Electronic Supplementary Information

Mechanism, Electronic and Ligand Effects for Reductive Elimination from ArylPd(II) Trifluoromethyl Complexes: a Systematic DFT Study

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Contents

1. Additional Computational Results

1.1 Computational methods effect using different DFT functionals

(a) Density functional theory method effects on optimized structures

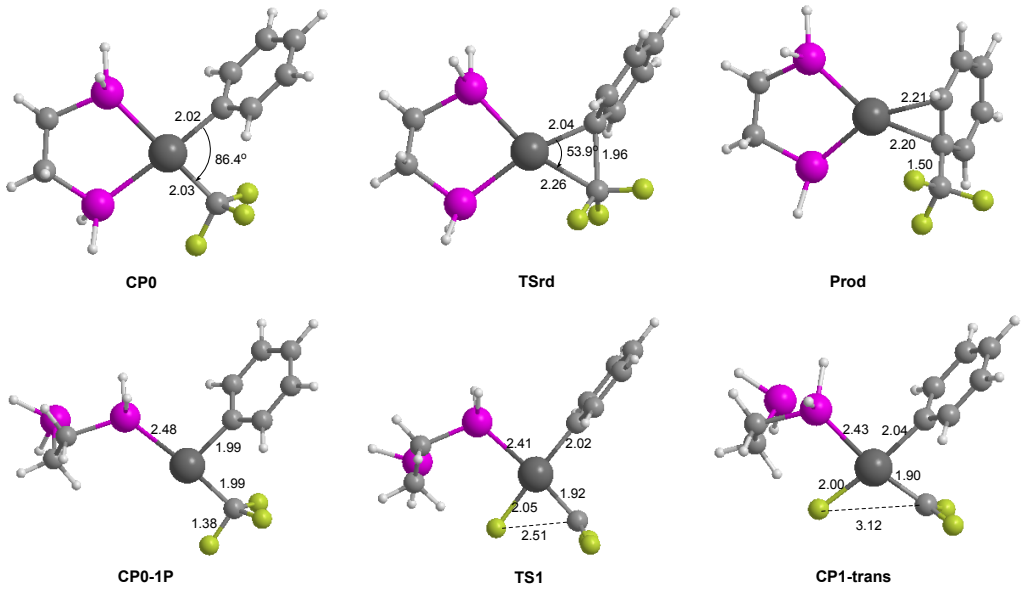


Fig. S1 Optimized intermediates and transition states involved in direct reductive elimination and α-fluoride elimination steps using B3P86 method.

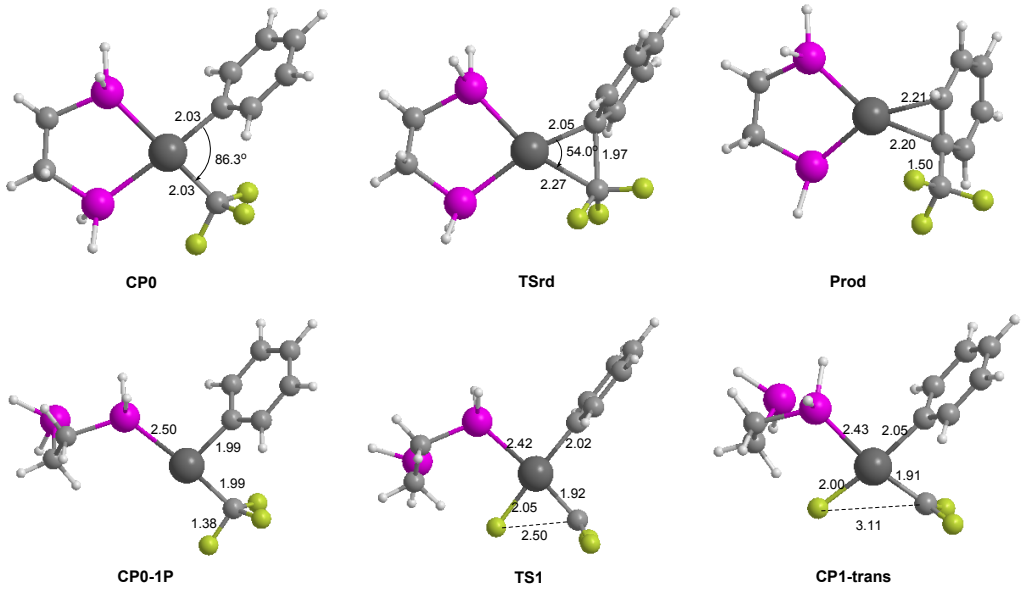


Fig. S2 Optimized intermediates and transition states involved in direct reductive elimination and α-fluoride elimination steps using B3PW91 method.

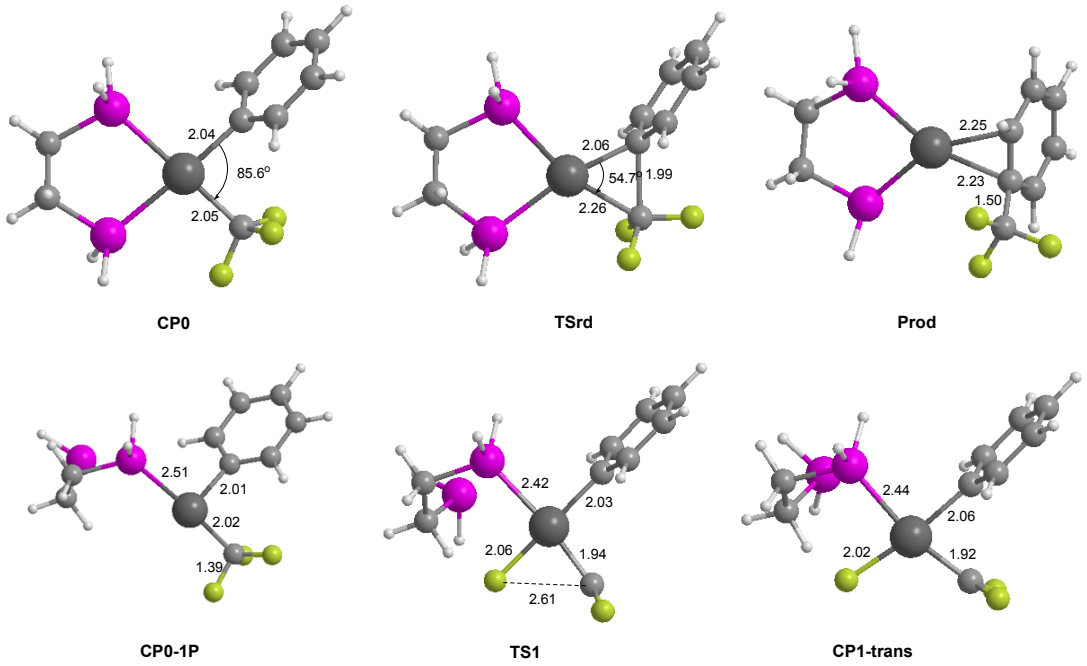


Fig. S3 Optimized intermediates and transition states involved in direct reductive elimination and α-fluoride elimination steps using M06 method.

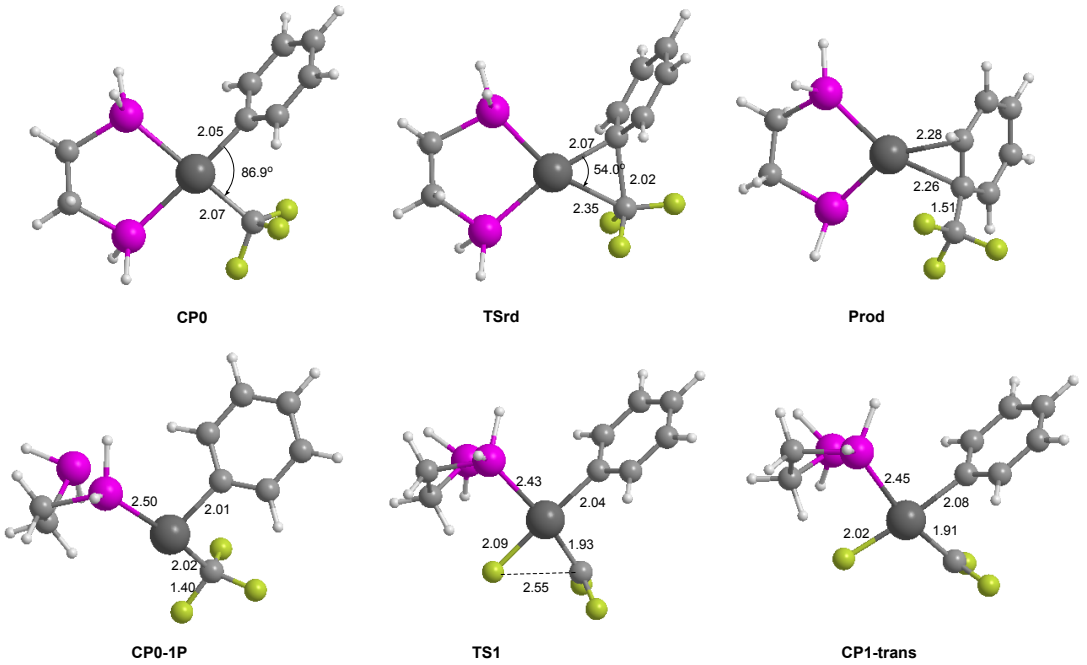


Fig. S4 Optimized intermediates and transition states involved in direct reductive elimination and α-fluoride elimination steps using B97D method.

As can be seen from Figs. S1-S4, for various DFT methods, there are only very minor differences for the key bond lengths and bond angles in the relevant key intermediates and transition states involved in direct reductive elimination mechanism and α-fluoride elimination step.

(b) Density functional effects on predicted energy profiles

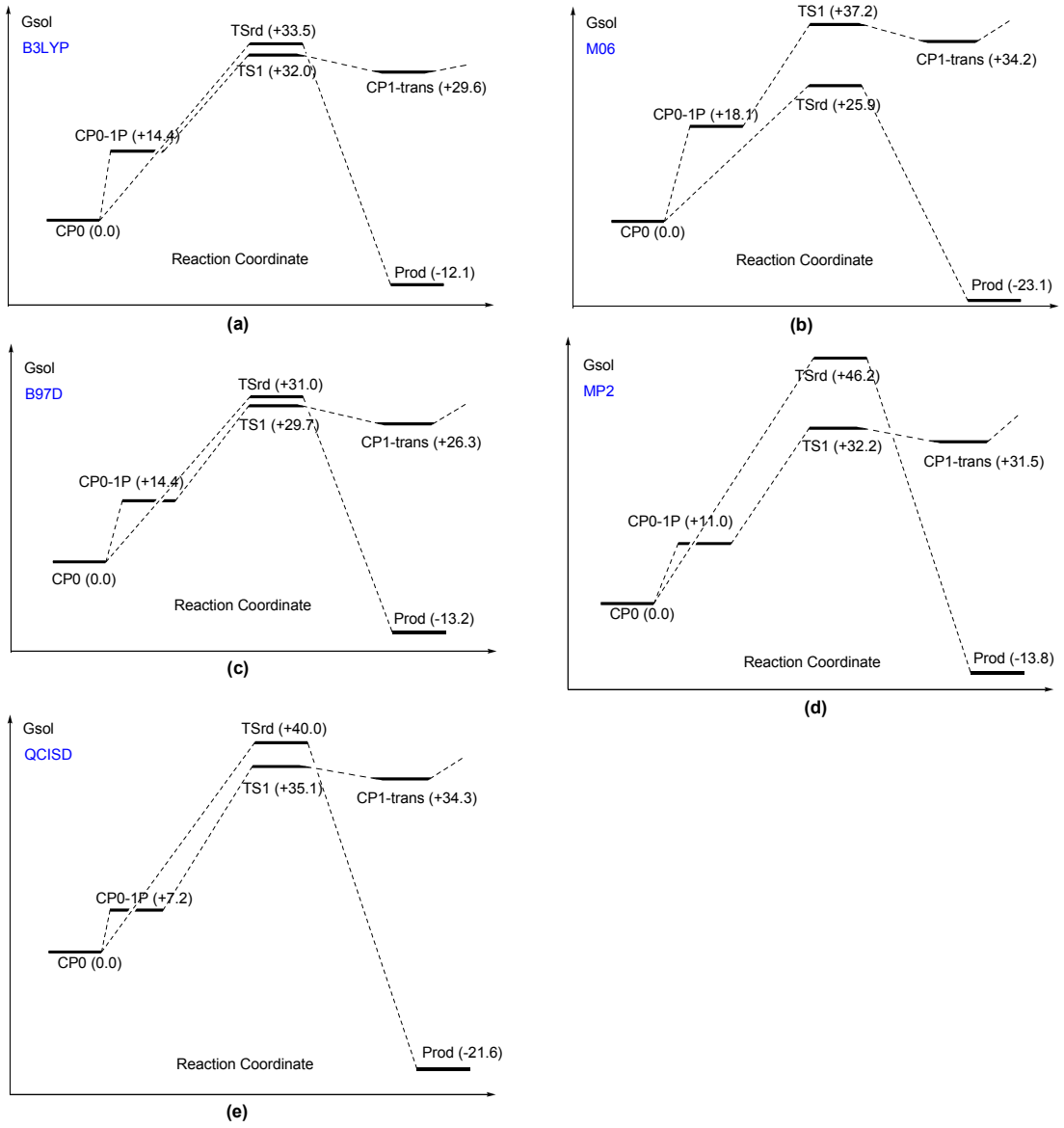


Figure S5. Reaction energy profiles for the key steps of direct reductive elimination

and α-fluoride elimination using different DFT functionals in combination with SMD solvation model on the B3LYP-based optimized geometries. Values in parentheses are relative Gibbs free energies in kcal/mol.

As can be seen, B3LYP, B97D, MP2 and QCISD methods gives similar shape of reaction profiles (especially with regard to the relative energy levels of **TSrd** and **TS1**) although there are some differences about the absolute values. Given the experimental conditions and observations, B97D functional in combination with SMD based on the B3LYP-optimized geometries should be a reasonable method.

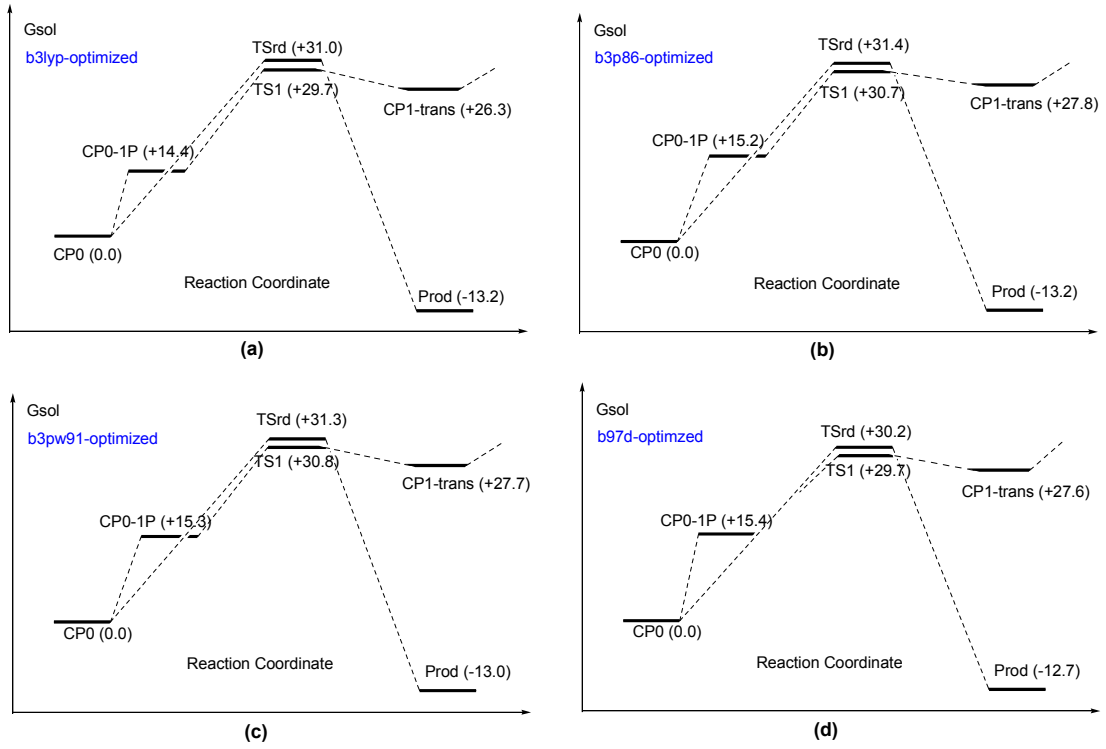


Fig. S6 Reaction energy profiles predicted by B97D/SMD based on optimized structures by different DFT functionals. Values in parentheses are relative Gibbs free energies in kcal/mol.

As can be seen, reaction profiles predicted by B97D/SMD method based on optimized geometries by these different DFT methods are of similar shape and magnitudes of values (especially regarding the relative energy levels of **TSrd** and **TS1**), and therefore essentially lead to the same conclusions.

(c) Solvation model examination

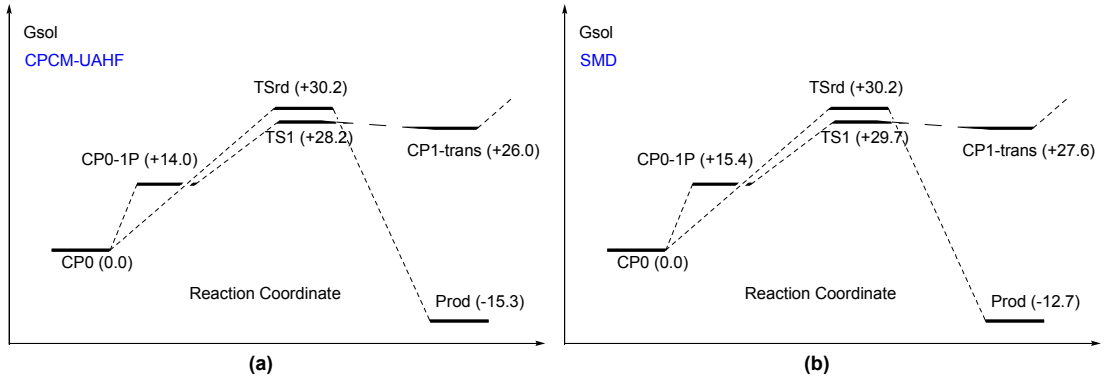
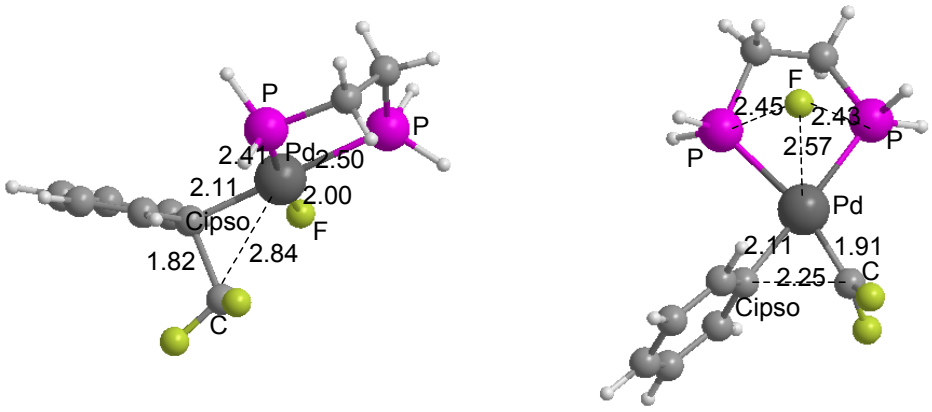


Figure S7. CPCM-UAHF and SMD solvation model effects on reaction profiles predicted by B97D method on B97D-optimized geometries.

As can be seen, there are very minor differences between CPCM-UAHF and SMD models, which essentially lead to the same conclusions.

1.2 Isomeric transition states for carbene insertion with bidentate phosphine ligand



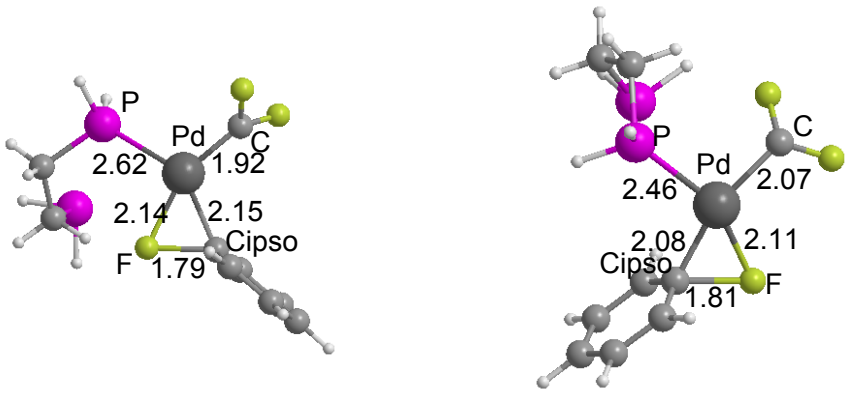
TS2-2P (+57.5) **TS2-2P-iso (+34.0)**

Fig. S8 Isomeric transition states for carbene insertion with bidentate phosphine ligand. Values in parentheses are Gibbs free energies in kcal/mol.

As can be seen, these transition states with bidentate phosphine ligand are much less stable than those reported in the main text which feature mono-phosphine ligation.

1.3 Side pathways with CP1 intermediates from α-Fluoride elimination (B3LYP/CPCM-UAHF results)

(a) Reductive elimination of Ph-F from CP1 intermediates



TSrd-PhF (+64.5) **TSrd-PhF-iso (+72.1)**

Fig. S9 Optimized transition states for Ph-F coupling from **CP1** intermediates. Values in parentheses are Gibbs free energies in kcal/mol.

(b) Reductive elimination of P-F products from CP1 intermediates

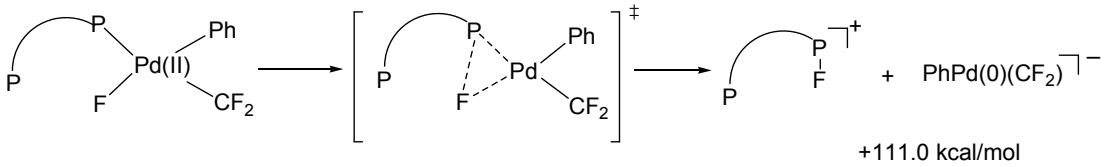


Fig. S10 P-F coupling from **CP1-trans** intermediate.

(c) Self-dimerization of difluorocarbene in CP1 intermediates

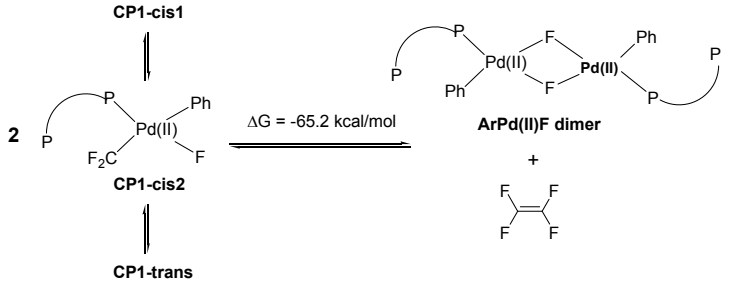


Fig. S11 self-dimerization of difluorocarbene in CP1 intermediates.

(d) Bimolecular disproportionation and transmetalation of CP1 intermediates

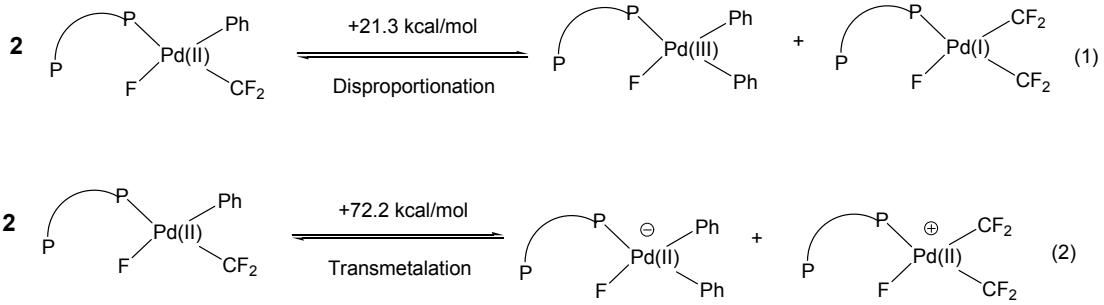


Fig. S12 Bimolecular disproportionation and transmetalation of **CP1** intermediates.

1.4 Side pathways from complex CP0 (B3LYP/CPCM-UAHF results)

(a) Bimolecular disproportionation mechanism

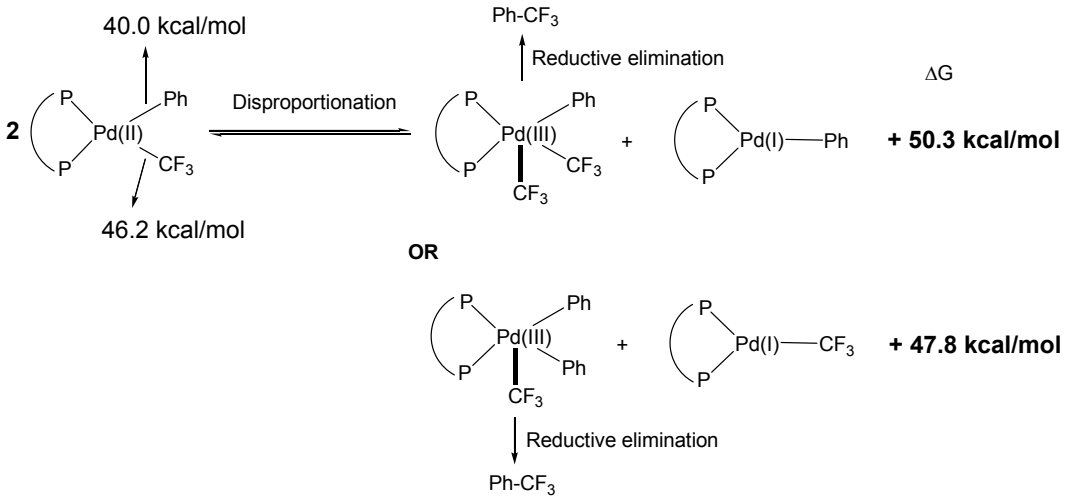


Fig. S13 Bimolecular disproportionation of **CP0**.

(b) Bimolecular transmetalation mechanism

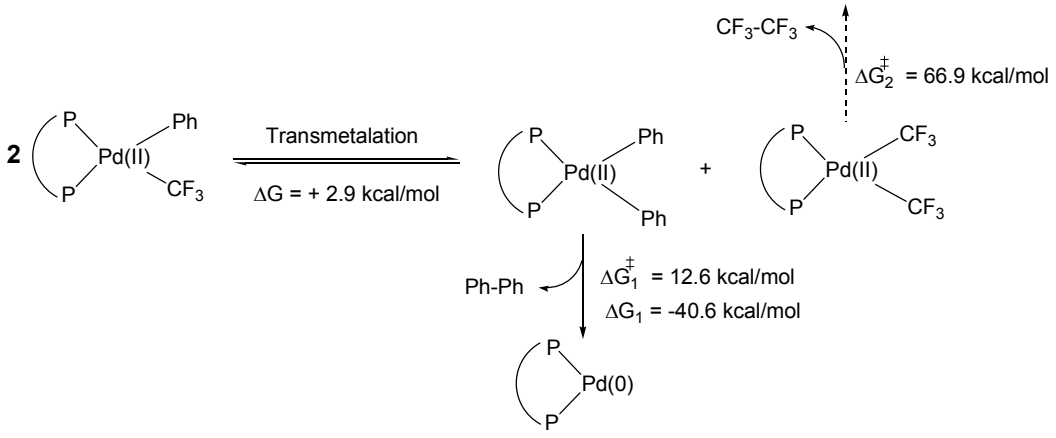


Fig. S14 Bimolecular transmetalation of **CP0**.

1.5 Reductive elimination from Pd(II) complex with Brettphos ligand

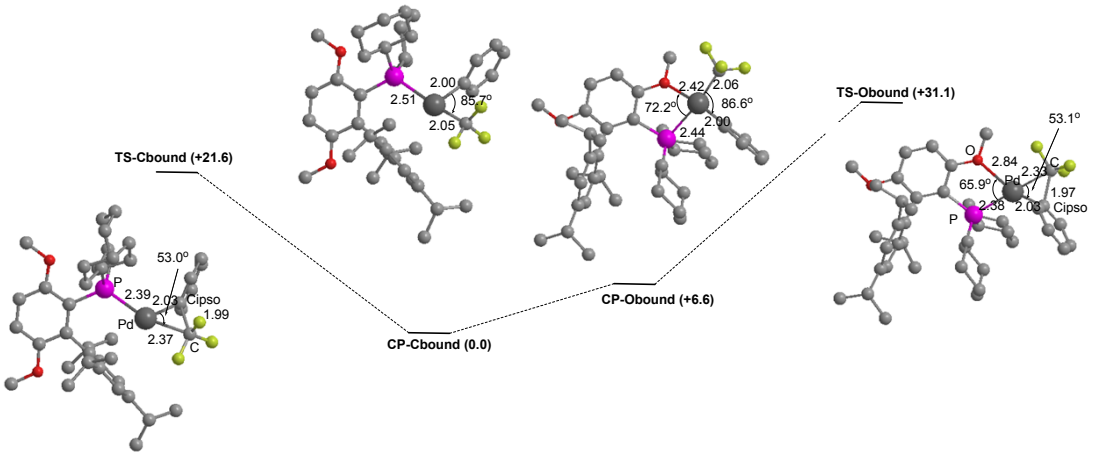


Fig. S15 Optimized structures and relative free energies for intermediates and transition states with Brettphos ligand using B97D functional. Values in parentheses are Gibbs free energies in kcal/mol. Values above the bonds or arrows are bond lengths in Å or angles in degree (°).

As can be seen, when Buchwald's Brettphos is used, C-bound precomplex **CP-Cbound** is more stable than O-bound one by 6.6 kcal/mol. Furthermore, the C-bound transition state **TS-Cbound** for reductive elimination of Ar-CF_3 from C-bound precomplex is much more stable than from O-bound isomer by 9.5 kcal/mol. Therefore, C-bound geometry should be more favorable for reductive elimination to occur for Brettphos ligand.

1.6 Reductive elimination from Pd(II) with P,O and P,N-donating ligands

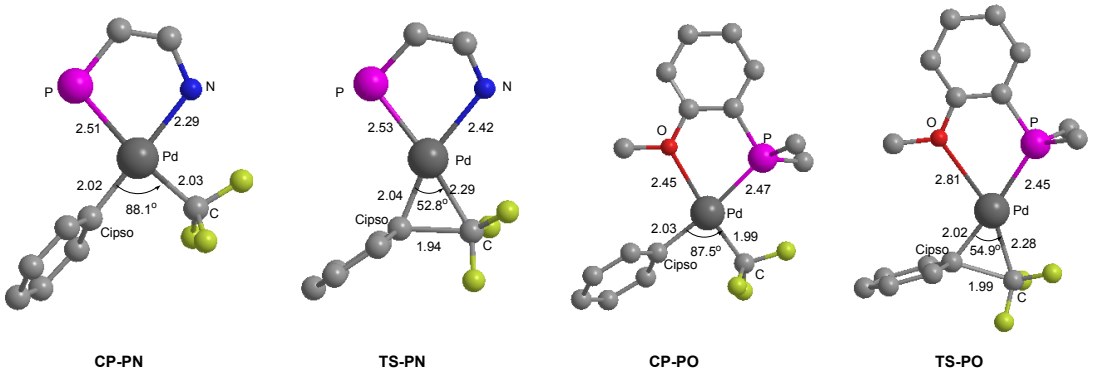
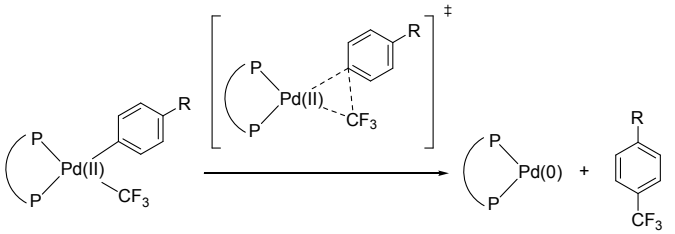


Fig. S16 Optimized pre-complexes and transition states. Hydrogen atoms are omitted for clarity. Values above the bonds or arrows are bond lengths in Å or angles in degree (°).

1.7 Electronic effect of the substituents on the aryl ligand (B3LYP/CPCM-UAHF results)

Table S1 Substituents effect of the aryl ligand for direct reductive elimination of Ar-CF_3



Entry	R =	$\Delta G^{\neq}$ *(kcal/mol)*
1	H	33.5
2	*p*-Me	32.3
3	*p*-OMe	33.7
4	*p*-NMe_2	32.0
5	*p*-Cl	34.6
6	*p*-Ac	33.6
7	*p*-CF_3	34.4
8	*p*-NO_2	33.8
9	*o*-Me	32.9
10	*o*-OMe	34.8

2. Computed Energies for Relevant Stationary Points

Table S2. Single Point Electronic Energies Corrected by Solvation Energies in Benzene predicted by B97D-SMD method, Zero-Point Vibrational Energies, and Thermal Corrections to Enthalpies and Gibbs Free Energies [a]

Complex	SP (a.u.)	ZPE (a.u.)	ΔH (a.u.)	ΔG (a.u.)
CP0	-1461.036232	0.1974	0.21628	0.148859
TSrd	-1460.985269	0.195599	0.214173	0.147323
Prod	-1461.058823	0.198264	0.216844	0.15033
CP0-1P	-1461.007978	0.196436	0.216156	0.143535
CP0-1P'	-1461.006631	0.196765	0.216371	0.145699
TSrd-1P	-1460.973277	0.195787	0.214838	0.144524
CP0-1P-iso	-1461.002974	0.196532	0.216097	0.144721
TS1	-1460.984114	0.195461	0.214802	0.144069
CP1-trans	-1460.987981	0.195564	0.215696	0.142469
TS1-iso	-1460.974196	0.195342	0.214599	0.144993
CP1-cis1	-1460.986774	0.195779	0.215786	0.142534
CP1-cis2	-1460.975998	0.195692	0.215663	0.144193
TS2-1P	-1460.982621	0.195217	0.214495	0.145492
TS2-1P-iso	-1460.984709	0.195066	0.214505	0.143918
CP2	-1461.019593	0.197417	0.216866	0.146903
TS3	-1460.987034	0.196628	0.2153	0.148017
Prod'	-1461.04568	0.198512	0.217603	0.147626
TS2-2P	-1460.941463	0.193761	0.212847	0.145759
TS2-2P-iso	-1460.98331	0.196787	0.215164	0.150034
Ligands effect				
PH_3-CP	-1040.452531	0.129864	0.144932	0.085982
PH_3-TS	-1040.420293	0.128962	0.143492	0.084919
PP-CP	-1459.79851	0.173458	0.191925	0.12533
PP-TS	-1459.737894	0.171814	0.190393	0.121543
PN-CP	-1173.181661	0.183791	0.201524	0.136345
PN-TS	-1173.124514	0.181564	0.199195	0.134549
PO-CP	-1232.316649	0.199021	0.218434	0.149342
PO-TS	-1232.271685	0.197547	0.216796	0.146323
$TS_{a\text{-}F}$-PO	-1232.282103	0.197274	0.216702	0.146004
PObenzene-CP	-1464.509102	0.305988	0.331164	0.248742
PObenzene-TS	-1464.460517	0.304426	0.329374	0.24422
$TS_{a\text{-}F}$-PObenzene	-1464.477241	0.304568	0.329594	0.248455

Xantphos-CP(B97D-opt)[b]	-2288.43045	0.68472	0.733975	0.601051
Xantphos-TS(B97D-opt)[b]	-2288.3828	0.681332	0.731179	0.592033
Xantphos-CP	-2959.959354	0.701943	0.750887	0.615175
Xantphos-TS	-2959.921941	0.700641	0.749177	0.614299
$TS_{a\text{-}F}$-Xantphos	-2959.916656	0.700126	0.749276	0.611935
OO-CP	-927.4980473	0.191891	0.209225	0.145393
OO-TS	-927.4438172	0.190429	0.207461	0.144364
NN-CP	-887.8048673	0.219572	0.236511	0.174221
NN-TS	-887.7358223	0.216929	0.23395	0.171104
ON-CP	-907.6507735	0.205675	0.222888	0.15778
ON-TS	-907.5926762	0.203649	0.220845	0.156796
CP-Obound(B97D-opt)[b]	-2217.50616	0.901296	0.955507	0.813123
TS-Obound(B97D-opt)[b]	-2217.46491	0.898998	0.953062	0.810956
CP-Cbound(B97D-opt)[b]	-2217.51828	0.900926	0.955184	0.81474
TS-Cbound(B97D-opt)[b]	-2217.48192	0.898993	0.952853	0.812767
CP-Obound	-2554.170452	0.922827	0.97693	0.833287
TS-Obound	-2554.118933	0.921103	0.974938	0.830955
CP-Cbound	-2554.176686	0.922461	0.976746	0.833671
TS-Cbound	-2554.133365	0.921256	0.974987	0.832201
$TS_{a\text{-}F}$-Brettphos	-2554.131182	0.921793	0.975594	0.834533
$PMe_2CH_2CH_2PMe_2$-CP	-1618.27569	0.315981	0.341533	0.260412
$PMe_2CH_2CH_2PMe_2$-TS	-1618.21349	0.313664	0.339234	0.25593
$P(CF_3)_2CH_2CH_2P(CF_3)_2$-CP	-2808.91123	0.222657	0.257059	0.149186
$P(CF_3)_2CH_2CH_2P(CF_3)_2$-TS	-2808.87232	0.221661	0.255487	0.148956
$TS_{a\text{-}F}$-$P(CF_3)_2CH_2CH_2P(CF_3)_2$	-2808.86297	0.221083	0.255698	0.146769

Note: a. SP: Single point electronic energy corrected by solvation energy in benzene predicted by B97D-SMD method;

ZPE: Zero-point vibrational energy;

ΔH: Thermal correction to enthalpy at 298.15 K;

ΔG: Thermal correction to Gibbs free energy at 298.15 K.

b. The geometries and energies are obtained by using B97D funcational for geometry optimization.

3. Cartesian Coordinates of Relevant Stationary Points

Direct reductive elimination mechanism:

CP0
SCF Done: E(RB+HF-LYP) = -790.001210656 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.199729	-1.088280	-1.090319
2	6	0	-1.642357	-0.416362	0.007857
3	6	0	-2.442353	-0.207112	1.139372
4	6	0	-3.758458	-0.680669	1.181436
5	6	0	-4.301603	-1.355022	0.086592
6	6	0	-3.518784	-1.553323	-1.052194
7	46	0	0.315768	0.142793	-0.021044
8	15	0	2.788532	0.679628	0.002612
9	6	0	3.742951	-0.924530	0.433416
10	6	0	3.096809	-2.149934	-0.224255
11	15	0	1.211429	-2.210104	0.121939
12	6	0	-0.352143	2.066598	-0.130361
13	9	0	-0.963354	2.499672	1.008387
14	9	0	0.709095	2.935461	-0.313996
15	9	0	-1.204056	2.339959	-1.149116
16	1	0	-2.050072	0.343762	1.989046
17	1	0	-4.362742	-0.510058	2.070073
18	1	0	-5.326647	-1.716274	0.117436
19	1	0	-3.933616	-2.068089	-1.916559
20	1	0	-1.610833	-1.251019	-1.990576
21	1	0	4.792623	-0.840035	0.136730
22	1	0	3.715330	-1.015106	1.524941
23	1	0	3.578333	-3.070532	0.118500
24	1	0	3.205342	-2.104723	-1.313545
25	1	0	1.182442	-2.904186	1.377880
26	1	0	0.810093	-3.298303	-0.720090
27	1	0	3.449577	1.083787	-1.205479
28	1	0	3.404266	1.615391	0.894650

TSrd
SCF Done: E(RB+HF-LYP) = -789.958720680 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.236313	1.749831	-0.024530
2	6	0	1.621994	-0.195094	-0.028271
3	9	0	1.051641	2.222304	1.238877
4	9	0	2.522636	2.061997	-0.337200
5	9	0	0.517233	2.554971	-0.877697
6	6	0	2.190348	-0.684632	-1.218949
7	6	0	3.226887	-1.615486	-1.166991
8	6	0	3.738618	-2.039084	0.064506
9	6	0	3.212729	-1.513918	1.246725
10	6	0	2.173069	-0.581894	1.204896
11	1	0	1.815207	-0.343181	-2.179864
12	1	0	3.643660	-2.006670	-2.092306
13	1	0	4.555278	-2.755207	0.099449
14	1	0	3.618938	-1.821359	2.207623
15	1	0	1.789003	-0.152271	2.125425
16	46	0	-0.412630	0.153405	-0.032631
17	15	0	-1.675369	-2.047358	-0.104461
18	15	0	-2.743391	1.124605	0.095179
19	6	0	-3.957549	-0.319273	-0.274218
20	1	0	-4.964647	-0.062127	0.067219
21	1	0	-3.993139	-0.419050	-1.364931
22	6	0	-3.491589	-1.628043	0.370568
23	1	0	-4.155285	-2.450290	0.087071
24	1	0	-3.511712	-1.547108	1.463200
25	1	0	-1.921348	-2.736046	-1.348430
26	1	0	-1.506016	-3.229691	0.703036
27	1	0	-3.294872	1.579969	1.345865
28	1	0	-3.341220	2.139808	-0.731327

Prod
SCF Done: E(RB+HF-LYP) = -790.037431038 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.164853	-1.363861	-0.468419
2	6	0	-1.821374	0.009027	0.042873
3	9	0	-1.830929	-2.338438	0.412234
4	9	0	-3.500611	-1.494429	-0.683466

5	9	0	-1.561177	-1.653672	-1.645715
6	6	0	-1.540043	1.069361	-0.879058
7	6	0	-1.713189	2.417541	-0.453772
8	6	0	-2.126326	2.709774	0.829397
9	6	0	-2.397709	1.661888	1.744713
10	6	0	-2.264951	0.345728	1.361708
11	1	0	-1.462192	0.853173	-1.940721
12	1	0	-1.533363	3.215714	-1.169505
13	1	0	-2.260495	3.743059	1.137845
14	1	0	-2.731732	1.898802	2.751365
15	1	0	-2.508861	-0.458758	2.049367
16	46	0	0.410912	0.211042	-0.142585
17	15	0	2.559104	1.193194	-0.915463
18	15	0	1.827832	-1.420622	1.078347
19	6	0	3.611874	-1.130355	0.414286
20	1	0	4.344092	-1.557447	1.106205
21	1	0	3.682391	-1.686693	-0.527273
22	6	0	3.902598	0.354395	0.182475
23	1	0	4.889192	0.482904	-0.272946
24	1	0	3.901511	0.899705	1.133048
25	1	0	3.104561	0.871428	-2.213305
26	1	0	3.071899	2.542473	-0.863093
27	1	0	2.093620	-1.301069	2.492554
28	1	0	1.821658	-2.861934	1.039413

monoP-ligation pathway of 1,2-bisphosphine ligand:

CP0-1P

SCF Done: E(RB+HF-LYP) = -789.982177196 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.334753	-2.807572	1.124793
2	6	0	1.398219	-1.775183	0.996896
3	6	0	1.586798	-0.779237	0.030985
4	6	0	2.722199	-0.802834	-0.784723
5	6	0	3.647027	-1.845566	-0.656616
6	6	0	3.456826	-2.848404	0.295576
7	46	0	0.146008	0.593700	-0.223413
8	6	0	1.431041	2.034656	0.313123
9	9	0	2.467775	2.287702	-0.525415
10	15	0	-1.643549	-1.019575	-1.008150
11	6	0	-3.424258	-0.456756	-1.419740
12	6	0	-4.092388	0.343148	-0.298313
13	15	0	-4.406229	-0.703852	1.292562
14	9	0	0.606055	3.148886	0.239894
15	9	0	1.939623	2.027097	1.563653
16	1	0	2.899110	-0.012011	-1.505506
17	1	0	4.524046	-1.862953	-1.299547
18	1	0	4.182014	-3.651673	0.396481
19	1	0	2.183417	-3.576396	1.879106
20	1	0	0.533493	-1.754894	1.654603
21	1	0	-5.034655	0.761858	-0.664723
22	1	0	-3.455517	1.182262	0.002585
23	1	0	-3.332193	0.171994	-2.312336
24	1	0	-4.019746	-1.332122	-1.699526
25	1	0	-1.325973	-1.716572	-2.219485
26	1	0	-1.877131	-2.159747	-0.175673
27	1	0	-5.602205	-1.372909	0.820789
28	1	0	-5.126746	0.317668	2.018982

CP0-1P'

SCF Done: E(RB+HF-LYP) = -789.984651344 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.854419	1.645102	-1.163706
2	6	0	4.892399	0.714414	-1.071137
3	6	0	4.634709	-0.561752	-0.568532
4	6	0	3.340927	-0.907193	-0.161047
5	6	0	2.288898	0.015480	-0.278181
6	6	0	2.560671	1.303502	-0.759906
7	46	0	0.459041	-0.747301	0.000441
8	6	0	0.075415	0.701953	1.331071
9	9	0	1.003197	0.927694	2.277504
10	15	0	-1.816012	-1.914995	-0.016101
11	6	0	-3.266161	-0.957020	-0.813536
12	6	0	-3.472721	0.415664	-0.176417
13	15	0	-4.967314	1.320054	-0.998230
14	9	0	-0.179706	1.897481	0.728876
15	9	0	-1.076345	0.379536	2.004747
16	1	0	-3.722635	0.315278	0.884529
17	1	0	1.766901	2.041307	-0.820576

18	1	0	4.052342	2.643327	-1.547724
19	1	0	5.898699	0.986093	-1.379708
20	1	0	5.440044	-1.287243	-0.478466
21	1	0	3.164662	-1.900431	0.248776
22	1	0	-2.567538	1.023052	-0.242127
23	1	0	-3.006542	-0.862087	-1.873641
24	1	0	-4.170874	-1.568449	-0.744253
25	1	0	-1.969537	-3.186785	-0.666720
26	1	0	-2.386697	-2.271988	1.249294
27	1	0	-4.758698	2.598019	-0.350206
28	1	0	-4.281791	1.706547	-2.216273

TSrd-1P

SCF Done: E(RB+HF-LYP) = -789.954729179 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.022481	2.253941	-0.329740
2	6	0	4.055517	1.044052	-1.026109
3	6	0	3.055759	0.087906	-0.824529
4	6	0	1.999421	0.367984	0.054073
5	6	0	1.990457	1.562984	0.793122
6	6	0	2.991200	2.511488	0.579367
7	46	0	0.182728	-0.257465	-0.557079
8	15	0	-2.001426	-0.888990	-1.457617
9	6	0	-3.539624	0.156636	-1.013791
10	6	0	-3.713864	0.280203	0.497999
11	1	0	-3.857523	-0.706518	0.951739
12	6	0	1.384042	-1.295189	1.060682
13	9	0	2.127494	-0.967005	2.146231
14	9	0	0.247975	-1.830709	1.619821
15	9	0	2.019034	-2.317579	0.441066
16	1	0	1.211043	1.745570	1.526844
17	1	0	2.974205	3.446652	1.133431
18	1	0	4.808475	2.989053	-0.480684
19	1	0	4.865840	0.836333	-1.720356
20	1	0	3.095871	-0.865834	-1.340394
21	15	0	-5.295577	1.300874	0.925946
22	1	0	-2.826408	0.728297	0.954187
23	1	0	-3.377368	1.139113	-1.470225
24	1	0	-4.421954	-0.290327	-1.481928
25	1	0	-2.171340	-0.976076	-2.882880
26	1	0	-2.497740	-2.199006	-1.137986
27	1	0	-5.027618	1.432710	2.343536
28	1	0	-4.748811	2.602781	0.594916

Prod'

SCF Done: E(RB+HF-LYP) = -790.032608075 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.168925	-0.065345	-1.022015
2	6	0	-1.773677	0.701705	0.110318
3	6	0	-2.325445	0.408273	1.381926
4	6	0	-3.232909	-0.630578	1.528743
5	6	0	-3.599298	-1.416104	0.422001
6	6	0	-3.069847	-1.143927	-0.834688
7	6	0	-1.069366	2.020487	-0.067436
8	46	0	-0.240625	-0.971979	-0.429514
9	15	0	1.926395	-1.876767	0.021057
10	6	0	3.002734	-0.954624	1.308227
11	6	0	3.080586	0.553916	1.067892
12	15	0	4.053170	1.010203	-0.534743
13	9	0	-0.413205	2.114181	-1.242128
14	9	0	-1.948558	3.052794	-0.027610
15	9	0	-0.171362	2.252975	0.924314
16	1	0	-2.043409	1.020030	2.233311
17	1	0	-3.656827	-0.840134	2.506690
18	1	0	-4.304962	-2.232611	0.546536
19	1	0	-3.377939	-1.726845	-1.697770
20	1	0	-1.927921	0.275776	-2.025157
21	1	0	3.544606	1.037506	1.933349
22	1	0	2.074050	0.967844	0.952579
23	1	0	2.518449	-1.143849	2.272522
24	1	0	3.996713	-1.413888	1.342829
25	1	0	2.078152	-3.212640	0.536049
26	1	0	2.855525	-2.001290	-1.066565
27	1	0	5.382234	0.911848	0.038947
28	1	0	3.971637	2.445403	-0.371350

α-fluoride elimination mechanism:

CP0-1P-iso
SCF Done: E(RB+HF-LYP) = -789.962495275 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.848698	-1.102977	-0.222933
2	6	0	-3.899099	-1.523724	-1.157132
3	6	0	-2.570890	-1.098761	-1.045640
4	6	0	-2.176967	-0.224755	-0.018298
5	6	0	-3.137872	0.163211	0.931186
6	6	0	-4.467191	-0.259367	0.823027
7	46	0	-0.367141	0.764846	-0.094658
8	15	0	0.551608	-0.988603	1.107081
9	6	0	2.421724	-0.992591	1.439371
10	6	0	3.284610	-1.112537	0.180988
11	15	0	3.083216	-2.800870	-0.728669
12	1	0	-2.857479	0.813156	1.759819
13	1	0	-5.201783	0.064491	1.557105
14	1	0	-5.879312	-1.439499	-0.303580
15	1	0	-4.190962	-2.186173	-1.969112
16	1	0	-1.843170	-1.445431	-1.778468
17	1	0	4.331046	-0.960670	0.461784
18	1	0	3.021130	-0.325057	-0.529541
19	1	0	2.620285	-0.031947	1.922336
20	1	0	2.628098	-1.793941	2.158173
21	1	0	0.007364	-1.103806	2.421782
22	1	0	0.277041	-2.287813	0.592560
23	1	0	3.979081	-3.567384	0.113495
24	1	0	4.069363	-2.553542	-1.754942
25	6	0	1.307410	1.974299	-0.279687
26	9	0	0.810634	3.233924	-0.546007
27	9	0	2.155077	2.138301	0.791053
28	9	0	2.137320	1.687773	-1.342672

TS1
SCF Done: E(RB+HF-LYP) = -789.944571388 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.093034	-1.106363	1.294976
2	6	0	1.816634	-0.506704	0.058809
3	6	0	2.714803	-0.693654	-1.000584
4	6	0	3.865304	-1.471456	-0.828156
5	6	0	4.132172	-2.069908	0.404702
6	6	0	3.243796	-1.884289	1.465590
7	46	0	0.121477	0.593244	-0.195001
8	15	0	-1.035431	-1.473427	-0.815403
9	6	0	-2.849542	-1.276393	-1.356126
10	6	0	-3.651097	-0.381023	-0.406500
11	15	0	-3.852323	-1.140255	1.349421
12	9	0	-1.549937	1.774390	-0.423278
13	1	0	2.525370	-0.234536	-1.968418
14	1	0	4.552209	-1.607092	-1.660648
15	1	0	5.025732	-2.674221	0.538111
16	1	0	3.443098	-2.344102	2.431024
17	1	0	1.413813	-0.972716	2.133933
18	1	0	-4.633222	-0.181194	-0.846296
19	1	0	-3.109642	0.565831	-0.290668
20	1	0	-2.801254	-0.801399	-2.342015
21	1	0	-3.290263	-2.271117	-1.486030
22	1	0	-0.477002	-2.220254	-1.900044
23	1	0	-1.072211	-2.499611	0.175686
24	1	0	-5.012732	-1.966431	1.078020
25	1	0	-4.613768	-0.053375	1.920307
26	6	0	0.818134	2.338990	0.268229
27	9	0	0.693687	2.910431	1.425807
28	9	0	1.153896	3.257514	-0.583511

TS1-iso
SCF Done: E(RB+HF-LYP) = -789.926070583 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.983006	-2.542199	-0.647516
2	6	0	-1.830380	-1.753475	-0.546113
3	6	0	-1.902510	-0.451448	-0.032522
4	6	0	-3.150163	0.059968	0.352416
5	6	0	-4.295026	-0.736547	0.270801
6	6	0	-4.214687	-2.039755	-0.227609
7	46	0	-0.332972	0.839354	0.082147
8	6	0	1.035105	2.319425	-0.198363

9	9	0	0.764955	3.582346	-0.143644
10	15	0	0.914885	-0.843264	1.254807
11	6	0	2.815807	-0.788278	1.351303
12	6	0	3.513879	-0.873569	-0.008719
13	15	0	3.259157	-2.574166	-0.885210
14	9	0	-1.544834	2.199270	-0.679053
15	9	0	2.183948	2.215859	-0.833938
16	1	0	-3.226473	1.091028	0.681037
17	1	0	-5.255651	-0.331240	0.580986
18	1	0	-5.108629	-2.654576	-0.298363
19	1	0	-2.913065	-3.547920	-1.056182
20	1	0	-0.885899	-2.165460	-0.894203
21	1	0	4.581919	-0.676191	0.124417
22	1	0	3.119171	-0.107577	-0.681940
23	1	0	3.057100	0.167228	1.830320
24	1	0	3.148480	-1.584198	2.026606
25	1	0	0.585161	-0.881077	2.646485
26	1	0	0.645388	-2.201054	0.911825
27	1	0	4.274154	-3.299053	-0.147619
28	1	0	4.113688	-2.300747	-2.018438

CP1-trans

SCF Done: E(RB+HF-LYP) = -789.946722306 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.813045	-2.301785	1.262263
2	6	0	1.806834	-1.334710	1.165712
3	6	0	1.670016	-0.566206	0.001762
4	6	0	2.575516	-0.759478	-1.050155
5	6	0	3.580882	-1.727525	-0.952518
6	6	0	3.700916	-2.501695	0.203125
7	46	0	0.098350	0.760073	-0.201256
8	6	0	1.430128	1.960086	0.483877
9	9	0	2.351436	2.564079	-0.211306
10	15	0	-1.330972	-1.051932	-1.061503
11	6	0	-3.144340	-0.557697	-1.344527
12	6	0	-3.808649	0.050639	-0.107429
13	15	0	-3.944185	-1.165709	1.376214
14	9	0	-1.529469	1.904588	-0.487211
15	9	0	1.679196	2.196661	1.739874
16	1	0	2.499881	-0.160845	-1.954992
17	1	0	4.271854	-1.871303	-1.780013
18	1	0	4.484366	-3.251057	0.280326
19	1	0	2.902315	-2.896393	2.168451
20	1	0	1.124971	-1.191736	2.000671
21	1	0	-4.802562	0.416157	-0.384214
22	1	0	-3.195161	0.903146	0.198777
23	1	0	-3.096105	0.209438	-2.123177
24	1	0	-3.687190	-1.422535	-1.741018
25	1	0	-0.967227	-1.570036	-2.345864
26	1	0	-1.398606	-2.280872	-0.336850
27	1	0	-5.137262	-1.868379	0.945676
28	1	0	-4.652565	-0.272061	2.264461

CP1-cis2

SCF Done: E(RB+HF-LYP) = -789.926538754 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.228990	1.800986	-0.093718
2	6	0	2.998881	2.423706	-0.306079
3	6	0	1.814032	1.680508	-0.245014
4	6	0	1.848274	0.302762	0.015096
5	6	0	3.092706	-0.322417	0.187389
6	6	0	4.271811	0.426101	0.152005
7	46	0	0.225510	-0.931466	0.075866
8	6	0	-1.275190	-2.285928	-0.167959
9	9	0	1.326368	-2.250414	-0.882048
10	15	0	-0.992208	0.662272	1.398729
11	6	0	-2.842334	0.945150	1.041001
12	6	0	-3.133476	1.338001	-0.409599
13	15	0	-2.423472	3.068878	-0.881081
14	1	0	3.133939	-1.398662	0.315058
15	1	0	5.228383	-0.070522	0.299628
16	1	0	5.148806	2.379723	-0.130106
17	1	0	2.954819	3.489452	-0.519863
18	1	0	0.873230	2.194848	-0.427475
19	1	0	-4.214300	1.314843	-0.578592
20	1	0	-2.677402	0.613603	-1.091693
21	1	0	-3.331964	-0.007483	1.267057
22	1	0	-3.223467	1.688789	1.749110
23	1	0	-1.038975	0.344430	2.793988

24	1	0	-0.457390	1.981740	1.470243
25	1	0	-3.509878	3.855704	-0.333727
26	1	0	-2.933413	3.091551	-2.232942
27	9	0	-2.575844	-2.068102	-0.231568
28	9	0	-1.096390	-3.509380	-0.539047

CP1-cis1
SCF Done: E(RB+HF-LYP) = -789.947579084 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.403266	-0.888901	-1.233732
2	6	0	-1.853934	-0.223051	-0.133321
3	6	0	-2.585509	-0.119409	1.053642
4	6	0	-3.869503	-0.671052	1.134270
5	6	0	-4.430105	-1.312516	0.029654
6	6	0	-3.694025	-1.419922	-1.152269
7	46	0	0.058649	0.416744	-0.342356
8	15	0	2.575631	0.753466	-0.893904
9	6	0	3.742747	-0.613610	-0.228888
10	6	0	2.989765	-1.901481	0.119608
11	15	0	2.020666	-1.732802	1.775214
12	6	0	-0.334779	2.095102	0.465473
13	9	0	0.568456	3.024879	0.676837
14	9	0	-1.471556	2.599758	0.849189
15	9	0	0.437148	-1.253168	-1.325948
16	1	0	-2.168796	0.374159	1.925870
17	1	0	-4.427755	-0.594234	2.064508
18	1	0	-5.431081	-1.732004	0.090737
19	1	0	-4.117621	-1.929676	-2.014650
20	1	0	-1.815806	-1.021778	-2.135245
21	1	0	4.499938	-0.803044	-0.996083
22	1	0	4.259373	-0.192785	0.640631
23	1	0	3.691630	-2.738564	0.175281
24	1	0	2.227232	-2.112586	-0.634039
25	1	0	3.043932	-2.286412	2.643877
26	1	0	1.274949	-2.964869	1.667161
27	1	0	2.743157	0.592501	-2.306338
28	1	0	3.403775	1.914910	-0.720302

TS2-1P
SCF Done: E(RB+HF-LYP) = -789.944374816 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.530572	-1.680047	0.552353
2	6	0	-1.803030	0.390632	0.029698
3	9	0	-1.814336	-1.793967	1.829021
4	9	0	-2.437515	-2.361969	-0.108717
5	9	0	1.564057	-1.931872	-0.372712
6	6	0	-2.670287	0.556810	-1.060604
7	6	0	-3.622977	1.577836	-1.053473
8	6	0	-3.733861	2.423068	0.053914
9	6	0	-2.896932	2.240833	1.158166
10	6	0	-1.943917	1.220130	1.152399
11	1	0	-2.599376	-0.107460	-1.917812
12	1	0	-4.282421	1.708596	-1.907709
13	1	0	-4.480266	3.212975	0.062088
14	1	0	-2.989678	2.889045	2.025795
15	1	0	-1.304757	1.076037	2.019280
16	46	0	-0.042784	-0.754491	-0.198551
17	15	0	1.473533	0.948970	-1.206981
18	15	0	3.893910	1.268202	1.390613
19	6	0	3.853389	-0.092096	0.032117
20	1	0	4.860094	-0.490432	-0.129315
21	1	0	3.206797	-0.904166	0.377003
22	6	0	3.290287	0.389080	-1.306387
23	1	0	3.271065	-0.460002	-1.995791
24	1	0	3.884175	1.191548	-1.756655
25	1	0	1.222569	1.288115	-2.577882
26	1	0	1.549828	2.276256	-0.677886
27	1	0	5.114920	1.928697	0.970586
28	1	0	4.541013	0.472577	2.409720

TS2-1P-iso
SCF Done: E(RB+HF-LYP) = -789.939588475 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.627595	0.536432	1.364751
2	6	0	2.197360	0.041166	0.128420

3	6	0	3.137502	-0.366351	-0.824706
4	6	0	4.500796	-0.327201	-0.521292
5	6	0	4.928193	0.140592	0.723645
6	6	0	3.991486	0.573909	1.665099
7	46	0	0.182190	-0.460196	-0.124554
8	15	0	-2.099107	-1.355937	-0.264461
9	6	0	-3.645983	-0.549407	-1.023694
10	6	0	-3.940503	0.854228	-0.486606
11	15	0	-4.495827	0.851281	1.362405
12	6	0	0.536007	1.282192	-0.781934
13	9	0	0.918866	1.597721	-1.998381
14	9	0	0.474929	2.405628	-0.103066
15	1	0	2.811682	-0.728725	-1.795668
16	1	0	5.227801	-0.659691	-1.258138
17	1	0	5.989259	0.174837	0.956683
18	1	0	4.321272	0.943376	2.632946
19	1	0	1.904115	0.876239	2.100434
20	1	0	-4.706833	1.329207	-1.106628
21	1	0	-3.039982	1.475668	-0.540436
22	1	0	-3.448078	-0.491503	-2.100184
23	1	0	-4.504512	-1.217300	-0.890075
24	1	0	-5.864928	0.439593	1.121841
25	1	0	-4.816368	2.260394	1.435571
26	9	0	0.306629	-2.269013	0.673864
27	1	0	-2.086746	-2.615529	-0.934692
28	1	0	-2.541930	-1.770099	1.024825

CP2

SCF Done: E(RB+HF-LYP) = -789.990378476 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.014172	-0.662707	1.328430
2	6	0	2.381211	0.272781	0.328855
3	6	0	3.276729	-0.115140	-0.697775
4	6	0	3.827634	-1.384858	-0.685452
5	6	0	3.470934	-2.309079	0.314960
6	6	0	2.568513	-1.954611	1.308403
7	6	0	1.605973	1.529593	0.259704
8	46	0	0.129349	0.292604	-0.230141
9	15	0	-1.596573	-1.527766	-0.733223
10	6	0	-3.279353	-0.818745	-1.294798
11	6	0	-3.785158	0.308859	-0.392475
12	15	0	-4.153042	-0.260766	1.407470
13	9	0	1.398272	2.169287	1.434316
14	9	0	2.022052	2.426580	-0.652266
15	9	0	-1.157760	1.682389	-0.853877
16	1	0	3.530765	0.601515	-1.471487
17	1	0	4.537622	-1.671680	-1.455956
18	1	0	3.908118	-3.303584	0.308592
19	1	0	2.299445	-2.663081	2.086269
20	1	0	1.394604	-0.342178	2.160473
21	1	0	-4.684600	0.746650	-0.837197
22	1	0	-3.003566	1.075393	-0.346313
23	1	0	-3.090554	-0.411476	-2.293538
24	1	0	-3.996313	-1.640642	-1.394787
25	1	0	-1.355141	-2.462442	-1.798152
26	1	0	-1.985539	-2.481469	0.264516
27	1	0	-5.482916	-0.794007	1.179719
28	1	0	-4.624777	1.014355	1.897998

TS3

SCF Done: E(RB+HF-LYP) = -789.955157464 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.250636	1.700041	0.089921
2	6	0	2.132121	0.556980	0.207835
3	9	0	0.741828	2.221393	1.193170
4	9	0	1.635319	2.633534	-0.757351
5	9	0	-0.501079	1.734094	-0.887309
6	6	0	3.097351	0.275853	-0.808002
7	6	0	3.903058	-0.837346	-0.701166
8	6	0	3.762767	-1.734185	0.382590
9	6	0	2.804551	-1.506745	1.353259
10	6	0	1.954994	-0.379285	1.281757
11	1	0	3.203940	0.964967	-1.638176
12	1	0	4.659449	-1.023565	-1.458397
13	1	0	4.412056	-2.602263	0.450444
14	1	0	2.696667	-2.188400	2.192118
15	1	0	1.355085	-0.103503	2.143742
16	46	0	0.106014	-0.277693	-0.169009
17	15	0	-1.690989	-1.902484	-0.237198

18	15	0	-3.942173	0.529236	1.132572
19	6	0	-3.437872	0.327357	-0.715750
20	1	0	-4.208736	0.760183	-1.361466
21	1	0	-2.515760	0.907377	-0.846770
22	6	0	-3.213954	-1.136344	-1.109152
23	1	0	-2.987488	-1.191925	-2.179889
24	1	0	-4.096897	-1.758417	-0.926205
25	1	0	-1.615354	-3.161587	-0.927051
26	1	0	-2.258521	-2.389531	0.985795
27	1	0	-5.363840	0.291170	0.966652
28	1	0	-4.066330	1.968922	1.118648

TS2-2P (outer attack of carbene to phenyl)
SCF Done: E(RB+HF-LYP) = -789.878455351 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.687572	-0.601862	1.668066
2	6	0	-1.542608	-0.034154	-0.053948
3	9	0	-1.085240	0.326698	2.461830
4	9	0	-2.985308	-0.553597	2.022243
5	9	0	0.018546	-2.393356	-0.254909
6	6	0	-2.213106	-0.917040	-0.957960
7	6	0	-3.273875	-0.482788	-1.732782
8	6	0	-3.734339	0.842007	-1.637259
9	6	0	-3.099850	1.733051	-0.771054
10	6	0	-2.007831	1.313441	-0.013881
11	1	0	-1.841838	-1.936180	-1.004162
12	1	0	-3.759196	-1.175208	-2.416537
13	1	0	-4.584730	1.168514	-2.230234
14	1	0	-3.455623	2.757109	-0.683569
15	1	0	-1.561497	2.003443	0.697141
16	46	0	0.520562	-0.469035	-0.105080
17	15	0	1.375058	1.784916	-0.015828
18	15	0	2.942396	-1.083818	-0.234564
19	6	0	3.895584	0.549247	-0.540235
20	1	0	4.953657	0.439533	-0.285335
21	1	0	3.832650	0.746182	-1.616005
22	6	0	3.268778	1.700760	0.255384
23	1	0	3.731227	2.655604	-0.012099
24	1	0	3.412315	1.551021	1.331045
25	1	0	1.276768	2.633374	-1.168769
26	1	0	0.989403	2.735249	0.984987
27	1	0	3.652428	-1.625586	0.890296
28	1	0	3.483722	-1.927606	-1.257692

TS2-2P-iso (F lies at the apical position)
SCF Done: E(RB+HF-LYP) = -789.924594350 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.910555	1.879489	0.029126
2	6	0	1.731930	-0.216685	-0.061285
3	9	0	1.370339	2.399365	1.140077
4	9	0	1.427323	2.570503	-0.958907
5	9	0	-1.881323	-0.509521	1.690060
6	6	0	2.474641	-0.394888	-1.234966
7	6	0	3.705516	-1.056398	-1.190744
8	6	0	4.208094	-1.519402	0.027278
9	6	0	3.481506	-1.316949	1.204081
10	6	0	2.251336	-0.656221	1.164240
11	1	0	2.095432	-0.025261	-2.183767
12	1	0	4.273044	-1.202760	-2.106435
13	1	0	5.168364	-2.027308	0.061644
14	1	0	3.873719	-1.669543	2.154734
15	1	0	1.689958	-0.498091	2.081019
16	46	0	-0.284638	0.391617	-0.111378
17	15	0	-1.302502	-1.857032	-0.273954
18	15	0	-2.648995	1.019690	-0.032710
19	6	0	-3.735626	-0.435386	-0.612936
20	1	0	-4.759937	-0.281356	-0.257700
21	1	0	-3.750498	-0.363116	-1.706177
22	6	0	-3.202483	-1.789207	-0.152918
23	1	0	-3.645858	-2.595635	-0.746513
24	1	0	-3.399524	-1.930297	0.907298
25	1	0	-1.099269	-2.737681	-1.406723
26	1	0	-0.914623	-2.755992	0.757120
27	1	0	-3.168821	1.485816	1.202950
28	1	0	-3.196037	2.037750	-0.906415

Pd-CF3 and Pd-Ph BDE calculations:

$L_2Pd(Ph)$•
SCF Done: E(UB+HF-LYP) = -452.355853493 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.772499	1.143734	-0.687546
2	6	0	2.389566	0.936246	-0.726848
3	6	0	1.787123	-0.125359	-0.029174
4	6	0	2.625900	-0.959691	0.732777
5	6	0	4.009665	-0.753955	0.780091
6	6	0	4.588106	0.298767	0.068181
7	46	0	-0.214809	-0.553396	-0.150277
8	15	0	-1.285390	1.716138	0.392498
9	6	0	-3.167713	1.503495	0.055752
10	6	0	-3.670292	0.114048	0.457282
11	15	0	-2.603083	-1.285819	-0.315091
12	1	0	2.203635	-1.789249	1.297986
13	1	0	4.635025	-1.417328	1.374963
14	1	0	5.662838	0.461233	0.104993
15	1	0	4.212842	1.968424	-1.245423
16	1	0	1.776612	1.614083	-1.318873
17	1	0	-4.717955	-0.012169	0.168094
18	1	0	-3.606935	-0.020051	1.542789
19	1	0	-3.734302	2.277073	0.582760
20	1	0	-3.305728	1.666724	-1.018899
21	1	0	-1.336831	2.103834	1.779194
22	1	0	-1.117863	3.045822	-0.145109
23	1	0	-3.255986	-1.418705	-1.590944
24	1	0	-3.216181	-2.421965	0.317001

CF_3•
SCF Done: E(UB+HF-LYP) = -337.547406910 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000006	0.000231	0.329042
2	9	0	1.108886	-0.607772	-0.073106
3	9	0	-1.080886	-0.656261	-0.073103
4	9	0	-0.028004	1.263879	-0.073153

$L_2Pd(CF_3)$•
SCF Done: E(UB+HF-LYP) = -558.349568309 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.224672	0.091608	-0.015767
2	9	0	-2.763830	0.227991	1.235049
3	46	0	-0.287117	-0.548428	0.020914
4	15	0	0.884348	1.736811	-0.030878
5	6	0	2.737572	1.362027	0.306157
6	6	0	3.195576	0.070637	-0.379962
7	15	0	2.068612	-1.423017	0.057526
8	9	0	-2.408504	1.308054	-0.625544
9	9	0	-3.045817	-0.778814	-0.681301
10	1	0	3.359434	2.200936	-0.020529
11	1	0	2.841961	1.278151	1.393536
12	1	0	4.231757	-0.156943	-0.112518
13	1	0	3.150007	0.175275	-1.469571
14	1	0	2.680823	-1.852503	1.285283
15	1	0	2.648678	-2.420258	-0.797251
16	1	0	0.997807	2.449615	-1.276352
17	1	0	0.715018	2.885788	0.819258

Ph•
SCF Done: E(UB+HF-LYP) = -231.561280746 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.226409	-0.771813	-0.000108
2	6	0	-0.000031	-1.400130	-0.000105
3	6	0	1.226444	-0.771757	0.000147
4	6	0	1.214254	0.632561	-0.000049
5	6	0	-0.000030	1.324677	-0.000060
6	6	0	-1.214220	0.632648	0.000137
7	1	0	2.162932	-1.323344	0.000183
8	1	0	2.154657	1.179161	-0.000133
9	1	0	0.000101	2.411240	-0.000111
10	1	0	-2.154737	1.179043	0.000200

11	1	0	-2.163004	-1.323213	0.000092

Ligand Effects

PH_3-CP
SCF Done: E(RB+HF-LYP) = -704.278604273 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.485858	-1.078165	0.858043
2	6	0	2.088194	-1.017105	0.896258
3	6	0	1.386421	-0.223245	-0.025813
4	6	0	2.104972	0.548850	-0.948837
5	6	0	3.500992	0.484906	-0.983077
6	6	0	4.193486	-0.328667	-0.082883
7	46	0	-0.586536	-0.537399	-0.098032
8	6	0	-0.902949	1.408231	0.271071
9	9	0	-0.487763	2.228242	-0.722625
10	15	0	-3.028411	-1.304878	-0.259295
11	9	0	-2.258812	1.603152	0.372604
12	9	0	-0.374738	1.872067	1.419670
13	1	0	1.580639	1.200026	-1.640637
14	1	0	4.048764	1.077001	-1.712712
15	1	0	5.279452	-0.369978	-0.108039
16	1	0	4.017795	-1.701655	1.573067
17	1	0	1.555087	-1.592409	1.650844
18	1	0	-3.852117	-0.658851	-1.234877
19	1	0	-3.404670	-2.658582	-0.545878
20	1	0	-3.868171	-1.102007	0.881721

PH_3-TS
SCF Done: E(RB+HF-LYP) = -704.249524701 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.769836	-0.286411	1.204175
2	6	0	1.118481	-0.089337	-0.021837
3	6	0	1.771206	-0.392460	-1.228654
4	6	0	3.037456	-0.977605	-1.196619
5	6	0	3.672143	-1.216433	0.026756
6	6	0	3.040673	-0.868628	1.222595
7	46	0	-0.861394	-0.459620	-0.021975
8	15	0	-3.225781	-1.082695	0.032776
9	6	0	0.012142	1.630526	-0.021187
10	9	0	-1.111695	2.150296	-0.615540
11	9	0	-0.024693	2.021002	1.274843
12	9	0	1.015807	2.323432	-0.612975
13	1	0	1.293176	-0.172863	-2.178580
14	1	0	3.535449	-1.234938	-2.128033
15	1	0	4.665274	-1.657217	0.045352
16	1	0	3.540147	-1.039189	2.172959
17	1	0	1.289872	0.014680	2.129515
18	1	0	-3.980493	-1.136638	-1.186341
19	1	0	-3.631024	-2.359188	0.550947
20	1	0	-4.147933	-0.282172	0.785056

PP-CP
SCF Done: E(RB+HF-LYP) = -788.764188801 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.611957	-0.387032	-0.003746
2	6	0	-2.404586	-0.198426	1.136190
3	6	0	-3.730916	-0.643487	1.164435
4	6	0	-4.290155	-1.268107	0.048318
5	6	0	-3.513622	-1.445327	-1.098118
6	6	0	-2.184481	-1.008567	-1.123433
7	46	0	0.359985	0.119374	-0.022695
8	15	0	2.845708	0.570115	-0.013826
9	6	0	3.739993	-1.077468	0.095385
10	6	0	3.065153	-2.228379	0.146119
11	15	0	1.186248	-2.254854	0.107580
12	6	0	-0.255184	2.061613	-0.090068
13	9	0	-1.060650	2.388121	-1.130073
14	9	0	0.837983	2.902970	-0.208207
15	9	0	-0.893891	2.478088	1.037996
16	1	0	-5.322906	-1.607339	0.069021
17	1	0	-1.600588	-1.152514	-2.030037
18	1	0	-3.940901	-1.921115	-1.978517
19	1	0	-4.330137	-0.490030	2.059529
20	1	0	-1.998338	0.312851	2.003772

21	1	0	0.906404	-3.098444	1.233877
22	1	0	0.953180	-3.230943	-0.919043
23	1	0	3.597987	-3.175329	0.210696
24	1	0	4.828297	-1.082584	0.118053
25	1	0	3.495929	1.297150	1.038208
26	1	0	3.535996	1.176648	-1.115864

PP-TS

SCF Done: E(RB+HF-LYP) = -788.714463327 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.723267	-0.428408	-0.875072
2	6	0	-3.854539	0.307981	-1.239117
3	6	0	-4.021536	1.614791	-0.776738
4	6	0	-3.059018	2.191399	0.058514
5	6	0	-1.927777	1.465861	0.433214
6	6	0	-1.740376	0.168598	-0.072999
7	46	0	0.166573	-0.253164	-0.578089
8	6	0	-0.898980	-1.175098	1.202915
9	9	0	0.300007	-1.442331	1.831205
10	15	0	2.410447	-0.733712	-1.417314
11	6	0	3.914305	0.236251	-0.879384
12	6	0	3.962960	1.072393	0.161097
13	15	0	2.582865	1.617112	1.317174
14	9	0	-1.372809	-2.371183	0.784412
15	9	0	-1.687130	-0.771590	2.229638
16	1	0	-4.908281	2.179232	-1.052584
17	1	0	-1.194058	1.902206	1.103983
18	1	0	-3.195006	3.204483	0.428456
19	1	0	-4.609791	-0.146521	-1.875333
20	1	0	-2.606264	-1.455015	-1.205907
21	1	0	2.902241	-2.076766	-1.263529
22	1	0	2.595452	-0.657605	-2.840873
23	1	0	4.808234	0.090402	-1.483303
24	1	0	4.903919	1.593044	0.335308
25	1	0	2.203399	0.338564	1.857528
26	1	0	3.466844	1.965865	2.408563

PN-CP

SCF Done: E(RB+HF-LYP) = -837.045346248 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.295092	-0.091611	-1.113127
2	6	0	3.636163	-0.489805	-1.143204
3	6	0	4.199953	-1.155686	-0.053652
4	6	0	3.412397	-1.421893	1.068083
5	6	0	2.068884	-1.032993	1.094352
6	6	0	1.490716	-0.371201	0.000250
7	46	0	-0.480132	0.053775	0.020603
8	6	0	0.014297	2.020375	0.105287
9	9	0	-1.161157	2.767795	0.191787
10	15	0	-1.442413	-2.256353	-0.136355
11	6	0	-3.267494	-1.850873	-0.170896
12	6	0	-3.658210	-0.579045	-0.085808
13	7	0	-2.720739	0.512892	0.041503
14	9	0	0.645975	2.508109	-0.996577
15	9	0	0.750657	2.413306	1.172221
16	1	0	5.244149	-1.457952	-0.075067
17	1	0	1.475425	-1.248771	1.980315
18	1	0	3.842516	-1.930948	1.928332
19	1	0	4.243003	-0.267409	-2.018556
20	1	0	1.884372	0.453515	-1.957698
21	1	0	-1.333529	-3.118375	-1.279305
22	1	0	-1.410737	-3.282450	0.869225
23	1	0	-4.008502	-2.640127	-0.261345
24	1	0	-4.718781	-0.324318	-0.109023
25	1	0	-2.853043	1.205569	-0.696628
26	1	0	-2.867456	1.026150	0.912200

PN-TS

SCF Done: E(RB+HF-LYP) = -836.995453472 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.125940	-1.470205	1.153746
2	6	0	-3.594318	-1.996765	-0.052067
3	6	0	-3.012390	-1.586751	-1.256903
4	6	0	-1.965444	-0.667389	-1.259011
5	6	0	-1.450533	-0.176701	-0.041384

6	6	0	-2.075549	-0.550497	1.163270
7	46	0	0.571276	0.086870	0.037447
8	15	0	2.117322	-1.909316	0.154788
9	6	0	3.750736	-1.098439	-0.259417
10	6	0	3.846317	0.234794	-0.261123
11	7	0	2.773357	1.079528	0.170827
12	6	0	-1.033002	1.713815	-0.037158
13	9	0	-0.910770	2.185864	1.236018
14	9	0	-2.270417	2.097724	-0.447329
15	9	0	-0.205241	2.491716	-0.830212
16	1	0	-4.420219	-2.703028	-0.056781
17	1	0	-1.538078	-0.333139	-2.200355
18	1	0	-3.383722	-1.978903	-2.200943
19	1	0	-3.585391	-1.768566	2.093308
20	1	0	-1.735319	-0.120902	2.100554
21	1	0	2.441656	-2.543159	1.410409
22	1	0	2.258937	-3.102585	-0.645654
23	1	0	4.601958	-1.699770	-0.564012
24	1	0	4.757262	0.724654	-0.607478
25	1	0	2.789376	1.229781	1.178302
26	1	0	2.800109	1.993743	-0.273538

PO-CP

SCF Done: E(RB+HF-LYP) = -896.207654855 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.117235	0.799722	1.155749
2	6	0	3.445026	1.244031	1.138624
3	6	0	4.233226	1.055491	0.001747
4	6	0	3.688756	0.413718	-1.112729
5	6	0	2.363597	-0.034285	-1.093721
6	6	0	1.553058	0.170458	0.032950
7	46	0	-0.431170	-0.215598	0.031735
8	6	0	0.023982	-2.160300	0.055814
9	9	0	-1.137117	-2.893680	0.126103
10	15	0	-2.957450	-0.286878	0.011061
11	6	0	-3.413089	1.507699	-0.068945
12	6	0	-2.446412	2.431789	-0.092750
13	8	0	-1.119009	2.127450	-0.025056
14	6	0	-0.206837	3.206987	-0.304973
15	9	0	0.772485	-2.567468	1.106468
16	9	0	0.654834	-2.592932	-1.066659
17	1	0	5.265668	1.396030	-0.011548
18	1	0	-0.270343	3.488374	-1.361111
19	1	0	0.787320	2.827726	-0.075962
20	1	0	-0.441139	4.066036	0.333111
21	1	0	1.967058	-0.556522	-1.959309
22	1	0	4.299301	0.251640	-1.998574
23	1	0	3.863981	1.727034	2.019068
24	1	0	1.524432	0.946481	2.056574
25	1	0	-4.447055	1.833370	-0.092812
26	1	0	-2.663929	3.497675	-0.148049
27	1	0	-3.740035	-0.845458	-1.054198
28	1	0	-3.760690	-0.756456	1.103743

PO-TS

SCF Done: E(RB+HF-LYP) = -896.167810312 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.790750	0.985468	-1.216139
2	6	0	-2.437754	2.221138	-1.169231
3	6	0	-2.804148	2.779731	0.060619
4	6	0	-2.525691	2.096518	1.246607
5	6	0	-1.872440	0.861084	1.211657
6	6	0	-1.464393	0.322515	-0.019012
7	46	0	0.348552	-0.550615	-0.015290
8	6	0	-1.628966	-1.679897	-0.038959
9	9	0	-1.069000	-2.736632	-0.713385
10	15	0	2.674681	-1.351266	0.044871
11	6	0	3.897953	0.045415	0.089069
12	6	0	3.503282	1.322802	0.004350
13	8	0	2.213149	1.688431	-0.161967
14	6	0	1.909297	3.074322	-0.002573
15	9	0	-2.880987	-1.619576	-0.566396
16	9	0	-1.777698	-2.072610	1.250543
17	1	0	-3.324350	3.733565	0.090902
18	1	0	2.070878	3.393417	1.034018
19	1	0	0.855024	3.183529	-0.257823
20	1	0	2.519425	3.687343	-0.678061
21	1	0	-1.682197	0.314448	2.129658
22	1	0	-2.826341	2.519022	2.202357

23	1	0	-2.670748	2.742398	-2.094697
24	1	0	-1.536923	0.537134	-2.172209
25	1	0	4.957590	-0.164481	0.185073
26	1	0	4.222348	2.142882	0.045798
27	1	0	3.169440	-2.161398	1.125321
28	1	0	3.217874	-2.153259	-1.019494

$TS_{a\text{-}F}$-PO
SCF Done: E(RB+HF-LYP) = -896.157364844 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.462711	-1.213514	1.606189
2	6	0	2.186244	-0.690720	1.370386
3	6	0	1.805768	-0.288104	0.082601
4	6	0	2.730519	-0.413981	-0.963181
5	6	0	4.006638	-0.937645	-0.727081
6	6	0	4.376196	-1.339407	0.557955
7	46	0	-0.071428	0.438886	-0.256799
8	6	0	0.328678	2.315031	-0.035517
9	9	0	0.508095	3.168444	-0.996803
10	15	0	-0.790381	-1.885220	-0.580393
11	6	0	-2.576087	-2.085847	-0.967894
12	6	0	-3.485953	-1.529478	-0.159530
13	8	0	-3.156582	-1.077129	1.064873
14	9	0	-1.956664	1.173962	-0.579678
15	9	0	0.156699	2.997187	1.056803
16	1	0	2.462847	-0.104718	-1.971180
17	1	0	4.711211	-1.029215	-1.550824
18	1	0	5.367677	-1.745505	0.741193
19	1	0	3.740273	-1.521670	2.611862
20	1	0	1.488822	-0.601008	2.200501
21	1	0	-4.543894	-1.467321	-0.426836
22	1	0	-2.863635	-2.520963	-1.917160
23	1	0	-0.166572	-2.590703	-1.654298
24	1	0	-0.492848	-2.791680	0.487523
25	6	0	-3.804851	0.141074	1.471974
26	1	0	-3.632712	0.233882	2.545945
27	1	0	-3.344580	0.961858	0.916193
28	1	0	-4.884886	0.082834	1.278407

PObenzene-CP
SCF Done: E(RB+HF-LYP) = -1128.51139297 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.084478	1.200451	-0.200050
2	6	0	4.252553	0.083475	-0.119852
3	6	0	2.863134	0.209562	-0.029839
4	6	0	2.298702	1.502232	-0.018032
5	6	0	3.127887	2.628460	-0.099920
6	6	0	4.511670	2.470342	-0.190194
7	15	0	1.730878	-1.279781	0.069431
8	6	0	2.268221	-2.366474	-1.369285
9	8	0	0.926293	1.605448	0.078172
10	6	0	0.343504	2.917156	0.114910
11	6	0	2.361026	-2.233623	1.564427
12	46	0	-0.557636	-0.340686	0.055349
13	6	0	-1.601299	-2.039301	-0.000771
14	6	0	-2.333113	0.646811	0.006311
15	1	0	2.106554	-1.823155	-2.303426
16	1	0	1.632734	-3.255794	-1.365083
17	1	0	6.161144	1.079114	-0.270001
18	1	0	2.709662	3.626977	-0.095491
19	1	0	5.139739	3.354638	-0.253290
20	1	0	0.726294	3.479989	0.973141
21	1	0	-0.728150	2.759295	0.219477
22	1	0	0.554945	3.456582	-0.814636
23	1	0	3.319552	-2.660212	-1.292439
24	1	0	3.417245	-2.500473	1.460113
25	1	0	1.758107	-3.140331	1.662575
26	1	0	2.224835	-1.622048	2.459595
27	1	0	4.695217	-0.909692	-0.128680
28	9	0	-2.478804	-2.218067	1.013111
29	9	0	-2.291532	-2.223282	-1.155276
30	9	0	-0.741175	-3.122375	0.075539
31	6	0	-3.055290	0.811851	-1.186523
32	6	0	-4.177944	1.644644	-1.239403
33	6	0	-4.613735	2.313706	-0.093397
34	6	0	-3.922278	2.140303	1.106997
35	6	0	-2.796748	1.308894	1.156529
36	1	0	-2.748900	0.279818	-2.083295
37	1	0	-4.718188	1.763691	-2.176468

38	1	0	-5.490301	2.955892	-0.133119
39	1	0	-4.263011	2.643171	2.009951
40	1	0	-2.280747	1.179827	2.106386

PObenzene-TS

SCF Done: E(RB+HF-LYP) = -1128.46928760 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.366927	0.543959	0.119874
2	6	0	-4.363820	-0.426651	0.091012
3	6	0	-3.010662	-0.084776	0.019923
4	6	0	-2.663000	1.283727	-0.024892
5	6	0	-3.665191	2.263962	0.006157
6	6	0	-5.007340	1.889312	0.077766
7	15	0	-1.662746	-1.402194	-0.017925
8	6	0	-2.144467	-2.509366	1.435114
9	8	0	-1.334508	1.581961	-0.100135
10	6	0	-0.924541	2.943826	-0.152455
11	6	0	-2.193019	-2.465604	-1.487302
12	46	0	0.601157	-0.454402	-0.030910
13	6	0	2.617826	-1.510237	-0.012687
14	6	0	2.392928	0.470215	-0.005368
15	1	0	-2.009866	-1.950544	2.364520
16	1	0	-1.471539	-3.371359	1.445782
17	1	0	-6.411139	0.251152	0.175137
18	1	0	-3.406281	3.315654	-0.025732
19	1	0	-5.771797	2.661417	0.100214
20	1	0	-1.336807	3.447645	-1.035715
21	1	0	0.163460	2.919466	-0.218405
22	1	0	-1.227926	3.484342	0.752804
23	1	0	-3.179942	-2.856839	1.364906
24	1	0	-3.229859	-2.804078	-1.394332
25	1	0	-1.528468	-3.332367	-1.543462
26	1	0	-2.081977	-1.880981	-2.403885
27	1	0	-4.646987	-1.475858	0.126000
28	9	0	3.897328	-1.412901	-0.469247
29	9	0	2.712206	-1.921848	1.277609
30	9	0	2.126331	-2.571350	-0.735119
31	6	0	2.758438	1.029616	1.230006
32	6	0	3.372125	2.284814	1.271003
33	6	0	3.654475	2.969956	0.086799
34	6	0	3.331004	2.393410	-1.146842
35	6	0	2.722849	1.138433	-1.199219
36	1	0	2.565473	0.482728	2.147456
37	1	0	3.638376	2.722350	2.230215
38	1	0	4.143843	3.939780	0.122059
39	1	0	3.566095	2.917029	-2.070488
40	1	0	2.502506	0.677488	-2.157770

$TS_{a\text{-}F}$-PObenzene

SCF Done: E(RB+HF-LYP) = -1128.46205605 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.009074	-1.381990	1.567742
2	6	0	2.859877	-0.609598	1.362302
3	6	0	2.362609	-0.388227	0.069201
4	6	0	3.054358	-0.950085	-1.014442
5	6	0	4.203607	-1.722955	-0.810601
6	6	0	4.683493	-1.943554	0.481806
7	46	0	0.677186	0.720736	-0.236974
8	6	0	1.556457	2.423697	-0.523267
9	9	0	2.056718	2.853884	-1.643482
10	15	0	-0.633561	-1.332808	0.019286
11	6	0	-2.456454	-1.018978	-0.181935
12	6	0	-3.050983	-0.078554	0.679239
13	8	0	-2.290304	0.364342	1.722668
14	9	0	-0.997710	1.848775	-0.576750
15	9	0	1.478649	3.443631	0.276522
16	1	0	2.701725	-0.786929	-2.030714
17	1	0	4.724124	-2.149189	-1.665590
18	1	0	5.576515	-2.542545	0.640648
19	1	0	4.377015	-1.540716	2.579179
20	1	0	2.353097	-0.177928	2.222750
21	6	0	-3.217926	-1.585587	-1.208404
22	6	0	-0.217853	-2.643496	-1.256781
23	6	0	-0.443679	-2.263618	1.641506
24	6	0	-2.344851	1.763728	2.043442
25	1	0	-1.646168	1.897742	2.872388
26	1	0	-2.014081	2.326817	1.167225
27	1	0	-3.345221	2.063528	2.376739
28	6	0	-4.552528	-1.219919	-1.391633

29	1	0	-2.769951	-2.309343	-1.882336
30	1	0	-5.133053	-1.666096	-2.193695
31	6	0	-5.127419	-0.273108	-0.543546
32	6	0	-4.385178	0.296605	0.490435
33	1	0	-6.164008	0.023104	-0.680751
34	1	0	-4.843959	1.022191	1.153290
35	1	0	-1.011761	-3.197994	1.608064
36	1	0	0.616755	-2.473425	1.802327
37	1	0	-0.821763	-1.629650	2.444878
38	1	0	-0.820897	-3.545044	-1.113006
39	1	0	-0.379122	-2.245952	-2.261881
40	1	0	0.841522	-2.887838	-1.146346

Xantphos-CP
SCF Done: E(RB97D) = -2288.43045019 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.323101	-3.283281	-1.127002
2	6	0	-3.016860	-2.574624	0.050646
3	6	0	-3.600058	-2.967765	1.269059
4	6	0	-4.480389	-4.061169	1.308040
5	6	0	-4.793305	-4.759658	0.132090
6	6	0	-4.213975	-4.365933	-1.084959
7	15	0	-1.857834	-1.073752	-0.045795
8	6	0	-1.692814	-0.593154	1.777005
9	6	0	-0.629778	-1.156745	2.504129
10	6	0	-0.462374	-0.845683	3.860878
11	6	0	-1.349222	0.038101	4.494093
12	6	0	-2.413307	0.600030	3.770516
13	6	0	-2.590422	0.279929	2.415568
14	6	0	-3.045382	0.247026	-0.703310
15	6	0	-2.597612	1.575235	-0.676963
16	6	0	-3.329318	2.656083	-1.194632
17	6	0	-4.570510	2.361010	-1.784896
18	6	0	-5.052392	1.042477	-1.822169
19	6	0	-4.302160	-0.010781	-1.274706
20	6	0	-2.755073	4.063664	-0.982081
21	6	0	-1.225832	3.973394	-1.096702
22	6	0	-0.600527	2.813554	-0.599135
23	8	0	-1.361260	1.782179	-0.088053
24	6	0	0.789394	2.631337	-0.578695
25	6	0	1.594601	3.687803	-1.042613
26	6	0	1.005654	4.856565	-1.545669
27	6	0	-0.391707	4.992909	-1.581452
28	6	0	-3.354716	5.094085	-1.957443
29	6	0	-3.093994	4.494094	0.479144
30	15	0	1.516439	0.976736	0.024884
31	6	0	3.246791	1.143302	-0.717118
32	6	0	4.411775	1.361978	0.031068
33	6	0	5.654977	1.446151	-0.619858
34	6	0	5.732582	1.339170	-2.015806
35	6	0	4.561060	1.142199	-2.766658
36	6	0	3.324638	1.034261	-2.118710
37	6	0	1.729896	1.272827	1.877011
38	6	0	2.595229	0.438237	2.611963
39	6	0	2.731555	0.614939	3.996922
40	6	0	1.990080	1.605224	4.660805
41	6	0	1.110282	2.419284	3.931266
42	6	0	0.983128	2.259845	2.543153
43	46	0	0.644174	-1.326047	-0.678410
44	6	0	2.552443	-2.012398	-0.425124
45	6	0	2.905192	-2.486238	0.854051
46	6	0	4.228564	-2.874188	1.140706
47	6	0	5.212423	-2.810274	0.142464
48	6	0	4.858000	-2.379968	-1.146778
49	6	0	3.535853	-2.000912	-1.430232
50	6	0	0.260454	-3.085335	-1.679284
51	9	0	-0.653888	-2.774587	-2.696377
52	9	0	-0.347059	-4.054294	-0.914007
53	9	0	1.279773	-3.716911	-2.332010
54	1	0	1.639098	5.666021	-1.912678
55	1	0	6.241102	-3.105668	0.362417
56	1	0	-0.830401	5.907083	-1.981542
57	1	0	3.275844	-1.679605	-2.437858
58	1	0	5.611856	-2.337363	-1.937087
59	1	0	4.481858	-3.232829	2.142537
60	1	0	2.153191	-2.543528	1.644719
61	1	0	2.678824	3.584401	-1.030664
62	1	0	-4.683479	-1.031431	-1.302379
63	1	0	-6.023748	0.834958	-2.274679
64	1	0	-5.172878	3.163523	-2.210952
65	1	0	4.360199	1.462763	1.114566
66	1	0	6.561035	1.601301	-0.030313
67	1	0	6.699932	1.407717	-2.517795

68	1	0	4.612532	1.054391	-3.853892
69	1	0	2.417634	0.847313	-2.697956
70	1	0	3.161094	-0.342168	2.104322
71	1	0	3.416207	-0.027536	4.555245
72	1	0	2.093203	1.737949	5.739915
73	1	0	0.520579	3.184460	4.440333
74	1	0	0.301056	2.900876	1.984888
75	1	0	0.069993	-1.827742	2.001430
76	1	0	0.375950	-1.271526	4.412839
77	1	0	-1.206264	0.294194	5.545721
78	1	0	-3.108095	1.286522	4.259941
79	1	0	-3.421576	0.710231	1.854811
80	1	0	-3.370535	-2.426518	2.186722
81	1	0	-4.922806	-4.362133	2.260270
82	1	0	-5.479291	-5.608842	0.164022
83	1	0	-4.442768	-4.909438	-2.004041
84	1	0	-2.853639	-3.006893	-2.067892
85	1	0	-4.445827	5.147520	-1.830428
86	1	0	-2.955118	6.096904	-1.746566
87	1	0	-3.130310	4.833824	-3.003097
88	1	0	-4.187004	4.539020	0.612356
89	1	0	-2.681828	3.773132	1.201067
90	1	0	-2.664482	5.487559	0.686697

Xantphos-TS

SCF Done: E(RB97D) = -2288.38280396 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.790654	-3.820747	-2.652950
2	6	0	-1.904651	-2.876873	-2.189744
3	6	0	-1.669067	-1.877694	-1.233483
4	8	0	-0.439472	-1.678046	-0.653869
5	6	0	0.661500	-2.373304	-1.097813
6	6	0	0.551161	-3.432921	-2.017707
7	6	0	-3.215355	-2.988925	-2.692970
8	6	0	-4.242607	-2.140400	-2.262414
9	6	0	-3.977846	-1.151146	-1.300011
10	6	0	-2.686237	-1.013347	-0.776032
11	6	0	1.729914	-4.125566	-2.347370
12	6	0	2.969110	-3.768403	-1.800675
13	6	0	3.051852	-2.678216	-0.921922
14	6	0	1.900336	-1.958790	-0.565541
15	15	0	-2.196114	0.298109	0.487359
16	6	0	-1.868494	-0.747189	2.022395
17	15	0	1.980738	-0.388108	0.516806
18	6	0	3.740233	0.175674	0.036190
19	46	0	-0.491446	1.859071	-0.192818
20	6	0	0.405190	2.070804	-2.320309
21	9	0	1.524447	2.562274	-2.950274
22	6	0	0.601180	3.449179	-0.786674
23	6	0	1.883584	3.558107	-0.203278
24	6	0	2.353034	4.819596	0.191106
25	6	0	1.579046	5.971163	-0.041106
26	6	0	0.331490	5.864384	-0.677774
27	6	0	-0.151677	4.607071	-1.077581
28	9	0	-0.657688	2.445814	-3.091176
29	9	0	0.552671	0.699413	-2.480652
30	6	0	-3.835807	1.147113	0.862763
31	6	0	2.272607	-1.118744	2.242352
32	1	0	-5.249001	-2.249749	-2.670275
33	1	0	1.958093	6.951831	0.254803
34	1	0	-3.428993	-3.760229	-3.434912
35	1	0	-1.101232	4.512837	-1.604591
36	1	0	-0.261560	6.760274	-0.877112
37	1	0	3.331945	4.903692	0.669390
38	1	0	2.492525	2.668017	-0.052403
39	1	0	-4.771740	-0.488548	-0.954038
40	1	0	4.016645	-2.367437	-0.519660
41	1	0	3.867961	-4.326404	-2.069072
42	1	0	1.670046	-4.958558	-3.050114
43	6	0	-0.662326	-3.740394	-4.200123
44	6	0	-1.155107	-5.274885	-2.241962
45	6	0	-4.840253	0.543692	1.641107
46	6	0	-6.046042	1.223162	1.875120
47	6	0	-6.250320	2.503018	1.331357
48	6	0	-5.245416	3.107167	0.558065
49	6	0	-4.036872	2.431490	0.325843
50	1	0	-4.672280	-0.446106	2.069507
51	1	0	-6.823685	0.756101	2.483549
52	1	0	-7.188670	3.030468	1.516197
53	1	0	-5.398992	4.105139	0.141884
54	1	0	-3.235460	2.891803	-0.259805
55	6	0	-1.023671	-0.212024	3.009578
56	6	0	-0.738673	-0.951460	4.166288

57	6	0	-1.284854	-2.233474	4.332581
58	6	0	-2.122456	-2.773904	3.343323
59	6	0	-2.415441	-2.032237	2.187961
60	1	0	-0.569167	0.768969	2.852801
61	1	0	-0.057668	-0.545448	4.913888
62	1	0	-1.043769	-2.816147	5.223943
63	1	0	-2.542172	-3.775049	3.466157
64	1	0	-3.052646	-2.455410	1.409001
65	6	0	2.571367	-0.220940	3.288982
66	6	0	2.751179	-0.688715	4.598535
67	6	0	2.601902	-2.056950	4.883676
68	6	0	2.280219	-2.949964	3.849991
69	6	0	2.125919	-2.486342	2.533289
70	1	0	2.670635	0.846619	3.076396
71	1	0	2.999232	0.015028	5.396553
72	1	0	2.732108	-2.421939	5.904799
73	1	0	2.157027	-4.013934	4.064691
74	1	0	1.890932	-3.187433	1.731424
75	6	0	4.864526	0.065813	0.874369
76	6	0	6.112640	0.554293	0.450280
77	6	0	6.248907	1.147907	-0.814025
78	6	0	5.129525	1.250549	-1.657234
79	6	0	3.881837	0.769058	-1.236200
80	1	0	4.771067	-0.400474	1.855563
81	1	0	6.979161	0.463542	1.109686
82	1	0	7.219196	1.528710	-1.140160
83	1	0	5.222673	1.712253	-2.642526
84	1	0	3.019101	0.862945	-1.894951
85	1	0	0.126726	-4.419665	-4.557036
86	1	0	-1.608622	-4.033199	-4.680394
87	1	0	-0.411626	-2.715161	-4.510702
88	1	0	-0.372915	-5.975014	-2.575305
89	1	0	-1.253687	-5.353688	-1.148445
90	1	0	-2.109767	-5.573175	-2.703207

OO-CP

SCF Done: E(RB+HF-LYP) = -926.259488151 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.399157	0.438430	-0.745448
2	6	0	3.749533	0.075566	-0.761063
3	6	0	4.191899	-1.038709	-0.045324
4	6	0	3.273296	-1.793711	0.685533
5	6	0	1.919974	-1.438555	0.697265
6	6	0	1.467757	-0.322224	-0.024292
7	46	0	-0.503616	-0.018153	-0.067947
8	6	0	-0.268070	1.932301	0.215160
9	9	0	-1.519378	2.413588	0.571229
10	8	0	-1.202928	-2.239258	-0.211495
11	6	0	-2.560525	-2.312268	0.254121
12	6	0	-3.430870	-1.226240	-0.370999
13	8	0	-2.842706	0.071401	-0.225971
14	9	0	0.085783	2.638062	-0.894488
15	9	0	0.565027	2.333686	1.200273
16	1	0	5.243681	-1.313947	-0.053643
17	1	0	1.220391	-2.043336	1.268953
18	1	0	3.606761	-2.660327	1.252749
19	1	0	4.458194	0.672677	-1.330968
20	1	0	2.076959	1.318373	-1.291984
21	1	0	-1.153448	-2.526823	-1.138469
22	1	0	-3.120141	0.501021	0.598892
23	1	0	-2.982117	-3.305558	0.051014
24	1	0	-2.492977	-2.180345	1.337413
25	1	0	-3.521859	-1.387683	-1.450710
26	1	0	-4.439825	-1.251730	0.059225

OO-TS

SCF Done: E(RB+HF-LYP) = -926.212598570 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.403188	-0.255798	-0.998284
2	6	0	3.648719	-0.830041	-0.733223
3	6	0	4.003359	-1.168815	0.574380
4	6	0	3.114126	-0.926939	1.627367
5	6	0	1.870139	-0.349831	1.377629
6	6	0	1.490062	-0.055908	0.052693
7	46	0	-0.399097	-0.537622	-0.372919
8	6	0	0.433098	1.573938	-0.171717
9	9	0	-0.871152	2.047028	0.082844
10	8	0	-2.827657	0.438495	1.595102
11	6	0	-3.850238	0.027720	0.714451

12	6	0	-3.561456	-1.300361	0.020675
13	8	0	-2.495730	-1.227831	-0.952427
14	9	0	0.713110	2.014672	-1.417269
15	9	0	1.161471	2.319289	0.691523
16	1	0	4.978396	-1.603578	0.777188
17	1	0	1.195509	-0.125806	2.198455
18	1	0	3.396753	-1.176668	2.646829
19	1	0	4.345224	-1.003294	-1.549627
20	1	0	2.138538	0.038275	-2.008481
21	1	0	-2.133155	0.890983	1.087071
22	1	0	-2.786358	-0.669217	-1.690589
23	1	0	-4.757950	-0.103374	1.317100
24	1	0	-4.075822	0.799562	-0.041946
25	1	0	-3.226399	-2.035990	0.754809
26	1	0	-4.466011	-1.678297	-0.475630

NN-CP

SCF Done: E(RB+HF-LYP) = -886.563594161 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.440802	-0.280480	-0.009459
2	6	0	2.275108	0.221409	-1.021315
3	6	0	3.636831	-0.096268	-1.056441
4	6	0	4.200616	-0.908913	-0.070456
5	6	0	3.390327	-1.400503	0.954051
6	6	0	2.026144	-1.088997	0.981679
7	46	0	-0.558521	-0.045167	-0.005773
8	7	0	-2.811830	-0.042387	0.010190
9	6	0	-3.296441	-1.354197	-0.461783
10	6	0	-2.414996	-2.471456	0.106126
11	7	0	-0.999884	-2.223068	-0.245823
12	6	0	-0.342344	1.940563	0.174299
13	9	0	0.310681	2.385766	1.277945
14	9	0	-1.609308	2.515870	0.257169
15	9	0	0.244572	2.565931	-0.887774
16	1	0	5.260757	-1.149309	-0.095746
17	1	0	1.420684	-1.471560	1.802761
18	1	0	3.818834	-2.021889	1.738255
19	1	0	4.261103	0.301614	-1.854138
20	1	0	1.865280	0.879881	-1.781003
21	1	0	-2.775723	-3.445704	-0.252135
22	1	0	-2.484893	-2.475216	1.199480
23	1	0	-3.229923	-1.355176	-1.555465
24	1	0	-4.345731	-1.542992	-0.195326
25	1	0	-3.112899	0.153642	0.963680
26	1	0	-3.141628	0.729795	-0.563881
27	1	0	-0.360097	-2.777697	0.320502
28	1	0	-0.811584	-2.464567	-1.218267

NN-TS

SCF Done: E(RB+HF-LYP) = -886.502413473 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.295177	-0.188183	-0.017058
2	6	0	-1.852415	-0.606407	1.212945
3	6	0	-2.856365	-1.574586	1.244644
4	6	0	-3.357798	-2.116070	0.057504
5	6	0	-2.854109	-1.668400	-1.169264
6	6	0	-1.853120	-0.700033	-1.212768
7	46	0	0.692616	0.118739	-0.027876
8	7	0	2.949456	0.761886	-0.037905
9	6	0	3.791895	-0.372310	0.377842
10	6	0	3.322213	-1.668756	-0.292052
11	7	0	1.915416	-1.936322	0.034591
12	6	0	-0.994012	1.694199	-0.026223
13	9	0	-2.298948	2.024313	-0.252607
14	9	0	-0.328406	2.457532	-0.961494
15	9	0	-0.717792	2.220191	1.203766
16	1	0	-4.149687	-2.859913	0.085669
17	1	0	-1.492854	-0.334581	-2.170877
18	1	0	-3.253207	-2.069769	-2.098446
19	1	0	-3.256883	-1.900759	2.202201
20	1	0	-1.493629	-0.162597	2.137227
21	1	0	4.001737	-2.485028	-0.001307
22	1	0	3.394222	-1.559828	-1.380729
23	1	0	3.695587	-0.471161	1.465295
24	1	0	4.859181	-0.220574	0.155280
25	1	0	3.186424	1.065549	-0.980878
26	1	0	3.085490	1.563153	0.572967
27	1	0	1.494542	-2.597535	-0.612006
28	1	0	1.814292	-2.322922	0.970702

ON-CP
SCF Done: E(RB+HF-LYP) = -906.411900779 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.457741	-0.269900	-0.005886
2	6	0	-2.314168	0.341342	0.922881
3	6	0	-3.666959	-0.008337	0.987402
4	6	0	-4.193661	-0.962090	0.114292
5	6	0	-3.356381	-1.567973	-0.824147
6	6	0	-2.001389	-1.224683	-0.883195
7	46	0	0.536453	-0.028876	-0.065823
8	7	0	2.801041	-0.053377	-0.045796
9	6	0	3.258201	-1.297162	0.600231
10	6	0	2.480271	-2.485184	0.033630
11	8	0	1.057918	-2.295598	0.117965
12	6	0	0.336056	1.949528	-0.156754
13	9	0	-0.388457	2.436986	-1.189420
14	9	0	1.602098	2.501222	-0.310801
15	9	0	-0.158006	2.537963	0.969433
16	1	0	-5.247175	-1.227253	0.161389
17	1	0	-1.367980	-1.712763	-1.621098
18	1	0	-3.756214	-2.307011	-1.515688
19	1	0	-4.312152	0.473799	1.719127
20	1	0	-1.929929	1.103234	1.592764
21	1	0	0.742690	-2.515405	1.009919
22	1	0	2.772825	-3.413747	0.538010
23	1	0	2.688618	-2.601692	-1.034551
24	1	0	3.062151	-1.202104	1.673752
25	1	0	4.336015	-1.478574	0.472573
26	1	0	3.155378	0.029143	-0.998099
27	1	0	3.102205	0.780318	0.452978

ON-TS
SCF Done: E(RB+HF-LYP) = -906.359201102 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.298000	-0.239187	-0.026245
2	6	0	-1.724273	-0.756317	1.212562
3	6	0	-2.623600	-1.824605	1.253939
4	6	0	-3.135211	-2.360664	0.070182
5	6	0	-2.751940	-1.819319	-1.162230
6	6	0	-1.859118	-0.750530	-1.215094
7	46	0	0.643149	0.236725	-0.140514
8	7	0	2.851262	0.755316	-0.167969
9	6	0	3.691770	-0.241525	0.524577
10	6	0	3.506497	-1.636803	-0.076132
11	8	0	2.155723	-2.068430	-0.139038
12	6	0	-1.097516	1.703271	0.056850
13	9	0	-2.403872	1.936088	-0.253051
14	9	0	-0.440649	2.633134	-0.720219
15	9	0	-0.954842	2.099377	1.350227
16	1	0	-3.844564	-3.183280	0.106048
17	1	0	-1.588315	-0.313088	-2.171790
18	1	0	-3.159092	-2.226679	-2.084574
19	1	0	-2.933789	-2.230268	2.214162
20	1	0	-1.359535	-0.312033	2.133613
21	1	0	1.793555	-2.134133	0.760316
22	1	0	4.131936	-2.348039	0.484606
23	1	0	3.856280	-1.643817	-1.114692
24	1	0	3.390789	-0.244202	1.578573
25	1	0	4.763475	0.011541	0.488150
26	1	0	3.152863	0.863182	-1.136127
27	1	0	2.949565	1.668372	0.270351

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reductive elimination of Brettphos
CP-Obound
SCF Done: E(RB97D) = -2217.50616228 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.874319	-0.029896	2.937698
2	6	0	0.623297	-0.654266	2.284194
3	6	0	0.640751	-2.182771	2.492206
4	6	0	0.674236	-2.519114	3.997487
5	6	0	1.894185	-1.877244	4.686795
6	6	0	1.922212	-0.355576	4.444561
7	15	0	0.585731	-0.150016	0.415472
8	6	0	-0.381100	1.493430	0.308014

9	6	0	0.179059	2.513782	1.321100
10	6	0	-0.569295	3.855920	1.165513
11	6	0	-0.458504	4.394753	-0.274762
12	6	0	-0.994944	3.361427	-1.286321
13	6	0	-0.254161	2.019783	-1.131465
14	46	0	2.809981	-0.309815	-0.567506
15	6	0	3.399743	1.587075	-0.336186
16	6	0	3.283131	2.505465	-1.397806
17	6	0	3.537475	3.872884	-1.189436
18	6	0	3.946958	4.335229	0.072026
19	6	0	4.122104	3.414512	1.117523
20	6	0	3.859345	2.047327	0.913342
21	1	0	4.145182	5.397344	0.232881
22	6	0	4.640373	-0.643321	-1.445163
23	9	0	5.700716	-0.689692	-0.565637
24	8	0	1.845035	-2.527640	-0.558445
25	6	0	2.693032	-3.689283	-0.603757
26	6	0	-0.362922	-1.593857	-0.392940
27	6	0	0.475988	-2.699350	-0.711703
28	6	0	-0.069229	-3.914348	-1.137922
29	6	0	-1.459614	-4.061524	-1.236002
30	6	0	-2.299545	-2.979328	-0.945855
31	6	0	-1.760345	-1.717658	-0.566357
32	8	0	-3.673031	-3.048384	-0.993237
33	6	0	-4.261101	-4.281634	-1.405823
34	6	0	-2.721238	-0.569366	-0.422473
35	6	0	-3.078751	0.182037	-1.575883
36	6	0	-3.966911	1.261212	-1.422420
37	6	0	-4.511834	1.613553	-0.180488
38	6	0	-4.169868	0.835704	0.936102
39	6	0	-3.287203	-0.251359	0.839651
40	6	0	-2.564309	-0.171908	-2.976105
41	6	0	-3.531541	-1.160578	-3.673763
42	6	0	-5.412763	2.833278	-0.040322
43	6	0	-4.694121	3.947371	0.755919
44	6	0	-2.956254	-1.067299	2.086489
45	6	0	-2.829484	-0.209393	3.364314
46	9	0	5.023773	0.202420	-2.453169
47	9	0	4.617839	-1.916107	-2.042258
48	6	0	-2.369443	1.043907	-3.912271
49	6	0	-6.767327	2.482160	0.612745
50	6	0	-4.009680	-2.179235	2.301741
51	1	0	0.571051	-4.758103	-1.387304
52	1	0	-1.866518	-5.022125	-1.546940
53	1	0	-4.231470	1.861884	-2.294179
54	1	0	-4.589627	1.095150	1.908724
55	1	0	2.329058	-4.440545	0.116236
56	1	0	3.689185	-3.329916	-0.336962
57	1	0	2.713974	-4.111807	-1.620237
58	1	0	-3.951628	-4.544989	-2.433070
59	1	0	-5.345065	-4.115945	-1.373885
60	1	0	-3.986132	-5.103005	-0.720296
61	1	0	-1.590239	-0.673194	-2.863116
62	1	0	-3.341623	1.459445	-4.224239
63	1	0	-1.845854	0.716015	-4.824183
64	1	0	-1.789066	1.852178	-3.447661
65	1	0	-4.513450	-0.678277	-3.813869
66	1	0	-3.680892	-2.068372	-3.079815
67	1	0	-3.138109	-1.436703	-4.666377
68	1	0	-5.613872	3.218695	-1.054997
69	1	0	-7.290734	1.699478	0.041179
70	1	0	-7.412422	3.374673	0.662354
71	1	0	-6.620410	2.113228	1.640962
72	1	0	-4.466082	3.600762	1.777401
73	1	0	-5.330698	4.844676	0.830719
74	1	0	-3.744938	4.226690	0.272660
75	1	0	-1.988657	-1.557388	1.916422
76	1	0	-4.997569	-1.727397	2.492029
77	1	0	-3.739577	-2.800855	3.172311
78	1	0	-4.090987	-2.818899	1.412710
79	1	0	-3.815353	0.143079	3.708176
80	1	0	-2.194374	0.675283	3.199532
81	1	0	-2.391049	-0.811353	4.176277
82	1	0	2.982222	2.156025	-2.385901
83	1	0	3.423493	4.574230	-2.020362
84	1	0	4.466251	3.755700	2.097722
85	1	0	3.997101	1.345945	1.735591
86	1	0	-1.435130	1.314905	0.545056
87	1	0	0.054525	2.138418	2.349708
88	1	0	1.255233	2.667571	1.143282
89	1	0	-1.634772	3.703960	1.416260
90	1	0	-0.162757	4.588580	1.882513
91	1	0	0.603326	4.599585	-0.497204
92	1	0	-1.008575	5.346675	-0.368072
93	1	0	-0.876042	3.736185	-2.317314
94	1	0	-2.073477	3.198824	-1.117625
95	1	0	0.811736	2.164416	-1.358506

96	1	0	-0.641762	1.269799	-1.832505
97	1	0	-0.282304	-0.238263	2.749934
98	1	0	1.540467	-2.590690	2.001824
99	1	0	-0.228124	-2.660294	2.016703
100	1	0	-0.251910	-2.142151	4.468720
101	1	0	0.684714	-3.613769	4.134012
102	1	0	1.885127	-2.096915	5.767507
103	1	0	2.815661	-2.323267	4.270331
104	1	0	2.825807	0.089739	4.893278
105	1	0	1.050067	0.108220	4.941405
106	1	0	2.763716	-0.444444	2.430626
107	1	0	1.902941	1.056621	2.782631

CP-Cbound

SCF Done: E(RB97D) = -2217.51827901 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.699988	0.198022	-0.286454
2	6	0	-3.133768	0.639387	0.922197
3	6	0	-1.931849	1.366259	0.967348
4	6	0	-1.279956	1.680584	-0.257185
5	6	0	-1.839763	1.264005	-1.486867
6	6	0	-3.041389	0.530164	-1.475519
7	6	0	-0.011311	2.481421	-0.245092
8	6	0	1.259412	1.888158	-0.100033
9	6	0	2.422382	2.702098	-0.146536
10	6	0	2.309337	4.088195	-0.316107
11	6	0	1.043180	4.682992	-0.436026
12	6	0	-0.111568	3.891506	-0.397535
13	15	0	1.374973	0.018216	0.205220
14	6	0	2.415764	-0.701883	-1.270803
15	6	0	3.866901	-1.095277	-0.941032
16	6	0	4.481784	-1.840177	-2.147865
17	6	0	4.421975	-0.979543	-3.426126
18	6	0	2.975368	-0.535828	-3.722768
19	6	0	2.367203	0.205466	-2.513521
20	8	0	3.627729	2.052259	-0.016697
21	6	0	4.819946	2.833292	-0.042480
22	8	0	-1.390775	4.390077	-0.493309
23	6	0	-1.537409	5.800929	-0.646367
24	6	0	-1.403129	1.861523	2.310437
25	6	0	-1.437469	0.781315	3.411371
26	6	0	-1.215461	1.638636	-2.829690
27	6	0	-2.025299	2.780949	-3.487190
28	6	0	-5.004985	-0.585611	-0.242601
29	6	0	-6.189428	0.383235	-0.011074
30	46	0	-0.691488	-1.326175	0.657245
31	6	0	-2.154621	-2.633834	1.259333
32	9	0	-2.932355	-2.029780	2.252641
33	6	0	-0.048068	-2.819324	-0.509136
34	6	0	0.901302	-3.768936	-0.095618
35	6	0	1.484761	-4.635681	-1.038848
36	6	0	1.102186	-4.580664	-2.389157
37	6	0	0.105769	-3.673785	-2.788500
38	6	0	-0.480017	-2.805390	-1.849936
39	1	0	1.560502	-5.251889	-3.118843
40	9	0	-1.694979	-3.792868	1.839441
41	9	0	-3.057598	-3.033995	0.296440
42	6	0	2.516882	-0.142304	1.755022
43	6	0	2.191419	0.919942	2.820647
44	6	0	3.089402	0.736545	4.062769
45	6	0	2.942752	-0.681972	4.647594
46	6	0	3.263147	-1.745259	3.579391
47	6	0	2.372522	-1.564929	2.332432
48	6	0	-2.197453	3.113888	2.749577
49	6	0	-1.097739	0.442411	-3.799680
50	6	0	-5.251729	-1.454192	-1.488747
51	1	0	2.236465	-5.359126	-0.711725
52	1	0	-0.223887	-3.641919	-3.830418
53	1	0	-1.255158	-2.106286	-2.162599
54	1	0	1.197087	-3.826888	0.951063
55	1	0	3.549428	0.008570	1.413063
56	1	0	1.870264	-1.623999	-1.506811
57	1	0	1.139138	0.817319	3.124357
58	1	0	2.316735	1.930676	2.405623
59	1	0	1.314017	-1.740402	2.596884
60	1	0	2.629617	-2.313698	1.568978
61	1	0	4.454731	-0.189813	-0.721284
62	1	0	3.905827	-1.742447	-0.052246
63	1	0	2.938791	1.126171	-2.314596
64	1	0	1.333481	0.501234	-2.733599
65	1	0	3.193805	4.722229	-0.354557
66	1	0	4.143534	0.902513	3.772936
67	1	0	2.836126	1.496574	4.821302

68	1	0	3.127316	-2.759749	3.989938
69	1	0	4.324547	-1.652335	3.283147
70	1	0	5.524375	-2.122502	-1.921919
71	1	0	3.914500	-2.773725	-2.309966
72	1	0	2.358679	-1.426448	-3.938415
73	1	0	2.944296	0.111305	-4.615974
74	1	0	0.980169	5.763235	-0.558150
75	1	0	4.926149	3.367134	-1.003632
76	1	0	5.643715	2.118531	0.078623
77	1	0	4.833653	3.566580	0.783471
78	1	0	1.902355	-0.822177	4.993465
79	1	0	3.598921	-0.806911	5.525248
80	1	0	5.051134	-0.080847	-3.284348
81	1	0	4.837648	-1.536350	-4.282876
82	1	0	-0.354885	2.164872	2.177203
83	1	0	-3.637005	0.384166	1.853374
84	1	0	-3.461376	0.201566	-2.425895
85	1	0	-0.199788	2.018098	-2.644499
86	1	0	-1.105462	6.341989	0.214838
87	1	0	-2.618342	5.981799	-0.696617
88	1	0	-1.054294	6.154069	-1.575266
89	1	0	-2.152776	3.889661	1.970949
90	1	0	-1.790226	3.522170	3.690085
91	1	0	-3.255946	2.852355	2.914773
92	1	0	-2.466547	0.481904	3.657618
93	1	0	-0.966126	1.169204	4.329535
94	1	0	-0.896095	-0.129104	3.102765
95	1	0	-0.554687	-0.397572	-3.343113
96	1	0	-0.560138	0.752420	-4.710964
97	1	0	-2.091628	0.079081	-4.106615
98	1	0	-3.051236	2.440724	-3.705459
99	1	0	-1.554898	3.090595	-4.435884
100	1	0	-2.086549	3.647893	-2.814177
101	1	0	-4.937421	-1.258365	0.626436
102	1	0	-5.422780	-0.829798	-2.382120
103	1	0	-6.149453	-2.074581	-1.339007
104	1	0	-4.394681	-2.116170	-1.677620
105	1	0	-6.040510	0.980138	0.903161
106	1	0	-7.134568	-0.176922	0.086181
107	1	0	-6.283894	1.079210	-0.861760

TS-Obound

SCF Done: E(RB97D) = -2217.46490992 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.939384	-0.488090	2.746290
2	6	0	0.593389	-0.945868	2.143347
3	6	0	0.432339	-2.466162	2.344196
4	6	0	0.477689	-2.813263	3.847342
5	6	0	1.790690	-2.329579	4.494893
6	6	0	1.999725	-0.821890	4.251044
7	15	0	0.520153	-0.406122	0.285939
8	6	0	-0.247777	1.347543	0.279201
9	6	0	0.425662	2.229706	1.350749
10	6	0	-0.159618	3.657572	1.284858
11	6	0	0.015364	4.271671	-0.118302
12	6	0	-0.614937	3.368234	-1.197634
13	6	0	-0.030767	1.944606	-1.121741
14	46	0	2.724797	-0.413703	-0.612948
15	6	0	3.898550	1.243317	-0.503808
16	6	0	3.697102	2.203421	-1.529436
17	6	0	3.711529	3.570462	-1.224877
18	6	0	3.984911	4.009468	0.083857
19	6	0	4.265255	3.063125	1.084558
20	6	0	4.247916	1.691060	0.794134
21	1	0	4.003719	5.076632	0.313327
22	6	0	5.014946	-0.287150	-1.049370
23	9	0	5.529208	-0.901453	0.061455
24	8	0	1.406523	-2.920014	-0.759028
25	6	0	2.165938	-3.890400	-1.486581
26	6	0	-0.636256	-1.701595	-0.499815
27	6	0	0.038881	-2.890090	-0.911603
28	6	0	-0.677777	-3.982036	-1.416039
29	6	0	-2.077142	-3.938487	-1.476958
30	6	0	-2.756002	-2.782743	-1.071042
31	6	0	-2.043035	-1.632974	-0.630337
32	8	0	-4.129737	-2.669447	-1.061653
33	6	0	-4.887368	-3.775461	-1.548116
34	6	0	-2.841362	-0.381128	-0.393179
35	6	0	-3.131867	0.472836	-1.493382
36	6	0	-3.871085	1.644583	-1.253915
37	6	0	-4.328785	1.995242	0.023321
38	6	0	-4.051822	1.123391	1.087192
39	6	0	-3.319960	-0.060496	0.903743

40	6	0	-2.692249	0.143698	-2.925002
41	6	0	-3.766505	-0.704815	-3.650256
42	6	0	-5.067087	3.306426	0.254624
43	6	0	-4.202280	4.276504	1.092685
44	6	0	-3.052739	-0.974365	2.096536
45	6	0	-2.774951	-0.206968	3.407272
46	9	0	6.023183	0.459769	-1.578881
47	9	0	4.830376	-1.295114	-2.006225
48	6	0	-2.399652	1.385283	-3.800410
49	6	0	-6.441998	3.086699	0.923057
50	6	0	-4.230191	-1.956785	2.298913
51	1	0	-0.158644	-4.885366	-1.733195
52	1	0	-2.618371	-4.811307	-1.838663
53	1	0	-4.086074	2.319369	-2.084074
54	1	0	-4.401771	1.383101	2.086977
55	1	0	2.035928	-4.899145	-1.056419
56	1	0	3.209034	-3.565260	-1.392520
57	1	0	1.868265	-3.901776	-2.549058
58	1	0	-4.645595	-3.988605	-2.605148
59	1	0	-5.938832	-3.474577	-1.459851
60	1	0	-4.704955	-4.682702	-0.944449
61	1	0	-1.770435	-0.456214	-2.865545
62	1	0	-1.748453	2.114272	-3.300509
63	1	0	-3.334833	1.899462	-4.076899
64	1	0	-1.914615	1.062705	-4.735374
65	1	0	-4.704240	-0.128750	-3.722999
66	1	0	-3.980593	-1.635592	-3.115554
67	1	0	-3.429519	-0.944891	-4.672758
68	1	0	-5.239241	3.772387	-0.731240
69	1	0	-7.069510	2.409418	0.322376
70	1	0	-6.970314	4.047257	1.040084
71	1	0	-6.322073	2.641668	1.924400
72	1	0	-4.001178	3.846233	2.087775
73	1	0	-4.721810	5.239190	1.232685
74	1	0	-3.234363	4.465463	0.602689
75	1	0	-2.161831	-1.572595	1.866629
76	1	0	-5.148710	-1.396945	2.542941
77	1	0	-4.013984	-2.648125	3.131047
78	1	0	-4.414759	-2.537847	1.385213
79	1	0	-3.694296	0.254536	3.803204
80	1	0	-2.032355	0.593136	3.260465
81	1	0	-2.396088	-0.902529	4.173014
82	1	0	3.498024	1.866492	-2.547540
83	1	0	3.512989	4.298473	-2.015398
84	1	0	4.498939	3.392947	2.100084
85	1	0	4.466539	0.957810	1.569400
86	1	0	-1.318249	1.297301	0.499879
87	1	0	0.260648	1.810107	2.356443
88	1	0	1.512800	2.267035	1.173691
89	1	0	-1.235079	3.613389	1.532853
90	1	0	0.328350	4.292098	2.044007
91	1	0	1.093951	4.378327	-0.325559
92	1	0	-0.432268	5.280016	-0.150603
93	1	0	-0.440159	3.793102	-2.201209
94	1	0	-1.707360	3.313680	-1.048736
95	1	0	1.052357	1.975267	-1.322024
96	1	0	-0.485084	1.290918	-1.878476
97	1	0	-0.231040	-0.428387	2.657053
98	1	0	1.254649	-2.978206	1.817864
99	1	0	-0.505935	-2.829755	1.900290
100	1	0	-0.377625	-2.327477	4.351987
101	1	0	0.358877	-3.901691	3.983104
102	1	0	1.791349	-2.551045	5.575543
103	1	0	2.635232	-2.884105	4.046811
104	1	0	2.967031	-0.494916	4.668429
105	1	0	1.210179	-0.254881	4.778320
106	1	0	2.748209	-1.011966	2.206218
107	1	0	2.104673	0.584868	2.583768

TS-Cbound
SCF Done: E(RB97D) = -2217.48191861 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.791066	0.095962	0.006294
2	6	0	-3.128971	0.588591	1.144888
3	6	0	-1.953265	1.353604	1.059404
4	6	0	-1.401523	1.620692	-0.224526
5	6	0	-2.040698	1.118985	-1.383108
6	6	0	-3.230113	0.378886	-1.244314
7	6	0	-0.167390	2.468497	-0.359472
8	6	0	1.145401	1.956445	-0.266011
9	6	0	2.250706	2.823552	-0.468178
10	6	0	2.048709	4.184691	-0.731433
11	6	0	0.744876	4.701477	-0.795375

12	6	0	-0.356367	3.856134	-0.609021
13	15	0	1.395964	0.136143	0.212190
14	6	0	2.367000	-0.714647	-1.233884
15	6	0	3.871847	-0.944584	-1.011032
16	6	0	4.446035	-1.783342	-2.175685
17	6	0	4.186412	-1.104076	-3.535811
18	6	0	2.680636	-0.839014	-3.736310
19	6	0	2.109736	-0.002213	-2.572930
20	8	0	3.496692	2.245418	-0.385360
21	6	0	4.637478	3.079978	-0.566263
22	8	0	-1.665805	4.280727	-0.643387
23	6	0	-1.903516	5.663641	-0.899026
24	6	0	-1.339937	1.928515	2.332116
25	6	0	-1.222583	0.884588	3.461678
26	6	0	-1.494618	1.374257	-2.785496
27	6	0	-2.337006	2.453147	-3.504548
28	6	0	-5.072578	-0.710308	0.192131
29	6	0	-6.194357	0.196715	0.753712
30	46	0	-0.551905	-1.183861	0.616615
31	6	0	-1.876764	-3.140086	0.818161
32	9	0	-2.879083	-2.972460	-0.101522
33	6	0	-0.130429	-3.029415	-0.126788
34	6	0	0.932340	-3.755728	0.471035
35	6	0	1.825079	-4.484891	-0.324520
36	6	0	1.651665	-4.555549	-1.720297
37	6	0	0.558742	-3.899019	-2.310451
38	6	0	-0.338971	-3.160344	-1.523795
39	1	0	2.345565	-5.133934	-2.333370
40	9	0	-2.362404	-2.605857	2.017882
41	9	0	-1.813120	-4.476819	1.079145
42	6	0	2.639372	0.176674	1.684757
43	6	0	2.339878	1.313019	2.677437
44	6	0	3.339925	1.275328	3.852220
45	6	0	3.298726	-0.090382	4.567522
46	6	0	3.572378	-1.237755	3.574281
47	6	0	2.586449	-1.194355	2.388225
48	6	0	-2.156658	3.158116	2.792696
49	6	0	-1.434127	0.085459	-3.636359
50	6	0	-5.558597	-1.421846	-1.082383
51	1	0	2.661280	-5.006232	0.148712
52	1	0	0.397590	-3.962561	-3.389636
53	1	0	-1.194823	-2.666393	-1.981712
54	1	0	1.067439	-3.712461	1.551596
55	1	0	3.642132	0.337865	1.265190
56	1	0	1.877015	-1.698066	-1.271268
57	1	0	1.321341	1.187945	3.073557
58	1	0	2.380683	2.287447	2.168388
59	1	0	1.553718	-1.364033	2.743135
60	1	0	2.804752	-2.003523	1.673873
61	1	0	4.389496	0.026001	-0.960575
62	1	0	4.047016	-1.468679	-0.059108
63	1	0	2.593277	0.988618	-2.553886
64	1	0	1.033123	0.158232	-2.714756
65	1	0	2.890293	4.858662	-0.885726
66	1	0	4.360146	1.451495	3.463799
67	1	0	3.115922	2.089467	4.562408
68	1	0	3.504038	-2.213731	4.083830
69	1	0	4.604369	-1.143036	3.188755
70	1	0	5.527718	-1.942982	-2.024869
71	1	0	3.959924	-2.774224	-2.167462
72	1	0	2.144301	-1.803218	-3.772717
73	1	0	2.502033	-0.323732	-4.695749
74	1	0	0.610299	5.763973	-0.991819
75	1	0	4.637064	3.544683	-1.568524
76	1	0	5.507122	2.418514	-0.463617
77	1	0	4.676095	3.874200	0.200713
78	1	0	2.295919	-0.231153	5.010605
79	1	0	4.027924	-0.115194	5.394821
80	1	0	4.728471	-0.140411	-3.567557
81	1	0	4.581261	-1.726711	-4.356618
82	1	0	-0.323809	2.276444	2.098329
83	1	0	-3.544267	0.364600	2.128464
84	1	0	-3.712181	0.000058	-2.144827
85	1	0	-0.469069	1.760302	-2.689989
86	1	0	-1.446021	6.298797	-0.118910
87	1	0	-2.994073	5.783466	-0.884941
88	1	0	-1.506165	5.961405	-1.886279
89	1	0	-2.215053	3.904826	1.986320
90	1	0	-1.693102	3.622328	3.679831
91	1	0	-3.183921	2.855740	3.056549
92	1	0	-2.212144	0.545165	3.805845
93	1	0	-0.696320	1.321044	4.326928
94	1	0	-0.661994	0.000878	3.112842
95	1	0	-0.909298	-0.720545	-3.102458
96	1	0	-0.906867	0.283319	-4.584122
97	1	0	-2.445981	-0.273725	-3.884768
98	1	0	-3.373472	2.099308	-3.634469

99	1	0	-1.918749	2.669925	-4.502286
100	1	0	-2.362607	3.380710	-2.915100
101	1	0	-4.850083	-1.483639	0.946694
102	1	0	-5.858139	-0.688418	-1.850309
103	1	0	-6.436371	-2.045735	-0.851714
104	1	0	-4.772409	-2.064815	-1.503210
105	1	0	-5.882103	0.686233	1.689560
106	1	0	-7.104483	-0.392977	0.954184
107	1	0	-6.444413	0.984616	0.023499

a-F elimination TS for Brettphos and Xantphos:

$TS_{a\text{-}F}$-Brettphos

SCF Done: E(RB+HF-LYP) = -2218.54542804 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.045978	-1.205475	2.124244
2	6	0	2.779960	0.185710	1.515367
3	6	0	2.314973	1.149938	2.621388
4	6	0	3.377554	1.247543	3.731155
5	6	0	3.726729	-0.129634	4.314673
6	6	0	4.135250	-1.113286	3.208295
7	15	0	1.487190	0.075569	0.075904
8	46	0	-0.110676	-1.699147	0.923892
9	6	0	-0.123104	-2.855342	-0.752901
10	6	0	0.972448	-3.701688	-0.989137
11	6	0	0.978918	-4.583015	-2.076976
12	6	0	-0.118277	-4.644722	-2.938002
13	6	0	-1.222608	-3.825780	-2.696570
14	6	0	-1.228326	-2.944560	-1.608365
15	6	0	0.981297	1.891814	-0.284825
16	6	0	-0.354802	2.345202	-0.362954
17	6	0	-0.594691	3.717122	-0.656908
18	6	0	0.452045	4.612096	-0.837597
19	6	0	1.768542	4.164526	-0.753518
20	6	0	2.033126	2.824924	-0.493521
21	6	0	-1.587974	1.495445	-0.167314
22	6	0	-2.187617	1.397026	1.114354
23	6	0	-3.368948	0.655994	1.244620
24	6	0	-3.997140	0.041695	0.160648
25	6	0	-3.420439	0.205719	-1.101787
26	6	0	-2.241191	0.934906	-1.294367
27	6	0	-5.284965	-0.748578	0.359343
28	6	0	-5.079407	-2.252820	0.096523
29	6	0	-1.669132	2.168302	2.332575
30	6	0	-2.439129	3.499137	2.488752
31	6	0	-1.781643	1.205751	-2.730642
32	6	0	-1.649544	-0.057954	-3.598443
33	8	0	3.313664	2.338917	-0.436183
34	6	0	4.397054	3.247789	-0.545119
35	8	0	-1.911371	4.088285	-0.751943
36	6	0	-2.212246	5.448006	-1.019007
37	6	0	2.457083	-0.530470	-1.505375
38	6	0	3.983968	-0.663453	-1.366026
39	6	0	4.573685	-1.356532	-2.609910
40	6	0	4.207422	-0.613826	-3.902522
41	6	0	2.687745	-0.433686	-4.023046
42	6	0	2.098034	0.254056	-2.778344
43	6	0	-1.736095	1.378544	3.652005
44	6	0	-2.734469	2.207946	-3.418687
45	6	0	-6.446566	-0.194520	-0.486821
46	6	0	-1.108191	-3.011867	1.915910
47	9	0	-2.203489	-2.770421	2.567867
48	9	0	0.009975	-0.965985	2.876712
49	9	0	-0.681946	-4.178744	2.300546
50	1	0	-0.116889	-5.331195	-3.780850
51	1	0	1.840837	-5.225779	-2.243149
52	1	0	-2.088333	-3.871633	-3.353947
53	1	0	-2.099294	-2.320943	-1.432818
54	1	0	1.833699	-3.682138	-0.324098
55	1	0	3.698348	0.567615	1.063658
56	1	0	2.049324	-1.539065	-1.623485
57	1	0	1.375318	0.760855	3.028289
58	1	0	2.121274	2.147450	2.211579
59	1	0	2.115669	-1.560022	2.579755
60	1	0	3.344418	-1.931134	1.356491
61	1	0	4.433525	0.329031	-1.254978
62	1	0	4.251040	-1.238616	-0.473378
63	1	0	2.490906	1.275540	-2.706478
64	1	0	1.013094	0.336201	-2.886086
65	1	0	2.574485	4.872182	-0.903529
66	1	0	4.289540	1.710142	3.322489
67	1	0	3.018315	1.915519	4.524893
68	1	0	4.317554	-2.109235	3.632709
69	1	0	5.083935	-0.786225	2.755346

70	1	0	5.664218	-1.432110	-2.507046
71	1	0	4.191282	-2.386226	-2.663310
72	1	0	2.212664	-1.417060	-4.149150
73	1	0	2.441709	0.151249	-4.918936
74	1	0	0.265158	5.657703	-1.050206
75	1	0	4.415798	3.739765	-1.526461
76	1	0	5.301563	2.648318	-0.427190
77	1	0	4.361433	4.010935	0.242707
78	1	0	2.848485	-0.529765	4.839758
79	1	0	4.528485	-0.036200	5.059171
80	1	0	4.691164	0.374629	-3.901361
81	1	0	4.598895	-1.152236	-4.775295
82	1	0	-0.616589	2.412977	2.153398
83	1	0	-3.826639	0.570855	2.226141
84	1	0	-3.916887	-0.219940	-1.970437
85	1	0	-0.793741	1.675505	-2.686632
86	1	0	-1.830799	6.109104	-0.229377
87	1	0	-3.301492	5.510517	-1.045059
88	1	0	-1.807284	5.769922	-1.987863
89	1	0	-2.400892	4.103543	1.579917
90	1	0	-2.021285	4.082983	3.318506
91	1	0	-3.494601	3.303925	2.716520
92	1	0	-2.772434	1.217689	3.975736
93	1	0	-1.244964	1.956459	4.445449
94	1	0	-1.230306	0.415205	3.553250
95	1	0	-0.977818	-0.796127	-3.153606
96	1	0	-1.261252	0.208292	-4.589404
97	1	0	-2.619262	-0.546336	-3.752917
98	1	0	-3.735301	1.775045	-3.536644
99	1	0	-2.362527	2.467121	-4.418077
100	1	0	-2.831865	3.124319	-2.832002
101	1	0	-5.568033	-0.638195	1.415156
102	1	0	-4.792572	-2.438660	-0.945619
103	1	0	-6.002230	-2.812185	0.293728
104	1	0	-4.290388	-2.658723	0.738739
105	1	0	-6.616369	0.867571	-0.278396
106	1	0	-7.374482	-0.738136	-0.271407
107	1	0	-6.245422	-0.296233	-1.559917

$TS_{a\text{-}F}$-Xantphos

SCF Done: E(RB+HF-LYP) = -2289.56079001 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.488519	-2.804203	-0.201842
2	6	0	2.104460	-2.603270	-0.131710
3	6	0	1.348337	-3.451985	0.692800
4	6	0	1.964414	-4.451072	1.454502
5	6	0	3.347525	-4.630141	1.390921
6	6	0	4.104727	-3.806575	0.556797
7	46	0	1.085380	-1.217240	-1.225022
8	6	0	0.558784	-2.453713	-2.615212
9	9	0	0.926686	-2.343144	-3.853777
10	15	0	-2.120123	-0.734359	0.240509
11	6	0	-2.871439	0.948027	-0.193620
12	6	0	-2.064650	2.091247	-0.257693
13	6	0	-2.564079	3.347454	-0.636523
14	6	0	-3.918476	3.432412	-0.972818
15	6	0	-4.747718	2.313298	-0.917712
16	6	0	-4.224538	1.083399	-0.527716
17	6	0	-1.635763	4.563559	-0.572639
18	6	0	-0.211098	4.095367	-0.881467
19	6	0	0.176608	2.814270	-0.463583
20	8	0	-0.733612	1.946448	0.086608
21	6	0	1.508158	2.376212	-0.533768
22	6	0	2.459891	3.234045	-1.092767
23	6	0	2.087488	4.488537	-1.572660
24	6	0	0.765897	4.913533	-1.458170
25	6	0	-2.090276	5.685998	-1.524117
26	6	0	-1.653209	5.110420	0.885137
27	15	0	1.961797	0.673383	0.127073
28	6	0	1.613115	0.823819	1.963665
29	6	0	1.223143	-0.310739	2.683394
30	6	0	0.956961	-0.213470	4.051117
31	6	0	1.079879	1.012511	4.705585
32	6	0	1.470872	2.146860	3.989997
33	6	0	1.734723	2.055130	2.622761
34	6	0	-3.207378	-1.806572	-0.882305
35	6	0	-2.939118	-1.726097	-2.259011
36	6	0	-3.687803	-2.482763	-3.160780
37	6	0	-4.696420	-3.335900	-2.703311
38	6	0	-4.954740	-3.427220	-1.335417
39	6	0	-4.216667	-2.661905	-0.426398
40	6	0	-2.852237	-1.064470	1.954550
41	6	0	-2.461922	-2.251862	2.595692

42	6	0	-2.909705	-2.554896	3.881750
43	6	0	-3.742348	-1.661715	4.560642
44	6	0	-4.124285	-0.471928	3.940178
45	6	0	-3.687308	-0.177274	2.645563
46	6	0	3.838689	0.683812	-0.007406
47	6	0	4.677149	0.871348	1.095639
48	6	0	6.065586	0.847274	0.935107
49	6	0	6.625348	0.644456	-0.326358
50	6	0	5.792031	0.456647	-1.432480
51	6	0	4.406196	0.466930	-1.272524
52	9	0	-0.194621	-0.167135	-2.507799
53	9	0	-0.379745	-3.349297	-2.568929
54	1	0	2.832847	5.141535	-2.017258
55	1	0	3.828085	-5.408103	1.978766
56	1	0	0.499797	5.904379	-1.809381
57	1	0	4.103461	-2.178709	-0.841367
58	1	0	5.182391	-3.940692	0.491234
59	1	0	1.358931	-5.092985	2.091011
60	1	0	0.267845	-3.336908	0.745018
61	1	0	3.495439	2.922307	-1.157878
62	1	0	-4.865306	0.207949	-0.501662
63	1	0	-5.797992	2.401189	-1.181178
64	1	0	-4.339925	4.384655	-1.275709
65	1	0	4.253495	1.030184	2.081749
66	1	0	6.707621	0.987915	1.800597
67	1	0	7.705019	0.628075	-0.448396
68	1	0	6.219456	0.292509	-2.418025
69	1	0	3.760942	0.300281	-2.132143
70	1	0	1.125083	-1.265345	2.178597
71	1	0	0.641255	-1.096898	4.598672
72	1	0	0.867094	1.086603	5.768750
73	1	0	1.566482	3.105065	4.493994
74	1	0	2.029124	2.941604	2.068464
75	1	0	-1.800656	-2.947438	2.083640
76	1	0	-2.603418	-3.484398	4.355254
77	1	0	-4.086792	-1.890720	5.565754
78	1	0	-4.769742	0.230920	4.461316
79	1	0	-3.999315	0.749756	2.175612
80	1	0	-4.434987	-2.733068	0.634889
81	1	0	-5.737114	-4.088424	-0.970475
82	1	0	-5.274591	-3.927373	-3.408827
83	1	0	-3.478769	-2.409729	-4.225486
84	1	0	-2.131618	-1.081940	-2.604625
85	1	0	-3.094528	6.033551	-1.265324
86	1	0	-1.434379	6.557671	-1.441165
87	1	0	-2.096837	5.353639	-2.567417
88	1	0	-2.665931	5.427588	1.159880
89	1	0	-1.331283	4.344324	1.597830
90	1	0	-0.979678	5.970538	0.979504

$PMe_2CH_2CH_2PMe_2$-CP

SCF Done: E(RB3LYP) = -947.304890997 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.071998	0.579173	-1.110725
2	6	0	2.686200	0.386035	-1.147925
3	6	0	1.988293	-0.096561	-0.028719
4	6	0	2.727969	-0.395994	1.125804
5	6	0	4.112408	-0.195901	1.169606
6	6	0	4.790524	0.294317	0.051988
7	46	0	-0.051296	-0.265305	-0.040996
8	6	0	0.199068	-2.296135	-0.088320
9	9	0	0.989798	-2.772769	-1.084923
10	15	0	-2.535319	-0.326603	0.015080
11	6	0	-3.134865	1.447195	0.392131
12	6	0	-2.245762	2.508455	-0.272586
13	15	0	-0.390272	2.185679	0.049687
14	9	0	0.701667	-2.812408	1.072655
15	9	0	-1.011403	-2.968460	-0.265255
16	1	0	2.227427	-0.809594	1.997282
17	1	0	4.662669	-0.435587	2.077541
18	1	0	5.867091	0.444187	0.083588
19	1	0	4.589577	0.948020	-1.994441
20	1	0	2.151778	0.609592	-2.069408
21	1	0	-4.179620	1.569631	0.082381
22	1	0	-3.106550	1.555142	1.483079
23	1	0	-2.518867	3.514175	0.068614
24	1	0	-2.375039	2.488000	-1.361416
25	6	0	-0.079271	3.000347	1.718290
26	6	0	0.468044	3.356397	-1.144323
27	6	0	-3.409328	-0.776168	-1.589928
28	6	0	-3.442822	-1.372375	1.285321
29	1	0	0.187514	4.397583	-0.955416
30	1	0	1.547987	3.234816	-1.027099

31	1	0	0.201152	3.084496	-2.169313
32	1	0	-0.350591	4.061188	1.701113
33	1	0	-0.659064	2.485497	2.488970
34	1	0	0.981391	2.894477	1.961507
35	1	0	-4.528456	-1.259654	1.201081
36	1	0	-3.158980	-2.413735	1.118554
37	1	0	-3.118795	-1.081597	2.288316
38	1	0	-4.497880	-0.720021	-1.485410
39	1	0	-3.081180	-0.103989	-2.387451
40	1	0	-3.113387	-1.794730	-1.853746

$PMe_2CH_2CH_2PMe_2$-TS
SCF Done: E(RB3LYP) = -947.253956465 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.606419	0.165974	1.224135
2	6	0	-2.004629	-0.124102	-0.015077
3	6	0	-2.633227	0.323019	-1.194836
4	6	0	-3.772594	1.122998	-1.125579
5	6	0	-4.332307	1.456668	0.112840
6	6	0	-3.748214	0.966770	1.283850
7	46	0	0.058242	-0.238835	-0.026675
8	15	0	2.482822	-0.960931	0.036913
9	6	0	3.469571	0.635486	-0.343205
10	6	0	2.876703	1.867873	0.351683
11	15	0	1.011286	2.086009	-0.024115
12	6	0	-1.434559	-1.999946	-0.071128
13	9	0	-0.705638	-2.658715	-1.034143
14	9	0	-1.093577	-2.523169	1.142884
15	9	0	-2.699653	-2.451686	-0.294062
16	1	0	-2.221112	0.049649	-2.162718
17	1	0	-4.232723	1.481567	-2.043883
18	1	0	-5.228538	2.069432	0.161659
19	1	0	-4.189227	1.200019	2.250566
20	1	0	-2.176965	-0.236452	2.137441
21	1	0	4.519876	0.498598	-0.056644
22	1	0	3.444109	0.762199	-1.432486
23	1	0	3.421314	2.774819	0.060224
24	1	0	2.966041	1.773023	1.440889
25	6	0	1.072498	3.059190	-1.646530
26	6	0	0.555478	3.455046	1.196988
27	6	0	3.238015	-1.477045	1.693002
28	6	0	3.318473	-2.184378	-1.136396
29	1	0	4.408510	-2.172912	-1.026137
30	1	0	2.943162	-3.189351	-0.924405
31	1	0	3.053066	-1.930815	-2.166483
32	1	0	4.329681	-1.550454	1.633299
33	1	0	2.963418	-0.746775	2.459217
34	1	0	2.823946	-2.446291	1.984485
35	1	0	1.669641	3.972495	-1.545253
36	1	0	1.501663	2.429112	-2.430681
37	1	0	0.052886	3.322929	-1.941016
38	1	0	1.225772	4.317413	1.109257
39	1	0	-0.472825	3.772623	1.003133
40	1	0	0.604595	3.056229	2.214031

$P(CF_3)_2CH_2CH_2P(CF_3)_2$-CP
SCF Done: E(RB3LYP) = -2138.08894094 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.155185	2.042515	-1.176672
2	6	0	-2.846105	1.548654	-1.175775
3	6	0	-2.031116	1.699648	-0.045913
4	6	0	-2.540452	2.362417	1.076512
5	6	0	-3.853548	2.846214	1.076641
6	6	0	-4.663618	2.689261	-0.049027
7	46	0	-0.173733	0.867721	-0.028356
8	6	0	0.547111	2.779510	-0.057757
9	9	0	0.100975	3.568886	-1.059928
10	15	0	2.056527	-0.307260	0.025428
11	6	0	1.748464	-2.145214	0.411928
12	6	0	0.482154	-2.662973	-0.282622
13	15	0	-0.995055	-1.498622	0.016571
14	9	0	0.331131	3.456275	1.101780
15	9	0	1.920756	2.746833	-0.205065
16	1	0	-1.915084	2.521040	1.949563
17	1	0	-4.236944	3.356637	1.957339
18	1	0	-5.681061	3.071941	-0.049611
19	1	0	-4.774805	1.920408	-2.062359
20	1	0	-2.472345	1.045110	-2.064195
21	1	0	2.621092	-2.734853	0.118546

22	1	0	1.646156	-2.211713	1.499888
23	1	0	0.231303	-3.670117	0.061781
24	1	0	0.622573	-2.702106	-1.367640
25	6	0	-1.690660	-2.234026	1.654874
26	6	0	-2.274156	-2.213376	-1.232399
27	6	0	3.084862	-0.465446	-1.596066
28	6	0	3.472634	0.069989	1.275598
29	9	0	-2.253799	-3.558864	-1.261272
30	9	0	-3.509763	-1.813030	-0.922078
31	9	0	-1.963466	-1.769380	-2.462538
32	9	0	-1.954055	-3.550518	1.550485
33	9	0	-0.755739	-2.077985	2.615951
34	9	0	-2.805475	-1.607751	2.031312
35	9	0	4.348593	-0.951616	1.350924
36	9	0	4.137811	1.172102	0.928073
37	9	0	2.935151	0.240846	2.493873
38	9	0	4.129620	-1.304744	-1.457540
39	9	0	2.278095	-0.972188	-2.553448
40	9	0	3.543103	0.718210	-1.999959

$P(CF_3)_2CH_2CH_2P(CF_3)_2$-TS
SCF Done: E(RB3LYP) = -2138.05310714 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.458453	-2.204784	1.210815
2	6	0	-1.906624	-1.990239	-0.059850
3	6	0	-2.738653	-1.971753	-1.190733
4	6	0	-4.120164	-2.082813	-1.034476
5	6	0	-4.677510	-2.249323	0.237727
6	6	0	-3.844251	-2.315250	1.355768
7	46	0	-0.218843	-0.787641	-0.108217
8	15	0	2.085548	0.156961	0.001884
9	6	0	1.932230	2.051495	-0.167178
10	6	0	0.681321	2.588752	0.536516
11	15	0	-0.885334	1.618515	0.037187
12	6	0	-0.204201	-3.060838	-0.267294
13	9	0	0.823843	-3.031908	-1.180257
14	9	0	0.332204	-3.354365	0.946094
15	9	0	-0.904632	-4.160201	-0.635347
16	1	0	-2.310731	-1.864405	-2.183515
17	1	0	-4.763445	-2.046024	-1.910202
18	1	0	-5.753625	-2.345972	0.352636
19	1	0	-4.269398	-2.463652	2.345339
20	1	0	-1.811169	-2.286664	2.078867
21	1	0	2.833767	2.527129	0.228326
22	1	0	1.888676	2.249795	-1.242981
23	1	0	0.541045	3.650598	0.316439
24	1	0	0.766984	2.474300	1.621767
25	6	0	-1.345151	2.569220	-1.579300
26	6	0	-2.147832	2.446376	1.239709
27	6	0	3.001501	0.058224	1.696735
28	6	0	3.592174	-0.126275	-1.169976
29	9	0	4.572237	0.779956	-0.985301
30	9	0	4.109806	-1.346438	-0.986933
31	9	0	3.169442	-0.017082	-2.441984
32	9	0	4.093412	0.845603	1.755381
33	9	0	2.152314	0.470124	2.663195
34	9	0	3.377261	-1.196559	1.964569
35	9	0	-1.318143	3.908986	-1.440740
36	9	0	-0.446598	2.243617	-2.533414
37	9	0	-2.565208	2.219036	-2.004980
38	9	0	-2.084872	3.792098	1.229906
39	9	0	-3.398253	2.083925	0.929182
40	9	0	-1.873354	2.032927	2.491124

$TS_{a\text{-}F}$-$P(CF_3)_2CH_2CH_2P(CF_3)_2$
SCF Done: E(RB3LYP) = -2138.03456472 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.769725	-0.698228	1.376905
2	6	0	-5.611892	-0.455444	0.011047
3	6	0	-4.421065	0.095863	-0.474298
4	6	0	-3.377287	0.404360	0.405530
5	6	0	-3.538779	0.162897	1.774615
6	6	0	-4.731532	-0.388137	2.256804
7	46	0	-1.649330	1.204843	-0.297386
8	9	0	0.030960	2.181172	-1.003732
9	6	0	-2.162214	3.077400	-0.320704
10	9	0	-2.532652	3.726820	-1.376692
11	15	0	-0.568195	-0.975895	-0.399618
12	6	0	-1.289671	-2.347164	-1.540329

13	9	0	-1.186026	-1.935228	-2.816235
14	9	0	-1.844877	3.943142	0.586587
15	6	0	1.232090	-0.917788	-0.973746
16	6	0	-0.452976	-1.953885	1.257584
17	9	0	-1.616047	-2.556093	1.530368
18	9	0	0.512406	-2.887784	1.221312
19	9	0	-0.164172	-1.097917	2.253526
20	9	0	-0.602510	-3.497420	-1.414056
21	9	0	-2.573592	-2.586926	-1.266718
22	1	0	-2.739595	0.395598	2.474338
23	1	0	-4.844693	-0.573468	3.322393
24	1	0	-6.695888	-1.124842	1.752774
25	1	0	-6.415488	-0.692342	-0.682336
26	1	0	-4.316690	0.281907	-1.540617
27	6	0	2.009796	0.131307	-0.174347
28	1	0	1.649286	-1.924462	-0.887514
29	1	0	1.186029	-0.644863	-2.032774
30	15	0	3.778250	0.341731	-0.855143
31	1	0	1.509403	1.101272	-0.301460
32	1	0	2.063858	-0.122231	0.887722
33	6	0	4.346226	1.704655	0.396879
34	6	0	4.605219	-1.151199	0.057298
35	9	0	5.940283	-1.106507	-0.066733
36	9	0	4.315485	-1.232621	1.371079
37	9	0	4.168775	-2.296452	-0.519766
38	9	0	5.688993	1.772445	0.428403
39	9	0	3.869421	2.894587	-0.008247
40	9	0	3.914998	1.501591	1.657480
