Supporting Information for

Computational modelling of Pd-catalysed alkoxycarbonylation of alkenes and alkynes†

Shahbaz Ahmad,[a] Michael Bühl*[a]

Contents

1. Methodology

Several studies involving homogenous catalysis validated the success of B3PW91[S1–S3] functional,[S4–S8] of which studies on (2-pyridyl)thiourea Pd(II) complexes[S8] are closely related to our systems. When coupled with Grimme's DFT-D3,[S9–S11] including Becke-Johnson damping,[S12,S13] B3PW91 benchmarks well against explicitly correlated CCSD(T).[S14]

We optimised the geometries of all transition states at the B3PW91/ECP1 level, where ECP1 corresponds with the 6-31G** basis set on all non-metal atoms in conjunction with SDD effective core potential (ECP)[S15–S18] on the metal atom. We used frequency calculations within the harmonic approximation to verify the nature of all transition states.

We computed harmonic frequencies analytically at 298.15 K to account for free energy and enthalpic corrections. Thermochemical correction term for each step, δE_G, was calculated as the difference of reaction energy ($\Delta E_{B3PW91/ECP1}$) and the corresponding free energy ($\Delta G_{B3PW91/ECP1}$):

$$\delta E_G = \Delta G_{B3PW9\ /ECP1} - \Delta E_{B3PW91/ECP1} \quad \text{(Eq. S1)}$$

Starting structures for most transition states were obtained by freezing respective coordinates and optimising the remaining geometric parameters with loose convergence criteria. Potential energy profile calculations were also performed to get starting structures for some transition states by increasing or decreasing the atom's distance of a coordinated moiety from one to the other ligand by 0.1 Å. The obtained structures from both methods were fully optimised to transition states. We carried out visual inspections of the imaginary frequency modes and performed intrinsic reaction coordinate (IRC) calculations to confirm the transition states.[S19,S20]

We used coordinates of the optimised transition states to refine energies at the B3PW91-D3/ECP2/PCM level of theory. ECP2 corresponds with 6-311+G** basis set on all non-metal atoms and SDD ECP on Pd. Methanol was used in the polarisable continuum (PCM)[S21–S23] model to account for the solvent effects, and missing dispersion was added with Grimme's DFT-D3,[S9–S11] including Becke-Johnson damping ($\boldsymbol{\delta_{D3}}$)[S12,S13] $\boldsymbol{\Delta\Delta G^{\ddagger}}$ and enthalpies $\boldsymbol{\Delta\Delta H^{\ddagger}}$ were calculated as:

$$\boldsymbol{\Delta\Delta G^{\ddagger}} = \Delta E + \delta E_{Solv} + \boldsymbol{\delta_{D3}} + \delta E_G \quad \text{(Eq. S2)}$$

$$\boldsymbol{\Delta\Delta H^{\ddagger}} = \Delta E + \delta E_{Solv} + \boldsymbol{\delta_{D3}} + \delta E_H \quad \text{(Eq. S3)}$$

where ΔE, and δE_{Solv} are computed at the B3PW91/ECP2 level, δE_G and δE_H are computed at the B3PW91/ECP1 level. All calculations were performed using Gaussian 09.[S24]

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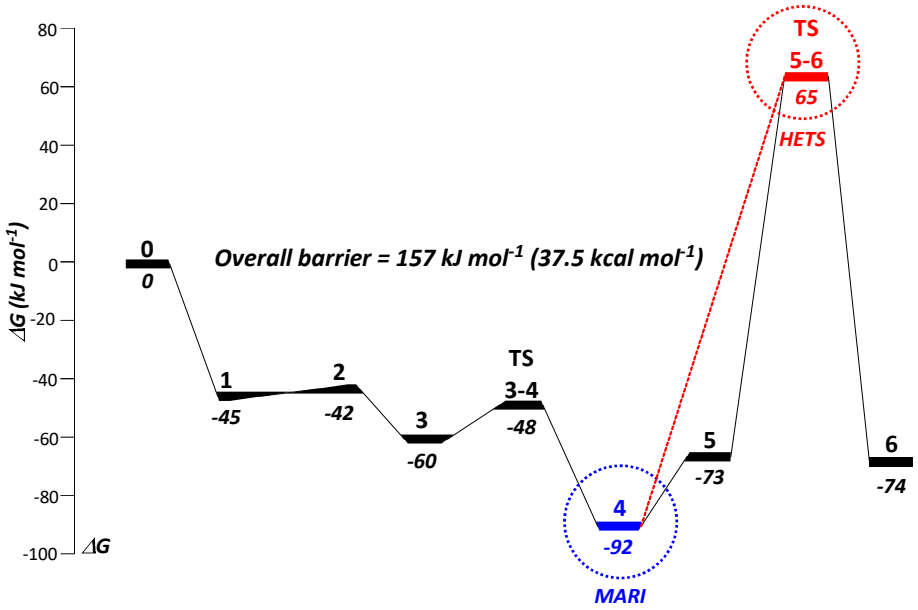
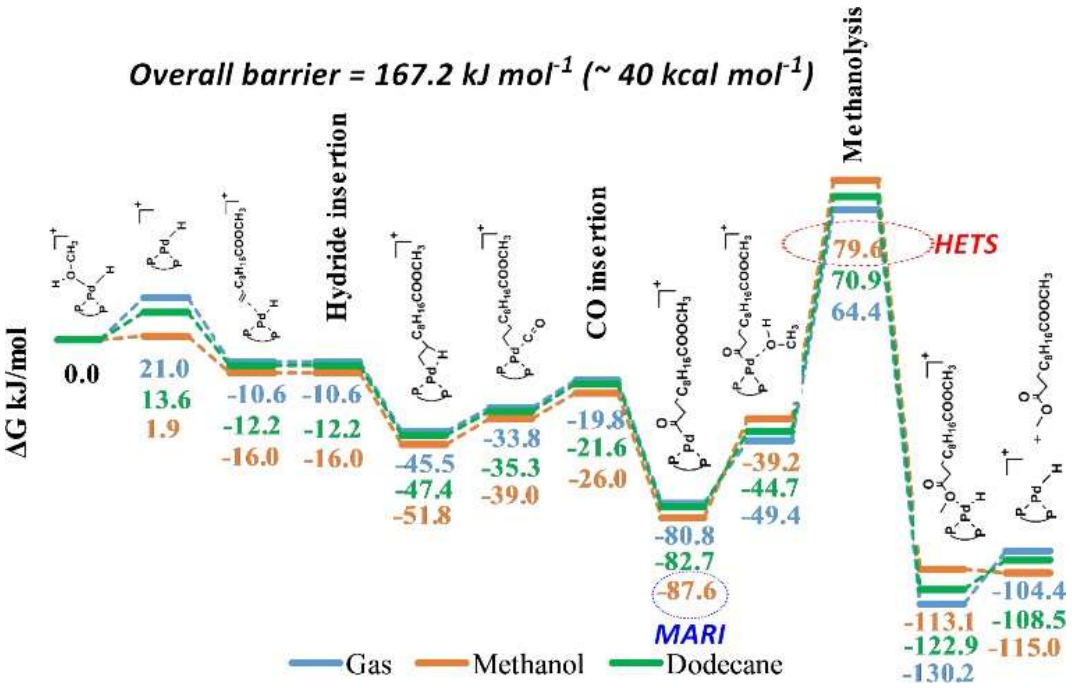


Scheme S1. Schematic reaction profile for Pd–catalysed methoxycarbonylation of *cis*-3-hexene with DMBPX (drawn from the data given in reference 100 in the main paper). The rate-limiting transition state, **TS5-6** (HETS, encircled in red), is 65 kJ mol^{-1} above the reactants (**0**, catalyst + substrates). This value is not the overall barrier of the catalytic cycle, however, which needs to be taken as the difference between the HETS and the lowest intermediate in the cycle (MARI, **4** in this case, encircled in blue). The resulting overall barrier is therefore 157 kJ mol^{-1}.



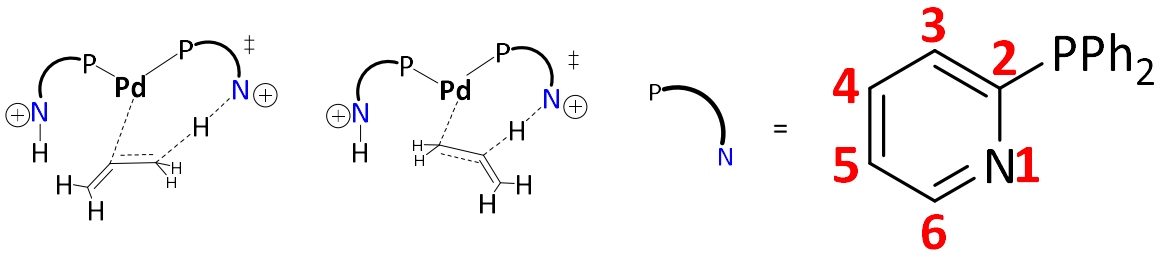
Scheme S2. Schematic profile for the Pd–catalysed methoxycarbonylation of methyl 10-undecenoate with DTBPX at PBE0-D3/def2-TZVP/COSMO. Looking at the data for methanol (orange energy levels), the overall barrier of the cycle is not the difference between the highest TS (HETS, encircled in red) and the reactants, i.e. 79.6 kJ mol^{-1}, but that between the HETS and the lowest intermediate (MARI, encircled in blue) and HETS (encircled in red), i.e. 0167.2 kJ mol^{-1}. Adapted from reference 103 in the main paper.

Table S1. Predicted branched:linear selectivities during carbonylation of propadiene with different ligands.

Ligand	$\Delta\Delta G^{\ddagger}$ (kcal mol^{-1})	% Branched (at 45 °C)
$PyPPh_2$	1.3	88.66
(6-Cl-Py)PPh_2	3.6	99.66
(6-Me-Py)PPh_2	1.1	85.07
(5,6-dichloro-Py)PPh_2	2.9	98.99
(6-Cl-5-NO_2-Py)PPh_2	0.6	72.09
(6-Cl-5-Me_2N-Py)PPh_2	2.3	97.44
(6-Cl-3-Me-Py)PPh_2	4.0	99.82

$\Delta\Delta G^{\ddagger} = \Delta G^{\ddagger}_{9L^+ \rightarrow 10L^+} - \Delta G^{\ddagger}_{9^+ \rightarrow 2ii^+}$ (see Scheme S1).

a) ***b)***



$TS9–2ii^+$ **$TS9L–10L^+$** **Numbering scheme of substituents**

Scheme S3. ***a)*** Transition states governing branched:linear selectivities, ***b)*** ligand with the numbering scheme of substituents.

3. **Atomic coordinates (in Å) of selected transition states, optimised at the B3PW91/ECP1 level, and corresponding SCF energies (in a.u.).**

TS9-2ii^{+} ($PyPPh_2$)

scf done: -2349.437491

Pd	0.057845	-1.194313	-0.462513
P	-2.023830	-0.015816	-0.045743
C	-3.286790	-0.961436	-1.026306
N	-2.902238	-2.202433	-1.349092
C	-4.544738	-0.484029	-1.390366
C	-3.725735	-3.028450	-2.002381
C	-5.411655	-1.334608	-2.078082
H	-6.397388	-0.986113	-2.371556
C	-5.002859	-2.630352	-2.383716
H	-5.651132	-3.317624	-2.916324
H	-4.839742	0.531842	-1.150111
H	-3.343521	-4.020177	-2.227878
C	-2.559509	-0.219149	1.688783
C	-3.908329	-0.151847	2.072631
C	-1.577002	-0.457362	2.661044
C	-4.261983	-0.313890	3.408874
H	-4.685840	0.021030	1.334671
C	-1.937535	-0.614575	3.998391
H	-0.531222	-0.529884	2.372945
C	-3.277843	-0.543627	4.372293
H	-5.307075	-0.264871	3.699163
H	-1.171044	-0.799179	4.744776
H	-3.559464	-0.672556	5.412997
C	-2.428743	1.718964	-0.508093
C	-2.864236	2.665694	0.431276
C	-2.284459	2.101878	-1.854788
C	-3.173712	3.966598	0.023579
H	-2.986317	2.384672	1.473199
C	-2.603321	3.396706	-2.256045
H	-1.942972	1.381145	-2.595005
C	-3.052929	4.330433	-1.317757
H	-3.529943	4.686660	0.754642
H	-2.511808	3.675487	-3.301736
H	-3.315132	5.335694	-1.634401
H	-1.538218	-2.503101	-1.043418
P	2.010527	-0.011282	-0.057469
C	2.521478	-0.110940	1.696981
C	3.331867	-0.453189	4.353551
C	3.185676	0.923965	2.372624
C	2.262762	-1.318266	2.366826
C	2.675546	-1.487127	3.686527
C	3.582987	0.751240	3.696845
H	3.403583	1.865774	1.878384
H	1.754725	-2.128045	1.849780
H	2.483680	-2.428482	4.192635
H	4.094834	1.557414	4.213580
H	3.649185	-0.585397	5.383471
C	1.953196	1.834786	-0.346248
C	1.642059	4.589360	-0.688023
N	0.762791	2.457972	-0.204258
C	3.047284	2.619799	-0.699767
C	2.893721	3.997218	-0.864690
C	0.569148	3.781555	-0.360411
H	4.011285	2.144752	-0.844328
H	3.751428	4.607421	-1.132578
H	-0.447290	4.136023	-0.229277
H	1.494766	5.655931	-0.813656
C	3.472693	-0.414096	-1.072355
C	5.662608	-0.980102	-2.706773
C	4.752080	-0.533498	-0.511787
C	3.292759	-0.591146	-2.453246
C	4.388470	-0.864589	-3.266328
C	5.842656	-0.819692	-1.333451
H	4.897058	-0.416129	0.558105
H	2.297248	-0.533876	-2.887140
H	4.247813	-1.002265	-4.334092
H	6.831716	-0.921998	-0.897325
H	6.514113	-1.205354	-3.341765
C	0.948590	-2.971834	-0.778803
C	-0.432893	-3.335350	-0.953352
H	-0.641303	-3.707013	-1.961893
H	-0.842335	-3.973798	-0.165743
C	2.151459	-3.519815	-0.770030
H	2.262218	-4.590513	-0.937845
H	3.062708	-2.952963	-0.615957
H	-0.056390	1.876214	-0.013651

TS9L-10L^{+} ($PyPPh_2$)

scf done: -2349.439679

Pd	0.048353	-1.088576	-0.317826
P	-1.995336	0.099654	-0.000839
C	-3.103560	-0.687861	-1.278947
N	-2.723346	-1.909345	-1.678850
C	-4.261300	-0.104496	-1.792285
C	-3.447508	-2.609674	-2.555957
C	-5.026230	-0.822094	-2.713962
H	-5.932317	-0.386349	-3.124423
C	-4.619455	-2.096157	-3.101818
H	-5.189244	-2.679408	-3.816998
H	-4.557218	0.893089	-1.485643
H	-3.064837	-3.591816	-2.820610
C	-2.810970	-0.244565	1.595000
C	-4.199475	-0.141836	1.774514
C	-2.001291	-0.624511	2.675453
C	-4.763137	-0.415011	3.017453
H	-4.845355	0.145738	0.950285
C	-2.571102	-0.889562	3.919584
H	-0.926771	-0.719846	2.538568
C	-3.950428	-0.787041	4.090010
H	-5.838171	-0.339427	3.149701
H	-1.939159	-1.182138	4.752607
H	-4.395396	-1.000259	5.057246
C	-2.253514	1.889699	-0.328782
C	-2.712495	2.766759	0.665201
C	-1.941297	2.397821	-1.602909
C	-2.876943	4.125278	0.380312
H	-2.966723	2.388987	1.651155
C	-2.117277	3.750349	-1.883569
H	-1.580889	1.732481	-2.384584
C	-2.588370	4.616517	-0.892897
H	-3.253844	4.792236	1.150392
H	-1.898693	4.127885	-2.878266
H	-2.739435	5.668338	-1.117463
H	-1.499869	-2.381161	-1.161341
P	2.111668	-0.082435	-0.025412
C	2.761121	-0.357421	1.662123
C	3.722823	-0.922858	4.228735
C	3.792073	0.416669	2.218535
C	2.214006	-1.412971	2.408434
C	2.698895	-1.695652	3.683633
C	4.266538	0.133294	3.496619
H	4.235302	1.238385	1.663662
H	1.412802	-2.015110	1.987428
H	2.276804	-2.520020	4.250395
H	5.064196	0.735912	3.920208
H	4.098657	-1.142112	5.223496
C	2.168336	1.779588	-0.140520
C	1.994848	4.564745	-0.144446
N	1.045015	2.440893	0.217995
C	3.257430	2.541049	-0.553977
C	3.173344	3.934183	-0.549103
C	0.919289	3.781300	0.230628
H	4.160765	2.035592	-0.878001
H	4.027346	4.528046	-0.861882
H	-0.049288	4.171878	0.522322
H	1.903555	5.644800	-0.134259
C	3.422127	-0.526817	-1.214162
C	5.338537	-1.223888	-3.122760
C	4.681408	-0.985153	-0.807215
C	3.122260	-0.432613	-2.583569
C	4.082342	-0.771049	-3.532013
C	5.633691	-1.334731	-1.765456
H	4.918628	-1.079813	0.247751

H	2.137074	-0.102644	-2.907395
H	3.849026	-0.693143	-4.589638
H	6.606527	-1.696726	-1.447001
H	6.083311	-1.497827	-3.863809
C	-0.482472	-3.145360	-0.629973
H	0.225454	1.871656	0.444226
C	-1.152821	-4.149701	-0.036686
H	-0.724241	-5.146049	0.057937
H	-2.181745	-4.026912	0.293376
C	0.883562	-2.913022	-0.955623
H	1.665394	-3.309927	-0.310305
H	1.179536	-2.788196	-1.997010

TS9-2ii^{+} (6-Cl-Py)PPh$_2$)

scf done: -3268.499531

Pd	-0.233132	-1.338323	-0.065406
P	-1.740980	0.496871	0.186892
C	-3.358647	-0.155239	-0.461409
N	-3.451311	-1.498064	-0.447133
C	-4.414864	0.631938	-0.904129
C	-4.588966	-2.096982	-0.806198
C	-5.599305	0.006456	-1.302007
H	-6.440058	0.596360	-1.654817
C	-5.701893	-1.376651	-1.240736
H	-6.605411	-1.899944	-1.531549
H	-4.313140	1.710608	-0.949394
C	-2.141888	0.955275	1.910978
C	-3.358245	1.541214	2.294716
C	-1.183649	0.665240	2.894013
C	-3.598742	1.845861	3.632223
H	-4.130440	1.748118	1.559998
C	-1.428421	0.971874	4.230925
H	-0.253994	0.178332	2.609694
C	-2.634788	1.564153	4.600668
H	-4.544528	2.294804	3.920047
H	-0.685677	0.734054	4.986716
H	-2.830684	1.794680	5.643442
C	-1.552736	2.038990	-0.783730
C	-1.982320	3.294482	-0.333120
C	-1.012161	1.916975	-2.076266
C	-1.902263	4.403627	-1.176811
H	-2.385118	3.408164	0.669138
C	-0.932389	3.029573	-2.912617
H	-0.683766	0.943431	-2.436421
C	-1.386303	4.272160	-2.465878
H	-2.250891	5.370723	-0.826226
H	-0.530169	2.924245	-3.916027
H	-1.338709	5.135536	-3.122948
H	-2.225516	-2.134454	-0.285508
P	1.982702	-0.667950	-0.038688
C	3.132052	-1.740805	0.888989
C	4.811110	-3.380497	2.403034
C	4.454575	-1.960021	0.478898
C	2.650337	-2.361460	2.053299
C	3.493862	-3.168400	2.812533
C	5.286600	-2.783408	1.235769
H	4.831693	-1.511373	-0.434532
H	1.611924	-2.234049	2.349666
H	3.117473	-3.648573	3.710669
H	6.306168	-2.962474	0.908375
H	5.463040	-4.022997	2.987150
C	2.355073	0.979376	0.765365
C	2.829666	3.535992	1.811488
N	1.967403	2.114689	0.122781
C	2.990700	1.124985	1.991785
C	3.220520	2.399707	2.514090
C	2.195511	3.363359	0.590586
H	3.320373	0.238610	2.520987
H	3.725922	2.509710	3.469291
H	3.014143	4.537224	2.182343
C	2.666290	-0.377965	-1.707468
C	3.684810	-0.076971	-4.296508
C	2.030734	-0.996892	-2.795118
C	3.819410	0.395857	-1.931110
C	4.321341	0.545173	-3.221148
C	2.543285	-0.847906	-4.082463
H	1.146486	-1.605751	-2.626667
H	4.339243	0.872468	-1.103647
H	5.214564	1.140056	-3.386395
H	2.051326	-1.337243	-4.917587
H	4.082610	0.037584	-5.300302
C	0.111781	-3.296464	-0.386003
H	1.486616	2.029348	-0.774703
C	1.118138	-4.132223	-0.579391
H	0.924561	-5.189250	-0.757815
H	2.157652	-3.824006	-0.557296
C	-1.322576	-3.262339	-0.350136
H	-1.790275	-3.548992	-1.295944
H	-1.773651	-3.747942	0.518963
Cl	-4.656149	-3.814378	-0.728464
Cl	1.702030	4.665401	-0.382437

TS9L-10L^{+} (6-Cl-Py)PPh$_2$)

scf done: -3268.500118

Pd	-0.269867	-1.060506	0.498000
P	-1.717219	0.748720	-0.003728
C	-3.215574	-0.149248	-0.674624
N	-3.305660	-1.449830	-0.336277
C	-4.198566	0.447031	-1.457333
C	-4.341374	-2.188712	-0.736338
C	-5.291084	-0.319446	-1.870739
H	-6.074049	0.126117	-2.477251
C	-5.373464	-1.657691	-1.509905
H	-6.199610	-2.287930	-1.818251
H	-4.110171	1.487133	-1.749630
C	-2.369023	1.643929	1.449710
C	-3.461788	2.522125	1.370889
C	-1.761061	1.411884	2.691659
C	-3.930220	3.157806	2.516649
H	-3.947683	2.716248	0.419257
C	-2.232354	2.053427	3.836282
H	-0.926847	0.717678	2.759838
C	-3.315732	2.925256	3.748908
H	-4.777038	3.834103	2.449801
H	-1.757795	1.868249	4.795252
H	-3.686150	3.422391	4.640367
C	-1.417755	2.007662	-1.300551
C	-1.278880	3.366813	-0.987986
C	-1.259349	1.591383	-2.633218
C	-1.010541	4.294485	-1.995640
H	-1.402396	3.708598	0.035154
C	-1.002109	2.523059	-3.635596
H	-1.362086	0.540987	-2.896345
C	-0.879315	3.877525	-3.318889
H	-0.926872	5.348041	-1.744951
H	-0.911662	2.193822	-4.666862
H	-0.694906	4.605146	-4.103823
H	-2.275173	-1.936341	0.455282
P	1.984828	-0.852997	0.037095
C	3.028166	-0.643162	1.522679
C	4.569234	-0.383632	3.845176
C	4.388142	-0.288915	1.437866
C	2.451089	-0.853692	2.784644
C	3.221413	-0.725715	3.939371
C	5.151086	-0.162336	2.595152
H	4.856883	-0.119843	0.471336
H	1.399871	-1.120126	2.856856
H	2.768786	-0.895050	4.911588
H	6.201134	0.104321	2.522409
H	5.168871	-0.287153	4.745223
C	2.509865	0.667419	-0.911526
C	3.127277	3.118018	-2.123898
N	2.585047	1.832457	-0.214843
C	2.757433	0.724419	-2.277079
C	3.069394	1.945627	-2.875997
C	2.878109	3.032494	-0.764198
H	2.723584	-0.190400	-2.857505
H	3.279759	1.986438	-3.940794
H	3.370986	4.076455	-2.566071
C	2.663867	-2.189813	-1.003508
C	3.554142	-4.257629	-2.660280
C	3.895866	-2.807747	-0.753953

C	1.868937	-2.631603	-2.075006
C	2.321210	-3.652203	-2.907363
C	4.332757	-3.841316	-1.581644
H	4.506874	-2.506006	0.090209
H	0.889875	-2.187873	-2.245154
H	1.704919	-3.987875	-3.736017
H	5.283457	-4.324468	-1.377913
H	3.900514	-5.063345	-3.300333
C	-1.453138	-2.543410	1.440357
H	2.454112	1.790517	0.795921
C	-2.291128	-2.648463	2.486654
H	-2.243512	-3.491019	3.174755
H	-3.110010	-1.947622	2.631469
C	-0.191742	-3.093698	1.085753
H	0.534941	-3.320296	1.863694
H	-0.100752	-3.705152	0.188653
Cl	2.938502	4.371356	0.284235
Cl	-4.360652	-3.848902	-0.287511

TS9-2ii^{+} (6-Me-Py)PPh$_2$)

scf done: -2428.063659

Pd	-0.058841	-1.342716	-0.169003
P	-1.870956	0.188441	0.130717
C	-3.342275	-0.703732	-0.569555
N	-3.215108	-2.039886	-0.606387
C	-4.506276	-0.070173	-0.992261
C	-4.236336	-2.825491	-0.999097
C	-5.570697	-0.861307	-1.425541
H	-6.494163	-0.400856	-1.764115
C	-5.440458	-2.243275	-1.411320
H	-6.257992	-2.881223	-1.730411
H	-4.578592	1.011990	-0.990192
C	-2.341849	0.491802	1.872026
C	-3.651227	0.797597	2.274063
C	-1.337265	0.381672	2.844984
C	-3.940431	1.006589	3.620445
H	-4.453457	0.859098	1.545021
C	-1.630870	0.591377	4.190697
H	-0.327514	0.113347	2.544575
C	-2.931940	0.906325	4.579168
H	-4.957224	1.238996	3.922292
H	-0.848931	0.494753	4.938204
H	-3.164005	1.061608	5.628448
C	-1.958159	1.795500	-0.750740
C	-2.564809	2.936510	-0.209300
C	-1.454863	1.841019	-2.062742
C	-2.698037	4.092131	-0.981811
H	-2.946511	2.921477	0.807357
C	-1.590181	2.997515	-2.830020
H	-0.985321	0.959723	-2.495895
C	-2.221851	4.121997	-2.293005
H	-3.186331	4.966185	-0.560490
H	-1.218742	3.016007	-3.850610
H	-2.343965	5.016887	-2.896127
H	-1.843103	-2.481850	-0.445031
P	2.003381	-0.304382	-0.052616
C	3.268245	-1.195843	0.915976
C	5.114814	-2.570465	2.499035
C	4.627451	-1.190362	0.573737
C	2.837532	-1.909609	2.046097
C	3.761782	-2.583184	2.840489
C	5.543648	-1.882319	1.364427
H	4.972997	-0.670714	-0.314090
H	1.778370	-1.958795	2.287483
H	3.423807	-3.134948	3.712415
H	6.593812	-1.887025	1.088824
H	5.833022	-3.108931	3.109946
C	2.056200	1.366866	0.778000
C	2.030745	3.939425	1.849367
N	1.537230	2.434625	0.115996
C	2.577096	1.591298	2.044452
C	2.556371	2.880369	2.581701
C	1.514150	3.708513	0.578400
H	3.009363	0.762884	2.593414
H	2.967748	3.058554	3.571086
H	2.024741	4.948401	2.246016
C	2.700107	0.110789	-1.689356
C	3.770313	0.602407	-4.228205
C	2.207466	-0.574245	-2.810886
C	3.734607	1.049729	-1.854067
C	4.263416	1.291971	-3.119072
C	2.745192	-0.329304	-4.073090
H	1.415426	-1.308173	-2.687901
H	4.142291	1.583346	-0.998973
H	5.067128	2.012347	-3.238589
H	2.364493	-0.869467	-4.934591
H	4.189127	0.790504	-5.212198
C	0.620903	-3.194244	-0.530484
H	1.146752	2.269732	-0.811253
C	1.754736	-3.850312	-0.712981
H	1.744676	-4.920356	-0.917123
H	2.727949	-3.374776	-0.655645
C	-0.803838	-3.418976	-0.524441
H	-1.188179	-3.770559	-1.485787
H	-1.159461	-4.010780	0.323075
C	-4.046365	-4.312650	-0.999938
H	-3.447674	-4.632844	-1.860229
H	-3.542719	-4.651077	-0.091397
H	-5.009422	-4.821661	-1.066369
C	0.988023	4.775198	-0.320575
H	1.764594	5.081944	-1.031844
H	0.118452	4.435551	-0.889722
H	0.703586	5.654933	0.258316

TS9L-10L^{+} (6-Me-Py)PPh$_2$)

scf done: -2428.064281

Pd	-0.047664	-1.120352	0.370157
P	-1.885326	0.332089	0.000898
C	-3.085743	-0.805883	-0.864906
N	-2.909073	-2.118418	-0.638640
C	-4.107572	-0.350739	-1.692840
C	-3.717208	-3.045066	-1.184978
C	-4.960610	-1.290241	-2.273941
H	-5.767910	-0.966632	-2.924413
C	-4.766392	-2.641108	-2.018182
H	-5.412013	-3.390363	-2.464116
H	-4.228979	0.709217	-1.887468
C	-2.758752	0.830362	1.527055
C	-4.122523	1.161789	1.546510
C	-2.024641	0.870125	2.721304
C	-4.733824	1.534553	2.740756
H	-4.712338	1.125454	0.635276
C	-2.639760	1.248867	3.913358
H	-0.974560	0.586630	2.717117
C	-3.993442	1.580944	3.923156
H	-5.790152	1.785804	2.749716
H	-2.065986	1.274984	4.834965
H	-4.475188	1.869407	4.852540
C	-1.881679	1.799849	-1.096996
C	-2.370426	3.047501	-0.687016
C	-1.352404	1.660735	-2.390941
C	-2.341727	4.134117	-1.564313
H	-2.792363	3.169202	0.306094
C	-1.334185	2.745067	-3.264092
H	-0.975091	0.696432	-2.724802
C	-1.828710	3.984610	-2.851876
H	-2.742930	5.091952	-1.245212
H	-0.947077	2.621108	-4.271429
H	-1.826401	4.826575	-3.537906
H	-1.784140	-2.448071	0.182568
P	2.102656	-0.365450	0.040155
C	2.980418	0.009741	1.599503
C	4.287469	0.503440	4.023698
C	4.194329	0.719402	1.619001
C	2.425704	-0.438318	2.807822
C	3.080439	-0.193472	4.013782
C	4.841950	0.961898	2.827040
H	4.642329	1.074678	0.694230
H	1.483708	-0.980652	2.799098
H	2.648708	-0.549189	4.944367
H	5.782513	1.504444	2.835389
H	4.798125	0.691353	4.963338

C	2.313817	1.273939	-0.826962
C	2.485808	3.845509	-1.888453
N	1.822054	2.369901	-0.192366
C	2.913822	1.468319	-2.062281
C	3.001238	2.759451	-2.589179
C	1.876568	3.641095	-0.654670
H	3.325587	0.617055	-2.591840
H	3.486836	2.917326	-3.547971
H	2.554463	4.852721	-2.283289
C	3.151815	-1.456727	-0.979138
C	4.642113	-3.174011	-2.605161
C	4.461032	-1.802262	-0.621103
C	2.585998	-1.993898	-2.147934
C	3.335175	-2.838182	-2.962969
C	5.198383	-2.662689	-1.434081
H	4.903650	-1.420209	0.292952
H	1.556806	-1.759790	-2.412812
H	2.895575	-3.246337	-3.868151
H	6.209416	-2.935212	-1.147087
H	5.221475	-3.843074	-3.234108
C	-0.886452	-2.931275	1.108024
H	1.390806	2.222877	0.717952
C	-1.656872	-3.320831	2.141706
H	-1.377945	-4.154063	2.785044
H	-2.632538	-2.873203	2.317775
C	0.485454	-3.123123	0.766970
H	1.222283	-3.253485	1.557683
H	0.747698	-3.604468	-0.174663
C	-3.454848	-4.487914	-0.875520
C	1.264049	4.717722	0.176738
H	-4.057383	-5.136243	-1.513424
H	-3.705541	-4.712655	0.166373
H	-2.400997	-4.740300	-1.020579
H	0.177539	4.726315	0.029423
H	1.652004	5.694717	-0.114474
H	1.464889	4.572143	1.242506

TS9-2ii^{+} (5,6-dichloro-Py)PPh$_2$)

scf done: -4187.555252

Pd	0.517880	-1.354087	-0.173784
P	1.361101	0.875574	-0.210627
C	3.166772	0.677125	0.180577
N	3.658762	-0.544615	-0.088519
C	3.995744	1.677139	0.677034
C	4.957587	-0.819486	0.049809
C	5.350095	1.408020	0.853707
H	6.023101	2.166613	1.240930
C	5.858453	0.152902	0.523684
H	3.591982	2.650492	0.933450
C	1.380726	1.702252	-1.841494
C	2.296234	2.706904	-2.192338
C	0.443342	1.270588	-2.792074
C	2.256364	3.279726	-3.461118
H	3.054684	3.036937	-1.488910
C	0.407572	1.845862	-4.060534
H	-0.243534	0.466308	-2.540889
C	1.311586	2.852611	-4.394771
H	2.970875	4.053548	-3.724807
H	-0.314204	1.498285	-4.793781
H	1.290528	3.295643	-5.385808
C	0.845809	2.104184	1.047410
C	0.843316	3.488197	0.827027
C	0.508877	1.607569	2.319616
C	0.543820	4.361318	1.874245
H	1.078385	3.887324	-0.155353
C	0.207537	2.485228	3.360287
H	0.512653	0.533811	2.500254
C	0.235180	3.863750	3.140213
H	0.558280	5.433230	1.699528
H	-0.033830	2.094544	4.344566
H	0.016642	4.548079	3.954674
H	2.676957	-1.495437	-0.265645
P	-1.780427	-1.414797	0.100805
C	-2.670511	-2.647937	-0.908973
C	-3.971831	-4.489149	-2.557706
C	-3.805000	-3.327472	-0.443331
C	-2.180618	-2.910302	-2.199048
C	-2.839315	-3.819350	-3.023117
C	-4.447341	-4.248961	-1.268751
H	-4.176929	-3.160130	0.562486
H	-1.271797	-2.424657	-2.546484
H	-2.456489	-4.021151	-4.018904
H	-5.317491	-4.783725	-0.900455
H	-4.475213	-5.209617	-3.195290
C	-2.726143	0.127387	-0.369960
C	-4.070774	2.534828	-0.923664
N	-2.617707	1.226595	0.419772
C	-3.530809	0.240372	-1.498471
C	-4.191767	1.433207	-1.775421
C	-3.255985	2.400715	0.205717
H	-3.651356	-0.618358	-2.148617
H	-4.827570	1.517379	-2.651984
C	-2.295525	-1.596395	1.843902
C	-3.007956	-2.006028	4.518236
C	-1.366161	-2.129751	2.750579
C	-3.587657	-1.267971	2.291951
C	-3.937371	-1.471628	3.624167
C	-1.725952	-2.335889	4.081079
H	-0.370246	-2.396178	2.406297
H	-4.329496	-0.867434	1.605437
H	-4.938081	-1.221301	3.963226
H	-1.004838	-2.757331	4.774826
H	-3.286576	-2.167959	5.555135
C	0.813610	-3.346759	-0.179125
H	-2.019706	1.175756	1.247712
C	0.133055	-4.473157	-0.049725
H	0.649917	-5.431542	-0.080467
H	-0.943870	-4.503891	0.075112
C	2.153047	-2.857762	-0.334572
H	2.812816	-3.116479	0.498005
H	2.600901	-3.041418	-1.314390
Cl	5.492490	-2.393190	-0.363958
Cl	-3.033149	3.626041	1.352302
Cl	7.522846	-0.185797	0.714409
Cl	-4.898925	3.989995	-1.243783

TS9L-10L^{+} (5,6-dichloro-Py)PPh$_2$)

scf done: -4187.556234

Pd	-0.499066	-1.134126	0.487079
P	-1.309307	1.085152	0.329340
C	-3.036618	0.804539	-0.327135
N	-3.529387	-0.435880	-0.162876
C	-3.808649	1.781947	-0.948243
C	-4.754343	-0.770389	-0.570073
C	-5.096120	1.464617	-1.371756
H	-5.722003	2.209363	-1.853543
C	-5.594082	0.175895	-1.186454
H	-3.409170	2.776056	-1.113931
C	-1.577314	1.922413	1.930113
C	-2.355125	3.083864	2.062409
C	-0.992654	1.352146	3.069966
C	-2.537230	3.662374	3.314925
H	-2.817950	3.542932	1.193773
C	-1.175594	1.937251	4.322067
H	-0.405090	0.441968	2.972566
C	-1.947609	3.090755	4.444410
H	-3.141758	4.559103	3.411603
H	-0.721577	1.489637	5.201074
H	-2.094846	3.544917	5.419660
C	-0.677783	2.355578	-0.829514
C	-0.125005	3.560898	-0.376226
C	-0.692911	2.082488	-2.207922
C	0.384732	4.484971	-1.289737
H	-0.110520	3.791473	0.684751
C	-0.192764	3.013253	-3.114694
H	-1.117777	1.152132	-2.578761
C	0.345975	4.217555	-2.656954
H	0.793655	5.424579	-0.929710
H	-0.235366	2.805074	-4.180017
H	0.723482	4.948752	-3.365630
H	-2.687636	-1.322967	0.467707
P	1.713323	-1.548863	-0.041577

C	2.756997	-1.921422	1.412873
C	4.275953	-2.561005	3.677607
C	4.161709	-1.987523	1.333259
C	2.129025	-2.166546	2.644161
C	2.887186	-2.487103	3.769012
C	4.912584	-2.307109	2.461081
H	4.672787	-1.800654	0.391788
H	1.046215	-2.108725	2.715943
H	2.392240	-2.681067	4.715676
H	5.994560	-2.364072	2.389785
H	4.865112	-2.814607	4.553685
C	2.680500	-0.121039	-0.751206
C	4.022407	2.206699	-1.579302
N	3.173484	0.794820	0.118984
C	2.870171	0.133353	-2.105386
C	3.538635	1.282148	-2.512855
C	3.823157	1.931049	-0.224835
H	2.510264	-0.583286	-2.834770
H	3.703772	1.474797	-3.568716
C	1.962106	-2.833274	-1.315385
C	2.198650	-4.767367	-3.319367
C	2.972549	-3.800610	-1.241521
C	1.054206	-2.856842	-2.387919
C	1.183254	-3.812901	-3.392343
C	3.083413	-4.764845	-2.242069
H	3.657680	-3.824343	-0.400986
H	0.236480	-2.139614	-2.424022
H	0.481003	-3.825565	-4.220482
H	3.861154	-5.519385	-2.174715
H	2.290066	-5.521825	-4.094780
C	-2.062432	-2.302156	1.304615
H	3.089869	0.590292	1.115652
C	-2.863023	-2.293826	2.384624
H	-3.073567	-3.202821	2.945920
H	-3.406345	-1.400448	2.683739
C	-1.053217	-3.157562	0.787281
H	-0.416520	-3.715041	1.471914
H	-1.184916	-3.623323	-0.188908
Cl	4.364685	2.923169	1.039361
Cl	-5.253274	-2.392443	-0.341438
Cl	-7.168076	-0.232152	-1.713383
Cl	4.845512	3.614127	-2.080195

TS9-2ii^{+} (6-Cl-5-NO2-Py)PPh$_2$)

scf done: -3677.274349

Pd	-0.535628	1.408240	-0.148792
P	-1.243994	-0.864232	-0.351130
C	-3.026578	-0.822848	0.193908
N	-3.598757	0.390626	0.113248
C	-3.761320	-1.936640	0.586731
C	-4.898672	0.573252	0.379439
C	-5.112232	-1.775896	0.874418
H	-5.741623	-2.612783	1.161613
C	-5.683952	-0.514206	0.781241
H	-3.290012	-2.909229	0.668098
C	-1.402454	-1.457966	-2.072315
C	-2.004227	-2.683010	-2.403763
C	-0.963141	-0.609556	-3.098911
C	-2.146694	-3.052718	-3.737919
H	-2.363020	-3.352645	-1.627695
C	-1.111322	-0.982274	-4.433836
H	-0.522594	0.352591	-2.847389
C	-1.700729	-2.204094	-4.753117
H	-2.612859	-4.001143	-3.987009
H	-0.776248	-0.316348	-5.223417
H	-1.820987	-2.494125	-5.792524
C	-0.569996	-2.236013	0.654643
C	0.048202	-3.357383	0.084566
C	-0.641852	-2.125952	2.054057
C	0.560715	-4.365656	0.903265
H	0.108262	-3.459855	-0.994808
C	-0.138987	-3.140602	2.864909
H	-1.108990	-1.257131	2.513185
C	0.458689	-4.264266	2.290060
H	1.024635	-5.239166	0.455011
H	-0.222455	-3.059328	3.944768
H	0.839002	-5.061178	2.922029
H	-2.688148	1.416368	-0.080690
P	1.759715	1.609480	0.068804
C	2.571047	2.708577	-1.142979
C	3.721359	4.330428	-3.106644
C	3.754075	3.410564	-0.870128
C	1.956161	2.844689	-2.398386
C	2.537726	3.644378	-3.378998
C	4.320876	4.220232	-1.851994
H	4.222112	3.355559	0.106549
H	1.006834	2.352072	-2.594027
H	2.056102	3.749582	-4.346370
H	5.230013	4.771550	-1.632484
H	4.167570	4.964806	-3.866443
C	2.678423	0.012958	-0.230607
C	3.892569	-2.481292	-0.494797
N	2.973372	-0.778731	0.830208
C	3.029230	-0.456003	-1.493753
C	3.645219	-1.694158	-1.618984
C	3.564499	-1.997827	0.767411
H	2.841132	0.162255	-2.363916
H	3.960744	-2.076422	-2.585707
C	2.324680	2.011946	1.758819
C	3.089089	2.722283	4.359712
C	1.370529	2.474614	2.679198
C	3.671664	1.903515	2.162323
C	4.046134	2.255935	3.456523
C	1.755170	2.830710	3.970581
H	0.332202	2.569069	2.374499
H	4.435517	1.556869	1.470062
H	5.086599	2.175957	3.756550
H	1.011049	3.195944	4.671674
H	3.386173	3.002145	5.365846
C	-0.940244	3.382794	-0.106953
H	2.779828	-0.402250	1.761569
C	-0.302296	4.540512	-0.076522
H	-0.861180	5.475404	-0.092420
H	0.779318	4.620256	-0.046816
C	-2.257233	2.818921	-0.153465
H	-2.852608	3.018442	0.741395
H	-2.802975	2.988640	-1.084881
Cl	-5.531090	2.143865	0.148743
Cl	3.910619	-2.731387	2.251642
N	-7.114191	-0.393200	1.129730
O	-7.810651	-1.341939	0.813355
O	-7.455285	0.611243	1.724698
N	4.510262	-3.807120	-0.705197
O	4.243356	-4.673074	0.107251
O	5.203594	-3.909295	-1.699777

TS9L-10L^{+} (6-Cl-5-NO$_2$-Py)PPh$_2$)

scf done: -3677.275362

Pd	0.474462	1.223064	0.546384
P	1.149351	-1.047306	0.478464
C	2.908784	-0.890216	-0.152012
N	3.457758	0.331943	-0.035990
C	3.641412	-1.942095	-0.694720
C	4.700098	0.599864	-0.454249
C	4.949725	-1.705817	-1.104727
H	5.575785	-2.497388	-1.505475
C	5.476689	-0.425396	-1.008312
H	3.201193	-2.926500	-0.802053
C	1.354981	-1.853623	2.103075
C	1.956147	-3.113714	2.257229
C	0.919001	-1.153835	3.237774
C	2.114048	-3.659285	3.527403
H	2.294191	-3.677433	1.392724
C	1.077931	-1.706595	4.507696
H	0.464738	-0.172630	3.121590
C	1.675825	-2.956960	4.652304
H	2.580647	-4.633019	3.641271
H	0.739102	-1.160074	5.382640
H	1.803124	-3.386861	5.641241
C	0.458714	-2.310486	-0.655410
C	-0.269185	-3.405676	-0.168139
C	0.588059	-2.137384	-2.044184

C	-0.834186	-4.324096	-1.054791
H	-0.374417	-3.560902	0.901521
C	0.032422	-3.063882	-2.923945
H	1.143739	-1.292685	-2.445136
C	-0.677655	-4.160725	-2.430883
H	-1.379557	-5.179009	-0.666290
H	0.166809	-2.938076	-3.994574
H	-1.095069	-4.892019	-3.116975
H	2.661649	1.277578	0.561851
P	-1.691493	1.737762	-0.090971
C	-2.790856	2.245025	1.275898
C	-4.393888	3.070010	3.418346
C	-4.185060	2.371636	1.114360
C	-2.217053	2.524096	2.526511
C	-3.016983	2.937736	3.590160
C	-4.977568	2.782559	2.182667
H	-4.654788	2.160495	0.156516
H	-1.144118	2.417721	2.661015
H	-2.564317	3.157666	4.552128
H	-6.050280	2.885179	2.049476
H	-5.015557	3.395289	4.246981
C	-2.643469	0.273573	-0.736964
C	-3.858126	-2.140799	-1.420101
N	-3.250442	-0.531437	0.172849
C	-2.683209	-0.128271	-2.068521
C	-3.304320	-1.323182	-2.405145
C	-3.844121	-1.720746	-0.094236
H	-2.241954	0.504888	-2.829509
H	-3.378962	-1.654002	-3.436641
C	-1.811869	2.919418	-1.473931
C	-1.842709	4.680229	-3.643320
C	-2.788588	3.921129	-1.549821
C	-0.834390	2.822302	-2.479251
C	-0.860700	3.691823	-3.566449
C	-2.796322	4.798496	-2.633027
H	-3.525752	4.038880	-0.762902
H	-0.042721	2.079817	-2.398181
H	-0.105106	3.612062	-4.342178
H	-3.548141	5.580122	-2.682939
H	-1.854996	5.368019	-4.483289
C	2.082148	2.323306	1.367037
H	-3.293977	-0.196188	1.137303
C	2.866191	2.293430	2.458339
H	3.133671	3.203740	2.992670
H	3.340360	1.374498	2.795276
C	1.140940	3.222040	0.801076
H	0.521845	3.834443	1.453910
H	1.322240	3.649133	-0.184710
Cl	-4.547607	-2.507459	1.229436
Cl	5.259925	2.199520	-0.246864
N	6.846974	-0.216568	-1.517222
O	7.620095	-1.139662	-1.329493
O	7.066084	0.827979	-2.100531
N	-4.438190	-3.430621	-1.845961
O	-4.807445	-3.482039	-3.004716
O	-4.462703	-4.325288	-1.021412

TS9-2ii^{+} (6-Cl-5-Me$_2$N-Py)PPh$_2$)

scf done: -3536.361513

Pd	-0.568085	1.384190	-0.276741
P	-1.234644	-0.902259	-0.213256
C	-3.059770	-0.839559	0.043813
N	-3.642627	0.321277	-0.303682
C	-3.853302	-1.887038	0.506527
C	-4.957901	0.495651	-0.251264
C	-5.222120	-1.712359	0.619567
H	-5.826344	-2.519298	1.017948
C	-5.849199	-0.494239	0.264857
H	-3.400120	-2.823939	0.813193
C	-1.016001	-1.835200	-1.773906
C	-1.891275	-2.842108	-2.206248
C	0.075847	-1.487229	-2.582883
C	-1.664208	-3.498758	-3.414018
H	-2.763086	-3.105448	-1.614998
C	0.300707	-2.146968	-3.789107
H	0.735513	-0.680318	-2.273627
C	-0.567935	-3.154899	-4.204882
H	-2.350963	-4.272938	-3.742897
H	1.142029	-1.862093	-4.414276
H	-0.401246	-3.661784	-5.150591
C	-0.708387	-2.011010	1.150896
C	-0.649513	-3.405974	1.027727
C	-0.439698	-1.418507	2.397272
C	-0.360219	-4.194897	2.141776
H	-0.836847	-3.876897	0.066685
C	-0.145869	-2.212315	3.505858
H	-0.492328	-0.336274	2.504189
C	-0.115607	-3.601952	3.380576
H	-0.332643	-5.276223	2.041839
H	0.045907	-1.746709	4.468208
H	0.097616	-4.220884	4.247128
H	-2.723710	1.350065	-0.499497
P	1.697953	1.636376	0.125079
C	2.538160	2.899874	-0.891610
C	3.778170	4.776656	-2.548359
C	3.549374	3.725970	-0.382344
C	2.141896	3.029476	-2.232159
C	2.769852	3.957439	-3.058596
C	4.161261	4.664764	-1.212197
H	3.849030	3.654190	0.658687
H	1.327552	2.422391	-2.620183
H	2.458421	4.055882	-4.094129
H	4.934652	5.312561	-0.810732
H	4.256106	5.511165	-3.189587
C	2.814878	0.182240	-0.195459
C	4.409301	-2.173521	-0.566530
N	2.655410	-0.948244	0.535822
C	3.842043	0.152407	-1.135912
C	4.608846	-0.985806	-1.316925
C	3.406567	-2.064979	0.433965
H	4.030214	1.032882	-1.738691
H	5.386084	-0.972455	-2.072599
C	2.069086	1.983604	1.881949
C	2.554397	2.629357	4.561167
C	1.057782	2.559940	2.665825
C	3.326929	1.731975	2.455152
C	3.563956	2.052388	3.789584
C	1.304778	2.884615	3.998219
H	0.085701	2.764628	2.224765
H	4.128854	1.297386	1.863896
H	4.539474	1.858403	4.225356
H	0.519929	3.338219	4.595988
H	2.744203	2.881827	5.600066
C	-1.020620	3.332910	-0.456228
H	1.932645	-0.964775	1.259628
C	-0.450576	4.524919	-0.390527
H	-1.045214	5.426695	-0.531532
H	0.610591	4.663016	-0.214159
C	-2.309894	2.725733	-0.645948
H	-3.037959	2.998016	0.122966
H	-2.709428	2.805005	-1.659839
Cl	-5.552994	1.960030	-0.956174
Cl	3.144198	-3.227857	1.657257
C	-8.057625	-1.498205	0.462871
C	-7.824534	0.915503	0.820439
H	-8.120644	-1.898541	1.484790
H	-9.063416	-1.208603	0.150317
H	-7.715239	-2.283678	-0.214815
H	-7.083941	1.618675	1.197624
H	-8.399838	1.393458	0.021765
H	-8.502762	0.678525	1.646852
C	6.442543	-3.170564	-1.460045
C	4.658361	-4.646961	-0.628475
H	6.975437	-2.265880	-1.158399
H	7.062471	-4.024384	-1.179556
H	6.321000	-3.179409	-2.551697
H	5.062298	-5.154513	0.252716
H	3.569878	-4.658264	-0.586904
H	4.956367	-5.206776	-1.520074
N	5.169835	-3.280859	-0.755696
N	-7.196517	-0.327687	0.369555

TS9L-10L^{+} (6-Cl-5-Me$_2$N-Py)PPh$_2$)

scf done: -3536.361731

Pd	-0.546461	-1.199299	0.466682
P	-1.246484	1.059430	0.500122
C	-2.938678	0.938506	-0.244272
N	-3.513917	-0.277655	-0.228087
C	-3.630894	1.997079	-0.830975
C	-4.727991	-0.501836	-0.709675
C	-4.918990	1.801632	-1.301759
H	-5.458411	2.642646	-1.722175
C	-5.560582	0.543369	-1.216593
H	-3.169670	2.975722	-0.908861
C	-1.510758	1.743876	2.175063
C	-2.363798	2.829698	2.426830
C	-0.838302	1.138110	3.245810
C	-2.530733	3.301802	3.725781
H	-2.901934	3.307994	1.613659
C	-1.005490	1.615990	4.544736
H	-0.196457	0.279708	3.060341
C	-1.850866	2.697396	4.784745
H	-3.194530	4.140452	3.913438
H	-0.483549	1.138966	5.368978
H	-1.986488	3.067109	5.796704
C	-0.501047	2.405961	-0.496094
C	-0.057887	3.607243	0.071302
C	-0.348022	2.202760	-1.877994
C	0.513603	4.594254	-0.734004
H	-0.172483	3.784393	1.136280
C	0.215181	3.193508	-2.677082
H	-0.691143	1.277351	-2.335353
C	0.646165	4.392923	-2.106032
H	0.839128	5.528559	-0.285927
H	0.306214	3.035277	-3.748002
H	1.073568	5.171112	-2.731600
H	-2.740360	-1.275938	0.344798
P	1.655226	-1.690824	-0.020105
C	2.618225	-2.166960	1.462910
C	4.014447	-2.949035	3.760218
C	4.022052	-2.241937	1.450044
C	1.926019	-2.477433	2.642848
C	2.623391	-2.869058	3.784548
C	4.712935	-2.632940	2.593579
H	4.578528	-2.004941	0.546658
H	0.841329	-2.412322	2.663251
H	2.079111	-3.112324	4.692059
H	5.796867	-2.695455	2.574198
H	4.556635	-3.255957	4.649513
C	2.756061	-0.345969	-0.683027
C	4.493069	1.817147	-1.403245
N	3.027496	0.698257	0.134076
C	3.324515	-0.282189	-1.951976
C	4.162282	0.764471	-2.297841
C	3.815564	1.753699	-0.157835
H	3.137029	-1.085492	-2.655275
H	4.619143	0.758778	-3.281072
C	1.880959	-2.983741	-1.292219
C	2.102874	-4.924746	-3.292022
C	2.806701	-4.026088	-1.159856
C	1.052645	-2.930799	-2.425502
C	1.173972	-3.891698	-3.426087
C	2.910637	-4.993934	-2.158306
H	3.432672	-4.098964	-0.276547
H	0.304964	-2.145501	-2.515558
H	0.532883	-3.844670	-4.301339
H	3.621990	-5.806413	-2.045152
H	2.187025	-5.682040	-4.065595
C	-2.209451	-2.344943	1.105780
H	2.594278	0.704347	1.056160
C	-3.038761	-2.400453	2.162896
H	-3.290872	-3.344128	2.644063
H	-3.562515	-1.516554	2.519350
C	-1.216271	-3.201945	0.554035
H	-0.640120	-3.851972	1.209847
H	-1.328091	-3.573378	-0.464021
Cl	3.838576	2.986604	1.027267
Cl	-5.191554	-2.165293	-0.826887
C	-7.438877	1.327307	-2.553721
C	-7.791205	-0.526072	-0.987579
H	-6.719977	1.663137	-3.304710
H	-8.264375	0.843409	-3.080314
H	-7.840530	2.198731	-2.017423
H	-7.397475	-0.887364	-0.039037
H	-8.694510	0.053379	-0.769117
H	-8.066252	-1.382224	-1.611058
C	6.286484	3.437651	-0.817914
C	5.641643	3.050994	-3.159306
H	6.362693	2.866244	0.106193
H	7.277252	3.437224	-1.282243
H	6.011491	4.470717	-0.584615
H	6.422751	2.379841	-3.541763
H	4.740595	2.946967	-3.768209
H	5.994950	4.078568	-3.267353
N	5.342728	2.817697	-1.751530
N	-6.831957	0.350243	-1.661389

TS9-2ii^{+} (6-Cl-3-Me-Py)PPh$_2$)

scf done: -3347.110482

Pd	-0.367290	-1.237304	-0.184790
P	-1.865200	0.595660	0.220501
C	-3.356609	0.262990	-0.867630
N	-3.445188	-1.061053	-1.137395
C	-4.342564	1.158430	-1.310913
C	-4.491164	-1.564875	-1.785441
C	-5.417588	0.603595	-2.030169
H	-6.200240	1.263361	-2.395770
C	-5.517655	-0.754314	-2.264198
H	-6.354962	-1.187383	-2.798957
C	-2.583116	0.536452	1.902554
C	-3.635538	1.364666	2.325268
C	-2.091601	-0.441823	2.780475
C	-4.165831	1.226322	3.604831
H	-4.051436	2.115795	1.662117
C	-2.627530	-0.579215	4.059854
H	-1.295799	-1.107626	2.451969
C	-3.662570	0.256675	4.473654
H	-4.979081	1.871936	3.922360
H	-2.242152	-1.342841	4.728774
H	-4.084017	0.149144	5.468539
C	-1.341044	2.312871	-0.127280
C	-1.302754	3.308160	0.858232
C	-0.921623	2.620627	-1.431536
C	-0.883592	4.599184	0.533085
H	-1.626070	3.087107	1.870989
C	-0.510657	3.912542	-1.751713
H	-0.940623	1.856866	-2.206370
C	-0.496201	4.906143	-0.770505
H	-0.882200	5.371144	1.297537
H	-0.216481	4.148642	-2.770495
H	-0.193971	5.917708	-1.025339
H	-2.276039	-1.815158	-0.836031
P	1.873389	-0.756964	0.176337
C	2.656885	-1.487667	1.653534
C	3.805212	-2.700022	3.897071
C	3.900562	-1.046920	2.138079
C	1.992851	-2.534485	2.308108
C	2.570813	-3.139803	3.422708
C	4.468586	-1.652237	3.255650
H	4.431692	-0.233117	1.650856
H	1.033506	-2.881507	1.935705
H	2.054792	-3.955470	3.919960
H	5.429950	-1.308325	3.625128
H	4.252319	-3.171385	4.767023
C	2.387835	1.035748	0.345615
C	3.249254	3.695299	0.280785
N	3.087019	1.560945	-0.693647
C	2.086439	1.869515	1.430402
C	2.537859	3.197139	1.366933
C	3.516104	2.836217	-0.771056
H	2.326897	3.861228	2.200571
H	3.595384	4.721225	0.242262
C	2.889260	-1.228617	-1.280388
C	4.337046	-1.923623	-3.574527

C	2.331785	-1.040962	-2.559196
C	4.176076	-1.777874	-1.164984
C	4.889801	-2.127756	-2.310398
C	3.059318	-1.376630	-3.699155
H	1.316504	-0.662114	-2.656508
H	4.611966	-1.955254	-0.187174
H	5.877985	-2.566834	-2.212521
H	2.620442	-1.232762	-4.681831
H	4.896879	-2.201172	-4.462503
C	-0.069451	-3.170150	-0.681668
H	3.308323	0.919070	-1.463234
C	0.901262	-4.062138	-0.783674
H	0.677496	-5.085273	-1.083038
H	1.942778	-3.829598	-0.588006
C	-1.484824	-3.026962	-0.863559
H	-1.803216	-3.171957	-1.898563
H	-2.113275	-3.553859	-0.141700
Cl	-4.572971	-3.269622	-2.033118
Cl	4.375297	3.291958	-2.168867
C	1.347171	1.377742	2.636746
H	0.542037	0.689602	2.366946
H	2.023732	0.838062	3.308129
H	0.915041	2.212793	3.191129
C	-4.348830	2.648916	-1.108335
H	-3.731036	2.982710	-0.278642
H	-3.976245	3.154091	-2.006823
H	-5.370997	2.998789	-0.941226

TS9L-10L^{+} (6-Cl-3-Me-Py)PPh$_2$)

scf done: -3347.111527

Pd	-0.336106	-1.006247	0.410834
P	-1.866450	0.770201	0.003179
C	-3.534359	-0.084661	-0.076141
N	-3.467611	-1.405024	0.195544
C	-4.749862	0.513290	-0.449809
C	-4.530460	-2.196030	0.094547
C	-5.867369	-0.337316	-0.535945
H	-6.828624	0.084451	-0.817435
C	-5.775260	-1.694779	-0.279799
H	-6.631273	-2.354851	-0.360616
C	-1.974399	1.952873	1.394342
C	-3.077503	2.013452	2.255545
C	-0.855126	2.758287	1.662396
C	-3.068348	2.876907	3.350510
H	-3.948492	1.389006	2.081620
C	-0.856900	3.629436	2.748572
H	0.017578	2.709331	1.015457
C	-1.963538	3.689217	3.596033
H	-3.930313	2.915989	4.009658
H	0.006576	4.260560	2.937571
H	-1.962593	4.364802	4.445833
C	-1.871066	1.730985	-1.560074
C	-1.713221	3.120925	-1.608670
C	-2.028897	1.012238	-2.755900
C	-1.719848	3.781342	-2.837812
H	-1.614736	3.694935	-0.692206
C	-2.051045	1.678656	-3.978660
H	-2.151840	-0.068746	-2.734962
C	-1.893510	3.065453	-4.021695
H	-1.611111	4.861713	-2.866178
H	-2.195724	1.117034	-4.897022
H	-1.917062	3.586077	-4.974444
H	-2.263431	-1.843359	0.759336
P	1.911086	-0.837359	-0.162582
C	2.900333	-1.135025	1.358113
C	4.283765	-1.552085	3.759424
C	3.991825	-2.014894	1.401274
C	2.496805	-0.478785	2.538677
C	3.196220	-0.678242	3.727959
C	4.672641	-2.222954	2.600617
H	4.300130	-2.552221	0.510515
H	1.617627	0.163608	2.532947
H	2.878177	-0.168190	4.632300
H	5.508767	-2.915141	2.627343
H	4.819361	-1.718696	4.689052
C	2.657559	0.793957	-0.708100
C	3.845186	3.273492	-1.229944
N	3.472465	1.424664	0.177496
C	2.406858	1.419313	-1.937883
C	3.020133	2.660346	-2.168014
C	4.062487	2.620125	-0.029397
H	2.846033	3.161966	-3.116286
H	4.314861	4.231856	-1.417061
C	2.546695	-1.943168	-1.466931
C	3.441270	-3.692669	-3.456862
C	3.864177	-1.853774	-1.947983
C	1.681057	-2.905743	-2.003498
C	2.130368	-3.779723	-2.991617
C	4.306468	-2.727772	-2.937299
H	4.550856	-1.109481	-1.552672
H	0.655908	-2.963690	-1.649495
H	1.455510	-4.526002	-3.399563
H	5.326664	-2.657536	-3.302319
H	3.790415	-4.373591	-4.227148
C	-1.329650	-2.367413	1.690622
H	3.649587	0.935726	1.062766
C	-2.021920	-2.347082	2.840787
H	-1.851530	-3.088931	3.618619
H	-2.840025	-1.650251	3.003718
C	-0.115862	-2.948655	1.239984
H	0.723241	-3.033085	1.927573
H	-0.144064	-3.702611	0.454300
Cl	5.045736	3.236273	1.217174
Cl	-4.322105	-3.873700	0.421672
C	-4.920300	1.971023	-0.769404
H	-4.289395	2.612322	-0.152732
H	-4.668261	2.167752	-1.816912
H	-5.959717	2.270959	-0.616179
C	1.549794	0.787763	-2.990516
H	2.129023	0.058125	-3.566917
H	0.697694	0.261955	-2.553061
H	1.164661	1.541885	-3.679068