Highly Active Catalysts of Bisphosphine Oxides for Asymmetric Heck Reaction

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Supporting information: DFT calculation

Computational Details

DFT calculations were carried out with the Gaussian 09 package [1]. Both olefin-catalyst complexes and transition structures are fully optimized by B3LYP [2] method using general basis set. The details of basis set are 6-31G+(d,p) [3] for H, C, O, F, and P, and LANL2DZ [4] with one f function for Pd. The LANL2 ECP is used for Pd. Harmonic frequency calculations are carried out to validate whether an optimized geometry is local minimum or transition state. All the geometries of the intermediates and transition states are also optimized in the dioxane solution using the PCM model [5].

References

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[2] (a) Backe, A. D. J. Chem. Phys., 98 (1993) 5648-52. (b) Lee, C., Yang, W. and Parr, R. G., Phys. Rev. B, 37 (1988) 785-89.

[3] (a) Hehre, W. J., Ditchfield, R., and Pople, J. A., J. Chem. Phys., 56 (1972) 2257. (b) Hariharan, P. C. and Pople, J. A., Theor. Chem. Acc., 28 (1973) 213-22. (c) Frisch, M. J., Pople, J. A., and Binkley, J. S., J. Chem. Phys., 80 (1984) 3265-69.
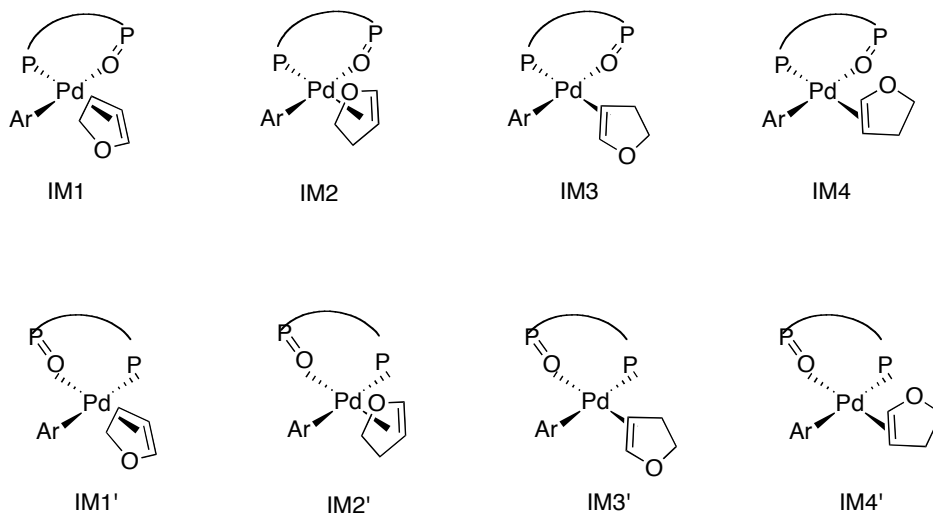
[4] Wadt, W. R. and Hay, P. J., J. Chem. Phys., 82 (1985) 284-98.

[5] Tomasi J., Mennucci B., and Cammi R., "Quantum mechanical continuum solvation models," Chem. Rev., 105 (2005) 2999-3093.
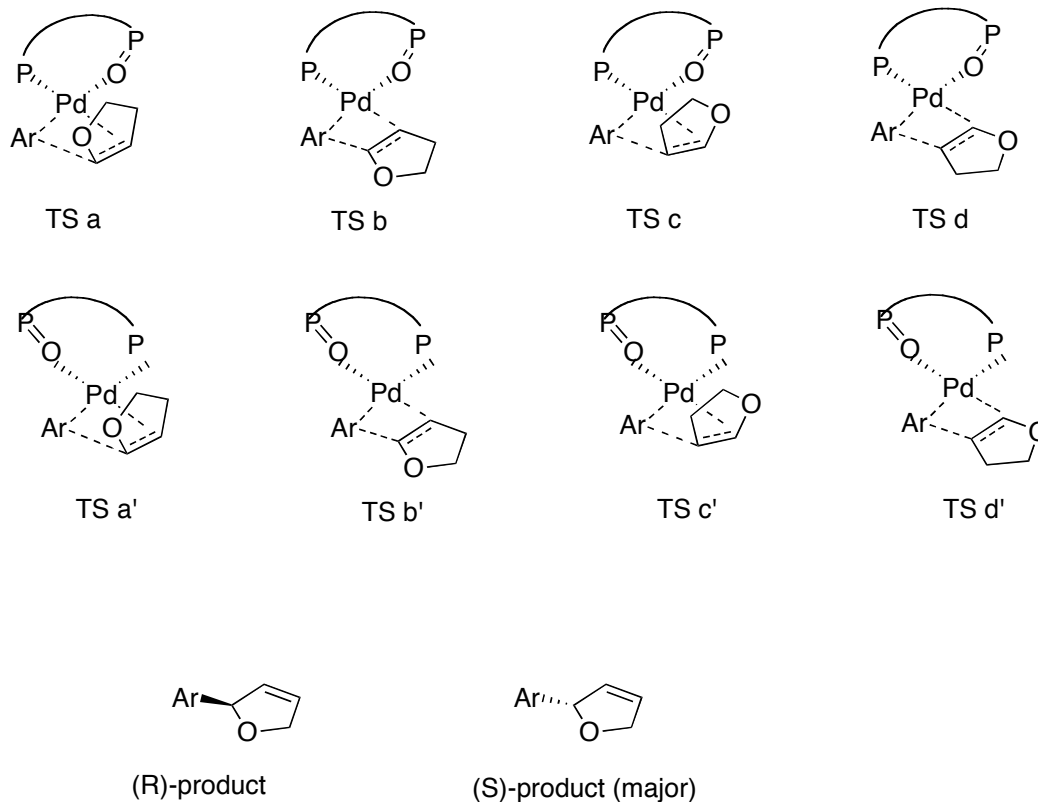
Computational Results and Discussions

Assuming the formation of olefin-complex was fast and reversible, our calculation indicated that IM1 and IM2 were two most stable species among oelfin complexes. Others were much high in energy. During olefin insertion, the barrier from IM1 to TSa was 2-3 kcal/mol higher than that from IM2 to TS2, both in gas phase and in dioxane solution. The calculation results showed that, among various pathways, the one from IM2 to TS2 was the most favorable to form the major enantiomer of the Heck product.

Table S1 Energy of cationic complexes of [(R)-Xyl-SDP(O)]Pd(p-CF$_3$C$_6$H$_4$)(2,3-dihydrofuran) in the gas phase and dioxane solution

Olefin Complexes	Energy+ZPE in gas phase (a.u.)	Relative Energy to IM1 in gas phase (kcal/mol)	Energy+ZPE in dioxane (a.u.)	Relative Energy to IM1 in dioxane (kcal/mol)
IM1	-2910.2657	0.0	-2910.2932	0.0
IM2	-2910.2647	0.6	-2910.2922	0.6
IM3	-2910.2611	2.9	-2910.2883	3.1
IM4	-2910.2595	3.9	-2910.2867	4.1
IM1'	-2910.2514	9.0	-2910.2790	8.9
IM2'	-2910.2536	7.6	-2910.2813	7.5
IM3'	-2910.2446	13.2	-2910.2721	13.2
IM4'	-2910.2479	11.2	-2910.2752	11.3

Table S2 Energy of olefin-insertion transition states of cationic complexes of [(R)-Xyl-SDP(O)]Pd(p-CF$_3$C$_6$H$_4$)(2,3-dihydrofuran) in the gas phase and dioxane solution

TS a   TS b   TS c   TS d

TS a'   TS b'   TS c'   TS d'

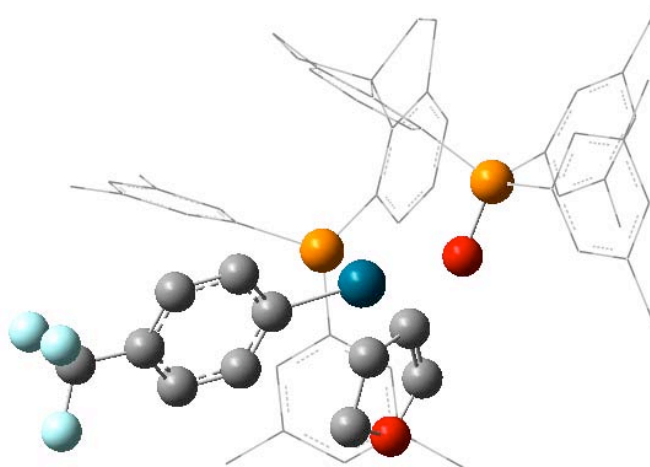(R)-product   (S)-product (major)

TSs	Energy+ZPE in gas phase (a.u.)	Relative Energy to IM1 in gas phase (kcal/mol)	Energy+ZPE in dioxane (a.u.)	Relative Energy to IM1 in dioxane solution (kcal/mol)	Product configuration
TS a	-2910.2308	21.3	-2910.2586	21.7	(R)
TS b	-2910.2354	18.4	-2910.2628	19.1	(S)
TS c	-2910.2305	22.1	-2910.2582	22.0	(S)
TS d	-2910.2312	21.7	-2910.2588	21.6	(R)
TS a'	-2910.2327	20.5	-2910.2607	20.4	(S)
TS b'	-2910.2352	18.5	-2910.2626	19.2	(R)
TS c'	-2910.2326	20.8	-2910.2604	20.6	(R)
TS d'	-2910.2302	22.3	-2910.2582	22.0	(S)

Cartesian coordinates for the optimal geometries in the gas phase.

IM1


```
Pd -0.537273  1.166819  0.399580
C    4.743043 -2.741160  3.277626
C    5.915905 -2.405336  1.051968
C    4.837180 -2.125575  1.899950
C    1.628521 -4.343495  1.480115
C    2.436659 -4.560547  0.363644
C    7.229116 -2.131946 -1.101387
C   -4.491095 -2.459382  4.395659
C    6.035475 -1.823100 -0.224622
C    3.837547 -1.243599  1.447116
C    0.671687 -3.324675  1.458908
C   -3.161100 -1.867462  3.983371
C   -2.293045 -1.312926  4.931927
C    2.281490 -3.738619 -0.750785
C   -3.704009 -5.754251 -0.765445
C    3.032258 -3.876720 -2.056476
C    5.034598 -0.939833 -0.648690
C   -2.762264 -1.885691  2.631385
C   -1.041983 -0.779835  4.569226
C   -0.131578 -0.178710  5.617792
C    3.936858 -0.664628  0.181524
C    0.486021 -2.494272  0.334103
C    1.329914 -2.690568 -0.785470
C   -1.523113 -1.364630  2.247691
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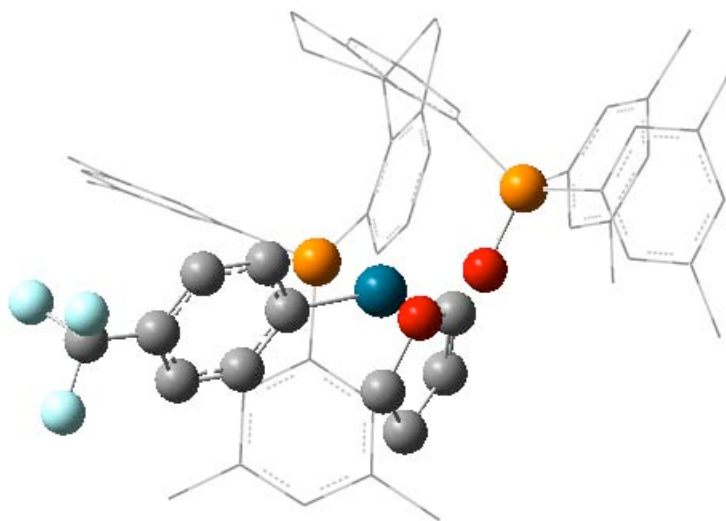
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C    2.693191  -2.572464  -2.802750
C   -4.353169  -3.564331  -1.867690
C   -2.343811  -2.179693  -0.512254
C    1.321355  -2.083022  -2.203455
C    4.500705   5.032153   2.206074
C    3.711068   3.021610   0.873641
C    3.739142   2.223937  -0.274883
C    4.543441   4.150846   0.977614
C    4.605572   2.537266  -1.332804
C    5.401051   4.447390  -0.091188
C    5.447616   3.656231  -1.252964
C   -4.206838  -2.189610  -2.088583
C   -3.185549  -1.503552  -1.400278
C    6.389263   4.005654  -2.383750
C    0.139201  -2.705969  -3.033936
C    1.190036  -0.577666  -2.498124
C    1.825855   0.554679  -1.938592
C   -5.123191  -1.446522  -3.036268
C   -0.127097  -1.720936  -4.190745
C    0.407295  -0.406797  -3.665317
C    1.628667   1.814236  -2.547836
C   -2.445053   1.581262  -0.023498
C   -3.477136   1.410578   0.914812
C   -2.756189   2.088856  -1.300320
C    0.843787   1.962305  -3.693203
C    0.227457   0.843417  -4.257617
C   -4.800662   1.718317   0.576673
C   -4.077227   2.400953  -1.639251
C   -5.100959   2.210989  -0.700248
C   -6.517948   2.438768  -1.096094
H    5.554229  -3.453493   3.453397
H    3.792401  -3.270813   3.408759
H    4.799029  -1.974205   4.060149
H    6.692560  -3.084359   1.394082
H    1.723906  -4.970745   2.360552
H    3.171280  -5.359627   0.357237
H   -4.838868  -2.039300   5.344335
H    7.314116  -3.207476  -1.298091
H    8.164412  -1.818603  -0.621878
H   -4.416806  -3.547159   4.527268
H    0.046838  -3.187278   2.331239
H   -4.676864  -5.967552  -0.305157
H   -2.594588  -1.291037   5.976044
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H    2.683106 -4.761010 -2.607701
H    0.838873  0.098233  5.193820
H   -3.432347 -2.308096  1.891071
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P    2.703789  0.660457 -0.271087
F   -7.097937  1.292686 -1.665882
F   -6.648352  3.444365 -2.049382
F   -7.325564  2.778528 -0.016504
C   -0.212030  2.990206  2.054132
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IM2


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Pd -0.547212   1.127561   0.561590
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C   7.232070  -2.096328  -1.111104
C  -4.523378  -2.812464   4.226159
C   6.031997  -1.817644  -0.233008
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C  -3.718225  -5.664466  -1.155785
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C   -2.771670  -2.111507   2.527651
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H    2.719234  -4.654610  -2.773503
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H   -0.391776   1.127079  -5.078246
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F   -7.066394   1.392170  -1.608517
F   -6.642330   3.579254  -1.743726
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C   -0.253791   3.045772   1.859638
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C    0.075399   3.604420   0.646076
H    0.968482   3.489010   0.053593
C   -1.886196   4.711482   1.244934
H   -2.813281   4.403363   0.765231
H   -1.918022   5.773356   1.488365
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H   -2.273093   3.124978   2.719268
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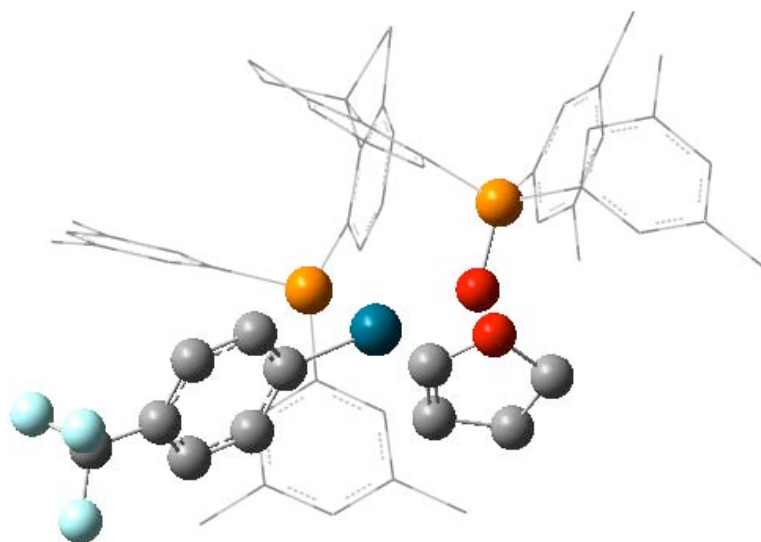
IM3


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C   -4.487122   2.322294   1.906446
C   -1.350294   4.404691   1.313482
C   -2.149910   4.623706   0.190617
C   -6.991016   2.437866  -0.999888
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C    4.710726   2.704827   4.126999
C   -5.780495   2.072975  -0.168770
C   -3.555001   1.384359   1.422844
C   -0.446279   3.338409   1.329732
C    3.392576   2.039548   3.796736
C    2.590895   1.495414   4.813165
C   -2.030129   3.763717  -0.898855
C    4.064473   5.302534  -1.296580
C   -2.788332   3.874640  -2.204263
C   -4.850410   1.128425  -0.620176
C    2.938856   1.965853   2.468009
C    1.355436   0.889769   4.535838
C    0.502745   0.304192   5.640180
C   -3.735520   0.802133   0.167948
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IM4

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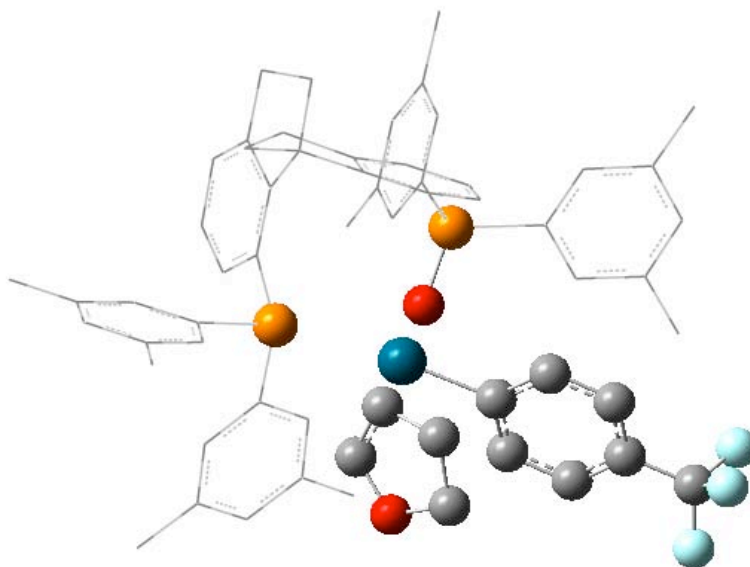
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IM1'


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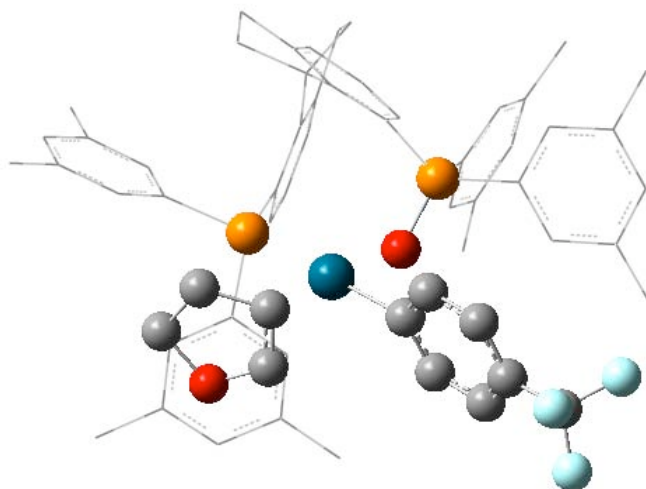
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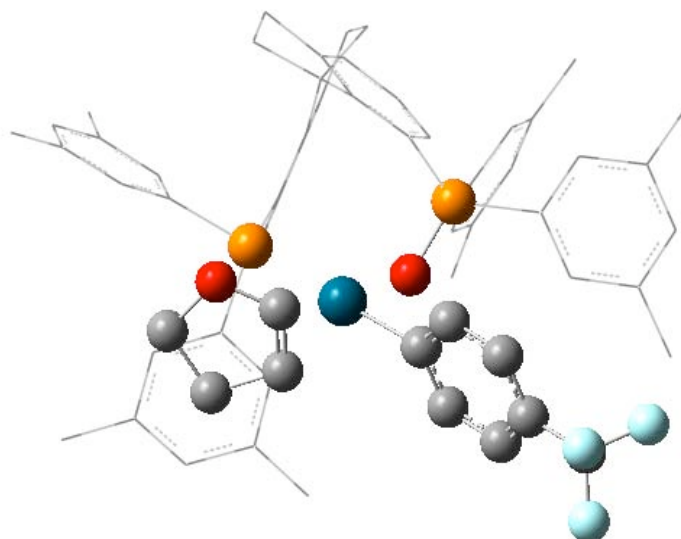
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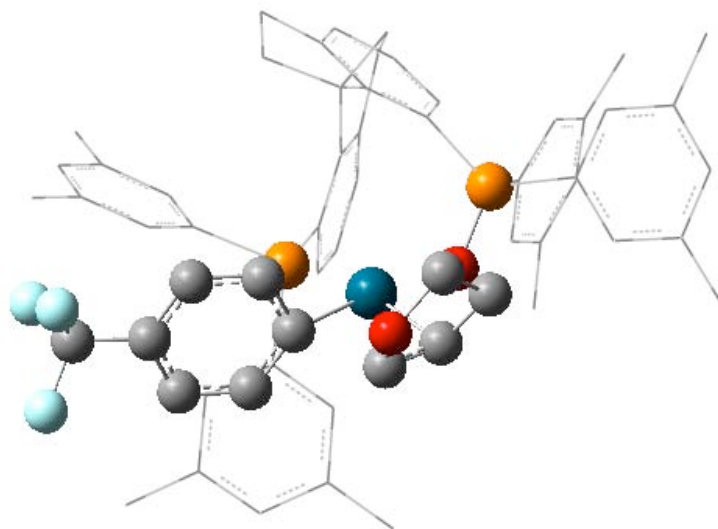
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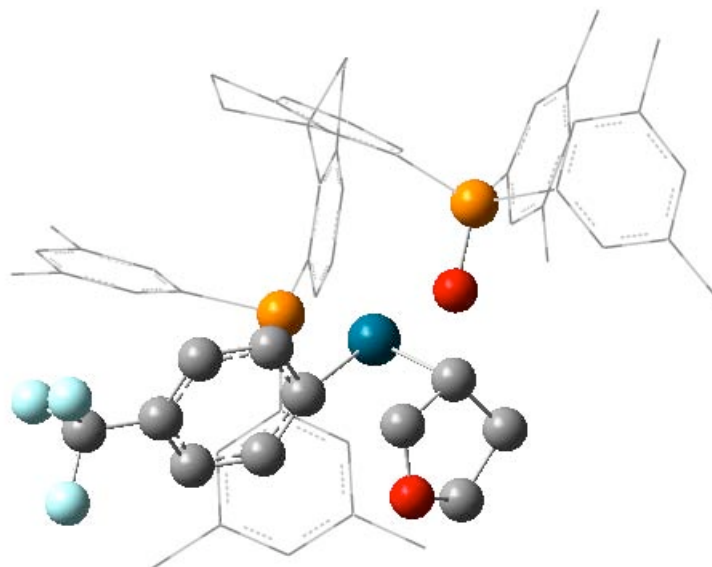
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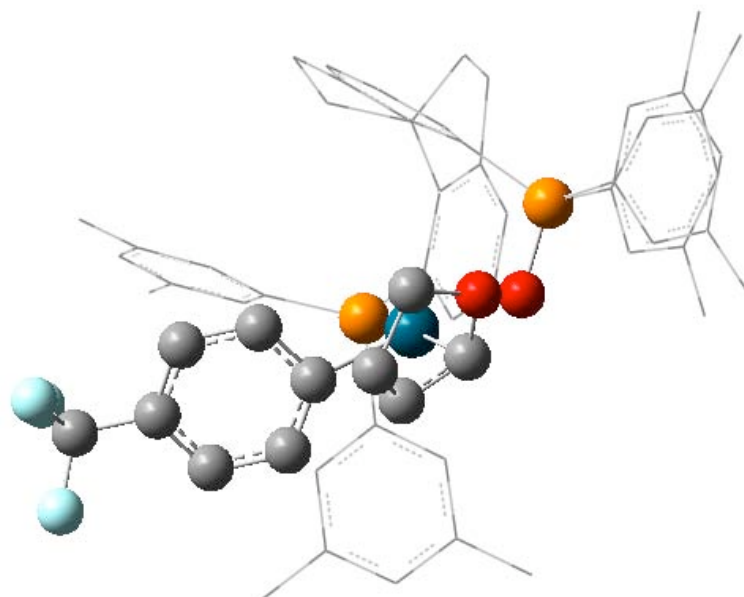
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TS c


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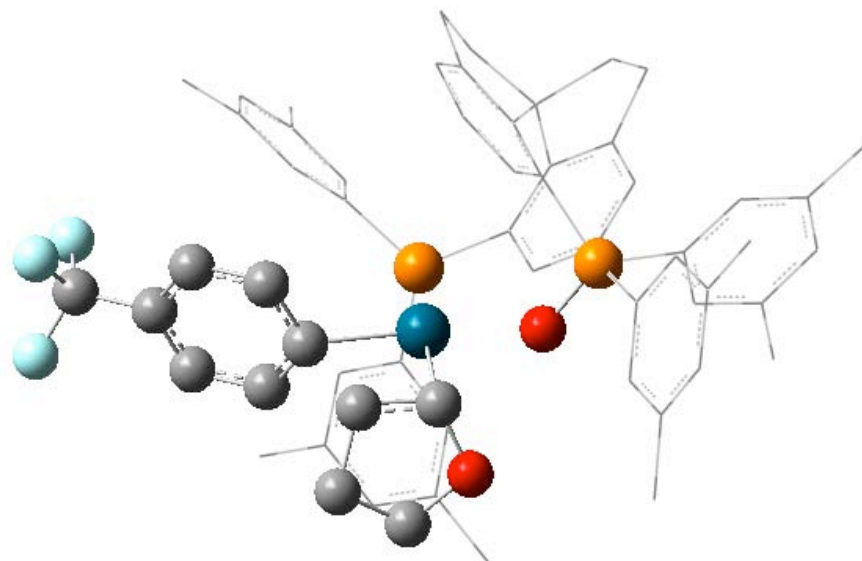
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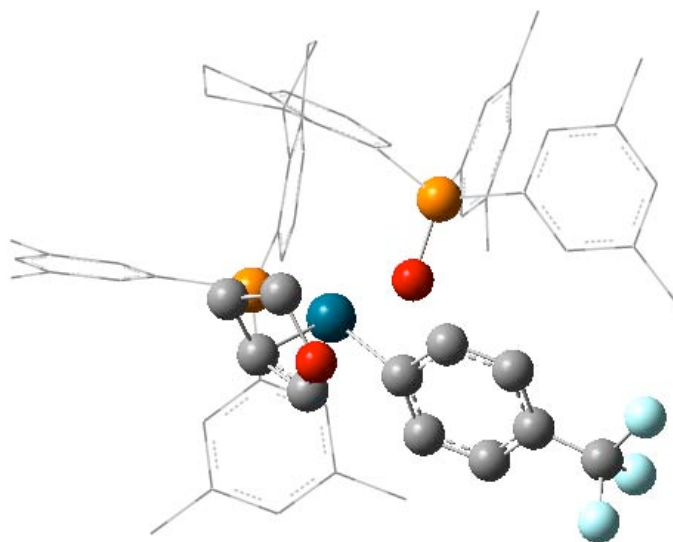
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C  -5.020107   1.323728  -0.367486
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C   -0.767522   2.680179   2.243170
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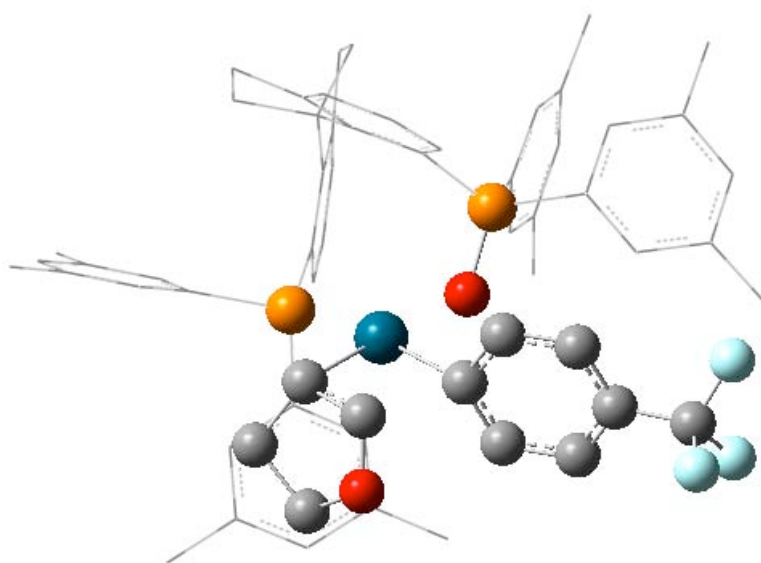
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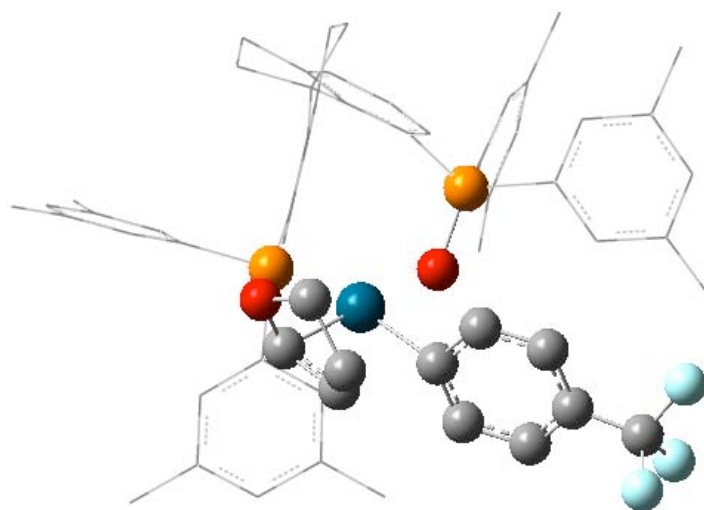
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H   3.019354  -1.478714  -2.469196
H  -6.461916   2.845871  -3.189176
H   4.188049  -1.879332  -4.557615
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H   5.538665  -2.896138  -4.041477
H  -1.417677  -3.572259   1.274304
H  -2.311729   0.621024  -2.672152
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H  -3.838367  -3.786887   1.730986
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P   2.248565 -0.419863  0.199514
P  -1.383663  1.456873 -0.170907
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F  -6.691118 -2.346176 -0.653856
F  -6.222352 -3.127849  1.397079
C   1.017164 -3.149546 -1.556341
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C  -0.204675 -3.918252 -1.532968
H  -0.860890 -4.067981 -2.376791
C   1.169888 -4.909702  0.068755
H   0.934467 -4.464219  1.039548
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C   2.051804 -4.001161 -0.799173
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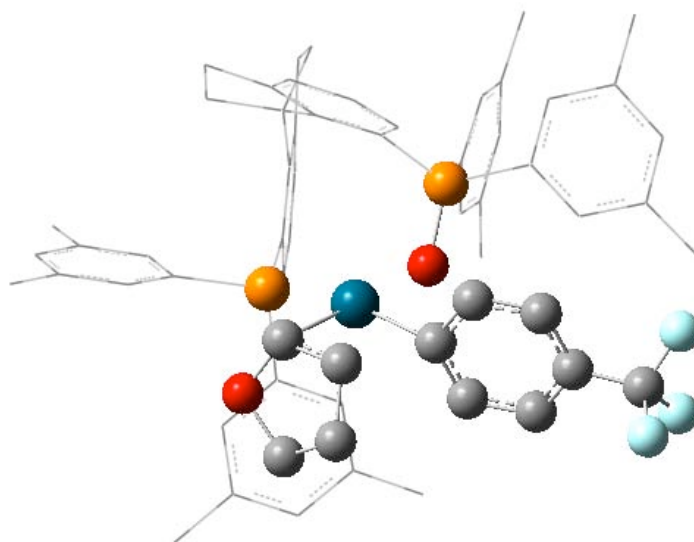
TS c'


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C   4.715730 -4.017636  3.678403
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C   2.404573 -3.130357  4.228695
C   2.425698  3.746147  0.750321
C   7.618535  0.054383  0.101671
C   2.261176  4.864260 -0.255478
C  -1.427047  4.252056  0.479634
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C   1.288176 -2.312488  3.973619
C   0.118461 -2.286791  4.933723
C  -1.086428  2.954809  0.893425
C   2.380516  1.317666  0.973308
C   2.200703  2.472114  0.176396
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C   6.342847 -0.451615 -0.535438
C   1.290652 -1.515753  2.819814
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C   6.379464 -1.128394 -1.768143
C   3.918762 -0.741166 -0.507729
C   1.966198  2.651126 -1.336602
C  -6.386537  0.486005  1.039504
C  -4.026756  0.967093  0.227211
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H    3.596874   1.334817  -4.012522
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H   -1.136677   0.031144  -4.925883
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F   -6.302445  -2.818922   1.808206
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H    1.983393  -3.423477  -0.431193
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TS d'

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C    2.707211   3.733978   2.395730
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C    4.570158  -4.313173   3.221311
C   -1.558875   5.179208   1.780825
C   -0.845433   2.519128   2.390410
C    2.676260   1.315785   2.375366
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C    2.253171  -3.454211   3.794635
C    2.338047   3.721791   1.052505
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C    2.160522   4.939052   0.171028
C   -1.542720   4.200402   0.778909
C    3.406756  -2.485219   1.903662
C    1.152316  -2.601671   3.589538
C   -0.043405  -2.651672   4.516507
C   -1.172378   2.881394   1.083441
C    2.320347   1.281876   1.011008
C    2.132066   2.513976   0.343809
C    2.325990  -1.627532   1.679652
C    6.357546  -0.289935  -0.524468
C    1.196232  -1.695906   2.519227
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C    1.483519   4.370027  -1.091812
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C    3.253541   2.715171  -1.927843
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