Supporting Information for:

A Surprising Mechanistic "Switch" in Lewis Acid Activation: A Bifunctional, Asymmetric Approach to α-Hydroxy Acid Derivatives

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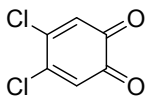
General. Unless otherwise stated, all reactions were carried out under anhydrous, air-free conditions. All solvents were dried and distilled by standard procedures. The ^{1}H and ^{13}C NMR spectra were acquired on a Bruker Avance 400 MHz spectrometer. The ^{1}H (400 MHz) and ^{13}C (101 MHz) chemical shifts are given in parts per million (δ) with respect to internal TMS standards and residual chloroform or DMSO. FT-IR spectra were recorded on a Bruker IFS-55 spectrometer and optical rotations were recorded on a Perkin Elmer 120 polarimeter at room temperature. Enantiomeric ratios were obtained by HPLC using the Chiracel OD or Whelk-01; compounds **7d, 7f, 7g, 10** and **11** were derivatized by benzylation prior to HPLC analysis. Benzoylquinidine **2a** was formed from quinidine (Sigma) and benzoyl chloride according to the method of Pracejus.[1] The $(Ph_3P)_2Pd(SbF_6)_2$ was made from $(Ph_3P)_2PdCl_2$ and $AgSbF_6$, and $(Ph_3P)_2CuClO_4$ was made in situ from $(ACN)_4CuClO_4$ and PPh_3.[2] All other chemicals were purchased from Aldrich Chemical Corporation, Alfa Aesar, and Acros Organics. Main paper references numbered (4),[3] (6),[4] and (7)[5] contain more than 15 authors and therefore are listed in their full form here.



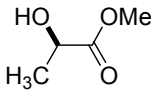
12

Procedure for 4,5-dichlorocyclohexa-3,5-diene-1,2-dione (12). 1.0 g (5.59 mmol) of 4,5-dichlorocatechol[6] and 0.396 g (6.15 mmol) of MnO_2 were added to 25 mL of THF at 0 ^oC. The reaction was allowed to warm up to room temperature over a period of 1 h and stirred until all the starting material was consumed by TLC. The reaction was filtered and the filtrate was concentrated *in vacuo*. The residue was crystallized using CH_2Cl_2/hexanes. Yellow crystalline solid: % yield = 52; mp = 81-83º C; ^1H NMR ($CDCl_3$) δ 7.41 (s, 2H) ppm; ^{13}C NMR ($CDCl_3$) δ 180.3, 158.2, 120.7 ppm; IR (CH_2Cl_2) 1705 cm^{-1}. Anal. Calcd. for $C_6H_2Cl_2O_2$ C, 40.72; H, 1.14. Found C, 40.68; H, 1.13.

General procedure for the synthesis of α-hydroxy oxygenated derivatives (7d, 7f, 7g, 7h): Benzoylquinidine **2a** (0.04 mmol) and *trans*-$(PPh_3)_2PdCl_2$ (0.04 mmol) were placed into a 25 mL round bottom flask equipped with a magnetic stir bar and were dissolved in 3 mL of THF. The flask was cooled to -78 ˚C and Hünig's base (0.4 mmol) was added to the reaction flask followed by propionyl chloride (0.4 mmol), as a solution in 2 mL of THF. *o*-Chloranil **4** (0.4 mmol) as a solution in 2 mL of THF was added via syringe pump for 6 h. The reaction (**7d**) was quenched using 3 mL of MeOH (**7f**, 3mL of H_20; **7g,** 1.0 eq. of NH_4OH; **7h,** 1.0 eq. thiophenol) and warmed to rt. Once the reaction was completed by TLC, 10 mL of CH_2Cl_2 was added to the reaction mixture and washed with 3 mL of H_2O (3X). The organic layer was dried using $MgSO_4$ and concentrated under reduced pressure. The residue was then dissolved in 2.6 mL of 4:1 (CH_3CN/H_2O) in a round bottom flask equipped with a magnetic stir bar. Cerium ammonium nitrate (0.14 mmol) was added to the reaction at 0 ºC and allowed to stir overnight to room temperature. Water was then added and the solution was extracted 3X with EtOAc. The organic layer was dried with $MgSO_4$ and concentrated *in vacuo*. The crude product was then columned using EtOAc/hexanes.

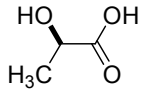
Note: Compounds **7d, 7f, 7g, 10** and **11** were derivatized by benzylation prior to HPLC analysis. **Representative derivatization procedure:** pure α-hydroxy derivative **7d** was stirred with benzyl chloride in DMF at 0 ºC, and 1 equiv. NaH (60% dispersion) was added to the solution and the mixture was stirred at 0 ºC until TLC indicated reaction

completion. Water was added and the product was extracted with diethyl ether, washed with dilute HCl and bicarbonate solutions successively, dried with $MgSO_4$ and filtered through a short plug of silica after partial dilution with hexanes to give pure product after solvent and excess benzyl chloride were removed under vacuum.



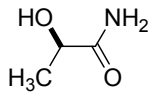
7d

(R)-methyl 2-hydroxypropanoate (7d).[7] Clear oil: % yield = 88; % ee = 96; $[\alpha]_D$ = +7.5º (c = 1.5, dioxane); ^{1}H NMR ($CDCl_3$) δ 4.28 (q, 1H), 3.79 (s, 3H), 3.02 (bs, 1H), 1.47 (d, 3H) ppm; ^{13}C NMR ($CDCl_3$) δ 179.8, 68.9, 54.6, 18.5 ppm; IR (CH_2Cl_2) 3511, 1744 cm^{-1}. HPLC (benzyl derivative, column = Whelk-01, 10% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 9.19, (S) = 10.56. Anal. Calcd. for $C_4H_8O_3$ C, 46.15; H, 7.75. Found C, 46.10; H, 7.73.



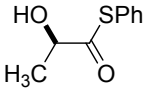
7f

(R)-2-hydroxypropanoic acid (7f).[8] Residue: % yield = 87; % ee = 97; $[\alpha]_D$ = +13.5º (c = 1.5, 1.5 N NaOH); ^{1}H NMR ($CDCl_3$) δ 4.27 (q, 1H), 3.00 (bs, 1H), 1.38 (d, 3H) ppm; ^{13}C NMR ($CDCl_3$) δ 180.7, 71.5, 22.6 ppm; IR (CH_2Cl_2) 3500-3400, 1724 cm^{-1}. HPLC (benzyl derivative, column = Whelk-01, 10% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 7.74, (S) = 8.92. Anal. Calcd. for $C_3H_6O_3$ C, 40.00; H, 6.71. Found C, 40.11; H, 6.73.



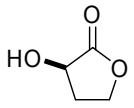
7g

(R)-2-hydroxypropanamide (7g).[9] White crystalline solid: % yield = 82; % ee = 80; mp= 51-52º C; $[\alpha]_D$ = +11.4º (c = 0.25, Methanol:Ethanol (1:1)); ^{1}H NMR (CH_3OD) δ 4.11 (q, 1H), 1.37 (d, 3H) ppm; ^{13}C NMR (CH_3OD) δ 177.3, 66.9, 18.7 ppm; IR (CH_2Cl_2) 3512, 3480, 1701 cm^{-1}. HPLC (benzyl derivative, column = Whelk-01, 20% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 10.09, (S) = 11.76. Anal. Calcd. for $C_3H_7NO_2$ C, 40.44; H, 7.92; N, 15.72. Found C, 40.46; H, 7.89; N, 15.68.



7h

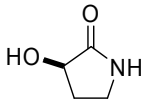
(R)-S-phenyl 2-hydroxypropanethioate (7h).[10] Clear oil: % yield = 80; % ee = 92; $[\alpha]_D$ = +13.5º (c = 1.5, 1.5 N NaOH); ^{1}H NMR ($CDCl_3$) δ 7.41-7.39 (m, 5H), 4.44 (q, 1H) 2.85 (bs, 1H), 1.51 (d, 3H) ppm; ^{13}C NMR ($CDCl_3$) δ 188.3, 138.4, 130.6, 130.5, 129.7, 129.5, 126.3, 69.5, 20.8 ppm; IR (CH_2Cl_2) 3418, 1710 cm^{-1}. HPLC (Whelk-01, 15% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 7.74, (S) = 8.92. Anal. Calcd. for $C_9H_{10}O_2S$ C, 59.32; H, 5.53. Found C, 59.28.6; H, 5.56.



10

Procedure for 3-hydroxy-dihydrofuran-2(3H)-one (10)[11]**:** Benzoylquinidine **2a** (0.04 mmol) and *trans*-$(PPh_3)_2PdCl_2$ (0.04 mmol) were placed into a 25 mL round bottom flask equipped with a magnetic stir bar and were dissolved in 3 mL of THF. The flask was cooled to -78 ˚C and Hünig's base (0.4 mmol) was added to the reaction flask followed by 4-benzyloxybutyryl chloride[12] (0.4 mmol), as a solution in 2 mL of THF. *o*-Chloranil **4** (0.4 mmol) as a solution in 2 mL of THF was added via syringe pump for 8 h. The reaction was quenched using 3 mL of H_2O and warmed to rt. Once the reaction was completed by TLC, 10 mL of EtOH was added to the reaction mixture followed by a

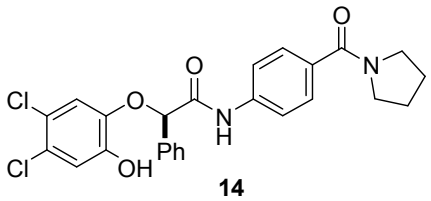
catalytic amount of acetic acid and Pd/C and hydrogenated for 8 h. The solution was filtered through celite and the filtrate was concentrated *in vacuo*. The residue was taken up in 10 mL of toluene and a catalytic amount of PTSA was added to the reaction mixture and refluxed for 10 h using a Dean-Stark trap. The reaction was concentrated under reduced pressure and the residue was dissolved in 2.6 mL of 4:1 (CH_3CN/H_2O) in a round bottom flask equipped with a magnetic stir bar. Cerium ammonium nitrate (0.14 mmol) was added to the reaction at 0º C and stirred overnight. Water was then added and the mixture was extracted 3X with EtOAc. The organic layer was dried with $MgSO_4$ and concentrated *in vacuo*. The crude product was then columned using 10% ETOAc/hexanes. Clear oil: % yield = 88; % ee = >99; $[\alpha]_D$ = +61.5º (c = 1.15, $CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 4.28 (m, 1H), 4.21-4.17 (m, 2H), 3.17 (bs, 1H), 2.2-2.8 (m, 2H) ppm; ^{13}C NMR ($CDCl_3$) δ 188.3, 68.3, 66.6, 25.4 ppm; IR (CH_2Cl_2) 3545, 1788 cm^{-1}. HPLC (benzyl derivative, column = Whelk-01, 5% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 12.60, (S) = 9.30. Anal. Calcd. for $C_4H_6O_3$ C, 47.06; H, 5.92. Found C, 47.07; H, 5.93.



11

Procedure for (S)-3-hydroxypyrrolidin-2-one (11)[13]: Benzoylquinidine **2a** (0.04 mmol) and *trans*-$(PPh_3)_2PdCl_2$ (0.04 mmol) were placed into a 25 mL round bottom flask equipped with a magnetic stir bar and were dissolved in 3 mL of THF. The flask was cooled to -78 ˚C and Hünig's base (0.4 mmol) was added to the reaction flask followed by 4-chlorobutyryl chloride (0.4 mmol), as a solution in 2 mL of THF. *o*-Chloranil **4** (0.4 mmol) as a solution in 2 mL of THF was added via syringe pump for 8 h. The reaction was quenched using NH_4OH (0.4 mmol) and warmed to rt. Once the reaction was completed by TLC, the reaction was concentrated *in vacuo*. The residue was dissolved in 3 mL of THF and NaH (0.4 mmol) followed by 15-crown-5 (0.04 mmol) were added to the solution at room temperature. After 5 h, the reaction was diluted with 10 mL of CH_2Cl_2 and washed 3X with H_2O in a separatory funnel. The organic layer was dried

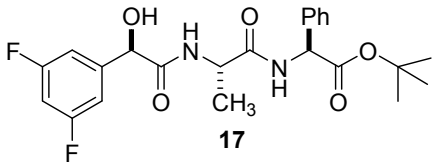
using $MgSO_4$ and concentrated *in vacuo*. The residue was then dissolved in 2.6 mL of 4:1 (CH_3CN/H_2O) in a round bottom flask equipped with a magnetic stir bar. Cerium ammonium nitrate (0.14 mmol) was added to the reaction at 0º C and stirred overnight. Water was then added and the mixture was extracted 3X with EtOAc. The organic layer was dried with $MgSO_4$ and concentrated *in vacuo*. The crude product was then columned using 50% ETOAc/hexanes. White crystalline solid: % yield = 82; % ee = >99; mp= 100-103º C; $[\alpha]_D$ = +61.5º (c = 120.4, $CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 7.22 (bs, 1H), 4.75 (bs, 1H), 4.30 (t, 1H), 3.32 (m, 2H), 2.45 (m, 1H), 2.08 (m, 1H) ppm; ^{13}C NMR ($CDCl_3$) δ 178.3, 69.8, 38.9, 30.0 ppm; IR (CH_2Cl_2) 3228, 1712 cm^{-1}; HPLC (benzyl derivative, column = Whelk-01, 1% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 7.35, (S) = 6.55. Anal. Calcd. for $C_4H_7NO_2$ C, 47.52; H, 6.98; N, 13.85. Found C, 47.58; H, 6.96; N, 13.81.



14

Prodecure for (R)-2-(4,5-dichloro-2-hydroxyphenoxy)-2-phenyl-N-(4-(pyrrolidine-1-carbonyl)-phenyl)acetamide (14)[14]: Benzoylquinidine **2a** (0.04 mmol) and *trans*-$(PPh_3)_2PdCl_2$ (0.04 mmol) were placed into a 25 mL round bottom flask equipped with a magnetic stir bar and were dissolved in 3 mL of THF. The flask was cooled to -78 ˚C and Hünig's base (0.4 mmol) was added to the reaction flask followed by phenylacetyl chloride (0.4 mmol), as a solution in 2 mL of THF. *o*-Quinone **12** (0.4 mmol) as a solution in 2 mL of THF was added via syringe pump for 8 h. The reaction was quenched using **13**[15] (0.4 mmol) in 2 mL of THF and then refluxed for 6 h. Once the reaction was completed by TLC, the reaction was concentrated *in vacuo*. The crude product was then columned using 30% EtOAc/hexanes. Light tan solid: % yield = 93; % ee = >99; mp= 181-183º C; $[\alpha]_D$ = +28.5º (c = 0.010, $CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 9.02 (s, 1H), 7.42-7.63 (m, 9H), 7.18 (s, 1H), 6.72 (d, 2H), 5.28 (s, 1H), 3.4-3.6 (m, 4H), 1.74-1.97 (m, 4H) ppm; ^{13}C NMR ($CDCl_3$) δ 168.3, 166.7, 148.3, 137.6, 131.0, 130.1, 129.4,

129.2, 128.5, 128.3, 126.9, 126.4, 125.9, 125.7, 124.8, 124.1, 123.5, 122.8, 121.7, 113.9, 76.6, 49.9, 46.3, 26.5, 24.5 ppm; IR (CH_2Cl_2) 3281, 1677, 1672 cm^{-1}. HPLC (Whelk-01, 10% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 8.84, (S) = 9.34. Anal. Calcd. for $C_{25}H_{22}Cl_2N_2O_4$ C, 61.87; H, 4.57; N, 5.77. Found C, 61.86; H, 4.55; N, 5.79.

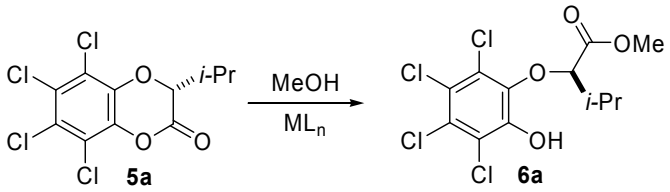


17

(S)-tert-butyl-2-((S)-2-((R)-2-(3,5-difluorophenyl)-2-hydroxyacetamido)-propanamido)-2-phenylacetate (17)[16]**:** Benzoylquinidine **2a** (0.04 mmol) and *trans*-$(PPh_3)_2PdCl_2$ (0.04 mmol) were placed into a 25 mL round bottom flask equipped with a magnetic stir bar and were dissolved in 3 mL of THF. The flask was cooled to -78 ˚C and Hünig's base (0.4 mmol) was added to the reaction flask followed by 3,5-(difluoro)phenylacetyl chloride[17] (0.4 mmol), as a solution in 2 mL of THF. *o*-Chloranil **4** (0.4 mmol) as a solution in 2 mL of THF was added via syringe pump for 8 h. The reaction was quenched using **16**[18] (0.4 mmol) in 2 mL of THF and then warmed to rt. Once the reaction was completed by TLC, the reaction was concentrated *in vacuo*. The reaction was diluted with 10 mL of CH_2Cl_2 and washed 3X with H_2O in a separatory funnel. The organic layer was dried using $MgSO_4$ and concentrated *in vacuo*. The residue was then dissolved in 2.6 mL of 4:1 (CH_3CN/H_2O) in a round bottom flask equipped with a magnetic stir bar. Cerium ammonium nitrate (0.14 mmol) was added to the reaction at 0º C and stirred overnight. Water was then added and the mixture was extracted 3X with EtOAc. The organic layer was dried with $MgSO_4$ and concentrated *in vacuo*. The crude product was then columned using 50% EtOAc/hexanes. Clear oil: % yield = 87; % ee = >99; $[\alpha]_D$ = -21.5º (c = 0.010, $CHCl_3$); ^{1}H NMR ($CDCl_3$) δ 7.18-7.42 (m, 6H), 6.60-7.25 (m, 3H), 5.36 (d, 1H), 4.90-5.02 (m, 2H), 4.51-4.58 (m, 1H), 4.31 (bs, 1H), 1.36-1.40 (m, 12H) ppm; ^{13}C NMR ($CDCl_3$) δ 176.3, 167.8, 166.7, 164.2 (doublet),

161.2 (doublet), 136.5 (triplet), 126.4, 125.9, 125.7, 124.8, 124.1, 123.5, 112.6 (doublet), 112.5 (doublet), 103.0 (triplet), 80.6, 79.6, 76.9, 46.3, 26.5, 19.5 ppm; IR (CH_2Cl_2) 3430, 3410, 3328, 1747, 1671, 1666 cm^{-1}. HPLC (Whelk-01, 1% *i*-PrOH/hexanes, 1.0 mL/min) (R) = 17.73, (S) = 19.38. Anal. Calcd. for $C_{23}H_{26}F_2N_2O_5$ C, 61.60; H, 5.84; N, 6.25. Found C, 61.68; H, 5.81; N, 6.22.

Rate of methanolysis forming 6a.[19]



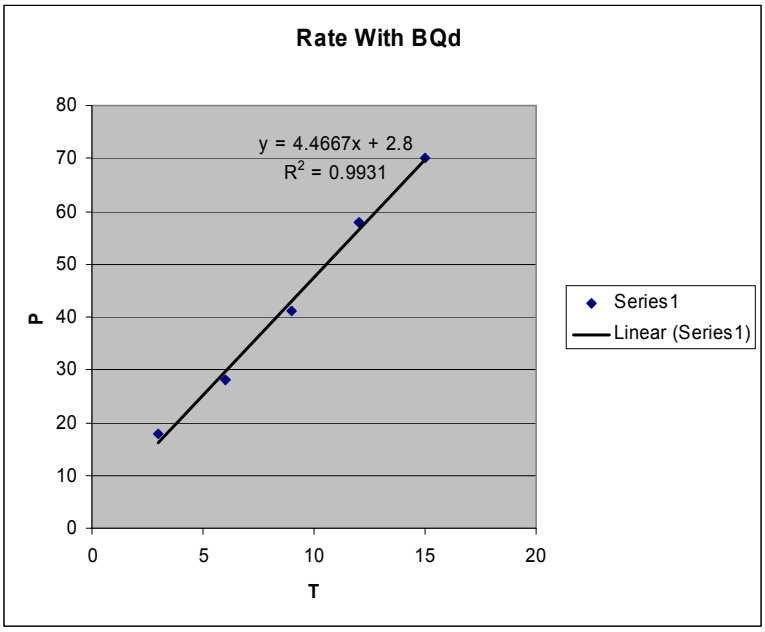
5a was formed: Benzoylquinidine **2a** (0.04 mmol) and *trans*-$(PPh_3)_2PdCl_2$ (0.04 mmol) were placed into a 25 mL round bottom flask equipped with a magnetic stir bar and were dissolved in 3 mL of THF. The flask was cooled to -78 ˚C and Hünig's base (0.4 mmol) was added to the reaction flask followed by isovaleryl chloride (0.4 mmol), as a solution in 2 mL of THF. *o*-Chloranil **4** (0.4 mmol) as a solution in 2 mL of THF was added via syringe pump for 6 h, and the reaction was maintained at -78 ˚C for an additional 6 h before warming to RT at which time the mixture was diluted with hexanes and filtered through a short plug of silica and washed through with hexanes. Pure **5a** is obtained after subjection to high vacuum.

Methanolysis: 5a (0.3 mmol, purified for accuracy) in 1 mL THF was added in one portion to a 10 mL round bottom flask containing catalysts as indicated below in a rapidly stirring solution of 2 mL THF and 3 mL MeOH. When the reaction was complete (by TLC) the solvent was rapidly evaporated (cold, under high vacuum). The catalysts were removed by dissolving the reaction mixture in CH_2Cl_2 and filtering through a plug of silica, washing with CH_2Cl_2. After removal of the solvent, the pure product was confirmed by ^1H NMR.[15]

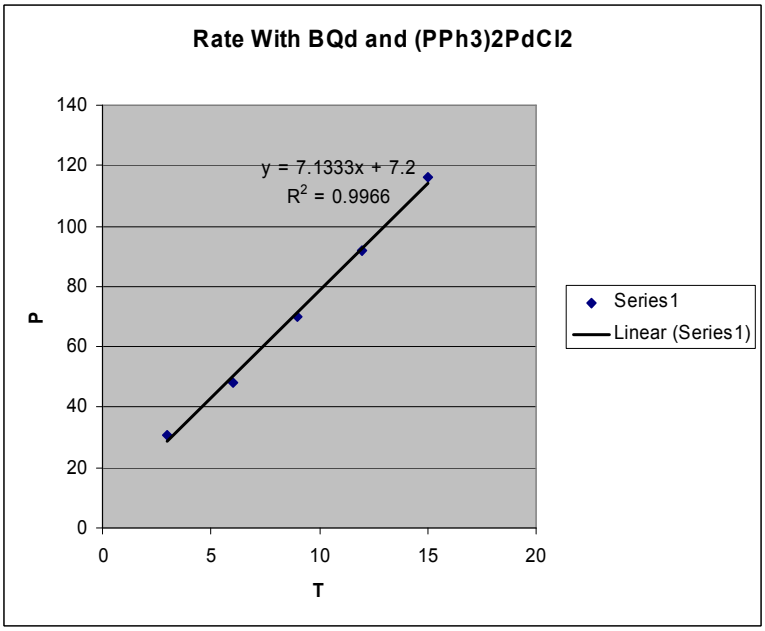
BQd	*trans*-$(PPh_3)_2PdCl_2$	$Sc(OTf)_3$	h
--	--	--	15
0.03mmol	--	--	13
0.015mmol	0.015mmol	--	12
0.01mmol	0.01mmol	0.01mmol	9
0.015mmol	--	0.015mmol	12
--	--	0.03mmol	12
--	0.015mmol	0.015mmol	12
--	0.03mmol	--	13

Rate Study with BQd vs. BQd and *trans*-$(PPh_3)_2PdCl_2$:

25-mL flasks were set up in the following manner: To a suspension of NaH (0.021 g, 0.875 mmol), **2a** (0.035 g, 0.0875 mmol), and 15-crown-5 (0.016 mL, 0.0875 mmol) in THF (8.0 mL) at -78°C was added phenylacetyl chloride **1b** (0.108 mL, 0.875 mmol) in a solution of THF (2.0 mL). The reaction was allowed to stir at -78 °C for 6 h. *o*-Chloranil **4** (0.200 mg, 0.875 mmol) was then added as a solution in 4 mL of THF to each reaction flask and allowed to react for 3, 6, 9, 12, and 15 min. The reactions were quenched at their respective times using 3.0 mL of 1M methanolic HCl. The resulting mixture was subjected to column chromatography using silica gel (1% EtOAc/hexanes). (Reactions performed in duplicate and averaged)



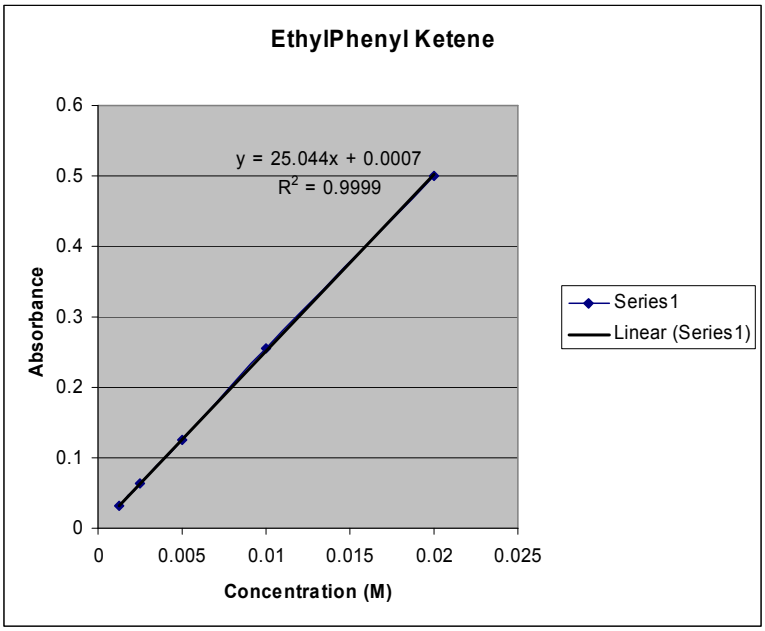
Procedure to determine rate effect of BQd and *trans*-$(PPh_3)_2PdCl_2$ is the same as stated above except with the addition of *trans*-$(PPh_3)_2PdCl_2$ (0.058 g, 0.0875 mmol) before adding phenylacetyl chloride **1b**.



The rate study showed a 1.6 fold increase in rate with BQd and *trans*-$(PPh_3)_2PdCl_2$ vs. BQd.

UV-Vis Study:

In a Schlenk tube, 0.137 mmol of ethylphenyl ketene was dissolved in 10 mL of THF and cooled to -78 ^{o}C. λ = 395 nm, A = 0.102835 was used to monitor ketene concentration vs. ketene enolate formation. 0.137 mmol of BQd was added to the solution and after 20 min. (absorbance was stabilized) A = 0.094842 at λ = 395 nm. 0.137 mmol of *trans*-$(PPh_3)_2PdCl_2$ was added to the Schlenk flask and after 20 min. (absorbance was stabilized) A = 0.091547 at λ = 395 nm.



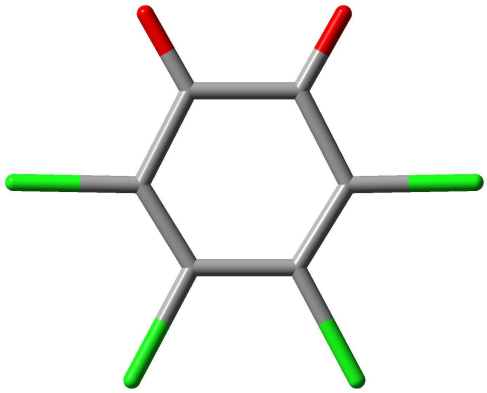
e = 125 $Lmol^{-1}cm^{-1}$

Initial Ketene Concentration = $4.10x10^{-3}$ M

Ketene Concentration with BQd = $3.76x10^{-3}$ M

Ketene Concentration with BQd and *trans*-$(PPh_3)_2PdCl_2$ = $3.63x10^{-3}$M

Figure 2A: *o*-chloranil



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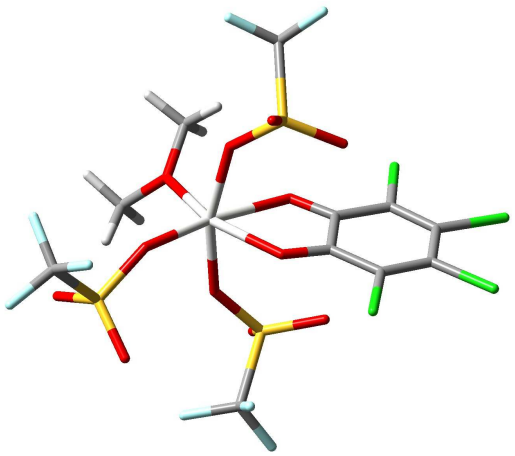
 Will use up to    4 processors via shared memory.
 %chk=/scratch/tdudding/Quinone-gv
 ---------------------------------------
 #opt=calcfc freq=noraman b3lyp/lanl2dz
 ---------------------------------------
 Zero-point correction=                          0.045879
(Hartree/Particle)
 Thermal correction to Energy=                    0.057013
 Thermal correction to Enthalpy=                  0.057958
 Thermal correction to Gibbs Free Energy=         0.006637
 Sum of electronic and zero-point Energies=           -438.650060
 Sum of electronic and thermal Energies=              -438.638925
 Sum of electronic and thermal Enthalpies=            -438.637981
 Sum of electronic and thermal Free Energies=         -438.689302
 C                  1.45559900    0.43142400    0.00000400
 C                 -1.45559200    0.43141500    0.00000300
 C                  0.77841900    1.75170200    0.00001300
 C                  0.73936500   -0.73102100    0.00000900
 C                 -0.73935300   -0.73102700    0.00001100
 C                 -0.77842600    1.75169700    0.00000700
 Cl                -3.24039200    0.46454500   -0.00002600
 Cl                -1.58001700   -2.31006800    0.00001200
 Cl                 1.58003700   -2.31005800    0.00000500
 Cl                 3.24037400    0.46456100   -0.00002700
 O                  1.39026400    2.83264100    0.00003000
 O                 -1.39027800    2.83263400    0.00001200
```

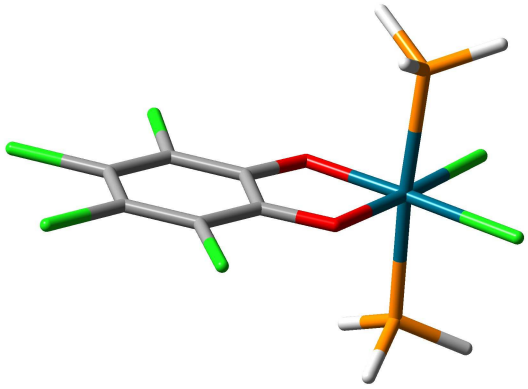
Figure 2B: *o*-chloranil-Sc(III) complex



```
*****************************************
 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               8-Oct-2008
 *****************************************
 %nosave
 %mem=2000mb
 %nproc=1
 Will use up to    1 processors via shared memory.
 ----------------------------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
geom=connectivity
 ----------------------------------------------------------
 Zero-point correction=                          0.202047
(Hartree/Particle)
 Thermal correction to Energy=                    0.249852
 Thermal correction to Enthalpy=                  0.250797
 Thermal correction to Gibbs Free Energy=         0.110478
 Sum of electronic and zero-point Energies=          -2359.815527
 Sum of electronic and thermal Energies=             -2359.767722
 Sum of electronic and thermal Enthalpies=           -2359.766778
 Sum of electronic and thermal Free Energies=        -2359.907097
```

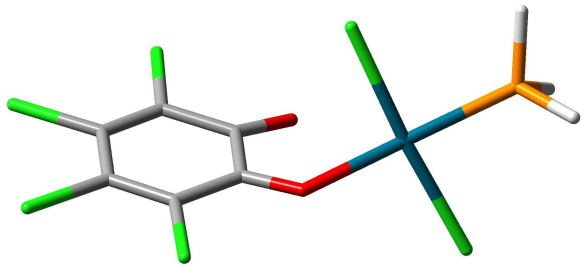
Sc	1.09920700	0.54399400	0.56725800	F	1.18716400	-3.75654500	-1.00645800
O	4.00622500	-1.76099700	-1.35865800	C	5.32738100	0.86209200	-1.48019400
O	1.21052800	-1.42068700	1.11306200	F	5.47538600	2.01200800	-0.73499200
O	0.38749400	2.38648600	0.01628600	F	4.67699600	1.14623200	-2.65810000
S	-0.84868200	3.02967100	-0.92951400	F	6.56834600	0.32467200	-1.75154800
O	-0.37049500	3.55167500	-2.36905800	O	4.97335200	-0.62396700	1.01926000
O	-2.18906600	2.09310600	-0.82244900	O	1.64349900	1.18505700	2.50806000
C	-1.25418000	4.63070100	0.21313600	C	2.71430100	0.50324100	3.28376000
F	-2.36857400	5.26798200	-0.27887300	H	3.34395100	-0.04110800	2.57866300
F	-0.17916200	5.48803400	0.20749200	H	2.24556100	-0.18239500	3.99731200
F	-1.49915600	4.20537000	1.50805300	H	3.30605300	1.26959500	3.79546900
S	4.26099200	-0.47498400	-0.42526100	C	0.85045800	2.13654200	3.31360000
O	2.87461500	0.49437100	-0.26720900	H	1.52411000	2.90330500	3.71088100
O	-0.22011100	-0.20198500	-1.04739200	H	0.35331400	1.59145900	4.12337200
O	-1.03298700	0.34072400	1.39430100	H	0.11354300	2.58551900	2.64923600
C	-1.91714700	-0.09512200	0.60970500				
C	-3.69944100	-1.11573400	-1.38725700				
C	-1.43881500	-0.42866900	-0.81518800				
C	-3.31951300	-0.28047900	0.93200200				
C	-4.16748300	-0.76912100	-0.02560700				
C	-2.39378200	-0.95658900	-1.77092300				
Cl	-3.83422500	0.14170000	2.58131300				
Cl	-5.88974900	-1.00513900	0.35515700				
Cl	-4.88886100	-1.75557300	-2.54511400				
Cl	-1.78542100	-1.35129400	-3.39113700				
S	0.21839600	-2.74783100	1.38683300				
O	0.19065600	-3.19857100	2.92885100				
O	-1.21071600	-2.56434600	0.59624600				
C	1.23130000	-4.11813400	0.31618600				
F	0.61585300	-5.33898300	0.49168600				
F	2.52389600	-4.17366100	0.76610800				

Figure 2C: *o*-chloranil-*trans*-$(Ph_3P)_2PdCl_2$



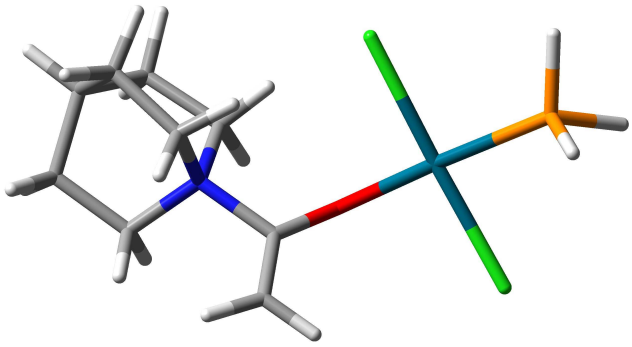
```
 ******************************************
 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               8-Oct-2008
 ******************************************
 %nosave
 %mem=2000mb
 %nproc=1
 Will use up to    1 processors via shared memory.
 ---------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ---------------------------------------
 Zero-point correction=                          0.103809
(Hartree/Particle)
 Thermal correction to Energy=                    0.126793
 Thermal correction to Enthalpy=                  0.127737
 Thermal correction to Gibbs Free Energy=         0.048010
 Sum of electronic and zero-point Energies=          -611.879804
 Sum of electronic and thermal Energies=             -611.856820
 Sum of electronic and thermal Enthalpies=           -611.855876
 Sum of electronic and thermal Free Energies=        -611.935603
 C                 -1.97188400    1.40738800   -0.00005900
 C                 -1.97181900   -1.40736900    0.00006900
 C                 -0.75541000    0.70830700   -0.00000600
 C                 -3.19373500    0.70444700   -0.00003900
 C                 -3.19370100   -0.70448200    0.00003200
 C                 -0.75537200   -0.70823500    0.00003200
 Cl                -1.90845300   -3.20517700    0.00014600
 Cl                -4.74660000   -1.61529600    0.00006700
 Cl                -4.74667100    1.61519600   -0.00009800
 Cl                -1.90859400    3.20519700   -0.00013500
 O                  0.46651600    1.36896700    0.00002700
 O                  0.46657700   -1.36883900    0.00001400
 Pd                 1.97751200    0.00007200    0.00000300
 Cl                 3.66010300    1.72814100   -0.00000800
 P                  2.06425700    0.00012700    2.40311400
 H                  1.44017300    1.12444800    3.00928600
 H                  3.38279000    0.00016600    2.92504700
 H                  1.44028200   -1.12421800    3.00936700
 P                  2.06428000   -0.00031900   -2.40310200
 H                  3.38282400    0.00101700   -2.92499200
 H                  1.43898000    1.12311800   -3.00966700
 H                  1.44155800   -1.12555300   -3.00898700
 Cl                 3.66001400   -1.72810800   -0.00002300
```

Figure 2D: *o*-chloranil-*trans*-Ph_3PPdCl_2 square planar



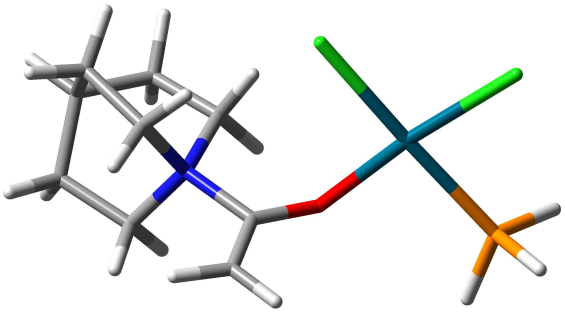
```
****************************************
 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               10-Oct-2008
 ****************************************
 %nosave
 %mem=2000mb
 %nproc=1
 Will use up to    1 processors via shared memory.
 ---------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ---------------------------------------
Zero-point correction=                          0.076762
(Hartree/Particle)
 Thermal correction to Energy=                  0.096949
 Thermal correction to Enthalpy=                0.097893
 Thermal correction to Gibbs Free Energy=       0.022472
 Sum of electronic and zero-point Energies=          -603.636052
 Sum of electronic and thermal Energies=             -603.615865
 Sum of electronic and thermal Enthalpies=           -603.614921
 Sum of electronic and thermal Free Energies=        -603.690342
 C                  2.12101900   -1.44623600   -0.37613100
 C                  1.75124000    1.42221700   -0.03045300
 C                  0.75112000   -0.90645300   -0.51474500
 C                  3.17722900   -0.61730600   -0.12210400
 C                  2.99127300    0.83950000    0.03028800
 C                  0.56087200    0.59847900   -0.22941000
 Cl                 1.49299900    3.17460900    0.17142600
 Cl                 4.43516500    1.84602000    0.31456800
 Cl                 4.83154900   -1.27777800    0.02205800
 Cl                 2.29792000   -3.20490600   -0.58880500
 O                 -0.22495900   -1.58176700   -0.88566400
 O                 -0.59581400    1.08643000   -0.18915400
 P                 -4.55969000   -0.76056500    0.51523300
 H                 -4.70710400   -1.46399800    1.74211700
 H                 -5.01636900   -1.70347000   -0.44624100
 H                 -5.63252600    0.17184200    0.55330600
 Cl                -3.47046700    0.95692800   -1.93241000
 Pd                -2.46427500    0.13741200    0.08750100
 Cl                -1.61318400   -0.74754200    2.15734800
```

Figure 4A: Pd(II)-enolate-*trans*-Ph_3



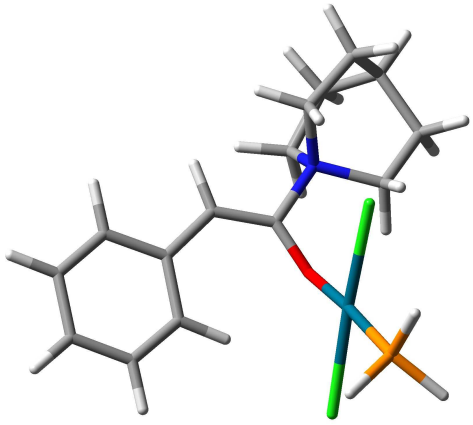
```
****************************************
 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               9-Oct-2008
****************************************
 %nosave
 %mem=2000mb
 %nproc=1
 Will use up to    1 processors via shared memory.
 ---------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ---------------------------------------
Zero-point correction=                          0.265674
(Hartree/Particle)
 Thermal correction to Energy=                  0.284270
 Thermal correction to Enthalpy=                0.285214
 Thermal correction to Gibbs Free Energy=       0.215825
 Sum of electronic and zero-point Energies=          -646.611432
 Sum of electronic and thermal Energies=             -646.592837
 Sum of electronic and thermal Enthalpies=           -646.591893
 Sum of electronic and thermal Free Energies=        -646.661282
N              2.22619900    0.56286500    0.06715500
 C             2.20447500   -0.26516700   -1.23195900
 C             2.38341400   -0.39850300    1.25798100
 C             3.42139900    1.51353800    0.01344100
 H             2.47266500    0.22904700    2.14867700
 H             1.45270900   -0.96833600    1.31651600
 H             3.30195300    2.10235000   -0.90031000
 H             3.34705800    2.19483800    0.86074600
 H             1.38683500   -0.97816500   -1.12434200
 H             1.93890900    0.42208000   -2.03702600
 C             3.62310600   -1.31300800    1.04463900
 H             3.30011200   -2.34488300    0.86480900
 H             4.24155200   -1.31552200    1.95051200
 C             3.58205300   -0.95076900   -1.44269400
 H             4.10698700   -0.50909600   -2.29941000
 H             3.42483500   -2.01144900   -1.66973700
 C             4.75137400    0.70441100    0.03834800
 H             5.41696800    1.06659800   -0.75410000
 H             5.27154200    0.85468400    0.99268800
 C             4.44034800   -0.79791400   -0.16526600
 H             5.37256700   -1.36570300   -0.26155900
 C             0.83886100    1.34210800    0.21593200
 O            -0.05283700    0.91192500   -0.63924400
 C             0.76273700    2.31718500    1.15386000
 H            -0.18100400    2.84084600    1.25887700
 H             1.57264500    2.59428700    1.81709900
 Pd           -1.80927600   -0.06368700   -0.14470100
 Cl           -0.61769900   -2.16762200    0.15752400
 P            -3.85979400   -1.10346900    0.30802800
 H            -4.88813900   -0.93269200   -0.66402400
 H            -3.86937800   -2.51811200    0.48758200
 H            -4.53368900   -0.66758500    1.48604600
 Cl           -3.10105400    1.97007600   -0.28099800
```

Figure 4B: Pd(II)-enolate-*cis*-Ph_3



```
*****************************************
 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               8-Oct-2008
 *****************************************
 %nosave
 %mem=2000mb
 %nproc=1
 Will use up to    1 processors via shared memory.
 ----------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ----------------------------------------
 Zero-point correction=                          0.265477  (Hartree/Particle)
 Thermal correction to Energy=                   0.283964
 Thermal correction to Enthalpy=                 0.284909
 Thermal correction to Gibbs Free Energy=        0.216764
 Sum of electronic and zero-point Energies=           -646.604516
 Sum of electronic and thermal Energies=              -646.586028
 Sum of electronic and thermal Enthalpies=            -646.585084
 Sum of electronic and thermal Free Energies=         -646.653229
 N            2.20370700    0.48355000    0.20380200
 C            1.91534600   -0.11292200   -1.18666900
 C            2.67912300   -0.64910600    1.13190900
 C            3.32144500    1.52201800    0.06221100
 H            2.99570900   -0.17624700    2.06453500
 H            1.80205900   -1.27034000    1.32715400
 H            2.98328500    2.23047800   -0.69995800
 H            3.39403900    2.05779300    1.00960800
 H            1.20102700   -0.92187100   -1.02177700
 H            1.41268800    0.66325900   -1.76402300
 C            3.83704500   -1.43327100    0.45496600
 H            3.48422000   -2.41955600    0.13169000
 H            4.64301300   -1.59596700    1.18076400
 C            3.23979000   -0.59807800   -1.83556000
 H            3.53399800    0.06231800   -2.66163300
 H            3.08509400   -1.59721900   -2.25857800
 C            4.65557200    0.82067100   -0.32411900
 H            5.13970500    1.37537900   -1.13658100
 H            5.34800900    0.82042700    0.52702300
 C            4.35604400   -0.63355500   -0.76527900
 H            5.26117400   -1.09939500   -1.17022800
 C            0.88594100    1.16283300    0.78926400
 O           -0.11732700    1.17744300   -0.05742800
 C            0.97778000    1.69257300    2.03224600
 H            0.09643200    2.14964800    2.46734100
 H            1.87075300    1.65181400    2.64369400
 Pd          -1.81306000   -0.07041800   -0.01401200
 Cl          -0.50913800   -2.02295700    0.54536200
 Cl          -3.86498700   -1.28185500   -0.09935300
 P           -3.16898100    1.80668600   -0.56919800
 H           -2.52267900    3.06957300   -0.75295400
 H           -3.93859200    1.72447500   -1.76718800
 H           -4.19021000    2.16480500    0.36044900
```

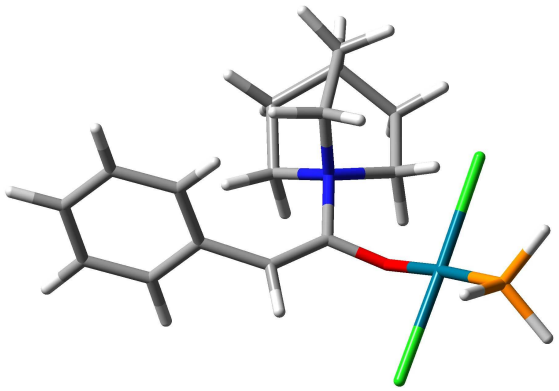
Figure 5A: Pd(II)-enolate-*Z*-Ph



```
 ****************************************
 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               14-Oct-2008
 ****************************************
 %nosave
 %mem=2000mb
 %nproc=2
 Will use up to    2 processors via shared memory.
 ----------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ----------------------------------------
 Zero-point correction=                           0.347932
(Hartree/Particle)
 Thermal correction to Energy=                    0.371011
 Thermal correction to Enthalpy=                  0.371955
 Thermal correction to Gibbs Free Energy=         0.292949
 Sum of electronic and zero-point Energies=           -877.555109
 Sum of electronic and thermal Energies=              -877.532029
 Sum of electronic and thermal Enthalpies=            -877.531085
 Sum of electronic and thermal Free Energies=         -877.610092
```

N	2.38201600	0.37963400	-0.25017600	C	-0.77740900	4.03764200	0.88330500
C	2.49428200	-1.06378000	-0.77197300	C	-1.85350900	2.31038100	-0.46170400
C	2.90977400	0.41174200	1.19270600	C	-1.97941700	4.75951000	0.93275500
C	3.25452000	1.27794800	-1.13436900	H	0.10502200	4.42950200	1.38851100
H	2.93255900	1.45987300	1.49953300	C	-3.05399600	3.03881800	-0.40974700
H	2.17037700	-0.11630500	1.79879900	H	-1.81555000	1.38120200	-1.01760700
H	2.91607200	1.11080700	-2.16111900	C	-3.12905900	4.26162800	0.28585200
H	3.03091300	2.31343800	-0.87432600	H	-2.02227200	5.70407100	1.47103800
H	1.95842400	-1.68433500	-0.05204600	H	-3.93098100	2.64639300	-0.91917600
H	1.94741100	-1.10115400	-1.71410700	H	-4.06273200	4.81843600	0.32120400
C	4.32148400	-0.23709900	1.25610400				
H	4.26860100	-1.20901300	1.76097100				
H	4.99235700	0.40014800	1.84495400				
C	3.98909200	-1.45870100	-0.91295800				
H	4.27738200	-1.51399400	-1.97043800				
H	4.13909100	-2.45624200	-0.48385100				
C	4.75747700	0.92947800	-0.93487900				
H	5.25156300	0.86471900	-1.91149200				
H	5.26234000	1.72123800	-0.36715600				
C	4.86924800	-0.41875200	-0.18062300				
H	5.91291900	-0.75084900	-0.15126300				
C	0.85280200	0.85722200	-0.32028500				
O	0.07191300	0.00158000	-0.91942500				
C	0.60411600	2.10544100	0.17678900				
H	1.42588200	2.65729500	0.62680900				
Pd	-1.26120400	-1.36496300	-0.05156900				
Cl	0.14861900	-1.78081800	1.88712200				
P	-2.85839400	-2.88097600	0.75459100				
H	-3.18218600	-3.98431600	-0.08798500				
H	-2.58689200	-3.53659400	1.99132000				
H	-4.15535100	-2.34257200	0.99853400				
Cl	-2.77301500	-1.10963700	-1.92172200				
C	-0.68912800	2.79833400	0.19186900				

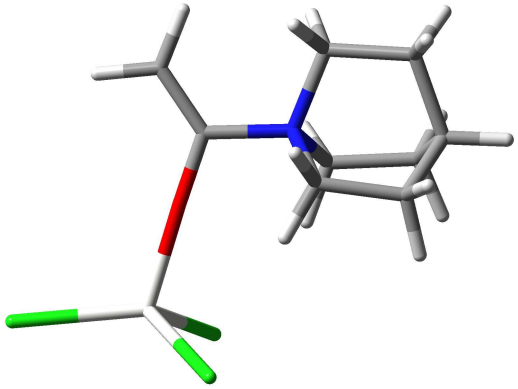
Figure 5B: Pd(II)-enolate-*E*-Ph



```
****************************************
 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
               9-Oct-2008
****************************************
 %nosave
 %mem=2000mb
 %nproc=1
 Will use up to    1 processors via shared memory.
 ----------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ----------------------------------------
Zero-point correction=                          0.347484
(Hartree/Particle)
 Thermal correction to Energy=                  0.370698
 Thermal correction to Enthalpy=                0.371642
 Thermal correction to Gibbs Free Energy=       0.290922
 Sum of electronic and zero-point Energies=          -877.540505
 Sum of electronic and thermal Energies=             -877.517291
 Sum of electronic and thermal Enthalpies=           -877.516347
 Sum of electronic and thermal Free Energies=        -877.597067
```

N	-1.38713900	1.17261500	-0.45305000	C	-0.53312500	-0.14166400	-0.70431000
				O	0.66840300	0.16127800	-1.14932500
C	-0.67934400	2.36104100	-1.14637400	C	-1.04339700	-1.39507100	-0.53692600
C	-1.44489300	1.47157200	1.05755900	Pd	2.42965900	-0.18979900	-0.12768100
C	-2.80750700	1.08238200	-1.01849400	Cl	2.17011200	1.87205600	1.14751800
H	-2.06926500	0.69363000	1.49809700	P	4.48610600	-0.63146900	0.91291300
H	-0.42161500	1.37998900	1.43002300	H	5.60407600	-0.84314400	0.05370000
H	-2.69518100	1.04619300	-2.10613400	H	5.00625200	0.34068000	1.81760000
H	-3.24713300	0.14340800	-0.69059300	H	4.54138300	-1.81167100	1.71064200
H	0.27854200	2.48046000	-0.64040000	Cl	2.73648500	-2.32816400	-1.21035800
H	-0.47463800	2.05055400	-2.17191000	H	-0.32216100	-2.15739700	-0.83559400
C	-2.02862300	2.89112200	1.29697800	C	-2.33239900	-1.91870200	0.00149400
H	-1.23371400	3.57856700	1.60919900	C	-3.22852800	-2.60055800	-0.86033400
H	-2.76587700	2.84993700	2.10797900	C	-2.65034700	-1.86787200	1.38127900
C	-1.57305800	3.62672200	-1.05755800	C	-4.41508200	-3.17423700	-0.36986200
H	-2.01976100	3.85878100	-2.03305800	H	-2.98497000	-2.67768200	-1.91779700
H	-0.94903700	4.48225000	-0.77425300	C	-3.83843900	-2.44057500	1.87529700
C	-3.64221700	2.30642300	-0.54640900	H	-1.94011900	-1.42230400	2.07386800
H	-4.23202000	2.69032100	-1.38734600	C	-4.73062800	-3.08940000	1.00108000
H	-4.34974000	2.00612900	0.23664200	H	-5.08720400	-3.69016200	-1.05201600
C	-2.68659000	3.39926900	-0.00906100	H	-4.05586800	-2.39539200	2.94023400
H	-3.23636000	4.32857800	0.17674100	H	-5.64582500	-3.53634200	1.38209200

Enolate-Sc(III) Complex



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geom=connectivity
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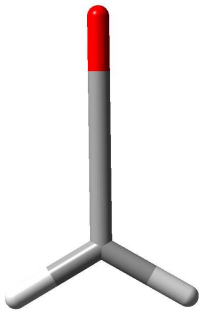
Zero-point correction=                          0.241176
(Hartree/Particle)
 Thermal correction to Energy=                    0.258048
 Thermal correction to Enthalpy=                  0.258992
 Thermal correction to Gibbs Free Energy=         0.193555
 Sum of electronic and zero-point Energies=           -573.256283
 Sum of electronic and thermal Energies=              -573.239411
 Sum of electronic and thermal Enthalpies=            -573.238467
 Sum of electronic and thermal Free Energies=         -573.303904
N              -1.79354600    0.69783400   -0.02796700
 C             -1.70326600   -0.18291700    1.24637900
 C             -1.73959700   -0.20569000   -1.28615600
 C             -3.13879200    1.42591800   -0.01996100
 H             -1.93133700    0.46112900   -2.13253500
 H             -0.72198100   -0.58722600   -1.37162000
 H             -3.18656700    1.99129700    0.91425800
 H             -3.13089900    2.12882700   -0.85589200
 H             -0.76447600   -0.73293600    1.18453200
 H             -1.62945200    0.51117700    2.08830100
 C             -2.79036000   -1.34085500   -1.16478300
 H             -2.28780200   -2.30156800   -1.00718100
 H             -3.35292400   -1.41820300   -2.10209400
 C             -2.94050600   -1.11605100    1.33784500
 H             -3.57701500   -0.82761500    2.18302000
 H             -2.60400300   -2.14234300    1.51905200
 C             -4.29977700    0.39703500   -0.14308400
 H             -5.05129500    0.60236400    0.62766500
 H             -4.79457900    0.50027000   -1.11591300
 C             -3.74283400   -1.03810100    0.01707500
 H             -4.56592000   -1.75985700    0.03420800
 C             -0.57519300    1.64071300   -0.04310600
 O              0.55169200    0.94400500   -0.06042400
 C             -0.70719200    2.98281000   -0.02758300
 H              0.19740200    3.58082300   -0.03193700
 H             -1.65360100    3.50341600   -0.00638300
 Cl             1.77672500   -1.61672000   -1.79123800
 Cl             4.08525500    1.19949200   -0.16710000
 Sc             2.16276300   -0.11912200   -0.00221400
 Cl             1.87936200   -1.27818700    2.03471600
```

Ketene



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Zero-point correction=                          0.031749
(Hartree/Particle)
 Thermal correction to Energy=                  0.035222
 Thermal correction to Enthalpy=                0.036166
 Thermal correction to Gibbs Free Energy=       0.008136
 Sum of electronic and zero-point Energies=          -152.541492
 Sum of electronic and thermal Energies=             -152.538019
 Sum of electronic and thermal Enthalpies=           -152.537075
 Sum of electronic and thermal Free Energies=        -152.565104
 C                  0.00000400   -1.22810300    0.00000000
 H                 -0.93663800   -1.77455200    0.00000000
 H                  0.93665100   -1.77454100    0.00000000
 C                  0.00000000    0.09539400    0.00000000
 O                 -0.00000400    1.29316800    0.00000000
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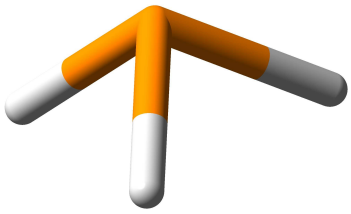
Phosphine



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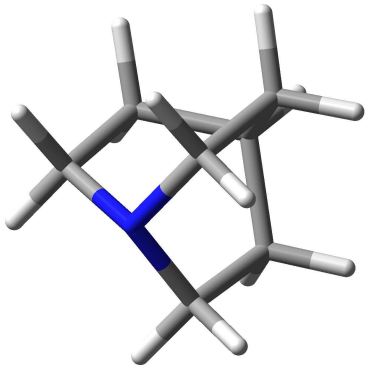
 ----------------------------------------
Zero-point correction=                          0.023288 (Hartree/Particle)
 Thermal correction to Energy=                  0.026193
 Thermal correction to Enthalpy=                0.027137
 Thermal correction to Gibbs Free Energy=       0.003234
 Sum of electronic and zero-point Energies=          -8.246579
 Sum of electronic and thermal Energies=             -8.243674
 Sum of electronic and thermal Enthalpies=           -8.242729
 Sum of electronic and thermal Free Energies=        -8.266633
 P                  0.00000000    0.00000000    0.12903200
 H                  0.00000000    1.22363800   -0.64515800
 H                  1.05970200   -0.61181900   -0.64515800
 H                 -1.05970200   -0.61181900   -0.64515800
```

Quinuclidine



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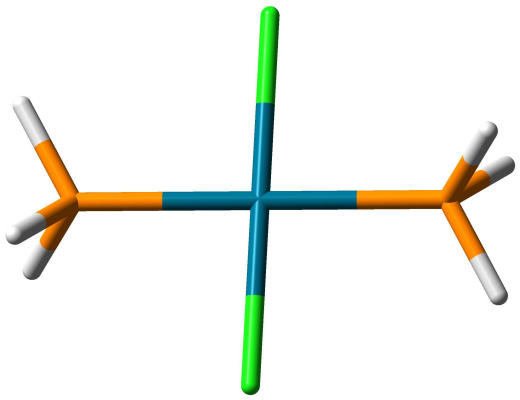
 Will use up to    2 processors via shared memory.
 ----------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ----------------------------------------
Zero-point correction=                          0.195826
(Hartree/Particle)
 Thermal correction to Energy=                  0.202390
 Thermal correction to Enthalpy=                0.203334
 Thermal correction to Gibbs Free Energy=       0.165264
 Sum of electronic and zero-point Energies=          -329.055242
 Sum of electronic and thermal Energies=             -329.048678
 Sum of electronic and thermal Enthalpies=           -329.047734
 Sum of electronic and thermal Free Energies=        -329.085804
 N            -1.29824700    0.00737500   -0.00177300
 C            -0.80808100   -0.31327700    1.36936500
 C            -0.79612000    1.34984400   -0.41190500
 C            -0.80835800   -1.02423700   -0.96108500
 H            -1.20408300    1.57349300   -1.40518500
 H            -1.20670600    2.09118300    0.28454100
 H            -1.22492900   -1.99241700   -0.65738400
 H            -1.21906500   -0.78743300   -1.95023400
 H            -1.21670700    0.43635400    2.05803000
 H            -1.22640200   -1.28513100    1.65862900
 C             0.77595500    1.39246800   -0.42277600
 H             1.15312000    2.15773600    0.26983000
 H             1.15497300    1.64583500   -1.42258900
 C             0.76384300   -0.33490800    1.42250800
 H             1.13244000   -1.31959700    1.74207200
 H             1.14280200    0.40217100    2.14409300
 C             0.76361000   -1.06973200   -0.99635600
 H             1.13384800   -2.06588800   -0.71658800
 H             1.13998800   -0.85664700   -2.00661900
 C             1.29797200   -0.00661300    0.00194800
 H             2.39552900   -0.01255600    0.00362700
```

trans-$(Ph_3)_2PdCl_2$



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 Gaussian 03:  IA32L-G03RevD.01 13-Oct-2005
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 Will use up to    2 processors via shared memory.
 ---------------------------------------
 # opt=calcfc freq=noraman b3lyp/lanl2dz
 ---------------------------------------
Zero-point correction=                          0.055935
(Hartree/Particle)
 Thermal correction to Energy=                  0.066926
 Thermal correction to Enthalpy=                0.067870
 Thermal correction to Gibbs Free Energy=       0.016476
 Sum of electronic and zero-point Energies=          -173.248526
 Sum of electronic and thermal Energies=             -173.237535
 Sum of electronic and thermal Enthalpies=           -173.236591
 Sum of electronic and thermal Free Energies=        -173.287985
 Pd             0.00000000   -0.00000200   -0.00014100
 P             -2.29324100    0.65684200    0.00011100
 H             -3.07821700    0.19433400   -1.09608700
 H             -3.07696200    0.19722000    1.09844200
 H             -2.59290100    2.05014300   -0.00149100
 P              2.29324300   -0.65683700    0.00009300
 H              2.59290900   -2.05013400   -0.00293300
 H              3.07873700   -0.19303200   -1.09519000
 H              3.07644100   -0.19851000    1.09933400
 Cl            -0.74973600   -2.28435300    0.00003900
 Cl             0.74973400    2.28435200    0.00004000
```

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