.05371	2.48675
C	-1.4464	1.55259	-0.31603
C	-2.39726	1.20122	0.59983
C	-1.67661	2.4368	-1.4793
C	-3.67718	1.95607	0.76577
C	-3.72767	3.3609	0.60425
C	-4.8776	1.27779	1.08929
C	-4.93747	4.05742	0.73324
H	-2.80196	3.90693	0.39639
C	-6.08663	1.97543	1.21462
H	-4.856	0.19219	1.22534
C	-6.12331	3.36854	1.03633
H	-4.95112	5.1459	0.6104
H	-7.00497	1.4278	1.45281
H	-7.06708	3.91403	1.1418
O	-2.42022	2.184	-2.42724
O	-0.87837	3.56334	-1.45068
C	-1.00729	4.40458	-2.61973
H	-2.05173	4.72799	-2.75808
H	-0.35708	5.2705	-2.43184
H	-0.68436	3.86698	-3.52659

Sum of electronic and thermal Enthalpies= -2446.268212
Sum of electronic and thermal Free Energies= -2446.400715
E(RM06L) = -2448.62177257
Imaginary frequency = -259.84 cm⁻¹

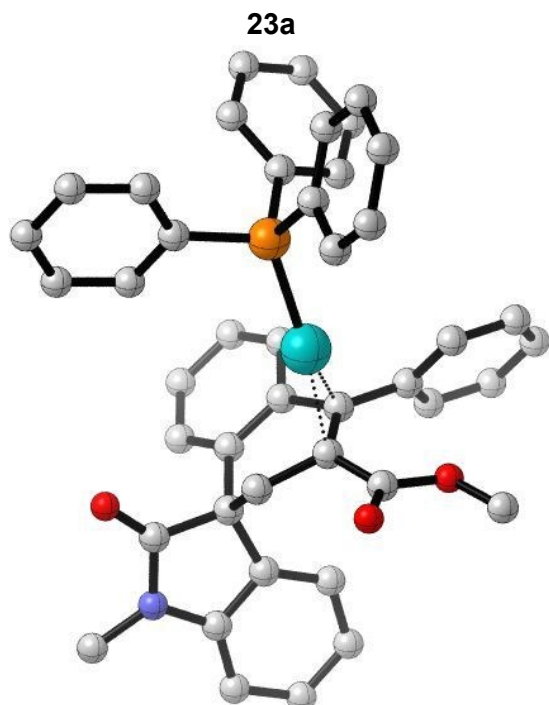
TS 22a-23a



Zero-point correction= 0.659890 (Hartree/Particle)
Thermal correction to Energy= 0.705886
Thermal correction to Enthalpy= 0.706830
Thermal correction to Gibbs Free Energy= 0.574328
Sum of electronic and zero-point Energies= -2446.315153
Sum of electronic and thermal Energies= -2446.269156

Pd	0.49939	0.49863	-0.38915
P	2.79527	0.04714	-0.01148
O	-0.27682	-3.45908	-0.12119
N	-2.49675	-3.87495	-0.65649
C	-2.05275	0.27683	1.56641
C	-2.11022	0.66059	2.92603
H	-2.23022	1.72255	3.1627
C	-2.00364	-0.27886	3.95968
H	-2.04032	0.04978	5.0037
C	-1.84832	-1.6346	3.64294
H	-1.76357	-2.38631	4.43448
C	-1.80509	-2.03361	2.29761
H	-1.68083	-3.09559	2.06928
C	-1.90166	-1.10246	1.24712
C	-1.94938	-1.58479	-0.2233
C	-1.10599	-0.74865	-1.21729
H	-1.70216	-0.4261	-2.08024
H	-0.23103	-1.32152	-1.58355
C	-3.4039	-1.7521	-0.68212
C	-4.41172	-0.81864	-0.93125
H	-4.21639	0.25133	-0.82555
C	-5.67775	-1.27161	-1.35983
H	-6.4695	-0.54325	-1.56046
C	-5.92576	-2.64123	-1.53893
H	-6.91394	-2.97819	-1.86901
C	-4.91368	-3.59504	-1.31453
H	-5.09819	-4.66201	-1.47202
C	-3.66488	-3.1247	-0.89473
C	-1.42773	-3.05772	-0.30922
C	-2.36096	-5.30615	-0.86225
H	-1.31517	-5.56498	-0.63944
H	-2.59455	-5.57807	-1.90709
H	-3.03324	-5.86622	-0.18888
C	3.85131	1.52565	-0.38218
C	3.40907	2.40221	-1.39753
H	2.45654	2.19649	-1.90126
C	4.16783	3.53094	-1.74207
H	3.81544	4.20307	-2.53171
C	5.36818	3.80595	-1.06632
H	5.95574	4.69224	-1.32849
C	5.80711	2.94796	-0.04488
H	6.73714	3.16382	0.49194
C	5.0547	1.81226	0.29656
H	5.39816	1.15234	1.0999
C	3.55153	-1.30984	-1.0189
C	4.7965	-1.18418	-1.66982
H	5.36098	-0.24926	-1.59463
C	5.31179	-2.25462	-2.42014
H	6.27693	-2.146	-2.92681
C	4.59351	-3.45632	-2.52081
H	4.99669	-4.28882	-3.10746
C	3.35294	-3.58503	-1.87289
H	2.78378	-4.51735	-1.95029
C	2.82582	-2.51744	-1.13103
H	1.84945	-2.62406	-0.64233
C	3.25601	-0.40009	1.72446
C	4.37073	-1.20609	2.04008
H	4.9882	-1.62053	1.23606
C	4.67985	-1.49122	3.37988
H	5.54416	-2.12154	3.61533
C	3.8806	-0.97658	4.4137
H	4.12112	-1.20434	5.45765
C	2.76451	-0.18105	4.10586
H	2.12885	0.20984	4.90711
C	2.44884	0.10024	2.76814
H	1.56302	0.69745	2.52083
C	-1.35005	1.26497	-0.59444
C	-2.15541	1.33283	0.51549
C	-1.56724	2.06022	-1.84107
C	-3.13402	2.44056	0.72993
C	-2.82096	3.77773	0.38721
C	-4.41133	2.17411	1.28333
C	-3.76124	4.80333	0.56279
H	-1.82461	4.00861	-0.00113
C	-5.35026	3.20061	1.45228
H	-4.66724	1.1489	1.56865
C	-5.03081	4.52045	1.09169
H	-3.49439	5.83212	0.29751
H	-6.33622	2.96813	1.86898
H	-5.76243	5.32319	1.23142

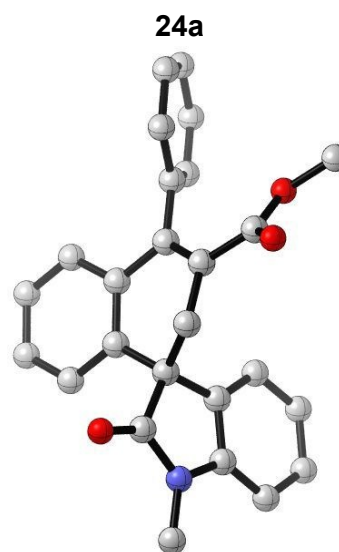
O	-2.42663	1.81167	-2.6828
O	-0.64643	3.06606	-1.99699
C	-0.80191	3.81986	-3.22405
H	-1.79711	4.29091	-3.26888
H	-0.01261	4.58348	-3.19882
H	-0.68204	3.1636	-4.10101



Zero-point correction= 0.662287 (Hartree/Particle)
 Thermal correction to Energy= 0.708469
 Thermal correction to Enthalpy= 0.709413
 Thermal correction to Gibbs Free Energy= 0.576343
 Sum of electronic and zero-point Energies= -2446.378808
 Sum of electronic and thermal Energies= -2446.332627
 Sum of electronic and thermal Enthalpies= -2446.331683
 Sum of electronic and thermal Free Energies= -2446.464753
 E(RM06L) = -2448.69513931

Pd	0.63945	0.21577	-0.66652
P	2.79573	-0.44461	-0.18636
O	-2.7146	-3.59303	-0.21853
N	-4.84435	-2.68356	-0.48045
C	-1.49603	0.16978	1.47976
C	-0.89442	0.37563	2.74569
H	-0.16061	1.17924	2.85331
C	-1.2075	-0.43575	3.84063
H	-0.71835	-0.26155	4.80455
C	-2.14641	-1.47022	3.69632
H	-2.40433	-2.10942	4.547
C	-2.75028	-1.68834	2.44968
H	-3.47172	-2.50398	2.33717
C	-2.43071	-0.89322	1.33534
C	-3.09243	-1.12855	-0.02462
C	-2.07143	-0.77993	-1.14335
H	-2.53476	-0.85337	-2.13941
H	-1.28442	-1.55833	-1.09827
C	-4.4415	-0.42994	-0.17508
C	-4.80742	0.91517	-0.09679
H	-4.0582	1.68674	0.10596
C	-6.15781	1.27429	-0.2957
H	-6.45105	2.32723	-0.23944
C	-7.1249	0.29318	-0.56437
H	-8.16939	0.58552	-0.71461
C	-6.77457	-1.0689	-0.64545
H	-7.52843	-1.83359	-0.85547
C	-5.43023	-1.40444	-0.4482
C	-3.47321	-2.62451	-0.23074
C	-5.53809	-3.92464	-0.77409
H	-4.78558	-4.72671	-0.73879
H	-5.9968	-3.89229	-1.7782
H	-6.32681	-4.12427	-0.02718

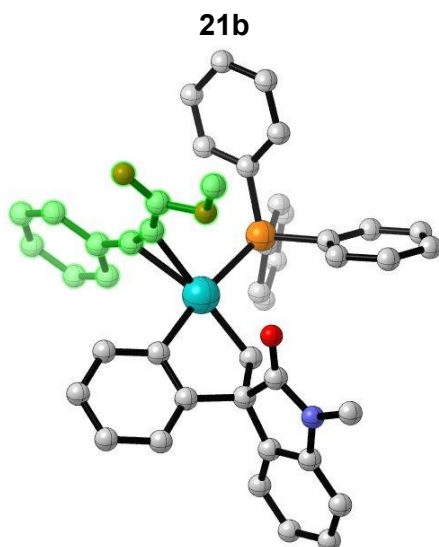
C	4.09164	0.15861	-1.36721
C	3.71145	0.33037	-2.71653
H	2.67416	0.12808	-3.01111
C	4.64382	0.76682	-3.66898
H	4.33572	0.89483	-4.71202
C	5.96418	1.05223	-3.28171
H	6.69005	1.40319	-4.02282
C	6.3475	0.89683	-1.94005
H	7.37326	1.12626	-1.6318
C	5.41801	0.45107	-0.98554
H	5.72157	0.34054	0.06078
C	3.00748	-2.28647	-0.21397
C	4.20552	-2.92129	-0.60566
H	5.06267	-2.3195	-0.92561
C	4.29629	-4.32293	-0.60338
H	5.22837	-4.80648	-0.91521
C	3.19515	-5.10147	-0.21139
C	3.26688	-6.19431	-0.21724
C	1.99758	-4.4766	0.1746
H	1.12953	-5.07629	0.46682
C	1.90124	-3.07709	0.16801
H	0.96133	-2.58617	0.44702
C	3.45427	0.05589	1.47263
C	4.31519	-0.7605	2.23622
H	4.60521	-1.74783	1.86212
C	4.79133	-0.31686	3.48138
H	5.45423	-0.96157	4.06848
C	4.41694	0.94351	3.97346
H	4.78778	1.28558	4.94551
C	3.55642	1.75962	3.21998
H	3.25216	2.73983	3.60213
C	3.07054	1.31588	1.98102
H	2.37633	1.93921	1.40596
C	-1.49114	0.6286	-0.9764
C	-1.18261	1.08969	0.34031
C	-1.60342	1.45889	-2.21766
C	-0.95707	2.53297	0.71783
C	0.14539	3.28695	0.25927
C	-1.88189	3.16432	1.58147
C	0.31181	4.62675	0.63783
H	0.87264	2.79081	-0.39744
C	-1.72158	4.50798	1.95361
H	-2.73346	2.5934	1.96619
C	-0.62281	5.24512	1.48568
H	1.17887	5.18784	0.27262
H	-2.45604	4.97567	2.61819
H	-0.49075	6.29022	1.78544
O	-1.67849	0.97085	-3.3465
O	-1.66396	2.80431	-1.99703
C	-1.7333	3.60001	-3.20015
H	-2.62464	3.33707	-3.7923
H	-1.78669	4.64169	-2.85516
H	-0.8383	3.44304	-3.82434



Zero-point correction= 0.394969 (Hartree/Particle)
 Thermal correction to Energy= 0.420914
 Thermal correction to Enthalpy= 0.421858
 Thermal correction to Gibbs Free Energy= 0.337629

Sum of electronic and zero-point Energies= -1283.494020
Sum of electronic and thermal Energies= -1283.468075
Sum of electronic and thermal Enthalpies= -1283.467131
Sum of electronic and thermal Free Energies= -1283.551360
E(RM06L) = -1284.17133851

O	3.02481	0.89823	-2.45947
N	3.9065	-0.18388	-0.59319
C	-0.54727	1.59549	-0.16316
C	-1.15756	2.84215	0.11548
H	-2.24799	2.89587	0.1712
C	-0.39383	3.99917	0.30735
H	-0.89173	4.95167	0.5149
C	1.00462	3.93184	0.22753
H	1.61308	4.82942	0.37755
C	1.62606	2.70687	-0.05837
H	2.71678	2.66181	-0.13764
C	0.87257	1.54202	-0.26778
C	1.54997	0.20206	-0.56328
C	0.61922	-0.64979	-1.46537
H	1.03168	-1.66127	-1.6017
H	0.61135	-0.17272	-2.46599
C	2.02203	-0.51347	0.70074
C	1.33174	-0.95581	1.82984
H	0.25111	-0.80601	1.91012
C	2.0422	-1.60623	2.86045
H	1.50721	-1.96018	3.74697
C	3.42819	-1.80122	2.75666
H	3.96821	-2.30629	3.56405
C	4.14238	-1.35555	1.62764
H	5.22302	-1.50606	1.5485
C	3.41918	-0.71458	0.6156
C	2.8837	0.38538	-1.35182
C	5.2841	-0.24038	-1.04868
H	5.31388	0.2486	-2.03373
H	5.62545	-1.28609	-1.14471
H	5.95405	0.29196	-0.3508
C	-0.7901	-0.73512	-0.91671
C	-1.3659	0.36853	-0.33695
C	-1.4456	-2.05579	-1.13669
C	-2.80232	0.42821	0.07662
C	-3.82755	0.30743	-0.88581
C	-3.16061	0.65332	1.42338
C	-5.17541	0.39091	-0.50886
H	-3.55725	0.1542	-1.93577
C	-4.50902	0.72496	1.80151
H	-2.37368	0.76411	2.17667
C	-5.52094	0.59456	0.83667
H	-5.95788	0.2999	-1.26956
H	-4.76961	0.88653	2.85277
H	-6.57357	0.65835	1.13116
O	-1.10245	-2.83386	-2.02606
O	-2.41663	-2.35309	-0.22426
C	-3.05763	-3.63075	-0.43876
H	-2.31772	-4.44672	-0.41062
H	-3.78358	-3.73208	0.37907
H	-3.5676	-3.6533	-1.41539

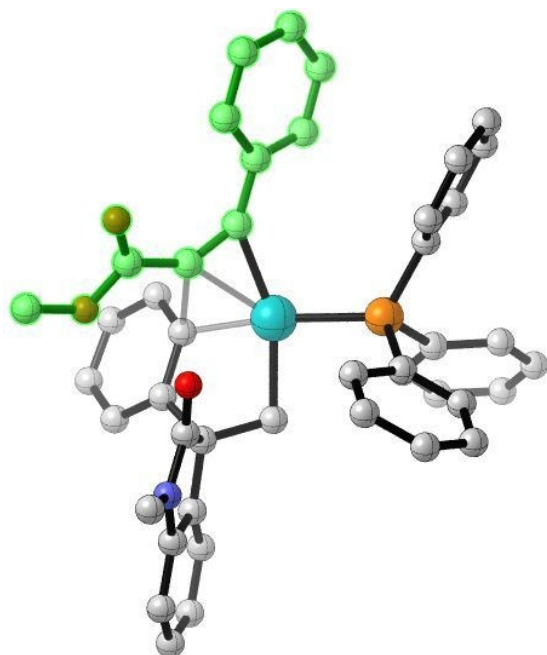


Zero-point correction= 0.657845 (Hartree/Particle)
Thermal correction to Energy= 0.705463
Thermal correction to Enthalpy= 0.706408
Thermal correction to Gibbs Free Energy= 0.569803
Sum of electronic and zero-point Energies= -2446.295245
Sum of electronic and thermal Energies= -2446.247627
Sum of electronic and thermal Enthalpies= -2446.246683
Sum of electronic and thermal Free Energies= -2446.383287
E(RM06L) = -2448.61365514

Pd	-0.03353	-0.70097	0.09682
P	-1.31174	1.35329	-0.36304
O	2.55296	0.47219	2.08461
N	4.5548	0.81784	0.95837
C	1.25982	-2.27435	0.38084
C	0.89513	-3.58254	0.75807
H	-0.15761	-3.84269	0.90993
C	1.87134	-4.5776	0.95027
H	1.56484	-5.58963	1.24025
C	3.23183	-4.27934	0.77288
H	3.99167	-5.05472	0.92071
C	3.61586	-2.98247	0.39931
H	4.6749	-2.74229	0.24793
C	2.6383	-1.99014	0.20043
C	2.95707	-0.55284	-0.18132
C	1.68236	0.01291	-0.86961
H	1.62864	-0.42069	-1.88557
H	1.71916	1.11182	-0.9588
C	4.22597	-0.3528	-0.99637
C	4.58909	-0.82954	-2.2566
H	3.90741	-1.47883	-2.81699
C	5.84484	-0.475	-2.79448
H	6.13741	-0.84499	-3.78229
C	6.72251	0.34608	-2.06793
H	7.69452	0.61462	-2.49505
C	6.37611	0.83146	-0.79082
H	7.06346	1.4682	-0.22535
C	5.12546	0.46718	-0.27805
C	3.27231	0.28071	1.1029
C	5.18317	1.6464	1.96955
H	4.47373	1.7182	2.80763
H	5.39908	2.65712	1.57869
C	6.12645	1.19289	2.32303
C	-1.84191	1.57325	-2.12788
C	-1.03357	1.01541	-3.14205
H	-0.14009	0.44791	-2.86325
C	-1.37023	1.18159	-4.49435
H	-0.73253	0.7442	-5.26985
C	-2.52413	1.89815	-4.85079
H	-2.79072	2.02186	-5.90572
C	-3.33855	2.45098	-3.84924
H	-4.24184	3.00796	-4.12034
C	-3.00086	2.2922	-2.49559
H	-3.64551	2.71857	-1.72072
C	-0.38038	2.90847	0.01694
C	-0.61347	4.12396	-0.66105
H	-1.34547	4.16557	-1.47388
C	0.09673	5.27969	-0.30197
H	-0.08666	6.21743	-0.83741
C	1.04081	5.23344	0.73775
H	1.59474	6.13691	1.01482
C	1.27813	4.02548	1.41264
H	2.02055	3.97729	2.21594
C	0.57831	2.86198	1.05239
H	0.79445	1.91413	1.55899
C	-2.89855	1.58391	0.5682
C	-3.03277	2.54809	1.58864
H	-2.20056	3.22198	1.81195
C	-4.23029	2.65281	2.31538
H	-4.31997	3.41009	3.10163
C	-5.30746	1.7991	2.03324
H	-6.24046	1.88323	2.60018
C	-5.18114	0.83265	1.02117
H	-6.01464	0.15913	0.79574
C	-3.98463	0.71946	0.29874
H	-3.89925	-0.04001	-0.48548
C	-1.51651	-1.41371	1.61283
C	-1.88262	-1.96103	0.53955
C	-1.52991	-1.11702	3.03653
C	-2.60085	-2.75626	-0.41205
C	-2.2812	-2.73622	-1.79167
C	-3.6622	-3.5814	0.04877
C	-3.00952	-3.52507	-2.69033
H	-1.45831	-2.09774	-2.12758
C	-4.3814	-4.3644	-0.86015
H	-3.90051	-3.59398	1.11661

C	-4.05854	-4.33885	-2.22931
H	-2.75703	-3.5063	-3.75532
H	-5.19669	-5.00024	-0.4999
H	-4.62448	-4.95525	-2.93548
O	-2.22052	-1.73583	3.84256
O	-0.69911	-0.09131	3.35225
C	-0.64308	0.21565	4.76485
H	-0.34182	-0.67412	5.33993
H	0.10907	1.00957	4.85571
H	-1.62588	0.55995	5.12593

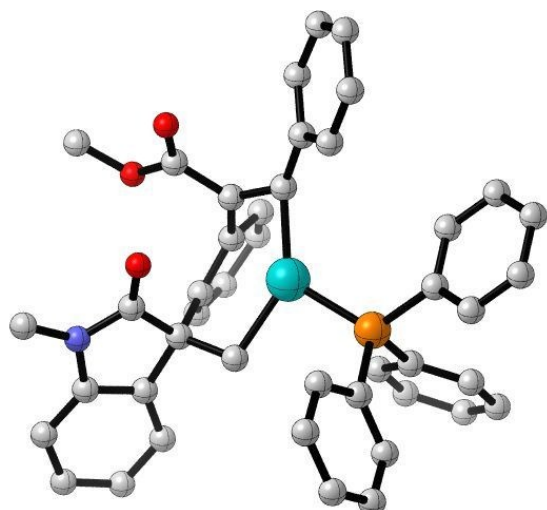
TS 21b-22b



Zero-point correction= 0.658182 (Hartree/Particle)
 Thermal correction to Energy= 0.704107
 Thermal correction to Enthalpy= 0.705051
 Thermal correction to Gibbs Free Energy= 0.575636
 Sum of electronic and zero-point Energies= -2446.262329
 Sum of electronic and thermal Energies= -2446.216405
 Sum of electronic and thermal Enthalpies= -2446.215461
 Sum of electronic and thermal Free Energies= -2446.344875
 E(RM06L) = -2448.57672852
 Imaginary frequency = -232.15cm⁻¹

Pd	-0.1311	0.33202	0.58456
P	-1.66047	-1.36665	0.02318
O	1.99997	0.91957	-1.90185
N	4.00821	-0.23067	-1.80356
C	1.36173	1.56428	1.43231
C	1.15329	2.42688	2.53169
H	0.15311	2.83491	2.70422
C	2.22013	2.80393	3.36393
H	2.04098	3.4784	4.20821
C	3.51239	2.3358	3.08871
H	4.35752	2.64984	3.71105
C	3.72479	1.42954	2.03384
H	4.72165	1.00427	1.87723
C	2.66326	1.00881	1.21725
C	2.77189	-0.16628	0.2475
C	1.49437	-1.03907	0.49556
H	1.62348	-1.53372	1.47448
H	1.39912	-1.82251	-0.27553
C	4.05228	-0.98311	0.3691
C	4.58407	-1.69847	1.44423
H	4.07174	-1.70036	2.41235
C	5.78804	-2.41414	1.27246
H	6.21069	-2.97529	2.11188
C	6.44568	-2.41199	0.03161
H	7.3788	-2.97193	-0.09037
C	5.92271	-1.7002	-1.06622
H	6.43397	-1.70204	-2.03371
C	4.72829	-0.99607	-0.87134

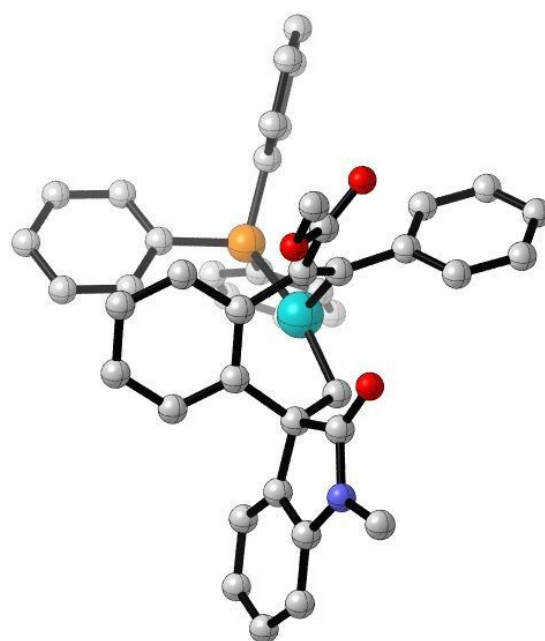
C	2.82772	0.27648	-1.25377
C	4.36511	-0.05343	-3.19877
H	3.57854	0.56752	-3.65294
H	4.41573	-1.02567	-3.72118
H	5.341	0.45452	-3.29599
C	-1.86144	-2.66484	1.32997
C	-1.01668	-2.62318	2.45865
H	-0.28239	-1.81423	2.53807
C	-1.12618	-3.59384	3.46775
H	-0.46494	-3.54618	4.33926
C	-2.08358	-4.61451	3.36315
H	-2.16921	-5.37122	4.15016
C	-2.94327	-4.65444	2.25249
H	-3.70355	-5.43876	2.17331
C	-2.83922	-3.68348	1.24514
H	-3.54015	-3.70085	0.40458
C	-1.07671	-2.24352	-1.50722
C	-1.33718	-3.60175	-1.78255
H	-1.8656	-4.22197	-1.05297
C	-0.90132	-4.17628	-2.98696
H	-1.10207	-5.23467	-3.18476
C	-0.21019	-3.40081	-3.93195
H	0.12557	-3.85196	-4.87182
C	0.06155	-2.05069	-3.65976
H	0.61577	-1.44094	-4.3807
C	-0.35762	-1.47479	-2.44962
H	-0.09403	-0.43614	-2.21621
C	-3.42403	-0.97114	-0.41099
C	-3.77234	-0.62429	-1.7334
H	-3.011	-0.63264	-2.51949
C	-5.09436	-0.28038	-2.0535
H	-5.34811	-0.01644	-3.08552
C	-6.08738	-0.28181	-1.06146
H	-7.11984	-0.02028	-1.31548
C	-5.74819	-0.61819	0.25848
H	-6.51506	-0.6215	1.04056
C	-4.42502	-0.95216	0.58497
H	-4.17422	-1.21253	1.61832
C	0.14339	2.4667	0.09823
C	-1.13059	2.2039	0.30651
C	0.92356	3.45345	-0.66873
C	-2.44034	2.81112	0.15674
C	-3.51495	2.38146	0.97403
C	-2.66584	3.86698	-0.76774
C	-4.77086	2.99419	0.88575
H	-3.33566	1.56892	1.68429
C	-3.92937	4.46307	-0.8604
H	-1.83047	4.20065	-1.39044
C	-4.98362	4.03472	-0.03408
H	-5.58796	2.65569	1.53142
H	-4.09225	5.27431	-1.57861
H	-5.9679	4.51011	-0.10761
O	0.38725	4.21561	-1.47697
O	2.25176	3.49007	-0.39398
C	2.98923	4.4393	-1.19235
H	2.59598	5.45915	-1.05245
H	4.02698	4.37064	-0.83842
H	2.92293	4.17592	-2.26047

22b'

Zero-point correction= 0.659089 (Hartree/Particle)
 Thermal correction to Energy= 0.705425
 Thermal correction to Enthalpy= 0.706369
 Thermal correction to Gibbs Free Energy= 0.574559
 Sum of electronic and zero-point Energies= -2446.287454
 Sum of electronic and thermal Energies= -2446.241118
 Sum of electronic and thermal Enthalpies= -2446.240174
 Sum of electronic and thermal Free Energies= -2446.371984
 E(RM06L) = -2448.60518984

Pd	0.24012	0.26545	-0.03382
P	1.96303	-1.1763	0.07862
O	-2.43091	1.36841	1.7534
N	-4.30227	0.01327	1.66088
C	-1.47392	1.27822	-1.54873
C	-1.17941	1.61714	-2.89651
H	-0.45176	2.41711	-3.06473
C	-1.82062	1.01878	-3.98594
H	-1.56965	1.32393	-5.00725
C	-2.81019	0.0604	-3.74118
H	-3.36504	-0.39664	-4.56755
C	-3.08151	-0.33601	-2.42195
H	-3.83093	-1.11301	-2.25782
C	-2.41438	0.20523	-1.3042
C	-2.57533	-0.51234	0.07726
C	-1.21401	-1.18308	0.47669
H	-1.10353	-2.11878	-0.09721
H	-1.18992	-1.4282	1.55207
C	-3.68438	-1.56923	0.11043
C	-3.80658	-2.80146	-0.54
H	-3.03799	-3.13313	-1.24635
C	-4.92448	-3.6218	-0.27929
H	-5.02312	-4.58246	-0.79438
C	-5.90485	-3.21566	0.63988
H	-6.76907	-3.85907	0.83504
C	-5.7859	-1.99412	1.33033
H	-6.53715	-1.68646	2.06388
C	-4.66783	-1.19706	1.05515
C	-3.04197	0.43774	1.23011
C	-4.99288	0.63458	2.77666
H	-4.38008	1.49158	3.09344
H	-5.09775	-0.07202	3.61982
H	-5.9964	0.98314	2.47599
C	2.10343	-2.24036	-1.43246
C	0.99979	-2.34342	-2.30477
H	0.08945	-1.77576	-2.08292
C	1.07809	-3.14373	-3.45548
H	0.21699	-3.20943	-4.12852
C	2.25878	-3.84455	-3.74858
H	2.3209	-4.46478	-4.64903
C	3.36693	-3.73645	-2.89201
H	4.29535	-4.26926	-3.12362
C	3.29423	-2.93492	-1.74214
H	4.1705	-2.83482	-1.09296
C	1.85765	-2.34727	1.50715
C	2.10881	-3.73027	1.40258
H	2.37827	-4.16593	0.43548
C	2.00525	-4.55505	2.53592
H	2.19589	-5.62948	2.44221
C	1.65596	-4.00743	3.77973

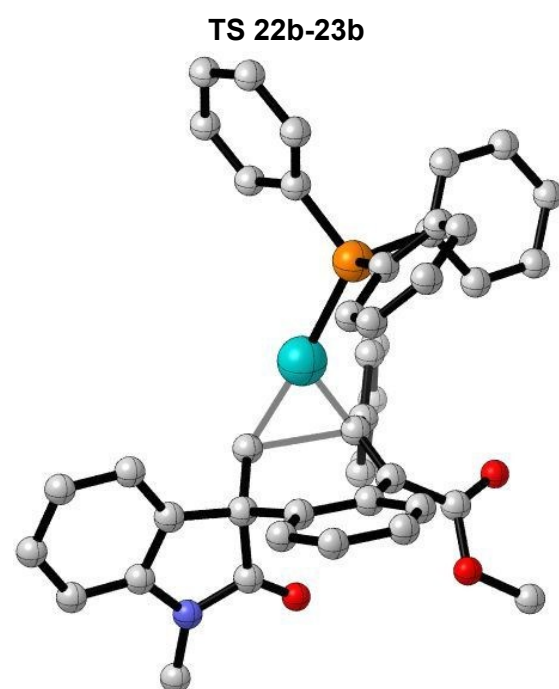
H	1.57456	-4.65297	4.66054
C	1.39865	-2.62981	3.88967
H	1.11368	-2.19799	4.85475
C	1.48898	-1.80552	2.75934
H	1.25457	-0.73719	2.83389
C	3.66766	-0.46527	0.2258
C	4.65595	-1.0252	1.06372
H	4.41938	-1.89522	1.68449
C	5.94386	-0.46589	1.10472
H	6.70423	-0.90507	1.75948
C	6.25508	0.6499	0.3114
H	7.25948	1.08497	0.34698
C	5.27124	1.21632	-0.5165
H	5.50247	2.09846	-1.12211
C	3.98035	0.66941	-0.55324
H	3.19751	1.13029	-1.16594
C	-0.85371	2.26019	-0.54562
C	0.5135	2.26918	-0.3081
C	-1.75933	3.31734	0.02984
C	1.37752	3.34939	0.11799
C	1.33783	4.61734	-0.52556
C	2.3554	3.14244	1.12677
C	2.23262	5.63043	-0.16883
H	0.59159	4.79018	-1.30719
C	3.22391	4.17158	1.50626
H	2.40321	2.16192	1.61049
C	3.17336	5.41721	0.85543
H	2.18851	6.59861	-0.67951
H	3.95544	3.9982	2.30278
H	3.86563	6.21638	1.14117
O	-1.43045	4.20639	0.80361
O	-3.02935	3.21111	-0.48391
C	-3.9517	4.18198	0.04972
H	-3.6019	5.20842	-0.14858
H	-4.90717	3.99222	-0.4596
H	-4.05656	4.05267	1.13947

22b

Zero-point correction= 0.659650 (Hartree/Particle)
 Thermal correction to Energy= 0.706209
 Thermal correction to Enthalpy= 0.707153
 Thermal correction to Gibbs Free Energy= 0.573626
 Sum of electronic and zero-point Energies= -2446.317292
 Sum of electronic and thermal Energies= -2446.270732
 Sum of electronic and thermal Enthalpies= -2446.269788
 Sum of electronic and thermal Free Energies= -2446.403315
 E(RM06L) = -2448.63109945

Pd	-0.25379	-0.19505	-0.74863
P	-2.53442	-0.5744	-0.06537
O	3.97755	1.52608	-0.20233
N	5.14334	-0.38976	-0.78853
C	1.59796	0.33062	1.71982
C	1.2257	0.2257	3.07953

H	0.68674	1.06275	3.53474
C	1.52319	-0.90341	3.85068
H	1.21001	-0.95003	4.89899
C	2.2286	-1.96193	3.26401
H	2.49199	-2.85095	3.84744
C	2.6134	-1.87586	1.91739
H	3.17681	-2.70187	1.47624
C	2.30061	-0.75588	1.11669
C	2.80165	-0.70591	-0.35335
C	1.71613	-0.32172	-1.41191
H	1.55237	-1.17058	-2.10827
H	2.01814	0.55484	-2.00449
C	3.49283	-1.99289	-0.80089
C	2.9825	-3.27225	-1.03466
H	1.92296	-3.48476	-0.85339
C	3.84372	-4.28984	-1.49728
H	3.44929	-5.29478	-1.67741
C	5.20242	-4.01896	-1.72767
H	5.86236	-4.81519	-2.08755
C	5.73317	-2.73293	-1.50898
C	6.78964	-2.52005	-1.69787
C	4.8603	-1.73894	-1.04831
C	3.99497	0.31501	-0.41759
C	6.43339	0.25198	-0.96577
H	6.29706	1.3143	-0.71395
H	6.78155	0.16213	-2.01049
H	7.19085	-0.1926	-0.29636
C	-3.65932	0.85247	0.27739
C	-3.15964	1.89373	1.09208
H	-2.12725	1.85095	1.45684
C	-3.97201	2.99117	1.41224
H	-3.57241	3.79478	2.03908
C	-5.28351	3.06753	0.91335
H	-5.9136	3.92931	1.15712
C	-5.7803	2.04319	0.09191
H	-6.79926	2.10234	-0.3054
C	-4.97395	0.93749	-0.22637
H	-5.36495	0.14249	-0.86958
C	-2.71254	-1.61007	1.45563
C	-3.92898	-1.71391	2.16649
H	-4.80429	-1.14404	1.8365
C	-4.01333	-2.52946	3.30522
H	-4.95951	-2.60335	3.85189
C	-2.88507	-3.24075	3.74871
H	-2.95248	-3.87128	4.64168
C	-1.66867	-3.12761	3.05725
H	-0.77869	-3.65696	3.41162
C	-1.57995	-2.31229	1.91794
H	-0.62267	-2.19296	1.39586
C	-3.39582	-1.52924	-1.39888
C	-4.25381	-2.62335	-1.16013
H	-4.45181	-2.94828	-0.13374
C	-4.84597	-3.30511	-2.23614
H	-5.50652	-4.15636	-2.03966
C	-4.59153	-2.90178	-3.55678
H	-5.05321	-3.43775	-4.39267
C	-3.73489	-1.8157	-3.80359
H	-3.52515	-1.50169	-4.83142
C	-3.13312	-1.13862	-2.7328
H	-2.44736	-0.30361	-2.92252
C	1.21564	1.585	0.998
C	0.48775	1.56342	-0.15678
C	1.57517	2.9041	1.61797
C	0.28213	2.66197	-1.11908
C	-1.00141	3.03649	-1.58276
C	1.41773	3.32032	-1.65881
C	-1.14708	4.05091	-2.53816
H	-1.88434	2.53808	-1.17327
C	1.26437	4.32274	-2.62487
H	2.41182	3.02671	-1.30621
C	-0.01618	4.69506	-3.06812
H	-2.14999	4.33862	-2.8723
H	2.15176	4.82006	-3.03188
H	-0.13238	5.48147	-3.82168
O	1.04592	3.98714	1.38482
O	2.60011	2.76708	2.52124
C	3.00895	4.00657	3.13322
H	2.16903	4.47938	3.66914
H	3.81301	3.73654	3.83226
H	3.3779	4.7142	2.37278

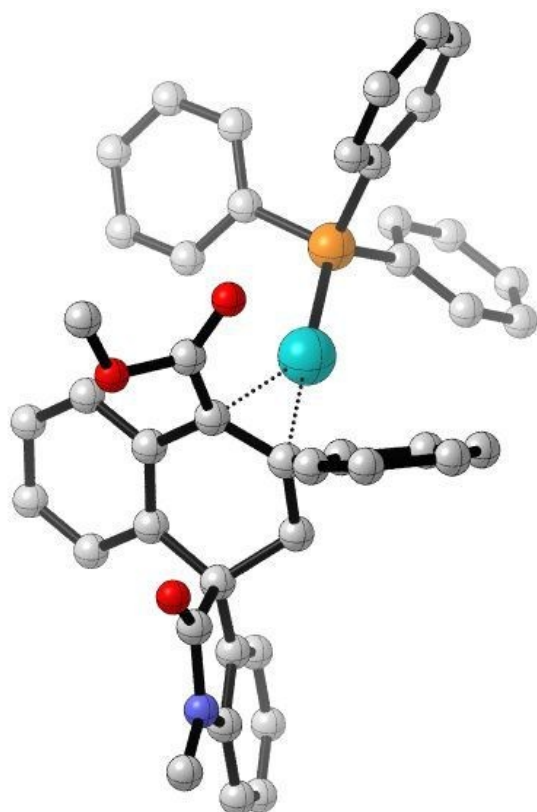


Zero-point correction= 0.658950 (Hartree/Particle)
 Thermal correction to Energy= 0.704959
 Thermal correction to Enthalpy= 0.705903
 Thermal correction to Gibbs Free Energy= 0.573712
 Sum of electronic and zero-point Energies= -2446.314998
 Sum of electronic and thermal Energies= -2446.268989
 Sum of electronic and thermal Enthalpies= -2446.268045
 Sum of electronic and thermal Free Energies= -2446.400236
 E(RM06L) = -2448.62703072
 Imaginary frequency = -210.67 cm⁻¹

Pd	-0.27998	-0.28095	-0.70108
P	-2.52826	-0.57095	-0.10054
O	4.22596	1.34947	-0.08888
N	5.18086	-0.66809	-0.72993
C	1.64254	0.3588	1.7495
C	1.28944	0.31968	3.11851
H	0.74697	1.16968	3.54378
C	1.60444	-0.77294	3.93415
H	1.30756	-0.77112	4.9882
C	2.29871	-1.86165	3.38898
H	2.56644	-2.72232	4.01117
C	2.66115	-1.8421	2.03356
H	3.213	-2.68882	1.61597
C	2.33564	-0.75694	1.19546
C	2.826	-0.74268	-0.27141
C	1.78174	-0.21463	-1.29399
H	1.45542	-1.02925	-1.9833
H	2.18032	0.59488	-1.91926
C	3.36752	-2.08737	-0.74692
C	2.71957	-3.30275	-0.9753
H	1.64629	-3.39975	-0.77701
C	3.46182	-4.40214	-1.45625
H	2.96143	-5.35873	-1.63595
C	4.83829	-4.27417	-1.70463
H	5.40504	-5.13315	-2.07868
C	5.50725	-3.05404	-1.48458
H	6.57841	-2.95518	-1.68431
C	4.75164	-1.97586	-1.00648
C	4.11982	0.14923	-0.33076
C	6.53383	-0.16977	-0.90114
H	6.52001	0.89332	-0.61797
H	6.86326	-0.26754	-1.95108
H	7.23979	-0.71677	-0.25163
C	-3.52148	0.98426	0.05134
C	-2.89302	2.11491	0.61946
H	-1.8383	2.06857	0.91163
C	-3.60767	3.31054	0.78606
H	-3.10283	4.17982	1.21902
C	-4.94951	3.39396	0.37876
H	-5.50336	4.33086	0.50104
C	-5.576	2.27763	-0.19855
H	-6.61926	2.34044	-0.52651

C	-4.8675	1.07595	-0.36339
H	-5.35911	0.21128	-0.82115
C	-2.79209	-1.40283	1.53243
C	-3.9631	-1.22133	2.29977
H	-4.74513	-0.54059	1.94685
C	-4.11889	-1.89434	3.52194
H	-5.02924	-1.7443	4.11219
C	-3.10756	-2.74932	3.99063
H	-3.22916	-3.26912	4.94692
C	-1.93394	-2.92319	3.23933
H	-1.13244	-3.57032	3.60958
C	-1.7734	-2.24896	2.01904
H	-0.8442	-2.35392	1.44636
C	-3.49376	-1.60613	-1.29884
C	-4.51454	-2.50194	-0.91675
H	-4.76818	-2.6203	0.14168
C	-5.19865	-3.25113	-1.88846
H	-5.98583	-3.94764	-1.58038
C	-4.87458	-3.11195	-3.24752
H	-5.40854	-3.69941	-4.00186
C	-3.8563	-2.22513	-3.63605
H	-3.59218	-2.1189	-4.69351
C	-3.16455	-1.48305	-2.66759
H	-2.35352	-0.80578	-2.96269
C	1.26142	1.55062	0.94296
C	0.72598	1.43965	-0.31707
C	1.35869	2.90763	1.57547
C	0.61717	2.543	-1.29969
C	-0.56882	2.79045	-2.02757
C	1.75987	3.3359	-1.57468
C	-0.62405	3.82275	-2.97353
H	-1.44956	2.17218	-1.82953
C	1.7032	4.35797	-2.53209
H	2.69149	3.1186	-1.04095
C	0.51135	4.60979	-3.23156
H	-1.55743	4.01126	-3.51507
H	2.59658	4.95889	-2.73479
H	0.46896	5.40933	-3.97906
O	0.5924	3.84902	1.3815
O	2.41669	2.98613	2.44419
C	2.54876	4.2664	3.09623
H	1.63131	4.52348	3.65119
H	3.40162	4.15932	3.78096
H	2.74262	5.06194	2.35815

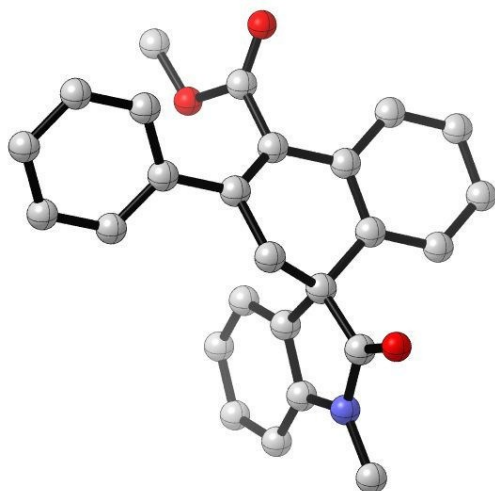
23b



Zero-point correction=	0.661814 (Hartree/Particle)
Thermal correction to Energy=	0.708185
Thermal correction to Enthalpy=	0.709129
Thermal correction to Gibbs Free Energy=	0.574662
Sum of electronic and zero-point Energies=	-2446.375593
Sum of electronic and thermal Energies=	-2446.329222
Sum of electronic and thermal Enthalpies=	-2446.328278
Sum of electronic and thermal Free Energies=	-2446.462746
E(RM06L) =	-2448.68921608

Pd	-0.64195	0.27234	-0.30113
P	-2.82981	-0.43715	-0.27732
O	4.32244	1.45387	0.85672
N	5.62043	-0.0773	-0.32043
C	1.5455	-0.33781	1.74417
C	0.93642	-0.74461	2.95416
H	0.08098	-0.17817	3.33372
C	1.40076	-1.85644	3.66588
H	0.91157	-2.14447	4.60236
C	2.48913	-2.59563	3.17606
H	2.86368	-3.46576	3.72511
C	3.09691	-2.21337	1.97042
H	3.94082	-2.7895	1.57802
C	2.63537	-1.10242	1.24369
C	3.31661	-0.66605	-0.05628
C	2.24932	-0.05277	-1.01511
H	1.60042	-0.88804	-1.34357
H	2.74329	0.34412	-1.91738
C	4.09997	-1.74662	-0.78256
C	3.69149	-2.96847	-1.31884
H	2.65529	-3.30428	-1.20268
C	4.63257	-3.77124	-1.99853
H	4.32285	-4.73256	-2.41984
C	5.96317	-3.34334	-2.13469
H	6.68474	-3.97439	-2.66394
C	6.392	-2.11212	-1.60016
H	7.42939	-1.78184	-1.70839
C	5.44324	-1.33072	-0.92936
C	4.43134	0.39257	0.24691
C	6.86988	0.6584	-0.24426
H	6.66077	1.58258	0.31509
H	7.24198	0.91325	-1.25241
H	7.64182	0.07239	0.2855
C	-4.03813	0.96593	-0.35299
C	-3.61916	2.20593	0.17962
H	-2.60391	2.3049	0.58557
C	-4.49063	3.3063	0.16603
H	-4.15653	4.26397	0.57898
C	-5.77533	3.18612	-0.38931
H	-6.44922	4.04952	-0.40781
C	-6.19073	1.95976	-0.93371
H	-7.18753	1.86465	-1.37806
C	-5.32711	0.85235	-0.91716
H	-5.65125	-0.09749	-1.35581
C	-3.32829	-1.3826	1.23697
C	-4.61383	-1.29485	1.81225
H	-5.36202	-0.62581	1.37467
C	-4.93233	-2.05189	2.9519
H	-5.93129	-1.97176	3.39414
C	-3.97465	-2.90452	3.52438
H	-4.22528	-3.49237	4.4139
C	-2.69042	-2.99076	2.96085
H	-1.93363	-3.64242	3.41016
C	-2.36497	-2.22748	1.82972
H	-1.35441	-2.26373	1.40635
C	-3.36687	-1.54396	-1.66778
C	-4.29473	-2.595	-1.51351
H	-4.72704	-2.79808	-0.52833
C	-4.65746	-3.38848	-2.61501
H	-5.37479	-4.20552	-2.48162
C	-4.10226	-3.13934	-3.87993
H	-4.38482	-3.76098	-4.73614
C	-3.1753	-2.09551	-4.0421
H	-2.73242	-1.90062	-5.02468
C	-2.80481	-1.30892	-2.94204
H	-2.06766	-0.50559	-3.06166
C	1.06259	0.86914	1.01316
C	1.41901	1.05596	-0.34885
C	0.54956	2.0412	1.82311
C	1.43324	2.38929	-1.03115
C	0.90216	2.5254	-2.33479
C	2.05205	3.50969	-0.43369
C	0.95172	3.75531	-3.00561
H	0.42659	1.6583	-2.80839
C	2.10319	4.7386	-1.10779
H	2.52848	3.39295	0.54413

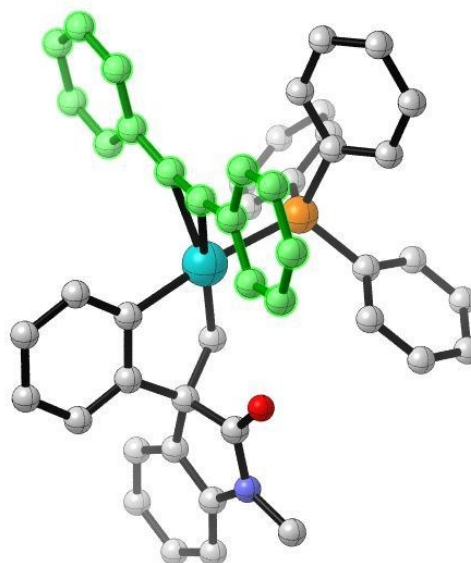
C	1.54889	4.86917	-2.39132
H	0.52092	3.8452	-4.00866
H	2.59	5.59639	-0.63093
H	1.59007	5.83029	-2.91481
O	-0.38746	2.78159	1.53864
O	1.29835	2.21159	2.95435
C	0.88242	3.32091	3.78255
H	-0.16132	3.19208	4.11263
H	1.5669	3.31443	4.64178
H	0.96075	4.27008	3.22847

24b

Zero-point correction= 0.395192 (Hartree/Particle)
 Thermal correction to Energy= 0.421003
 Thermal correction to Enthalpy= 0.421947
 Thermal correction to Gibbs Free Energy= 0.338756
 Sum of electronic and zero-point Energies= -1283.494128
 Sum of electronic and thermal Energies= -1283.468317
 Sum of electronic and thermal Enthalpies= -1283.467373
 Sum of electronic and thermal Free Energies= -1283.550564
 E(RM06L) = -1284.17119449

O	-2.86709	-0.0348	-2.6423
N	-3.51574	-1.12513	-0.687
C	0.07148	2.03989	-0.22845
C	0.23384	3.43278	-0.04078
H	1.24125	3.83188	0.10041
C	-0.86865	4.29541	-0.06688
H	-0.71703	5.37072	0.07208
C	-2.15707	3.78365	-0.27732
H	-3.02394	4.45168	-0.30033
C	-2.33237	2.40466	-0.4664
H	-3.33717	2.00744	-0.64141
C	-1.23756	1.52727	-0.45077
C	-1.42066	0.01507	-0.60422
C	-0.18671	-0.57204	-1.33776
H	-0.22785	-0.21961	-2.38916
H	-0.2623	-1.67137	-1.37799
C	-1.73724	-0.68089	0.71887
C	-1.03377	-0.75109	1.92294
H	-0.06925	-0.2464	2.03177
C	-1.58237	-1.48674	2.99493
H	-1.037	-1.5503	3.94148
C	-2.82083	-2.13271	2.85817
H	-3.23544	-2.69759	3.69942
C	-3.54659	-2.06599	1.65298
H	-4.51329	-2.56736	1.54844
C	-2.98562	-1.33477	0.60009
C	-2.66707	-0.34156	-1.46898
C	-4.76316	-1.67362	-1.1884
H	-4.86713	-1.33029	-2.22846
H	-5.62065	-1.31476	-0.5925
H	-4.74811	-2.77756	-1.16365
C	1.21962	1.1048	-0.17768
C	1.12868	-0.15358	-0.71232
C	2.4726	1.57315	0.50956
C	2.26777	-1.10031	-0.8011
C	3.54296	-0.66651	-1.2374
C	2.0975	-2.47	-0.48825

C	4.61125	-1.56788	-1.33993
H	3.68322	0.38135	-1.52067
C	3.16907	-3.3673	-0.58452
H	1.12555	-2.8255	-0.13037
C	4.42983	-2.92138	-1.01344
H	5.58592	-1.21303	-1.691
H	3.01904	-4.41969	-0.32177
H	5.26356	-3.6258	-1.09879
O	3.14354	2.55176	0.19552
O	2.75715	0.78509	1.5869
C	3.97368	1.14473	2.28671
H	3.94545	2.20061	2.59799
H	4.01576	0.47806	3.15813
H	4.84911	0.98675	1.63648

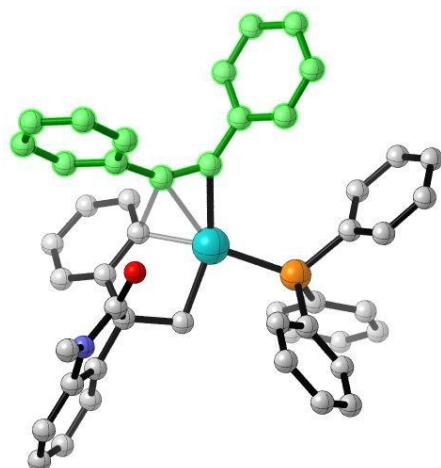
37a

Zero-point correction= 0.695492 (Hartree/Particle)
 Thermal correction to Energy= 0.743028
 Thermal correction to Enthalpy= 0.743973
 Thermal correction to Gibbs Free Energy= 0.609177
 Sum of electronic and zero-point Energies= -2449.440530
 Sum of electronic and thermal Energies= -2449.392994
 Sum of electronic and thermal Enthalpies= -2449.392049
 Sum of electronic and thermal Free Energies= -2449.526845
 E(RM06L) = -2451.78947649

Pd	0.01384	0.6345	0.24746
P	-1.24806	-1.46393	0.13599
O	2.56147	0.145	-2.13131
N	4.57226	-0.5353	-1.19818
C	1.29555	2.23478	0.36975
C	0.91654	3.59197	0.41563
H	-0.14288	3.86808	0.39237
C	1.88481	4.61051	0.48787
H	1.56743	5.6594	0.52625
C	3.25186	4.28988	0.51049
H	4.00516	5.08341	0.56784
C	3.65075	2.94534	0.46519
H	4.71518	2.68365	0.49416
C	2.68099	1.92788	0.40158
C	3.0153	0.44548	0.33081
C	1.76629	-0.31594	0.86531
H	1.7633	-0.21231	1.96655
H	1.80591	-1.39027	0.61803
C	4.30559	0.02388	1.01807
C	4.70435	0.11769	2.35202
H	4.04281	0.57948	3.09315
C	5.9702	-0.37805	2.73075
H	6.29149	-0.30752	3.77481
C	6.82166	-0.95788	1.77609
H	7.80155	-1.33931	2.08192
C	6.43811	-1.05642	0.42341
H	7.10393	-1.50583	-0.3197
C	5.17853	-0.55757	0.07185
C	3.29788	0.02973	-1.14665
C	5.16983	-1.03216	-2.42346

H	4.44272	-0.8518	-3.22919
H	5.38239	-2.11391	-2.35148
H	6.11017	-0.49825	-2.64901
C	-0.35958	-2.82121	-0.76077
C	0.5503	-2.45115	-1.77462
H	0.76387	-1.39236	-1.96066
C	1.21003	-3.43879	-2.52462
H	1.9114	-3.13711	-3.30931
C	0.98212	-4.79832	-2.25991
H	1.50329	-5.56728	-2.84033
C	0.09036	-5.17145	-1.24012
H	-0.08368	-6.23063	-1.02205
C	-0.58	-4.18966	-0.49473
H	-1.26888	-4.48919	0.3015
C	-2.8899	-1.40885	-0.72385
C	-3.08454	-1.96635	-2.00424
H	-2.26599	-2.49954	-2.49683
C	-4.32641	-1.84724	-2.64987
H	-4.46236	-2.28804	-3.64318
C	-5.38784	-1.17449	-2.026
H	-6.35647	-1.08737	-2.52952
C	-5.20095	-0.61215	-0.75172
H	-6.02299	-0.08519	-0.25551
C	-3.96025	-0.72096	-0.10744
H	-3.82638	-0.27711	0.88434
C	-1.68182	-2.22034	1.77382
C	-2.79595	-3.07152	1.95005
H	-3.46617	-3.27172	1.10795
C	-3.06001	-3.64577	3.2036
H	-3.92861	-4.30152	3.32692
C	-2.21798	-3.37801	4.29539
H	-2.42744	-3.82521	5.27284
C	-1.11225	-2.52878	4.13079
H	-0.45564	-2.30966	4.97945
C	-0.84847	-1.9493	2.88
H	0.0061	-1.27692	2.75501
C	-1.56247	1.81848	-0.95833
C	-1.90093	1.92329	0.24741
C	-1.48338	1.91775	-2.38601
C	-2.63426	2.33734	-3.10689
C	-0.2881	1.6287	-3.09215
C	-2.58282	2.46984	-4.49819
H	-3.55892	2.54911	-2.56168
C	-0.25426	1.76709	-4.48599
H	0.60143	1.30242	-2.54178
C	-1.39343	2.18628	-5.19331
H	-3.47523	2.79457	-5.04374
H	0.67485	1.54523	-5.02098
H	-1.35764	2.29178	-6.28283
C	-2.55631	2.28691	1.46998
C	-1.98028	2.00355	2.73398
C	-3.81203	2.95177	1.42112
C	-2.6397	2.37771	3.91107
H	-1.01158	1.49429	2.75899
C	-4.46179	3.3188	2.60474
H	-4.26053	3.17503	0.4483
C	-3.88079	3.03409	3.85355
H	-2.18118	2.15568	4.88029
H	-5.42758	3.83263	2.55298
H	-4.39371	3.32395	4.77637

TS 37a-38a'

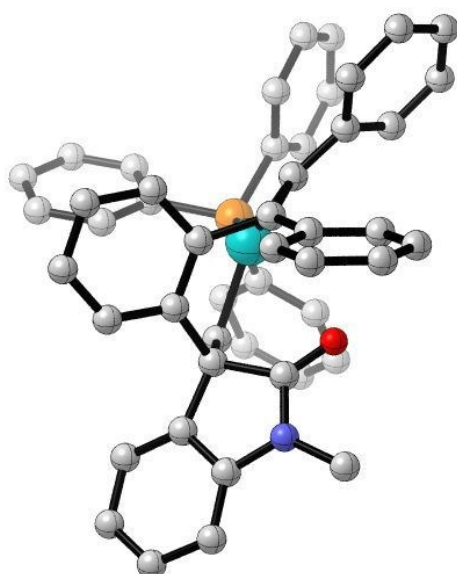


Zero-point correction=	0.694714 (Hartree/Particle)
Thermal correction to Energy=	0.741199
Thermal correction to Enthalpy=	0.742143
Thermal correction to Gibbs Free Energy=	0.610454
Sum of electronic and zero-point Energies=	-2449.397205
Sum of electronic and thermal Energies=	-2449.350720
Sum of electronic and thermal Enthalpies=	-2449.349776
Sum of electronic and thermal Free Energies=	-2449.481464
E(RM06L) =	-2451.73940632
Imaginary frequency =	-206.78 cm ⁻¹

Pd	0.14666	0.15213	-0.44048
P	1.91189	-1.31454	0.04549
O	-2.11455	0.66233	1.82516
N	-4.031	-0.64449	1.76948
C	-1.42397	0.9903	-1.5603
C	-1.24933	1.69838	-2.76931
H	-0.29156	2.19129	-2.96096
C	-2.30161	1.8164	-3.69605
H	-2.14838	2.37341	-4.62677
C	-3.54943	1.24566	-3.40587
H	-4.38572	1.3597	-4.10395
C	-3.72034	0.48847	-2.23138
H	-4.66975	-0.02737	-2.05302
C	-2.66464	0.31993	-1.31927
C	-2.67337	-0.72616	-0.20358
C	-1.27838	-1.42793	-0.28435
H	-1.27401	-2.05958	-1.18955
H	-1.11431	-2.08064	0.59034
C	-3.83989	-1.70417	-0.26436
C	-4.21362	-2.62499	-1.2451
H	-3.63353	-2.70991	-2.1704
C	-5.34516	-3.44164	-1.03381
H	-5.64296	-4.16607	-1.79844
C	-6.08951	-3.33046	0.15178
H	-6.96588	-3.96892	0.30539
C	-5.72691	-2.40901	1.1544
H	-6.30634	-2.32579	2.0789
C	-4.60026	-1.61013	0.92364
C	-2.85813	-0.11148	1.22375
C	-4.49575	-0.31397	3.1039
H	-3.79437	0.43	3.51037
H	-4.50532	-1.20733	3.75437
H	-5.51275	0.1155	3.0733
C	1.55111	-2.38429	1.51549
C	0.77844	-1.81108	2.55053
H	0.36549	-0.80332	2.4205
C	0.50924	-2.53998	3.71952
H	-0.08965	-2.08434	4.51494
C	0.99042	-3.852	3.8594
H	0.77199	-4.42384	4.76755
C	1.74054	-4.43472	2.82506
H	2.10561	-5.46272	2.92261
C	2.0232	-3.70537	1.65899
H	2.60237	-4.17213	0.8563
C	3.6162	-0.67521	0.40746
C	4.24455	-0.83904	1.65906
H	3.73098	-1.3757	2.46246
C	5.53523	-0.32592	1.87556
H	6.01391	-0.46281	2.85126
C	6.21159	0.34646	0.84628
H	7.2198	0.73909	1.01523
C	5.58693	0.51996	-0.40071
H	6.10191	1.05609	-1.20438
C	4.29514	0.02225	-0.61657
H	3.80927	0.17456	-1.58633
C	2.27983	-2.47013	-1.35963
C	3.4725	-3.22813	-1.39964
H	4.21523	-3.11764	-0.60275
C	3.72505	-4.09902	-2.47031
H	4.65233	-4.68154	-2.48883
C	2.79891	-4.21237	-3.52082
H	3.00077	-4.88734	-4.3593
C	1.62374	-3.44534	-3.50032
H	0.90727	-3.5141	-4.32568
C	1.36506	-2.5773	-2.42721
H	0.46182	-1.95881	-2.41403
C	-0.43567	2.32526	-0.31029
C	0.86347	2.17654	-0.3136
C	-1.43925	3.23438	0.25143
C	-1.11606	3.85818	1.48364
C	-2.6477	3.58986	-0.38946
C	-1.96879	4.81532	2.04549
H	-0.18909	3.57439	1.98939
C	-3.5009	4.54331	0.18403

H	-2.91233	3.13143	-1.3444
C	-3.16832	5.16067	1.40028
H	-1.69956	5.28559	2.99745
H	-4.43139	4.80894	-0.32937
H	-3.83929	5.90412	1.84385
C	2.02045	3.04271	-0.169
C	2.14752	4.18787	-1.00074
C	3.01974	2.81076	0.80821
C	3.22722	5.06642	-0.85164
H	1.38051	4.37838	-1.75822
C	4.08737	3.70531	0.96361
H	2.93974	1.93109	1.45258
C	4.2018	4.83357	0.13447
H	3.3029	5.94422	-1.50299
H	4.84045	3.51179	1.73486
H	5.04279	5.52472	0.25405

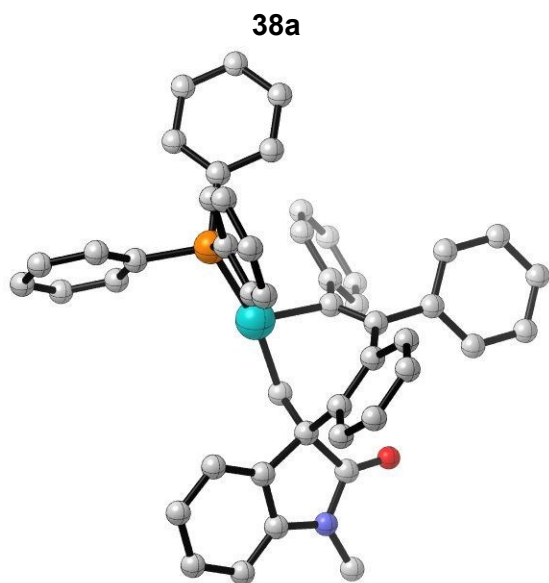
38a'



Zero-point correction= 0.696359 (Hartree/Particle)
 Thermal correction to Energy= 0.742915
 Thermal correction to Enthalpy= 0.743859
 Thermal correction to Gibbs Free Energy= 0.611964
 Sum of electronic and zero-point Energies= -2449.420461
 Sum of electronic and thermal Energies= -2449.373905
 Sum of electronic and thermal Enthalpies= -2449.372961
 Sum of electronic and thermal Free Energies= -2449.504856
 E(RM06L) = -2451.76617649

Pd	-0.26258	0.08535	0.06739
P	-2.32147	-0.79119	-0.11499
O	2.22919	0.53892	-1.77402
N	4.03874	-0.90001	-1.60336
C	1.567	0.59755	1.62287
C	1.29135	0.90486	2.98436
H	0.77252	1.84721	3.18593
C	1.70842	0.09442	4.04575
H	1.48568	0.3818	5.07862
C	2.4482	-1.05908	3.76028
H	2.83151	-1.69297	4.56711
C	2.68307	-1.42201	2.42428
H	3.22295	-2.3505	2.22697
C	2.23334	-0.65539	1.32956
C	2.2284	-1.33019	-0.08953
C	0.75152	-1.71842	-0.41237
H	0.45889	-2.57416	0.22047
H	0.62864	-1.99725	-1.47243
C	3.19039	-2.51703	-0.199
C	3.14041	-3.80434	0.34257
H	2.30073	-4.10419	0.97888
C	4.17203	-4.72372	0.05377
H	4.13607	-5.73079	0.48087
C	5.23714	-4.35524	-0.78261
H	6.03401	-5.07456	-0.99858
C	5.28796	-3.07555	-1.36977
H	6.1015	-2.79709	-2.04625
C	4.25172	-2.18224	-1.07284
C	2.7844	-0.41098	-1.22572

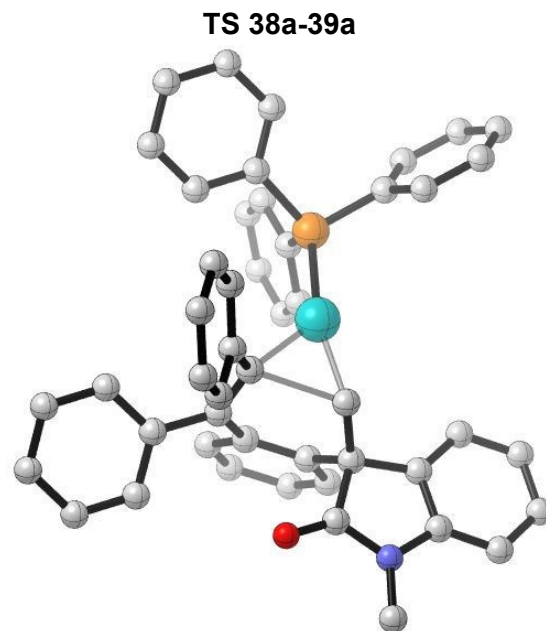
C	4.82161	-0.29443	-2.66639
H	4.3367	0.65989	-2.91845
H	4.84655	-0.94112	-3.56286
H	5.85575	-0.10755	-2.33001
C	-2.51113	-1.95029	-1.54623
C	-1.9172	-1.56868	-2.77026
H	-1.34554	-0.63476	-2.81991
C	-2.03331	-2.3882	-3.90191
H	-1.56905	-2.08035	-4.84469
C	-2.72749	-3.60766	-3.82066
H	-2.80892	-4.25309	-4.70159
C	-3.30581	-4.0013	-2.60413
H	-3.83905	-4.9553	-2.5323
C	-3.20205	-3.17712	-1.47048
H	-3.65442	-3.49414	-0.52556
C	-3.74768	0.37608	-0.30844
C	-4.81996	0.13038	-1.19258
H	-4.81504	-0.76475	-1.82247
C	-5.89425	1.03266	-1.26497
H	-6.72159	0.83565	-1.9553
C	-5.90821	2.18009	-0.45591
H	-6.74638	2.88256	-0.51519
C	-4.83844	2.4327	0.41928
H	-4.83442	3.33608	1.03754
C	-3.75743	1.54182	0.48676
H	-2.90103	1.7522	1.13701
C	-2.81658	-1.76743	1.38168
C	-4.16961	-2.05952	1.66467
H	-4.95901	-1.68504	1.00447
C	-4.50865	-2.80978	2.80162
H	-5.56081	-3.02886	3.0127
C	-3.50458	-3.26703	3.67106
H	-3.77237	-3.84649	4.56098
C	-2.15929	-2.96636	3.40412
H	-1.3734	-3.30504	4.08722
C	-1.81583	-2.21757	2.26762
H	-0.7716	-1.9565	2.06529
C	1.30142	1.79625	0.69323
C	-0.00934	2.1029	0.38127
C	2.50364	2.60368	0.31916
C	2.50362	3.43922	-0.8243
C	3.67033	2.57351	1.1195
C	3.61525	4.22976	-1.13638
H	1.62738	3.44742	-1.47646
C	4.78501	3.36579	0.80297
H	3.70053	1.93295	2.00639
C	4.76321	4.20097	-0.32404
H	3.59057	4.86527	-2.02853
H	5.67241	3.32961	1.44469
H	5.6327	4.81906	-0.57259
C	-0.59038	3.37504	-0.01144
C	-0.31838	4.56039	0.72892
C	-1.50355	3.46644	-1.09607
C	-0.92553	5.77539	0.39237
H	0.37984	4.50667	1.5705
C	-2.08873	4.68966	-1.44457
H	-1.73264	2.55714	-1.66081
C	-1.80842	5.84959	-0.70036
H	-0.70335	6.67358	0.97936
H	-2.77811	4.73732	-2.29459
H	-2.27776	6.80279	-0.96609



Zero-point correction= 0.697117 (Hartree/Particle)
 Thermal correction to Energy= 0.743840
 Thermal correction to Enthalpy= 0.744785
 Thermal correction to Gibbs Free Energy= 0.611244
 Sum of electronic and zero-point Energies= -2449.453118
 Sum of electronic and thermal Energies= -2449.406395
 Sum of electronic and thermal Enthalpies= -2449.405451
 Sum of electronic and thermal Free Energies= -2449.538991
 E(RM06L) = -2451.79365824

Pd	-0.28931	-0.24626	-0.75222
P	-2.54393	-0.40166	0.09497
O	4.53798	0.2648	-0.65215
N	4.71236	-2.03149	-0.98191
C	1.88459	0.52475	1.51134
C	1.80265	0.83141	2.89319
H	1.51137	1.84825	3.17457
C	2.07118	-0.1114	3.89045
H	1.98421	0.16686	4.94616
C	2.45637	-1.40667	3.51747
H	2.69123	-2.16304	4.2743
C	2.56091	-1.72726	2.15688
H	2.88174	-2.7341	1.87481
C	2.27279	-0.7955	1.13305
C	2.54441	-1.23729	-0.32729
C	1.63902	-0.61992	-1.43364
H	1.40448	-1.3784	-2.20775
H	2.13129	0.23304	-1.92051
C	2.57526	-2.75167	-0.50528
C	1.56487	-3.70691	-0.38441
H	0.56067	-3.40698	-0.06303
C	1.85322	-5.05875	-0.66904
H	1.06667	-5.8139	-0.57343
C	3.14366	-5.43917	-1.07256
H	3.35696	-6.49075	-1.29129
C	4.1748	-4.48806	-1.2037
H	5.17857	-4.78635	-1.52108
C	3.86725	-3.15234	-0.91512
C	4.03208	-0.85696	-0.65312
C	6.1112	-2.04849	-1.3702
H	6.46581	-1.00779	-1.3265
H	6.23369	-2.43689	-2.39714
H	6.70653	-2.67124	-0.67904
C	-2.66992	-0.91497	1.86544
C	-1.51751	-1.43867	2.48801
H	-0.57636	-1.48649	1.9267
C	-1.56738	-1.863	3.82536
H	-0.66121	-2.25401	4.29824
C	-2.76364	-1.76018	4.55269
H	-2.79995	-2.0842	5.59827
C	-3.91205	-1.22542	3.94371
H	-4.84322	-1.1319	4.51276
C	-3.86719	-0.80065	2.60702
H	-4.75773	-0.365	2.14132
C	-3.37435	-1.75611	-0.85968
C	-4.25506	-2.69873	-0.28806
H	-4.49004	-2.64856	0.77987
C	-4.82129	-3.70896	-1.0818

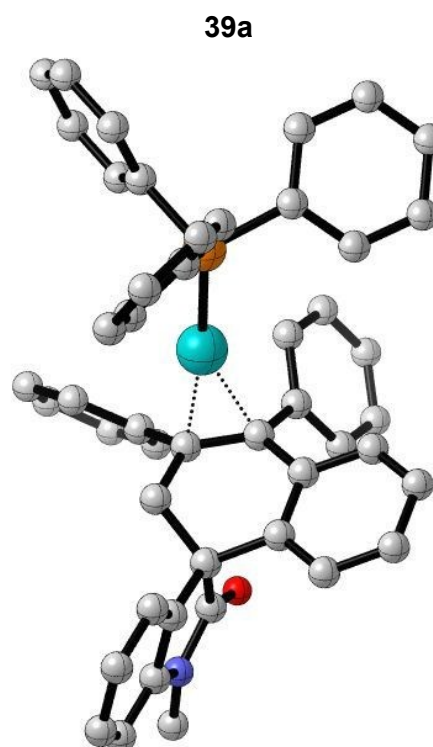
H	-5.49953	-4.43867	-0.62676
C	-4.5191	-3.78798	-2.45132
H	-4.96107	-4.57946	-3.06561
C	-3.64153	-2.85575	-3.02887
H	-3.39487	-2.91651	-4.09396
C	-3.06608	-1.85019	-2.23697
H	-2.36526	-1.13131	-2.68081
C	-3.7331	1.01486	0.00532
C	-4.91313	0.98314	-0.76501
H	-5.1746	0.08009	-1.32533
C	-5.75719	2.10578	-0.81138
H	-6.67206	2.06941	-1.41244
C	-5.43443	3.265	-0.08948
H	-6.09461	4.13773	-0.12714
C	-4.25782	3.30385	0.67884
H	-3.99753	4.20651	1.24143
C	-3.40789	2.18986	0.72205
H	-2.48781	2.22749	1.316
C	1.54295	1.64192	0.57288
C	0.673	1.49581	-0.46622
C	2.13076	2.98087	0.91264
C	1.32777	4.13605	1.04127
C	3.52557	3.10035	1.12062
C	1.90021	5.37678	1.35983
H	0.24701	4.05145	0.88958
C	4.09478	4.34242	1.43494
H	4.15506	2.21344	0.99647
C	3.28601	5.48531	1.55904
H	1.25988	6.26039	1.45813
H	5.17816	4.41912	1.5798
H	3.73298	6.45342	1.80964
C	0.45454	2.45424	-1.56999
C	-0.84301	2.84915	-1.97887
C	1.56838	2.96612	-2.28575
C	-1.02016	3.73153	-3.05288
H	-1.7104	2.46183	-1.43628
C	1.38536	3.8401	-3.36576
H	2.57589	2.66965	-1.97735
C	0.09204	4.22767	-3.75491
H	-2.03247	4.03255	-3.34419
H	2.2589	4.22163	-3.90574
H	-0.0484	4.9113	-4.59906



Zero-point correction= 0.696378 (Hartree/Particle)
 Thermal correction to Energy= 0.742564
 Thermal correction to Enthalpy= 0.743508
 Thermal correction to Gibbs Free Energy= 0.611485
 Sum of electronic and zero-point Energies= -2449.451205
 Sum of electronic and thermal Energies= -2449.405019
 Sum of electronic and thermal Enthalpies= -2449.404075
 Sum of electronic and thermal Free Energies= -2449.536097
 E(RM06L) = -2451.79006138
 Imaginary frequency = -205.82 cm⁻¹

Pd	0.39038	0.23757	-0.64958
P	2.64483	0.29653	0.0082
O	-4.47289	-0.18448	-0.39513
N	-4.70494	2.09358	-0.79018
C	-1.8181	-0.33265	1.60669
C	-1.63006	-0.61772	2.98045
H	-1.38945	-1.64594	3.26735
C	-1.73129	0.37334	3.96427
H	-1.56914	0.11643	5.01652
C	-2.04289	1.68781	3.58911
H	-2.1411	2.47691	4.34237
C	-2.25084	1.98822	2.23374
H	-2.515	3.01009	1.94686
C	-2.13652	1.00492	1.23054
C	-2.48958	1.3634	-0.22992
C	-1.59435	0.6839	-1.30367
H	-1.07038	1.44558	-1.92737
H	-2.17221	0.0481	-1.98652
C	-2.5532	2.86319	-0.49611
C	-1.54989	3.83411	-0.49254
H	-0.52072	3.55908	-0.23522
C	-1.87867	5.16672	-0.81971
H	-1.09888	5.93465	-0.81691
C	-3.19997	5.51186	-1.14835
H	-3.44385	6.54896	-1.40127
C	-4.22337	4.54366	-1.16196
H	-5.25102	4.81416	-1.42255
C	-3.87581	3.2276	-0.83271
C	-3.98512	0.94316	-0.46451
C	-6.12439	2.07219	-1.09587
H	-6.45641	1.02841	-0.99228
H	-6.31207	2.41882	-2.12774
H	-6.68938	2.71163	-0.39483
C	2.93088	0.59829	1.81148
C	1.91246	1.24157	2.54596
H	0.9733	1.50636	2.04573
C	2.08937	1.51449	3.91131
H	1.2861	2.00479	4.47015
C	3.27758	1.13729	4.55752
H	3.41099	1.34207	5.62516
C	4.28981	0.48184	3.83646
H	5.2126	0.17424	4.34001
C	4.11886	0.21072	2.46986
H	4.90343	-0.31496	1.91504
C	3.59634	1.64563	-0.83903
C	4.62154	2.38698	-0.21511
H	4.88758	2.17906	0.8261
C	5.29344	3.3986	-0.92082
H	6.08362	3.97215	-0.42449
C	4.95301	3.67737	-2.25427
H	5.47705	4.46886	-2.80037
C	3.93146	2.94543	-2.88261
H	3.65516	3.16366	-3.91957
C	3.25145	1.94129	-2.17729
H	2.43758	1.3815	-2.65487
C	3.65212	-1.22422	-0.3144
C	4.91759	-1.1986	-0.93561
H	5.34811	-0.24513	-1.25765
C	5.62675	-2.39392	-1.14361
H	6.60767	-2.36328	-1.63005
C	5.08434	-3.62018	-0.72917
H	5.63973	-4.54969	-0.89249
C	3.8227	-3.65242	-0.11021
H	3.39079	-4.6066	0.20929
C	3.10591	-2.46376	0.08834
H	2.11352	-2.48796	0.55297
C	-1.66718	-1.44918	0.62783
C	-0.99468	-1.27178	-0.55402
C	-2.21396	-2.77983	1.04222
C	-1.4502	-3.9646	0.93809
C	-3.5241	-2.87035	1.57091
C	-1.97927	-5.20002	1.33918
H	-0.43282	-3.90777	0.5392
C	-4.05203	-4.10655	1.96811
H	-4.13089	-1.96229	1.63334
C	-3.28217	-5.2771	1.85728
H	-1.36778	-6.10496	1.25276
H	-5.07302	-4.15675	2.36247
H	-3.69444	-6.24138	2.17335
C	-1.02097	-2.21734	-1.69783
C	0.16036	-2.6291	-2.35807
C	-2.26579	-2.68841	-2.18695
C	0.10305	-3.50573	-3.45067
H	1.12381	-2.25584	-1.99561
C	-2.31944	-3.55547	-3.2872
H	-3.18486	-2.35805	-1.6918

C	-1.13665	-3.97151	-3.92132
H	1.03066	-3.82272	-3.9399
H	-3.29094	-3.9072	-3.65158
H	-1.18062	-4.64941	-4.78059

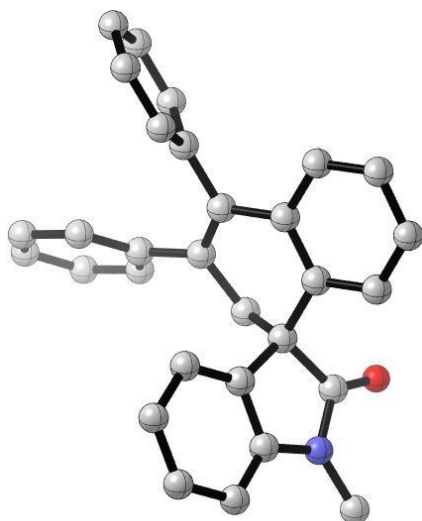


Zero-point correction= 0.698969 (Hartree/Particle)
 Thermal correction to Energy= 0.745583
 Thermal correction to Enthalpy= 0.746527
 Thermal correction to Gibbs Free Energy= 0.611689
 Sum of electronic and zero-point Energies= -2449.511440
 Sum of electronic and thermal Energies= -2449.464826
 Sum of electronic and thermal Enthalpies= -2449.463882
 Sum of electronic and thermal Free Energies= -2449.598720
 E(RM06L) = -2451.85401605

Pd	-0.66065	0.24976	-0.27752
P	-2.79229	-0.57508	-0.17273
O	4.3928	1.36975	0.41314
N	5.52957	-0.49507	-0.38882
C	1.57656	0.15627	1.77112
C	1.00843	0.19518	3.06687
H	0.2601	0.96273	3.28723
C	1.3849	-0.72216	4.05533
H	0.92556	-0.67125	5.04833
C	2.35234	-1.69916	3.77189
H	2.65789	-2.41882	4.53838
C	2.93609	-1.744	2.49589
H	3.69758	-2.49727	2.26998
C	2.5559	-0.83698	1.49289
C	3.21768	-0.83839	0.11516
C	2.15153	-0.44129	-0.95365
H	1.43403	-1.28267	-1.00929
H	2.62974	-0.36391	-1.94421
C	3.904	-2.12719	-0.30119
C	3.40733	-3.4229	-0.451
H	2.36512	-3.6473	-0.1996
C	4.26877	-4.44131	-0.91256
H	3.89057	-5.46176	-1.02808
C	5.60786	-4.15247	-1.22139
H	6.2667	-4.95056	-1.57914
C	6.12506	-2.84968	-1.07753
H	7.16904	-2.62847	-1.31863
C	5.25537	-1.85436	-0.61588
C	4.40442	0.18314	0.08893
C	6.82064	0.1477	-0.55842
H	6.69319	1.20021	-0.26411
H	7.15365	0.09604	-1.61005
H	7.58514	-0.32504	0.08355

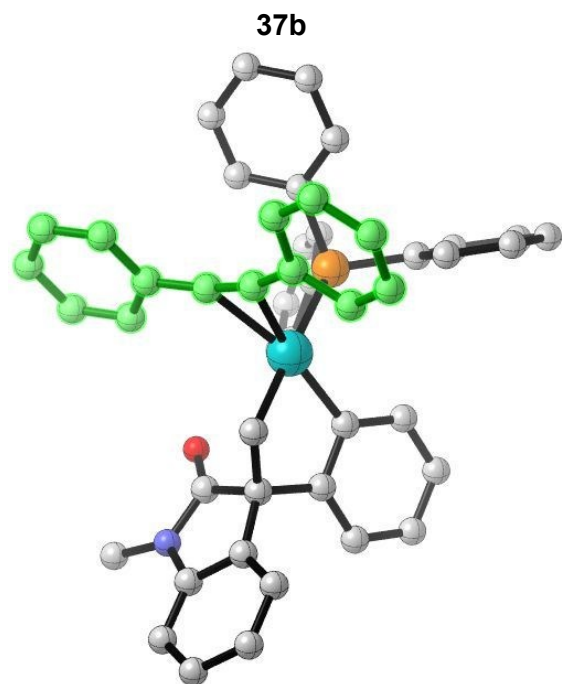
C	-3.70483	-0.14948	1.38512
C	-2.98373	-0.21164	2.59849
H	-1.92133	-0.48151	2.5772
C	-3.61575	0.08401	3.81469
H	-3.04732	0.02971	4.74922
C	-4.9687	0.46448	3.8337
H	-5.45796	0.70757	4.78286
C	-5.6876	0.54185	2.63092
H	-6.74021	0.84491	2.63794
C	-5.06217	0.23272	1.41097
H	-5.62991	0.29495	0.47725
C	-2.9449	-2.42402	-0.25371
C	-3.89556	-3.15671	0.48746
H	-4.5757	-2.63411	1.16808
C	-3.96605	-4.55484	0.36531
H	-4.70419	-5.11337	0.95103
C	-3.09483	-5.23395	-0.50068
H	-3.15095	-6.32373	-0.59315
C	-2.14311	-4.51147	-1.2408
H	-1.45466	-5.03616	-1.91196
C	-2.06255	-3.11762	-1.11038
H	-1.30453	-2.55121	-1.66482
C	-3.93394	-0.01542	-1.52505
C	-5.05034	-0.76605	-1.9528
H	-5.26253	-1.73714	-1.49294
C	-5.88224	-0.27892	-2.97384
H	-6.74358	-0.87109	-3.3014
C	-5.60873	0.95964	-3.57745
H	-6.25699	1.33522	-4.37634
C	-4.49562	1.70919	-3.1626
H	-4.27064	2.6701	-3.63739
C	-3.65897	1.22178	-2.14669
H	-2.77264	1.78624	-1.8324
C	1.18129	1.16743	0.74183
C	1.44373	0.8861	-0.62012
C	0.87608	2.55049	1.25624
C	-0.30971	3.24633	0.94119
C	1.83142	3.18561	2.08558
C	-0.53407	4.54233	1.43127
H	-1.05505	2.73992	0.31366
C	1.60631	4.48092	2.5731
H	2.76376	2.66152	2.3174
C	0.42189	5.16464	2.24971
H	-1.46401	5.06282	1.17794
H	2.36155	4.95895	3.20662
H	0.24428	6.1739	2.63662
C	1.45146	1.9107	-1.71533
C	0.89332	1.58553	-2.97572
C	2.08114	3.16676	-1.56642
C	0.92983	2.49744	-4.03958
H	0.40933	0.61022	-3.10564
C	2.11992	4.07663	-2.63395
H	2.55826	3.41537	-0.6158
C	1.54072	3.75172	-3.8711
H	0.48014	2.22796	-5.0015
H	2.61549	5.04413	-2.49772
H	1.57228	4.46624	-4.70066

26



Zero-point correction= 0.432340 (Hartree/Particle)
Thermal correction to Energy= 0.458326
Thermal correction to Enthalpy= 0.459271
Thermal correction to Gibbs Free Energy= 0.375634
Sum of electronic and zero-point Energies= -1286.629441
Sum of electronic and thermal Energies= -1286.603455
Sum of electronic and thermal Enthalpies= -1286.602511
Sum of electronic and thermal Free Energies= -1286.686147
E(RM06L) = -1287.33452376

O	3.139	0.18252	-2.57683
N	3.95404	-0.59604	-0.53723
C	-0.19851	1.83063	-0.41149
C	-0.62354	3.18107	-0.3934
H	-1.69345	3.39797	-0.33395
C	0.29401	4.23656	-0.46035
H	-0.06653	5.27031	-0.45033
C	1.66717	3.96558	-0.544
H	2.39417	4.78248	-0.59305
C	2.10664	2.63374	-0.57706
H	3.17719	2.42056	-0.66102
C	1.19582	1.56795	-0.52711
C	1.67425	0.11596	-0.55049
C	0.60012	-0.76288	-1.24564
H	0.88949	-1.82293	-1.15748
H	0.63314	-0.50362	-2.32418
C	2.10126	-0.38922	0.82603
C	1.41001	-0.49006	2.03374
H	0.36558	-0.17159	2.09876
C	2.07173	-1.01115	3.1653
H	1.53436	-1.09815	4.11456
C	3.41291	-1.41621	3.08235
H	3.91568	-1.8176	3.96818
C	4.12952	-1.31285	1.87441
H	5.17613	-1.62496	1.81115
C	3.45394	-0.79614	0.76328
C	2.98267	-0.05825	-1.38157
C	5.28923	-0.93963	-0.99255
H	5.33874	-0.67966	-2.06046
H	5.48381	-2.01924	-0.86561
H	6.05594	-0.37115	-0.43735
C	-0.79953	-0.55313	-0.68952
C	-1.17881	0.71658	-0.32356
C	-1.66276	-1.76111	-0.61305
C	-1.6246	-2.72105	-1.65445
C	-2.48812	-2.03195	0.50471
C	-2.39886	-3.88767	-1.59392
H	-0.99423	-2.54116	-2.53178
C	-3.25102	-3.2047	0.57019
H	-2.51758	-1.31893	1.33293
C	-3.21537	-4.13686	-0.47988
H	-2.36087	-4.6058	-2.4199
H	-3.87287	-3.3943	1.4515
H	-3.81391	-5.05208	-0.42689
C	-2.57364	1.05072	0.10698
C	-2.82193	1.64817	1.36419
C	-3.6716	0.80107	-0.74545
C	-4.12875	1.96273	1.76508
H	-1.97897	1.86328	2.02965
C	-4.97718	1.12229	-0.34771
H	-3.49053	0.34812	-1.72501
C	-5.21156	1.70023	0.91027
H	-4.30091	2.41598	2.74711
H	-5.81444	0.92244	-1.02462
H	-6.23139	1.94974	1.22096

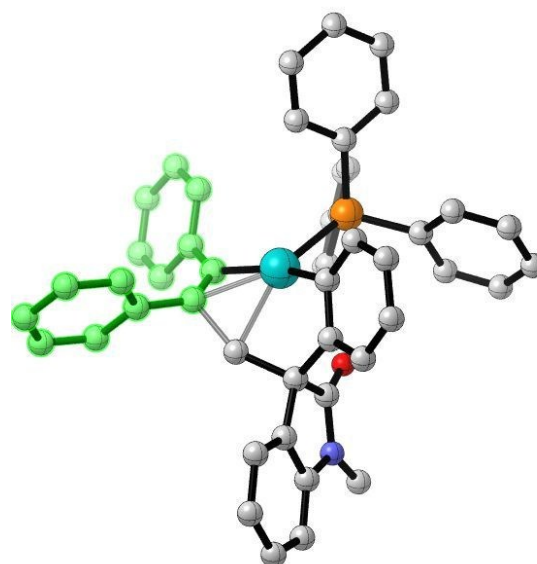


Zero-point correction= 0.695568 (Hartree/Particle)
 Thermal correction to Energy= 0.743020
 Thermal correction to Enthalpy= 0.743964
 Thermal correction to Gibbs Free Energy= 0.610049
 Sum of electronic and zero-point Energies= -2449.438196
 Sum of electronic and thermal Energies= -2449.390745
 Sum of electronic and thermal Enthalpies= -2449.389800
 Sum of electronic and thermal Free Energies= -2449.523716
 E(RM06L) = -2451.78506445

Pd	-0.21938	0.13263	-0.3803
P	1.96235	0.55464	0.68633
O	-2.50293	-0.84337	1.93887
N	-4.68971	-0.90904	1.16183
C	-1.17918	1.82881	0.30853
C	-0.58499	3.04074	0.71957
H	0.50279	3.1548	0.71055
C	-1.36607	4.13378	1.1401
H	-0.87425	5.06366	1.44922
C	-2.7657	4.03685	1.16462
H	-3.37488	4.88724	1.49073
C	-3.38385	2.84445	0.75726
H	-4.47712	2.76188	0.7559
C	-2.60062	1.75942	0.3249
C	-3.18214	0.4288	-0.12579
C	-2.14597	-0.18135	-1.10848
H	-2.21111	0.35481	-2.07183
H	-2.31252	-1.25763	-1.28992
C	-4.59438	0.46012	-0.68712
C	-5.12478	1.11917	-1.79706
H	-4.48681	1.76282	-2.41237
C	-6.49061	0.95331	-2.11086
H	-6.91529	1.46832	-2.97841
C	-7.3086	0.13372	-1.31614
H	-8.36691	0.01229	-1.57006
C	-6.79117	-0.538	-0.19023
H	-7.43039	-1.1744	0.42937
C	-5.43437	-0.35742	0.10217
C	-3.35657	-0.50165	1.11503
C	-5.21564	-1.78622	2.19151
H	-4.37851	-2.02906	2.86275
H	-5.61856	-2.71589	1.75161
H	-6.01652	-1.28654	2.76538
C	2.75856	2.17546	0.25251
C	2.74494	2.56175	-1.10748
H	2.25791	1.91953	-1.84999
C	3.33989	3.76649	-1.51164
H	3.32607	4.04887	-2.56963
C	3.93412	4.61349	-0.56175
H	4.38716	5.55975	-0.87567
C	3.93352	4.24704	0.79329
H	4.3846	4.90763	1.54148
C	3.35372	3.03417	1.20003
H	3.35349	2.76226	2.25981

C	3.33516	-0.65693	0.35895
C	4.41661	-0.36864	-0.49921
H	4.49901	0.61843	-0.96372
C	5.40282	-1.33657	-0.75188
H	6.23983	-1.09248	-1.41497
C	5.32284	-2.6033	-0.1538
H	6.09479	-3.35513	-0.3496
C	4.24654	-2.90047	0.69872
H	4.17092	-3.88634	1.16916
C	3.25863	-1.93791	0.9512
H	2.42612	-2.18344	1.61794
C	1.8758	0.5282	2.5349
C	3.04047	0.446	3.33385
H	4.02462	0.37936	2.85817
C	2.94005	0.42829	4.73257
H	3.84805	0.36593	5.34204
C	1.67718	0.48092	5.34813
H	1.60001	0.46191	6.44065
C	0.51764	0.54431	4.56074
H	-0.46971	0.56952	5.0331
C	0.61113	0.56752	3.15888
H	-0.29634	0.59796	2.54639
C	0.62211	-1.23402	-1.9785
C	0.40844	-2.03303	-1.03072
C	1.00155	-0.71062	-3.26128
C	0.62349	0.58954	-3.68287
C	1.76781	-1.52144	-4.1411
C	0.99818	1.05867	-4.94872
H	0.03212	1.20667	-2.99805
C	2.13718	-1.04104	-5.40203
H	2.06666	-2.52328	-3.81853
C	1.75526	0.24893	-5.81217
H	0.6938	2.06235	-5.26367
H	2.72772	-1.67699	-6.06994
H	2.04655	0.61959	-6.80036
C	0.25862	-3.20148	-0.21582
C	-0.39388	-3.15884	1.04263
C	0.77918	-4.43903	-0.68434
C	-0.51592	-4.32809	1.8056
H	-0.8153	-2.2121	1.39743
C	0.64715	-5.59741	0.08827
H	1.28457	-4.47338	-1.6542
C	0.00185	-5.54732	1.33741
H	-1.02422	-4.28287	2.77439
H	1.05074	-6.54475	-0.28484
H	-0.09744	-6.45624	1.94011

TS 37b-38b'



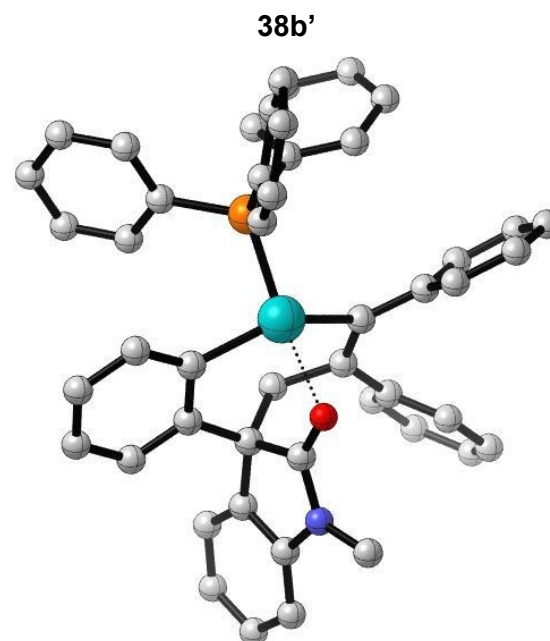
Zero-point correction= 0.695357 (Hartree/Particle)
 Thermal correction to Energy= 0.741783
 Thermal correction to Enthalpy= 0.742727
 Thermal correction to Gibbs Free Energy= 0.611275
 Sum of electronic and zero-point Energies= -2449.387812
 Sum of electronic and thermal Energies= -2449.341387
 Sum of electronic and thermal Enthalpies= -2449.340442
 Sum of electronic and thermal Free Energies= -2449.471895

E(RM06L) = -2451.73298278

Imaginary frequency = -228.96 cm⁻¹

Pd	0.01525	0.17452	-0.51519
P	-2.00955	-0.84549	-0.07593
O	0.97812	-1.14356	1.97642
N	3.24801	-1.43085	2.34139
C	0.77971	-1.47512	-1.47577
C	0.27581	-2.25138	-2.5366
H	-0.68763	-1.98854	-2.99171
C	0.99321	-3.35311	-3.03955
H	0.58693	-3.93714	-3.87423
C	2.22607	-3.70537	-2.46935
H	2.78269	-4.57164	-2.84323
C	2.76109	-2.9272	-1.42977
H	3.74053	-3.18108	-1.00917
C	2.05576	-1.80502	-0.95032
C	2.64061	-0.85065	0.09785
C	2.3428	0.65522	-0.30306
H	2.75455	0.80431	-1.31008
H	2.91436	1.27475	0.40545
C	4.15174	-0.96861	0.27605
C	5.19526	-0.78647	-0.63317
H	4.98006	-0.53727	-1.67748
C	6.527	-0.94088	-0.1931
H	7.35177	-0.80014	-0.89851
C	6.79917	-1.27712	1.14295
H	7.83663	-1.39634	1.47236
C	5.75807	-1.4675	2.07333
H	5.97284	-1.73187	3.11309
C	4.44499	-1.30552	1.61598
C	2.13389	-1.15315	1.54747
C	3.14976	-1.75945	3.75195
H	2.07974	-1.75575	4.00687
H	3.67934	-1.01269	4.37022
H	3.57498	-2.75827	3.95487
C	-1.998	-2.64592	0.38036
C	-2.07714	-3.64536	-0.61433
H	-2.18495	-3.36761	-1.66559
C	-2.02165	-5.00325	-0.26555
H	-2.08771	-5.76398	-1.05052
C	-1.87901	-5.38428	1.07754
H	-1.83702	-6.44469	1.34805
C	-1.78923	-4.3967	2.0709
H	-1.67715	-4.68183	3.12242
C	-1.84611	-3.03784	1.72729
H	-1.77476	-2.28133	2.51268
C	-3.19794	-0.75902	-1.48959
C	-4.38128	-1.53018	-1.54598
H	-4.60302	-2.24821	-0.74995
C	-5.26402	-1.39393	-2.62867
H	-6.17799	-1.99639	-2.6627
C	-4.97416	-0.49326	-3.66769
H	-5.66352	-0.39181	-4.51259
C	-3.79418	0.26604	-3.62689
H	-3.55632	0.95863	-4.44098
C	-2.90809	0.1311	-2.54573
H	-1.97051	0.70023	-2.51073
C	-2.89667	-0.08443	1.36571
C	-4.29157	0.11449	1.40039
H	-4.90823	-0.14777	0.53567
C	-4.89891	0.66605	2.54016
H	-5.98249	0.82584	2.55101
C	-4.12354	1.01462	3.65651
H	-4.59995	1.44557	4.54347
C	-2.73308	0.82023	3.62643
H	-2.11992	1.10098	4.48924
C	-2.11757	0.28602	2.48445
H	-1.03021	0.15604	2.44764
C	1.07016	2.14839	-0.31966
C	-0.13501	2.13145	0.22191
C	1.87637	3.17087	-1.01192
C	2.06795	3.11291	-2.41299
C	2.44085	4.24917	-0.29339
C	2.78712	4.11614	-3.07557
H	1.63236	2.27744	-2.97272
C	3.15485	5.25508	-0.96271
H	2.31231	4.29515	0.79219
C	3.3325	5.19223	-2.35359
H	2.91882	4.0605	-4.16153
H	3.57881	6.08803	-0.3916
H	3.89373	5.97579	-2.87316
C	-1.0675	3.13807	0.69407
C	-0.68303	4.07275	1.69162
C	-2.38841	3.21418	0.18311
C	-1.57851	5.05023	2.14454

H	0.32257	4.00769	2.11917
C	-3.27128	4.20696	0.62349
H	-2.70298	2.49183	-0.57632
C	-2.87455	5.12851	1.60843
H	-1.26011	5.75872	2.91731
H	-4.28137	4.25595	0.20256
H	-3.57222	5.89585	1.9599



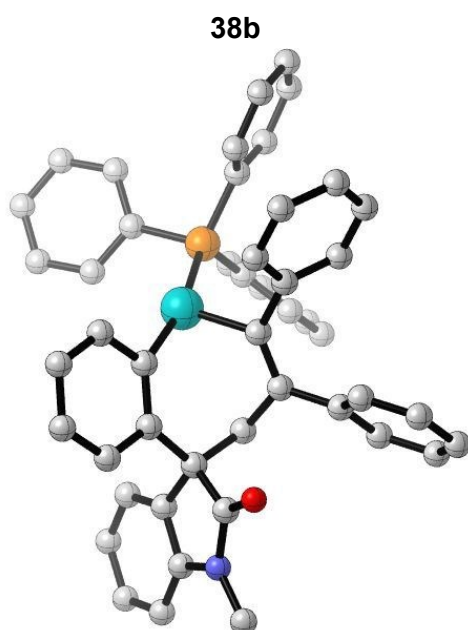
Zero-point correction= 0.697988 (Hartree/Particle)
 Thermal correction to Energy= 0.743951
 Thermal correction to Enthalpy= 0.744895
 Thermal correction to Gibbs Free Energy= 0.615513
 Sum of electronic and zero-point Energies= -2449.430885
 Sum of electronic and thermal Energies= -2449.384922
 Sum of electronic and thermal Enthalpies= -2449.383978
 Sum of electronic and thermal Free Energies= -2449.513360
 E(RM06L) = -2451.78076100

Pd	-0.31929	-0.33857	0.67142
P	-2.39124	-0.27725	-0.1895
O	1.45539	-0.33395	2.01397
N	3.70974	-0.85194	1.80284
C	0.00875	-2.40374	0.60982
C	-0.78861	-3.53689	0.85288
H	-1.81848	-3.40648	1.20718
C	-0.30615	-4.84394	0.65348
H	-0.95109	-5.70564	0.86332
C	0.99937	-5.03624	0.1836
H	1.38894	-6.04625	0.01532
C	1.82089	-3.92397	-0.0653
H	2.84562	-4.08336	-0.41614
C	1.34241	-2.61324	0.13677
C	2.31882	-1.38952	-0.06044
C	1.79131	-0.30467	-1.12461
H	0.83401	-0.67819	-1.52615
H	2.51758	-0.32137	-1.95438
C	3.77302	-1.75662	-0.31696
C	4.40851	-2.29539	-1.43828
H	3.83023	-2.55691	-2.33098
C	5.80304	-2.50657	-1.40685
H	6.30615	-2.93301	-2.28017
C	6.54969	-2.17342	-0.2652
H	7.63143	-2.34094	-0.25494
C	5.93	-1.61583	0.87024
H	6.51337	-1.34347	1.75469
C	4.54736	-1.41637	0.81463
C	2.41676	-0.78487	1.34818
C	4.14108	-0.38789	3.1121
H	3.25579	-0.00268	3.63733
H	4.88739	0.41857	3.00988
H	4.58017	-1.21773	3.69223
C	-3.57571	-0.2381	1.23529
C	-3.17655	-0.82297	2.45714
H	-2.16757	-1.24657	2.53589
C	-4.05162	-0.83971	3.55363

H	-3.72894	-1.29196	4.49733
C	-5.33085	-0.2695	3.44474
H	-6.01095	-0.27729	4.30312
C	-5.73255	0.31926	2.23496
H	-6.72567	0.77258	2.14692
C	-4.86118	0.33723	1.1336
H	-5.17388	0.81452	0.19958
C	-2.93911	-1.72581	-1.21262
C	-4.26791	-2.19853	-1.1832
H	-4.99685	-1.74079	-0.50718
C	-4.66015	-3.26206	-2.01166
H	-5.69226	-3.62641	-1.97264
C	-3.73457	-3.8563	-2.88418
H	-4.04241	-4.68577	-3.5296
C	-2.40993	-3.39134	-2.9184
H	-1.67889	-3.85919	-3.58583
C	-2.01135	-2.33959	-2.0796
H	-0.96904	-2.00632	-2.07592
C	-2.92669	1.15749	-1.23434
C	-3.25658	1.00374	-2.59779
H	-3.22477	0.01297	-3.06031
C	-3.63556	2.11696	-3.36518
H	-3.89018	1.9824	-4.42195
C	-3.69591	3.39145	-2.78071
H	-3.99509	4.25787	-3.3801
C	-3.36622	3.55165	-1.42474
H	-3.3952	4.54246	-0.9609
C	-2.97642	2.44552	-0.65589
H	-2.70428	2.58855	0.39407
C	1.61162	1.15798	-0.64211
C	0.5042	1.51605	0.0855
C	2.75149	2.08253	-0.94898
C	3.30177	2.91985	0.05164
C	3.33095	2.13696	-2.24011
C	4.37762	3.77397	-0.22667
H	2.86953	2.89168	1.0565
C	4.4052	2.99397	-2.52115
H	2.91817	1.51669	-3.04394
C	4.93671	3.81661	-1.51493
H	4.78503	4.4075	0.56919
H	4.8257	3.02158	-3.53263
H	5.7784	4.4828	-1.73204
C	0.14231	2.87082	0.51969
C	-0.32075	3.09154	1.84417
C	0.16711	3.98436	-0.36127
C	-0.70692	4.36679	2.2769
H	-0.37538	2.23326	2.52332
C	-0.23577	5.25622	0.06866
H	0.50361	3.83527	-1.39164
C	-0.6699	5.45879	1.39012
H	-1.04973	4.50908	3.30808
H	-0.21046	6.09677	-0.6343
H	-0.98357	6.45377	1.72379

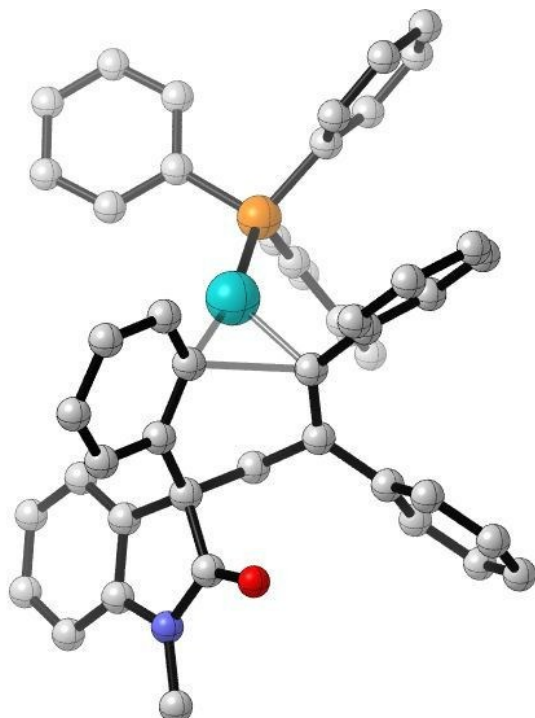
Zero-point correction= 0.697371 (Hartree/Particle)
 Thermal correction to Energy= 0.744199
 Thermal correction to Enthalpy= 0.745143
 Thermal correction to Gibbs Free Energy= 0.610848
 Sum of electronic and zero-point Energies= -2449.453503
 Sum of electronic and thermal Energies= -2449.406675
 Sum of electronic and thermal Enthalpies= -2449.405731
 Sum of electronic and thermal Free Energies= -2449.540026
 E(RM06L) = -2451.79672685

Pd	0.54443	-0.38336	-0.89854
P	2.61387	-0.64971	0.31314
O	-4.47336	1.27267	-0.71978
N	-5.3126	-0.62193	0.34155
C	-1.09087	-0.60123	-2.07005
C	-0.72357	-0.73603	-3.43337
H	0.30819	-0.52105	-3.74011
C	-1.64536	-1.14905	-4.40853
H	-1.3318	-1.25351	-5.45342
C	-2.97134	-1.40968	-4.02996
H	-3.71072	-1.72561	-4.77362
C	-3.35146	-1.24977	-2.69272
H	-4.39027	-1.45519	-2.40647
C	-2.43606	-0.83231	-1.69739
C	-2.99854	-0.71181	-0.26852
C	-2.03239	-0.09837	0.80741
H	-1.20219	-0.81639	0.93866
H	-2.59463	-0.06297	1.75672
C	-3.5041	-2.04647	0.27515
C	-2.84502	-3.25841	0.47393
H	-1.79776	-3.36985	0.17226
C	-3.54742	-4.3383	1.05093
H	-3.04065	-5.29598	1.2064
C	-4.89321	-4.19102	1.42364
H	-5.4284	-5.03525	1.87103
C	-5.5749	-2.973	1.22814
H	-6.62495	-2.86253	1.5155
C	-4.86086	-1.91508	0.65139
C	-4.3093	0.13976	-0.27784
C	-6.66077	-0.12401	0.54211
H	-6.67874	0.90556	0.15358
H	-6.92704	-0.1196	1.61405
H	-7.39793	-0.73823	-0.00587
C	3.96718	0.5918	0.11725
C	3.92749	1.4284	-1.01784
H	3.08417	1.35007	-1.71304
C	4.94281	2.37216	-1.23647
H	4.89616	3.02203	-2.11581
C	5.99745	2.49629	-0.31787
H	6.7854	3.23859	-0.48398
C	6.03407	1.67766	0.82365
H	6.84905	1.78071	1.54808
C	5.02319	0.72934	1.04391
H	5.04736	0.10286	1.9417
C	3.35144	-2.23555	-0.29849
C	4.7087	-2.38535	-0.65049
H	5.39689	-1.54173	-0.53819
C	5.17792	-3.61153	-1.15084
H	6.23357	-3.7159	-1.42325
C	4.30103	-4.69689	-1.30491
H	4.67015	-5.64945	-1.69904
C	2.94622	-4.55543	-0.95941
H	2.25514	-5.3957	-1.08311
C	2.47311	-3.33181	-0.46457
H	1.41318	-3.21855	-0.20303
C	2.48405	-0.89909	2.1403
C	3.2715	-1.83285	2.84715
H	3.98265	-2.46697	2.30712
C	3.13425	-1.96219	4.23876
H	3.74639	-2.69257	4.77861
C	2.21332	-1.16257	4.93483
H	2.10668	-1.26701	6.01966
C	1.42115	-0.23693	4.23534
H	0.694	0.38082	4.77262
C	1.54828	-0.10955	2.84386
H	0.9113	0.59126	2.29182
C	-1.46141	1.27042	0.46284
C	-0.3758	1.33352	-0.35095
C	-2.10537	2.48441	1.05518
C	-2.42488	3.61566	0.26979
C	-2.4081	2.52711	2.43666
C	-3.01207	4.74878	0.84743
H	-2.23031	3.58644	-0.80507
C	-2.99418	3.66292	3.01546
H	-2.16526	1.66636	3.07039
C	-3.29759	4.78104	2.22291



H	-3.26002	5.60869	0.21576
H	-3.21175	3.67357	4.08934
H	-3.759	5.66731	2.67149
C	0.33927	2.51768	-0.86514
C	0.41197	2.77709	-2.25745
C	0.9864	3.41538	0.02051
C	1.09064	3.90371	-2.74065
H	-0.07954	2.08358	-2.94734
C	1.66654	4.53913	-0.46893
H	0.93775	3.22805	1.09759
C	1.72329	4.78984	-1.84991
H	1.12375	4.09325	-3.81928
H	2.15701	5.22148	0.23371
H	2.25518	5.66858	-2.22985

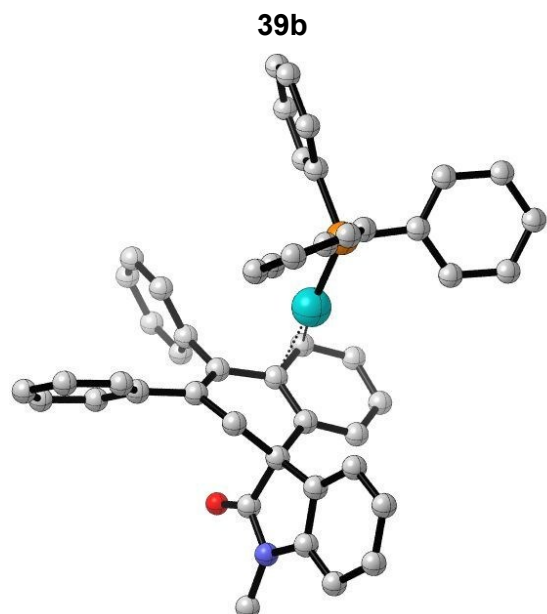
TS 38b-39b



Zero-point correction= 0.696992 (Hartree/Particle)
 Thermal correction to Energy= 0.743168
 Thermal correction to Enthalpy= 0.744112
 Thermal correction to Gibbs Free Energy= 0.611454
 Sum of electronic and zero-point Energies= -2449.450906
 Sum of electronic and thermal Energies= -2449.404730
 Sum of electronic and thermal Enthalpies= -2449.403786
 Sum of electronic and thermal Free Energies= -2449.536444
 E(RM06L) = -2451.79128096
 Imaginary frequency = -148.20 cm⁻¹

Pd	0.59486	-0.17553	-0.88478
P	2.64576	-0.61654	0.21595
O	-4.64403	0.94177	-0.41631
N	-5.19628	-1.19032	0.34161
C	-1.11138	-0.12189	-2.01365
C	-0.75958	0.09483	-3.36933
H	0.18752	0.5918	-3.60835
C	-1.60101	-0.32152	-4.41319
H	-1.30109	-0.16416	-5.45525
C	-2.82974	-0.92795	-4.10755
H	-3.50337	-1.25189	-4.90788
C	-3.20584	-1.0957	-2.76902
H	-4.17665	-1.55019	-2.53729
C	-2.37013	-0.68955	-1.7047
C	-2.90684	-0.86915	-0.27836
C	-1.99514	-0.25301	0.84046
H	-1.09257	-0.89026	0.90747
H	-2.54034	-0.34251	1.79509
C	-3.20528	-2.32034	0.08138
C	-2.3763	-3.44031	0.11625
H	-1.32896	-3.35647	-0.19387
C	-2.90675	-4.67657	0.54322
H	-2.26562	-5.56323	0.57121

C	-4.25296	-4.77486	0.93048
H	-4.65388	-5.73892	1.26075
C	-5.10489	-3.65253	0.8997
H	-6.154	-3.73308	1.19994
C	-4.55992	-2.43592	0.4706
C	-4.32158	-0.2136	-0.15676
C	-6.59314	-0.91738	0.62566
H	-6.7637	0.14292	0.38486
H	-6.82428	-1.09596	1.69093
H	-7.25587	-1.54811	0.00629
C	3.9732	0.66027	0.04191
C	3.94923	1.47179	-1.11208
H	3.13178	1.34823	-1.83218
C	4.94562	2.43741	-1.32014
H	4.91552	3.06393	-2.21744
C	5.96558	2.61133	-0.37012
H	6.73839	3.37113	-0.52775
C	5.98555	1.8195	0.79003
H	6.77243	1.96132	1.5386
C	4.99394	0.84745	0.99822
H	5.00525	0.24039	1.90961
C	3.43908	-2.1707	-0.41144
C	4.83359	-2.33594	-0.54664
C	5.50836	-1.51654	-0.27871
C	5.3592	-3.54287	-1.037
H	6.44333	-3.65819	-1.14173
C	4.50151	-4.59464	-1.39647
H	4.91464	-5.53252	-1.78222
C	3.11109	-4.43616	-1.27145
H	2.43573	-5.24797	-1.56111
C	2.58328	-3.22988	-0.7888
H	1.49711	-3.09651	-0.70977
C	2.52861	-0.88179	2.04458
C	3.31359	-1.82447	2.74161
H	4.01767	-2.46049	2.19486
C	3.18565	-1.95944	4.134
H	3.79549	-2.6982	4.66505
C	2.27852	-1.15478	4.84179
H	2.18019	-1.26296	5.92706
C	1.49003	-0.21814	4.15262
H	0.77481	0.40669	4.69776
C	1.60625	-0.08727	2.76075
H	0.97019	0.62133	2.21703
C	-1.58773	1.18787	0.56427
C	-0.65144	1.40098	-0.40235
C	-2.21855	2.27539	1.36765
C	-2.68025	3.47647	0.78036
C	-2.36918	2.12304	2.76758
C	-3.25803	4.48448	1.56313
H	-2.60561	3.60282	-0.30196
C	-2.94456	3.13398	3.55106
H	-2.01348	1.20689	3.25272
C	-3.39179	4.32226	2.95228
H	-3.61778	5.40001	1.08106
H	-3.04144	2.99209	4.63324
H	-3.84569	5.11167	3.56077
C	-0.11865	2.68707	-0.90493
C	-0.51325	3.22219	-2.15616
C	0.80599	3.42317	-0.12288
C	-0.00711	4.45198	-2.60024
H	-1.22843	2.66636	-2.76953
C	1.30469	4.65465	-0.56901
H	1.12243	3.01918	0.8437
C	0.90371	5.17463	-1.81104
H	-0.33203	4.85113	-3.5675
H	2.01194	5.2093	0.05708
H	1.2968	6.13521	-2.16061

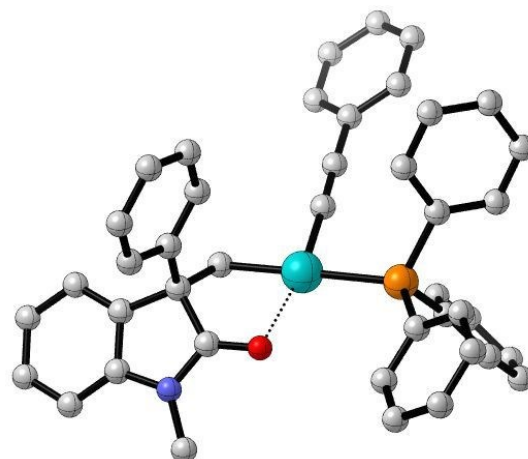


Zero-point correction= 0.698916 (Hartree/Particle)
 Thermal correction to Energy= 0.745636
 Thermal correction to Enthalpy= 0.746580
 Thermal correction to Gibbs Free Energy= 0.610322
 Sum of electronic and zero-point Energies= -2449.510024
 Sum of electronic and thermal Energies= -2449.463304
 Sum of electronic and thermal Enthalpies= -2449.462360
 Sum of electronic and thermal Free Energies= -2449.598618
 E(RM06L) = -2451.85465108

Pd	0.7955	0.05512	-0.8426
P	2.82031	-0.18789	0.14647
•	-4.73309	-0.20342	-1.1388
N	-4.87277	-2.37766	-0.31554
C	-1.32249	0.28758	-1.58762
C	-0.47951	0.5812	-2.71557
H	-0.17285	1.61589	-2.89431
C	-0.22006	-0.40314	-3.70202
H	0.40215	-0.1413	-4.56387
C	-0.77648	-1.68009	-3.58736
H	-0.59631	-2.4343	-4.36013
C	-1.5524	-2.00633	-2.45594
H	-1.96024	-3.01676	-2.34724
C	-1.80144	-1.06522	-1.44825
C	-2.69387	-1.39245	-0.25623
C	-2.33658	-0.45524	0.93564
H	-1.32644	-0.75788	1.28263
H	-3.03911	-0.63922	1.76507
C	-2.67397	-2.84176	0.19837
C	-1.62308	-3.64201	0.6468
H	-0.60044	-3.24936	0.66172
C	-1.89699	-4.96093	1.06791
H	-1.08045	-5.59928	1.41928
C	-3.21022	-5.45793	1.03699
H	-3.4104	-6.48289	1.36646
C	-4.28229	-4.66191	0.58619
H	-5.30379	-5.05316	0.56276
C	-3.99033	-3.35665	0.17169
C	-4.20119	-1.19402	-0.64511
C	-6.29929	-2.5512	-0.52164
H	-6.67679	-1.60616	-0.9404
H	-6.81402	-2.76492	0.43182
H	-6.50037	-3.37512	-1.22948
C	3.90411	1.31982	0.16964
C	3.79129	2.22418	-0.90844
H	3.05329	2.02137	-1.69374
C	4.59859	3.37005	-0.96311
H	4.50124	4.06395	-1.80489
C	5.51769	3.63424	0.06645
H	6.14075	4.53418	0.02906
C	5.62685	2.74731	1.14956
H	6.33487	2.95365	1.95956
C	4.82565	1.59465	1.20235
H	4.90905	0.91146	2.0542
C	3.91315	-1.48035	-0.61897
C	5.32288	-1.4139	-0.60851

H	5.82536	-0.55699	-0.14759
C	6.08532	-2.43491	-1.19981
H	7.17875	-2.36946	-1.19141
C	5.45019	-3.53203	-1.80377
H	6.04704	-4.32484	-2.26725
C	4.0471	-3.60264	-1.8234
H	3.54574	-4.44972	-2.30383
C	3.28327	-2.57926	-1.24267
H	2.18748	-2.60805	-1.28075
C	2.76803	-0.68106	1.93787
C	3.66186	-1.60393	2.52009
H	4.4339	-2.07655	1.90433
C	3.56069	-1.92648	3.88431
H	4.25672	-2.64972	4.32303
C	2.5733	-1.32725	4.6816
H	2.49579	-1.58113	5.7441
C	1.67845	-0.40668	4.10912
H	0.9025	0.06058	4.72492
C	1.76863	-0.09311	2.7453
H	1.05833	0.60696	2.28825
C	-2.33564	1.01695	0.54923
C	-1.794	1.36199	-0.66465
C	-2.91108	1.9688	1.53102
C	-3.76676	3.02763	1.14071
C	-2.66389	1.7938	2.91569
C	-4.3312	3.88499	2.09408
H	-4.00481	3.15711	0.08199
C	-3.22137	2.65911	3.86763
H	-2.01226	0.97771	3.24725
C	-4.05812	3.71085	3.46142
H	-4.99791	4.68994	1.76634
H	-3.00275	2.50911	4.9306
H	-4.50036	4.38344	4.20392
C	-1.6506	2.77812	-1.12567
C	-2.31832	3.22137	-2.29031
C	-0.83729	3.69303	-0.42245
C	-2.18824	4.54826	-2.7281
H	-2.95521	2.51913	-2.83884
C	-0.7043	5.01811	-0.864
H	-0.31007	3.35327	0.47431
C	-1.38032	5.45107	-2.01658
H	-2.72167	4.87804	-3.62626
H	-0.06773	5.71349	-0.30642
H	-1.27652	6.4858	-2.36019

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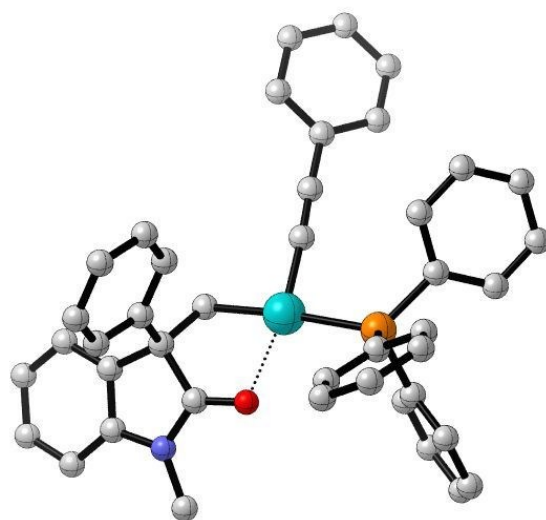


Zero-point correction= 0.618064 (Hartree/Particle)
 Thermal correction to Energy= 0.660692
 Thermal correction to Enthalpy= 0.661637
 Thermal correction to Gibbs Free Energy= 0.534957
 Sum of electronic and zero-point Energies= -2218.467351
 Sum of electronic and thermal Energies= -2218.424723
 Sum of electronic and thermal Enthalpies= -2218.423779
 Sum of electronic and thermal Free Energies= -2218.550459
 E(RM06L) = -2220.68056119

C	-7.04295	1.02163	-1.83887
C	-6.34547	-0.20094	-1.75855
C	-5.07759	-0.17505	-1.17245
C	-4.49291	1.01019	-0.67091

C	-5.20197	2.20917	-0.74914
C	-6.48129	2.20991	-1.34349
H	-8.03826	1.039	-2.2941
H	-6.78432	-1.12715	-2.14167
H	-4.76797	3.1346	-0.35701
H	-7.04259	3.1465	-1.41801
C	-2.99695	-0.80502	-0.46654
C	-3.11759	0.67748	-0.09337
C	-1.89615	1.33491	-0.78401
H	-1.75368	2.38072	-0.47668
H	-2.01008	1.29782	-1.88144
C	-3.11739	0.81905	1.44954
C	-4.17992	0.27043	2.20014
C	-2.08085	1.48424	2.13231
C	-4.20498	0.37857	3.59728
H	-5.00371	-0.2368	1.68586
C	-2.11348	1.60121	3.53337
H	-1.23977	1.90251	1.57259
C	-3.16979	1.04825	4.27098
H	-5.03794	-0.05664	4.15981
H	-1.30295	2.13082	4.04541
H	-3.19019	1.13934	5.36214
•	-1.93362	-1.47027	-0.38428
N	-4.17218	-1.25998	-1.00197
C	-4.36518	-2.60068	-1.5344
H	-5.21441	-3.09839	-1.03622
H	-4.55678	-2.56128	-2.62076
H	-3.44401	-3.16952	-1.34593
Pd	-0.28468	0.05846	-0.36508
P	1.64262	-1.36278	-0.04511
C	2.90917	-0.67193	1.10906
C	4.29466	-0.8522	0.91674
C	2.45464	0.05189	2.23183
C	5.21065	-0.32457	1.84204
H	4.65727	-1.39641	0.03851
C	3.37188	0.56931	3.15836
H	1.38071	0.22268	2.36144
C	4.7511	0.38302	2.96476
H	6.28507	-0.46463	1.68188
H	3.00966	1.13268	4.02461
H	5.46695	0.79623	3.68331
C	2.56642	-1.62273	-1.62908
C	3.09967	-2.87337	-2.00665
C	2.72704	-0.51207	-2.48887
C	3.78615	-3.00991	-3.22486
H	2.97533	-3.74121	-1.35148
C	3.42122	-0.65478	-3.69929
H	2.3055	0.45793	-2.19962
C	3.94934	-1.90258	-4.0718
H	4.19328	-3.98601	-3.5102
H	3.54299	0.21282	-4.35641
H	4.48402	-2.01208	-5.02146
C	1.37977	-3.08467	0.5912
C	2.26321	-3.70324	1.50198
C	0.25098	-3.80208	0.13491
C	2.02818	-5.01724	1.93815
H	3.13509	-3.15567	1.87276
C	0.02611	-5.11771	0.56746
H	-0.4616	-3.31934	-0.54063
C	0.91293	-5.72885	1.46922
H	2.72038	-5.48398	2.64717
H	-0.8516	-5.66463	0.20638
H	0.73104	-6.75338	1.81085
C	0.84747	1.62365	-0.44586
C	1.54683	2.64726	-0.47288
C	2.38374	3.80452	-0.48309
C	1.94471	5.02171	-1.07079
C	3.67987	3.77293	0.10004
C	2.76741	6.15496	-1.07323
H	0.94851	5.05765	-1.52295
C	4.49522	4.9113	0.09361
H	4.02787	2.8416	0.55721
C	4.04616	6.10809	-0.49153
H	2.40805	7.08291	-1.53205
H	5.49076	4.86513	0.54934
H	4.687	6.99621	-0.49436

28a



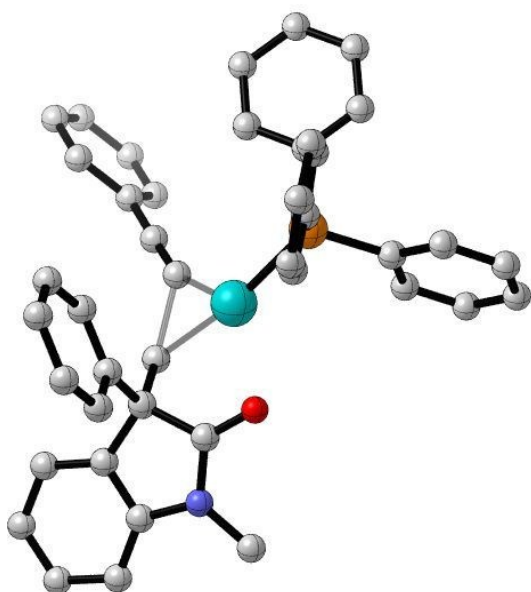
Zero-point correction= 0.618026 (Hartree/Particle)
 Thermal correction to Energy= 0.660624
 Thermal correction to Enthalpy= 0.661568
 Thermal correction to Gibbs Free Energy= 0.535364
 Sum of electronic and zero-point Energies= -2218.466964
 Sum of electronic and thermal Energies= -2218.424367
 Sum of electronic and thermal Enthalpies= -2218.423423
 Sum of electronic and thermal Free Energies= -2218.549627
 E(RM06L) = -2220.67960583

C	6.87891	1.06255	1.94393
C	6.1624	-0.14897	1.86416
C	4.91021	-0.11024	1.24583
C	4.35952	1.07702	0.71139
C	5.08692	2.26496	0.79067
C	6.3506	2.25273	1.41733
H	7.86278	1.06987	2.42363
H	6.57522	-1.07683	2.2714
H	4.67908	3.19168	0.37434
H	6.92606	3.18063	1.49259
C	2.83854	-0.71523	0.49477
C	2.99453	0.75997	0.10274
C	1.77201	1.45992	0.75139
H	1.65838	2.4985	0.40962
H	1.86488	1.45292	1.85108
C	3.03338	0.86946	-1.44302
C	1.98474	1.46644	-2.1696
C	4.13809	0.34871	-2.15202
C	2.04551	1.54216	-3.57243
H	1.11164	1.86141	-1.64219
C	4.19311	0.41922	-3.55079
H	4.97108	-0.10485	-1.6037
C	3.14451	1.01903	-4.26824
H	1.2218	2.01382	-4.11875
H	5.05985	0.00915	-4.08035
H	3.18714	1.07903	-5.36093
O	1.76886	-1.3699	0.39302
N	3.99031	-1.18151	1.06783
C	4.14178	-2.51919	1.62248
H	4.98505	-3.0456	1.14406
H	4.31982	-2.46662	2.71044
H	3.20772	-3.0661	1.43061
Pd	0.14762	0.20471	0.32815
P	-1.66113	-1.36805	0.00367
C	-3.3986	-0.7548	-0.11269
C	-4.47477	-1.39506	0.53787
C	-3.64828	0.38982	-0.90152
C	-5.78224	-0.9034	0.39223
H	-4.29077	-2.27621	1.16064
C	-4.95759	0.87293	-1.04782
H	-2.81375	0.91715	-1.37223
C	-6.02578	0.22831	-0.40236
H	-6.61028	-1.40643	0.90317
H	-5.13856	1.76581	-1.65463
H	-7.04557	0.61262	-0.51171
C	-1.69401	-2.53416	1.44059
C	-1.9566	-3.91411	1.3137
C	-1.43003	-1.99573	2.7202

C	-1.96497	-4.73931	2.45049
H	-2.14996	-4.34242	0.32482
C	-1.44762	-2.82216	3.85358
H	-1.20108	-0.92764	2.81478
C	-1.71412	-4.19553	3.72059
H	-2.16797	-5.8102	2.34167
H	-1.24508	-2.3939	4.84102
H	-1.72096	-4.84156	4.605
C	-1.49866	-2.47665	-1.4724
C	-2.61497	-2.95611	-2.19089
C	-0.19955	-2.84357	-1.88989
C	-2.43375	-3.79534	-3.30235
H	-3.62531	-2.66665	-1.8853
C	-0.02559	-3.68682	-2.99759
H	0.67059	-2.46224	-1.34534
C	-1.1407	-4.16348	-3.70664
H	-3.30713	-4.15857	-3.85465
H	0.98593	-3.96276	-3.31418
H	-1.00208	-4.81444	-4.57646
C	-0.9434	1.79435	0.38941
C	-1.59176	2.85088	0.42394
C	-2.38165	4.03922	0.45949
C	-1.89425	5.2606	-0.08018
C	-3.68125	4.03671	1.03613
C	-2.67327	6.42362	-0.04318
H	-0.89476	5.27624	-0.52634
C	-4.45193	5.20539	1.07181
H	-4.06849	3.10161	1.4518
C	-3.95525	6.40514	0.53324
H	-2.2762	7.35346	-0.46577
H	-5.44988	5.18037	1.52399
H	-4.56099	7.31705	0.56272

H	-4.9106	1.95626	0.54334
H	-7.26699	1.90352	-0.31589
C	-2.63378	-1.47799	-0.8112
C	-2.9131	-0.14584	-0.06581
C	-2.03749	1.017	-0.6938
C	-2.50073	1.94042	-0.32713
H	-2.15345	1.00005	-1.78842
C	-2.746	-0.32868	1.45584
C	-2.04199	0.59643	2.25102
C	-3.37172	-1.42568	2.08761
C	-1.96271	0.42074	3.64377
H	-1.53694	1.44671	1.78458
C	-3.28304	-1.60448	3.47427
H	-3.93962	-2.14658	1.48832
C	-2.5773	-0.67817	4.26032
H	-1.40817	1.14919	4.2447
H	-3.77007	-2.46675	3.9421
H	-2.50754	-0.81425	5.34458
•	-1.53595	-2.05772	-0.91067
N	-3.79997	-1.91304	-1.40931
C	-3.87547	-3.10207	-2.24382
H	-4.6189	-3.81312	-1.84433
H	-4.15336	-2.83488	-3.27833
H	-2.87938	-3.56765	-2.23981
Pd	-0.07049	-0.15227	-0.40592
P	2.11458	-0.88182	-0.12379
C	3.42912	0.39409	0.1338
C	4.77697	0.18763	-0.23449
C	3.0517	1.61818	0.72473
C	5.73413	1.18611	0.00446
H	5.07503	-0.74983	-0.71594
C	4.01332	2.6131	0.96192
H	1.99763	1.79556	0.96157
C	5.35426	2.39813	0.60553
H	6.77718	1.01884	-0.28556
H	3.70645	3.56472	1.40773
H	6.10173	3.17879	0.78347
C	2.74687	-1.86628	-1.56256
C	3.55649	-3.01312	-1.42109
C	2.38424	-1.43701	-2.85874
C	4.0028	-3.71	-2.55646
H	3.83148	-3.36515	-0.42137
C	2.83881	-2.13	-3.99013
H	1.73399	-0.56098	-2.96813
C	3.64862	-3.26887	-3.84132
H	4.62794	-4.60126	-2.43448
H	2.55228	-1.78593	-4.98974
H	3.99635	-3.8151	-4.72464
C	2.31955	-2.04327	1.30608
C	3.4392	-2.03151	2.16345
C	1.28302	-2.97532	1.54021
C	3.52415	-2.94151	3.23069
H	4.24253	-1.30668	1.99853
C	1.37783	-3.88972	2.59914
H	0.3978	-2.97141	0.8932
C	2.4976	-3.87358	3.44842
H	4.39616	-2.91918	3.89333
H	0.56858	-4.60772	2.76968
H	2.56537	-4.58076	4.28203
C	-0.35876	1.78167	-0.4066
C	-0.07467	3.00067	-0.37577
C	0.28375	4.37122	-0.3275
C	0.30536	5.0819	0.90856
C	0.62944	5.08723	-1.51066
C	0.65541	6.43583	0.95248
H	0.04129	4.54848	1.82746
C	0.97526	6.44138	-1.45321
H	0.62188	4.55624	-2.4676
C	0.9921	7.12697	-0.2251
H	0.66433	6.95854	1.91563
H	1.23741	6.96886	-2.37724
H	1.26485	8.18659	-0.18639

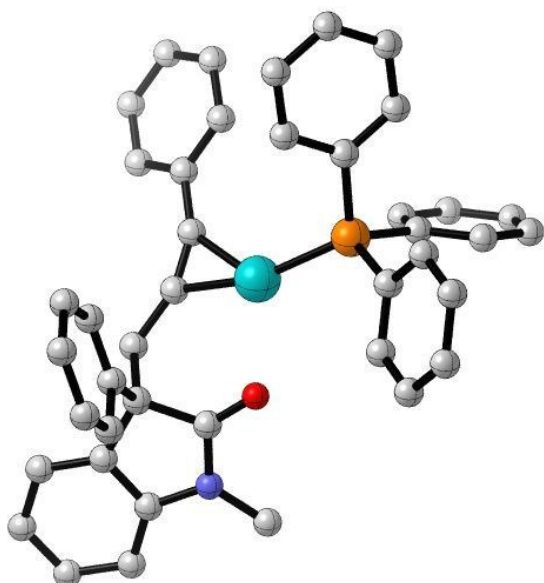
TS 28-29



Zero-point correction= 0.616372 (Hartree/Particle)
 Thermal correction to Energy= 0.658940
 Thermal correction to Enthalpy= 0.659885
 Thermal correction to Gibbs Free Energy= 0.532699
 Sum of electronic and zero-point Energies= -2218.436629
 Sum of electronic and thermal Energies= -2218.394060
 Sum of electronic and thermal Enthalpies= -2218.393116
 Sum of electronic and thermal Free Energies= -2218.520301
 E(RM06L) = -2220.64402574
 Imaginary frequency = -307.34 cm⁻¹

C	-7.02059	0.0212	-1.36126
C	-6.1584	-1.04226	-1.69707
C	-4.8487	-0.98457	-1.21147
C	-4.38405	0.08645	-0.41738
C	-5.25214	1.12746	-0.08611
C	-6.57751	1.09171	-0.56714
H	-8.05291	0.00591	-1.72514
H	-6.50598	-1.87768	-2.31219

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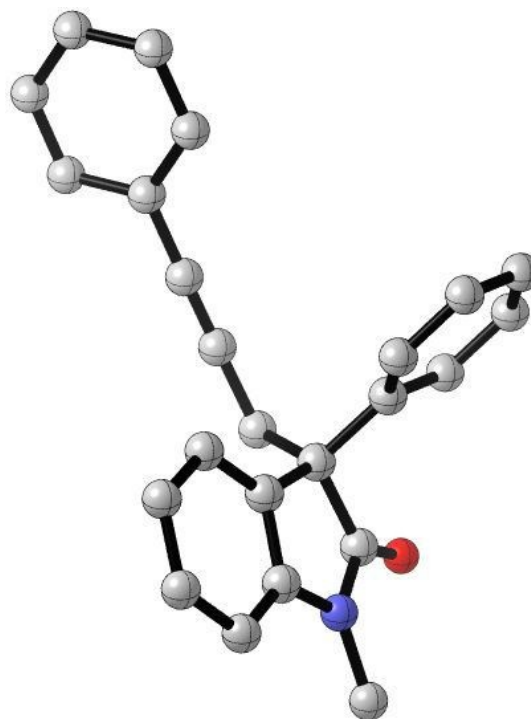


Zero-point correction= 0.619076 (Hartree/Particle)
 Thermal correction to Energy= 0.661447
 Thermal correction to Enthalpy= 0.662391
 Thermal correction to Gibbs Free Energy= 0.535798
 Sum of electronic and zero-point Energies= -2218.497332
 Sum of electronic and thermal Energies= -2218.454962
 Sum of electronic and thermal Enthalpies= -2218.454018
 Sum of electronic and thermal Free Energies= -2218.580611
 E(RM06L) = -2220.70965828

C	-7.32084	-0.32045	-1.65754
C	-6.21361	-1.1162	-2.01298
C	-4.99431	-0.84078	-1.38383
C	-4.85712	0.18842	-0.42763
C	-5.96386	0.96364	-0.08186
C	-7.20298	0.70475	-0.70483
H	-8.28857	-0.51152	-2.13243
H	-6.30904	-1.91748	-2.75165
H	-5.87428	1.75358	0.67135
H	-8.07898	1.30488	-0.4403
C	-2.77411	-0.93962	-0.74307
C	-3.4042	0.25907	0.03444
C	-2.77761	1.5972	-0.49857
H	-3.2862	2.42684	0.03138
H	-3.07221	1.69424	-1.56201
C	-3.26591	0.05082	1.55101
C	-2.58775	0.95625	2.38876
C	-3.86469	-1.08749	2.1345
C	-2.51576	0.72957	3.77443
H	-2.0895	1.83223	1.9658
C	-3.78609	-1.31749	3.5139
H	-4.40793	-1.79762	1.50039
C	-3.11121	-0.40511	4.34245
H	-1.98328	1.44716	4.40757
H	-4.25673	-2.20839	3.94304
H	-3.05	-0.58023	5.42162
•	-1.60772	-1.35762	-0.69596
N	-3.75412	-1.48847	-1.55936
C	-3.51206	-2.60442	-2.45929
H	-4.12597	-3.47767	-2.17677
H	-3.74642	-2.32159	-3.50003
H	-2.44641	-2.86273	-2.38035
Pd	0.1663	0.27748	-0.23407
P	2.20816	-0.8106	-0.07774
C	3.44294	-0.06117	1.09314
C	4.83799	-0.08274	0.88063
C	2.93677	0.56412	2.25358
C	5.70811	0.49926	1.81801
H	5.24408	-0.5469	-0.02441
C	3.80809	1.13512	3.19338
H	1.85045	0.61198	2.39575
C	5.19618	1.10438	2.97706
H	6.78882	0.48151	1.6391
H	3.40188	1.61669	4.08938
H	5.8763	1.55961	3.70504
C	3.155	-0.90091	-1.67569

C	3.98414	-1.98545	-2.03265
C	3.01259	0.1777	-2.57649
C	4.6663	-1.98448	-3.26095
H	4.08704	-2.83807	-1.35325
C	3.70267	0.18061	-3.79791
H	2.34354	1.00472	-2.31104
C	4.53043	-0.90104	-4.14352
H	5.30244	-2.83528	-3.52897
H	3.5843	1.02446	-4.48621
H	5.06112	-0.9033	-5.10176
C	2.16687	-2.58819	0.47233
C	3.18554	-3.19987	1.23391
C	1.03508	-3.34974	0.10532
C	3.08051	-4.54984	1.60839
H	4.05926	-2.61713	1.54399
C	0.93789	-4.70016	0.47436
H	0.22293	-2.87137	-0.45335
C	1.95948	-5.30378	1.22635
H	3.87632	-5.01116	2.20351
H	0.05456	-5.27982	0.18465
H	1.87787	-6.35535	1.52197
C	-1.30619	1.72765	-0.38765
C	-0.19286	2.36836	-0.34564
C	0.58085	3.58961	-0.36341
C	-0.04804	4.82291	-0.68276
C	1.96574	3.59517	-0.06937
C	0.68774	6.01347	-0.70632
H	-1.11761	4.82945	-0.9175
C	2.69493	4.79123	-0.09056
H	2.44768	2.64531	0.1812
C	2.06264	6.00474	-0.41052
H	0.18662	6.95463	-0.95848
H	3.76496	4.775	0.14307
H	2.63593	6.93761	-0.43114

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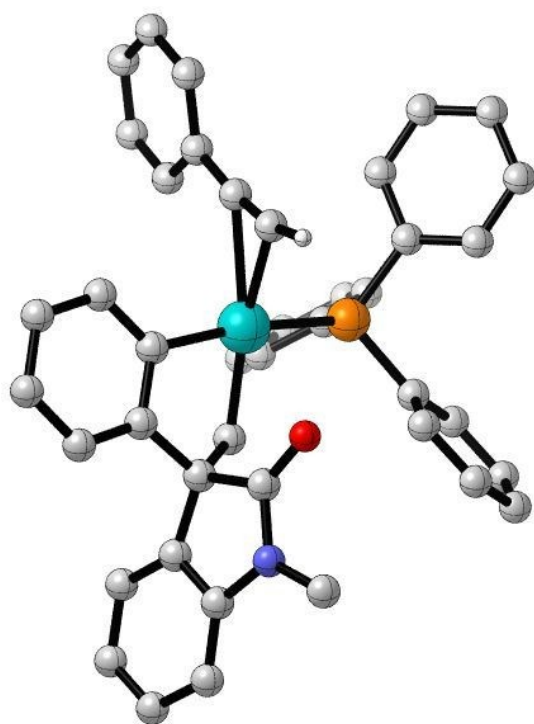


Zero-point correction= 0.351586 (Hartree/Particle)
 Thermal correction to Energy= 0.374006
 Thermal correction to Enthalpy= 0.374950
 Thermal correction to Gibbs Free Energy= 0.297354
 Sum of electronic and zero-point Energies= -1055.599078
 Sum of electronic and thermal Energies= -1055.576657
 Sum of electronic and thermal Enthalpies= -1055.575713
 Sum of electronic and thermal Free Energies= -1055.653310
 E(RM06L) = -1056.18051589

C	2.601	-3.23029	1.66532
C	3.48488	-2.43663	0.90866
C	2.94679	-1.34098	0.22473
C	1.57164	-1.01525	0.28529

C	0.70753	-1.82342	1.02795
C	1.23018	-2.93593	1.72137
H	2.99441	-4.09406	2.21098
H	4.5508	-2.67625	0.85358
H	-0.36272	-1.59954	1.05877
H	0.55928	-3.57305	2.30551
C	2.72816	0.46584	-1.20014
C	1.31652	0.21363	-0.57342
C	0.33423	-0.08531	-1.76614
H	0.68707	-0.99504	-2.28852
H	0.43192	0.74516	-2.49075
C	0.88292	1.47929	0.19542
C	0.79645	2.70974	-0.49195
C	0.57123	1.45194	1.5679
C	0.39163	3.87417	0.17456
H	1.08175	2.75744	-1.54652
C	0.16331	2.61958	2.23359
H	0.65204	0.51469	2.12469
C	0.0675	3.83424	1.54022
H	0.33344	4.81834	-0.37718
H	-0.07575	2.57465	3.30152
H	-0.25116	4.7441	2.05948
O	3.01979	1.29486	-2.06138
N	3.61478	-0.44035	-0.62524
C	5.02334	-0.49512	-0.97554
H	5.65616	-0.34953	-0.08296
H	5.27737	-1.46377	-1.44135
H	5.20676	0.31681	-1.6946
C	-1.05831	-0.24706	-1.36124
C	-2.23063	-0.36616	-1.02177
C	-3.59607	-0.48918	-0.61809
C	-4.48322	-1.35356	-1.30843
C	-4.08696	0.2572	0.48383
C	-5.81956	-1.46378	-0.90598
H	-4.10855	-1.93018	-2.15931
C	-5.42444	0.13721	0.87913
H	-3.40439	0.92675	1.01531
C	-6.29551	-0.72141	0.1877
H	-6.49417	-2.13379	-1.44914
H	-5.79041	0.71936	1.73131
H	-7.34119	-0.81101	0.49922

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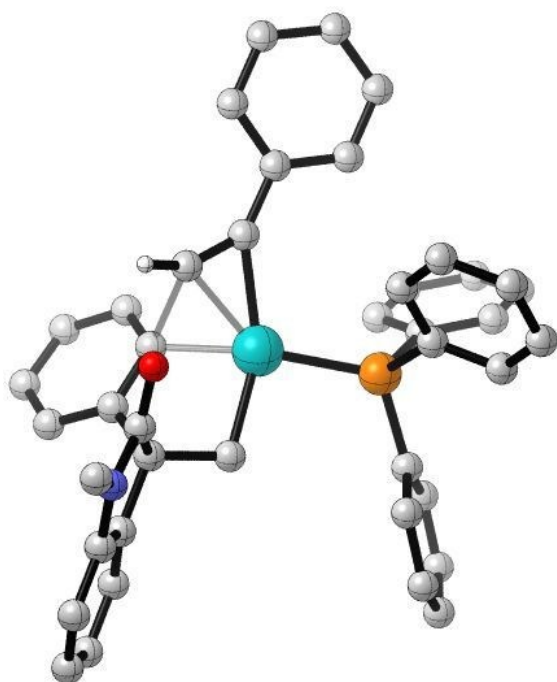


Zero-point correction=	0.615748 (Hartree/Particle)
Thermal correction to Energy=	0.658518
Thermal correction to Enthalpy=	0.659463
Thermal correction to Gibbs Free Energy=	0.535181
Sum of electronic and zero-point Energies=	-2218.455862
Sum of electronic and thermal Energies=	-2218.413092

Sum of electronic and thermal Enthalpies=	-2218.412147
Sum of electronic and thermal Free Energies=	-2218.536429
E(RM06L) =	-2220.66820116

Pd	-0.06177	-0.76481	0.31013
P	-1.35297	1.28452	-0.06543
O	2.43725	0.27172	2.25666
N	4.46531	0.66408	1.1973
C	1.20638	-2.37186	0.44089
C	0.82752	-3.70036	0.71513
H	-0.22687	-3.95348	0.86962
C	1.7941	-4.72079	0.79495
H	1.48076	-5.75105	1.00217
C	3.15464	-4.42526	0.61118
H	3.90569	-5.22051	0.67466
C	3.5511	-3.10671	0.33627
H	4.60932	-2.86926	0.17577
C	2.58199	-2.09178	0.24332
C	2.88969	-0.6308	-0.05451
C	1.61037	-0.05448	-0.72551
H	1.54121	-0.47731	-1.74425
H	1.64464	1.04575	-0.79802
C	4.1679	-0.37275	-0.83719
C	4.54972	-0.76167	-2.12188
H	3.87536	-1.36744	-2.73688
C	5.81417	-0.37344	-2.61391
H	6.12145	-0.67357	-3.62077
C	6.68195	0.39212	-1.81826
H	7.66112	0.68655	-2.21051
C	6.31643	0.78893	-0.51616
H	6.99589	1.38293	0.10278
C	5.05693	0.39402	-0.05032
C	3.1781	0.12924	1.28047
C	5.07829	1.42231	2.27155
H	4.35485	1.44305	3.10039
H	5.30514	2.45515	1.951
H	6.01356	0.94198	2.61024
C	-0.38016	2.84054	0.18683
C	0.62618	2.82471	1.17792
H	0.85496	1.89411	1.71184
C	1.35929	3.9904	1.4547
H	2.1355	3.96676	2.22663
C	1.11097	5.17065	0.73597
H	1.69078	6.07571	0.94662
C	0.12353	5.18517	-0.26319
H	-0.06751	6.10006	-0.8343
C	-0.62209	4.02779	-0.5357
H	-1.38796	4.04657	-1.3174
C	-2.85304	1.57331	0.98785
C	-2.86151	2.52373	2.03039
H	-1.98756	3.16141	2.195
C	-3.98938	2.66404	2.85583
H	-3.98126	3.40987	3.65792
C	-5.12222	1.86183	2.65038
H	-6.00184	1.97551	3.29268
C	-5.12069	0.91034	1.61659
H	-5.99842	0.27715	1.4492
C	-3.99364	0.76092	0.79561
H	-4.00506	0.01269	-0.00367
C	-2.02459	1.44265	-1.7862
C	-3.16152	2.22008	-2.10102
H	-3.70734	2.73534	-1.30416
C	-3.60675	2.3205	-3.4287
H	-4.49084	2.92447	-3.65954
C	-2.92455	1.6483	-4.4563
H	-3.27554	1.72697	-5.49068
C	-1.79672	0.86929	-4.1518
H	-1.26434	0.33683	-4.94704
C	-1.35163	0.76317	-2.82473
H	-0.48159	0.14471	-2.57935
C	-1.96133	-1.97888	1.24395
C	-1.22424	-1.4315	2.08687
H	-0.77066	-1.10209	3.00797
C	-2.9144	-2.68893	0.44385
C	-2.88919	-2.61382	-0.97126
C	-3.90729	-3.48317	1.07626
C	-3.83695	-3.31225	-1.73041
H	-2.11511	-2.00444	-1.44891
C	-4.84618	-4.17854	0.30584
H	-3.92716	-3.54478	2.16845
C	-4.81671	-4.09541	-1.09764
H	-3.80764	-3.24643	-2.82286
H	-5.60593	-4.79014	0.80366
H	-5.554	-4.64167	-1.69487

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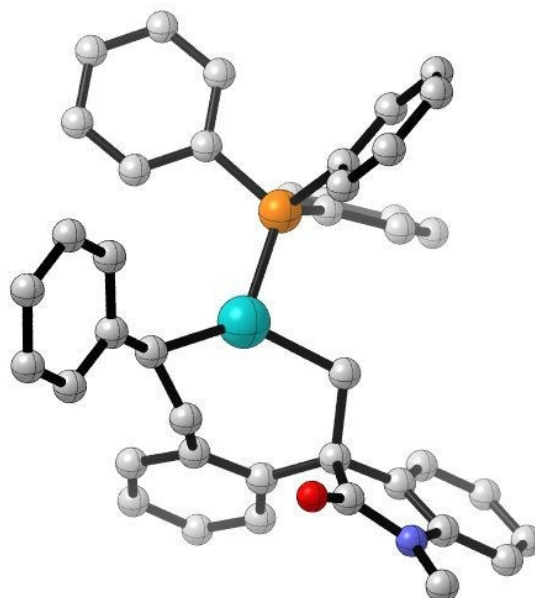


Zero-point correction= 0.615278 (Hartree/Particle)
 Thermal correction to Energy= 0.656970
 Thermal correction to Enthalpy= 0.657915
 Thermal correction to Gibbs Free Energy= 0.536356
 Sum of electronic and zero-point Energies= -2218.428623
 Sum of electronic and thermal Energies= -2218.386930
 Sum of electronic and thermal Enthalpies= -2218.385986
 Sum of electronic and thermal Free Energies= -2218.507545
 E(RM06L) = -2220.63199906
 Imaginary frequency = -268.39 cm⁻¹

Pd	-0.02439	-0.61122	-0.24151
P	-1.36039	1.32488	-0.11339
O	2.14715	-1.55946	2.21328
N	4.22186	-0.53321	2.04221
C	1.22948	-2.13955	-0.9914
C	0.85152	-3.06577	-1.98943
H	-0.20771	-3.31223	-2.10881
C	1.81827	-3.70479	-2.78314
H	1.50476	-4.42417	-3.54759
C	3.17968	-3.43913	-2.57385
H	3.94161	-3.95582	-3.16726
C	3.56858	-2.48102	-1.62071
H	4.62632	-2.21713	-1.51397
C	2.61178	-1.80245	-0.84743
C	2.93834	-0.59438	0.02233
C	1.79682	0.45093	-0.23049
H	1.95554	0.90258	-1.22545
H	1.82215	1.25766	0.52279
C	4.30996	0.03196	-0.18663
C	4.90206	0.58277	-1.3249
H	4.37467	0.56111	-2.28464
C	6.1859	1.16035	-1.22622
H	6.65843	1.58875	-2.11579
C	6.85956	1.18963	0.00578
H	7.85455	1.64241	0.07078
C	6.27622	0.64364	1.16665
H	6.80189	0.6673	2.1261
C	5.00463	0.0707	1.04408
C	2.99692	-0.97818	1.53633
C	4.60751	-0.70389	3.43074
H	3.77356	-1.21826	3.9315
H	4.78438	0.27262	3.91606
H	5.52364	-1.31533	3.51576
C	-0.55186	2.93284	-0.55269
C	0.28626	3.57507	0.38697
H	0.39061	3.16354	1.39638
C	0.97323	4.74874	0.04245
H	1.61406	5.23772	0.78372
C	0.84279	5.29203	-1.24613
H	1.38126	6.20692	-1.51445

C	0.0199	4.65511	-2.1881
H	-0.08918	5.07257	-3.19476
C	-0.67342	3.4832	-1.846
H	-1.3166	2.99799	-2.58674
C	-2.10091	1.66856	1.5478
C	-2.58737	2.94347	1.91753
H	-2.49382	3.7874	1.22613
C	-3.16711	3.1405	3.18027
H	-3.54049	4.13231	3.4569
C	-3.26023	2.07254	4.08851
H	-3.70853	2.2304	5.07519
C	-2.7675	0.80724	3.73296
H	-2.82635	-0.02627	4.44032
C	-2.18649	0.60474	2.47091
H	-1.78813	-0.37793	2.19524
C	-2.7903	1.24923	-1.29145
C	-3.95912	2.0259	-1.1432
H	-4.07137	2.69049	-0.28085
C	-4.99113	1.93515	-2.09003
H	-5.89835	2.53528	-1.96207
C	-4.86365	1.0781	-3.19611
H	-5.67158	1.01004	-3.93226
C	-3.70409	0.30137	-3.34934
H	-3.60358	-0.37703	-4.2029
C	-2.67559	0.37946	-2.39719
H	-1.77893	-0.24621	-2.48753
C	-1.29948	-2.33907	0.25381
C	-0.04562	-2.6414	0.45963
H	0.65047	-3.13927	1.1294
C	-2.63031	-2.8544	0.48705
C	-3.77597	-2.02044	0.43466
C	-2.82411	-4.23761	0.76353
C	-5.05446	-2.5386	0.6786
H	-3.64625	-0.96176	0.19397
C	-4.10438	-4.75107	0.99469
H	-1.9508	-4.89754	0.78972
C	-5.22754	-3.90431	0.95891
H	-5.92322	-1.87258	0.63859
H	-4.22906	-5.81881	1.20663
H	-6.22895	-4.3089	1.13981

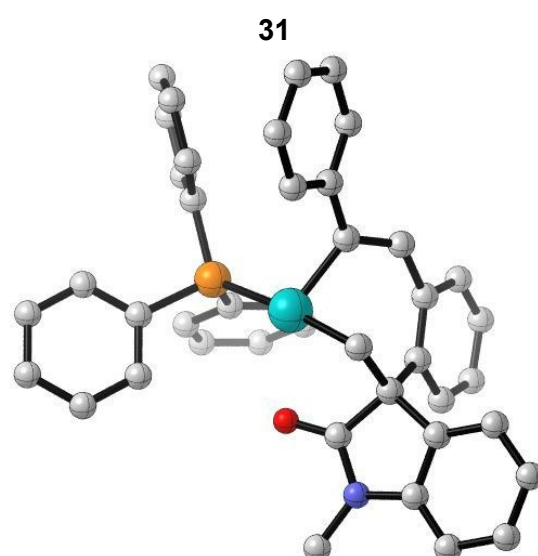
31a



Zero-point correction= 0.618072 (Hartree/Particle)
 Thermal correction to Energy= 0.659677
 Thermal correction to Enthalpy= 0.660621
 Thermal correction to Gibbs Free Energy= 0.539273
 Sum of electronic and zero-point Energies= -2218.456814
 Sum of electronic and thermal Energies= -2218.415209
 Sum of electronic and thermal Enthalpies= -2218.414265
 Sum of electronic and thermal Free Energies= -2218.535613
 E(RM06L) = -2220.66117463

Pd	-0.31961	-0.58321	-0.17335
P	-1.61113	1.3003	0.05344
O	2.62082	-2.55907	1.49144

N	4.43393	-1.13523	1.61409
C	1.40953	-1.94346	-1.65186
C	1.16483	-2.30812	-2.99792
H	0.29846	-2.9443	-3.20495
C	2.02233	-1.92068	-4.03531
H	1.81173	-2.2296	-5.06489
C	3.16221	-1.16501	-3.73421
H	3.86358	-0.8743	-4.52343
C	3.40081	-0.75951	-2.41005
H	4.27544	-0.13844	-2.19969
C	2.53233	-1.09536	-1.35431
C	2.73125	-0.47107	0.05364
C	1.45182	0.29889	0.57133
H	1.49307	1.32367	0.16779
H	1.44405	0.35025	1.67393
C	3.89012	0.52802	0.12653
C	4.08136	1.75694	-0.51305
H	3.34727	2.12088	-1.23973
C	5.22961	2.52142	-0.21895
H	5.3876	3.47875	-0.72558
C	6.16894	2.06289	0.71948
H	7.05585	2.66559	0.9414
C	5.98569	0.83694	1.38732
H	6.71185	0.48319	2.12541
C	4.84205	0.09126	1.07411
C	3.19402	-1.53669	1.10857
C	5.14129	-1.88245	2.638
H	4.54407	-2.78284	2.84512
H	5.24478	-1.28819	3.56374
H	6.14649	-2.17562	2.28721
C	-0.93039	2.891	-0.6043
C	0.03998	3.60848	0.13245
H	0.31855	3.27706	1.13787
C	0.639	4.7567	-0.40908
H	1.38204	5.30619	0.17848
C	0.28697	5.19895	-1.69461
H	0.75488	6.09497	-2.11562
C	-0.66748	4.48548	-2.4375
H	-0.94744	4.82274	-3.44115
C	-1.27173	3.33909	-1.89892
H	-2.01707	2.7924	-2.48491
C	-1.98269	1.66919	1.8301
C	-2.379	2.94388	2.29083
H	-2.42169	3.78935	1.59647
C	-2.68752	3.14245	3.64569
H	-2.98971	4.13621	3.99312
C	-2.60312	2.07369	4.55331
H	-2.84261	2.23235	5.61012
C	-2.19912	0.80575	4.10491
H	-2.11807	-0.02807	4.81005
C	-1.88617	0.60453	2.7516
H	-1.54845	-0.37524	2.39179
C	-3.27815	1.19274	-0.76547
C	-4.26335	2.19064	-0.59731
H	-4.06242	3.06264	0.03285
C	-5.50762	2.06933	-1.23239
H	-6.26688	2.84625	-1.09243
C	-5.77989	0.9545	-2.04481
H	-6.75294	0.86238	-2.5391
C	-4.80485	-0.0395	-2.21676
H	-5.01187	-0.91159	-2.84602
C	-3.55852	0.07538	-1.57725
H	-2.79215	-0.70392	-1.68595
C	-0.8544	-2.52308	-0.54483
C	0.5456	-2.5616	-0.59518
H	1.10093	-3.10549	0.18454
C	-1.71953	-3.53772	0.01795
C	-2.96947	-3.1824	0.59661
C	-1.3799	-4.91969	-0.04427
C	-3.82172	-4.15806	1.12227
H	-3.24414	-2.12242	0.61803
C	-2.24322	-5.89489	0.46617
H	-0.42705	-5.20496	-0.50257
C	-3.46394	-5.51822	1.05597
H	-4.7752	-3.86483	1.57472
H	-1.96611	-6.95332	0.41066
H	-4.13937	-6.28311	1.454

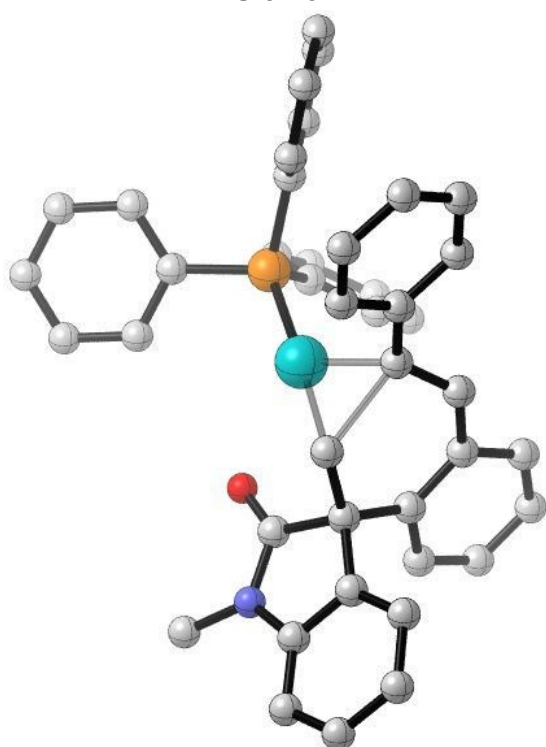


Zero-point correction= 0.619572 (Hartree/Particle)
 Thermal correction to Energy= 0.660765
 Thermal correction to Enthalpy= 0.661709
 Thermal correction to Gibbs Free Energy= 0.542778
 Sum of electronic and zero-point Energies= -2218.494846
 Sum of electronic and thermal Energies= -2218.453653
 Sum of electronic and thermal Enthalpies= -2218.452709
 Sum of electronic and thermal Free Energies= -2218.571640
 E(RM06L) = -2220.70312550

Pd	-0.09032	0.32997	-0.68504
P	1.92285	-0.82993	-0.03177
•	-1.53397	-1.69561	-0.86725
N	-3.84894	-1.69796	-1.1029
C	-1.75107	1.47834	1.84368
C	-1.82074	1.6053	3.26069
H	-1.18075	2.36113	3.73093
C	-2.62593	0.79418	4.06354
H	-2.62623	0.92524	5.15099
C	-3.42734	-0.1849	3.45675
H	-4.06623	-0.84153	4.05623
C	-3.4239	-0.29181	2.06175
H	-4.09577	-1.01904	1.59237
C	-2.62036	0.51839	1.22728
C	-2.86816	0.33219	-0.30008
C	-1.92732	1.13034	-1.22519
H	-2.08277	2.21232	-1.12258
H	-2.08061	0.84228	-2.28277
C	-4.35797	0.50353	-0.61153
C	-5.19946	1.61124	-0.50682
H	-4.81124	2.56658	-0.13844
C	-6.55364	1.48108	-0.87913
H	-7.22124	2.34536	-0.80551
C	-7.05399	0.25238	-1.3408
H	-8.108	0.16608	-1.62391
C	-6.21971	-0.87912	-1.44458
H	-6.61045	-1.83705	-1.80113
C	-4.88053	-0.72453	-1.074
C	-2.64299	-1.13741	-0.73866
C	-3.98	-3.03668	-1.65606
H	-2.98561	-3.50443	-1.62314
H	-4.33288	-2.99441	-2.70163
H	-4.69032	-3.63672	-1.06182
C	2.47953	-2.03909	-1.32564
C	1.48371	-2.75691	-2.02774
H	0.42622	-2.59444	-1.79076
C	1.84647	-3.67927	-3.02055
H	1.06729	-4.23104	-3.55753
C	3.20017	-3.8893	-3.33338
H	3.47964	-4.60426	-4.11458
C	4.19273	-3.17506	-2.64452
H	5.24994	-3.3316	-2.88473
C	3.83668	-2.25487	-1.64434
H	4.61545	-1.69941	-1.11255
C	1.63756	-1.8964	1.45492
C	2.25936	-3.15127	1.63106
H	2.93528	-3.53714	0.86073
C	2.00595	-3.90937	2.78554
H	2.48986	-4.88402	2.91171

C	1.13248	-3.42278	3.77226
H	0.93365	-4.0186	4.66965
C	0.50784	-2.17649	3.60089
H	-0.18534	-1.79455	4.35728
C	0.75366	-1.4181	2.44614
H	0.24812	-0.45699	2.30198
C	3.47543	0.08966	0.38082
C	4.29787	-0.25287	1.47475
H	4.0178	-1.08552	2.12733
C	5.47261	0.47243	1.73193
H	6.10119	0.19945	2.58649
C	5.83895	1.54241	0.90003
H	6.75377	2.10891	1.10462
C	5.02355	1.89009	-0.18966
H	5.29068	2.73353	-0.83415
C	3.84541	1.17286	-0.44556
H	3.19887	1.46807	-1.27805
C	0.05482	2.13987	0.14331
C	-0.76661	2.38281	1.20307
H	-0.65289	3.34586	1.7301
C	0.96487	3.16498	-0.4034
C	1.61681	4.1077	0.43258
C	1.20198	3.24452	-1.79876
C	2.44773	5.09818	-0.10798
H	1.48323	4.04181	1.51738
C	2.02524	4.24234	-2.3389
H	0.72037	2.50065	-2.44414
C	2.65389	5.17573	-1.49628
H	2.94651	5.809	0.56039
H	2.18046	4.28922	-3.42255
H	3.30505	5.94999	-1.9159

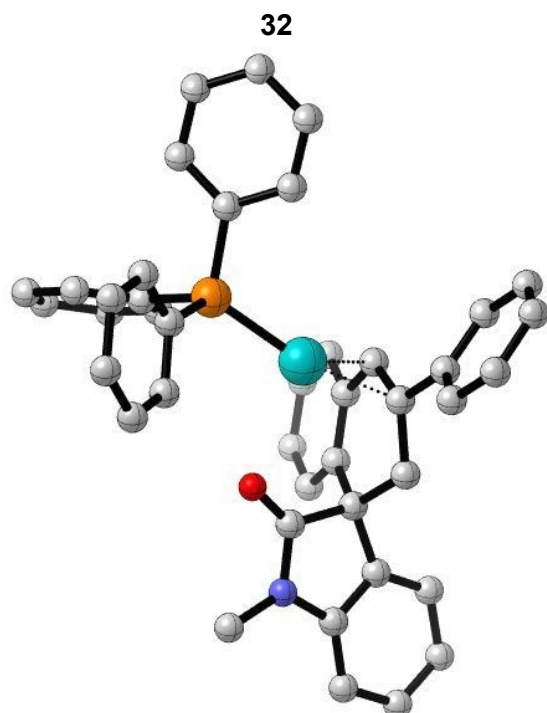
TS 31-32



Zero-point correction= 0.618024 (Hartree/Particle)
 Thermal correction to Energy= 0.659172
 Thermal correction to Enthalpy= 0.660116
 Thermal correction to Gibbs Free Energy= 0.539611
 Sum of electronic and zero-point Energies= -2218.485335
 Sum of electronic and thermal Energies= -2218.444186
 Sum of electronic and thermal Enthalpies= -2218.443242
 Sum of electronic and thermal Free Energies= -2218.563747
 E(RM06L) = -2220.69023173
 Imaginary frequency = -291.59 cm⁻¹

Pd	0.05485	0.24045	-0.45702
P	2.19555	-0.61828	-0.11312
•	-1.55779	-2.04705	-0.8731
N	-3.81587	-1.86535	-1.39266
C	-2.02667	0.76805	2.19871

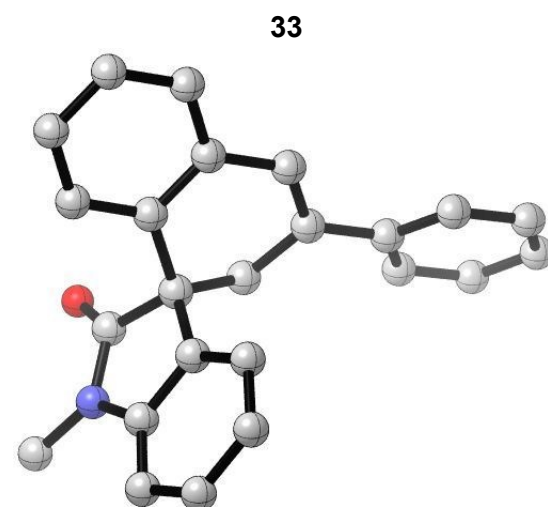
C	-2.1124	0.63909	3.61159
H	-1.58369	1.37667	4.22711
C	-2.8215	-0.39789	4.22297
H	-2.8527	-0.47188	5.31531
C	-3.49173	-1.33934	3.42465
H	-4.05174	-2.16217	3.88038
C	-3.45675	-1.20278	2.03054
H	-4.0202	-1.91351	1.41515
C	-2.74406	-0.16597	1.39628
C	-2.88589	-0.04859	-0.14098
C	-1.94419	0.96553	-0.84342
H	-2.40526	1.95976	-0.89699
H	-1.75445	0.6649	-1.89909
C	-4.34921	0.20042	-0.5165
C	-5.19003	1.28086	-0.25021
H	-4.82639	2.13484	0.33151
C	-6.51524	1.25346	-0.7336
H	-7.18381	2.09606	-0.5315
C	-6.98339	0.1516	-1.46781
H	-8.01443	0.14246	-1.83599
C	-6.1477	-0.9505	-1.73959
H	-6.5147	-1.80878	-2.31054
C	-4.8374	-0.90136	-1.25191
C	-2.63018	-1.43657	-0.80776
C	-3.92463	-3.09977	-2.15142
H	-2.94683	-3.60007	-2.09492
H	-4.17247	-2.89256	-3.20762
H	-4.70196	-3.75668	-1.72377
C	2.73164	-1.77314	-1.46389
C	1.75032	-2.63744	-2.00236
H	0.72196	-2.5965	-1.62289
C	2.08771	-3.53739	-3.02404
H	1.32124	-4.20486	-3.43251
C	3.39797	-3.57583	-3.53109
H	3.6561	-4.27316	-4.3353
C	4.37272	-2.71099	-3.00966
H	5.39396	-2.73084	-3.40556
C	4.04383	-1.8136	-1.97959
H	4.8075	-1.13829	-1.5803
C	2.36793	-1.65475	1.41319
C	3.26495	-2.7405	1.50734
H	3.88064	-3.01429	0.64383
C	3.35638	-3.4818	2.69647
H	4.05272	-4.32518	2.75853
C	2.55209	-3.14914	3.79883
H	2.62124	-3.73238	4.72338
C	1.64841	-2.07762	3.70739
H	1.00423	-1.82525	4.55603
C	1.5514	-1.33661	2.51974
H	0.82748	-0.51821	2.4334
C	3.58959	0.59491	0.00969
C	4.75885	0.3547	0.76319
H	4.86129	-0.57574	1.33137
C	5.78612	1.31151	0.79907
H	6.68743	1.11748	1.39066
C	5.65646	2.51447	0.08561
H	6.45722	3.26108	0.11962
C	4.49219	2.76306	-0.6595
H	4.37409	3.70594	-1.20307
C	3.46078	1.81231	-0.69257
H	2.53803	2.0162	-1.2474
C	-0.64184	1.93874	0.43594
C	-1.24243	1.88252	1.66315
H	-1.14665	2.75084	2.33225
C	-0.01875	3.17848	-0.08704
C	0.60875	4.10204	0.78857
C	-0.0127	3.47928	-1.47194
C	1.19617	5.27667	0.30124
H	0.66153	3.87634	1.85814
C	0.5661	4.66093	-1.95635
H	-0.46026	2.76684	-2.1717
C	1.17354	5.56897	-1.07319
H	1.68373	5.96473	1.00063
H	0.54672	4.8693	-3.03169
H	1.63232	6.48834	-1.45179



Zero-point correction= 0.620804 (Hartree/Particle)
 Thermal correction to Energy= 0.662295
 Thermal correction to Enthalpy= 0.663239
 Thermal correction to Gibbs Free Energy= 0.539661
 Sum of electronic and zero-point Energies= -2218.549780
 Sum of electronic and thermal Energies= -2218.508289
 Sum of electronic and thermal Enthalpies= -2218.507345
 Sum of electronic and thermal Free Energies= -2218.630923
 E(RM06L) = -2220.75615974

Pd	0.34333	0.57592	0.03501
P	2.39132	-0.46042	-0.12582
O	-1.37361	-1.1096	-1.29671
N	-3.61298	-1.40037	-1.82588
C	-1.72933	-0.00803	2.20907
C	-1.3995	-0.56079	3.47061
H	-0.58805	-0.10043	4.04644
C	-2.08317	-1.66914	3.98379
H	-1.80752	-2.07609	4.96261
C	-3.12464	-2.24934	3.24175
H	-3.66744	-3.11753	3.62913
C	-3.47571	-1.70185	1.99682
H	-4.30262	-2.13987	1.42785
C	-2.79949	-0.5881	1.47099
C	-3.18292	-0.02738	0.09029
C	-2.73188	1.45712	-0.08941
H	-3.50814	2.09705	0.37935
H	-2.76	1.70527	-1.16412
C	-4.67339	-0.15232	-0.2094
C	-5.7803	0.3977	0.43759
H	-5.6475	1.01704	1.33123
C	-7.07196	0.13571	-0.06603
H	-7.9466	0.56284	0.43409
C	-7.24122	-0.67178	-1.20258
H	-8.24853	-0.86832	-1.58399
C	-6.13431	-1.23861	-1.86484
H	-6.26865	-1.86799	-2.74955
C	-4.86227	-0.96338	-1.34871
C	-2.56491	-0.89866	-1.05417
C	-3.40461	-2.24169	-2.99141
H	-2.31995	-2.39822	-3.08504
H	-3.78779	-1.75361	-3.90509
H	-3.90855	-3.21629	-2.86765
C	2.97679	-0.62419	-1.88227
C	2.00527	-0.97135	-2.84955
H	0.96509	-1.12233	-2.53547
C	2.36779	-1.11433	-4.19703
H	1.60812	-1.38611	-4.93811
C	3.697	-0.89687	-4.59898
H	3.97657	-0.99901	-5.65309
C	4.66335	-0.53797	-3.64627
H	5.69927	-0.35958	-3.95495

C	4.30743	-0.40298	-2.29345
H	5.06455	-0.11794	-1.55557
C	2.51343	-2.2011	0.50444
C	3.39984	-3.15989	-0.0321
H	4.04434	-2.89411	-0.87704
C	3.44663	-4.45859	0.50064
H	4.13543	-5.19601	0.07399
C	2.60939	-4.81319	1.57111
H	2.64463	-5.82792	1.98211
C	1.71691	-3.86748	2.10264
H	1.04909	-4.14196	2.92607
C	1.66344	-2.57106	1.56842
H	0.94728	-1.83761	1.95723
C	3.79951	0.40753	0.71621
C	4.93471	-0.25393	1.23114
H	5.0095	-1.3442	1.16103
C	5.96278	0.47809	1.84847
H	6.83595	-0.04681	2.25129
C	5.8709	1.87532	1.95341
H	6.67282	2.44315	2.43746
C	4.74132	2.54076	1.44743
H	4.65829	3.62933	1.53605
C	3.70762	1.81102	0.84168
H	2.80467	2.3151	0.47448
C	-1.39456	1.84017	0.53815
C	-0.98356	1.15347	1.70247
H	-0.27464	1.61529	2.39896
C	-0.87178	3.19894	0.20661
C	-0.4052	4.08613	1.20937
C	-0.85425	3.66003	-1.13548
C	0.0828	5.35787	0.88307
H	-0.44611	3.77708	2.25893
C	-0.36782	4.93339	-1.46018
H	-1.19842	2.99762	-1.93682
C	0.10685	5.79073	-0.45386
H	0.43227	6.0225	1.681
H	-0.35563	5.25566	-2.50709
H	0.48294	6.78741	-0.70678

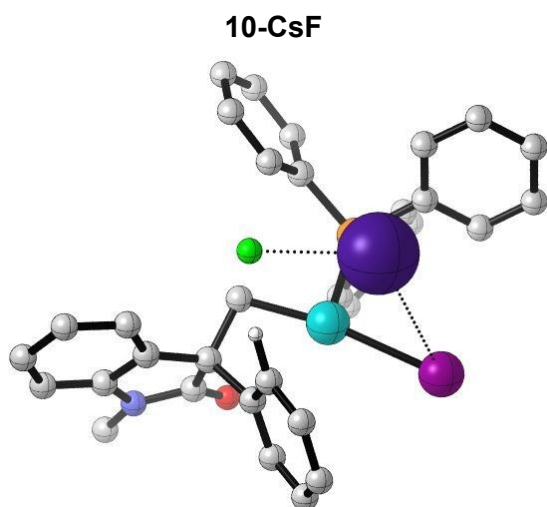


Zero-point correction= 0.354192 (Hartree/Particle)
 Thermal correction to Energy= 0.375156
 Thermal correction to Enthalpy= 0.376100
 Thermal correction to Gibbs Free Energy= 0.304258
 Sum of electronic and zero-point Energies= -1055.659927
 Sum of electronic and thermal Energies= -1055.638963
 Sum of electronic and thermal Enthalpies= -1055.638019
 Sum of electronic and thermal Free Energies= -1055.709860
 E(RM06L) = -1056.23628180

•	-1.91168	-0.06482	-2.77104
N	-2.60324	-1.47882	-1.05233
C	0.02396	2.30191	0.28025
C	-0.19015	3.64207	0.67713
H	0.6651	4.2318	1.02668
C	-1.46394	4.2187	0.61477
H	-1.60958	5.25976	0.92052
C	-2.55011	3.45726	0.15528
H	-3.55003	3.89904	0.09849

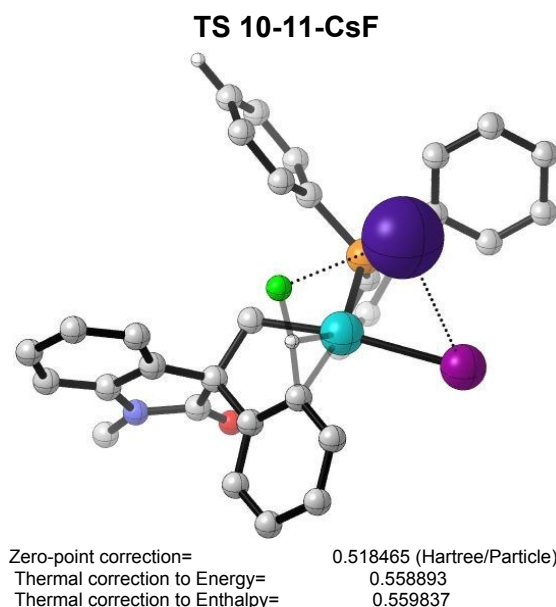
C	-2.35449	2.12134	-0.23228
H	-3.20672	1.53331	-0.58839
C	-1.08204	1.5346	-0.17853
C	-0.85415	0.05509	-0.50828
C	0.58287	-0.17927	-1.05862
H	0.59081	0.18882	-2.10557
H	0.76992	-1.26593	-1.09907
C	-1.21031	-0.84283	0.67602
C	-0.70812	-0.90185	1.97622
H	0.0858	-0.21848	2.29123
C	-1.23566	-1.85275	2.87466
H	-0.84435	-1.90938	3.89498
C	-2.25982	-2.72307	2.47008
H	-2.66229	-3.45519	3.17764
C	-2.78549	-2.67053	1.16441
H	-3.58668	-3.34669	0.85167
C	-2.24618	-1.72275	0.28751
C	-1.83666	-0.45397	-1.60752
C	-3.60115	-2.2137	-1.8087
H	-3.60898	-1.78872	-2.82347
H	-4.60153	-2.10495	-1.35409
H	-3.34673	-3.28712	-1.85914
C	1.66622	0.5236	-0.25905
C	1.35841	1.71279	0.33548
H	2.14143	2.3009	0.82811
C	3.02961	-0.04873	-0.23159
C	3.48434	-0.8974	-1.27061
C	3.92684	0.23358	0.8288
C	4.78476	-1.42008	-1.26157
H	2.82074	-1.1313	-2.10888
C	5.22397	-0.29097	0.83828
H	3.58656	0.84749	1.66888
C	5.6624	-1.11979	-0.20858
H	5.11346	-2.06454	-2.08366
H	5.89311	-0.0637	1.67495
H	6.67554	-1.53427	-0.19767

H	-1.4734	1.93305	0.34726
C	-2.41579	-1.11476	-0.81815
C	-2.65774	-1.44742	-2.17721
C	-1.91425	-2.11788	0.06414
C	-2.46296	-2.75594	-2.63125
H	-2.99886	-0.67412	-2.87062
C	-1.7454	-3.43173	-0.41508
H	-1.66995	-1.85339	1.11859
C	-2.0259	-3.75793	-1.74695
H	-2.65519	-2.99701	-3.68163
H	-1.39786	-4.2147	0.27088
H	-1.88936	-4.78318	-2.10625
O	-2.86811	1.68475	-2.25936
N	-4.77871	1.38783	-0.95933
C	-5.66036	2.23515	-1.74168
H	-6.54403	1.6705	-2.08718
H	-6.00139	3.1044	-1.15093
H	-5.08238	2.58543	-2.60995
Pd	-0.10822	-0.22788	-0.59933
I	1.50015	-2.00156	-2.09725
P	1.40953	1.34401	0.05751
C	1.6002	2.64229	-1.23898
C	2.77131	3.42562	-1.34494
C	0.52942	2.8627	-2.13266
C	2.86429	4.42362	-2.3271
H	3.61247	3.24662	-0.66742
C	0.62941	3.86681	-3.10871
H	-0.37557	2.24491	-2.07305
C	1.79278	4.64656	-3.20795
H	3.77695	5.02381	-2.4063
H	-0.20463	4.02765	-3.79914
H	1.86968	5.42261	-3.97694
C	3.14098	0.74205	0.35866
C	3.68202	0.67323	1.66223
C	3.92523	0.30356	-0.73326
C	4.97779	0.16713	1.86971
H	3.09912	1.03768	2.51439
C	5.22406	-0.18296	-0.52145
H	3.51405	0.33094	-1.74603
C	5.75215	-0.26048	0.77846
H	5.38846	0.13279	2.88506
H	5.81959	-0.51331	-1.37861
H	6.7656	-0.64361	0.93907
C	1.03619	2.24391	1.63571
C	1.32518	3.61919	1.77201
C	0.50736	1.52371	2.7351
C	1.11046	4.26932	2.99709
H	1.71331	4.18628	0.92037
C	0.30415	2.19001	3.9566
H	0.17708	0.46535	2.6518
C	0.60628	3.55392	4.09508
H	1.3344	5.33749	3.08942
H	-0.12155	1.63112	4.79712
H	0.43509	4.06291	5.04995
Cs	1.47681	-2.51753	1.79987
F	-0.89593	-1.09659	2.58028



Zero-point correction= 0.523559 (Hartree/Particle)
 Thermal correction to Energy= 0.564425
 Thermal correction to Enthalpy= 0.565369
 Thermal correction to Gibbs Free Energy= 0.445182
 Sum of electronic and zero-point Energies= -2042.039668
 Sum of electronic and thermal Energies= -2041.998803
 Sum of electronic and thermal Enthalpies= -2041.997858
 Sum of electronic and thermal Free Energies= -2042.118046
 E(RM06L) = -2330.85710797

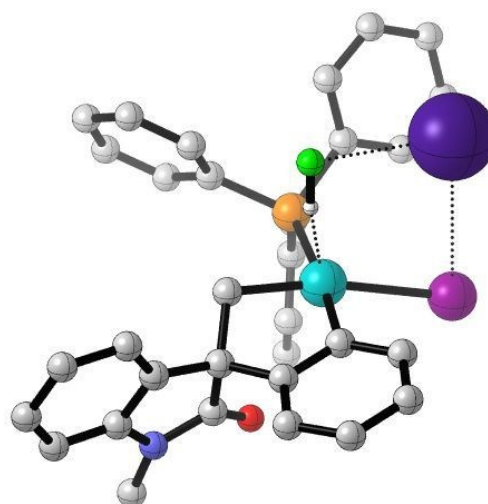
C	-6.35229	0.21713	2.24472
C	-6.31422	0.84096	0.98009
C	-5.10437	0.79287	0.27973
C	-3.97037	0.13175	0.79795
C	-3.99884	-0.44456	2.06985
C	-5.21411	-0.40251	2.78786
H	-7.28561	0.23692	2.81777
H	-7.1942	1.34973	0.57454
H	-3.07242	-0.85937	2.49956
H	-5.26642	-0.84814	3.78668
C	-3.43782	1.19013	-1.28023
C	-2.82891	0.25944	-0.20336
C	-1.55954	0.84005	0.42497
H	-1.40964	0.43303	1.4414



Thermal correction to Gibbs Free Energy= 0.439785
 Sum of electronic and zero-point Energies= -2042.034251
 Sum of electronic and thermal Energies= -2041.993823
 Sum of electronic and thermal Enthalpies= -2041.992879
 Sum of electronic and thermal Free Energies= -2042.112931
 E(RM06L) = -2330.83422687
 Imaginary frequency = -404.48 cm⁻¹

C	-6.27545	-0.15129	2.53351
C	-6.30606	0.65057	1.37289
C	-5.17847	0.62263	0.54447
C	-4.05544	-0.17456	0.84986
C	-4.02685	-0.95782	2.00377
C	-5.15609	-0.94044	2.85011
H	-7.14427	-0.15106	3.2006
H	-7.17812	1.26859	1.13768
H	-3.12519	-1.54271	2.22914
H	-5.16164	-1.546	3.76241
C	-3.65707	1.06488	-1.15369
C	-2.99896	0.00251	-0.23042
C	-1.66433	0.54626	0.35178
H	-1.5589	0.21231	1.39148
H	-1.61717	1.6447	0.29131
C	-2.75068	-1.31411	-0.96733
C	-3.68144	-1.83987	-1.88281
C	-1.54632	-2.0115	-0.6629
C	-3.4368	-3.07367	-2.50016
H	-4.59968	-1.28817	-2.11439
C	-1.32473	-3.25067	-1.32206
H	-1.09035	-1.92045	0.56119
C	-2.25717	-3.7873	-2.21582
H	-4.16732	-3.48074	-3.20834
H	-0.39173	-3.79325	-1.1349
H	-2.06512	-4.74811	-2.70596
O	-3.17035	1.61641	-2.14274
N	-4.93603	1.33151	-0.65071
C	-5.82205	2.31948	-1.23815
H	-6.78153	1.86254	-1.53886
H	-6.02676	3.14137	-0.52845
H	-5.30985	2.71955	-2.12628
Pd	-0.02246	-0.386	-0.55656
I	1.96634	-1.83825	-2.00443
P	1.26562	1.43888	0.00259
C	1.13045	2.86263	-1.16463
C	2.11087	3.878	-1.24452
C	-0.00297	2.92278	-2.00452
C	1.94972	4.94443	-2.14247
H	3.00815	3.82449	-0.61902
C	-0.15913	3.99646	-2.89544
H	-0.7628	2.13287	-1.97103
C	0.81306	5.00654	-2.9663
H	2.7167	5.72414	-2.20203
H	-1.04325	4.02957	-3.53976
H	0.69237	5.83779	-3.66928
C	3.09799	1.196	0.19596
C	3.71302	1.13854	1.46672
C	3.89245	0.99608	-0.95639
C	5.09144	0.88363	1.58269
H	3.11953	1.32325	2.36823
C	5.27013	0.75882	-0.83603
H	3.43031	1.022	-1.94656
C	5.87317	0.69465	0.43102
H	5.5567	0.86137	2.57481
H	5.87043	0.61049	-1.73939
H	6.94857	0.50701	0.5202
C	0.82382	2.11303	1.67959
C	0.95476	3.48037	1.99905
C	0.39703	1.20894	2.68128
C	0.68235	3.93667	3.29874
H	1.26133	4.19297	1.22677
C	0.13484	1.67147	3.98169
H	0.21154	0.15321	2.43477
C	0.27991	3.03276	4.29488
H	0.78068	5.00261	3.53033
H	-0.21164	0.96618	4.74498
H	0.06353	3.39081	5.30702
Cs	2.07161	-2.50493	1.75114
F	-0.78955	-1.93322	1.83767

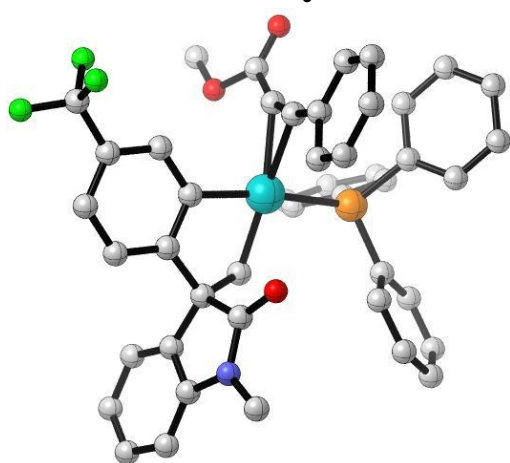
11d-CsF



Zero-point correction= 0.520201 (Hartree/Particle)
 Thermal correction to Energy= 0.561506
 Thermal correction to Enthalpy= 0.562450
 Thermal correction to Gibbs Free Energy= 0.439964
 Sum of electronic and zero-point Energies= -2042.054004
 Sum of electronic and thermal Energies= -2042.012699
 Sum of electronic and thermal Enthalpies= -2042.011755
 Sum of electronic and thermal Free Energies= -2042.134241
 E(RM06L) = -2330.84885490

C	6.98442	0.42902	-1.79763
C	6.6034	0.84024	-0.50441
C	5.32796	0.47331	-0.05865
C	4.43893	-0.28073	-0.85902
C	4.83604	-0.68443	-2.1343
C	6.11668	-0.32386	-2.6054
H	7.97634	0.70198	-2.17328
H	7.28304	1.42406	0.1239
H	4.15972	-1.27938	-2.75774
H	6.4364	-0.63538	-3.60497
C	3.41658	0.25876	1.23276
C	3.14209	-0.50812	-0.09905
C	1.89678	0.10894	-0.79021
H	1.85341	-0.26141	-1.82896
H	1.94191	1.21039	-0.81621
C	2.78772	-1.96146	0.1878
C	3.73018	-3.00076	0.28622
C	1.40251	-2.2026	0.37558
C	3.29918	-4.31052	0.54967
H	4.79561	-2.7881	0.1389
C	0.99129	-3.52399	0.64364
H	-0.10523	-0.98199	-1.66503
C	1.93021	-4.56954	0.72451
H	4.0295	-5.12465	0.61689
H	-0.06662	-3.73591	0.83298
H	1.58906	-5.58983	0.93894
O	2.65084	0.43739	2.18072
N	4.719	0.76362	1.17466
C	5.31419	1.53979	2.24634
H	6.23228	1.05485	2.62335
H	5.56379	2.56123	1.90669
H	4.56825	1.59309	3.05341
Pd	0.20975	-0.53986	0.25737
I	-1.77141	-1.55684	2.07119
P	-1.03692	1.52467	-0.05834
C	-1.12132	2.54955	1.47339
C	-2.07009	3.58006	1.65957
C	-0.1698	2.28709	2.48272
C	-2.06325	4.3409	2.83861
H	-2.81854	3.7824	0.88605
C	-0.16616	3.05746	3.65708
H	0.56145	1.47953	2.35307
C	-1.10963	4.08096	3.83766
H	-2.8044	5.13544	2.97754
H	0.57188	2.84287	4.43657
H	-1.10838	4.6732	4.75914
C	-2.82471	1.36881	-0.57224
C	-3.22439	1.46499	-1.92442
C	-3.80111	1.0362	0.39853
C	-4.55821	1.2239	-2.30054

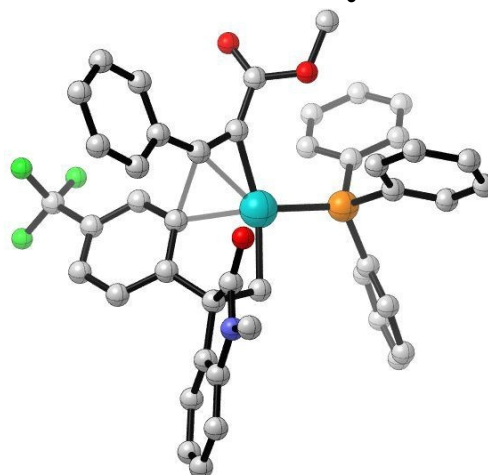
H	-2.494	1.74765	-2.68866
C	-5.13481	0.80396	0.0206
H	-3.51343	0.95106	1.44996
C	-5.51953	0.88948	-1.32959
H	-4.8491	1.32427	-3.35243
H	-5.87556	0.56134	0.79037
H	-6.56279	0.72167	-1.61934
C	-0.36607	2.67506	-1.35537
C	-0.16405	4.05184	-1.12581
C	-0.01972	2.13171	-2.61558
C	0.35566	4.87272	-2.14006
H	-0.40669	4.4841	-0.15052
C	0.48635	2.96055	-3.62925
H	-0.13319	1.0561	-2.79443
C	0.67578	4.3322	-3.39513
H	0.51167	5.93913	-1.94466
H	0.74959	2.52661	-4.5999
H	1.08235	4.97435	-4.18361
Cs	-3.04799	-2.26405	-1.40347
F	-0.50192	-1.12705	-2.57673

21a-CF₃

Zero-point correction=	0.662353 (Hartree/Particle)
Thermal correction to Energy=	0.713729
Thermal correction to Enthalpy=	0.714673
Thermal correction to Gibbs Free Energy=	0.569033
Sum of electronic and zero-point Energies=	-2783.333345
Sum of electronic and thermal Energies=	-2783.281969
Sum of electronic and thermal Enthalpies=	-2783.281025
Sum of electronic and thermal Free Energies=	-2783.426665
E(RM06L) =	-2785.76188734

Pd	-0.01547	-0.25533	-0.30798
P	-2.2406	0.77946	-0.26662
O	1.59187	1.34382	2.30299
N	3.00504	3.06654	1.65571
C	1.94068	-0.8724	-0.35518
C	2.37459	-2.20308	-0.4891
H	1.64979	-3.01456	-0.60113
C	3.74868	-2.51572	-0.49227
C	4.71175	-1.50063	-0.3577
H	5.77545	-1.75356	-0.36812
C	4.29556	-0.16905	-0.22798
H	5.04008	0.63059	-0.14274
C	2.92384	0.14345	-0.23066
C	2.37168	1.55281	-0.08462
C	0.95781	1.54535	-0.73383
H	1.08576	1.53291	-1.83215
H	0.37844	2.44188	-0.45913
C	3.27065	2.66778	-0.59625
C	3.76343	2.93102	-1.87502
H	3.52149	2.26164	-2.7077
C	4.58128	4.06257	-2.07921
H	4.97232	4.27738	-3.07868
C	4.89923	4.91278	-1.00743
H	5.53505	5.78778	-1.17817
C	4.41544	4.65919	0.2918
H	4.66712	5.32134	1.12586
C	3.60573	3.53167	0.46986
C	2.2461	1.92001	1.42849
C	3.11727	3.69862	2.9576
H	2.5247	3.09384	3.66004

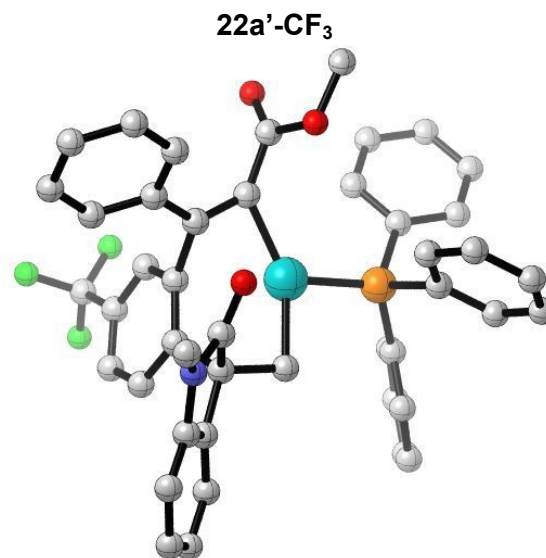
H	2.72273	4.73014	2.93189
H	4.16917	3.72781	3.29287
C	-2.96349	0.9907	-1.95814
C	-2.07757	1.10333	-3.05141
H	-0.99921	1.02484	-2.87644
C	-2.57337	1.29911	-4.35002
H	-1.87589	1.38569	-5.18985
C	-3.95785	1.37494	-4.57204
H	-4.34448	1.52194	-5.58605
C	-4.84702	1.25271	-3.49139
H	-5.92792	1.30332	-3.66036
C	-4.35511	1.06162	-2.19059
H	-5.05258	0.95416	-1.35377
C	-2.28149	2.47864	0.46885
C	-3.11959	3.50501	-0.01419
H	-3.75916	3.32537	-0.88378
C	-3.1323	4.76112	0.6125
H	-3.78258	5.55286	0.22546
C	-2.31596	5.00226	1.72944
H	-2.32925	5.98289	2.21698
C	-1.47596	3.98564	2.21222
H	-0.82862	4.16838	3.07618
C	-1.44789	2.73143	1.58149
H	-0.76115	1.95522	1.93911
C	-3.58982	-0.09818	0.65705
C	-4.11344	0.40736	1.86559
H	-3.75759	1.36524	2.25617
C	-5.09524	-0.30753	2.57057
H	-5.49282	0.10194	3.50533
C	-5.568	-1.53376	2.07943
H	-6.335	-2.08902	2.62951
C	-5.05026	-2.04591	0.87812
H	-5.40868	-3.00286	0.48469
C	-4.06492	-1.33933	0.17311
H	-3.67417	-1.76231	-0.75692
C	-0.9024	-2.30192	-0.5446
C	-0.75072	-2.19311	0.70046
C	-1.30085	-2.92601	-1.79493
C	-0.71085	-2.41026	2.11343
C	0.03965	-1.57029	2.97447
C	-1.43403	-3.50981	2.65027
C	0.06276	-1.83797	4.34905
H	0.59232	-0.72136	2.55615
C	-1.39551	-3.763	4.02464
H	-2.01348	-4.14817	1.97709
C	-0.64877	-2.92882	4.87665
H	0.64447	-1.18887	5.01122
H	-1.95037	-4.61316	4.43459
H	-0.62293	-3.13155	5.9526
O	-2.22077	-3.73861	-1.8804
O	-0.54619	-2.50706	-2.84562
C	-0.89387	-3.12665	-4.10776
H	-1.93029	-2.87844	-4.38727
H	-0.18366	-2.71322	-4.83561
H	-0.79246	-4.22153	-4.04266
C	4.17649	-3.95832	-0.57863
F	5.4619	-4.09338	-1.0229
F	4.11528	-4.58274	0.63813
F	3.37964	-4.68059	-1.42272

TS 21a-22a-CF₃

Zero-point correction= 0.661757 (Hartree/Particle)
 Thermal correction to Energy= 0.711963
 Thermal correction to Enthalpy= 0.712907
 Thermal correction to Gibbs Free Energy= 0.570976
 Sum of electronic and zero-point Energies= -2783.297230
 Sum of electronic and thermal Energies= -2783.247024
 Sum of electronic and thermal Enthalpies= -2783.246080
 Sum of electronic and thermal Free Energies= -2783.388011
 E(RM06L) = -2785.72129083
 Imaginary frequency = -221.15 cm⁻¹

Pd	-0.27786	-0.15675	-0.1046
P	-2.5553	0.23043	-0.32597
O	1.14658	1.2183	2.43764
N	2.03603	3.32991	2.06771
C	1.81553	-0.47353	-0.47707
C	2.35653	-1.47206	-1.31535
H	1.82461	-2.42	-1.4323
C	3.59439	-1.29179	-1.95642
C	4.31611	-0.10546	-1.75684
H	5.29376	0.02623	-2.22878
C	3.74658	0.93406	-1.0057
H	4.26355	1.89698	-0.94596
C	2.48782	0.79319	-0.39503
C	1.69232	2.00079	0.10768
C	0.25297	1.83756	-0.48975
H	0.30288	1.99176	-1.58192
H	-0.43233	2.58936	-0.06279
C	2.28069	3.3672	-0.22108
C	2.59608	3.96186	-1.44526
H	2.47108	3.40282	-2.37875
C	3.08051	5.28687	-1.46619
H	3.33459	5.75667	-2.42148
C	3.23583	6.00628	-0.27006
H	3.61167	7.03433	-0.29877
C	2.9117	5.42802	0.97329
H	3.02704	5.99148	1.90414
C	2.4364	4.11143	0.9705
C	1.58106	2.07352	1.66468
C	2.02726	3.76257	3.45374
H	1.63586	2.92358	4.04815
H	1.37707	4.64543	3.58781
H	3.04667	4.01446	3.79572
C	-3.44104	-1.19476	-1.11315
C	-2.69837	-2.0515	-1.95257
H	-1.62061	-1.88565	-2.06479
C	-3.32703	-3.11831	-2.61462
H	-2.73834	-3.77758	-3.26072
C	-4.70063	-3.34621	-2.43384
H	-5.19024	-4.18325	-2.94267
C	-5.44378	-2.50335	-1.5905
H	-6.51355	-2.68267	-1.43863
C	-4.82028	-1.4301	-0.93545
H	-5.40658	-0.78603	-0.27297
C	-3.04272	1.66142	-1.39776
C	-3.34547	1.47551	-2.7634
H	-3.37024	0.46547	-3.18434
C	-3.62525	2.57791	-3.58597
H	-3.86431	2.41601	-4.64237
C	-3.60557	3.87891	-3.05874
H	-3.82588	4.73716	-3.702
C	-3.3035	4.07356	-1.70139
H	-3.28689	5.08429	-1.28023
C	-3.02012	2.97482	-0.87607
H	-2.7981	3.13849	0.18331
C	-3.43259	0.56805	1.26458
C	-4.70488	1.18214	1.31525
H	-5.191	1.51475	0.39221
C	-5.33794	1.39472	2.5496
H	-6.32333	1.87183	2.57919
C	-4.70536	1.00552	3.74221
H	-5.19883	1.17772	4.7047
C	-3.43575	0.40761	3.69865
H	-2.93223	0.11483	4.62572
C	-2.79837	0.19083	2.46665
H	-1.80481	-0.2662	2.42517
C	-0.14301	-2.12051	0.64534
C	1.07794	-1.71239	0.90866
C	-0.95392	-3.28477	0.9734
C	2.20817	-2.13465	1.74417
C	3.15679	-1.25957	2.31524
C	2.32196	-3.52884	1.98765
C	4.18403	-1.76295	3.1242
H	3.06566	-0.18732	2.14067
C	3.35342	-4.01987	2.7979

H	1.5979	-4.21087	1.53037
C	4.28964	-3.1419	3.36901
H	4.90818	-1.07056	3.56687
H	3.43033	-5.09821	2.9738
H	5.09952	-3.53021	3.99562
O	-0.6473	-4.45418	0.72847
O	-2.14156	-2.93396	1.55743
C	-2.99845	-4.053	1.87633
H	-2.4836	-4.76526	2.54132
H	-3.87247	-3.61513	2.37723
H	-3.3032	-4.58105	0.95841
C	4.17571	-2.40802	-2.78874
F	5.01607	-1.93449	-3.7558
F	4.90088	-3.28236	-2.03066
F	3.20425	-3.13593	-3.41118



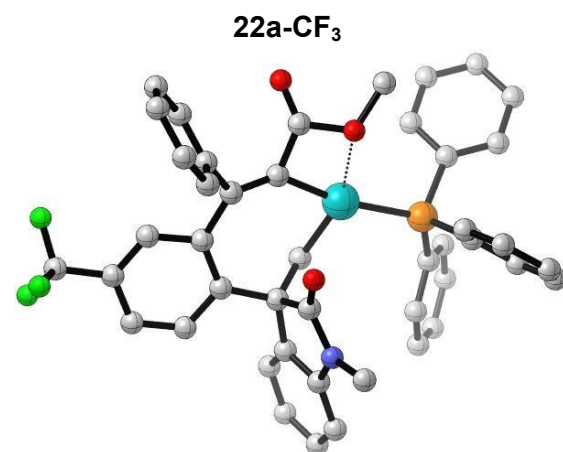
Zero-point correction= 0.663627 (Hartree/Particle)
 Thermal correction to Energy= 0.714005
 Thermal correction to Enthalpy= 0.714949
 Thermal correction to Gibbs Free Energy= 0.572496
 Sum of electronic and zero-point Energies= -2783.317233
 Sum of electronic and thermal Energies= -2783.266855
 Sum of electronic and thermal Enthalpies= -2783.265911
 Sum of electronic and thermal Free Energies= -2783.408364
 E(RM06L) = -2785.74404214

Pd	-0.41011	-0.08372	0.08901
P	-2.57839	0.45173	-0.14082
O	1.58705	0.62436	2.43119
N	3.22765	2.20969	2.01699
C	1.78906	-0.89365	-0.63497
C	1.87934	-1.76721	-1.75334
H	1.51413	-2.78953	-1.62286
C	2.44944	-1.38109	-2.9703
C	2.97444	-0.08686	-3.0938
H	3.45567	0.22852	-4.02389
C	2.84025	0.81353	-2.0319
H	3.21262	1.8301	-2.16974
C	2.22866	0.47614	-0.80451
C	1.82888	1.65918	0.14925
C	0.29699	1.88891	-0.03627
H	0.10185	2.31345	-1.03486
H	-0.10999	2.54843	0.7485
C	2.63367	2.94074	-0.08554
C	2.61187	3.8706	-1.12888
H	1.93834	3.73165	-1.9814
C	3.45488	5.00127	-1.07242
H	3.44434	5.72683	-1.89157
C	4.29939	5.20167	0.03052
H	4.95218	6.08007	0.06384
C	4.30784	4.29796	1.11099
H	4.94389	4.46929	1.98444
C	3.46044	3.18596	1.03584
C	2.16278	1.38072	1.65302
C	3.77385	2.22894	3.36324
H	3.30453	1.3997	3.91241
H	3.54351	3.18288	3.87182

H	4.86799	2.08757	3.34229
C	-3.71803	-0.98491	-0.41698
C	-3.17909	-2.24023	-0.76049
H	-2.09116	-2.35622	-0.82322
C	-4.02973	-3.33518	-0.98864
H	-3.5972	-4.30737	-1.24468
C	-5.41974	-3.18339	-0.87266
H	-6.08219	-4.03837	-1.04495
C	-5.96246	-1.93375	-0.52524
H	-7.0465	-1.81274	-0.4266
C	-5.11813	-0.83775	-0.29736
H	-5.54946	0.12835	-0.01621
C	-2.96757	1.58918	-1.54518
C	-3.4808	1.086	-2.75989
H	-3.72822	0.0237	-2.84842
C	-3.68076	1.94181	-3.85447
H	-4.0811	1.53714	-4.78996
C	-3.37485	3.30786	-3.75078
H	-3.53508	3.97407	-4.60484
C	-2.86189	3.81667	-2.54586
H	-2.62294	4.88165	-2.45556
C	-2.65205	2.96456	-1.4515
H	-2.25108	3.3713	-0.5178
C	-3.24299	1.30182	1.36006
C	-4.31196	2.22297	1.30765
H	-4.75101	2.50009	0.34378
C	-4.80133	2.80377	2.48863
H	-5.6274	3.52109	2.43807
C	-4.23065	2.47048	3.72755
H	-4.6115	2.92816	4.64672
C	-3.16631	1.55551	3.78452
H	-2.71259	1.29816	4.74723
C	-2.66887	0.97477	2.60797
H	-1.83311	0.26678	2.64647
C	0.05158	-1.97858	0.75392
C	1.37968	-1.66416	0.63911
C	-0.64193	-3.02167	1.49913
C	2.48129	-2.10451	1.53928
C	3.81827	-2.16552	1.08134
C	2.21018	-2.50409	2.87027
C	4.84415	-2.63429	1.91586
H	4.05502	-1.85928	0.05766
C	3.23493	-2.97662	3.69794
H	1.1909	-2.41192	3.2549
C	4.55807	-3.04654	3.22632
H	5.87034	-2.68243	1.53541
H	3.00275	-3.27961	4.72489
H	5.35841	-3.41335	3.8778
O	-0.78421	-4.17765	1.09525
O	-1.24913	-2.55977	2.65022
C	-2.06008	-3.55104	3.32096
H	-1.46129	-4.43724	3.58732
H	-2.44019	-3.05529	4.2252
H	-2.89542	-3.87145	2.67722
C	2.58605	-2.37538	-4.09737
F	2.56937	-1.75918	-5.3154
F	3.76435	-3.06354	-4.02015
F	1.58494	-3.29841	-4.0882

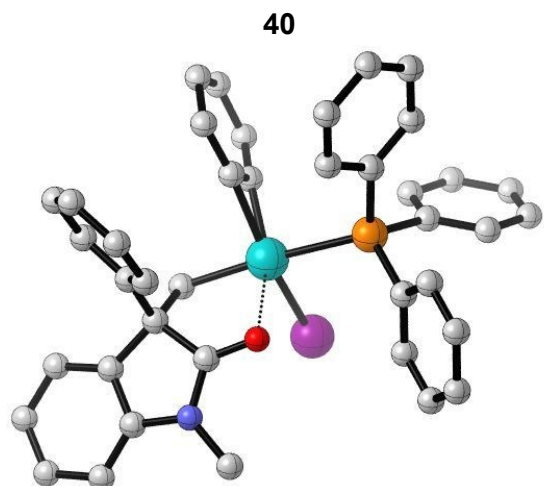
Sum of electronic and zero-point Energies= -2783.346913
 Sum of electronic and thermal Energies= -2783.296768
 Sum of electronic and thermal Enthalpies= -2783.295824
 Sum of electronic and thermal Free Energies= -2783.438108
 E(RM06L) = -2785.77146461

Pd	-0.68305	-0.83406	-0.32112
P	-3.02201	-0.31189	-0.28785
O	0.9098	0.34032	2.21496
N	0.19088	2.54031	2.1463
C	3.09749	0.05921	-0.29559
C	4.48076	-0.00791	-0.61945
H	4.94067	-0.99247	-0.72035
C	5.28449	1.11659	-0.82412
C	4.7266	2.39003	-0.66751
H	5.33465	3.29018	-0.7931
C	3.36639	2.48913	-0.36326
H	2.93869	3.48707	-0.25117
C	2.5149	1.37156	-0.20959
C	1.02082	1.67158	0.0599
C	0.08131	0.9408	-0.95357
H	0.63397	0.76077	-1.89058
H	-0.78831	1.57704	-1.17488
C	0.64638	3.15714	-0.02402
C	0.63517	4.03605	-1.11095
H	1.01747	3.71152	-2.08439
C	0.14454	5.34743	-0.93919
H	0.15054	6.0434	-1.78377
C	-0.34797	5.76422	0.30896
H	-0.72167	6.78596	0.43379
C	-0.36922	4.88495	1.40953
H	-0.76076	5.20561	2.3796
C	0.13016	3.58924	1.21773
C	0.71134	1.37198	1.57882
C	-0.17092	2.635	3.54951
H	0.05697	1.65897	4.00265
H	-1.24673	2.85409	3.66873
H	0.41504	3.42348	4.05424
C	-3.93544	-1.66867	-1.15773
C	-3.29172	-2.27667	-2.25953
H	-2.28701	-1.93837	-2.54235
C	-3.92341	-3.30926	-2.97025
H	-3.4155	-3.77153	-3.82311
C	-5.1971	-3.75446	-2.5793
H	-5.68664	-4.56618	-3.12759
C	-5.83816	-3.16279	-1.47819
H	-6.82805	-3.5125	-1.16631
C	-5.21337	-2.12368	-0.7701
H	-5.71605	-1.67391	0.09219
C	-3.66348	1.23558	-1.06753
C	-4.53537	1.22805	-2.17614
H	-4.89336	0.27705	-2.58221
C	-4.94983	2.43719	-2.75856
H	-5.63034	2.41801	-3.61648
C	-4.49664	3.66272	-2.24563
H	-4.81839	4.60307	-2.70527
C	-3.62428	3.67884	-1.14455
H	-3.25165	4.62669	-0.74392
C	-3.20724	2.47398	-0.56037
H	-2.52609	2.49925	0.29708
C	-3.75414	-0.2677	1.41046
C	-4.97846	0.37242	1.70312
H	-5.51905	0.9027	0.91199
C	-5.49458	0.34558	3.00841
H	-6.44436	0.84518	3.22733
C	-4.79369	-0.3151	4.03138
H	-5.19773	-0.3319	5.04912
C	-3.5692	-0.94289	3.74976
H	-3.01168	-1.44587	4.54673
C	-3.0472	-0.91591	2.44683
H	-2.07934	-1.38224	2.22752
C	1.16808	-1.65137	-0.25706
C	2.47183	-1.29027	-0.0829
C	0.6996	-3.05719	-0.20909
C	3.42904	-2.33143	0.4592
C	3.82492	-2.23001	1.81202
C	3.93861	-3.3888	-0.32279
C	4.70553	-3.1682	2.36997
H	3.42473	-1.41124	2.41923
C	4.82682	-4.32162	0.23721
H	3.62769	-3.48321	-1.36638
C	5.21274	-4.21549	1.58249
H	4.99699	-3.08023	3.42236
H	5.21551	-5.13645	-0.38309
H	5.90472	-4.94554	2.01595
O	1.10463	-4.08137	-0.73325



Zero-point correction= 0.664537 (Hartree/Particle)
 Thermal correction to Energy= 0.714682
 Thermal correction to Enthalpy= 0.715626
 Thermal correction to Gibbs Free Energy= 0.573342

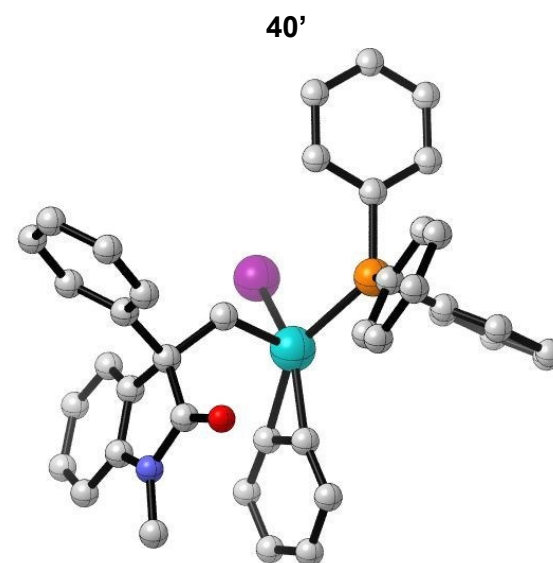
O	-0.56757	-3.04146	0.45783
C	-1.33247	-4.26747	0.34766
H	-0.75301	-5.10603	0.76257
H	-2.24821	-4.09821	0.92975
H	-1.57817	-4.47875	-0.70543
C	6.75368	0.95814	-1.12792
F	7.21266	1.96701	-1.92741
F	7.51148	0.98592	0.00946
F	7.02699	-0.2191	-1.7576



Zero-point correction= 0.596547 (Hartree/Particle)
 Thermal correction to Energy= 0.639389
 Thermal correction to Enthalpy= 0.640334
 Thermal correction to Gibbs Free Energy= 0.514506
 Sum of electronic and zero-point Energies= -2153.111392
 Sum of electronic and thermal Energies= -2153.068550
 Sum of electronic and thermal Enthalpies= -2153.067606
 Sum of electronic and thermal Free Energies= -2153.193433
 E(RM06L) = -2441.74924345

C	-6.72306	-1.95516	-0.04715
C	-5.63657	-2.29165	0.78449
C	-4.47578	-1.52342	0.6669
C	-4.36821	-0.43956	-0.23437
C	-5.45399	-0.12159	-1.05053
C	-6.63431	-0.88834	-0.95513
H	-7.64667	-2.53894	0.0183
H	-5.70283	-3.12399	1.49131
H	-5.39563	0.70914	-1.7604
H	-7.48754	-0.64813	-1.59686
C	-2.33046	-0.77159	0.93467
C	-2.9759	0.19051	-0.07808
C	-2.09692	0.13337	-1.35345
H	-2.23969	1.00818	-2.00178
H	-2.23937	-0.80208	-1.91061
C	-3.09997	1.61462	0.50912
C	-2.79389	1.90939	1.85225
C	-3.58892	2.65409	-0.30934
C	-2.97237	3.20635	2.36227
H	-2.39313	1.12985	2.50682
C	-3.77102	3.94782	0.19889
H	-3.82397	2.45595	-1.36
C	-3.46478	4.23063	1.54024
H	-2.72547	3.41149	3.40953
H	-4.15148	4.73739	-0.45771
H	-3.60805	5.24036	1.93889
O	-1.12627	-0.75087	1.27505
N	-3.25274	-1.68802	1.364
C	-2.93295	-2.7956	2.25357
H	-3.52311	-2.73282	3.18388
H	-3.14138	-3.75651	1.75383
H	-1.86076	-2.72917	2.4871
Pd	-0.08306	0.07778	-0.67114
I	0.099	-2.55032	-1.65827
P	2.19952	-0.0566	0.41245
C	2.82287	1.59389	0.96926
C	4.11086	2.07103	0.65341
C	1.9542	2.40977	1.72978
C	4.52597	3.33767	1.09774
H	4.79107	1.45184	0.06126

C	2.37938	3.66549	2.18638
H	0.94252	2.05808	1.95944
C	3.66574	4.13408	1.86852
H	5.52787	3.69845	0.84178
H	1.7003	4.2844	2.78241
H	3.99322	5.11927	2.21708
C	3.59183	-0.746	-0.58379
C	4.68349	-1.4075	0.018
C	3.56857	-0.57842	-1.98417
C	5.73952	-1.88718	-0.77248
H	4.70215	-1.55289	1.10272
C	4.63049	-1.05265	-2.76871
H	2.71114	-0.0879	-2.4538
C	5.71551	-1.70888	-2.16532
H	6.57997	-2.40503	-0.29817
H	4.60132	-0.92295	-3.8555
H	6.5381	-2.08861	-2.78063
C	2.22545	-1.06504	1.96747
C	2.77866	-0.58589	3.17416
C	1.68356	-2.36923	1.92582
C	2.78926	-1.39889	4.32
H	3.20142	0.42194	3.22126
C	1.70783	-3.17843	3.07103
H	1.24287	-2.74249	0.99381
C	2.25611	-2.69598	4.2716
H	3.22113	-1.01486	5.25051
H	1.29342	-4.19131	3.02306
H	2.26888	-3.32912	5.16537
C	-0.03535	3.56854	-0.98394
C	0.33634	4.16795	-2.21937
C	0.70633	3.40416	-3.34215
C	0.73227	1.98135	-3.31326
C	0.39078	1.47216	-2.06856
C	0.03041	2.17926	-0.99551
H	-0.34578	4.17067	-0.12528
H	0.32802	5.26125	-2.30019
H	0.97905	3.9173	-4.27145
H	0.9966	1.38571	-4.19173

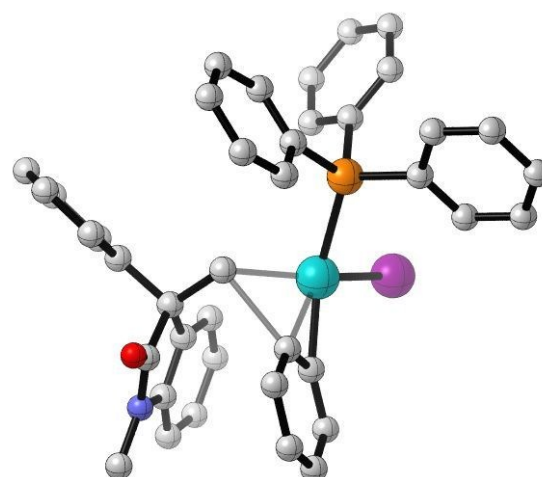


Zero-point correction= 0.596590 (Hartree/Particle)
 Thermal correction to Energy= 0.639611
 Thermal correction to Enthalpy= 0.640555
 Thermal correction to Gibbs Free Energy= 0.514574
 Sum of electronic and zero-point Energies= -2153.107237
 Sum of electronic and thermal Energies= -2153.064216
 Sum of electronic and thermal Enthalpies= -2153.063272
 Sum of electronic and thermal Free Energies= -2153.189254
 E(RM06L) = -2441.74580484

C	5.29145	-1.85524	1.4799
C	5.2138	-1.55344	0.10533
C	4.22549	-0.65284	-0.30307
C	3.34131	-0.03963	0.61378
C	3.41197	-0.37027	1.96799
C	4.39681	-1.28525	2.39906
H	6.05464	-2.55868	1.82907

H	5.89124	-2.02189	-0.61451
H	2.69019	0.03872	2.68239
H	4.45338	-1.55633	3.45748
C	2.79231	0.57154	-1.63506
C	2.44997	0.91864	-0.15424
C	0.94844	0.93076	0.13445
H	0.42311	1.51864	-0.63011
H	0.73943	1.28251	1.15383
C	2.83001	2.42137	0.07844
C	2.41656	3.39857	-0.85589
C	3.5201	2.8358	1.23612
C	2.70148	4.75446	-0.63907
H	1.89758	3.08114	-1.765
C	3.80106	4.19411	1.44819
H	3.85582	2.09288	1.9641
C	3.39249	5.15915	0.5142
H	2.38246	5.49655	-1.37865
H	4.3468	4.49578	2.34851
H	3.61337	6.21836	0.68292
O	2.22209	0.97733	-2.65171
N	3.90914	-0.25148	-1.61598
C	4.52018	-0.77999	-2.8238
H	5.6001	-0.55327	-2.84485
H	4.37171	-1.87183	-2.88882
H	4.0231	-0.29305	-3.67542
Pd	-0.14403	-0.87331	0.17413
I	-0.4388	-1.06301	2.93292
P	-2.24903	0.26164	-0.31093
C	-3.16251	1.25114	0.95069
C	-4.55738	1.1338	1.12942
C	-2.43867	2.17172	1.73777
C	-5.21748	1.93772	2.07256
H	-5.12451	0.4098	0.53578
C	-3.10312	2.97634	2.67416
H	-1.35316	2.24849	1.62651
C	-4.49272	2.86096	2.84283
H	-6.29983	1.83841	2.20643
H	-2.53139	3.68372	3.2834
H	-5.00861	3.48397	3.58092
C	-3.37093	-1.15419	-0.68742
C	-4.04886	-1.28156	-1.91767
C	-3.49993	-2.17032	0.28939
C	-4.85233	-2.40617	-2.1644
H	-3.94944	-0.50242	-2.67945
C	-4.30796	-3.28819	0.03512
H	-2.96313	-2.08322	1.24197
C	-4.98372	-3.40946	-1.19074
H	-5.37708	-2.49646	-3.12144
H	-4.40251	-4.06904	0.79676
H	-5.60932	-4.28632	-1.38801
C	-2.27524	1.33268	-1.81824
C	-3.29788	2.2812	-2.04433
C	-1.23283	1.20248	-2.76196
C	-3.28395	3.07132	-3.20348
H	-4.10026	2.40461	-1.30996
C	-1.22181	1.9997	-3.91789
H	-0.41701	0.49423	-2.58165
C	-2.24715	2.93165	-4.142
H	-4.08218	3.80242	-3.37013
H	-0.39824	1.89689	-4.6313
H	-2.23485	3.55664	-5.04129
C	2.07597	-3.42192	-0.33419
C	2.27648	-4.02333	-1.59998
C	1.676	-3.51553	-2.77572
C	0.83665	-2.3749	-2.75923
C	0.6371	-1.84568	-1.48264
C	1.21685	-2.32355	-0.36967
H	2.56016	-3.7998	0.57065
H	2.91117	-4.91456	-1.67254
H	1.85687	-4.02874	-3.72779
H	0.38856	-1.98103	-3.67699

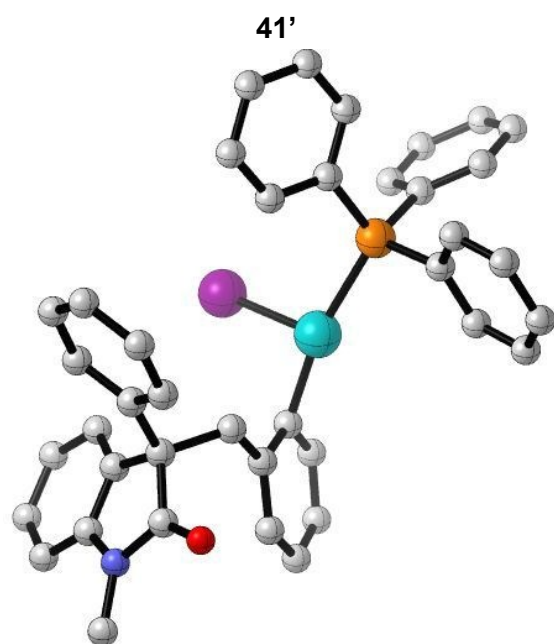
TS 40'-41'



Zero-point correction= 0.595956 (Hartree/Particle)
 Thermal correction to Energy= 0.638292
 Thermal correction to Enthalpy= 0.639236
 Thermal correction to Gibbs Free Energy= 0.514970
 Sum of electronic and zero-point Energies= -2153.099972
 Sum of electronic and thermal Energies= -2153.057636
 Sum of electronic and thermal Enthalpies= -2153.056691
 Sum of electronic and thermal Free Energies= -2153.180958
 E(RM06L) = -2441.74033786
 Imaginary frequency = -192.85 cm⁻¹

C	4.3984	-2.35208	2.1868
C	4.96184	-1.83768	1.00219
C	4.28758	-0.79038	0.36618
C	3.09197	-0.24099	0.88236
C	2.53946	-0.7744	2.04827
C	3.19904	-1.83679	2.7017
H	4.90183	-3.17584	2.7034
H	5.88579	-2.25399	0.59009
H	1.58985	-0.3978	2.44112
H	2.76065	-2.26793	3.60621
C	3.65816	0.77145	-1.21337
C	2.64057	0.88601	-0.03176
C	1.17858	0.85698	-0.53216
H	1.07198	1.36897	-1.49708
H	0.53068	1.35337	0.20756
C	2.83244	2.30015	0.59537
C	2.74505	3.44123	-0.23476
C	3.05287	2.48392	1.97548
C	2.86928	4.72857	0.30673
H	2.61578	3.3082	-1.31225
C	3.17538	3.77536	2.51328
H	3.14546	1.61462	2.63191
C	3.08111	4.90292	1.68383
H	2.80597	5.59929	-0.3547
H	3.35202	3.8956	3.58761
H	3.17851	5.90886	2.10571
O	3.64781	1.40709	-2.26988
N	4.6228	-0.15646	-0.84524
C	5.73313	-0.52235	-1.70659
H	6.69622	-0.37959	-1.18646
H	5.64728	-1.57449	-2.03007
H	5.68717	0.13617	-2.58644
Pd	-0.17376	-0.90524	-0.18383
I	-1.21462	-2.76341	1.52613
P	-2.18578	0.46296	-0.21029
C	-3.00373	0.82156	1.40641
C	-4.39619	1.00717	1.5298
C	-2.1853	0.94319	2.54905
C	-4.9565	1.32255	2.77759
H	-5.04267	0.89506	0.65378
C	-2.74724	1.2712	3.79165
H	-1.10952	0.75775	2.46253
C	-4.13403	1.45998	3.90756
H	-6.03971	1.45668	2.86645
H	-2.10315	1.36086	4.6724
H	-4.57482	1.70337	4.87998
C	-3.50582	-0.27264	-1.27931
C	-4.43119	0.5446	-1.96801
C	-3.60238	-1.67577	-1.39681
C	-5.43892	-0.03553	-2.7539

H	-4.35764	1.63438	-1.89739
C	-4.6125	-2.24852	-2.18553
H	-2.89234	-2.31424	-0.86024
C	-5.53089	-1.4326	-2.8648
H	-6.15024	0.60745	-3.28313
H	-4.67599	-3.33837	-2.26906
H	-6.315	-1.88307	-3.48258
C	-1.95244	2.13931	-0.96285
C	-2.16792	3.33613	-0.24999
C	-1.48183	2.20885	-2.29528
C	-1.92827	4.57844	-0.86231
H	-2.52902	3.29881	0.78224
C	-1.2511	3.45005	-2.90412
H	-1.304	1.28455	-2.85687
C	-1.47342	4.63938	-2.18771
H	-2.10196	5.50045	-0.29755
H	-0.89403	3.48897	-3.93858
H	-1.28979	5.60871	-2.66259
C	1.94542	-3.33348	-1.24874
C	2.55317	-3.31107	-2.52986
C	2.47026	-2.18895	-3.38152
C	1.78463	-1.00617	-3.00481
C	1.21573	-1.09085	-1.73707
C	1.27691	-2.1569	-0.92198
H	1.98889	-4.21478	-0.6028
H	3.0878	-4.2022	-2.87928
H	2.94747	-2.22881	-4.36708
H	1.75131	-0.12587	-3.65138

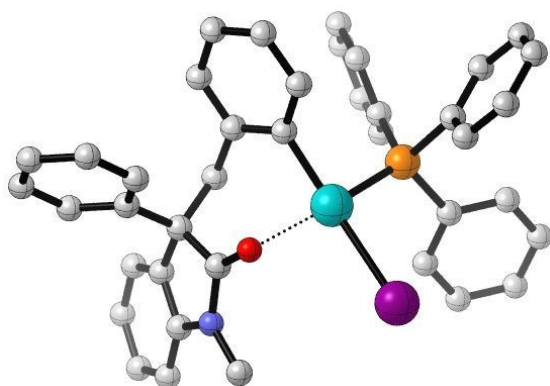


Zero-point correction= 0.598787 (Hartree/Particle)
 Thermal correction to Energy= 0.641443
 Thermal correction to Enthalpy= 0.642387
 Thermal correction to Gibbs Free Energy= 0.513609
 Sum of electronic and zero-point Energies= -2153.176296
 Sum of electronic and thermal Energies= -2153.133640
 Sum of electronic and thermal Enthalpies= -2153.132696
 Sum of electronic and thermal Free Energies= -2153.261474
 E(RM06L) = -2441.80899534

C	5.89834	-2.00066	1.75121
C	6.33832	-1.27583	0.62576
C	5.42651	-0.40247	0.02381
C	4.11316	-0.22333	0.51572
C	3.68632	-0.96734	1.61753
C	4.58932	-1.8585	2.2367
H	6.58898	-2.69391	2.24266
H	7.35197	-1.40252	0.23393
H	2.65796	-0.88249	1.98529
H	4.25844	-2.44787	3.09719
C	4.43867	1.03559	-1.49069
C	3.40236	0.81067	-0.34246
C	2.01238	0.3673	-0.91785
H	1.77888	1.06888	-1.74018

H	1.25705	0.53302	-0.12835
C	3.20217	2.1778	0.36612
C	2.83394	3.30758	-0.39873
C	3.33013	2.32217	1.76142
C	2.59066	4.54234	0.22034
H	2.77273	3.21948	-1.48746
C	3.08315	3.55948	2.37943
H	3.62851	1.46472	2.37064
C	2.70985	4.67432	1.61384
H	2.31283	5.40678	-0.39247
H	3.19005	3.64795	3.46602
H	2.52328	5.63987	2.09618
O	4.2762	1.67996	-2.52962
N	5.61204	0.37801	-1.13443
C	6.80562	0.39131	-1.96125
H	7.66915	0.7875	-1.39895
H	7.04967	-0.62443	-2.32117
H	6.59373	1.04455	-2.82082
Pd	-0.84745	-1.00845	-0.35808
I	-0.32621	-1.89888	2.08722
P	-2.92883	0.21104	-0.22198
C	-2.9686	1.64739	0.93589
C	-4.16372	2.16279	1.48119
C	-1.73757	2.24824	1.27463
C	-4.12348	3.27195	2.34095
H	-5.12195	1.69016	1.24154
C	-1.70163	3.36169	2.12703
H	-0.80594	1.82967	0.87782
C	-2.89526	3.87411	2.66126
H	-5.0544	3.66335	2.76486
H	-0.73865	3.81716	2.37883
H	-2.86843	4.73709	3.33498
C	-4.48622	-0.71966	0.12586
C	-5.70329	-0.44353	-0.53346
C	-4.43863	-1.74392	1.09734
C	-6.85837	-1.17685	-0.21727
H	-5.74459	0.33847	-1.29881
C	-5.59797	-2.46835	1.41267
H	-3.49052	-1.97302	1.59762
C	-6.80808	-2.18727	0.7567
H	-7.79815	-0.95891	-0.73579
H	-5.55195	-3.26083	2.16691
H	-7.70972	-2.7595	0.99941
C	-3.20743	0.95243	-1.89535
C	-3.59162	2.29345	-2.10186
C	-2.96357	0.12555	-3.01674
C	-3.73444	2.79426	-3.40649
H	-3.77206	2.94627	-1.24199
C	-3.11175	0.62785	-4.31755
H	-2.657	-0.91751	-2.86535
C	-3.4963	1.96507	-4.51418
H	-4.03036	3.83804	-3.55609
H	-2.91905	-0.0226	-5.17696
H	-3.60417	2.36096	-5.52933
C	0.74337	-3.26018	-1.31533
C	1.65424	-3.78226	-2.25005
C	2.65848	-2.9534	-2.77635
C	2.76956	-1.6189	-2.35852
C	1.88624	-1.07088	-1.40048
C	0.82821	-1.90183	-0.95527
H	-0.03483	-3.89653	-0.88266
H	1.5806	-4.8315	-2.55633
H	3.37014	-3.35155	-3.50751
H	3.54922	-0.98172	-2.78989

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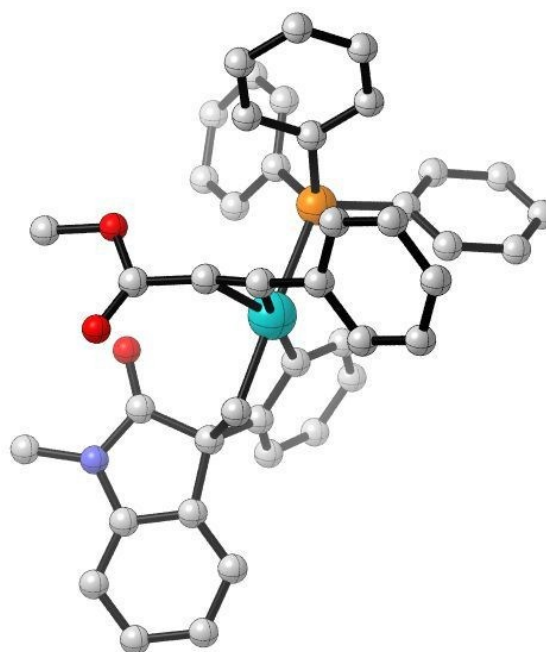


Zero-point correction= 0.600550 (Hartree/Particle)
 Thermal correction to Energy= 0.642085
 Thermal correction to Enthalpy= 0.643030
 Thermal correction to Gibbs Free Energy= 0.521825
 Sum of electronic and zero-point Energies= -2153.196712
 Sum of electronic and thermal Energies= -2153.155176
 Sum of electronic and thermal Enthalpies= -2153.154232
 Sum of electronic and thermal Free Energies= -2153.275437
 E(RM06L) = -2441.84018725

C	4.92151	-3.16558	2.54622
C	4.26812	-3.34749	1.31199
C	3.71926	-2.21524	0.70125
C	3.82068	-0.92437	1.26345
C	4.44993	-0.76768	2.50071
C	5.00453	-1.89646	3.14102
H	5.36033	-4.03221	3.0509
H	4.18431	-4.33866	0.85751
H	4.51404	0.21792	2.97403
H	5.5023	-1.78003	4.10857
C	2.48818	-0.87914	-0.70075
C	3.14927	0.07766	0.33306
C	2.08795	0.94857	1.11515
H	2.63147	1.41014	1.95882
H	1.3401	0.25558	1.54151
C	4.17741	0.95688	-0.43452
C	3.80603	1.59958	-1.63666
C	5.48608	1.15317	0.05242
C	4.71775	2.41579	-2.32287
H	2.80341	1.44767	-2.04256
C	6.39399	1.9766	-0.63284
H	5.81057	0.64935	0.96653
C	6.01471	2.61185	-1.82425
H	4.40658	2.89897	-3.25499
H	7.40494	2.11114	-0.23321
H	6.72477	3.24891	-2.36218
O	1.69732	-0.58745	-1.63069
N	2.95773	-2.15354	-0.48414
C	2.59227	-3.30513	-1.30152
H	3.48067	-3.69886	-1.82495
H	2.15845	-4.09523	-0.66725
H	1.82978	-2.97878	-2.02339
Pd	-0.36874	-0.13852	-0.82972
I	-1.25401	-2.53075	-1.95576
P	-2.2164	0.31025	0.41727
C	-1.99483	1.39303	1.91159
C	-1.97807	0.82852	3.20575
C	-1.79918	2.78655	1.77385
C	-1.77058	1.63809	4.33418
H	-2.13234	-0.24613	3.33678
C	-1.60325	3.59127	2.9055
H	-1.78911	3.24432	0.78128
C	-1.58548	3.02091	4.18899
H	-1.76121	1.18158	5.32958
H	-1.45679	4.66888	2.77872
H	-1.42785	3.65184	5.0701
C	-3.01769	-1.1852	1.15292
C	-4.41113	-1.2342	1.3592
C	-2.21135	-2.2551	1.59379
C	-4.98825	-2.34102	2.00187
H	-5.04797	-0.41585	1.00952
C	-2.79141	-3.35021	2.25082
H	-1.13489	-2.23575	1.39652
C	-4.18053	-3.39634	2.45329
H	-6.07318	-2.37723	2.14573

H	-2.15788	-4.17793	2.58554
H	-4.63361	-4.25871	2.95348
C	-3.5354	1.12945	-0.58091
C	-4.45871	2.03909	-0.01994
C	-3.64	0.78504	-1.94704
C	-5.47022	2.597	-0.81827
H	-4.38328	2.31807	1.03548
C	-4.65552	1.3453	-2.73668
H	-2.931	0.06668	-2.37705
C	-5.56947	2.25262	-2.17593
H	-6.18016	3.30391	-0.37599
H	-4.72899	1.0707	-3.79394
H	-6.35763	2.69246	-2.79616
C	1.87989	3.35459	0.36244
C	1.30114	4.37628	-0.40427
C	0.22396	4.07935	-1.25286
C	-0.2869	2.768	-1.30079
C	0.28146	1.74787	-0.51269
C	1.3912	2.02934	0.31544
H	2.74014	3.57821	1.00501
H	1.69809	5.39531	-0.34723
H	-0.22878	4.86261	-1.87148
H	-1.1418	2.5481	-1.95046

42a

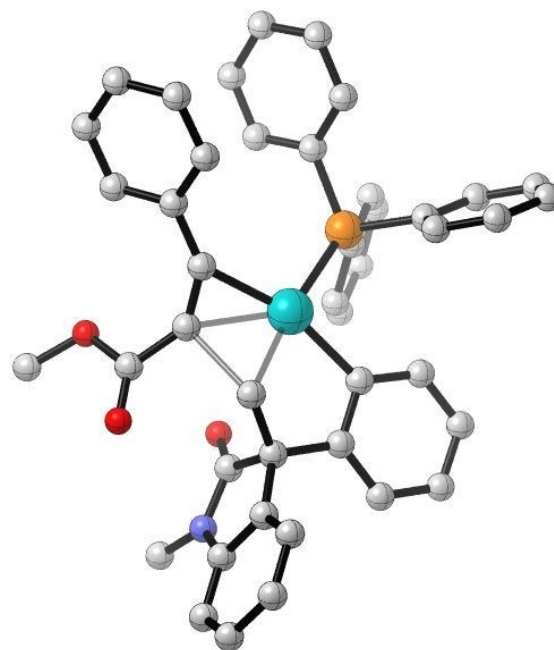


Zero-point correction= 0.658301 (Hartree/Particle)
 Thermal correction to Energy= 0.705714
 Thermal correction to Enthalpy= 0.706658
 Thermal correction to Gibbs Free Energy= 0.572896
 Sum of electronic and zero-point Energies= -2446.294054
 Sum of electronic and thermal Energies= -2446.246642
 Sum of electronic and thermal Enthalpies= -2446.245698
 Sum of electronic and thermal Free Energies= -2446.379459
 E(RM06L) = -2448.61477080

Pd	0.224	0.34117	-0.201
P	-1.96422	-0.78691	-0.05775
O	2.62051	-1.07454	1.7126
N	4.76694	-0.29394	1.28259
C	1.15643	-1.02799	-1.42518
C	0.54105	-1.96814	-2.27789
H	-0.54874	-2.00578	-2.3663
C	1.30616	-2.86749	-3.04394
H	0.80069	-3.58387	-3.70224
C	2.70746	-2.84968	-2.96756
H	3.30353	-3.5506	-3.5625
C	3.34424	-1.91646	-2.13491
H	4.43873	-1.8763	-2.08498
C	2.57877	-1.00889	-1.381
C	3.17905	0.05119	-0.47295
C	2.12194	1.18452	-0.39962
H	2.10979	1.72127	-1.36564
H	2.31864	1.89719	0.41899

C	4.56235	0.55935	-0.84616
C	5.02768	1.1769	-2.00791
H	4.35241	1.33379	-2.85608
C	6.37609	1.58682	-2.07866
H	6.75057	2.07045	-2.98648
C	7.24036	1.37741	-0.99158
H	8.28418	1.70216	-1.05684
C	6.78854	0.75263	0.1882
H	7.46425	0.59048	1.03346
C	5.44827	0.35146	0.23449
C	3.42833	-0.52147	0.96165
C	5.35728	-0.67431	2.552
H	4.57817	-1.19762	3.12526
H	5.69444	0.21399	3.11526
H	6.21781	-1.3497	2.39842
C	-2.77245	-1.01584	-1.71061
C	-2.68548	0.06576	-2.61667
H	-2.13863	0.96995	-2.32507
C	-3.27796	-0.02054	-3.88511
H	-3.20482	0.82522	-4.57684
C	-3.94581	-1.19444	-4.27262
H	-4.39702	-1.26669	-5.26783
C	-4.02155	-2.27919	-3.38473
H	-4.53102	-3.20093	-3.68546
C	-3.44213	-2.19159	-2.10811
H	-3.49911	-3.045	-1.42542
C	-3.31173	0.02717	0.93083
C	-4.54095	0.43083	0.36917
H	-4.73892	0.25817	-0.69281
C	-5.51942	1.04972	1.16601
H	-6.47139	1.35045	0.71525
C	-5.2823	1.27543	2.53046
H	-6.04687	1.75472	3.15118
C	-4.05743	0.88015	3.09689
H	-3.86267	1.05255	4.16091
C	-3.07658	0.26421	2.30534
H	-2.12426	-0.03174	2.75768
C	-1.90994	-2.4661	0.71734
C	-3.08366	-3.12794	1.14592
H	-4.05763	-2.6396	1.0335
C	-3.00437	-4.3986	1.73471
H	-3.91921	-4.9043	2.06201
C	-1.7535	-5.01455	1.91329
H	-1.69274	-6.00479	2.37764
C	-0.58362	-4.35325	1.50889
H	0.39462	-4.82135	1.6599
C	-0.65612	-3.08253	0.91414
H	0.25709	-2.55729	0.61501
C	-0.68483	2.34481	0.77327
C	-0.08062	1.63703	1.60924
C	-1.4576	3.24972	-0.01878
C	-2.73233	3.67955	0.4328
C	-0.95195	3.7413	-1.25067
C	-3.47092	4.59217	-0.33001
H	-3.12763	3.28516	1.37306
C	-1.70428	4.65021	-2.0033
H	0.02694	3.39642	-1.59577
C	-2.96268	5.08015	-1.54597
H	-4.45282	4.92051	0.02583
H	-1.30592	5.02708	-2.9509
H	-3.54678	5.7924	-2.13784
C	0.74886	1.29035	2.76139
O	0.18802	0.28835	3.48754
O	1.81186	1.83951	3.02616
C	1.03029	-0.21232	4.55843
H	0.41904	-0.96253	5.07732
H	1.92835	-0.67129	4.11759
H	1.31697	0.60295	5.24117

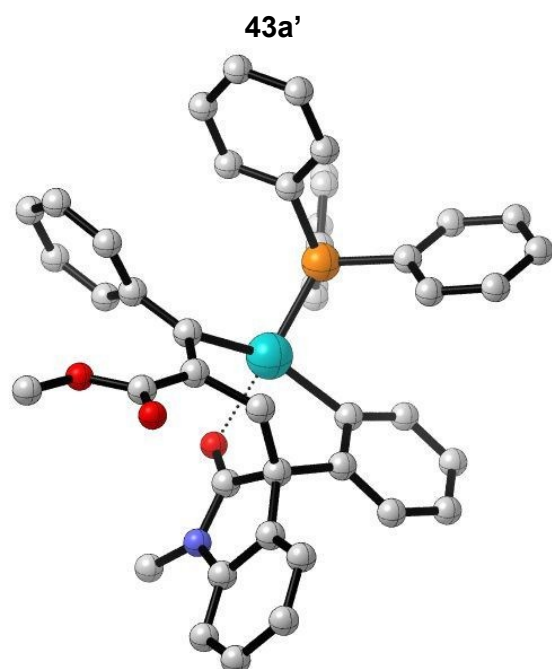
TS 42a-43b'



Zero-point correction= 0.658120 (Hartree/Particle)
 Thermal correction to Energy= 0.704147
 Thermal correction to Enthalpy= 0.705092
 Thermal correction to Gibbs Free Energy= 0.575304
 Sum of electronic and zero-point Energies= -2446.258420
 Sum of electronic and thermal Energies= -2446.212392
 Sum of electronic and thermal Enthalpies= -2446.211448
 Sum of electronic and thermal Free Energies= -2446.341236
 E(RM06L) = -2448.57963926
 Imaginary frequency = -245.73 mc^{-1}

Pd	0.03693	-0.037	-0.40074
P	-2.08692	-0.83564	0.11088
O	2.55806	0.34576	2.00565
N	4.73094	0.31724	1.18143
C	0.98605	-1.90517	-0.12505
C	0.43294	-3.18978	0.06799
H	-0.65216	-3.32609	0.09561
C	1.23197	-4.33678	0.22659
H	0.7558	-5.31405	0.36981
C	2.62906	-4.22879	0.19977
H	3.26157	-5.11522	0.31983
C	3.2122	-2.96858	0.00728
H	4.30347	-2.87023	-0.02677
C	2.40496	-1.82618	-0.16083
C	3.04179	-0.44628	-0.3355
C	2.09249	0.4708	-1.12051
H	1.69105	-0.02041	-2.02925
H	2.60589	1.38368	-1.44697
C	4.42745	-0.44797	-0.96931
C	4.84499	-0.81301	-2.24954
H	4.12122	-1.19084	-2.97955
C	6.21061	-0.70081	-2.58628
H	6.54897	-0.98494	-3.58763
C	7.13753	-0.22972	-1.64209
H	8.19503	-0.14678	-1.91437
C	6.7333	0.13834	-0.3435
H	7.45819	0.50534	0.38929
C	5.37347	0.0223	-0.03077
C	3.35229	0.12629	1.09305
C	5.37286	0.86311	2.36194
H	4.59062	0.97351	3.12759
H	5.81907	1.85005	2.14518
H	6.16062	0.18401	2.7331
C	-2.59986	-2.24057	-0.98597
C	-2.13817	-2.21638	-2.31959
H	-1.45503	-1.41799	-2.63207
C	-2.52304	-3.21833	-3.22331
H	-2.15585	-3.18975	-4.25452
C	-3.35873	-4.26452	-2.79972
H	-3.64905	-5.05376	-3.50111
C	-3.81017	-4.30315	-1.47049
H	-4.45162	-5.12349	-1.13144

C	-3.43825	-3.29452	-0.56725
H	-3.78537	-3.34045	0.46938
C	-3.56674	0.28157	0.01901
C	-4.59229	0.09802	-0.93033
H	-4.53266	-0.72689	-1.64638
C	-5.70086	0.96106	-0.95248
H	-6.49401	0.80254	-1.69113
C	-5.79575	2.01319	-0.02998
H	-6.66204	2.68282	-0.04598
C	-4.77367	2.20572	0.91523
H	-4.83648	3.02932	1.63347
C	-3.66471	1.34997	0.9383
H	-2.87209	1.50854	1.67694
C	-2.21553	-1.42242	1.86422
C	-3.47105	-1.7013	2.45351
H	-4.39144	-1.55448	1.87856
C	-3.54773	-2.13462	3.78525
H	-4.52482	-2.35106	4.23021
C	-2.37588	-2.2748	4.54819
H	-2.43752	-2.60625	5.59032
C	-1.13008	-1.97295	3.97728
H	-0.21483	-2.06187	4.57137
C	-1.04472	-1.54781	2.64126
H	-0.07371	-1.30321	2.19798
C	-0.31673	2.06337	-0.5812
C	0.9445	1.99873	-0.24514
C	-1.38003	3.0202	-0.83736
C	-1.51534	4.20615	-0.06951
C	-2.27951	2.80171	-1.91033
C	-2.51099	5.14112	-0.37958
H	-0.82403	4.37526	0.75953
C	-3.25973	3.7501	-2.22668
H	-2.18377	1.88137	-2.49429
C	-3.3813	4.92222	-1.46128
H	-2.60346	6.05222	0.22198
H	-3.93763	3.56989	-3.06732
H	-4.15293	5.66037	-1.70472
C	1.99774	2.87649	0.30062
O	1.43304	3.81137	1.12752
O	3.20481	2.84093	0.0696
C	2.37994	4.75599	1.67956
H	1.78093	5.44043	2.29567
H	3.12779	4.23276	2.29602
H	2.89963	5.30479	0.8777

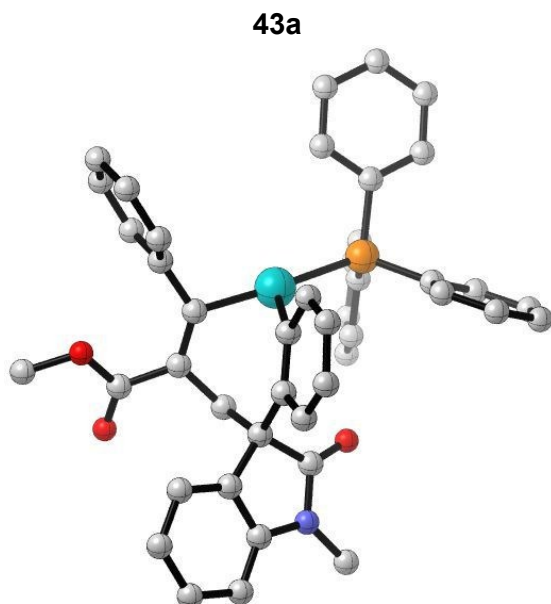


Zero-point correction=	0.660926 (Hartree/Particle)
Thermal correction to Energy=	0.706721
Thermal correction to Enthalpy=	0.707666
Thermal correction to Gibbs Free Energy=	0.578449
Sum of electronic and zero-point Energies=	-2446.302038
Sum of electronic and thermal Energies=	-2446.256243
Sum of electronic and thermal Enthalpies=	-2446.255298

Sum of electronic and thermal Free Energies= -2446.384515
 E(RM06L) = -2448.62276789

Pd	-0.09833	-0.20353	0.60449
P	-2.20181	-0.53407	-0.12673
O	1.68917	0.12539	1.88205
N	3.98637	-0.09378	1.62814
C	0.51516	-2.20089	0.63516
C	-0.11013	-3.41873	0.95774
H	-1.1357	-3.41497	1.34651
C	0.5416	-4.65552	0.79383
H	0.02821	-5.58624	1.0631
C	1.84476	-4.68921	0.28228
H	2.36396	-5.64329	0.13987
C	2.49708	-3.48784	-0.04138
H	3.52263	-3.52093	-0.42283
C	1.84997	-2.24632	0.12385
C	2.63992	-0.91174	-0.16507
C	1.94244	0.02828	-1.2604
H	1.04703	-0.49869	-1.6294
H	2.64818	0.12606	-2.10202
C	4.12515	-1.09075	-0.4471
C	4.80226	-1.59294	-1.56058
H	4.24498	-1.96381	-2.42708
C	6.21253	-1.61747	-1.55707
H	6.74908	-2.01226	-2.42525
C	6.93263	-1.13622	-0.45184
H	8.02699	-1.16036	-0.46328
C	6.26863	-0.60956	0.67334
H	6.82915	-0.22145	1.52891
C	4.87123	-0.59559	0.64494
C	2.68791	-0.22635	1.20979
C	4.37923	0.48301	2.90461
H	3.46249	0.78361	3.43098
H	5.01975	1.36788	2.74822
H	4.92657	-0.2576	3.51286
C	-2.52788	-2.06457	-1.12459
C	-1.54944	-2.50512	-2.03991
H	-0.58701	-1.98676	-2.09203
C	-1.79208	-3.61783	-2.85937
H	-1.02307	-3.94896	-3.56485
C	-3.00729	-4.31459	-2.75989
H	-3.19202	-5.18986	-3.39158
C	-3.98005	-3.89192	-1.83998
H	-4.92575	-4.43684	-1.74949
C	-3.74535	-2.77049	-1.02867
H	-4.50934	-2.44965	-0.31376
C	-3.06312	0.76951	-1.12377
C	-3.46299	0.54477	-2.45851
H	-3.27631	-0.42461	-2.92932
C	-4.11055	1.55765	-3.18388
H	-4.41742	1.3691	-4.21822
C	-4.37116	2.79995	-2.58485
H	-4.88188	3.58655	-3.15046
C	-3.96827	3.03274	-1.25975
H	-4.14978	4.00337	-0.78807
C	-3.30895	2.02972	-0.53431
H	-2.98383	2.2309	0.4909
C	-3.28797	-0.70418	1.36637
C	-4.669	-0.41037	1.32901
H	-5.12256	-0.03271	0.40714
C	-5.45946	-0.58148	2.47703
H	-6.52848	-0.34658	2.43814
C	-4.88154	-1.0432	3.67069
H	-5.49981	-1.17108	4.56555
C	-3.50735	-1.33	3.71641
H	-3.04859	-1.68009	4.64707
C	-2.71264	-1.15964	2.57254
H	-1.63477	-1.36149	2.60085
C	0.42592	1.71674	-0.09372
C	1.55119	1.46398	-0.84046
C	-0.14947	3.01401	0.26607
C	-0.44646	3.30597	1.62286
C	-0.50217	3.97854	-0.71253
C	-1.03095	4.52536	1.98739
H	-0.20105	2.55721	2.38388
C	-1.10842	5.18798	-0.34648
H	-0.30152	3.76031	-1.76609
C	-1.37091	5.47328	1.00427
H	-1.23366	4.73452	3.0438
H	-1.37656	5.91432	-1.1222
H	-1.84176	6.4204	1.28876
C	2.54318	2.47896	-1.31728
O	2.47899	3.67023	-0.64776
O	3.37646	2.27403	-2.20362
C	3.39701	4.6716	-1.13025

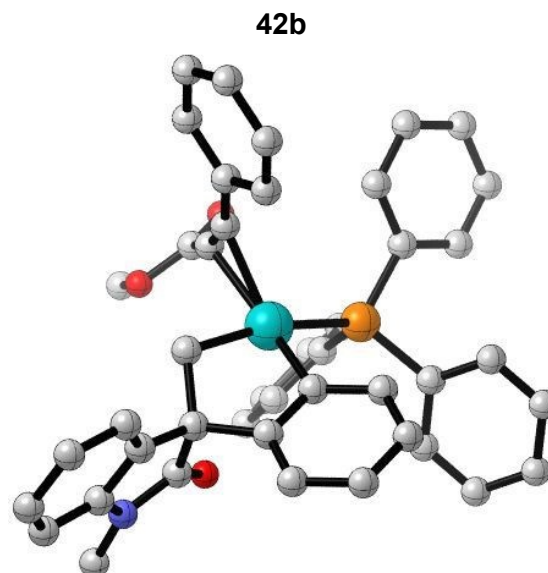
H	3.20228	5.56358	-0.5186
H	4.44159	4.33847	-1.01229
H	3.22123	4.88747	-2.19713



Zero-point correction= 0.660558 (Hartree/Particle)
 Thermal correction to Energy= 0.707243
 Thermal correction to Enthalpy= 0.708187
 Thermal correction to Gibbs Free Energy= 0.573491
 Sum of electronic and zero-point Energies= -2446.324122
 Sum of electronic and thermal Energies= -2446.277437
 Sum of electronic and thermal Enthalpies= -2446.276493
 Sum of electronic and thermal Free Energies= -2446.411189
 E(RM06L) = -2448.63412438

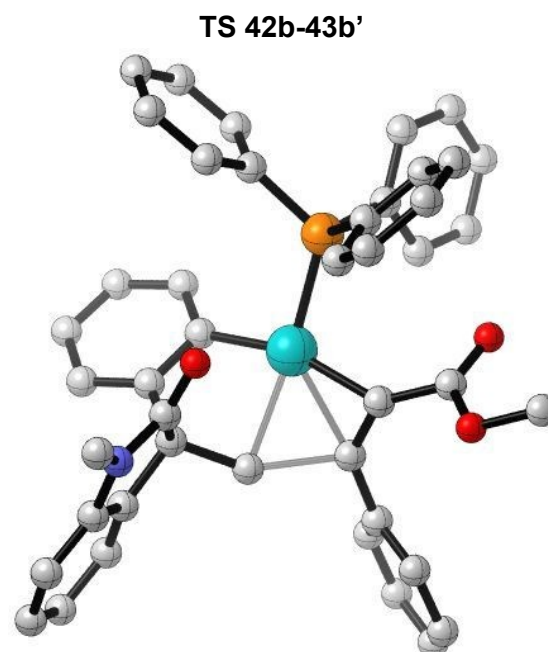
Pd	-0.5369	0.76113	-0.05447
P	-2.66375	-0.40551	0.10862
O	0.88745	-2.93325	0.80716
N	3.16444	-3.35891	0.59945
C	0.65256	-0.00324	-1.50076
C	0.17941	0.27504	-2.80363
H	-0.67116	0.95229	-2.93635
C	0.77062	-0.3149	-3.93275
H	0.38063	-0.09202	-4.93236
C	1.8592	-1.18302	-3.76247
H	2.33304	-1.66121	-4.62614
C	2.35806	-1.41666	-2.47647
H	3.23176	-2.06592	-2.35521
C	1.79328	-0.81733	-1.32122
C	2.46855	-1.13927	0.03278
C	2.12054	-0.18122	1.22346
H	2.82329	-0.39296	2.0464
H	1.10275	-0.44184	1.55876
C	3.97665	-1.31803	-0.1053
C	4.97536	-0.4265	-0.49894
H	4.71738	0.59428	-0.79782
C	6.317	-0.86155	-0.51874
H	7.10722	-0.16785	-0.82224
C	6.6458	-2.17653	-0.15212
H	7.69134	-2.50123	-0.17174
C	5.6497	-3.09234	0.2404
H	5.9057	-4.11824	0.52176
C	4.32524	-2.63927	0.25461
C	2.02464	-2.56259	0.51113
C	3.1289	-4.74164	1.04108
H	2.0756	-4.98508	1.24548
H	3.72513	-4.87754	1.96087
H	3.51982	-5.41684	0.25934
C	-4.13839	0.63791	-0.29731
C	-3.96921	2.03965	-0.28746
H	-2.97847	2.46114	-0.07388
C	-5.05055	2.89028	-0.56414
H	-4.9049	3.97544	-0.55332
C	-6.30953	2.34795	-0.86922
H	-7.15202	3.01003	-1.09538
C	-6.48386	0.95416	-0.89487

H	-7.46206	0.52768	-1.1414
C	-5.40587	0.10153	-0.60967
H	-5.54573	-0.98395	-0.64063
C	-2.88003	-0.84623	1.89327
C	-3.95543	-0.38704	2.68094
H	-4.73871	0.23159	2.23148
C	-4.02484	-0.72286	4.04379
H	-4.86284	-0.35965	4.64842
C	-3.02817	-1.52077	4.62644
H	-3.08446	-1.7804	5.68892
C	-1.95571	-1.98239	3.84344
H	-1.17415	-2.60423	4.29256
C	-1.87105	-1.64415	2.48499
H	-1.02663	-2.00383	1.88282
C	-2.97761	-2.00016	-0.76887
C	-3.77674	-3.01912	-0.20628
H	-4.19439	-2.89243	0.798
C	-4.02165	-4.20017	-0.92395
H	-4.64107	-4.98659	-0.47962
C	-3.4678	-4.37587	-2.20282
H	-3.65568	-5.3005	-2.75889
C	-2.66161	-3.37058	-2.76043
H	-2.21234	-3.51019	-3.74917
C	-2.41233	-2.18806	-2.04718
H	-1.75822	-1.41928	-2.47067
C	1.12528	1.86916	0.23815
C	2.17033	1.30235	0.8998
C	0.8639	3.2685	-0.13817
C	0.40521	4.19584	0.83256
C	0.99087	3.70456	-1.48141
C	0.10036	5.51635	0.47213
H	0.30492	3.86909	1.87309
C	0.69328	5.02698	-1.8312
H	1.32834	2.99114	-2.23943
C	0.24403	5.93958	-0.85926
H	-0.24796	6.21871	1.23753
H	0.80976	5.34919	-2.87188
H	0.00611	6.97115	-1.13931
C	3.35634	2.03783	1.43424
O	3.5386	3.26368	0.85505
O	4.10893	1.59776	2.30321
C	4.64708	4.01379	1.39492
H	4.6642	4.95608	0.83023
H	4.50252	4.20868	2.47042
H	5.59314	3.46311	1.26546



Zero-point correction= 0.658137 (Hartree/Particle)
 Thermal correction to Energy= 0.705606
 Thermal correction to Enthalpy= 0.706550
 Thermal correction to Gibbs Free Energy= 0.571587
 Sum of electronic and zero-point Energies= -2446.287945
 Sum of electronic and thermal Energies= -2446.240476
 Sum of electronic and thermal Enthalpies= -2446.239531
 Sum of electronic and thermal Free Energies= -2446.374494
 E(RM06L) = -2448.60303213

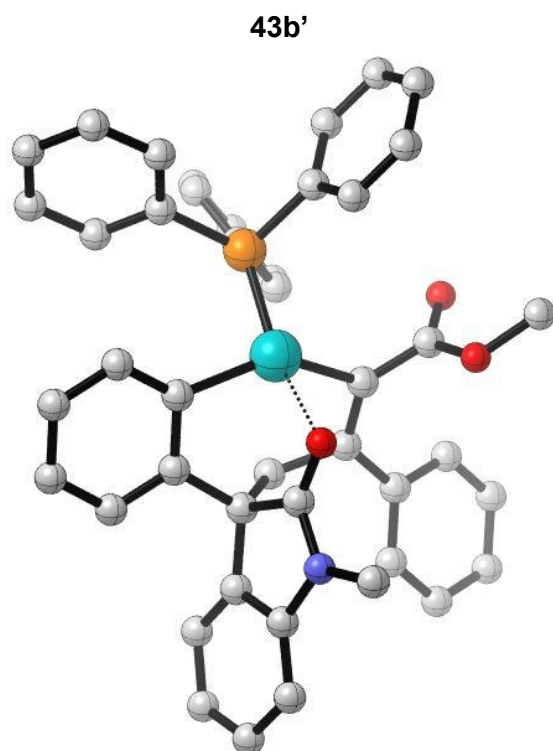
Pd	0.18773	0.40821	-0.09452
P	-2.11267	-0.6167	-0.2848
O	1.8574	-2.07611	1.32057
N	4.15617	-1.79121	1.47329
C	1.11412	-0.54947	-1.65195
C	0.53105	-0.8698	-2.89198
H	-0.51899	-0.63251	-3.08674
C	1.28173	-1.50604	-3.89877
H	0.80805	-1.74728	-4.85733
C	2.62774	-1.83661	-3.67649
H	3.20998	-2.33616	-4.45868
C	3.23381	-1.50896	-2.45273
H	4.29274	-1.73507	-2.28189
C	2.48808	-0.8537	-1.45781
C	3.05001	-0.39433	-0.12122
C	2.19305	0.83658	0.28227
H	2.48773	1.7019	-0.33337
H	2.28405	1.09704	1.35071
C	4.54572	-0.12835	-0.0722
C	5.33903	0.77137	-0.7851
H	4.88871	1.42197	-1.54237
C	6.7247	0.82545	-0.52368
H	7.35555	1.52794	-1.07733
C	7.29894	-0.01769	0.44153
H	8.37537	0.03374	0.63615
C	6.51391	-0.93608	1.16762
H	6.9651	-1.59373	1.91683
C	5.14213	-0.97245	0.8919
C	2.89152	-1.51465	0.95297
C	4.38671	-2.78069	2.50976
H	3.41108	-3.23299	2.74187
H	4.80205	-2.31227	3.41999
H	5.08353	-3.56348	2.16108
C	-2.32625	-2.04504	-1.45519
C	-2.82321	-1.83448	-2.7615
H	-3.15833	-0.83736	-3.06552
C	-2.90758	-2.89763	-3.67388
H	-3.30315	-2.7166	-4.67912
C	-2.48809	-4.18423	-3.30067
H	-2.55323	-5.01345	-4.01285
C	-1.98266	-4.39959	-2.00898
H	-1.65068	-5.39876	-1.70779
C	-1.90061	-3.33999	-1.0926
H	-1.50784	-3.52494	-0.08833
C	-3.61768	0.40652	-0.63566
C	-4.87043	-0.17265	-0.94908
H	-4.96603	-1.26065	-1.02143
C	-5.98907	0.6389	-1.19069
H	-6.95188	0.17642	-1.43311
C	-5.87366	2.03772	-1.12584
H	-6.74731	2.66967	-1.31764
C	-4.63518	2.62076	-0.81941
H	-4.53608	3.71	-0.76965
C	-3.51364	1.81164	-0.57579
H	-2.55255	2.27107	-0.33256
C	-2.44303	-1.40243	1.36533
C	-3.72359	-1.46766	1.95212
H	-4.5798	-1.00266	1.4555
C	-3.90539	-2.11401	3.18426
H	-4.90479	-2.15512	3.6305
C	-2.81306	-2.70253	3.84344
H	-2.95998	-3.21392	4.8011
C	-1.53217	-2.62434	3.27291
H	-0.67062	-3.06852	3.7824
C	-1.33994	-1.96819	2.04507
H	-0.32931	-1.89855	1.62282
C	-0.17665	2.46301	0.55827
C	-0.58595	1.86746	1.59508
C	0.15969	3.61579	-0.24709
C	0.54626	3.49531	-1.60276
C	0.07371	4.9062	0.33737
C	0.84168	4.64065	-2.35395
H	0.61167	2.49406	-2.04154
C	0.3728	6.04236	-0.42276
H	-0.22552	4.99892	1.38589
C	0.75723	5.91516	-1.76953
H	1.13996	4.53562	-3.40219
H	0.3073	7.0331	0.0391
H	0.99027	6.80752	-2.35966
C	-1.29583	1.57248	2.82263
O	-0.44871	1.12245	3.79248
O	-2.50716	1.71836	2.97051
C	-1.10306	0.80353	5.04448
H	-0.28979	0.54614	5.73651
H	-1.67479	1.66834	5.41736
H	-1.78491	-0.05163	4.91132



Zero-point correction= 0.658044 (Hartree/Particle)
 Thermal correction to Energy= 0.704475
 Thermal correction to Enthalpy= 0.705420
 Thermal correction to Gibbs Free Energy= 0.573411
 Sum of electronic and zero-point Energies= -2446.255699
 Sum of electronic and thermal Energies= -2446.209267
 Sum of electronic and thermal Enthalpies= -2446.208323
 Sum of electronic and thermal Free Energies= -2446.340332
 E(RM06L) = -2448.57108084
 Imaginary frequency = -217.49 cm⁻¹

Pd	-0.0309	0.10544	-0.42814
P	-2.23031	-0.45789	-0.05898
O	1.06748	-1.2736	1.98652
N	3.35077	-1.62351	2.1704
C	0.53717	-1.61285	-1.37964
C	-0.11159	-2.4079	-2.34179
H	-1.11163	-2.13329	-2.69466
C	0.50011	-3.55908	-2.87043
H	-0.02461	-4.1598	-3.62276
C	1.77629	-3.94123	-2.4298
H	2.25262	-4.84499	-2.82514
C	2.45351	-3.14846	-1.49007
H	3.46218	-3.42821	-1.16634
C	1.85052	-1.9792	-0.98349
C	2.579	-1.03692	-0.01979
C	2.32631	0.48105	-0.40961
H	2.64556	0.60113	-1.45336
C	3.00444	1.06454	0.23137
H	4.09221	-1.2281	0.02719
C	5.06009	-1.10781	-0.97159
H	4.76755	-0.86194	-1.99776
C	6.416	-1.32286	-0.6462
H	7.18157	-1.2329	-1.423
C	6.78754	-1.65492	0.66676
H	7.84281	-1.82127	0.90691
C	5.82374	-1.78162	1.6869
H	6.11564	-2.04296	2.70842
C	4.48501	-1.56179	1.34225
C	2.18603	-1.312	1.46989
C	3.35935	-1.94787	3.58567
H	2.31543	-1.90744	3.92978
H	3.96399	-1.21929	4.15438
H	3.76543	-2.96073	3.75545
C	-2.66438	-2.26011	0.02309
C	-3.22144	-2.94487	-1.07842
H	-3.46368	-2.40192	-1.99649
C	-3.4828	-4.3224	-1.0034
H	-3.92124	-4.83587	-1.86573
C	-3.18272	-5.03634	0.16605
H	-3.38693	-6.11065	0.22351
C	-2.61544	-4.36495	1.26154

H	-2.37352	-4.91348	2.17796
C	-2.35606	-2.98895	1.19218
H	-1.91022	-2.48091	2.05193
C	-3.3965	0.24864	-1.30133
C	-4.75141	-0.14807	-1.3888
H	-5.13835	-0.93116	-0.72883
C	-5.60291	0.44572	-2.33313
H	-6.64994	0.13019	-2.39313
C	-5.1129	1.43771	-3.19886
H	-5.77874	1.89779	-3.93673
C	-3.76928	1.83533	-3.11796
H	-3.38259	2.60888	-3.78929
C	-2.91426	1.2452	-2.1746
H	-1.86631	1.55339	-2.09857
C	-2.79496	0.16733	1.59539
C	-4.08977	0.6767	1.81618
H	-4.79726	0.76225	0.98683
C	-4.47015	1.10664	3.09749
H	-5.47581	1.51115	3.25451
C	-3.5652	1.02913	4.16786
H	-3.86536	1.36397	5.1667
C	-2.26993	0.53188	3.94914
H	-1.55284	0.4813	4.77551
C	-1.87746	0.11267	2.66796
H	-0.856	-0.24262	2.49121
C	1.15861	2.0514	-0.24353
C	0.00286	2.03208	0.38451
C	1.98968	3.10071	-0.85981
C	2.30595	3.08886	-2.2381
C	2.44678	4.17486	-0.06026
C	3.05802	4.12834	-2.80215
H	1.93857	2.26999	-2.8662
C	3.19816	5.21154	-0.63226
H	2.18805	4.19052	1.00254
C	3.51102	5.19049	-2.00141
H	3.28805	4.11057	-3.87278
H	3.5437	6.03877	-0.00296
H	4.10206	5.99925	-2.4436
C	-0.93137	3.04878	0.8499
O	-0.40523	3.76732	1.90123
O	-2.06313	3.24016	0.40925
C	-1.32032	4.74063	2.45456
H	-0.79328	5.18363	3.31137
H	-1.56671	5.5157	1.71039
H	-2.25359	4.25384	2.78027

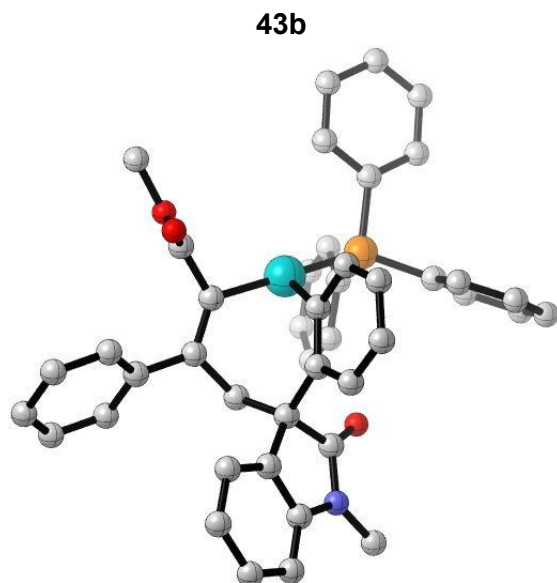


Zero-point correction=	0.661469 (Hartree/Particle)
Thermal correction to Energy=	0.707142
Thermal correction to Enthalpy=	0.708086

Thermal correction to Gibbs Free Energy=	0.579784
Sum of electronic and zero-point Energies=	-2446.301784
Sum of electronic and thermal Energies=	-2446.256111
Sum of electronic and thermal Enthalpies=	-2446.255166
Sum of electronic and thermal Free Energies=	-2446.383468
E(RM06L) =	-2448.62332374

Pd	-0.32551	-0.35722	0.67449
P	-2.39477	-0.10268	-0.19051
O	1.41911	-0.48236	2.01926
N	3.68281	-0.9425	1.80045
C	0.0182	-2.38513	0.40589
C	-0.76894	-3.53621	0.57036
H	-1.78796	-3.44311	0.96044
C	-0.27794	-4.81715	0.25165
H	-0.91226	-5.69886	0.4011
C	1.02063	-4.95773	-0.25276
H	1.41344	-5.94585	-0.51611
C	1.83518	-3.8233	-0.40517
H	2.85875	-3.94516	-0.77338
C	1.35468	-2.53846	-0.08042
C	2.33189	-1.30285	-0.13647
C	1.83206	-0.1185	-1.09701
H	0.88018	-0.45316	-1.54585
H	2.56154	-0.05204	-1.92179
C	3.79256	-1.64836	-0.39291
C	4.45425	-2.07816	-1.54631
H	3.89693	-2.24996	-2.47325
C	5.84764	-2.29584	-1.50235
H	6.37047	-2.6392	-2.40023
C	6.56756	-2.07539	-0.31689
H	7.64835	-2.24802	-0.29713
C	5.92257	-1.62448	0.8515
H	6.4853	-1.43915	1.77116
C	4.54138	-1.4165	0.78355
C	2.39847	-0.84638	1.32898
C	4.08045	-0.60582	3.15923
H	3.18734	-0.24111	3.68567
H	4.84893	0.18564	3.14962
H	4.47801	-1.49439	3.67927
C	-3.46143	-1.61596	-0.25946
C	-3.26799	-2.5569	-1.29619
H	-2.51759	-2.36919	-2.07061
C	-4.03654	-3.72858	-1.34417
H	-3.88067	-4.44438	-2.15797
C	-4.99117	-3.98945	-0.34641
H	-5.58677	-4.90766	-0.38224
C	-5.17361	-3.0706	0.69851
H	-5.91328	-3.26719	1.48183
C	-4.41587	-1.88842	0.74215
H	-4.5738	-1.17284	1.55472
C	-2.61837	0.6215	-1.88045
C	-3.77665	0.35444	-2.6465
H	-4.54265	-0.32641	-2.26381
C	-3.94497	0.95017	-3.90604
H	-4.84523	0.73334	-4.49092
C	-2.9627	1.81548	-4.41437
H	-3.09368	2.27546	-5.3997
C	-1.81391	2.088	-3.65545
H	-1.04532	2.76502	-4.04211
C	-1.63935	1.49652	-2.39456
H	-0.75198	1.7211	-1.79549
C	-3.32289	1.02275	0.95014
C	-4.42465	1.78854	0.51706
H	-4.7304	1.76493	-0.53353
C	-5.12069	2.59841	1.4277
H	-5.9693	3.19714	1.08044
C	-4.7274	2.6479	2.77484
H	-5.27235	3.28242	3.48186
C	-3.62781	1.89045	3.21122
H	-3.3114	1.93008	4.25883
C	-2.92266	1.08652	2.30201
H	-2.04476	0.513	2.62555
C	1.60241	1.30731	-0.51868
C	0.495	1.54215	0.24753
C	2.61147	2.34628	-0.88661
C	2.23846	3.69537	-1.11185
C	3.9792	2.00994	-1.04132
C	3.19478	4.6618	-1.45267
H	1.18501	3.97995	-1.03948
C	4.93466	2.97975	-1.37879
H	4.30638	0.9768	-0.88261
C	4.54925	4.31354	-1.58563
H	2.87453	5.69476	-1.62924
H	5.986	2.68822	-1.48062
H	5.29326	5.07046	-1.8558

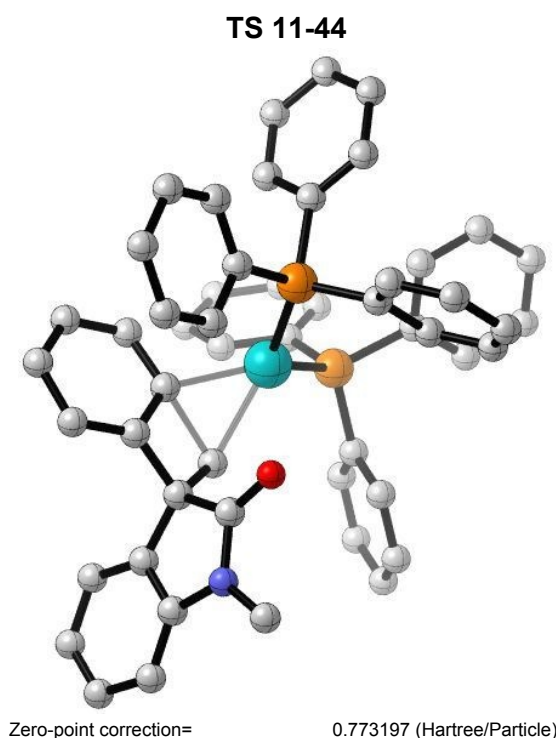
C	0.01221	2.8031	0.81306
O	0.47775	3.02679	2.08759
O	-0.80401	3.55634	0.26805
C	-0.07223	4.20556	2.71461
H	0.39448	4.2527	3.70898
H	0.16812	5.11124	2.13354
H	-1.1683	4.12686	2.80419



Zero-point correction= 0.660700 (Hartree/Particle)
 Thermal correction to Energy= 0.707308
 Thermal correction to Enthalpy= 0.708253
 Thermal correction to Gibbs Free Energy= 0.573783
 Sum of electronic and zero-point Energies= -2446.321476
 Sum of electronic and thermal Energies= -2446.274868
 Sum of electronic and thermal Enthalpies= -2446.273924
 Sum of electronic and thermal Free Energies= -2446.408393
 E(RM06L) = -2448.63030119

Pd	-0.6015	0.91626	-0.1906
P	-2.76857	-0.09684	0.15501
O	0.42603	-2.66277	1.03788
N	2.59924	-3.44453	0.77208
C	0.39263	-0.11366	-1.59973
C	-0.13992	0.0518	-2.89672
H	-0.941	0.77794	-3.06561
C	0.33432	-0.71272	-3.97467
H	-0.09873	-0.57498	-4.97166
C	1.3649	-1.63894	-3.75935
H	1.74888	-2.24911	-4.58351
C	1.92513	-1.76164	-2.48328
H	2.7544	-2.46005	-2.331
C	1.47888	-0.99007	-1.37989
C	2.19177	-1.22278	-0.02612
C	2.04363	-0.08195	1.04363
H	2.76726	-0.30875	1.84512
H	1.03125	-0.17651	1.47192
C	3.65153	-1.6329	-0.19614
C	4.74629	-0.9428	-0.71991
H	4.62502	0.07206	-1.10957
C	6.00994	-1.5698	-0.73649
H	6.87379	-1.03322	-1.14077
C	6.16721	-2.87329	-0.23864
H	7.15365	-3.34832	-0.25881
C	5.07274	-3.58622	0.28955
H	5.19462	-4.60281	0.67558
C	3.82851	-2.9449	0.29921
C	1.58311	-2.50085	0.64607
C	2.39309	-4.75464	1.36332
H	1.33187	-4.81466	1.64715
H	3.02445	-4.88665	2.26001
H	2.62867	-5.55571	0.64046
C	-3.20248	-1.80439	-0.39929
C	-2.71997	-2.25593	-1.64595
H	-2.05598	-1.61862	-2.23879
C	-3.07003	-3.53116	-2.11553

H	-2.68597	-3.87477	-3.08166
C	-3.89433	-4.36767	-1.3458
H	-4.16059	-5.36468	-1.71264
C	-4.36733	-3.92796	-0.09871
H	-5.0025	-4.58001	0.5104
C	-4.02273	-2.65279	0.37571
H	-4.38069	-2.31928	1.35517
C	-4.18637	0.94056	-0.43013
C	-5.49093	0.43407	-0.61294
H	-5.69504	-0.62479	-0.42353
C	-6.52258	1.2802	-1.04876
H	-7.53062	0.87698	-1.19297
C	-6.26394	2.63742	-1.30381
H	-7.0705	3.29372	-1.64734
C	-4.96795	3.14862	-1.12724
H	-4.75938	4.20362	-1.33345
C	-3.93274	2.30315	-0.69918
H	-2.9134	2.69267	-0.58045
C	-2.97312	-0.16956	1.99371
C	-3.9825	0.52873	2.68739
H	-4.72281	1.11349	2.13262
C	-4.04096	0.47375	4.09027
H	-4.82748	1.02077	4.62113
C	-3.09909	-0.27991	4.80742
H	-3.14694	-0.32074	5.9008
C	-2.09237	-0.97924	4.11891
H	-1.35496	-1.56867	4.67415
C	-2.01827	-0.9222	2.71956
H	-1.22762	-1.46551	2.18649
C	2.23316	1.33953	0.51708
C	1.17313	1.8879	-0.13585
C	3.51688	2.04797	0.79195
C	4.14899	2.8415	-0.19824
C	4.14324	1.94265	2.05817
C	5.35724	3.49983	0.07432
H	3.6846	2.92965	-1.18447
C	5.34615	2.60889	2.32904
H	3.66883	1.35299	2.84986
C	5.96201	3.38928	1.33682
H	5.8313	4.09946	-0.71056
H	5.8033	2.51939	3.32059
H	6.90539	3.90474	1.54616
C	1.06807	3.20471	-0.80471
O	0.21584	4.03579	-0.10359
O	1.57382	3.54286	-1.87354
C	0.01384	5.3278	-0.71985
H	-0.64737	5.87897	-0.03663
H	0.97251	5.85777	-0.84054
H	-0.45362	5.22083	-1.71289

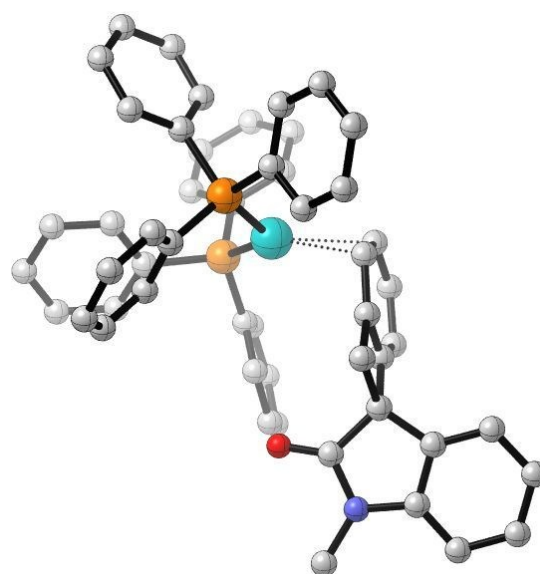


Thermal correction to Energy= 0.826006
 Thermal correction to Enthalpy= 0.826950
 Thermal correction to Gibbs Free Energy= 0.678619
 Sum of electronic and zero-point Energies= -2946.176522
 Sum of electronic and thermal Energies= -2946.123714
 Sum of electronic and thermal Enthalpies= -2946.122770
 Sum of electronic and thermal Free Energies= -2946.271101
 E(RM06L) = -2948.62581598
 Imaginary frequency = -345.91 cm⁻¹

Pd	0.00519	-0.05594	-0.32105
P	1.28781	-2.07611	-0.03709
P	1.09764	2.01364	0.14784
O	-2.43064	1.26445	1.81391
N	-4.53235	0.2713	1.88313
C	-1.64301	0.47785	-1.60796
C	-1.1062	0.78276	-2.8825
H	-0.16521	0.34354	-3.23064
C	-1.79404	1.70531	-3.69681
H	-1.35747	1.98953	-4.66146
C	-3.02989	2.25777	-3.30971
H	-3.54377	2.9601	-3.97413
C	-3.63884	1.85063	-2.10629
H	-4.65316	2.17655	-1.8498
C	-2.93831	0.95831	-1.29254
C	-3.34625	0.02686	-0.16814
C	-2.12579	-0.9328	-0.43094
H	-2.40082	-1.73519	-1.12993
H	-1.71873	-1.394	0.49202
C	-4.71226	-0.62403	-0.2323
C	-5.35914	-1.30456	-1.26428
H	-4.87256	-1.42187	-2.23865
C	-6.64971	-1.82901	-1.0395
H	-7.16547	-2.36553	-1.84199
C	-7.27719	-1.66311	0.20588
H	-8.2792	-2.07394	0.36807
C	-6.64175	-0.97068	1.25633
H	-7.13541	-0.83824	2.22383
C	-5.36181	-0.45987	1.01293
C	-3.32754	0.61966	1.26727
C	-4.8616	0.64978	3.24529
H	-4.00682	1.22394	3.63326
H	-5.02389	-0.24239	3.87599
H	-5.77095	1.2763	3.27332
C	1.67706	-2.85311	-1.68135
C	0.74229	-2.6798	-2.72654
H	-0.15891	-2.08376	-2.54091
C	0.96628	-3.25053	-3.98843
H	0.23042	-3.10907	-4.78734
C	2.13716	-3.98903	-4.22896
H	2.31862	-4.42635	-5.21656
C	3.07721	-4.15826	-3.19973
H	3.99373	-4.73001	-3.38192
C	2.8494	-3.59753	-1.93193
H	3.58682	-3.7345	-1.13459
C	0.33034	-3.41176	0.82884
C	0.17175	-4.72004	0.3243
H	0.6535	-5.00157	-0.61741
C	-0.59927	-5.66422	1.0228
H	-0.71472	-6.67512	0.61671
C	-1.21652	-5.31895	2.23563
H	-1.81747	-6.05713	2.77709
C	-1.06574	-4.01895	2.74711
H	-1.54754	-3.73877	3.69002
C	-0.30719	-3.07007	2.04514
H	-0.20611	-2.05182	2.43949
C	2.93065	-2.17438	0.82999
C	3.28708	-3.22673	1.70149
H	2.57803	-4.03781	1.89464
C	4.547	-3.23973	2.32275
H	4.8082	-4.06096	2.99926
C	5.46852	-2.20935	2.07667
H	6.44986	-2.22148	2.56294
C	5.1227	-1.15928	1.20973
H	5.8291	-0.34552	1.01588
C	3.86049	-1.13654	0.59787
H	3.59016	-0.30514	-0.06146
C	1.46111	2.30238	1.94612
C	1.43518	3.58179	2.54215
H	1.17953	4.45729	1.93712
C	1.72417	3.73513	3.90802
H	1.69591	4.7333	4.35871
C	2.04575	2.61653	4.69355
H	2.26889	2.7389	5.75898
C	2.07388	1.33978	4.10849

H	2.32017	0.46145	4.71483
C	1.77738	1.18324	2.74633
H	1.78544	0.18801	2.28931
C	2.77127	2.20619	-0.64428
C	3.88306	2.77959	0.00893
H	3.77954	3.14683	1.03491
C	5.12239	2.87709	-0.64667
H	5.97751	3.32124	-0.12518
C	5.26554	2.41226	-1.96392
H	6.23238	2.48888	-2.47274
C	4.16374	1.84207	-2.62446
H	4.26836	1.47141	-3.64984
C	2.92972	1.73161	-1.9662
H	2.07626	1.26408	-2.47002
C	0.26883	3.60226	-0.34164
C	-1.08115	3.77178	0.04169
H	-1.58723	2.97501	0.59913
C	-1.76474	4.95067	-0.28991
H	-2.80933	5.07321	0.01647
C	-1.12274	5.96401	-1.02187
H	-1.66303	6.87949	-1.28672
C	0.21354	5.79557	-1.41634
H	0.72204	6.57976	-1.98822
C	0.90895	4.62333	-1.07533
H	1.95358	4.50548	-1.37924

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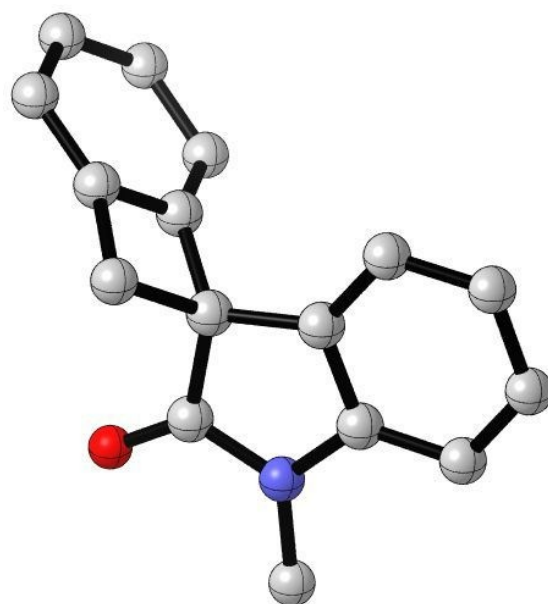


Zero-point correction= 0.775470 (Hartree/Particle)
 Thermal correction to Energy= 0.828565
 Thermal correction to Enthalpy= 0.829509
 Thermal correction to Gibbs Free Energy= 0.679740
 Sum of electronic and zero-point Energies= -2946.219727
 Sum of electronic and thermal Energies= -2946.166633
 Sum of electronic and thermal Enthalpies= -2946.165689
 Sum of electronic and thermal Free Energies= -2946.315457
 E(RM06L) = -2948.67374474

Pd	-0.55001	0.08668	-0.74647
P	-1.58875	2.0557	0.01413
P	-1.31418	-2.05069	-0.11531
O	3.34939	-0.52901	2.04898
N	5.62762	-0.32137	1.60497
C	2.35684	0.90925	-1.15089
C	1.20511	0.99768	-1.97283
H	0.7523	1.95391	-2.25245
C	0.90688	-0.21562	-2.6877
H	0.12157	-0.19503	-3.45218
C	1.74824	-1.36573	-2.61585
H	1.47841	-2.24225	-3.21489
C	2.9029	-1.40095	-1.82239
H	3.54646	-2.28443	-1.78998
C	3.15322	-0.23133	-1.08346
C	4.17135	0.39997	-0.12525
C	3.23622	1.70509	-0.19664
H	3.75622	2.58763	-0.60853

H	2.7787	1.963	0.77467
C	5.6182	0.53558	-0.53558
C	6.20431	0.98486	-1.71867
H	5.57724	1.30308	-2.55864
C	7.61157	1.01388	-1.81998
H	8.08277	1.36496	-2.74332
C	8.41033	0.59101	-0.74512
H	9.50122	0.61761	-0.83641
C	7.83405	0.12558	0.45427
H	8.46004	-0.20859	1.2872
C	6.43705	0.10528	0.53461
C	4.26924	-0.20845	1.29375
C	6.1069	-0.8398	2.87294
H	5.21836	-1.07357	3.47858
H	6.72475	-0.09017	3.39838
H	6.70646	-1.75616	2.72667
C	-1.15368	3.6556	-0.83174
C	0.15203	4.17356	-0.65575
H	0.84282	3.67321	0.03257
C	0.56474	5.32871	-1.33502
H	1.57515	5.72037	-1.17435
C	-0.31206	5.9802	-2.21979
H	0.01163	6.87917	-2.75474
C	-1.60417	5.46789	-2.41307
H	-2.2968	5.96933	-3.09801
C	-2.02428	4.31749	-1.7243
H	-3.03911	3.93707	-1.87665
C	-1.34569	2.50655	1.79979
C	-1.4691	3.8255	2.29219
H	-1.69987	4.64444	1.6029
C	-1.27912	4.09562	3.65675
H	-1.37482	5.12288	4.02533
C	-0.96286	3.05426	4.5453
H	-0.81019	3.26787	5.60872
C	-0.83301	1.74164	4.06415
H	-0.57647	0.92623	4.74841
C	-1.0185	1.46939	2.69944
H	-0.90346	0.44974	2.31576
C	-3.43954	2.02703	-0.18601
C	-4.33086	2.73938	0.64384
H	-3.94285	3.33821	1.47418
C	-5.71574	2.67469	0.4195
H	-6.39748	3.22545	1.07689
C	-6.22691	1.90877	-0.64136
H	-7.30754	1.8605	-0.81313
C	-5.34788	1.19596	-1.47345
H	-5.73867	0.58697	-2.29552
C	-3.96432	1.24674	-1.24025
H	-3.27126	0.66286	-1.85904
C	-2.30525	-2.21415	1.45357
C	-2.06026	-3.20536	2.42762
H	-1.24985	-3.92538	2.27766
C	-2.84893	-3.27052	3.58929
H	-2.64345	-4.04202	4.33959
C	-3.89459	-2.3555	3.78794
H	-4.50763	-2.40883	4.6941
C	-4.14561	-1.36576	2.82217
H	-4.95432	-0.64244	2.97065
C	-3.35135	-1.28978	1.66907
H	-3.53667	-0.50559	0.92733
C	-2.42892	-2.89975	-1.3404
C	-3.4408	-3.80986	-0.96561
H	-3.60225	-4.03486	0.09355
C	-4.24533	-4.4216	-1.94113
H	-5.02883	-5.12354	-1.63519
C	-4.04977	-4.1348	-3.30185
H	-4.68027	-4.61108	-4.06032
C	-3.04764	-3.22794	-3.68506
H	-2.89372	-2.99368	-4.74413
C	-2.24837	-2.61101	-2.71055
H	-1.47644	-1.88923	-2.99936
C	0.02974	-3.30234	0.16196
C	1.19804	-2.86023	0.82149
H	1.30623	-1.80876	1.11136
C	2.2405	-3.75769	1.09836
H	3.12837	-3.39176	1.62351
C	2.14497	-5.09961	0.69383
H	2.96333	-5.79802	0.90073
C	0.99795	-5.54118	0.01401
H	0.91888	-6.58445	-0.3115
C	-0.05758	-4.65107	-0.24558
H	-0.95265	-5.00841	-0.76516

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Zero-point correction= 0.241372 (Hartree/Particle)
 Thermal correction to Energy= 0.255827
 Thermal correction to Enthalpy= 0.256771
 Thermal correction to Gibbs Free Energy= 0.199881
 Sum of electronic and zero-point Energies= -747.268466
 Sum of electronic and thermal Energies= -747.254011
 Sum of electronic and thermal Enthalpies= -747.253067
 Sum of electronic and thermal Free Energies= -747.309957
 E(RM06L) = -747.667109048

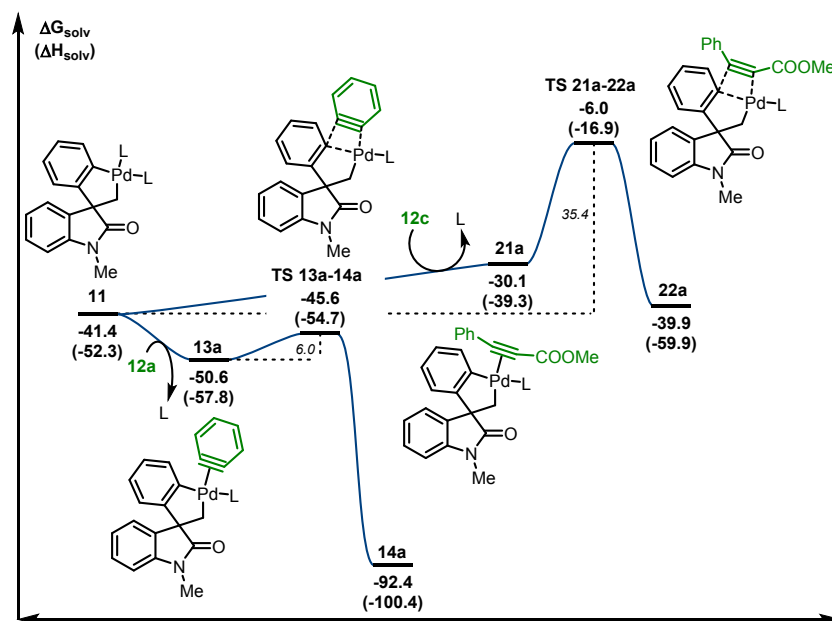
C	3.41482	1.94853	-0.21115
C	3.3423	0.54604	-0.32601
C	2.10149	-0.05894	-0.09679
C	0.95245	0.6951	0.23997
C	1.03974	2.08313	0.3406
C	2.28283	2.71146	0.11651
H	4.37367	2.4478	-0.38438
H	4.22581	-0.04446	-0.58574
H	0.15247	2.67684	0.58558
H	2.36356	3.79984	0.19548
C	0.42176	-1.63954	0.1457
C	-0.21127	-0.25028	0.41711
C	-1.06804	-0.20701	1.77277
H	-0.75499	0.59499	2.46246
H	-1.08069	-1.17314	2.30519
C	-1.543	0.0395	-0.29278
C	-2.28132	0.07937	0.89615
C	-2.11448	0.23967	-1.54951
C	-3.65611	0.31828	0.90723
C	-3.50404	0.4855	-1.55033
H	-1.54237	0.2113	-2.48227
C	-4.2535	0.52293	-0.35531
H	-4.25273	0.35018	1.82497
H	-4.01846	0.65084	-2.50299
H	-5.32991	0.71712	-0.41341
O	-0.12409	-2.73847	0.19953
N	1.77265	-1.42551	-0.15164
C	2.69264	-2.50781	-0.44912
H	3.11936	-2.39868	-1.46189
H	3.51743	-2.54035	0.28466
H	2.11339	-3.44159	-0.39262

5 – Selected Discussions Based on the Energy Span Model

The discussion reported herein applies the Energy Span Model proposed by Shaik and Kozuch (S. Kozuch and S. Shaik, Acc. Chem. Res., 2011, 44, 101).

The application of this method to the system under study would not provide reliable results due to the complexity of the reaction mechanism. For this reason, we prefer a *qualitative* treatment of the results instead of a *quantitative* one (possible with this model). Several association, dissociation, and ligand exchange processes as well as the treatment of salts as isolated molecules provides intrinsic errors that affects the correct estimation of the Gibbs free energy changes. Herein we present a short discussion on the application of the Energy Span model to selected steps of the full reaction mechanism.

- 1) *Comparison of the most favorable pathways for the migratory insertion step in the case of benzyne **12a** (Figure 4 in the paper) and the internal alkyne **12c** (Figure 7 in the paper).*

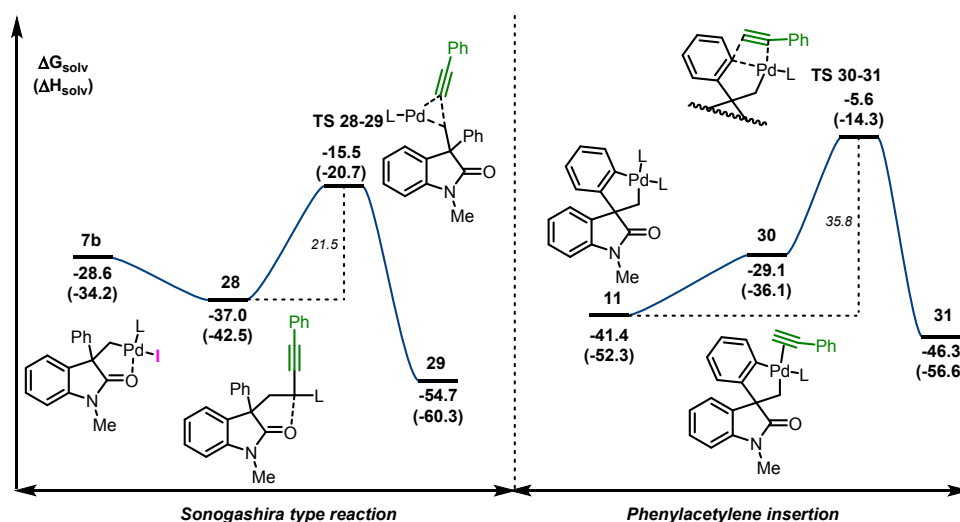


Energetically favored substitution of a ligand in **11** by benzyne **12a** provides structure **13a** with a decrease of energy of -9.2 kcal mol⁻¹. The subsequent migratory insertion step requires 6.0 kcal mol⁻¹, providing intermediate **14a**. On the contrary, ligand substitution in **11** by alkyne **12c** generates **21a** with an overall increase in energy of +11.3 kcal mol⁻¹. The subsequent migratory insertion step requires in this case 24.1 kcal mol⁻¹ and generates **22a**. The overall energy required for the insertion of alkyne **12c** is 35.4 kcal mol⁻¹ and, according to the energy span model, a difference of 29.4 kcal mol⁻¹ in comparison with the energy span calculated for the benzyne insertion (6.0 kcal mol⁻¹). Although qualitative consistent with the experiments, the high energy span required for the alkyne insertion seems to be in contrast with the experimental reaction conditions (100 °C) and the span energy difference would not account for the 80 °C required for the reaction in the case of benzyne reactants.

Several points should be taken into account in this evaluation:

- Due to its high reactivity, benzyne **12a** is formed *in situ* from the corresponding precursor (by treatment with CsF). The rate for the formation of this intermediate is unknown.
- The *in situ* formation of benzyne **12a** requires the presence of CsF in the reaction media whereas in the case of alkyne **12c** this salt is not necessary.
- Solubility of the salts involved in the reaction mechanism are not taken into account in this model and in DFT studies in general.
- Although the ligand exchange in both cases is a equimolecular process, intrinsic errors may still be present.

2) Comparison between the Sonogashira-type reaction and the migratory insertion of terminal alkyne **12e** (Figure 8 in the paper)



In analogy to the previous discussion, formation of the alkyne complex **28** from intermediate **7b** is thermodynamically favored ($\Delta G = -8.4$ kcal mol⁻¹). The subsequent C(sp³)–C(sp) bond-forming reductive elimination requires 21.5 kcal mol⁻¹. In the case of the migratory insertion mechanism, ligand exchange in **11** generates intermediate **30** with an increase of energy of +12.3 kcal mol⁻¹. The subsequent migratory insertion requires additional 23.5 kcal mol⁻¹ resulting in an overall energy span of 35.8 kcal mol⁻¹. This energy span is 14.3 kcal mol⁻¹ higher than the activation energy computed for the Sonogashira-type reaction. This results suggests that the Sonogashira-type reaction is even more kinetically favored to the corresponding migratory insertion mechanism when comparing the difference in energy between the two corresponding transition states **TS 28-29** and **TS 30-31**, respectively.