Perfluorinated TADDOL Phosphoramidite as an L,Z-Ligand on Rh(I) and Co(-1): Evidence for Bidentate Coordination via Metal-C_6F_5 Interaction

Derek M. Dalton, Anthony K. Rappé and Tomislav Rovis*

Department of Chemistry, Colorado State University, Ft. Collins, CO 80523

rovis@lamar.colostate.edu

Supporting Information

1. General Methods

Toluene, tetrahydrofuran, ether, and dichloromethane were degassed with argon and passed through one column of neutral alumina and one column of Q5 reactant. Triethylamine (peptide synthesis grade) was purchased from Fisher Scientific, dried over calcium hydride and freshly distilled prior to use. Flash column chromatography was carried out on silica gel (60 Å, 230 - 400 mesh, obtained from Silicycle Inc.) and was performed with reagent grade solvents. Analytical thin-layer chromatography (TLC) was performed on Silicycle glass-backed silica gel plates (60 Å, 0.25 mm, purchased from Silicycle Inc.) and visualized with a UV lamp (254 nm), and potassium permanganate or cerric ammonium molybdate.

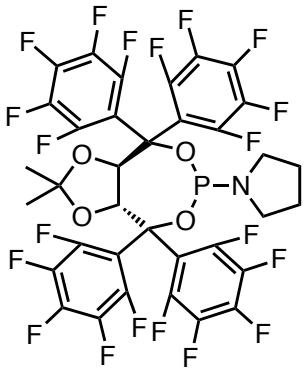
Infrared spectra (IR) were obtained on a Nicolet Avatar 320 FT-IR spectrometer and Bruker Tensor 27 FT-IR spectrometer. ^{1}H NMR and ^{13}C NMR were obtained on Varian Unity 300 and Unity 400 spectrometers. Chemical shifts are expressed in parts per million values (δ, ppm). Proton chemical shifts in CDCl3 were referenced to 7.26 ppm (CHCl3). Carbon chemical shifts were referenced to 77.2 ppm (CDCl3). Peak multiplicities are designated by the following abbreviations: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublets; dt, doublet of triplets; b, broad; *J*, coupling constant in Hz. Low resolution mass spectra (MS) and high resolution mass spectra (HRMS) were recorded on a Fisons VG Autospec spectrometer. HPLC spectra were obtained on an Agilent 1100 series system. Optical rotation was obtained with an Autopol-III automatic polarimeter. Melting points were obtained on a Fisher-Johns melting point apparatus and are uncorrected. References following the compound names indicate literature articles where the compound has been previously been reported.

Unless indicated, commercially available starting materials were purchased from Aldrich Chemicals and used without further purification. $[Rh(ethylene)_2Cl]_2$ and cobalt carbonyl were purchased from Strem Chemicals or Alfa Aesar and used without further purification.

2. General Procedure for Ligand Synthesis

Taddol diols were prepared from diethyl-tartrate according to literature procedures.[1]

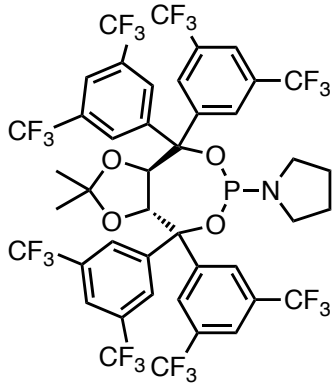
To a flame-dried round bottom flask equipped with a magnetic stirbar under an Ar atmosphere was added the desired amine (pyrrolidine: 0.20 ml, 2.42 mmol, 1 equiv.) and tetrahydrofuran (THF, anhydrous, 40 ml). The reaction vessel is cooled to 0 °C and *n*-butyl lithium (1.6 ml, 1.6 M in hexanes) is added dropwise via syringe. The solution is stirred for 30 minutes at 0 °C before phosphorous trichloride (0.22 ml, 2.52 mmol, 1.0 equiv.) is added in one portion via syringe. After stirring an additional 15 minutes, a solution of Taddol diol (2.0 g, 2.42 mmol, 1 equiv.), and triethylamine (1.0 ml, 7.19 mmol, 3.0 equiv.) in THF (10 ml) is added via syringe. The flask is allowed to warm to room temperature, stirred for 3 hours, and solvent is removed by rotary evaporation. Toluene (50 ml) is then added to the resultant residue and the slurry is filtered through alumina and washed with toluene (2x). Solvent is removed from the combined filtrates by rotary evaporation. If necessary, the product can be further purified by column chromatography (19:1 Hexanes/EtOAc) to yield a white foam powder (1.1g, 51% yield, CKPhos).



[1] For the synthesis of the Taddol diol precursors see: Seebach, D.; Beck, A.K.; Keckel, A. *Angew. Chem. Int. Ed.* **2001**, *40*, 92. Burks, H.E.; Shubin, L.; Morken, J.P. *J. Am. Chem. Soc.* **2007**, 129, 28, 8766.

1-((3aR,8aR)-2,2-dimethyl-4,4,8,8-tetrakis(perfluorophenyl)tetrahydro-[1,3]dioxolo[4,5-e][1,3,2]dioxaphosphepin-6-yl)pyrrolidine (CKphos).

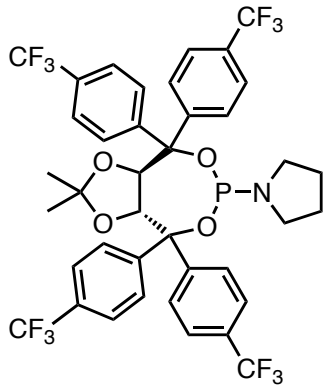
General procedure yielded a white solid (51 %). $[\alpha]^{20}_{D}$ = -109°, c = 0.01 g/ml $CHCl_3$. Rf = 0.46 (19:1, Hex/EtOAc). ^{1}H-NMR (400 MHz; $CDCl_3$): δ 5.59 (1H, d, *J* = 7.8 Hz), 5.31 (1H, d, *J* = 8.2 Hz), 3.12 (2H, dd, *J* = 9.7, 5.7 Hz), 2.79 (2H, dd, *J* = 9.4, 5.4 Hz), 1.70-1.59 (4H, m), 1.08 (3H, s), 0.72 (3H, s). ^{13}C-NMR (100 MHZ; $CDCl_3$): δ 146.3, 143.8, 142.3, 139.7, 139.0, 136.5, 117.7, 113.3, 80.6, 80.5, 80.4, 45.6, 45.4, 45.1, 26.3, 26.2, 26.0, 25.9, 25.8. ^{31}P-NMR (75 MHz; $CDCl_3$): δ 138.6. ^{19}F-NMR (376 MHz; $CDCl_3$): δ −131.2 (1F, d), -133.7 (1F, m), -135.8 (1F, d), -137.6 (2F, m), -139.2 (1F, d), -140.1 (1F, d), -151.8 (1F, t), -152.1 (1F, t), -152.3 (1F, t), -152.9 (1F, t), -160.4 (1F, m), -160.7 (1F, m), -161.1 to -161.4 (5F, m), -161.8 (1F, dt), -162.1 (1F, m). IR (Thin Film) v 2988, 2876, 1651, 1525, 1487, 1409, 1384, 1374, 1346, 1308, 1240, 1131, 985, 862, 807, 743, 703. HRMS (ESI) m/z $[C_{35}H_{17}F_{20}NO_4P]$+ calculated 925.0498, found 925.0508.



1-((3aR,8aR)-4,4,8,8-tetrakis(3,5-bistrifluoromethylphenyl)-2,2-dimethyltetrahydro-[1,3]dioxolo[4,5-e][1,3,2]dioxaphosphepin-6-yl)pyrollidine (T8)

General procedure yielded a white solid (72 %). $[\alpha]^{20}_{D}$ = -65°, c = 0.01 g/ml $CHCl_3$. Rf = 0.5 (19:1, Hex/EtOAc). ^{1}H-NMR (400 MHz; $CDCl_3$): δ 8.26 (2H, s), 8.01 (2H, s), 7.84 (8H, q, J =

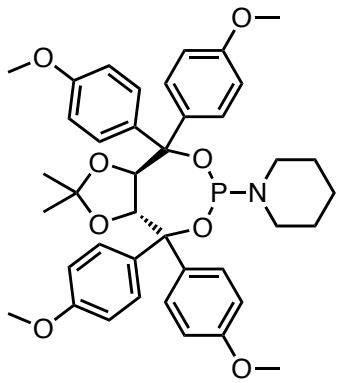
8.7 Hz), 4.96-4.93 (1H, dd, J = 8.7, 3.8 Hz), 4.30 (dd, J = 8.7, 1.1 Hz), 3.41 (2H, quintet, J = 6.9 Hz), 3.30 (2H, quintet, J = 7.0 Hz), 1.97-1.89 (4H, m) 1.49 (3H, s) 0.310 (3H, s). ^{13}C-NMR (100 MHz; $CDCl_3$): δ 147.3, 146.4, 142.6, 141.8, 131.8 (m), 128.5 (d), 126.9, 126.6, 124.3, 122.7 (m), 122.3 (m), 121.6, 118.9, 82.8, 81.8, 81.5, 80.0, 79.9, 79.3, 45.0, 26.9, 26.0, 25.1. ^{19}F-NMR (376 MHz; $CDCl_3$): δ 63.1 (q). ^{31}P-NMR (75 MHz; $CDCl_3$) δ 139.4. IR (Thin Film) v 3103, 2969, 2879, 1625, 1467, 1374, 1338, 1279, 1176, 1133, 1047, 1014, 904, 879, 848, 779, 709, 683. HRMS (ESI) *m/z* $[C_{43}H_{29}F_{24}NO_4P]^+$ calculated 1109.1373, found 1109.1364.



1-((3aR,8aR)-2,2-dimethyl-4,4,8,8-tetrakis(4-(trifluoromethyl)phenyl)tetrahydro-[1,3]dioxolo[4,5-e][1,3,2]dioxaphosphepin-6-yl)pyrrolidine (T7)

General procedure yielded a white solid (56%). $[\alpha]^{20}_D$ = -87°, c = 0.01 g/ml $CHCl_3$. Rf = 0.34 (19:1, Hex/EtOAc). ^{1}H-NMR (400 MHz; $CDCl_3$): δ 7.87 (2H, d, *J* = 8.3 Hz), 7.70 (2H, d, *J* = 8.4 Hz), 7.63-7.50 (12H, m), 5.12 (1H, dd, *J* = 8.6, 3.4 Hz), 4.64 (1H, d, *J* = 8.6 Hz), 3.40 (2H, quintet, 7.2 Hz), 3.26 (2H, quintet, 7.3 Hz), 1.87 (4H, m), 1.34 (3H, s), 0.32 (3H, s). ^{13}C-NMR (100 MHz; $CDCl_3$): δ 147.8, 147.1, 143.3, 142.7, 128.4, 128.2, 128.1, 128.0, 127.9 127.8, 127.7, 127.6, 127.3, 127.0, 126.9, 126.7, 125.8 125.4, 125.3, 123.5, 123.5, 123.4, 123.3, 123.0, 123.0, 122.9, 122.9, 122.8, 122.3, 122.3, 120.7, 120.6, 110.4, 80.3, 80.3, 80.1, 79.8, 79.0, 18.7, 78.6,

43.1, 43.0, 25.5, 24.1, 24.0, 23.3. ^{19}F-NMR (376 MHz; $CDCl_3$): δ -62.7 (q). ^{31}P-NMR (75 MHz; $CDCl_3$): δ 139.0. IR (Thin Film) v 2991, 2939, 2876, 1929, 1619, 1458, 1375, 1166, 1126, 1070, 1009, 909, 881, 851, 780, 733. HRMS (ESI) *m/z* $[C_{39}H_{33}F_{12}NO_4P]^+$ calculated 837.1877, found 837.1877.



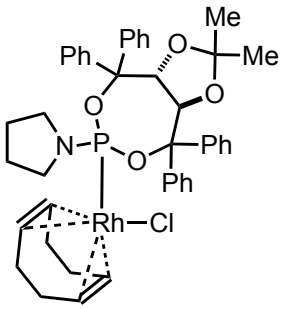
1-((3a*R*,8a*R*)-4,4,8,8-tetrakis(4-methoxyphenyl)-2,2-dimethyltetrahydro-[1,3]dioxolo[4,5-*e*][1,3,2]dioxaphosphepin-6-yl)piperidine (T4)

Synthesized according to the general ligand procedure with the following modifications to yield a white solid (35 %). After removal of THF, the product was further purified by column chromatography on neutral alumina (19:1 to 9:1 Hex/EtOAc). $[\alpha]^{20}_D$ = -94.5°, c = 0.01 g/ml $CHCl_3$. Rf = 0.10 (9:1, Hex/EtOAc). ^{1}H-NMR (400 MHz; $CDCl_3$): δ 7.69 (2H, d, *J* = 8.8 Hz), 7.51 (2H, d, *J* = 8.8 Hz), 7.34 (4H, dd, *J* = 18.0, 8.8 Hz), 6.81 (8H, td, *J* = 9.6, 5.9 Hz), 5.06 (1H, dd, *J* = 8.5, 3.3 Hz), 4.70 (1H, d, *J* = 8.5 Hz), 3.78 (12H, m), 3.27 (2H, m), 3.16 (2H, m), 1.59 (3H, s), 1.33 (3H, s). ^{13}C-NMR (100 MHZ; $CDCl_3$): δ 158.6, 158.5, 158.4, 158.3, 139.7, 139.3, 134.7, 134.4, 130.1, 130.0, 129.9, 128.2, 113.3, 112.9, 112.7, 112.4, 111.3, 98.3, 82.9, 82.8, 82.6, 82.4, 55.1, 45.0, 44.9, 27.6, 27.0, 25.5, 25.2. ^{31}P-NMR (75 MHZ; $CDCl_3$): δ 138.6. IR (Thin

Film) v 2994, 2934, 2836, 1609, 1582, 1509, 1462, 1372, 1301, 1251, 1214, 1176, 1092, 1035, 949, 880, 787, 739, 712. MS (LR-ES) *m/z* $[C_{40}H_{46}NO_8P]^+$ calculated 700.3, found 700.4.

3. Synthesis of Rh(cod)Cl·Phosphoramidite Complexes

To an oven-dried 3 ml vial flushed with argon was added rhodium(cod)chloride dimer (1 equiv.) and phosphoramidite ligand (2 equiv.). Solids were dissolved in $CDCl_3$ and stirred until homogenous under argon. Spectra were collected promptly after the solution was made. Complex in solution slowly decomposed over time (hours) when exposed to air.



Rh(cod)Cl•T4 Complex

General procedure yielded a yellow solution. ^{1}H-NMR (400 MHz; $CDCl_3$): δ 7.96 (2H, d, *J* = 7.3 Hz) 7.51 (2H, t, *J* = 7.6 Hz) 7.42 (3H, m) 7.31 (2H, t, 7.6 Hz) 7.22 (3H, m) 7.13 (6H, m) 7.00 (2H, dt, *J* = 2.4, 5.0 Hz) 5.42 (1H, d, *J* = 8.0 Hz) 5.38 (1H, dd, *J* = 4.0, 7.5 Hz) 5.19 (1H, d, *J* = 8.0 Hz) 5.04 (1H, m) 4.00 (1H, m) 3.46 (1H, t, *J* = 6.9 Hz) 3.36 (2H, bs) 3.03 (2H, t, *J* = 6.7 Hz) 2.27 (1H, m) 2.17 (1H, m) 1.87 (2H, dd, *J* = 5.7, 13.2 Hz) 1.80 (1H, t, *J* = 9.0 Hz) 1.68 (2H, t, *J* = 9.0 Hz) 1.50 (1H, m) 1.33 (2H, m) 1.17 (2H, m) 0.44 (3H, s) 0.38 (3H, s). ^{13}C-NMR (100 MHz; $CDCl_3$): δ 144.6, 143.6, 142.0, 141.7, 129.2, 128.5, 128.0, 127.01, 126.83, 115.0, 109.1, 106.3, 98.4, 86.9, 86.1, 80.7, 78.7, 68.3, 67.6, 48.4, 33.3, 32.4, 28.6, 26.8, 26.4, 25.6. ^{31}P-NMR (75 MHz; $CDCl_3$): δ 144.6, 143.6.

Rh(cod)Cl•CKphos Complex

General procedure yielded a yellow solution. ^{1}H-NMR (400 MHz; $CDCl_3$): δ 5.76 (1H, d, *J* = 7.6 Hz) 5.64 (1H, d, *J* = 7.6 Hz) 5.49 (1H, m) 4.79 (1H, m) 4.13 (1H, bs) 3.84 (1H, bs) 3.02 (2H, bs)

2.41 (2H, m) 2.28 (1H, m) 2.18 (1H, dd J = 5.7, 15 Hz) 2.09 (3H, q, J = 7.4 Hz) 1.97 (1H, dt, J = 6.1, 13.0 Hz) 1.86 (1H, dt, J = 7.0, 14.2 Hz) 1.68 (1H, q, J = 7.8 Hz) 1.49 (6H, bs) 0.80 (3H, s) 0.73 (3H, s). ^{13}C-NMR (100 MHz; $CDCl_3$): δ 146.1, 143.6, 142.3, 138.9, 136.4, 116.0, 115.2, 113.4, 112.7, 109.7, 85.2, 83.3, 79.1, 78.7, 71.7, 69.2, 49.6, 34.4, 32.0, 30.8, 27.7, 26.4, 26.1. ^{31}P-NMR (75 MHz; $CDCl_3$): δ 116.5 (1P, dd, J = 5, 243 Hz). ^{19}F-NMR (376 MHz; $CDCl_3$): δ ^{19}F-NMR (376 MHz; $CDCl_3$): δ -124.63 (dd, J = 24.9, 4.8 Hz, 1F), -129.52 (d, J = 23.0 Hz, 1F), -131.90 (d, J = 23.0 Hz, 1F), -134.13 (d, J = 22.2 Hz, 1F), -138.01 (d, J = 22.0 Hz, 1F), -139.33 (d, J = 18.1 Hz, 1F), -140.30--140.34 (m, 1F), -143.66 (d, J = 22.8 Hz, 1F), -151.43--151.63 (m, 3F), -152.39 (t, J = 21.7 Hz, 1F), -157.19 (td, J = 23.3, 6.7 Hz, 1F), -160.44 (td, J = 22.2, 5.2 Hz, 1F), -160.68 (td, J = 21.7, 5.2 Hz, 1F), -160.89 (td, J = 21.5, 5.2 Hz, 1F), -161.71 (dddd, J = 40.0, 21.8, 20.3, 6.8 Hz, 3F), -162.99 (td, J = 22.3, 5.2 Hz, 1F).

4. General Procedure for Rhodium Catalyzed [2+2+2] Cycloadditions

Isocyanates and vinylogous amide indolizinone products not listed below were synthesized according to previously reported literature procedures.[2]

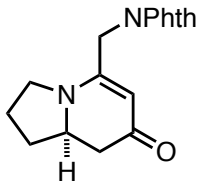
An oven-dried round bottom flask was charged with $[Rh(C_2H_4)_2Cl]_2$ (4 mg, 0.01 mmol) and ligand (20 mg, 0.02 mmol) and fitted with an oven-dried reflux condenser in an inert atmosphere (Ar) glove box. Upon removal from the glove box, 2 ml of toluene was added via syringe and the resulting yellow solution was stirred at ambient temperature for 5 min. To this solution, alkyne **1** (0.20 mmol, 1 equiv) and isocyanate **2** (0.26 mmol, 1.3 equiv) in 6 ml of toluene was added via syringe. An additional 2 ml of toluene was used to wash down the residue and added to the reaction mixture. The reaction mixture was heated to 110 °C in an oil bath and kept at reflux for 16 h. The reaction mixture was cooled to 23 °C, concentrated in *vacuo*, and purified by flash column chromatography (19:1 EtOAc:MeOH). Evaporation of solvent afforded the analytically pure products. Absolute stereochemistry was established as previously reported.[3,4]

---

[2] a) Dalton, D. M.; Oberg, K. M.; Yu, R. T.; Lee, E. E.; Perreault, S.; Oinen, M. E.; Pease, M. L.; Malik, G.; Rovis, T. *J. Am. Chem. Soc.* **2009**, *131,* 43, 15717-15728. b) Yu, R. T.; Lee, E. E.; Malik, G.; Rovis, T. *Angew. Chem. Int. Ed.* **2009**, *48*, 2379-2382. c) Lee, E. E.; Rovis, T. *Org. Lett.* **2008**, 10, 6, 1231-1234.

[3] Yu, R. T.; Rovis, T. *J. Am. Chem. Soc.* **2006**, *128*, 12370-12371

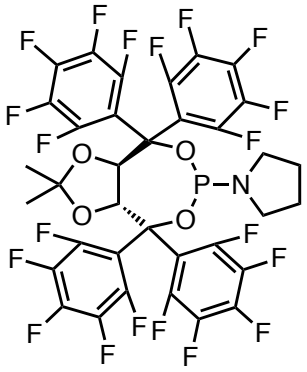
[4] Yu, R. T.; Lee, E. E.; Malik, G.; Rovis, T. *Angew. Chem. Int. Ed.* **2009**, *48*, 2379-2382.

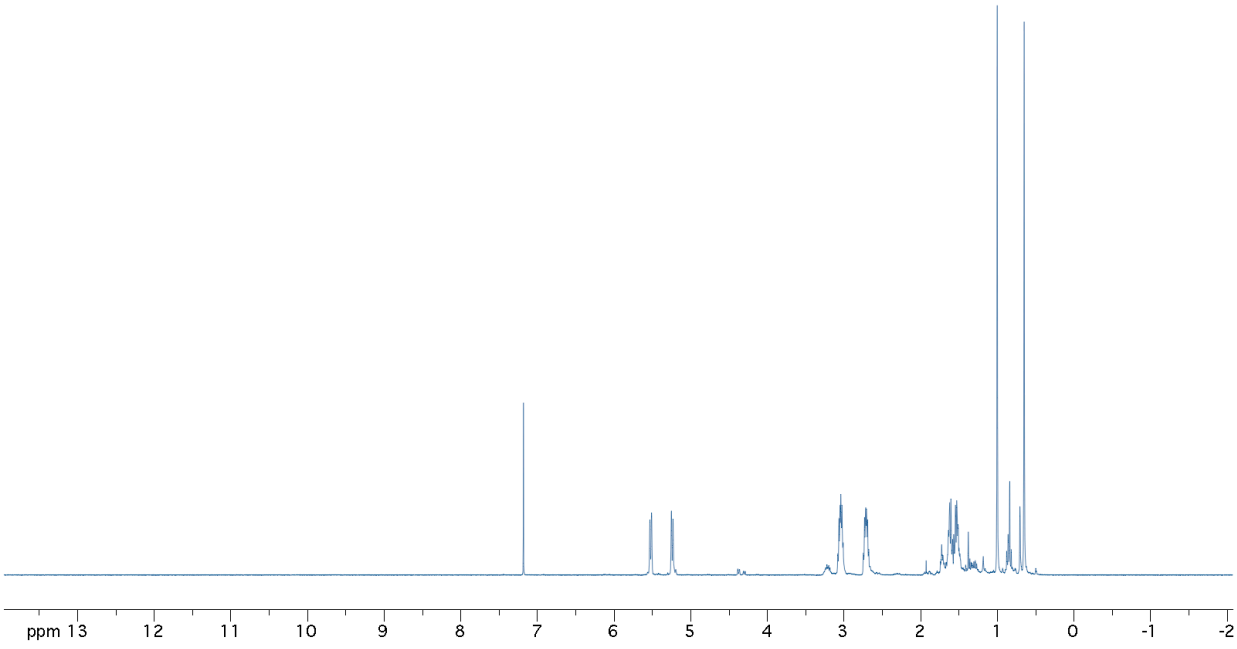


2-((7-oxo-1,2,3,7,8,8a-hexahydroindolizin-5-yl)methyl)isoindoline-1,3-dione (4f)

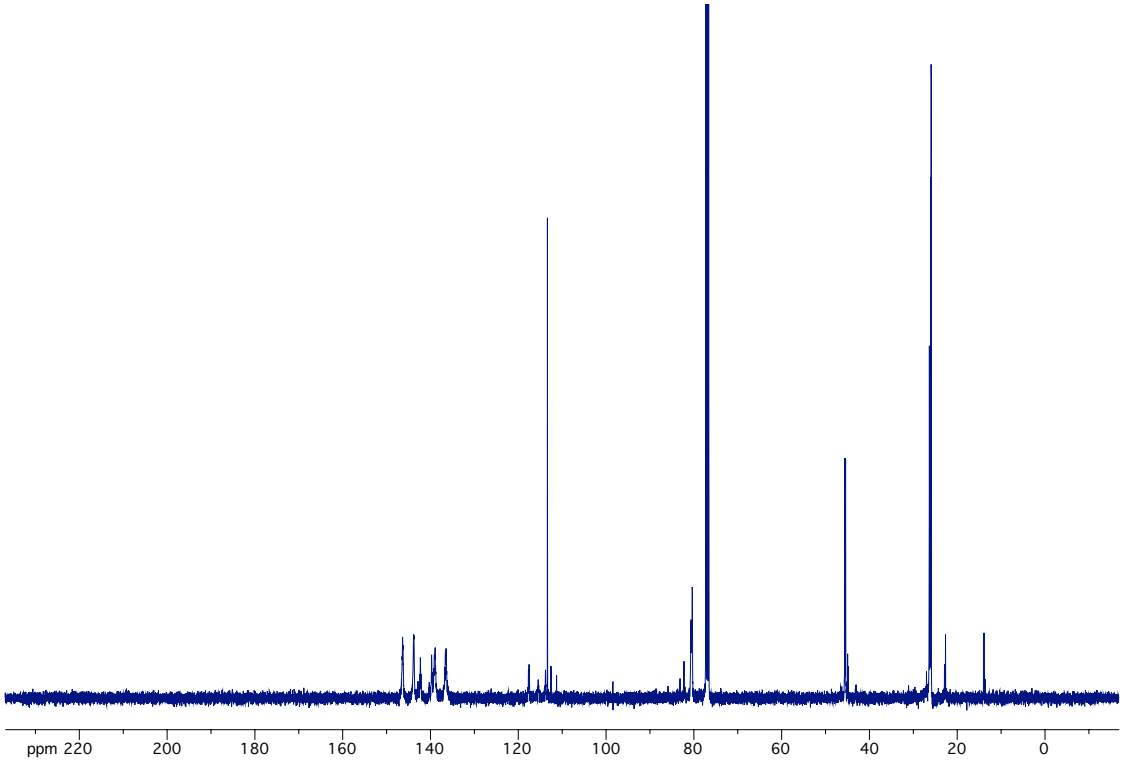
General procedure yielded a brown solid (71%). 98% ee by HPLC (Chiralcel ODH, Hex:iPrOH 70:30, 1 ml/min, RTmajor = 41.6 min, RTminor = 26.8 min). $[\alpha]^{20}_{D} = 152°$, c = 0.01 g/ml $CHCl_3$. Rf = 0.14 (EtOAc). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (2H, dd, *J* = 5.4, 3.1 Hz), 7.69 (2H, dd, *J* = 5.4, 3.0 Hz), 4.66 (1H, s), 4.41 (2H, q, *J* = 13.6 Hz), 3.75 (1H, ddt, *J* = 15.5, 10.3, 5.2 Hz), 3.61 (2H, dq, *J* = 24.9, 8.5 Hz), 2.34 (1H, dd, *J* = 16.0, 5.0 Hz), 2.24 (2H m), 2.13 (1H, dt, *J* = 12.7, 6.4 Hz), 1.90 (1H, m), 1.64 (1H, m). ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.7, 167.3, 157.3, 134.4, 131.7, 123.7, 98.3, 94.7, 59.5, 46.5, 41.2, 37.9, 32.2, 24.1. IR (Thin Film) v 2964, 2875, 2360, 1778, 1716, 1620, 1562, 1500, 1469, 1422, 1394, 1351, 1330, 1300, 1273, 1250, 1198, 1167, 1112, 1086, 989, 952, 859, 756. HRMS (ESI) *m/z* $[C_{17}H_{17}N_2O_3]^+$ calculated 297.1234, found 297.1234.

5. ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR, and ^{31}P-NMR Spectra

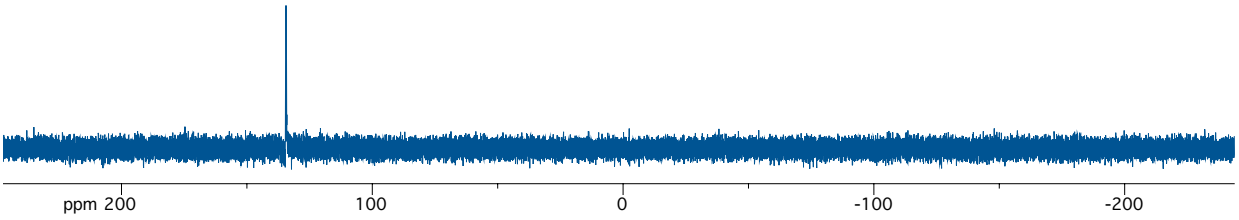




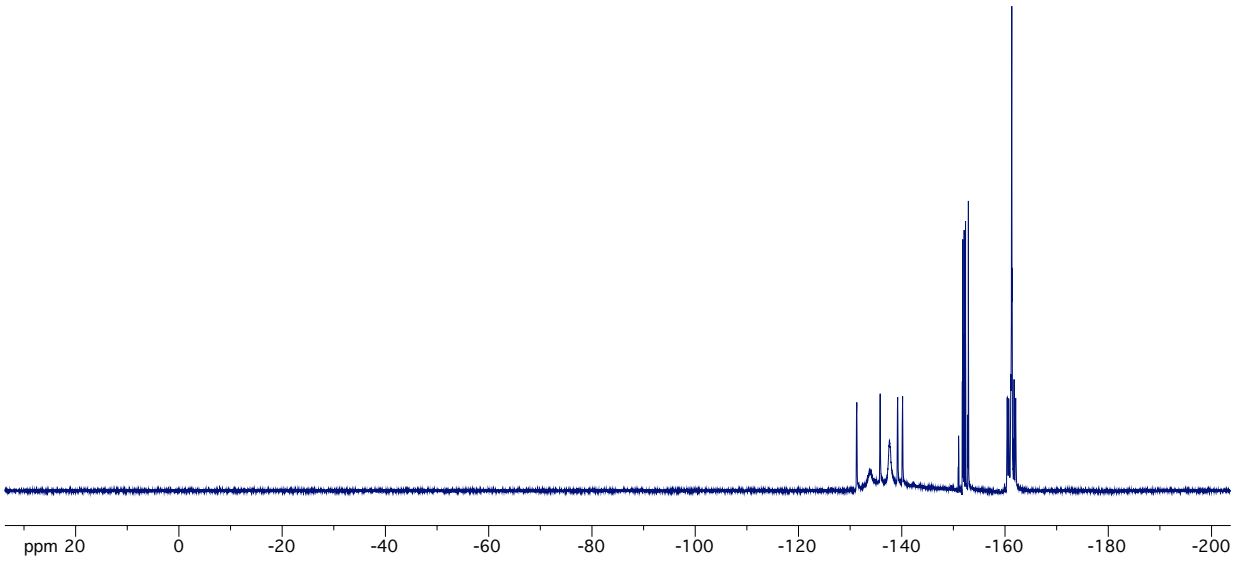
^{1}HNMR CKphos



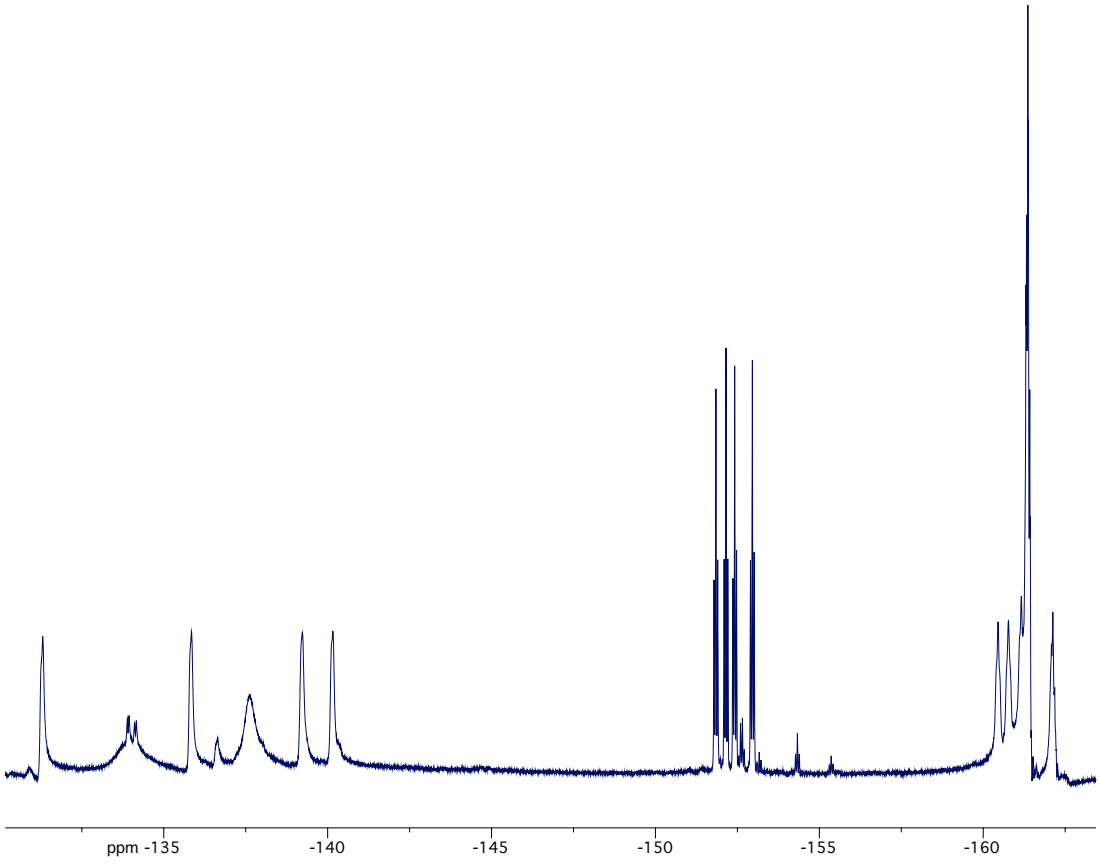
^{13}CNMR



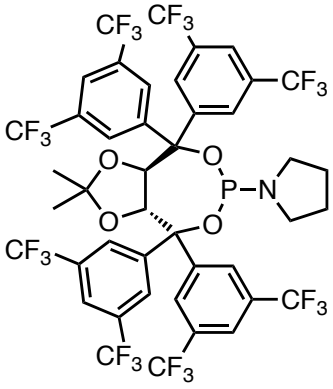
^{31}PNMR

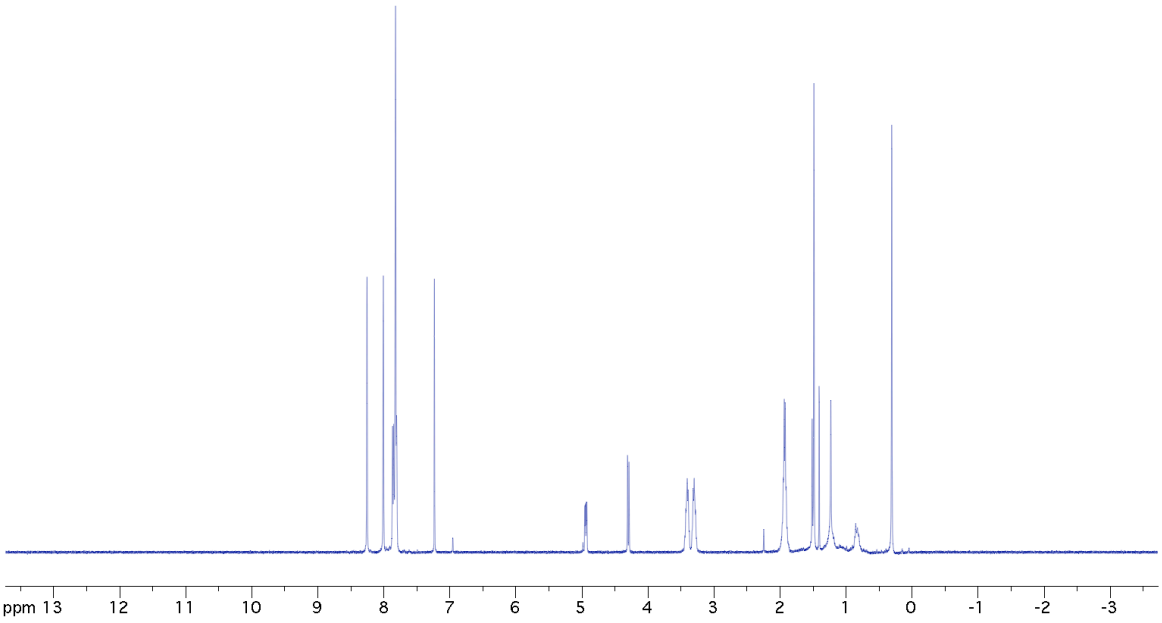


^{19}FNMR

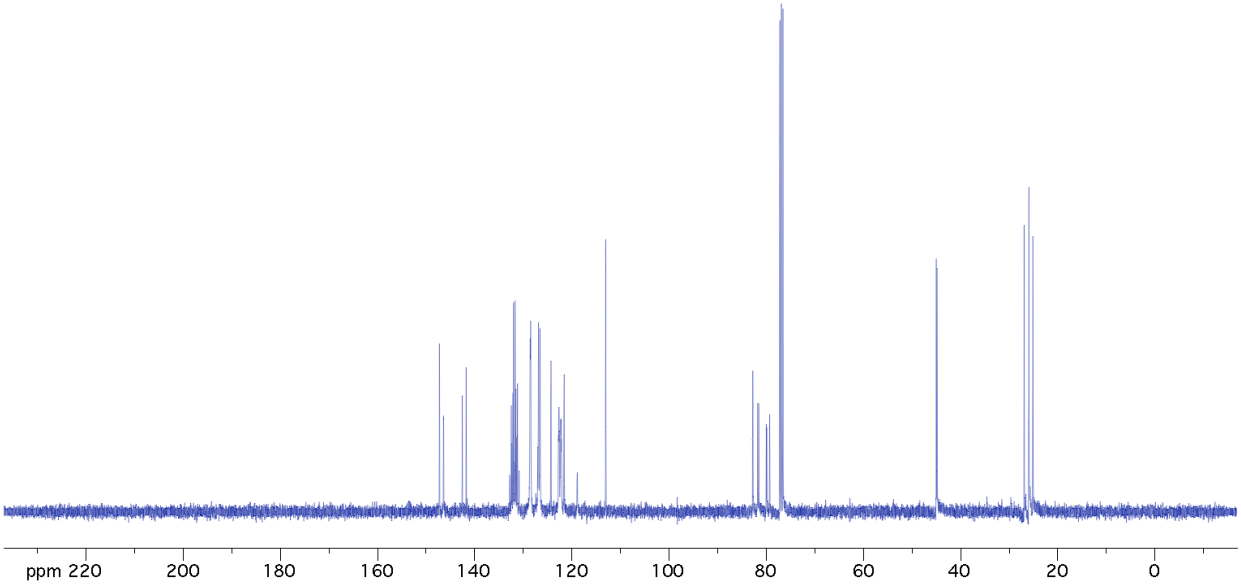


^{19}FNMR

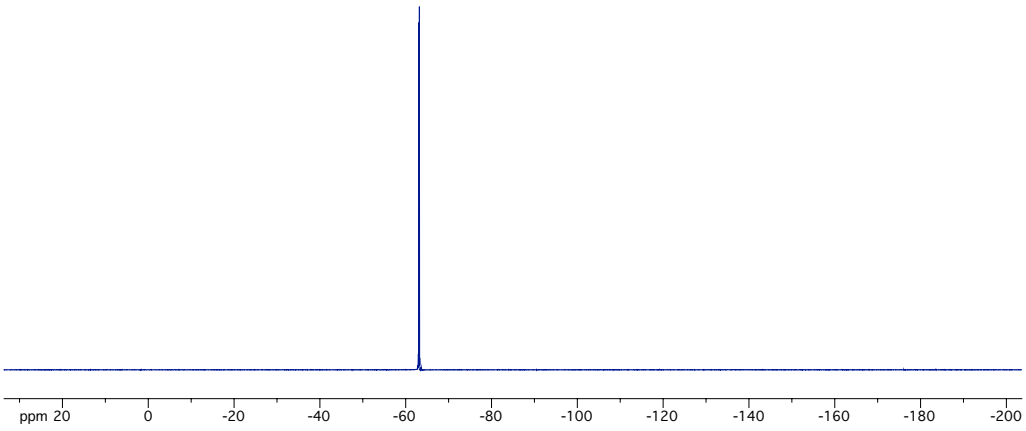

CF3
CF3
CF3
CF3
O
O
P
N
O
O
CF3
CF3
CF3
CF3


ppm 13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3

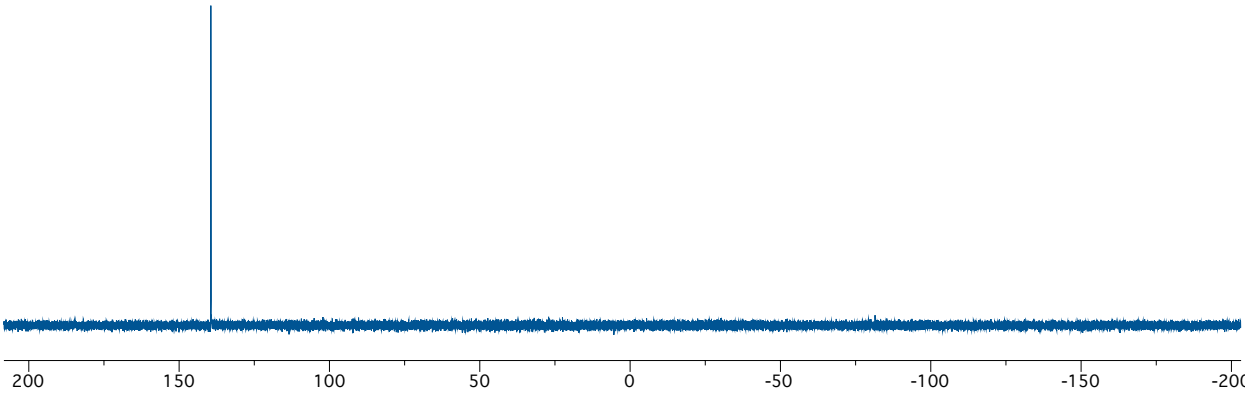
^{1}H-NMR



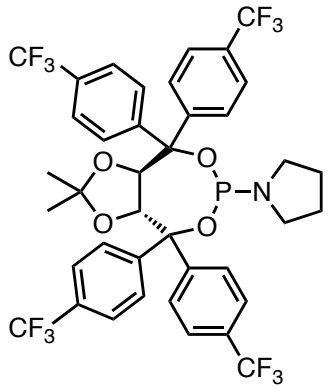
^{13}CNMR

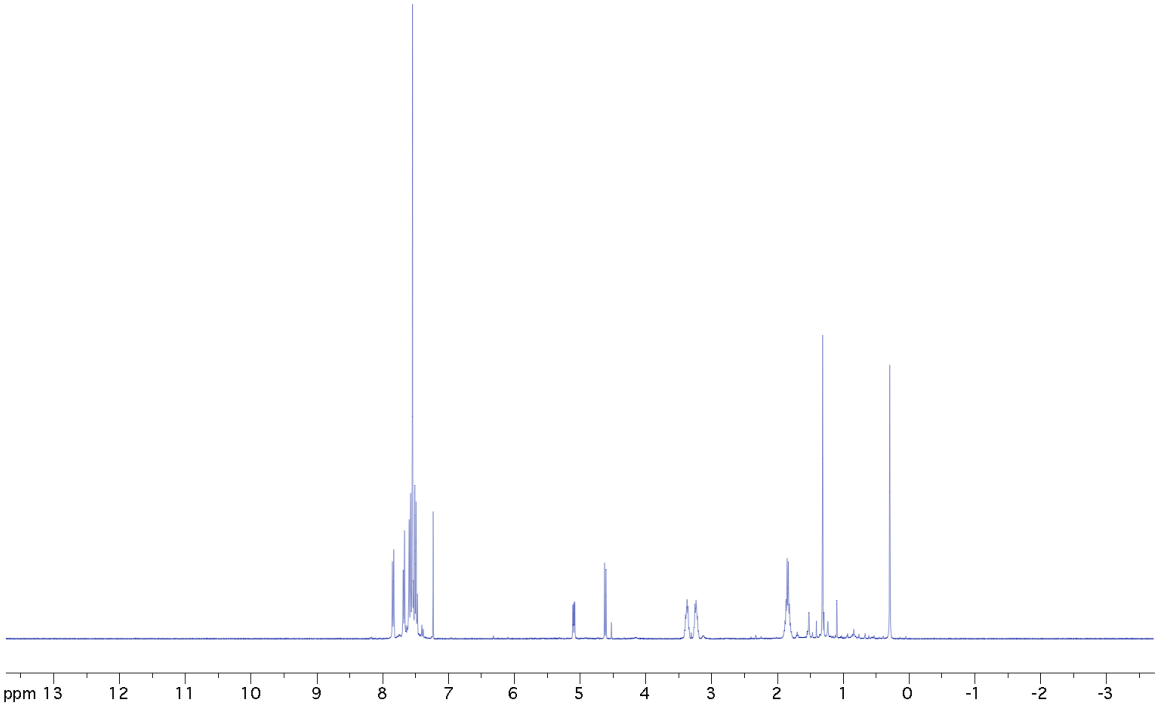


^{19}FNMR

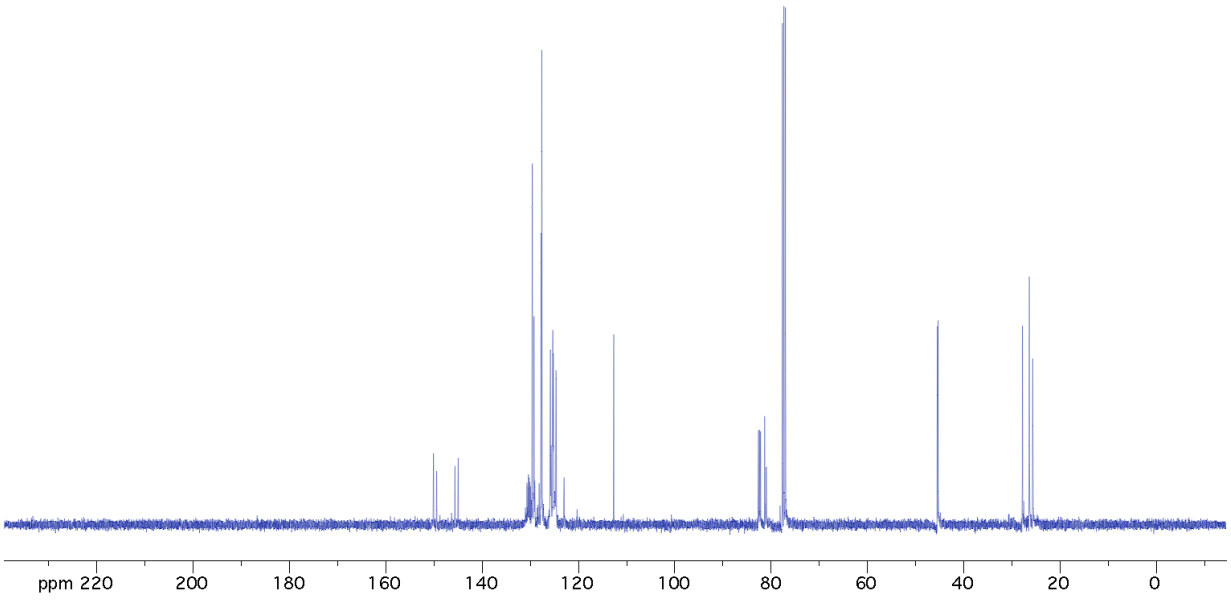


^{31}PNMR

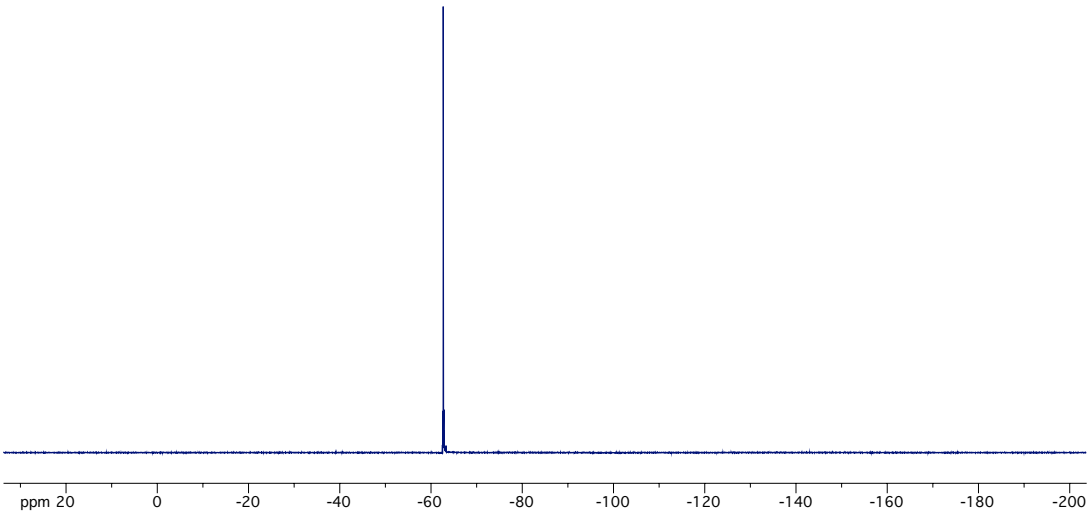




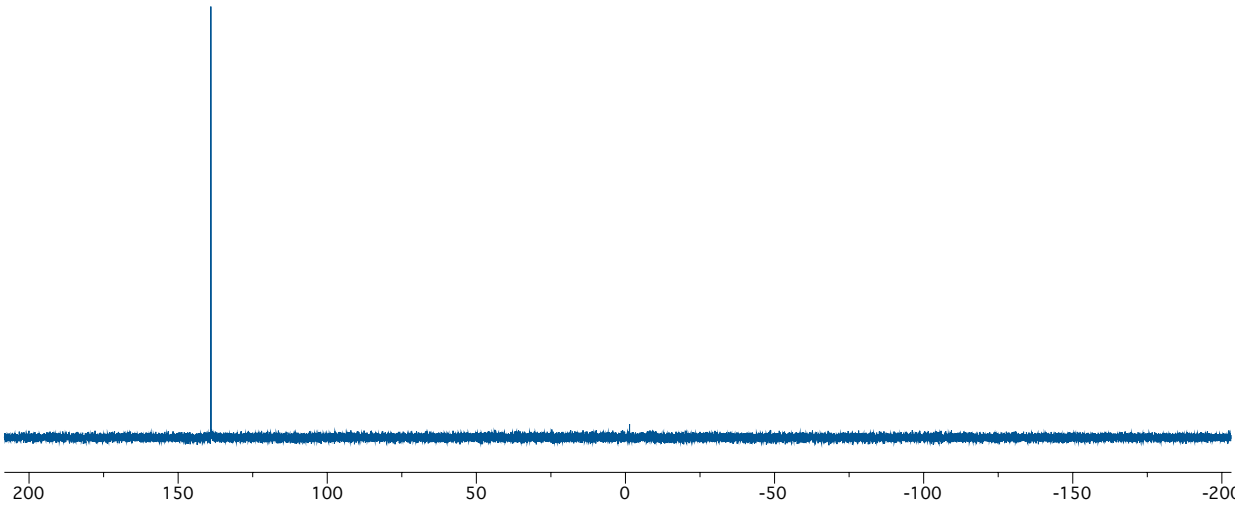
^{1}HNMR



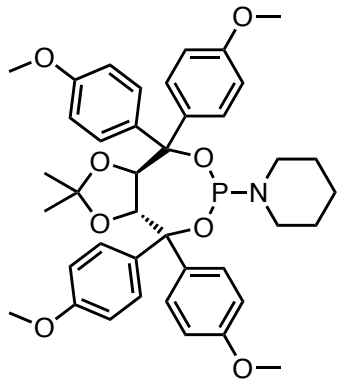
^{13}CNMR

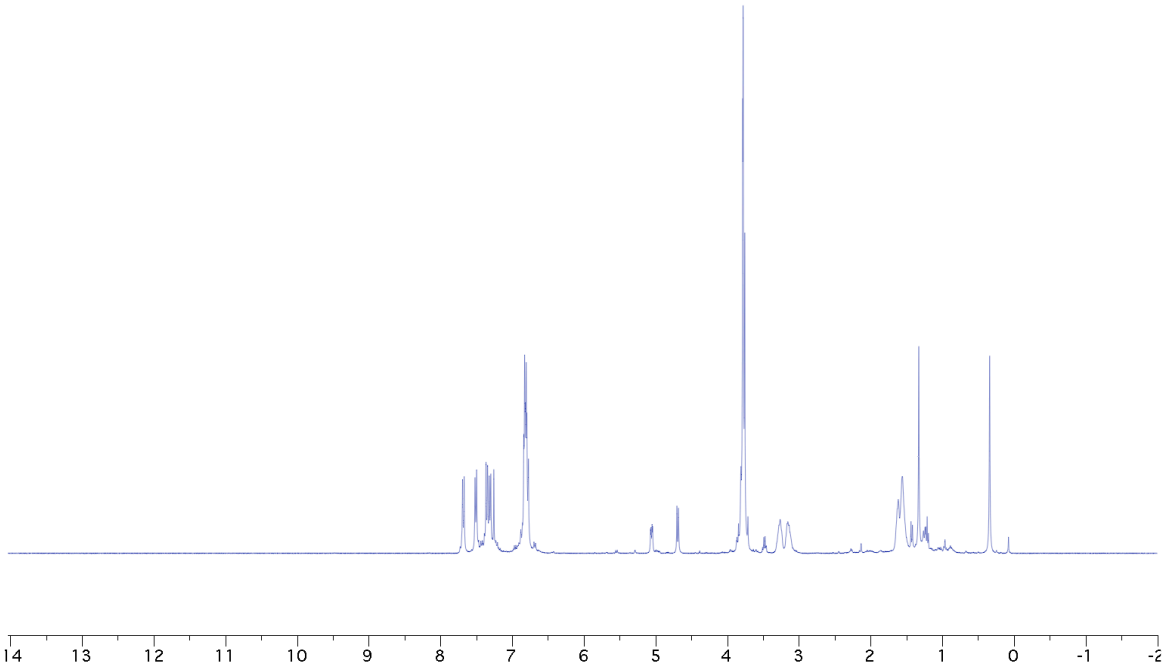


^{19}FNMR

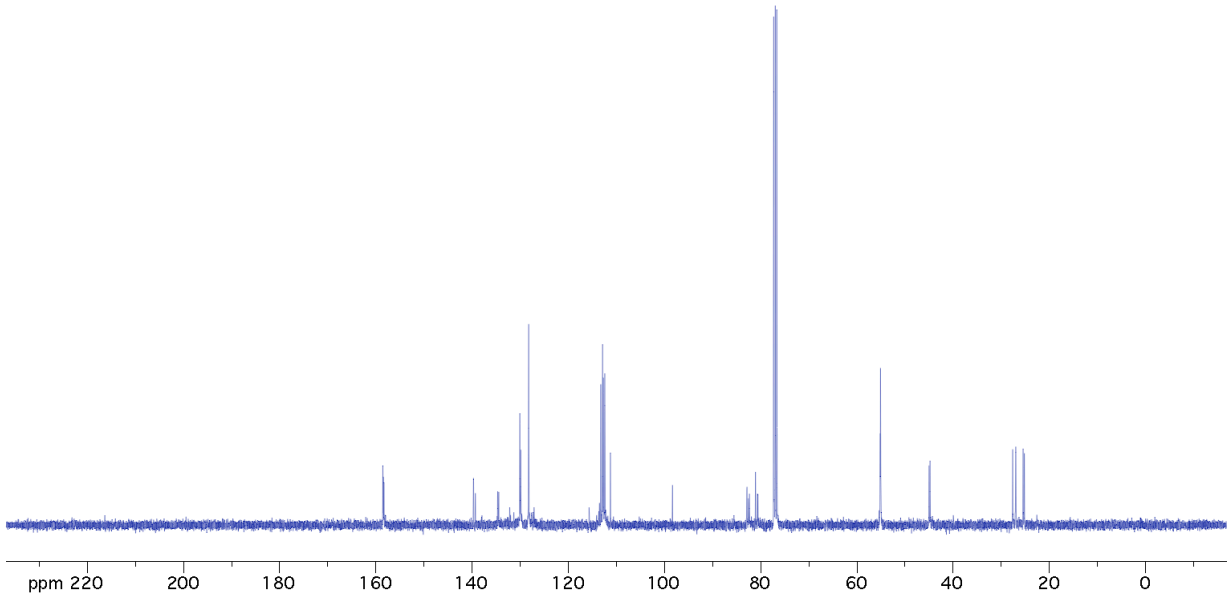


^{31}PNMR

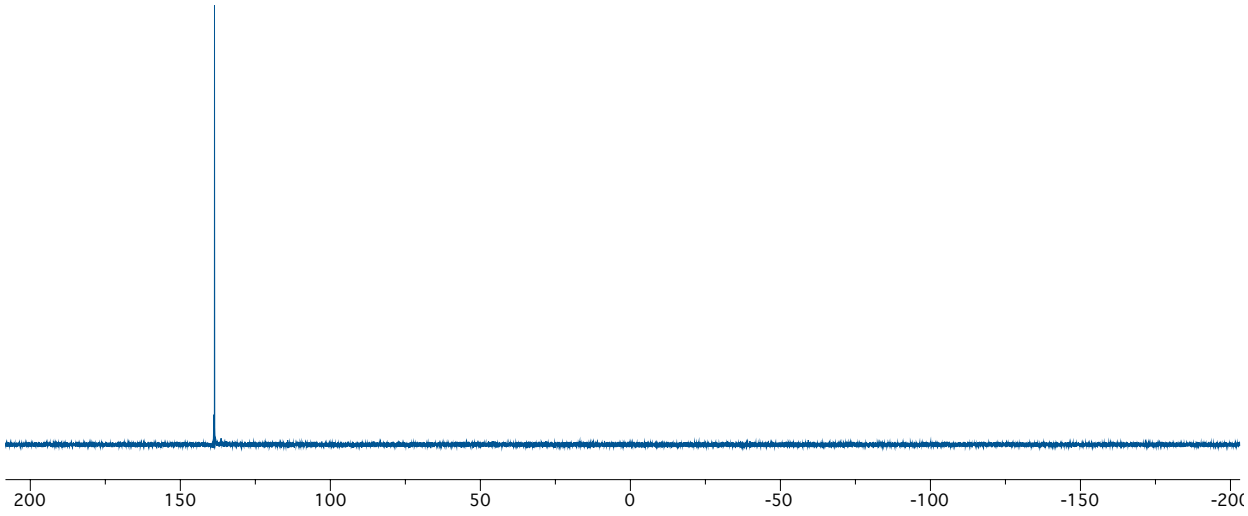




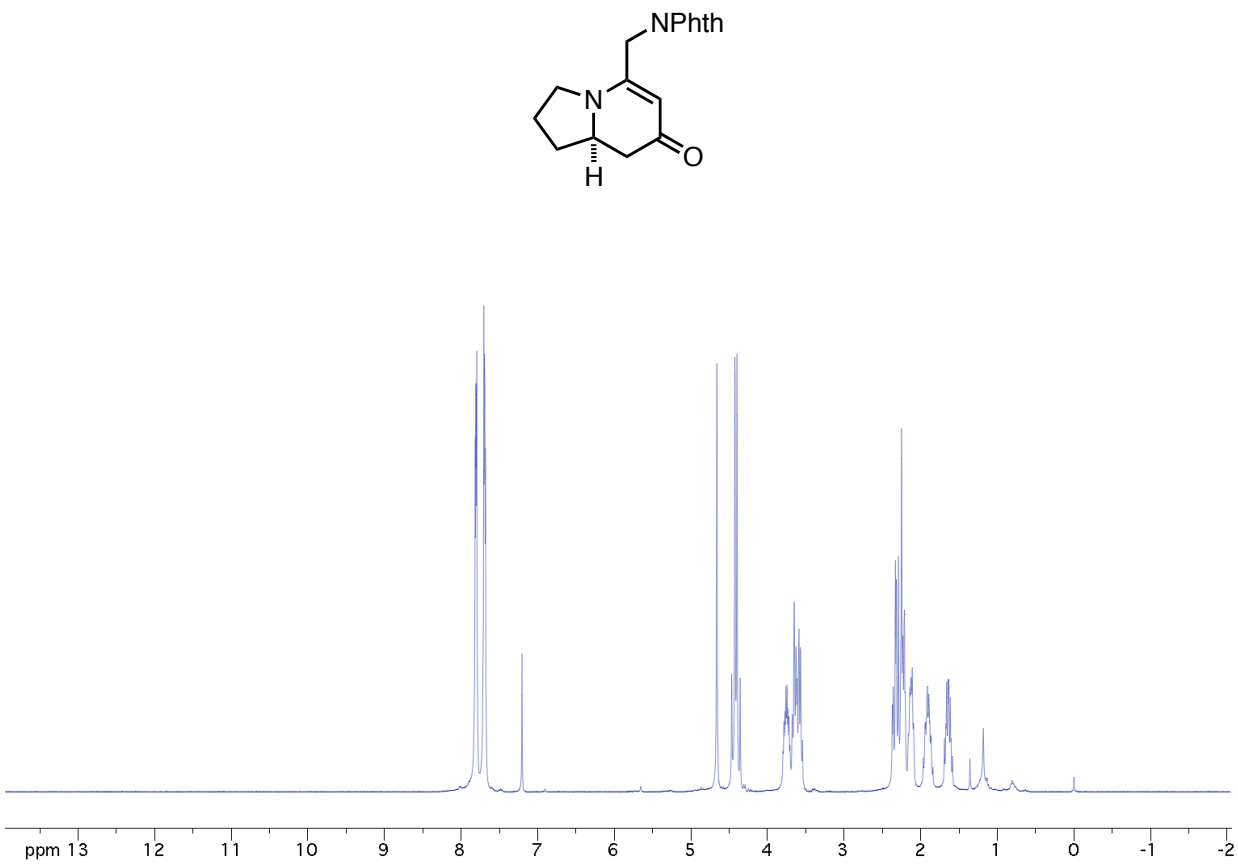
^{1}HNMR



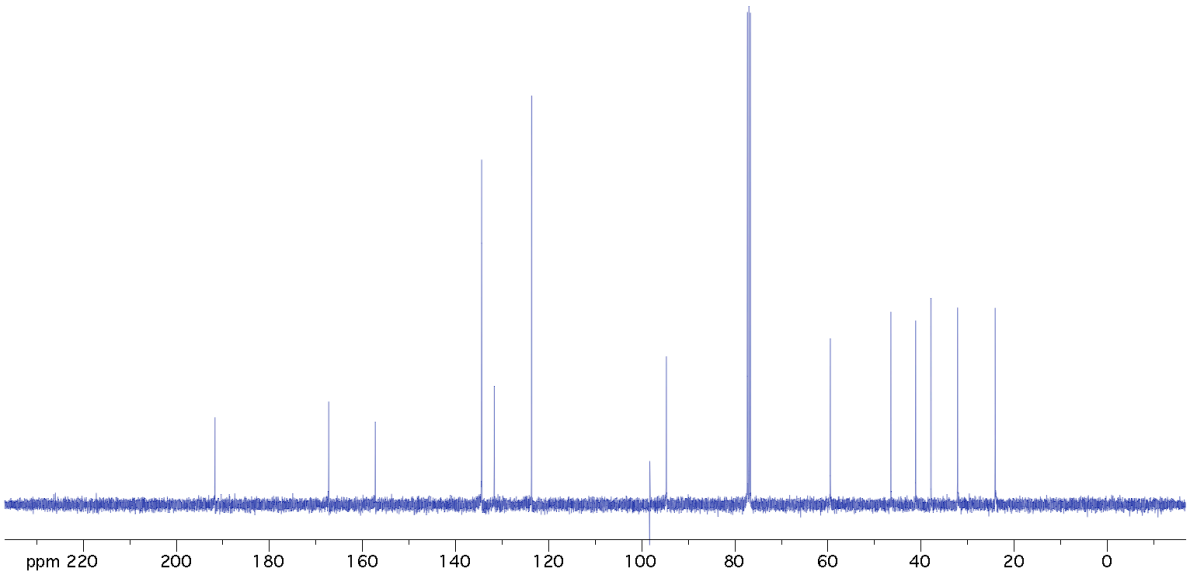
^{13}CNMR

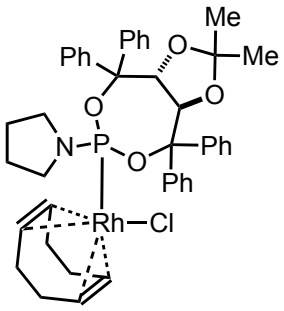


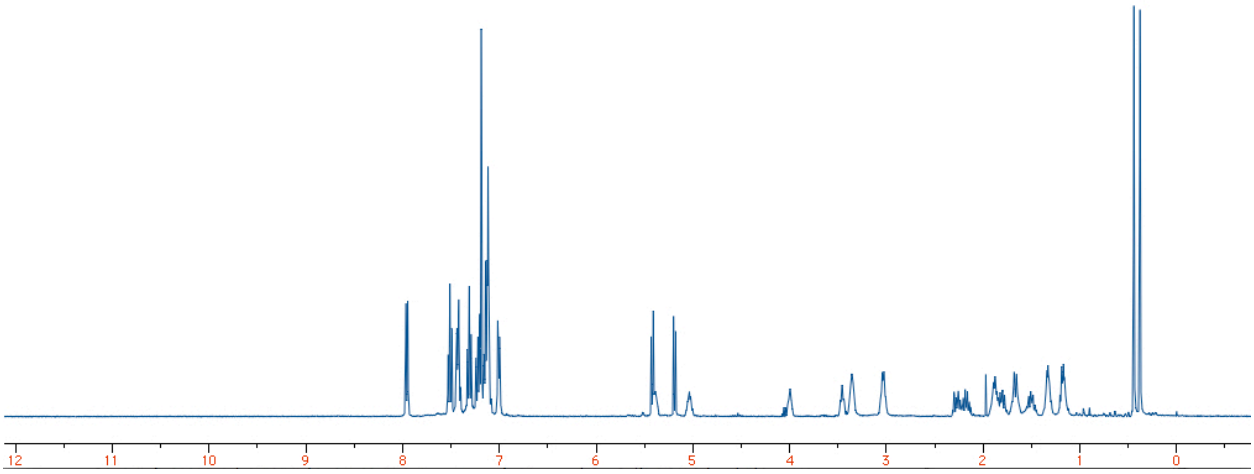
^{31}PNMR


NPhth
N
O
H
ppm 13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2

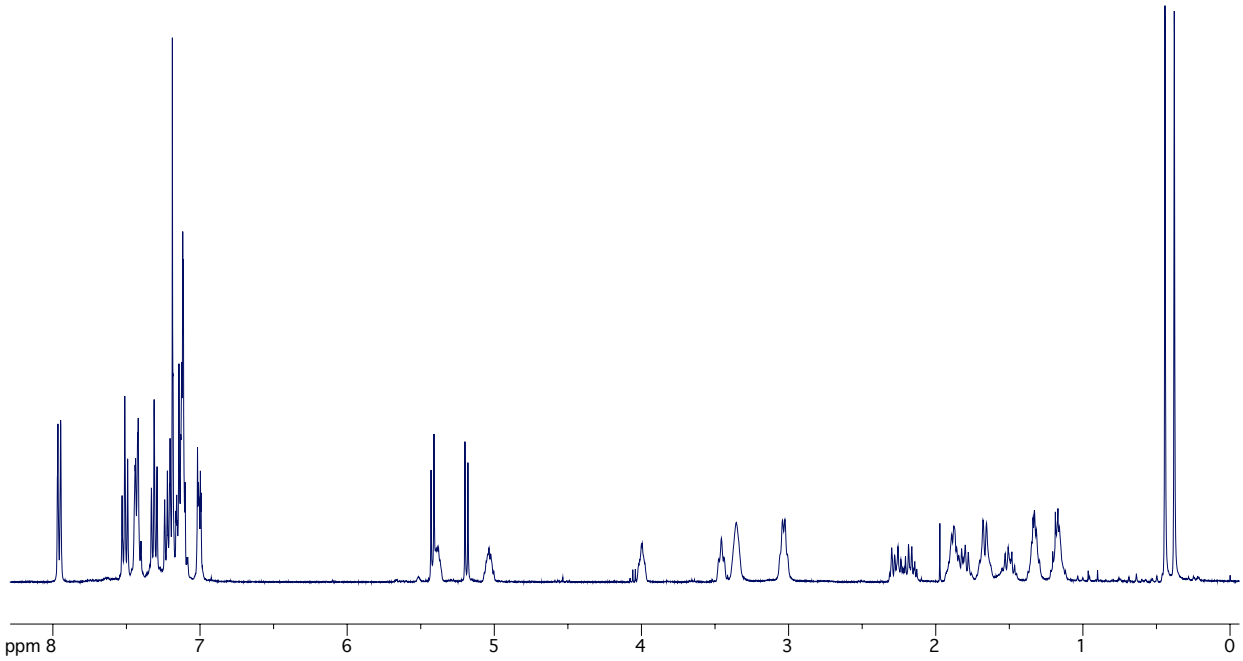
^{1}HNMR


ppm 220
200
180
160
140
120
100
80
60
40
20
0

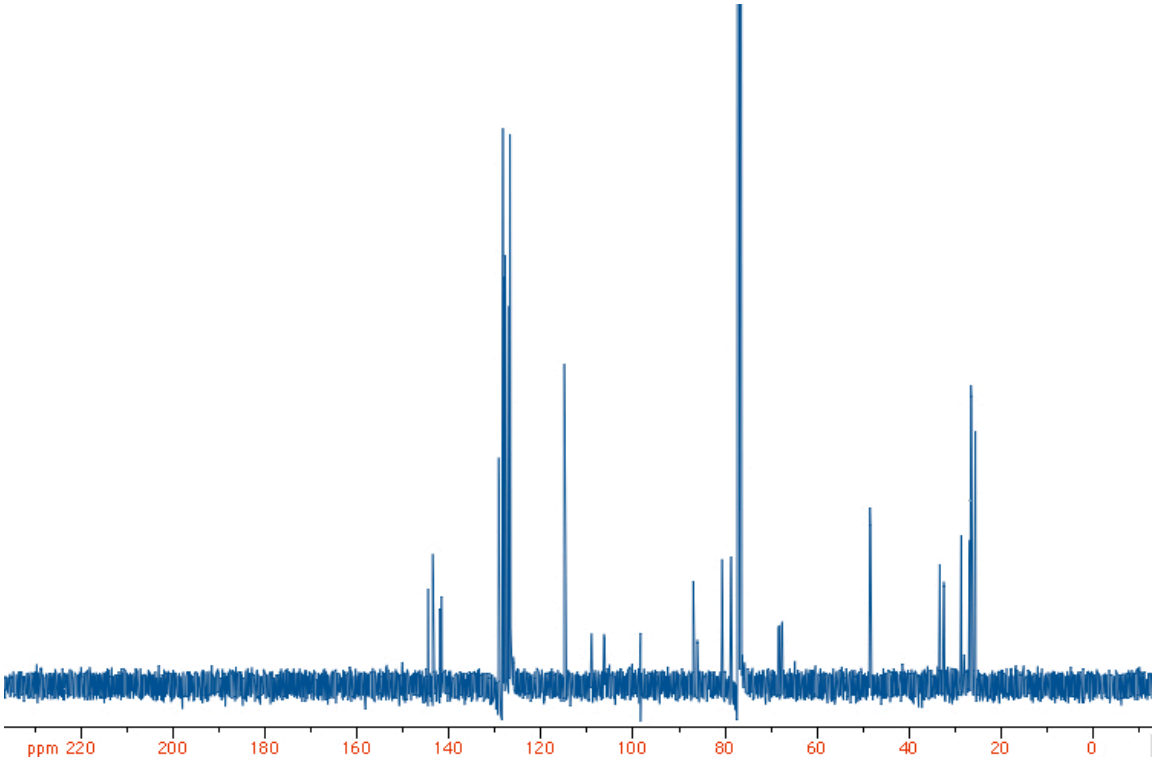




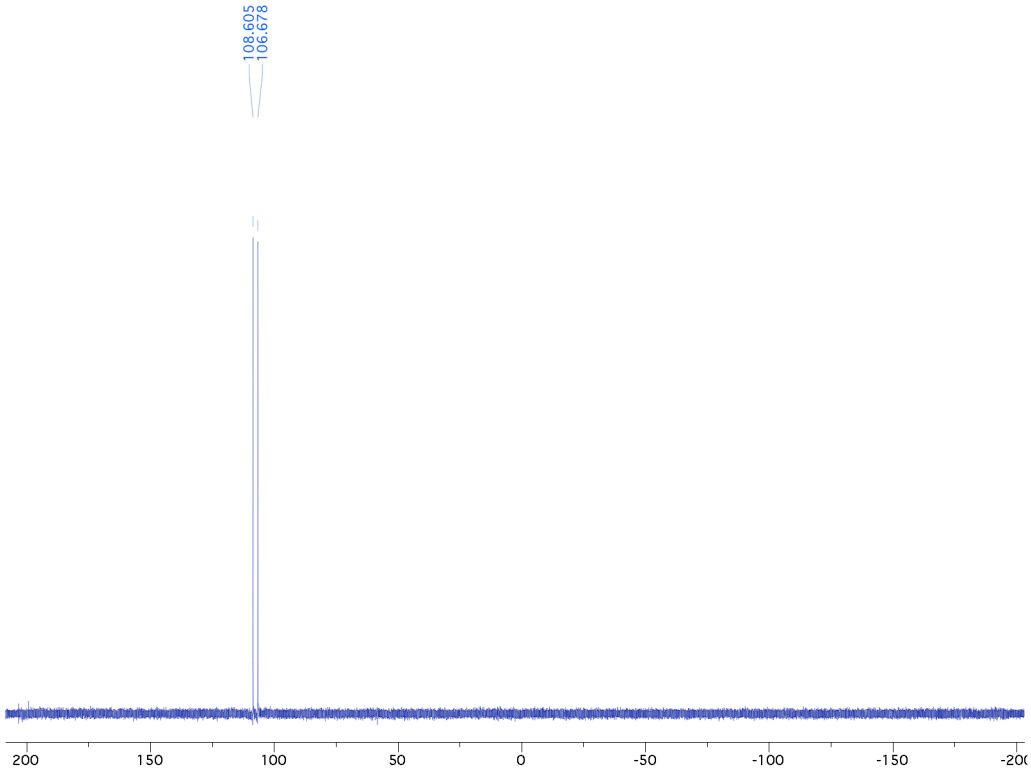
^{1}H-NMR Rh(cod)Cl•**T1**



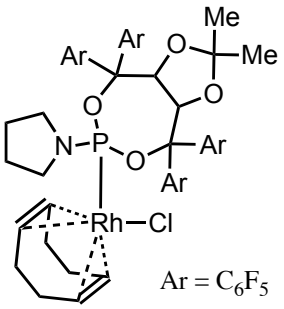
^{1}H-NMR Rh(cod)Cl•**T1**

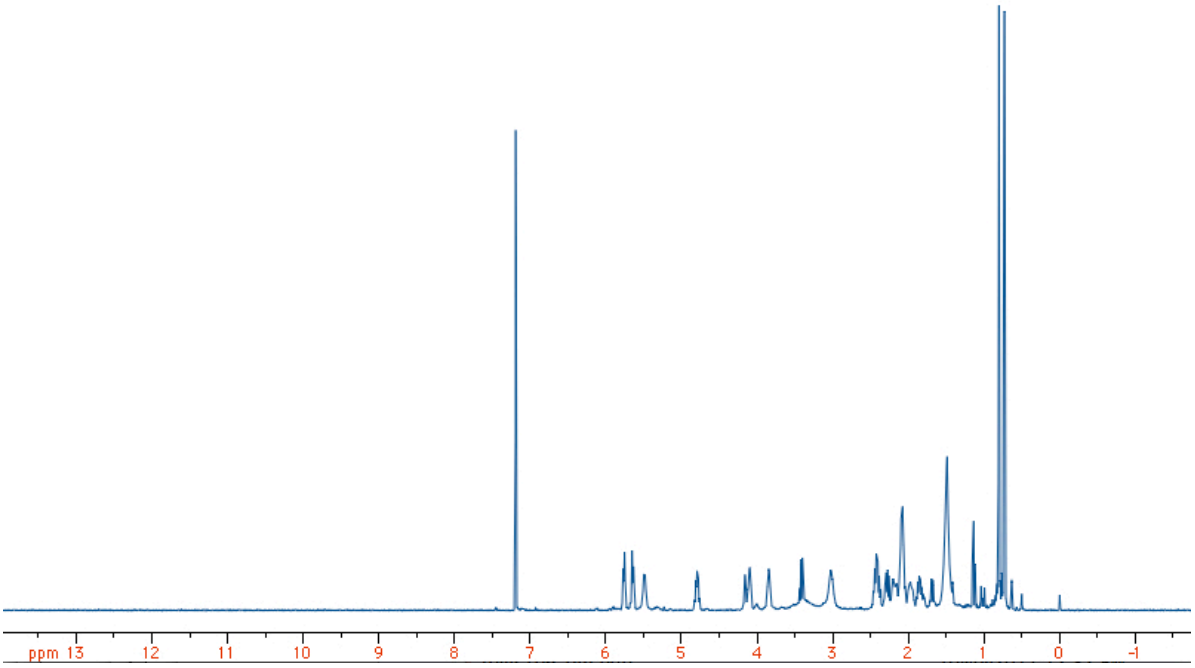


^{13}CNMR Rh(cod)Cl•**T1**

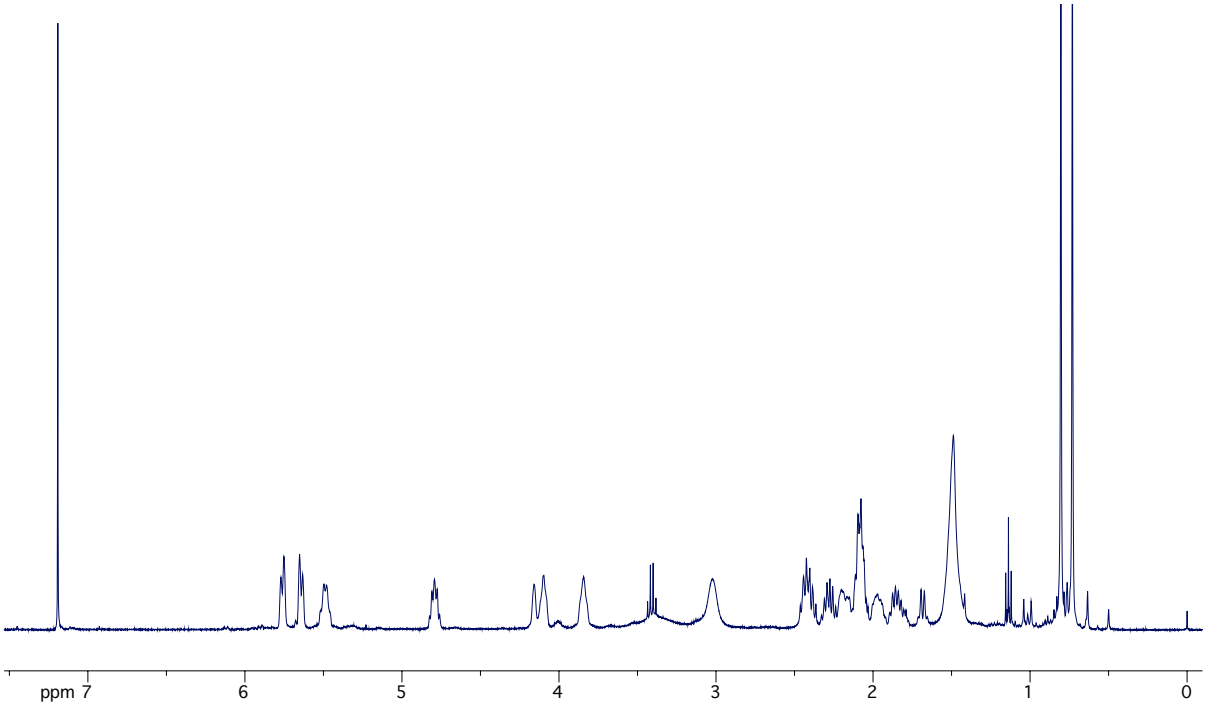


^{31}P-NMR Rh(cod)Cl•**T1**

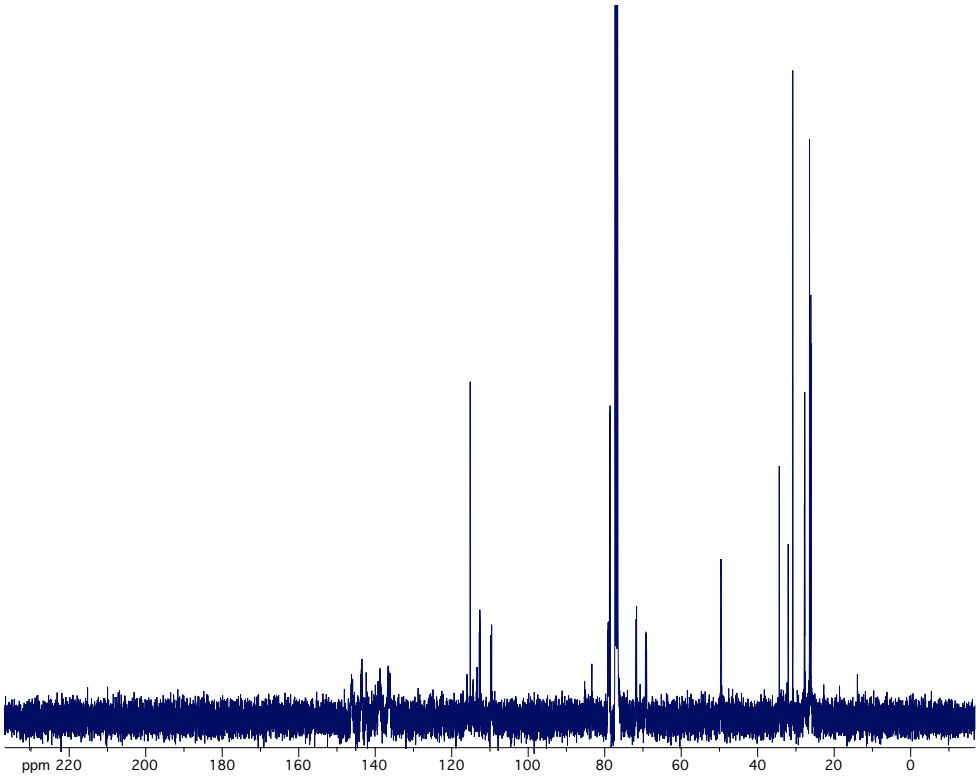




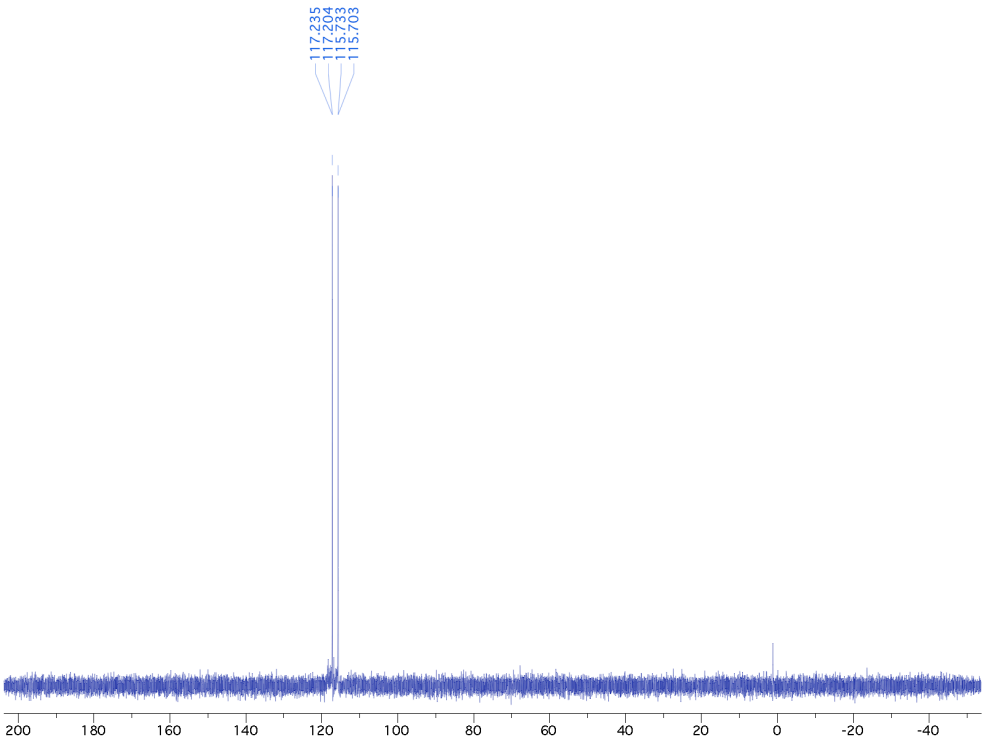
^{1}HNMR Rh(cod)Cl•CKphos



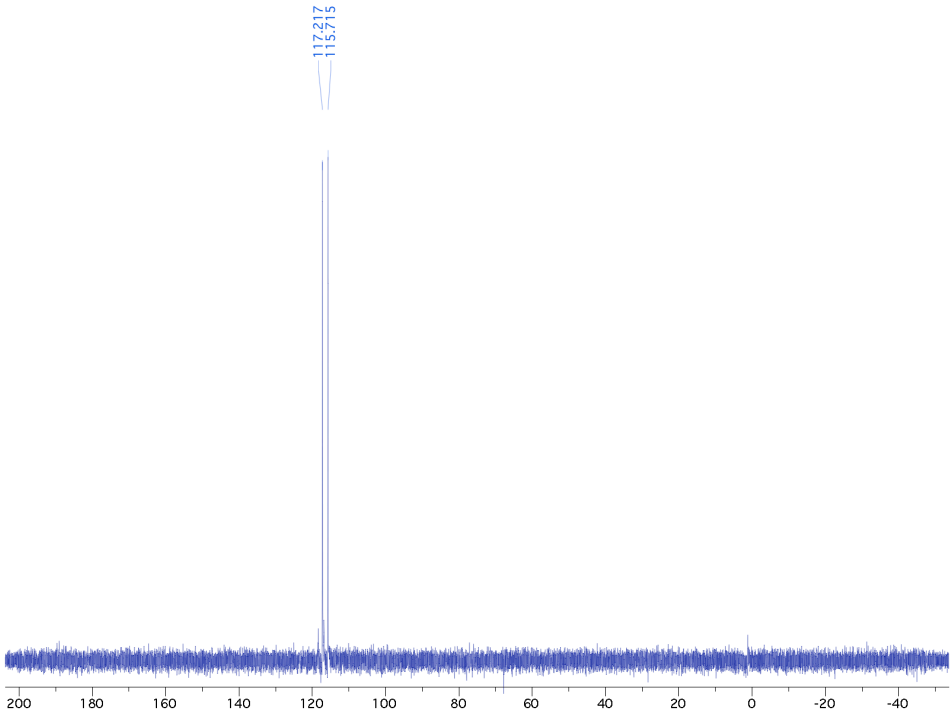
^{1}HNMR of Rh(cod)Cl•CKphos



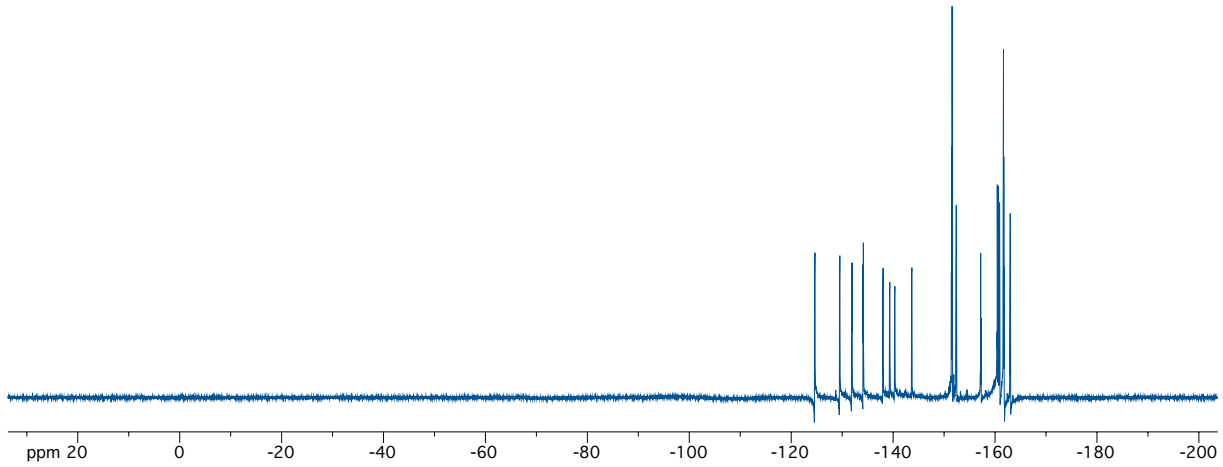
^{13}CNMR of Rh(cod)Cl•CKphos



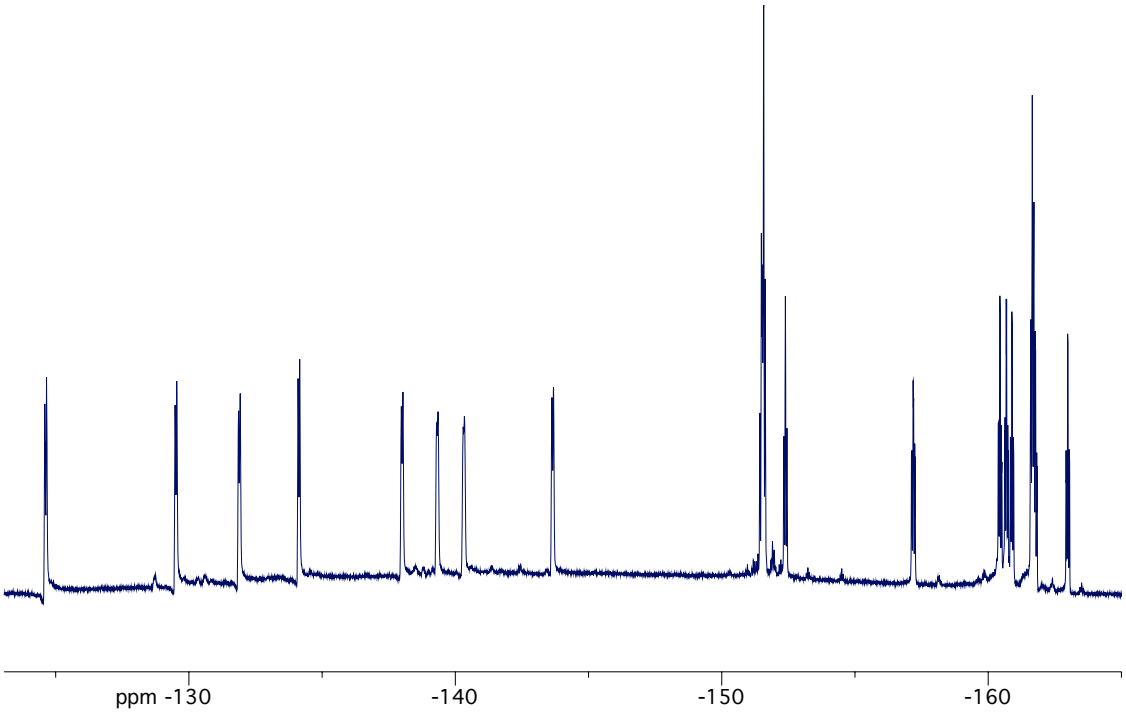
^{31}P-NMR Rh(cod)Cl•CKphos



^{19}F-decoupled ^{31}P-NMR Rh(cod)Cl-CKphos



^{19}FNMR Rh(cod)Cl•CKphos



^{19}FNMR Rh(cod)Cl•CKphos

5. X-ray Crystallography Data

All single crystals were coated in oil, transferred to a goniometer head, and mounted on a Bruker Kappa Apex CCD diffractometer under a stream of N_2. All data collections were performed with Mo Kα radiation and a graphite monochromator. Data sets were taken with complete coverage and fourfold redundancy at 120 °K. Data was integrated and corrected for absorption effects with the Apex 2 software package.[5] Structures were solved with the SHELXTL software package.[6] All non-hydrogen atoms were refined with anisotropic thermal parameters and hydrogen atoms placed in idealized positions. Crystal data and structure parameters are provided as CIF files. Rhodium alkene bond distances were generated in XP using the cent/x, join and bang commands.

Rh(cod)X-CKphos complexes were synthesized by adding Rh(cod)Cl (1 equiv.), racemic CKphos (1 equiv), and Ag salt of desired counterion (OTs, OTf, 1 equiv) to an oven dried vial equipped with a magnetic stirbar in an Ar atmosphere glove box. After removal of the vial from the glove box, DCM (1 ml) is added and the solution stirred at rt under Ar flow for 1 h. A white precipitate forms and the solution is filtered through a plug of cotton or glass wool. The clear yellow solution is layered with hexanes and slow evaporation provided yellow X-ray quality crystals.

---

[5] Bruker AXS Inc., 5465 East Chervl Parkway, Madison, WI 53711-5373 USA

[6] Sheldrick, G. (1997) *SHELXL-97 Program for Crystal Structure Refinement*, Institüt für Anorganische Chemie der Universität, Göttingen, Germany.

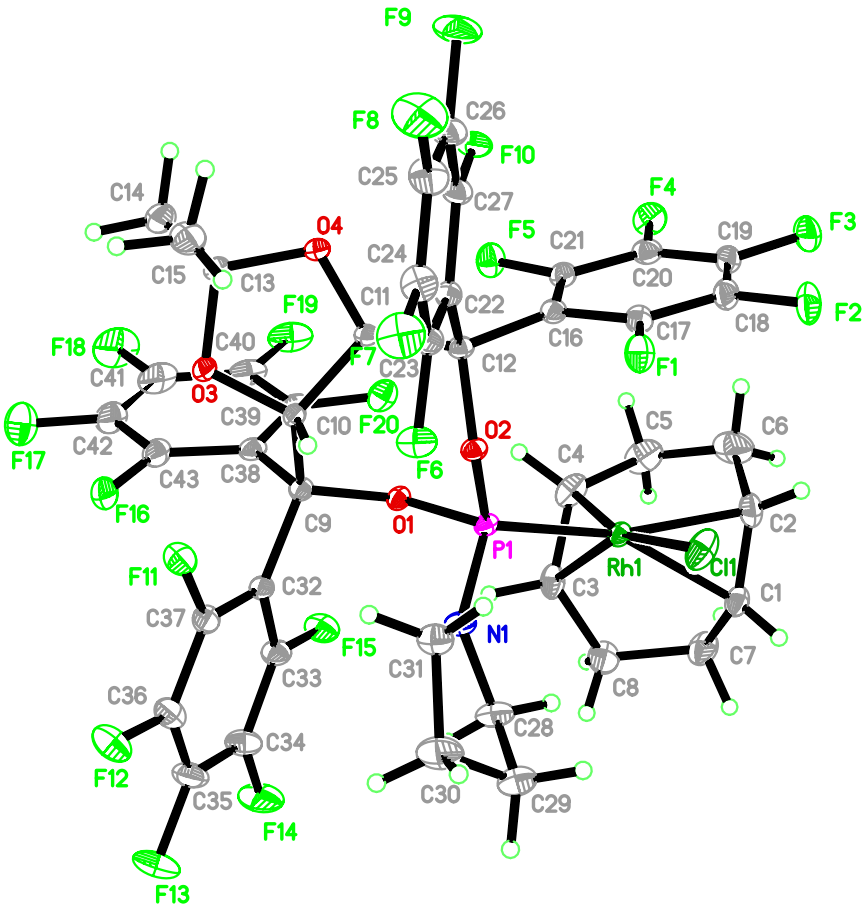


Table 1. Crystal data and structure refinement for Rh(cod)Cl•CKphos.

Identification code	rovis106_0m	
Empirical formula	C_{44} H_{28} Cl_3 F_{20} N O_4 P Rh	
Formula weight	1254.90	
Temperature	120 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P*-1	
Unit cell dimensions	a = 11.5246(6) Å	α = 68.867(2)°
	b = 12.6819(7) Å	β = 84.990(3)°
	c = 17.2832(9) Å	ɣ = 77.050(3)°
Volume	2296.1(2) $Å^3$	
Z	2	
Density (calculated)	1.815 Mg/m^3	
Absorption coefficient	0.709 mm^{-1}	

F_{000}	1244
Crystal size	0.37 x 0.11 x 0.09 mm^3
Theta range for data collection	1.76 to 33.21°.
Index ranges	-17≤h≤17, -18≤k≤19, -26≤l≤26
Reflections collected	64119
Independent reflections	17541 [R_{int} = 0.0432]
Completeness to theta = 33.21°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9364 and 0.7794
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17541 / 0 / 669
Goodness-of-fit on F^2	1.091
Final R indices [I>2sigma(I)]	R1 = 0.0495, wR2 = 0.1323
R indices (all data)	R1 = 0.0742, wR2 = 0.1536
Largest diff. peak and hole	2.036 and -1.839 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Rh(cod)Cl•CKphos. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4215(2)	3155(2)	5437(1)	22(1)
C(2)	4982(3)	3691(3)	4861(2)	30(1)
C(3)	4116(3)	1588(2)	4622(2)	24(1)
C(4)	5032(2)	2038(2)	4109(2)	26(1)
C(5)	6208(3)	2072(3)	4432(2)	36(1)
C(6)	6184(3)	3148(4)	4630(2)	43(1)
C(7)	4521(3)	1876(3)	5951(2)	30(1)
C(8)	4092(3)	1137(2)	5561(2)	30(1)
C(9)	2301(2)	2121(2)	2253(1)	16(1)
C(10)	2061(2)	3257(2)	1476(1)	15(1)
C(11)	3153(2)	3821(2)	1330(1)	15(1)
C(12)	2900(2)	4844(2)	1672(1)	15(1)
C(13)	2593(2)	3737(2)	86(1)	19(1)
C(14)	3383(3)	2983(3)	-338(2)	28(1)

C(15)	1716(3)4729(2)	-493(2)	29(1)
C(16)	3968(2)5123(2)	1982(1)	17(1)
C(17)	3728(2)6064(2)	2257(1)	19(1)
C(18)	4585(3)6379(2)	2584(2)	23(1)
C(19)	5745(2)5761(2)	2644(2)	23(1)
C(20)	6016(2)4830(2)	2381(1)	21(1)
C(21)	5150(2)4528(2)	2047(1)	19(1)
C(22)	2279(2)5951(2)	985(1)	16(1)
C(23)	1076(2)6441(2)	946(1)	19(1)
C(24)	591(2) 7454(2)	310(2)	26(1)
C(25)	1315(3)7995(2)	-314(2)	30(1)
C(26)	2517(3)7530(2)	-300(2)	27(1)
C(27)	2979(2)6527(2)	338(2)	21(1)
C(28)	860(2) 2786(3)	4453(2)	27(1)
C(29)	-301(3)3470(3)	4655(2)	32(1)
C(30)	-996(3)3863(3)	3871(2)	36(1)
C(31)	-75(2) 4188(2)	3184(2)	25(1)
C(32)	1214(2)1632(2)	2677(1)	17(1)
C(33)	1400(2) 693(2)	3418(2)	22(1)
C(34)	496(3) 164(2)	3853(2)	29(1)
C(35)	-644(3) 557(3)	3543(2)	30(1)
C(36)	-864(2)1468(2)	2803(2)	25(1)
C(37)	58(2) 1988(2)	2380(1)	20(1)
C(38)	3175(2)1182(2)	2003(1)	20(1)
C(39)	4401(2) 873(2)	2125(2)	22(1)
C(40)	5130(3) 43(2)	1858(2)	29(1)
C(41)	4655(3)-504(3)	1447(2)	37(1)
C(42)	3455(3)-227(3)	1304(2)	35(1)
C(43)	2738(3) 597(2)	1576(2)	25(1)
C(44)	10079(4)7388(3)	2918(3)	52(1)
Cl(1)	2435(1)5221(1)	4101(1)	31(1)
Cl(2)	10362(2)8710(1)	2406(2)	125(1)
Cl(3)	8680(1)7327(2)	3385(1)	83(1)
F(1)	2630(1)6712(1)	2198(1)	25(1)
F(2)	4298(2)7288(2)	2833(1)	32(1)
F(3)	6594(2)6073(2)	2938(1)	32(1)

F(4)	7144(1)4236(2)	2425(1)	30(1)
F(5)	5523(1)3643(1)	1774(1)	26(1)
F(6)	295(1) 5971(1)	1516(1)	26(1)
F(7)	-576(2)7899(2)	320(1)	36(1)
F(8)	858(2) 8970(2)	-924(1)	45(1)
F(9)	3238(2)8038(2)	-899(1)	40(1)
F(10)	4152(1)6120(1)	315(1)	26(1)
F(11)	-224(1)2841(1)	1651(1)	25(1)
F(12)	-1956(2)1832(2)	2482(1)	34(1)
F(13)	-1516(2) 44(2)	3954(1)	42(1)
F(14)	735(2) -729(2)	4565(1)	41(1)
F(15)	2499(1) 247(1)	3738(1)	27(1)
F(16)	1577(2) 824(2)	1411(1)	29(1)
F(17)	2985(2)-762(2)	905(1)	52(1)
F(18)	5365(2)-1320(2)	1197(2)	56(1)
F(19)	6302(2)-233(2)	2013(1)	37(1)
F(20)	4959(1)1366(1)	2506(1)	26(1)
N(1)	1041(2)3395(2)	3551(1)	19(1)
O(1)	2876(1)2383(1)	2852(1)	15(1)
O(2)	2093(1)4566(1)	2365(1)	15(1)
O(3)	1987(2)3016(2)	750(1)	20(1)
O(4)	3328(2)4200(2)	462(1)	20(1)
P(1)	2405(1)3440(1)	3210(1)	14(1)
Rh(1)	3618(1)3408(1)	4168(1)	16(1)

Table 3. Bond lengths [Å] and angles [°] for Rh(cod)Cl•CKphos.

C(1)-C(2)	1.365(4)	C(4)-C(5)	1.524(4)
C(1)-C(7)	1.518(4)	C(4)-Rh(1)	2.125(3)
C(1)-Rh(1)	2.245(2)	C(5)-C(6)	1.516(5)
C(2)-C(6)	1.491(5)	C(7)-C(8)	1.515(4)
C(2)-Rh(1)	2.219(3)	C(9)-O(1)	1.445(3)
C(3)-C(4)	1.403(4)	C(9)-C(32)	1.533(3)
C(3)-C(8)	1.514(4)	C(9)-C(38)	1.541(3)
C(3)-Rh(1)	2.110(3)	C(9)-C(10)	1.564(3)

C(10)-O(3)	1.409(3)	C(30)-C(31)	1.525(4)
C(10)-C(11)	1.541(3)	C(31)-N(1)	1.473(3)
C(11)-O(4)	1.413(3)	C(32)-C(37)	1.388(4)
C(11)-C(12)	1.571(3)	C(32)-C(33)	1.392(3)
C(12)-O(2)	1.440(2)	C(33)-F(15)	1.344(3)
C(12)-C(16)	1.541(3)	C(33)-C(34)	1.383(3)
C(12)-C(22)	1.545(3)	C(34)-F(14)	1.338(3)
C(13)-O(3)	1.425(3)	C(34)-C(35)	1.378(4)
C(13)-O(4)	1.441(3)	C(35)-F(13)	1.332(3)
C(13)-C(14)	1.511(4)	C(35)-C(36)	1.377(4)
C(13)-C(15)	1.518(4)	C(36)-F(12)	1.334(3)
C(16)-C(21)	1.394(3)	C(36)-C(37)	1.389(3)
C(16)-C(17)	1.401(3)	C(37)-F(11)	1.339(3)
C(17)-F(1)	1.336(3)	C(38)-C(39)	1.393(4)
C(17)-C(18)	1.376(4)	C(38)-C(43)	1.407(4)
C(18)-F(2)	1.336(3)	C(39)-F(20)	1.337(3)
C(18)-C(19)	1.382(4)	C(39)-C(40)	1.383(4)
C(19)-F(3)	1.333(3)	C(40)-F(19)	1.343(4)
C(19)-C(20)	1.377(4)	C(40)-C(41)	1.371(5)
C(20)-F(4)	1.341(3)	C(41)-F(18)	1.344(3)
C(20)-C(21)	1.381(4)	C(41)-C(42)	1.371(5)
C(21)-F(5)	1.341(3)	C(42)-F(17)	1.339(4)
C(22)-C(23)	1.384(3)	C(42)-C(43)	1.376(4)
C(22)-C(27)	1.397(3)	C(43)-F(16)	1.337(3)
C(23)-F(6)	1.341(3)	C(44)-Cl(2)	1.681(4)
C(23)-C(24)	1.392(3)	C(44)-Cl(3)	1.743(4)
C(24)-F(7)	1.337(3)	Cl(1)-Rh(1)	2.3645(7)
C(24)-C(25)	1.376(4)	N(1)-P(1)	1.636(2)
C(25)-F(8)	1.336(3)	O(1)-P(1)	1.6390(17)
C(25)-C(26)	1.378(4)	O(2)-P(1)	1.6309(16)
C(26)-F(9)	1.337(3)	P(1)-Rh(1)	2.2423(6)
C(26)-C(27)	1.379(3)	C(2)-C(1)-C(7)	122.2(3)
C(27)-F(10)	1.337(3)	C(2)-C(1)-Rh(1)	71.18(15)
C(28)-N(1)	1.489(3)	C(7)-C(1)-Rh(1)	110.13(17)
C(28)-C(29)	1.511(4)	C(1)-C(2)-C(6)	127.1(3)
C(29)-C(30)	1.500(5)	C(1)-C(2)-Rh(1)	73.21(16)

C(6)-C(2)-Rh(1)	108.7(2)	C(21)-C(16)-C(12)	127.8(2)
C(4)-C(3)-C(8)	126.5(3)	C(17)-C(16)-C(12)	116.8(2)
C(4)-C(3)-Rh(1)	71.24(15)	F(1)-C(17)-C(18)	116.8(2)
C(8)-C(3)-Rh(1)	109.84(18)	F(1)-C(17)-C(16)	120.1(2)
C(3)-C(4)-C(5)	123.8(2)	C(18)-C(17)-C(16)	123.0(2)
C(3)-C(4)-Rh(1)	70.06(15)	F(2)-C(18)-C(17)	120.1(2)
C(5)-C(4)-Rh(1)	113.3(2)	F(2)-C(18)-C(19)	120.2(2)
C(6)-C(5)-C(4)	114.1(3)	C(17)-C(18)-C(19)	119.7(2)
C(2)-C(6)-C(5)	114.1(3)	F(3)-C(19)-C(20)	120.4(2)
C(8)-C(7)-C(1)	112.7(2)	F(3)-C(19)-C(18)	120.6(2)
C(3)-C(8)-C(7)	114.5(2)	C(20)-C(19)-C(18)	119.0(2)
O(1)-C(9)-C(32)	107.81(17)	F(4)-C(20)-C(19)	119.4(2)
O(1)-C(9)-C(38)	108.55(19)	F(4)-C(20)-C(21)	119.9(2)
C(32)-C(9)-C(38)	108.55(18)	C(19)-C(20)-C(21)	120.8(2)
O(1)-C(9)-C(10)	106.04(17)	F(5)-C(21)-C(20)	115.8(2)
C(32)-C(9)-C(10)	116.94(19)	F(5)-C(21)-C(16)	122.1(2)
C(38)-C(9)-C(10)	108.68(17)	C(20)-C(21)-C(16)	122.1(2)
O(3)-C(10)-C(11)	104.46(17)	C(23)-C(22)-C(27)	115.7(2)
O(3)-C(10)-C(9)	111.13(19)	C(23)-C(22)-C(12)	126.0(2)
C(11)-C(10)-C(9)	108.50(19)	C(27)-C(22)-C(12)	118.2(2)
O(4)-C(11)-C(10)	104.44(18)	F(6)-C(23)-C(22)	122.3(2)
O(4)-C(11)-C(12)	112.39(17)	F(6)-C(23)-C(24)	115.4(2)
C(10)-C(11)-C(12)	110.19(18)	C(22)-C(23)-C(24)	122.4(2)
O(2)-C(12)-C(16)	106.41(17)	F(7)-C(24)-C(25)	120.8(2)
O(2)-C(12)-C(22)	108.60(18)	F(7)-C(24)-C(23)	119.3(2)
C(16)-C(12)-C(22)	107.92(18)	C(25)-C(24)-C(23)	119.9(3)
O(2)-C(12)-C(11)	107.52(16)	F(8)-C(25)-C(24)	120.3(3)
C(16)-C(12)-C(11)	117.72(19)	F(8)-C(25)-C(26)	120.1(3)
C(22)-C(12)-C(11)	108.39(18)	C(24)-C(25)-C(26)	119.5(2)
O(3)-C(13)-O(4)	106.27(17)	F(9)-C(26)-C(25)	120.7(2)
O(3)-C(13)-C(14)	107.8(2)	F(9)-C(26)-C(27)	119.8(3)
O(4)-C(13)-C(14)	109.0(2)	C(25)-C(26)-C(27)	119.6(2)
O(3)-C(13)-C(15)	110.9(2)	F(10)-C(27)-C(26)	116.6(2)
O(4)-C(13)-C(15)	108.9(2)	F(10)-C(27)-C(22)	120.5(2)
C(14)-C(13)-C(15)	113.6(2)	C(26)-C(27)-C(22)	122.9(2)
C(21)-C(16)-C(17)	115.4(2)	N(1)-C(28)-C(29)	104.0(2)

C(30)-C(29)-C(28)	102.7(2)	F(17)-C(42)-C(43)	120.4(3)
C(29)-C(30)-C(31)	103.9(2)	C(41)-C(42)-C(43)	119.6(3)
N(1)-C(31)-C(30)	103.6(2)	F(16)-C(43)-C(42)	116.3(3)
C(37)-C(32)-C(33)	115.5(2)	F(16)-C(43)-C(38)	120.6(2)
C(37)-C(32)-C(9)	126.9(2)	C(42)-C(43)-C(38)	123.2(3)
C(33)-C(32)-C(9)	117.5(2)	Cl(2)-C(44)-Cl(3)	116.8(2)
F(15)-C(33)-C(34)	116.7(2)	C(31)-N(1)-C(28)	109.80(19)
F(15)-C(33)-C(32)	120.2(2)	C(31)-N(1)-P(1)	128.56(16)
C(34)-C(33)-C(32)	123.1(3)	C(28)-N(1)-P(1)	117.95(17)
F(14)-C(34)-C(35)	120.5(2)	C(9)-O(1)-P(1)	127.67(15)
F(14)-C(34)-C(33)	120.0(3)	C(12)-O(2)-P(1)	123.75(14)
C(35)-C(34)-C(33)	119.5(2)	C(10)-O(3)-C(13)	109.76(17)
F(13)-C(35)-C(36)	120.6(3)	C(11)-O(4)-C(13)	110.40(16)
F(13)-C(35)-C(34)	120.0(3)	O(2)-P(1)-N(1)	97.71(9)
C(36)-C(35)-C(34)	119.4(2)	O(2)-P(1)-O(1)	102.68(8)
F(12)-C(36)-C(35)	120.0(2)	N(1)-P(1)-O(1)	108.16(10)
F(12)-C(36)-C(37)	120.1(2)	O(2)-P(1)-Rh(1)	120.99(7)
C(35)-C(36)-C(37)	119.9(3)	N(1)-P(1)-Rh(1)	112.80(8)
F(11)-C(37)-C(32)	121.3(2)	O(1)-P(1)-Rh(1)	112.84(7)
F(11)-C(37)-C(36)	116.1(2)	C(3)-Rh(1)-C(4)	38.69(11)
C(32)-C(37)-C(36)	122.6(2)	C(3)-Rh(1)-C(2)	95.88(11)
C(39)-C(38)-C(43)	114.7(2)	C(4)-Rh(1)-C(2)	81.07(12)
C(39)-C(38)-C(9)	126.2(2)	C(3)-Rh(1)-P(1)	93.08(8)
C(43)-C(38)-C(9)	119.0(2)	C(4)-Rh(1)-P(1)	99.74(8)
F(20)-C(39)-C(40)	115.2(3)	C(2)-Rh(1)-P(1)	166.24(8)
F(20)-C(39)-C(38)	122.2(2)	C(3)-Rh(1)-C(1)	81.50(10)
C(40)-C(39)-C(38)	122.7(3)	C(4)-Rh(1)-C(1)	89.82(10)
F(19)-C(40)-C(41)	120.2(3)	C(2)-Rh(1)-C(1)	35.60(10)
F(19)-C(40)-C(39)	119.7(3)	P(1)-Rh(1)-C(1)	157.25(7)
C(41)-C(40)-C(39)	120.1(3)	C(3)-Rh(1)-Cl(1)	155.33(8)
F(18)-C(41)-C(42)	120.3(3)	C(4)-Rh(1)-Cl(1)	164.91(8)
F(18)-C(41)-C(40)	120.0(3)	C(2)-Rh(1)-Cl(1)	89.33(9)
C(42)-C(41)-C(40)	119.7(3)	P(1)-Rh(1)-Cl(1)	86.84(2)
F(17)-C(42)-C(41)	120.0(3)	C(1)-Rh(1)-Cl(1)	89.08(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Rh(cod)Cl•CKphos. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	31(1)	20(1)	16(1)	-7(1)	-4(1)	-5(1)
C(2)	35(2)	34(2)	29(1)	-16(1)	-5(1)	-16(1)
C(3)	32(1)	15(1)	25(1)	-9(1)	-8(1)	0(1)
C(4)	23(1)	28(1)	22(1)	-10(1)	-5(1)	8(1)
C(5)	20(1)	52(2)	30(1)	-13(1)	-5(1)	3(1)
C(6)	28(2)	66(2)	34(2)	-7(2)	-4(1)	-20(2)
C(7)	42(2)	27(1)	18(1)	-5(1)	-6(1)	-5(1)
C(8)	46(2)	18(1)	24(1)	-2(1)	-3(1)	-9(1)
C(9)	21(1)	12(1)	13(1)	-3(1)	1(1)	-4(1)
C(10)	21(1)	14(1)	12(1)	-5(1)	2(1)	-6(1)
C(11)	18(1)	14(1)	13(1)	-4(1)	2(1)	-6(1)
C(12)	17(1)	13(1)	13(1)	-3(1)	1(1)	-3(1)
C(13)	26(1)	19(1)	13(1)	-6(1)	3(1)	-9(1)
C(14)	33(1)	29(1)	26(1)	-16(1)	9(1)	-10(1)
C(15)	32(1)	25(1)	23(1)	0(1)	-5(1)	-7(1)
C(16)	20(1)	14(1)	15(1)	-4(1)	0(1)	-4(1)
C(17)	23(1)	15(1)	18(1)	-4(1)	-2(1)	-4(1)
C(18)	34(1)	17(1)	20(1)	-7(1)	-2(1)	-8(1)
C(19)	28(1)	28(1)	17(1)	-7(1)	-2(1)	-14(1)
C(20)	20(1)	25(1)	17(1)	-4(1)	-1(1)	-6(1)
C(21)	21(1)	19(1)	16(1)	-5(1)	1(1)	-5(1)
C(22)	21(1)	13(1)	15(1)	-3(1)	-1(1)	-4(1)
C(23)	23(1)	17(1)	18(1)	-5(1)	0(1)	-4(1)
C(24)	25(1)	21(1)	27(1)	-4(1)	-7(1)	0(1)
C(25)	41(2)	15(1)	25(1)	5(1)	-10(1)	-4(1)
C(26)	34(1)	21(1)	21(1)	3(1)	-2(1)	-10(1)
C(27)	25(1)	19(1)	18(1)	-1(1)	-1(1)	-9(1)
C(28)	21(1)	33(2)	21(1)	-4(1)	6(1)	-3(1)

C(29)	28(1)	38(2)	29(1)	-13(1)	9(1)	-6(1)
C(30)	20(1)	43(2)	38(2)	-10(1)	6(1)	-2(1)
C(31)	20(1)	27(1)	24(1)	-5(1)	-1(1)	-2(1)
C(32)	23(1)	15(1)	14(1)	-4(1)	2(1)	-7(1)
C(33)	28(1)	18(1)	18(1)	-2(1)	2(1)	-7(1)
C(34)	36(2)	24(1)	22(1)	1(1)	5(1)	-13(1)
C(35)	30(1)	29(1)	31(1)	-9(1)	12(1)	-16(1)
C(36)	21(1)	24(1)	32(1)	-11(1)	2(1)	-7(1)
C(37)	25(1)	16(1)	18(1)	-5(1)	0(1)	-6(1)
C(38)	29(1)	14(1)	16(1)	-5(1)	6(1)	-7(1)
C(39)	29(1)	16(1)	17(1)	-4(1)	5(1)	-2(1)
C(40)	35(2)	16(1)	28(1)	-5(1)	12(1)	1(1)
C(41)	56(2)	18(1)	38(2)	-17(1)	20(2)	-5(1)
C(42)	54(2)	26(2)	32(1)	-19(1)	14(1)	-16(1)
C(43)	37(1)	18(1)	21(1)	-9(1)	5(1)	-9(1)
C(44)	55(2)	38(2)	57(2)	-13(2)	12(2)	-7(2)
Cl(1)	46(1)	18(1)	24(1)	-10(1)	-6(1)	7(1)
Cl(2)	118(1)	32(1)	198(2)	-25(1)	73(1)	-15(1)
Cl(3)	50(1)	118(1)	85(1)	-43(1)	16(1)	-22(1)
F(1)	26(1)	19(1)	30(1)	-12(1)	-6(1)	1(1)
F(2)	44(1)	25(1)	36(1)	-17(1)	-7(1)	-9(1)
F(3)	33(1)	41(1)	31(1)	-15(1)	-6(1)	-17(1)
F(4)	19(1)	42(1)	30(1)	-13(1)	-2(1)	-4(1)
F(5)	21(1)	27(1)	34(1)	-18(1)	0(1)	-1(1)
F(6)	20(1)	27(1)	23(1)	-2(1)	0(1)	-1(1)
F(7)	28(1)	31(1)	37(1)	-4(1)	-10(1)	7(1)
F(8)	51(1)	26(1)	38(1)	13(1)	-14(1)	-2(1)
F(9)	45(1)	34(1)	27(1)	10(1)	1(1)	-19(1)
F(10)	22(1)	28(1)	22(1)	-2(1)	2(1)	-10(1)
F(11)	26(1)	23(1)	23(1)	0(1)	-6(1)	-7(1)
F(12)	22(1)	34(1)	46(1)	-11(1)	-1(1)	-10(1)
F(13)	35(1)	40(1)	46(1)	-4(1)	14(1)	-22(1)
F(14)	46(1)	35(1)	28(1)	11(1)	4(1)	-16(1)
F(15)	27(1)	23(1)	23(1)	3(1)	-3(1)	-6(1)
F(16)	40(1)	28(1)	27(1)	-13(1)	2(1)	-16(1)
F(17)	76(2)	45(1)	59(1)	-43(1)	16(1)	-26(1)

F(18)	72(2)	34(1)	68(1)	-37(1)	31(1)	-5(1)
F(19)	32(1)	27(1)	39(1)	-6(1)	13(1)	6(1)
F(20)	23(1)	28(1)	26(1)	-13(1)	-1(1)	2(1)
N(1)	16(1)	19(1)	16(1)	-2(1)	1(1)	-2(1)
O(1)	19(1)	13(1)	13(1)	-5(1)	0(1)	-2(1)
O(2)	17(1)	14(1)	12(1)	-3(1)	1(1)	-3(1)
O(3)	31(1)	21(1)	12(1)	-5(1)	2(1)	-14(1)
O(4)	27(1)	22(1)	13(1)	-6(1)	5(1)	-12(1)
P(1)	16(1)	12(1)	12(1)	-4(1)	1(1)	-2(1)
Rh(1)	19(1)	13(1)	13(1)	-5(1)	0(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Rovis106_0m.

	x	y	z	U(eq)
H(1)	3701	3640	5715	27
H(2)	4909	4503	4795	35
H(3)	3668	1216	4377	28
H(4)	5101	1922	3575	31
H(5A)	6420	1400	4930	43
H(5B)	6824	2019	4021	43
H(6A)	6725	2950	5083	52
H(6B)	6474	3711	4150	52
H(7A)	5377	1634	6019	36
H(7B)	4164	1752	6498	36
H(8A)	4585	365	5759	36
H(8B)	3283	1077	5748	36
H(10)	1339	3788	1556	18
H(11)	3850	3244	1607	18
H(14A)	2901	2650	-574	41
H(14B)	3917	2378	59	41
H(14C)	3835	3442	-770	41
H(15A)	1186	5122	-177	43
H(15B)	1265	4433	-779	43

H(15C)	2143	5260	-889	43
H(28A)	1508	2791	4774	33
H(28B)	806	1992	4564	33
H(29A)	-702	2989	5121	38
H(29B)	-176	4122	4780	38
H(30A)	-1632	4524	3838	43
H(30B)	-1335	3247	3837	43
H(31A)	-276	4074	2691	30
H(31B)	-15	4988	3042	30
H(44A)	10676	6974	3345	62
H(44B)	10177	6977	2532	62

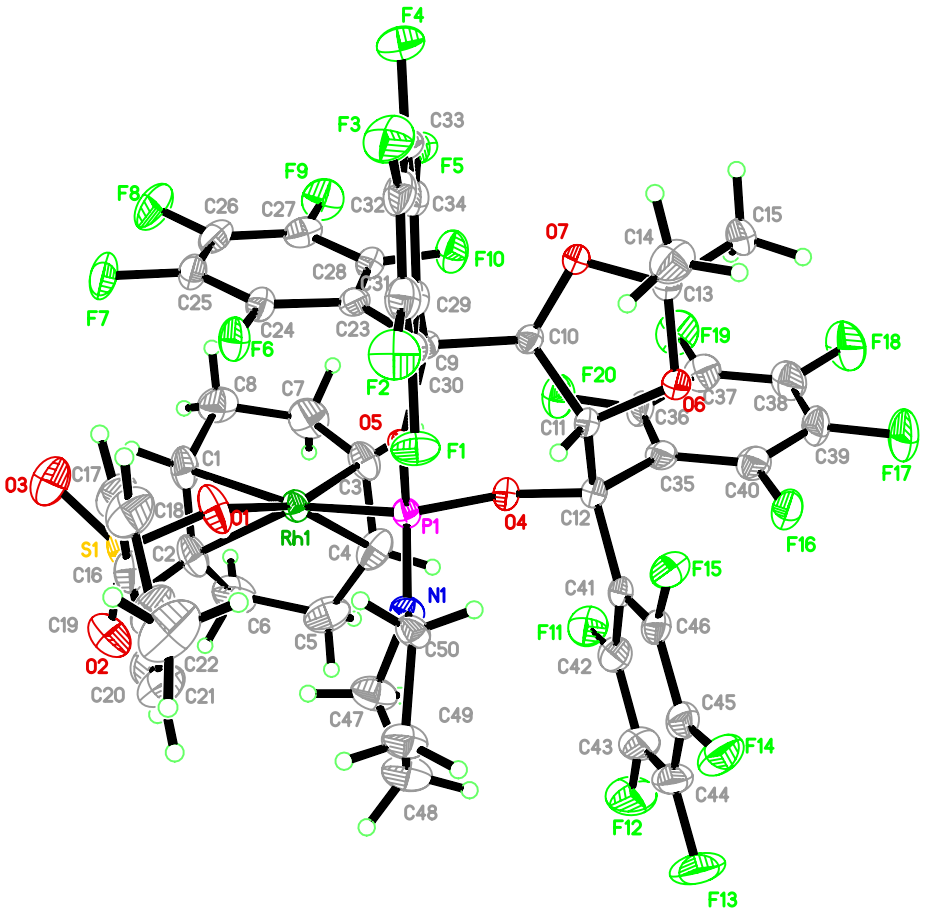


Table 6. Crystal data and structure refinement for Rh(cod)OTs·CKphos.

Identification code	Rovis117_0m	
Empirical formula	C_{50} H_{33} F_{20} N O_7 P Rh S	
Formula weight	1305.71	
Temperature	120 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* -1	
Unit cell dimensions	*a* = 11.7155(4) Å	α = 70.901(2)°.
	b = 12.1131(4) Å	β = 89.025(2)°.
	c = 18.2303(6) Å	γ = 83.198(2)°.
Volume	2426.82(14) $Å^3$	
Z	2	
Density (calculated)	1.787 Mg/m^3	
Absorption coefficient	0.561 mm^{-1}	
F_{000}	1304	

Crystal size	0.29 x 0.13 x 0.07 mm^3
Theta range for data collection	1.75 to 26.52°.
Index ranges	$-14 \le h \le 14$, $-15 \le k \le 15$, $-22 \le l \le 22$
Reflections collected	36213
Independent reflections	9971 [R_{int} = 0.0596]
Completeness to theta = 26.52°	98.8 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9597 and 0.8538
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9971 / 0 / 733
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0457, wR2 = 0.1109
R indices (all data)	R1 = 0.0782, wR2 = 0.1451
Largest diff. peak and hole	0.740 and -1.029 e.$Å^{-3}$

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for Rh(cod)OTs·CKphos. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9955(4)	8455(4)	5518(3)	32(1)
C(2)	9206(4)	8425(4)	4954(3)	33(1)
C(3)	9865(4)	6004(4)	6177(2)	29(1)
C(4)	8957(4)	6007(4)	5686(3)	33(1)
C(5)	8938(4)	6495(4)	4805(3)	41(1)
C(6)	9476(5)	7642(5)	4471(3)	42(1)
C(7)	11032(4)	6404(4)	5907(3)	40(1)
C(8)	11091(4)	7704(4)	5751(3)	36(1)
C(9)	7958(3)	6393(3)	8449(2)	18(1)
C(10)	8051(3)	5016(3)	8765(2)	19(1)
C(11)	6914(3)	4585(3)	8627(2)	19(1)
C(12)	7028(3)	4175(3)	7902(2)	20(1)
C(13)	7459(4)	3732(3)	9927(2)	24(1)

C(14)	6685(4)	4193(4)	10454(3)	37(1)
C(15)	8130(4)	2543(3)	10323(3)	33(1)
C(16)	5996(4)	10401(3)	6383(2)	27(1)
C(17)	6073(4)	10656(4)	7070(3)	36(1)
C(18)	5093(4)	10811(4)	7467(3)	41(1)
C(19)	4013(4)	10768(4)	7181(3)	36(1)
C(20)	3948(4)	10554(4)	6485(3)	39(1)
C(21)	4916(4)	10360(4)	6090(3)	33(1)
C(22)	2962(5)	10933(5)	7623(3)	54(2)
C(23)	9072(3)	6931(3)	8169(2)	21(1)
C(24)	9007(4)	8167(3)	7898(2)	23(1)
C(25)	9936(4)	8761(3)	7603(2)	27(1)
C(26)	10979(4)	8147(4)	7568(2)	28(1)
C(27)	11093(4)	6940(4)	7832(2)	27(1)
C(28)	10152(4)	6352(3)	8133(2)	24(1)
C(29)	7445(3)	6876(3)	9080(2)	19(1)
C(30)	6311(3)	7337(3)	9111(2)	22(1)
C(31)	5911(4)	7751(4)	9702(2)	26(1)
C(32)	6646(4)	7711(3)	10290(2)	28(1)
C(33)	7771(4)	7260(4)	10286(2)	27(1)
C(34)	8153(4)	6855(3)	9689(2)	23(1)
C(35)	7766(4)	2964(3)	8133(2)	23(1)
C(36)	8931(4)	2760(3)	8022(2)	26(1)
C(37)	9546(4)	1659(4)	8316(3)	31(1)
C(38)	9008(4)	709(4)	8741(3)	36(1)
C(39)	7858(4)	868(4)	8856(3)	33(1)
C(40)	7252(4)	1968(4)	8559(2)	28(1)
C(41)	5900(4)	4088(3)	7514(2)	21(1)
C(42)	5962(4)	3875(4)	6803(3)	28(1)
C(43)	5001(4)	3757(4)	6423(3)	35(1)
C(44)	3952(4)	3829(4)	6736(3)	35(1)
C(45)	3852(4)	4014(4)	7441(3)	30(1)
C(46)	4809(4)	4143(3)	7818(2)	24(1)
C(47)	5788(4)	7086(4)	5831(2)	35(1)
C(48)	4530(4)	7033(5)	5785(3)	41(1)
C(49)	4034(4)	7417(4)	6430(3)	33(1)

C(50)	4991(3)	7160(4)	7043(2)	23(1)
F(1)	5517(2)	7395(2)	8573(1)	30(1)
F(2)	4813(2)	8215(2)	9687(1)	35(1)
F(3)	6264(2)	8131(2)	10856(1)	37(1)
F(4)	8511(2)	7237(2)	10843(1)	38(1)
F(5)	9269(2)	6428(2)	9719(1)	28(1)
F(6)	8016(2)	8811(2)	7939(1)	29(1)
F(7)	9812(2)	9940(2)	7358(2)	38(1)
F(8)	11884(2)	8716(2)	7289(2)	42(1)
F(9)	12113(2)	6333(2)	7806(2)	38(1)
F(10)	10377(2)	5175(2)	8406(2)	33(1)
F(11)	6991(2)	3755(2)	6480(1)	36(1)
F(12)	5119(3)	3567(3)	5737(2)	52(1)
F(13)	3018(3)	3714(3)	6375(2)	55(1)
F(14)	2821(2)	4058(2)	7768(2)	40(1)
F(15)	4644(2)	4294(2)	8509(1)	28(1)
F(16)	6125(2)	2043(2)	8712(1)	31(1)
F(17)	7315(3)	-46(2)	9265(2)	46(1)
F(18)	9611(3)	-360(2)	9034(2)	49(1)
F(19)	10677(2)	1518(2)	8181(2)	44(1)
F(20)	9548(2)	3624(2)	7621(2)	34(1)
N(1)	6022(3)	6783(3)	6670(2)	22(1)
O(1)	7647(3)	8838(2)	6361(2)	35(1)
O(2)	6922(3)	10208(3)	5127(2)	41(1)
O(3)	8068(3)	10843(3)	5986(2)	44(1)
O(4)	7644(2)	5019(2)	7334(2)	20(1)
O(5)	7160(2)	6791(2)	7790(1)	18(1)
O(6)	6794(2)	3630(2)	9305(2)	23(1)
O(7)	8242(2)	4566(2)	9576(2)	25(1)
P(1)	7347(1)	6446(1)	7004(1)	19(1)
Rh(1)	8577(1)	7393(1)	6135(1)	22(1)
S(1)	7254(1)	10085(1)	5906(1)	29(1)

Table 8. Bond lengths [Å] and angles [°] for Rh(cod)OTs·CKphos.

C(1)-C(2)	1.376(6)	C(23)-C(24)	1.407(5)
C(1)-C(8)	1.503(6)	C(24)-F(6)	1.335(5)
C(1)-Rh(1)	2.239(4)	C(24)-C(25)	1.380(6)
C(2)-C(6)	1.496(6)	C(25)-F(7)	1.340(5)
C(2)-Rh(1)	2.269(4)	C(25)-C(26)	1.365(6)
C(3)-C(4)	1.401(6)	C(26)-F(8)	1.335(5)
C(3)-C(7)	1.525(6)	C(26)-C(27)	1.372(6)
C(3)-Rh(1)	2.105(4)	C(27)-F(9)	1.335(5)
C(4)-C(5)	1.517(6)	C(27)-C(28)	1.391(6)
C(4)-Rh(1)	2.098(4)	C(28)-F(10)	1.342(4)
C(5)-C(6)	1.529(7)	C(29)-C(30)	1.387(6)
C(7)-C(8)	1.515(7)	C(29)-C(34)	1.390(6)
C(9)-O(5)	1.449(4)	C(30)-F(1)	1.342(4)
C(9)-C(23)	1.534(5)	C(30)-C(31)	1.383(6)
C(9)-C(29)	1.535(5)	C(31)-F(2)	1.338(5)
C(9)-C(10)	1.567(5)	C(31)-C(32)	1.372(6)
C(10)-O(7)	1.410(4)	C(32)-F(3)	1.341(5)
C(10)-C(11)	1.541(5)	C(32)-C(33)	1.367(6)
C(11)-O(6)	1.409(4)	C(33)-F(4)	1.338(5)
C(11)-C(12)	1.556(5)	C(33)-C(34)	1.379(6)
C(12)-O(4)	1.447(4)	C(34)-F(5)	1.343(5)
C(12)-C(41)	1.540(5)	C(35)-C(36)	1.380(6)
C(12)-C(35)	1.545(5)	C(35)-C(40)	1.402(6)
C(13)-O(7)	1.431(5)	C(36)-F(20)	1.346(4)
C(13)-O(6)	1.433(5)	C(36)-C(37)	1.380(6)
C(13)-C(14)	1.503(6)	C(37)-F(19)	1.345(5)
C(13)-C(15)	1.512(6)	C(37)-C(38)	1.376(6)
C(16)-C(17)	1.390(6)	C(38)-F(18)	1.344(5)
C(16)-C(21)	1.394(6)	C(38)-C(39)	1.360(7)
C(16)-S(1)	1.765(4)	C(39)-F(17)	1.340(5)
C(17)-C(18)	1.374(7)	C(39)-C(40)	1.375(6)
C(18)-C(19)	1.390(7)	C(40)-F(16)	1.343(5)
C(19)-C(20)	1.381(7)	C(41)-C(46)	1.387(6)
C(19)-C(22)	1.490(7)	C(41)-C(42)	1.401(6)
C(20)-C(21)	1.370(7)	C(42)-F(11)	1.347(5)
C(23)-C(28)	1.384(6)	C(42)-C(43)	1.377(6)

C(43)-F(12)	1.345(5)	C(1)-C(8)-C(7)	113.9(4)
C(43)-C(44)	1.351(7)	O(5)-C(9)-C(23)	106.8(3)
C(44)-F(13)	1.332(5)	O(5)-C(9)-C(29)	108.1(3)
C(44)-C(45)	1.376(6)	C(23)-C(9)-C(29)	109.1(3)
C(45)-F(14)	1.340(5)	O(5)-C(9)-C(10)	107.2(3)
C(45)-C(46)	1.376(6)	C(23)-C(9)-C(10)	116.5(3)
C(46)-F(15)	1.339(5)	C(29)-C(9)-C(10)	108.8(3)
C(47)-N(1)	1.474(5)	O(7)-C(10)-C(11)	104.9(3)
C(47)-C(48)	1.487(6)	O(7)-C(10)-C(9)	112.0(3)
C(48)-C(49)	1.485(6)	C(11)-C(10)-C(9)	110.9(3)
C(49)-C(50)	1.529(6)	O(6)-C(11)-C(10)	104.0(3)
C(50)-N(1)	1.475(5)	O(6)-C(11)-C(12)	110.9(3)
N(1)-P(1)	1.632(3)	C(10)-C(11)-C(12)	109.0(3)
O(1)-S(1)	1.487(3)	O(4)-C(12)-C(41)	107.9(3)
O(1)-Rh(1)	2.104(3)	O(4)-C(12)-C(35)	108.4(3)
O(2)-S(1)	1.434(3)	C(41)-C(12)-C(35)	108.7(3)
O(3)-S(1)	1.441(3)	O(4)-C(12)-C(11)	106.4(3)
O(4)-P(1)	1.629(3)	C(41)-C(12)-C(11)	116.6(3)
O(5)-P(1)	1.624(3)	C(35)-C(12)-C(11)	108.4(3)
P(1)-Rh(1)	2.2421(10)	O(7)-C(13)-O(6)	106.4(3)
		O(7)-C(13)-C(14)	109.1(3)
C(2)-C(1)-C(8)	125.9(4)	O(6)-C(13)-C(14)	109.9(4)
C(2)-C(1)-Rh(1)	73.4(2)	O(7)-C(13)-C(15)	109.3(4)
C(8)-C(1)-Rh(1)	107.8(3)	O(6)-C(13)-C(15)	107.4(3)
C(1)-C(2)-C(6)	122.1(4)	C(14)-C(13)-C(15)	114.4(4)
C(1)-C(2)-Rh(1)	71.0(2)	C(17)-C(16)-C(21)	119.3(4)
C(6)-C(2)-Rh(1)	110.6(3)	C(17)-C(16)-S(1)	120.3(3)
C(4)-C(3)-C(7)	125.0(4)	C(21)-C(16)-S(1)	120.4(3)
C(4)-C(3)-Rh(1)	70.3(3)	C(18)-C(17)-C(16)	119.7(4)
C(7)-C(3)-Rh(1)	113.8(3)	C(17)-C(18)-C(19)	121.4(5)
C(3)-C(4)-C(5)	125.8(4)	C(20)-C(19)-C(18)	118.1(5)
C(3)-C(4)-Rh(1)	70.8(2)	C(20)-C(19)-C(22)	121.4(4)
C(5)-C(4)-Rh(1)	109.5(3)	C(18)-C(19)-C(22)	120.5(5)
C(4)-C(5)-C(6)	114.5(4)	C(21)-C(20)-C(19)	121.6(4)
C(2)-C(6)-C(5)	111.1(4)	C(20)-C(21)-C(16)	119.9(4)
C(8)-C(7)-C(3)	114.3(4)	C(28)-C(23)-C(24)	114.7(4)

C(28)-C(23)-C(9)	128.0(3)	C(36)-C(35)-C(12)	126.4(4)
C(24)-C(23)-C(9)	117.2(4)	C(40)-C(35)-C(12)	118.3(4)
F(6)-C(24)-C(25)	117.4(3)	F(20)-C(36)-C(37)	115.2(4)
F(6)-C(24)-C(23)	119.5(3)	F(20)-C(36)-C(35)	122.3(4)
C(25)-C(24)-C(23)	123.0(4)	C(37)-C(36)-C(35)	122.5(4)
F(7)-C(25)-C(26)	120.3(4)	F(19)-C(37)-C(38)	120.1(4)
F(7)-C(25)-C(24)	119.8(4)	F(19)-C(37)-C(36)	119.5(4)
C(26)-C(25)-C(24)	120.0(4)	C(38)-C(37)-C(36)	120.4(4)
F(8)-C(26)-C(25)	120.3(4)	F(18)-C(38)-C(39)	120.6(4)
F(8)-C(26)-C(27)	120.3(4)	F(18)-C(38)-C(37)	120.3(5)
C(25)-C(26)-C(27)	119.4(4)	C(39)-C(38)-C(37)	119.1(4)
F(9)-C(27)-C(26)	119.8(4)	F(17)-C(39)-C(38)	120.1(4)
F(9)-C(27)-C(28)	120.1(4)	F(17)-C(39)-C(40)	119.8(4)
C(26)-C(27)-C(28)	120.1(4)	C(38)-C(39)-C(40)	120.1(4)
F(10)-C(28)-C(23)	122.3(3)	F(16)-C(40)-C(39)	115.9(4)
F(10)-C(28)-C(27)	114.8(4)	F(16)-C(40)-C(35)	121.3(4)
C(23)-C(28)-C(27)	122.8(4)	C(39)-C(40)-C(35)	122.8(4)
C(30)-C(29)-C(34)	115.1(4)	C(46)-C(41)-C(42)	115.4(4)
C(30)-C(29)-C(9)	126.0(3)	C(46)-C(41)-C(12)	126.3(4)
C(34)-C(29)-C(9)	118.9(4)	C(42)-C(41)-C(12)	118.2(4)
F(1)-C(30)-C(31)	115.2(4)	F(11)-C(42)-C(43)	118.0(4)
F(1)-C(30)-C(29)	122.2(4)	F(11)-C(42)-C(41)	119.7(4)
C(31)-C(30)-C(29)	122.6(4)	C(43)-C(42)-C(41)	122.3(4)
F(2)-C(31)-C(32)	120.2(4)	F(12)-C(43)-C(44)	120.4(4)
F(2)-C(31)-C(30)	119.8(4)	F(12)-C(43)-C(42)	119.2(5)
C(32)-C(31)-C(30)	120.0(4)	C(44)-C(43)-C(42)	120.4(4)
F(3)-C(32)-C(33)	120.5(4)	F(13)-C(44)-C(43)	120.9(4)
F(3)-C(32)-C(31)	120.0(4)	F(13)-C(44)-C(45)	119.6(5)
C(33)-C(32)-C(31)	119.4(4)	C(43)-C(44)-C(45)	119.4(4)
F(4)-C(33)-C(32)	120.5(4)	F(14)-C(45)-C(46)	119.6(4)
F(4)-C(33)-C(34)	119.8(4)	F(14)-C(45)-C(44)	120.1(4)
C(32)-C(33)-C(34)	119.7(4)	C(46)-C(45)-C(44)	120.3(4)
F(5)-C(34)-C(33)	116.5(4)	F(15)-C(46)-C(45)	116.6(4)
F(5)-C(34)-C(29)	120.2(4)	F(15)-C(46)-C(41)	121.1(3)
C(33)-C(34)-C(29)	123.2(4)	C(45)-C(46)-C(41)	122.2(4)
C(36)-C(35)-C(40)	115.1(4)	N(1)-C(47)-C(48)	103.4(4)

C(49)-C(48)-C(47)	105.4(4)	C(4)-Rh(1)-C(1)	96.45(17)
C(48)-C(49)-C(50)	106.9(4)	O(1)-Rh(1)-C(1)	92.95(15)
N(1)-C(50)-C(49)	104.0(3)	C(3)-Rh(1)-C(1)	81.22(16)
C(47)-N(1)-C(50)	109.5(3)	C(4)-Rh(1)-P(1)	93.91(12)
C(47)-N(1)-P(1)	119.7(3)	O(1)-Rh(1)-P(1)	80.50(8)
C(50)-N(1)-P(1)	128.5(3)	C(3)-Rh(1)-P(1)	101.05(12)
S(1)-O(1)-Rh(1)	136.05(19)	C(1)-Rh(1)-P(1)	165.74(13)
C(12)-O(4)-P(1)	128.1(2)	C(4)-Rh(1)-C(2)	81.08(17)
C(9)-O(5)-P(1)	124.5(2)	O(1)-Rh(1)-C(2)	96.39(14)
C(11)-O(6)-C(13)	109.5(3)	C(3)-Rh(1)-C(2)	89.00(16)
C(10)-O(7)-C(13)	110.3(3)	C(1)-Rh(1)-C(2)	35.55(16)
O(5)-P(1)-O(4)	103.02(14)	P(1)-Rh(1)-C(2)	157.25(13)
O(5)-P(1)-N(1)	98.25(16)	O(2)-S(1)-O(3)	116.2(2)
O(4)-P(1)-N(1)	109.15(16)	O(2)-S(1)-O(1)	111.50(19)
O(5)-P(1)-Rh(1)	117.86(10)	O(3)-S(1)-O(1)	110.6(2)
O(4)-P(1)-Rh(1)	115.15(11)	O(2)-S(1)-C(16)	107.4(2)
N(1)-P(1)-Rh(1)	111.79(12)	O(3)-S(1)-C(16)	107.2(2)
C(4)-Rh(1)-O(1)	159.38(16)	O(1)-S(1)-C(16)	102.97(18)
C(4)-Rh(1)-C(3)	38.94(17)		
O(1)-Rh(1)-C(3)	161.58(15)		

Symmetry transformations used to generate equivalent atoms:

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Rh(cod)OTs•CKphos. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	28(2)	24(2)	36(3)	0(2)	13(2)	-9(2)
C(2)	34(3)	27(2)	27(2)	4(2)	9(2)	-1(2)
C(3)	31(3)	25(2)	26(2)	-4(2)	6(2)	3(2)
C(4)	31(3)	34(3)	43(3)	-23(2)	12(2)	-10(2)
C(5)	41(3)	55(3)	39(3)	-30(3)	1(2)	-7(3)
C(6)	45(3)	57(3)	21(2)	-9(2)	7(2)	-7(3)
C(7)	24(3)	45(3)	45(3)	-9(2)	5(2)	-1(2)

C(8)	25(2)	48(3)	35(3)	-13(2)	4(2)	-10(2)
C(9)	17(2)	16(2)	21(2)	-5(2)	-2(2)	-3(2)
C(10)	20(2)	15(2)	22(2)	-7(2)	-2(2)	-2(2)
C(11)	22(2)	14(2)	21(2)	-3(2)	-2(2)	-5(2)
C(12)	21(2)	18(2)	21(2)	-5(2)	0(2)	-6(2)
C(13)	31(2)	21(2)	20(2)	-4(2)	-2(2)	-9(2)
C(14)	39(3)	45(3)	35(3)	-21(2)	8(2)	-13(2)
C(15)	45(3)	19(2)	30(3)	1(2)	-10(2)	-7(2)
C(16)	33(3)	18(2)	30(2)	-7(2)	4(2)	-3(2)
C(17)	30(3)	30(2)	53(3)	-21(2)	-1(2)	-4(2)
C(18)	46(3)	37(3)	50(3)	-30(2)	4(3)	-2(2)
C(19)	35(3)	34(3)	50(3)	-26(2)	8(2)	-10(2)
C(20)	32(3)	43(3)	51(3)	-23(2)	-2(2)	-10(2)
C(21)	36(3)	32(2)	34(3)	-15(2)	3(2)	-7(2)
C(22)	40(3)	63(4)	74(4)	-43(3)	16(3)	-14(3)
C(23)	21(2)	23(2)	20(2)	-7(2)	-1(2)	-6(2)
C(24)	26(2)	19(2)	25(2)	-8(2)	2(2)	-5(2)
C(25)	35(3)	21(2)	26(2)	-6(2)	1(2)	-10(2)
C(26)	31(3)	33(2)	27(2)	-15(2)	5(2)	-16(2)
C(27)	24(2)	37(3)	26(2)	-16(2)	2(2)	-7(2)
C(28)	27(2)	19(2)	28(2)	-7(2)	-3(2)	-6(2)
C(29)	24(2)	12(2)	22(2)	-6(2)	4(2)	-4(2)
C(30)	23(2)	21(2)	21(2)	-5(2)	0(2)	-5(2)
C(31)	28(2)	24(2)	26(2)	-8(2)	8(2)	-6(2)
C(32)	41(3)	19(2)	28(2)	-13(2)	8(2)	-9(2)
C(33)	36(3)	26(2)	20(2)	-9(2)	-5(2)	-9(2)
C(34)	23(2)	17(2)	28(2)	-7(2)	1(2)	-2(2)
C(35)	26(2)	19(2)	24(2)	-9(2)	-5(2)	0(2)
C(36)	33(3)	17(2)	30(2)	-10(2)	1(2)	-7(2)
C(37)	30(3)	26(2)	41(3)	-18(2)	0(2)	4(2)
C(38)	49(3)	19(2)	39(3)	-9(2)	-7(2)	4(2)
C(39)	47(3)	17(2)	34(3)	-6(2)	-1(2)	-9(2)
C(40)	31(3)	24(2)	30(2)	-13(2)	-2(2)	-3(2)
C(41)	27(2)	12(2)	24(2)	-4(2)	-4(2)	-5(2)
C(42)	34(3)	24(2)	30(2)	-12(2)	-1(2)	-4(2)
C(43)	52(3)	32(2)	29(3)	-19(2)	-11(2)	-5(2)

C(44)	38(3)	29(2)	41(3)	-14(2)	-18(2)	-1(2)
C(45)	28(3)	19(2)	41(3)	-6(2)	-5(2)	-2(2)
C(46)	27(2)	15(2)	30(2)	-7(2)	-3(2)	-3(2)
C(47)	31(3)	49(3)	24(2)	-10(2)	-2(2)	-1(2)
C(48)	31(3)	52(3)	36(3)	-14(2)	-7(2)	3(2)
C(49)	25(2)	44(3)	28(2)	-9(2)	-2(2)	-2(2)
C(50)	16(2)	25(2)	23(2)	-2(2)	0(2)	2(2)
F(1)	21(1)	44(2)	28(1)	-17(1)	-1(1)	-1(1)
F(2)	31(2)	41(2)	37(2)	-19(1)	9(1)	2(1)
F(3)	48(2)	40(2)	33(2)	-25(1)	7(1)	-5(1)
F(4)	45(2)	43(2)	31(1)	-19(1)	-7(1)	-9(1)
F(5)	26(1)	32(1)	29(1)	-12(1)	-5(1)	-5(1)
F(6)	31(1)	18(1)	37(1)	-8(1)	5(1)	-2(1)
F(7)	51(2)	22(1)	44(2)	-9(1)	7(1)	-17(1)
F(8)	37(2)	46(2)	52(2)	-22(1)	17(1)	-27(1)
F(9)	21(1)	44(2)	49(2)	-17(1)	5(1)	0(1)
F(10)	23(1)	22(1)	50(2)	-8(1)	2(1)	1(1)
F(11)	46(2)	39(2)	29(1)	-19(1)	6(1)	-8(1)
F(12)	72(2)	57(2)	38(2)	-28(2)	-15(2)	-8(2)
F(13)	48(2)	57(2)	69(2)	-30(2)	-30(2)	-5(2)
F(14)	24(1)	38(2)	63(2)	-21(1)	-5(1)	-6(1)
F(15)	26(1)	35(1)	29(1)	-15(1)	3(1)	-10(1)
F(16)	30(1)	23(1)	39(2)	-9(1)	3(1)	-9(1)
F(17)	57(2)	19(1)	58(2)	-4(1)	6(2)	-9(1)
F(18)	56(2)	19(1)	63(2)	-9(1)	-5(2)	15(1)
F(19)	33(2)	37(2)	64(2)	-22(1)	1(1)	7(1)
F(20)	29(1)	25(1)	47(2)	-10(1)	7(1)	-1(1)
N(1)	21(2)	26(2)	19(2)	-6(2)	0(1)	-1(2)
O(1)	46(2)	21(2)	30(2)	0(1)	8(2)	7(1)
O(2)	47(2)	38(2)	30(2)	-4(2)	-1(2)	4(2)
O(3)	42(2)	41(2)	54(2)	-16(2)	8(2)	-18(2)
O(4)	22(2)	16(1)	22(2)	-6(1)	3(1)	-4(1)
O(5)	18(1)	16(1)	18(1)	-4(1)	-3(1)	1(1)
O(6)	28(2)	21(1)	19(2)	-4(1)	-2(1)	-9(1)
O(7)	32(2)	20(1)	22(2)	-2(1)	-6(1)	-10(1)
P(1)	19(1)	18(1)	19(1)	-5(1)	1(1)	-2(1)

Rh(1)	21(1)	20(1)	22(1)	-4(1)	2(1)	-3(1)
S(1)	31(1)	20(1)	30(1)	-1(1)	3(1)	-1(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Rh(cod)OTs·CKphos.

	x	y	z	U(eq)
H(1)	9925	9226	5587	38
H(2)	8736	9173	4690	39
H(3)	9905	5355	6671	35
H(4)	8493	5357	5898	40
H(5A)	8147	6629	4619	50
H(5B)	9344	5908	4609	50
H(6A)	10303	7465	4452	50
H(6B)	9185	8048	3945	50
H(7A)	11610	5957	6301	48
H(7B)	11222	6222	5436	48
H(8A)	11383	7810	6216	43
H(8B)	11634	7973	5342	43
H(10)	8676	4685	8507	22
H(11)	6269	5207	8559	23
H(14A)	6204	4885	10151	56
H(14B)	7144	4387	10816	56
H(14C)	6214	3603	10733	56
H(15A)	7607	1970	10527	50
H(15B)	8595	2586	10739	50
H(15C)	8616	2318	9954	50
H(17)	6785	10721	7259	43
H(18)	5154	10947	7937	49
H(20)	3231	10541	6279	47
H(21)	4852	10201	5628	40
H(22A)	2293	11066	7295	80
H(22B)	2994	11599	7794	80
H(22C)	2922	10241	8066	80
H(47A)	6219	6524	5624	42
H(47B)	5979	7869	5548	42
H(48A)	4207	7554	5289	49

H(48B)	4376	6238	5848	49
H(49A)	3392	6988	6648	40
H(49B)	3762	8251	6243	40
H(50A)	5090	7859	7172	27
H(50B)	4825	6541	7512	27

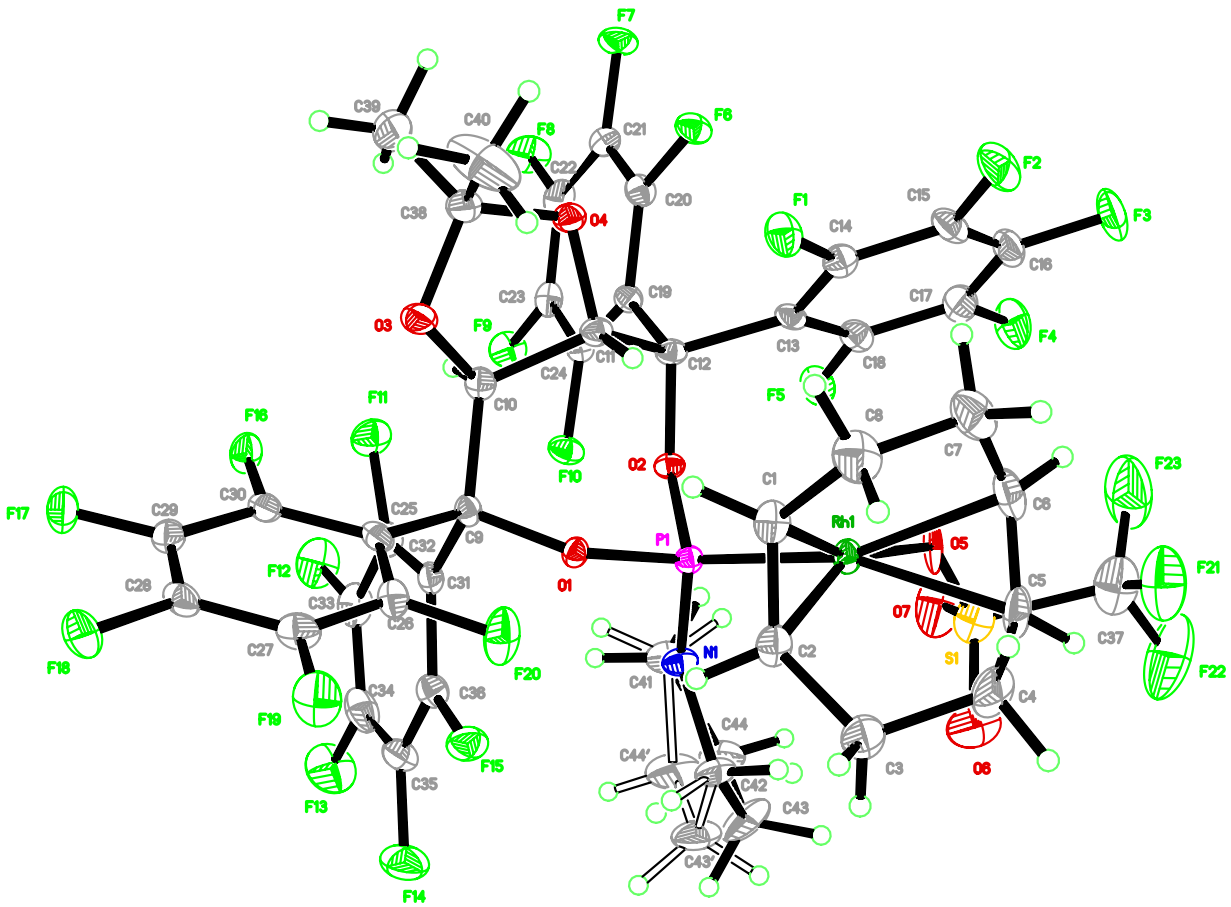


Table 11. Crystal data and structure refinement for Rh(cod)OTf·CKphos.

Identification code	Rovis107	
Empirical formula	C_{44} H_{28} F_{23} N O_7 P Rh S	
Formula weight	1285.61	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	*a* = 10.4903(10) Å	α= 78.012(3)°.
	b = 14.3946(14) Å	β= 84.045(3)°.
	c = 15.5781(15) Å	γ = 72.010(4)°.
Volume	2186.6(4) $Å^3$	
Z	2	
Density (calculated)	1.953 Mg/m^3	
Absorption coefficient	0.630 mm^{-1}	
F_{000}	1276	

Crystal size	0.23 x 0.06 x 0.06 mm^3
Theta range for data collection	1.82 to 27.10°.
Index ranges	$-13 \le h \le 13$, $-17 \le k \le 18$, $-19 \le l \le 19$
Reflections collected	40057
Independent reflections	9632 [R_{int} = 0.0482]
Completeness to theta = 27.10°	99.9 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9626 and 0.8687
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9632 / 43 / 725
Goodness-of-fit on F^2	1.124
Final R indices [I>2sigma(I)]	R1 = 0.0453, wR2 = 0.1260
R indices (all data)	R1 = 0.0687, wR2 = 0.1592
Largest diff. peak and hole	0.851 and -1.335 e.$Å^{-3}$

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for Rh(cod)OTf·CKphos. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5764(4)	5050(3)	7868(3)	18(1)
C(2)	4816(4)	5209(3)	7231(3)	19(1)
C(3)	4769(5)	4485(3)	6663(3)	28(1)
C(4)	6143(5)	3908(3)	6330(3)	30(1)
C(5)	7091(5)	4542(3)	6092(3)	25(1)
C(6)	7983(4)	4555(3)	6655(3)	25(1)
C(7)	8166(5)	3970(3)	7597(3)	30(1)
C(8)	6850(5)	4068(3)	8136(3)	29(1)
C(9)	3468(4)	7979(3)	8467(2)	13(1)
C(10)	4657(4)	8066(3)	8935(2)	14(1)
C(11)	6086(4)	7476(3)	8664(2)	14(1)
C(12)	6672(4)	7965(3)	7810(2)	13(1)
C(13)	8014(4)	7311(3)	7454(3)	14(1)

C(14)	8764(4)	6368(3)	7861(3)	17(1)
C(15)	9997(4)	5879(3)	7511(3)	21(1)
C(16)	10511(4)	6314(3)	6741(3)	23(1)
C(17)	9789(4)	7240(3)	6310(3)	23(1)
C(18)	8569(4)	7712(3)	6670(3)	18(1)
C(19)	6879(4)	8954(3)	7897(2)	13(1)
C(20)	7976(4)	8942(3)	8352(3)	16(1)
C(21)	8224(4)	9793(3)	8470(3)	17(1)
C(22)	7384(4)	10710(3)	8112(3)	18(1)
C(23)	6322(4)	10758(3)	7642(2)	16(1)
C(24)	6068(4)	9901(3)	7545(2)	13(1)
C(25)	2480(4)	7575(3)	9137(3)	15(1)
C(26)	2124(4)	6716(3)	9156(3)	17(1)
C(27)	1138(4)	6464(3)	9723(3)	19(1)
C(28)	455(4)	7074(3)	10309(3)	17(1)
C(29)	782(4)	7920(3)	10319(3)	18(1)
C(30)	1780(4)	8156(3)	9743(2)	15(1)
C(31)	2573(4)	8971(3)	7936(2)	15(1)
C(32)	2514(4)	9929(3)	7983(3)	21(1)
C(33)	1618(5)	10765(3)	7507(3)	24(1)
C(34)	727(5)	10646(3)	6985(3)	26(1)
C(35)	726(4)	9703(3)	6946(3)	23(1)
C(36)	1611(4)	8902(3)	7418(3)	17(1)
C(37)	8636(6)	6410(4)	4253(4)	42(1)
C(38)	5945(4)	7383(4)	10160(3)	25(1)
C(39)	6022(6)	8122(6)	10673(4)	62(2)
C(40)	6330(6)	6317(5)	10675(4)	56(2)
N(1)	4050(3)	8110(2)	6186(2)	15(1)
C(41)	4019(4)	9137(3)	5739(3)	21(1)
C(42)	3390(4)	7647(3)	5662(3)	21(1)
C(43)	3253(19)	8356(9)	4782(6)	32(4)
C(44)	3631(15)	9152(9)	4811(6)	24(3)
C(43')	2675(15)	8529(8)	4989(9)	31(3)
C(44')	3044(17)	9338(9)	5013(9)	35(4)
F(1)	8347(2)	5891(2)	8616(2)	23(1)
F(2)	10689(3)	4987(2)	7930(2)	31(1)

F(3)	11703(3)	5845(2)	6403(2)	33(1)
F(4)	10265(3)	7667(2)	5560(2)	33(1)
F(5)	7906(2)	8609(2)	6232(2)	21(1)
F(6)	8883(2)	8081(2)	8676(2)	18(1)
F(7)	9280(2)	9722(2)	8917(2)	23(1)
F(8)	7614(3)	11543(2)	8212(2)	28(1)
F(9)	5515(2)	11640(2)	7287(2)	22(1)
F(10)	5010(2)	10042(2)	7073(2)	18(1)
F(11)	3288(3)	10147(2)	8505(2)	24(1)
F(12)	1626(3)	11661(2)	7590(2)	33(1)
F(13)	-154(3)	11441(2)	6540(2)	39(1)
F(14)	-172(3)	9581(2)	6454(2)	33(1)
F(15)	1495(2)	7998(2)	7382(2)	23(1)
F(16)	2050(2)	8998(2)	9767(2)	20(1)
F(17)	111(2)	8532(2)	10851(2)	25(1)
F(18)	-528(2)	6848(2)	10848(2)	26(1)
F(19)	821(3)	5642(2)	9703(2)	29(1)
F(20)	2700(3)	6078(2)	8606(2)	28(1)
F(21)	8884(4)	5441(2)	4542(2)	53(1)
F(22)	8554(5)	6556(3)	3386(2)	74(1)
F(23)	9662(4)	6681(3)	4427(3)	72(1)
O(1)	4020(3)	7278(2)	7885(2)	12(1)
O(2)	5682(3)	8198(2)	7157(2)	13(1)
O(3)	4632(3)	7603(2)	9843(2)	24(1)
O(4)	6807(3)	7445(2)	9391(2)	15(1)
O(5)	7268(3)	6760(2)	5631(2)	22(1)
O(6)	6076(4)	6755(3)	4470(3)	51(1)
O(7)	7034(4)	8114(3)	4477(3)	50(1)
P(1)	4970(1)	7402(1)	6991(1)	12(1)
Rh(1)	6259(1)	5936(1)	6698(1)	14(1)
S(1)	7073(1)	7101(1)	4755(1)	33(1)

Table 13. Bond lengths [Å] and angles [°] for Rh(cod)OTf·CKphos.

C(1)-C(2)	1.412(6)	C(1)-C(8)	1.526(6)

C(1)-Rh(1)	2.113(4)	C(21)-F(7)	1.335(4)
C(2)-C(3)	1.515(5)	C(21)-C(22)	1.381(6)
C(2)-Rh(1)	2.104(4)	C(22)-F(8)	1.336(4)
C(3)-C(4)	1.523(6)	C(22)-C(23)	1.373(6)
C(4)-C(5)	1.518(7)	C(23)-F(9)	1.332(4)
C(5)-C(6)	1.352(6)	C(23)-C(24)	1.379(5)
C(5)-Rh(1)	2.282(4)	C(24)-F(10)	1.335(4)
C(6)-C(7)	1.532(7)	C(25)-C(30)	1.390(5)
C(6)-Rh(1)	2.244(4)	C(25)-C(26)	1.392(6)
C(7)-C(8)	1.523(7)	C(26)-F(20)	1.349(4)
C(9)-O(1)	1.443(4)	C(26)-C(27)	1.374(6)
C(9)-C(25)	1.548(5)	C(27)-F(19)	1.332(5)
C(9)-C(10)	1.558(5)	C(27)-C(28)	1.388(6)
C(9)-C(31)	1.564(5)	C(28)-F(18)	1.337(5)
C(10)-O(3)	1.435(5)	C(28)-C(29)	1.367(6)
C(10)-C(11)	1.542(5)	C(29)-F(17)	1.326(4)
C(11)-O(4)	1.412(4)	C(29)-C(30)	1.383(6)
C(11)-C(12)	1.533(5)	C(30)-F(16)	1.336(4)
C(12)-O(2)	1.444(4)	C(31)-C(32)	1.378(6)
C(12)-C(19)	1.540(5)	C(31)-C(36)	1.395(5)
C(12)-C(13)	1.553(5)	C(32)-F(11)	1.348(5)
C(13)-C(18)	1.389(6)	C(32)-C(33)	1.399(6)
C(13)-C(14)	1.397(6)	C(33)-F(12)	1.325(5)
C(14)-F(1)	1.337(5)	C(33)-C(34)	1.370(6)
C(14)-C(15)	1.384(6)	C(34)-F(13)	1.339(5)
C(15)-F(2)	1.333(5)	C(34)-C(35)	1.373(6)
C(15)-C(16)	1.372(7)	C(35)-F(14)	1.346(5)
C(16)-F(3)	1.337(5)	C(35)-C(36)	1.364(6)
C(16)-C(17)	1.383(7)	C(36)-F(15)	1.356(5)
C(17)-F(4)	1.327(5)	C(37)-F(23)	1.322(7)
C(17)-C(18)	1.373(6)	C(37)-F(21)	1.324(6)
C(18)-F(5)	1.340(5)	C(37)-F(22)	1.331(7)
C(19)-C(24)	1.397(5)	C(37)-S(1)	1.828(6)
C(19)-C(20)	1.408(5)	C(38)-O(4)	1.428(5)
C(20)-F(6)	1.344(4)	C(38)-O(3)	1.431(5)
C(20)-C(21)	1.379(5)	C(38)-C(39)	1.482(7)

C(38)-C(40)	1.527(7)	O(1)-C(9)-C(31)	109.3(3)
N(1)-C(42)	1.488(5)	C(25)-C(9)-C(31)	104.6(3)
N(1)-C(41)	1.489(5)	C(10)-C(9)-C(31)	115.8(3)
N(1)-P(1)	1.629(3)	O(3)-C(10)-C(11)	98.9(3)
C(41)-C(44')	1.527(10)	O(3)-C(10)-C(9)	110.3(3)
C(41)-C(44)	1.537(10)	C(11)-C(10)-C(9)	117.3(3)
C(42)-C(43')	1.515(10)	O(4)-C(11)-C(12)	110.9(3)
C(42)-C(43)	1.520(10)	O(4)-C(11)-C(10)	101.1(3)
C(43)-C(44)	1.333(12)	C(12)-C(11)-C(10)	114.7(3)
C(43')-C(44')	1.344(12)	O(2)-C(12)-C(11)	106.4(3)
O(1)-P(1)	1.639(3)	O(2)-C(12)-C(19)	106.9(3)
O(2)-P(1)	1.623(3)	C(11)-C(12)-C(19)	111.9(3)
O(5)-S(1)	1.366(3)	O(2)-C(12)-C(13)	108.1(3)
O(5)-Rh(1)	2.210(3)	C(11)-C(12)-C(13)	115.3(3)
O(6)-S(1)	1.431(4)	C(19)-C(12)-C(13)	107.9(3)
O(7)-S(1)	1.421(4)	C(18)-C(13)-C(14)	115.8(4)
P(1)-Rh(1)	2.2366(10)	C(18)-C(13)-C(12)	117.5(3)
C(2)-C(1)-C(8)	124.0(4)	C(14)-C(13)-C(12)	126.6(4)
C(2)-C(1)-Rh(1)	70.1(2)	F(1)-C(14)-C(15)	116.1(4)
C(8)-C(1)-Rh(1)	113.7(3)	F(1)-C(14)-C(13)	122.2(4)
C(1)-C(2)-C(3)	126.5(4)	C(15)-C(14)-C(13)	121.7(4)
C(1)-C(2)-Rh(1)	70.8(2)	F(2)-C(15)-C(16)	120.1(4)
C(3)-C(2)-Rh(1)	109.8(3)	F(2)-C(15)-C(14)	119.6(4)
C(2)-C(3)-C(4)	114.0(4)	C(16)-C(15)-C(14)	120.3(4)
C(5)-C(4)-C(3)	112.3(4)	F(3)-C(16)-C(15)	120.4(4)
C(6)-C(5)-C(4)	122.8(4)	F(3)-C(16)-C(17)	119.8(4)
C(6)-C(5)-Rh(1)	71.1(2)	C(15)-C(16)-C(17)	119.8(4)
C(4)-C(5)-Rh(1)	109.2(3)	F(4)-C(17)-C(18)	120.5(4)
C(5)-C(6)-C(7)	126.1(4)	F(4)-C(17)-C(16)	120.6(4)
C(5)-C(6)-Rh(1)	74.2(2)	C(18)-C(17)-C(16)	118.9(4)
C(7)-C(6)-Rh(1)	107.1(3)	F(5)-C(18)-C(17)	116.9(4)
C(8)-C(7)-C(6)	113.2(4)	F(5)-C(18)-C(13)	119.6(3)
C(7)-C(8)-C(1)	114.5(4)	C(17)-C(18)-C(13)	123.5(4)
O(1)-C(9)-C(25)	108.0(3)	C(24)-C(19)-C(20)	114.9(3)
O(1)-C(9)-C(10)	107.7(3)	C(24)-C(19)-C(12)	125.6(3)
C(25)-C(9)-C(10)	111.2(3)	C(20)-C(19)-C(12)	119.5(3)

F(6)-C(20)-C(21)	115.7(3)	F(11)-C(32)-C(31)	123.3(4)
F(6)-C(20)-C(19)	121.0(3)	F(11)-C(32)-C(33)	113.9(4)
C(21)-C(20)-C(19)	123.2(4)	C(31)-C(32)-C(33)	122.8(4)
F(7)-C(21)-C(20)	119.8(3)	F(12)-C(33)-C(34)	121.2(4)
F(7)-C(21)-C(22)	120.9(3)	F(12)-C(33)-C(32)	118.9(4)
C(20)-C(21)-C(22)	119.3(4)	C(34)-C(33)-C(32)	119.8(4)
F(8)-C(22)-C(23)	120.3(4)	F(13)-C(34)-C(33)	120.4(4)
F(8)-C(22)-C(21)	120.3(4)	F(13)-C(34)-C(35)	120.6(4)
C(23)-C(22)-C(21)	119.5(4)	C(33)-C(34)-C(35)	119.0(4)
F(9)-C(23)-C(22)	119.8(3)	F(14)-C(35)-C(36)	120.8(4)
F(9)-C(23)-C(24)	119.6(4)	F(14)-C(35)-C(34)	119.3(4)
C(22)-C(23)-C(24)	120.6(4)	C(36)-C(35)-C(34)	119.8(4)
F(10)-C(24)-C(23)	115.1(3)	F(15)-C(36)-C(35)	116.1(4)
F(10)-C(24)-C(19)	122.4(3)	F(15)-C(36)-C(31)	119.9(3)
C(23)-C(24)-C(19)	122.5(3)	C(35)-C(36)-C(31)	123.9(4)
C(30)-C(25)-C(26)	115.2(4)	F(23)-C(37)-F(21)	108.6(5)
C(30)-C(25)-C(9)	118.0(3)	F(23)-C(37)-F(22)	108.9(5)
C(26)-C(25)-C(9)	126.6(3)	F(21)-C(37)-F(22)	106.5(4)
F(20)-C(26)-C(27)	114.9(4)	F(23)-C(37)-S(1)	111.1(4)
F(20)-C(26)-C(25)	122.5(4)	F(21)-C(37)-S(1)	110.9(4)
C(27)-C(26)-C(25)	122.6(4)	F(22)-C(37)-S(1)	110.7(4)
F(19)-C(27)-C(26)	120.1(4)	O(4)-C(38)-O(3)	105.2(3)
F(19)-C(27)-C(28)	119.7(4)	O(4)-C(38)-C(39)	108.6(4)
C(26)-C(27)-C(28)	120.2(4)	O(3)-C(38)-C(39)	111.8(4)
F(18)-C(28)-C(29)	120.2(4)	O(4)-C(38)-C(40)	109.5(4)
F(18)-C(28)-C(27)	120.6(4)	O(3)-C(38)-C(40)	107.9(4)
C(29)-C(28)-C(27)	119.2(4)	C(39)-C(38)-C(40)	113.5(5)
F(17)-C(29)-C(28)	120.2(4)	C(42)-N(1)-C(41)	111.3(3)
F(17)-C(29)-C(30)	120.2(4)	C(42)-N(1)-P(1)	118.7(3)
C(28)-C(29)-C(30)	119.5(4)	C(41)-N(1)-P(1)	128.2(3)
F(16)-C(30)-C(29)	117.4(3)	N(1)-C(41)-C(44')	101.8(5)
F(16)-C(30)-C(25)	119.3(4)	N(1)-C(41)-C(44)	101.4(5)
C(29)-C(30)-C(25)	123.4(4)	C(44')-C(41)-C(44)	25.1(5)
C(32)-C(31)-C(36)	114.5(4)	N(1)-C(42)-C(43')	102.3(5)
C(32)-C(31)-C(9)	127.9(3)	N(1)-C(42)-C(43)	102.2(5)
C(36)-C(31)-C(9)	117.2(3)	C(43')-C(42)-C(43)	25.0(5)

C(44)-C(43)-C(42)	111.7(8)	O(5)-Rh(1)-P(1)	87.94(7)
C(43)-C(44)-C(41)	111.4(8)	C(2)-Rh(1)-C(6)	96.47(16)
C(44')-C(43')-C(42)	111.3(8)	C(1)-Rh(1)-C(6)	81.63(17)
C(43')-C(44')-C(41)	111.6(8)	O(5)-Rh(1)-C(6)	89.65(14)
C(9)-O(1)-P(1)	128.2(2)	P(1)-Rh(1)-C(6)	162.45(12)
C(12)-O(2)-P(1)	122.9(2)	C(2)-Rh(1)-C(5)	81.26(16)
C(38)-O(3)-C(10)	108.0(3)	C(1)-Rh(1)-C(5)	89.16(16)
C(11)-O(4)-C(38)	108.1(3)	O(5)-Rh(1)-C(5)	90.24(14)
S(1)-O(5)-Rh(1)	134.0(2)	P(1)-Rh(1)-C(5)	162.54(12)
O(2)-P(1)-N(1)	97.64(15)	C(6)-Rh(1)-C(5)	34.76(16)
O(2)-P(1)-O(1)	102.58(13)	O(5)-S(1)-O(7)	113.5(2)
N(1)-P(1)-O(1)	109.63(16)	O(5)-S(1)-O(6)	111.1(2)
O(2)-P(1)-Rh(1)	118.95(11)	O(7)-S(1)-O(6)	119.4(3)
N(1)-P(1)-Rh(1)	114.40(12)	O(5)-S(1)-C(37)	102.5(2)
O(1)-P(1)-Rh(1)	112.18(10)	O(7)-S(1)-C(37)	104.4(3)
C(2)-Rh(1)-C(1)	39.13(16)	O(6)-S(1)-C(37)	103.7(3)
C(2)-Rh(1)-O(5)	154.66(14)		
C(1)-Rh(1)-O(5)	165.46(14)		
C(2)-Rh(1)-P(1)	93.09(11)		
C(1)-Rh(1)-P(1)	96.87(11)		

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Rh(cod)OTf•CKphos. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(2)	12(2)	19(2)	-1(2)	2(2)	-5(2)
C(2)	21(2)	16(2)	24(2)	-7(2)	4(2)	-10(2)
C(3)	26(2)	27(2)	38(3)	-16(2)	2(2)	-13(2)
C(4)	36(3)	22(2)	40(3)	-19(2)	4(2)	-12(2)
C(5)	27(2)	17(2)	33(2)	-15(2)	11(2)	-5(2)
C(6)	17(2)	17(2)	41(3)	-11(2)	8(2)	-3(2)
C(7)	25(2)	18(2)	41(3)	-3(2)	-4(2)	1(2)
C(8)	32(3)	18(2)	29(2)	3(2)	-4(2)	-1(2)
C(9)	13(2)	10(2)	16(2)	-5(2)	2(2)	-3(2)

C(10)	15(2)	14(2)	16(2)	-4(2)	2(2)	-6(2)
C(11)	15(2)	12(2)	15(2)	-3(2)	-4(2)	-3(2)
C(12)	14(2)	11(2)	15(2)	-2(1)	-4(2)	-4(2)
C(13)	11(2)	13(2)	22(2)	-6(2)	-4(2)	-4(2)
C(14)	19(2)	15(2)	17(2)	-3(2)	-2(2)	-6(2)
C(15)	14(2)	15(2)	34(2)	-6(2)	-6(2)	-1(2)
C(16)	12(2)	26(2)	35(2)	-15(2)	2(2)	-6(2)
C(17)	19(2)	31(2)	24(2)	-10(2)	6(2)	-14(2)
C(18)	15(2)	15(2)	23(2)	-4(2)	-2(2)	-5(2)
C(19)	12(2)	15(2)	14(2)	-3(2)	1(1)	-6(2)
C(20)	16(2)	13(2)	17(2)	-1(2)	-1(2)	-2(2)
C(21)	18(2)	18(2)	17(2)	-5(2)	-1(2)	-6(2)
C(22)	25(2)	11(2)	23(2)	-7(2)	3(2)	-10(2)
C(23)	20(2)	12(2)	14(2)	0(2)	3(2)	-3(2)
C(24)	13(2)	14(2)	12(2)	-3(2)	-1(1)	-4(2)
C(25)	10(2)	17(2)	17(2)	-2(2)	-2(2)	-3(2)
C(26)	15(2)	16(2)	18(2)	-5(2)	2(2)	-2(2)
C(27)	21(2)	19(2)	21(2)	0(2)	-2(2)	-12(2)
C(28)	13(2)	24(2)	15(2)	2(2)	0(2)	-9(2)
C(29)	16(2)	21(2)	15(2)	-4(2)	-2(2)	-2(2)
C(30)	12(2)	17(2)	15(2)	-2(2)	-2(2)	-5(2)
C(31)	12(2)	16(2)	14(2)	-4(2)	1(2)	-1(2)
C(32)	20(2)	24(2)	19(2)	-6(2)	2(2)	-7(2)
C(33)	29(2)	16(2)	25(2)	-2(2)	3(2)	-5(2)
C(34)	19(2)	25(2)	25(2)	3(2)	2(2)	2(2)
C(35)	14(2)	31(2)	23(2)	-5(2)	-3(2)	-5(2)
C(36)	16(2)	16(2)	19(2)	-3(2)	0(2)	-4(2)
C(37)	49(3)	36(3)	45(3)	-13(3)	13(3)	-18(3)
C(38)	16(2)	43(3)	16(2)	-6(2)	0(2)	-9(2)
C(39)	25(3)	116(6)	63(4)	-71(4)	0(3)	-11(3)
C(40)	28(3)	78(5)	41(3)	38(3)	-7(2)	-18(3)
N(1)	18(2)	14(2)	16(2)	-2(1)	-5(1)	-7(1)
C(41)	26(2)	14(2)	21(2)	3(2)	-8(2)	-9(2)
C(42)	23(2)	21(2)	22(2)	-7(2)	-6(2)	-10(2)
C(43)	57(10)	27(6)	11(5)	-1(4)	-13(5)	-7(6)
C(44)	27(6)	28(6)	17(5)	7(4)	-7(4)	-15(5)

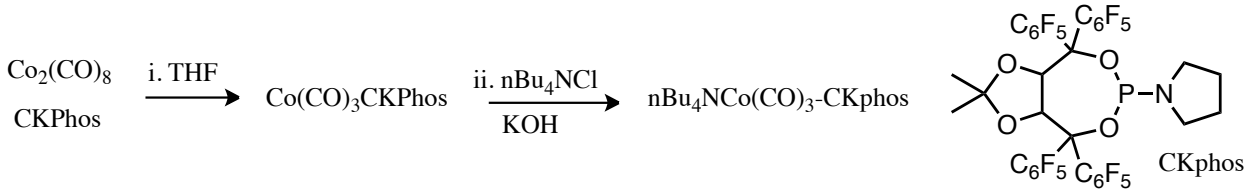
C(43')	32(7)	30(6)	31(7)	-5(5)	-19(5)	-4(5)
C(44')	41(8)	31(6)	26(6)	9(5)	-25(6)	-3(6)
F(1)	22(1)	15(1)	25(1)	-1(1)	0(1)	0(1)
F(2)	23(1)	17(1)	45(2)	-5(1)	-5(1)	5(1)
F(3)	16(1)	33(2)	49(2)	-18(1)	10(1)	-1(1)
F(4)	25(1)	41(2)	29(1)	-5(1)	14(1)	-12(1)
F(5)	20(1)	18(1)	21(1)	2(1)	2(1)	-5(1)
F(6)	16(1)	13(1)	24(1)	-3(1)	-6(1)	-2(1)
F(7)	18(1)	23(1)	31(1)	-10(1)	-9(1)	-8(1)
F(8)	34(2)	15(1)	40(2)	-7(1)	-8(1)	-12(1)
F(9)	28(1)	11(1)	25(1)	0(1)	-6(1)	-2(1)
F(10)	16(1)	15(1)	23(1)	-1(1)	-7(1)	-2(1)
F(11)	29(1)	18(1)	28(1)	-8(1)	-3(1)	-9(1)
F(12)	42(2)	14(1)	38(2)	-4(1)	0(1)	-5(1)
F(13)	37(2)	25(2)	44(2)	6(1)	-12(1)	5(1)
F(14)	26(1)	40(2)	30(1)	-1(1)	-12(1)	-7(1)
F(15)	23(1)	21(1)	27(1)	-7(1)	-4(1)	-9(1)
F(16)	22(1)	20(1)	23(1)	-10(1)	6(1)	-11(1)
F(17)	23(1)	30(1)	24(1)	-12(1)	9(1)	-10(1)
F(18)	20(1)	33(2)	26(1)	-4(1)	7(1)	-14(1)
F(19)	33(2)	24(1)	38(2)	-9(1)	9(1)	-20(1)
F(20)	34(2)	19(1)	36(2)	-15(1)	15(1)	-14(1)
F(21)	59(2)	35(2)	62(2)	-14(2)	21(2)	-11(2)
F(22)	114(4)	62(3)	36(2)	-16(2)	31(2)	-19(2)
F(23)	48(2)	77(3)	109(3)	-53(3)	36(2)	-34(2)
O(1)	13(1)	12(1)	13(1)	-5(1)	2(1)	-5(1)
O(2)	13(1)	13(1)	13(1)	-2(1)	-2(1)	-6(1)
O(3)	14(2)	44(2)	12(1)	-3(1)	-1(1)	-10(1)
O(4)	14(1)	19(1)	12(1)	-1(1)	-2(1)	-6(1)
O(5)	22(2)	12(1)	35(2)	-11(1)	25(1)	-12(1)
O(6)	43(2)	75(3)	45(2)	-25(2)	-7(2)	-19(2)
O(7)	70(3)	32(2)	39(2)	-3(2)	10(2)	-8(2)
P(1)	13(1)	11(1)	13(1)	-3(1)	0(1)	-4(1)
Rh(1)	15(1)	12(1)	17(1)	-5(1)	1(1)	-3(1)
S(1)	35(1)	34(1)	31(1)	-11(1)	2(1)	-9(1)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Rh(cod)OTf·CKphos.

	x	y	z	U(eq)
H(1)	5415	5415	8349	22
H(2)	3936	5663	7356	23
H(3A)	4230	4849	6163	33
H(3B)	4328	4016	7000	33
H(4A)	6532	3340	6779	36
H(4B)	6037	3661	5816	36
H(5)	7371	4660	5469	30
H(6)	8803	4682	6365	30
H(7A)	8603	3274	7580	36
H(7B)	8751	4205	7886	36
H(8A)	7027	3994	8749	35
H(8B)	6511	3527	8083	35
H(10)	4601	8768	8885	17
H(11)	6106	6801	8622	17
H(39A)	5735	8777	10323	93
H(39B)	6930	7982	10835	93
H(39C)	5450	8086	11194	93
H(40A)	5803	6287	11216	83
H(40B)	7264	6108	10799	83
H(40C)	6166	5886	10333	83
H(41A)	4889	9243	5731	25
H(41B)	3354	9632	6017	25
H(41C)	4900	9166	5499	25
H(41D)	3689	9605	6137	25
H(42A)	2520	7617	5924	25
H(42B)	3943	6984	5604	25
H(42C)	2760	7347	6025	25
H(42D)	4045	7148	5383	25
H(43A)	3800	8010	4337	39
H(43B)	2327	8568	4616	39

H(44A)	2902	9748	4629	28
H(44B)	4391	9169	4403	28
H(43C)	2882	8365	4407	37
H(43D)	1713	8673	5103	37
H(44C)	2253	9878	5111	42
H(44D)	3465	9542	4451	42

6. Synthesis and X-ray of $Co(CO)_3$n-BuN_4·CKPhos



In an Ar atmosphere glove box to an oven-dried 20 ml scintillation vial equipped with a magnetic stirbar was added Co_2CO_8 (15 mg, 0.044 mmol, 1 equiv), racemic CKPhos (55 mg, 0.059 mmol) and THF (2 ml). Bubbling (release of CO) occurs and the resultant dark brown solution is stirred 30 minutes at room temperature. *n*-Bu_4NCl (37 mg, 0.133 mmol) and KOH (10 mg, 0.178 mmol) are then added and the heterogeneous solution is stirred overnight. Reaction mixture is then filtered through a plug of cotton in a glass pipette. THF was removed under reduced pressure and DCM was added to the solid residue. Layering with hexanes and slow evaporation provided tan crystals of X-ray quality (50 mg, 43% yield).

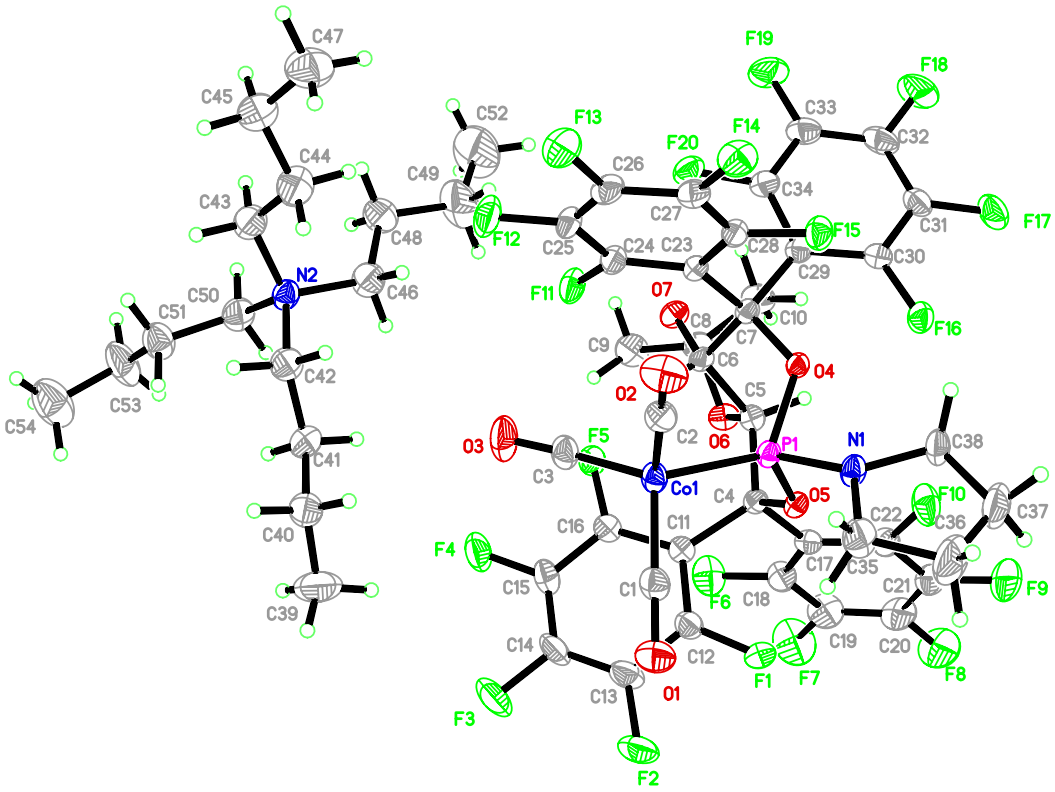


Table 16. Crystal data and structure refinement for $Co(CO)_3$*n*-Bu_4N·CKphos.

Identification code	rovis141r_0m-sr	
Empirical formula	C_{54} H_{52} Co F_{20} N_2 O_7 P	
Formula weight	1310.88	
Temperature	120 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* -1	
Unit cell dimensions	*a* = 13.4123(5) Å	α= 94.268(2)°
	b = 14.8876(6) Å	β= 90.340(2)°
	c = 16.7728(7) Å	ɣ = 97.344(2)°
Volume	3312.1(2) $Å^3$	
Z	2	
Density (calculated)	1.314 Mg/m^3	
Absorption coefficient	0.385 mm^{-1}	
F_{000}	1336	
Crystal size	0.56 x 0.21 x 0.05 mm^3	
Theta range for data collection	1.22 to 26.45°.	

Index ranges	$-16 \le h \le 15$, $-18 \le k \le 18$, $-20 \le l \le 20$
Reflections collected	48968
Independent reflections	13496 [R_{int} = 0.0482]
Completeness to theta = 26.45°	98.8 %
Absorption correction	multi-scan
Max. and min. transmission	0.9795 and 0.8137
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13496 / 0 / 772
Goodness-of-fit on F^2	0.934
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1458
R indices (all data)	R1 = 0.1172, wR2 = 0.1645
Largest diff. peak and hole	0.535 and -0.318 e.$Å^{-3}$

Table 17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Co(CO)_3$n-Bu_4N•CKphos. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1347(3)	3478(2)	4123(2)	63(1)
C(2)	2441(3)	2324(2)	5031(2)	61(1)
C(3)	3367(3)	3303(2)	3786(2)	65(1)
C(4)	1574(2)	1869(2)	1843(2)	45(1)
C(5)	2393(2)	1244(2)	1700(2)	45(1)
C(6)	3280(2)	1306(2)	2299(2)	45(1)
C(7)	3085(2)	620(2)	2959(2)	43(1)
C(8)	3808(3)	1090(2)	982(2)	60(1)
C(9)	4583(3)	1708(3)	529(2)	84(1)
C(10)	3709(3)	97(3)	644(2)	76(1)
C(11)	1846(3)	2913(2)	1951(2)	49(1)
C(12)	1070(3)	3420(2)	2136(2)	61(1)
C(13)	1207(4)	4354(3)	2260(3)	79(1)
C(14)	2139(4)	4818(2)	2205(3)	85(1)
C(15)	2920(3)	4355(3)	2008(2)	73(1)
C(16)	2786(3)	3421(2)	1897(2)	56(1)

C(17)	825(3)	1642(2)	1123(2)	51(1)
C(18)	890(3)	2108(3)	446(2)	71(1)
C(19)	217(4)	1922(3)	-188(3)	92(2)
C(20)	-560(4)	1253(4)	-148(3)	90(2)
C(21)	-634(3)	754(3)	475(3)	75(1)
C(22)	63(3)	936(3)	1092(2)	61(1)
C(23)	3739(2)	846(2)	3721(2)	43(1)
C(24)	4556(3)	1497(2)	3850(2)	54(1)
C(25)	5051(3)	1677(2)	4569(2)	60(1)
C(26)	4742(3)	1197(3)	5200(2)	64(1)
C(27)	3948(3)	525(2)	5113(2)	58(1)
C(28)	3473(2)	358(2)	4376(2)	51(1)
C(29)	3219(2)	-340(2)	2617(2)	47(1)
C(30)	2449(3)	-1025(2)	2385(2)	51(1)
C(31)	2622(3)	-1861(2)	2057(2)	65(1)
C(32)	3580(4)	-2053(3)	1947(3)	81(1)
C(33)	4373(3)	-1404(3)	2179(3)	76(1)
C(34)	4185(3)	-580(2)	2508(2)	58(1)
C(35)	-136(3)	1495(3)	4340(3)	89(1)
C(36)	-1098(4)	916(4)	4325(4)	145(3)
C(37)	-1009(4)	104(4)	3846(4)	145(3)
C(38)	26(3)	113(2)	3551(2)	67(1)
C(39)	4645(5)	6448(4)	3510(4)	157(3)
C(40)	5267(3)	5971(3)	4012(3)	91(1)
C(41)	6051(3)	5517(3)	3546(3)	88(1)
C(42)	6737(3)	5105(3)	4048(3)	77(1)
C(43)	8287(3)	4400(3)	4275(3)	84(1)
C(44)	7878(4)	3750(3)	4855(3)	99(2)
C(45)	8584(4)	3563(4)	5483(3)	110(2)
C(46)	7054(3)	3759(3)	3187(3)	85(1)
C(47)	8192(4)	2849(4)	6013(3)	123(2)
C(48)	7704(4)	3147(3)	2787(3)	102(2)
C(49)	7164(5)	2306(4)	2381(4)	149(3)
C(50)	8127(3)	5216(3)	3064(3)	83(1)
C(51)	8563(4)	6143(3)	3357(3)	90(1)
C(52)	7691(6)	1695(5)	1896(5)	207(4)

C(53)	9021(4)	6702(3)	2746(4)	132(2)
C(54)	9303(5)	7652(4)	2919(4)	156(3)
Co(1)	2237(1)	2737(1)	4102(1)	51(1)
F(1)	118(2)	3014(1)	2181(1)	77(1)
F(2)	416(2)	4792(2)	2430(2)	114(1)
F(3)	2280(2)	5726(2)	2326(2)	130(1)
F(4)	3855(2)	4802(2)	1936(2)	101(1)
F(5)	3610(2)	3040(1)	1711(1)	67(1)
F(6)	1656(2)	2786(2)	367(1)	96(1)
F(7)	338(3)	2436(2)	-817(2)	147(1)
F(8)	-1230(2)	1084(2)	-759(2)	132(1)
F(9)	-1388(2)	66(2)	496(2)	112(1)
F(10)	-78(2)	359(2)	1675(1)	94(1)
F(11)	4929(2)	1986(1)	3250(1)	71(1)
F(12)	5847(2)	2321(2)	4653(2)	95(1)
F(13)	5232(2)	1361(2)	5912(1)	92(1)
F(14)	3645(2)	36(2)	5723(1)	79(1)
F(15)	2718(2)	-339(1)	4315(1)	64(1)
F(16)	1485(2)	-906(1)	2448(1)	65(1)
F(17)	1842(2)	-2491(1)	1834(1)	89(1)
F(18)	3754(2)	-2866(2)	1603(2)	118(1)
F(19)	5317(2)	-1582(2)	2067(2)	108(1)
F(20)	4996(2)	20(1)	2723(1)	72(1)
N(1)	543(2)	1016(2)	3850(2)	52(1)
N(2)	7549(2)	4620(2)	3657(2)	60(1)
O(1)	742(2)	3977(2)	4140(2)	97(1)
O(2)	2590(2)	2062(2)	5646(2)	91(1)
O(3)	4117(2)	3728(2)	3621(2)	105(1)
O(4)	2074(1)	626(1)	3198(1)	41(1)
O(5)	1021(1)	1602(1)	2529(1)	44(1)
O(6)	2864(2)	1417(2)	965(1)	56(1)
O(7)	4102(2)	1149(2)	1808(1)	55(1)
P(1)	1533(1)	1552(1)	3437(1)	43(1)

Table 18. Bond lengths [Å] and angles [°] for $Co(CO)_3$n-Bu_4N·CKphos.

C(1)-O(1)	1.167(4)	C(17)-C(18)	1.371(5)
C(1)-Co(1)	1.726(4)	C(18)-F(6)	1.360(4)
C(2)-O(2)	1.153(4)	C(18)-C(19)	1.379(6)
C(2)-Co(1)	1.750(4)	C(19)-F(7)	1.349(5)
C(3)-O(3)	1.164(4)	C(19)-C(20)	1.350(6)
C(3)-Co(1)	1.743(4)	C(20)-C(21)	1.325(6)
C(4)-O(5)	1.427(4)	C(20)-F(8)	1.346(5)
C(4)-C(5)	1.537(4)	C(21)-F(9)	1.347(4)
C(4)-C(11)	1.548(4)	C(21)-C(22)	1.379(5)
C(4)-C(17)	1.555(4)	C(22)-F(10)	1.348(4)
C(5)-O(6)	1.413(3)	C(23)-C(24)	1.372(4)
C(5)-C(6)	1.542(4)	C(23)-C(28)	1.386(4)
C(6)-O(7)	1.414(3)	C(24)-F(11)	1.346(4)
C(6)-C(7)	1.562(4)	C(24)-C(25)	1.366(5)
C(7)-O(4)	1.417(3)	C(25)-F(12)	1.341(4)
C(7)-C(29)	1.532(4)	C(25)-C(26)	1.357(5)
C(7)-C(23)	1.537(4)	C(26)-F(13)	1.350(4)
C(8)-O(6)	1.415(4)	C(26)-C(27)	1.364(5)
C(8)-O(7)	1.430(4)	C(27)-F(14)	1.336(4)
C(8)-C(10)	1.532(5)	C(27)-C(28)	1.377(5)
C(8)-C(9)	1.541(5)	C(28)-F(15)	1.352(3)
C(11)-C(12)	1.386(5)	C(29)-C(30)	1.388(4)
C(11)-C(16)	1.392(5)	C(29)-C(34)	1.397(5)
C(12)-F(1)	1.346(4)	C(30)-F(16)	1.332(4)
C(12)-C(13)	1.378(5)	C(30)-C(31)	1.371(5)
C(13)-F(2)	1.337(4)	C(31)-F(17)	1.343(4)
C(13)-C(14)	1.355(6)	C(31)-C(32)	1.363(6)
C(14)-F(3)	1.341(4)	C(32)-F(18)	1.350(4)
C(14)-C(15)	1.355(6)	C(32)-C(33)	1.377(6)
C(15)-F(4)	1.354(4)	C(33)-F(19)	1.338(4)
C(15)-C(16)	1.376(5)	C(33)-C(34)	1.361(5)
C(16)-F(5)	1.333(4)	C(34)-F(20)	1.345(4)
C(17)-C(22)	1.367(5)	C(35)-N(1)	1.449(5)

C(35)-C(36)	1.456(6)	O(7)-C(6)-C(5)	103.4(2)
C(36)-C(37)	1.419(7)	O(7)-C(6)-C(7)	113.4(3)
C(37)-C(38)	1.475(6)	C(5)-C(6)-C(7)	112.7(2)
C(38)-N(1)	1.482(4)	O(4)-C(7)-C(29)	108.7(2)
C(39)-C(40)	1.465(7)	O(4)-C(7)-C(23)	106.5(2)
C(40)-C(41)	1.513(6)	C(29)-C(7)-C(23)	108.6(3)
C(41)-C(42)	1.464(6)	O(4)-C(7)-C(6)	107.1(2)
C(42)-N(2)	1.509(5)	C(29)-C(7)-C(6)	110.2(2)
C(43)-C(44)	1.481(6)	C(23)-C(7)-C(6)	115.5(2)
C(43)-N(2)	1.511(5)	O(6)-C(8)-O(7)	105.6(2)
C(44)-C(45)	1.477(6)	O(6)-C(8)-C(10)	110.3(3)
C(45)-C(47)	1.484(6)	O(7)-C(8)-C(10)	109.6(3)
C(46)-C(48)	1.470(6)	O(6)-C(8)-C(9)	109.8(3)
C(46)-N(2)	1.526(5)	O(7)-C(8)-C(9)	109.0(3)
C(48)-C(49)	1.480(6)	C(10)-C(8)-C(9)	112.3(3)
C(49)-C(52)	1.432(7)	C(12)-C(11)-C(16)	114.7(3)
C(50)-C(51)	1.476(5)	C(12)-C(11)-C(4)	117.0(3)
C(50)-N(2)	1.532(5)	C(16)-C(11)-C(4)	128.2(3)
C(51)-C(53)	1.458(6)	F(1)-C(12)-C(13)	116.1(4)
C(53)-C(54)	1.423(6)	F(1)-C(12)-C(11)	120.7(3)
Co(1)-P(1)	2.1254(8)	C(13)-C(12)-C(11)	123.2(4)
N(1)-P(1)	1.644(3)	F(2)-C(13)-C(14)	120.7(4)
O(4)-P(1)	1.663(2)	F(2)-C(13)-C(12)	119.4(4)
O(5)-P(1)	1.676(2)	C(14)-C(13)-C(12)	119.9(4)
O(1)-C(1)-Co(1)	179.6(4)	F(3)-C(14)-C(15)	120.5(4)
O(2)-C(2)-Co(1)	178.9(4)	F(3)-C(14)-C(13)	120.2(4)
O(3)-C(3)-Co(1)	175.0(3)	C(15)-C(14)-C(13)	119.2(4)
O(5)-C(4)-C(5)	108.3(2)	F(4)-C(15)-C(14)	120.5(4)
O(5)-C(4)-C(11)	107.0(2)	F(4)-C(15)-C(16)	118.6(4)
C(5)-C(4)-C(11)	121.0(3)	C(14)-C(15)-C(16)	120.9(4)
O(5)-C(4)-C(17)	105.7(2)	F(5)-C(16)-C(15)	115.6(3)
C(5)-C(4)-C(17)	105.9(2)	F(5)-C(16)-C(11)	122.3(3)
C(11)-C(4)-C(17)	108.1(3)	C(15)-C(16)-C(11)	122.1(4)
O(6)-C(5)-C(4)	109.3(2)	C(22)-C(17)-C(18)	113.6(3)
O(6)-C(5)-C(6)	103.7(2)	C(22)-C(17)-C(4)	123.1(3)
C(4)-C(5)-C(6)	119.7(2)	C(18)-C(17)-C(4)	123.3(3)

F(6)-C(18)-C(17)	120.2(3)	F(16)-C(30)-C(31)	115.2(3)
F(6)-C(18)-C(19)	116.3(4)	F(16)-C(30)-C(29)	122.0(3)
C(17)-C(18)-C(19)	123.5(4)	C(31)-C(30)-C(29)	122.8(3)
F(7)-C(19)-C(20)	122.1(4)	F(17)-C(31)-C(32)	119.9(3)
F(7)-C(19)-C(18)	118.6(5)	F(17)-C(31)-C(30)	119.8(4)
C(20)-C(19)-C(18)	119.3(4)	C(32)-C(31)-C(30)	120.3(4)
C(21)-C(20)-F(8)	120.8(5)	F(18)-C(32)-C(31)	120.5(4)
C(21)-C(20)-C(19)	119.8(4)	F(18)-C(32)-C(33)	120.1(4)
F(8)-C(20)-C(19)	119.4(5)	C(31)-C(32)-C(33)	119.4(4)
C(20)-C(21)-F(9)	119.5(4)	F(19)-C(33)-C(34)	120.8(4)
C(20)-C(21)-C(22)	119.9(4)	F(19)-C(33)-C(32)	119.8(4)
F(9)-C(21)-C(22)	120.6(4)	C(34)-C(33)-C(32)	119.4(4)
F(10)-C(22)-C(17)	122.4(3)	F(20)-C(34)-C(33)	116.1(3)
F(10)-C(22)-C(21)	113.9(4)	F(20)-C(34)-C(29)	120.3(3)
C(17)-C(22)-C(21)	123.7(4)	C(33)-C(34)-C(29)	123.6(4)
C(24)-C(23)-C(28)	114.4(3)	N(1)-C(35)-C(36)	107.1(4)
C(24)-C(23)-C(7)	128.1(3)	C(37)-C(36)-C(35)	108.6(4)
C(28)-C(23)-C(7)	117.5(3)	C(36)-C(37)-C(38)	110.3(4)
F(11)-C(24)-C(25)	116.2(3)	C(37)-C(38)-N(1)	104.3(3)
F(11)-C(24)-C(23)	120.5(3)	C(39)-C(40)-C(41)	113.0(5)
C(25)-C(24)-C(23)	123.2(3)	C(42)-C(41)-C(40)	113.7(4)
F(12)-C(25)-C(26)	119.8(3)	C(41)-C(42)-N(2)	119.2(4)
F(12)-C(25)-C(24)	120.2(4)	C(44)-C(43)-N(2)	115.9(4)
C(26)-C(25)-C(24)	120.1(3)	C(45)-C(44)-C(43)	116.2(4)
F(13)-C(26)-C(25)	120.6(4)	C(44)-C(45)-C(47)	115.5(5)
F(13)-C(26)-C(27)	119.3(4)	C(48)-C(46)-N(2)	118.4(4)
C(25)-C(26)-C(27)	120.1(3)	C(46)-C(48)-C(49)	114.8(4)
F(14)-C(27)-C(26)	120.9(3)	C(52)-C(49)-C(48)	120.8(6)
F(14)-C(27)-C(28)	120.8(3)	C(51)-C(50)-N(2)	117.9(3)
C(26)-C(27)-C(28)	118.3(3)	C(53)-C(51)-C(50)	115.0(4)
F(15)-C(28)-C(27)	115.7(3)	C(54)-C(53)-C(51)	120.4(5)
F(15)-C(28)-C(23)	120.3(3)	C(1)-Co(1)-C(3)	108.34(18)
C(27)-C(28)-C(23)	124.0(3)	C(1)-Co(1)-C(2)	113.38(17)
C(30)-C(29)-C(34)	114.5(3)	C(3)-Co(1)-C(2)	108.66(18)
C(30)-C(29)-C(7)	125.8(3)	C(1)-Co(1)-P(1)	104.31(12)
C(34)-C(29)-C(7)	119.8(3)	C(3)-Co(1)-P(1)	120.39(11)

C(2)-Co(1)-P(1)	101.83(11)	C(5)-O(6)-C(8)	107.5(2)
C(35)-N(1)-C(38)	109.6(3)	C(6)-O(7)-C(8)	110.4(2)
C(35)-N(1)-P(1)	121.9(2)	N(1)-P(1)-O(4)	95.44(12)
C(38)-N(1)-P(1)	124.7(2)	N(1)-P(1)-O(5)	97.57(12)
C(42)-N(2)-C(43)	110.8(3)	O(4)-P(1)-O(5)	95.50(10)
C(42)-N(2)-C(46)	108.6(3)	N(1)-P(1)-Co(1)	115.64(10)
C(43)-N(2)-C(46)	111.2(3)	O(4)-P(1)-Co(1)	124.99(8)
C(42)-N(2)-C(50)	110.3(3)	O(5)-P(1)-Co(1)	121.56(8)
C(43)-N(2)-C(50)	108.3(3)		
C(46)-N(2)-C(50)	107.6(3)		
C(7)-O(4)-P(1)	125.24(17)		
C(4)-O(5)-P(1)	124.50(18)		

Symmetry transformations used to generate equivalent atoms:

Table 19. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $Co(CO)_3$n-Bu_4N·CKphos. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	68(3)	58(2)	62(2)	-12(2)	11(2)	4(2)
C(2)	62(2)	60(2)	58(3)	-12(2)	2(2)	12(2)
C(3)	66(3)	56(2)	68(3)	-13(2)	-1(2)	-2(2)
C(4)	43(2)	47(2)	45(2)	-1(2)	0(2)	7(2)
C(5)	51(2)	47(2)	36(2)	-1(1)	5(2)	6(2)
C(6)	36(2)	48(2)	50(2)	-4(2)	8(2)	10(1)
C(7)	35(2)	48(2)	46(2)	0(2)	2(2)	5(1)
C(8)	54(2)	73(2)	54(2)	3(2)	12(2)	18(2)
C(9)	83(3)	91(3)	80(3)	12(2)	33(2)	15(2)
C(10)	87(3)	78(3)	65(3)	-12(2)	15(2)	29(2)
C(11)	54(2)	50(2)	43(2)	3(2)	5(2)	7(2)
C(12)	63(3)	50(2)	69(3)	2(2)	9(2)	9(2)
C(13)	89(3)	56(3)	95(3)	3(2)	25(3)	29(2)
C(14)	100(4)	36(2)	119(4)	1(2)	23(3)	9(2)
C(15)	84(3)	52(2)	79(3)	4(2)	12(2)	-12(2)
C(16)	62(2)	53(2)	53(2)	5(2)	8(2)	8(2)
C(17)	55(2)	51(2)	47(2)	1(2)	-2(2)	14(2)
C(18)	78(3)	69(3)	65(3)	6(2)	-6(2)	6(2)
C(19)	117(4)	106(4)	55(3)	18(3)	-26(3)	15(3)
C(20)	96(4)	106(4)	68(3)	-14(3)	-42(3)	20(3)
C(21)	72(3)	74(3)	76(3)	-11(2)	-17(2)	7(2)
C(22)	69(3)	61(2)	52(2)	-1(2)	-15(2)	7(2)
C(23)	38(2)	47(2)	44(2)	2(2)	0(2)	5(1)
C(24)	45(2)	58(2)	57(2)	5(2)	-3(2)	1(2)
C(25)	46(2)	64(2)	67(3)	-3(2)	-14(2)	-4(2)
C(26)	63(3)	73(3)	56(2)	-11(2)	-23(2)	16(2)
C(27)	59(2)	64(2)	52(2)	5(2)	-4(2)	16(2)
C(28)	43(2)	50(2)	58(2)	-1(2)	-2(2)	5(2)

C(29)	48(2)	47(2)	48(2)	2(2)	-1(2)	10(2)
C(30)	55(2)	49(2)	50(2)	5(2)	0(2)	13(2)
C(31)	82(3)	43(2)	69(3)	2(2)	-9(2)	9(2)
C(32)	109(4)	53(2)	83(3)	-10(2)	-3(3)	35(3)
C(33)	75(3)	74(3)	87(3)	-1(2)	5(2)	35(2)
C(34)	55(2)	63(2)	57(2)	0(2)	-4(2)	16(2)
C(35)	72(3)	81(3)	112(4)	-7(3)	41(3)	2(2)
C(36)	67(4)	135(5)	222(7)	-19(5)	54(4)	-13(3)
C(37)	58(3)	87(4)	277(8)	-33(4)	47(4)	-17(3)
C(38)	54(2)	60(2)	80(3)	5(2)	9(2)	-15(2)
C(39)	139(5)	150(5)	191(7)	-44(5)	-56(5)	88(5)
C(40)	73(3)	81(3)	117(4)	-20(3)	9(3)	13(2)
C(41)	58(3)	86(3)	118(4)	1(3)	-4(3)	10(2)
C(42)	62(3)	78(3)	91(3)	4(2)	17(2)	8(2)
C(43)	74(3)	89(3)	88(3)	-7(3)	-3(3)	13(2)
C(44)	95(4)	108(4)	91(3)	18(3)	-3(3)	0(3)
C(45)	110(4)	110(4)	113(4)	15(3)	-25(3)	17(3)
C(46)	82(3)	87(3)	84(3)	-18(2)	1(2)	15(2)
C(47)	136(5)	132(5)	110(4)	40(4)	-5(4)	30(4)
C(48)	105(4)	83(3)	117(4)	-23(3)	-4(3)	25(3)
C(49)	155(6)	103(4)	179(6)	-60(4)	50(5)	14(4)
C(50)	64(3)	87(3)	96(3)	-5(3)	16(2)	11(2)
C(51)	86(3)	79(3)	104(4)	-3(3)	20(3)	1(3)
C(52)	209(8)	152(6)	250(9)	-96(6)	23(7)	44(6)
C(53)	130(5)	66(3)	193(6)	3(3)	61(4)	-18(3)
C(54)	161(6)	103(5)	197(7)	7(4)	72(5)	-6(4)
Co(1)	52(1)	48(1)	50(1)	-10(1)	2(1)	0(1)
F(1)	50(1)	70(1)	114(2)	4(1)	7(1)	19(1)
F(2)	105(2)	72(2)	173(3)	7(2)	30(2)	45(2)
F(3)	148(3)	42(1)	196(3)	1(2)	30(2)	8(2)
F(4)	94(2)	61(1)	139(2)	4(1)	16(2)	-21(1)
F(5)	53(1)	61(1)	87(2)	4(1)	18(1)	2(1)
F(6)	121(2)	101(2)	63(2)	24(1)	-5(1)	-11(2)
F(7)	214(4)	154(3)	74(2)	40(2)	-42(2)	3(3)
F(8)	143(3)	154(3)	98(2)	-9(2)	-64(2)	23(2)
F(9)	95(2)	116(2)	111(2)	-18(2)	-36(2)	-22(2)

F(10)	110(2)	80(2)	81(2)	8(1)	-31(1)	-29(1)
F(11)	53(1)	81(1)	75(2)	16(1)	-3(1)	-17(1)
F(12)	73(2)	98(2)	104(2)	3(1)	-33(1)	-27(1)
F(13)	103(2)	102(2)	69(2)	-7(1)	-41(1)	9(1)
F(14)	85(2)	98(2)	57(1)	21(1)	-4(1)	14(1)
F(15)	60(1)	67(1)	62(1)	18(1)	-5(1)	-9(1)
F(16)	57(1)	55(1)	78(1)	-11(1)	-5(1)	-2(1)
F(17)	111(2)	46(1)	105(2)	-10(1)	-13(2)	0(1)
F(18)	145(3)	66(2)	147(2)	-26(2)	-1(2)	47(2)
F(19)	85(2)	101(2)	145(2)	-17(2)	6(2)	53(2)
F(20)	47(1)	79(1)	90(2)	-8(1)	0(1)	18(1)
N(1)	43(2)	55(2)	55(2)	-7(1)	16(1)	-2(1)
N(2)	47(2)	65(2)	65(2)	-3(2)	6(2)	3(2)
O(1)	88(2)	80(2)	127(3)	-5(2)	14(2)	32(2)
O(2)	122(3)	100(2)	57(2)	6(2)	2(2)	38(2)
O(3)	80(2)	89(2)	131(3)	-6(2)	21(2)	-32(2)
O(4)	34(1)	40(1)	48(1)	-2(1)	4(1)	3(1)
O(5)	37(1)	50(1)	43(1)	-1(1)	1(1)	4(1)
O(6)	60(2)	69(2)	42(1)	4(1)	10(1)	19(1)
O(7)	45(1)	69(2)	53(2)	2(1)	11(1)	12(1)
P(1)	38(1)	45(1)	43(1)	-3(1)	4(1)	1(1)

Table 20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $Co(CO)_3$n-Bu_4N·CKphos.

	x	y	z	U(eq)
H(5)	2065	614	1656	54
H(6)	3401	1925	2555	53
H(9A)	4361	1712	-16	126
H(9B)	5222	1482	540	126
H(9C)	4650	2314	779	126
H(10A)	3192	-255	922	113
H(10B)	4336	-136	712	113
H(10C)	3536	62	85	113

H(35A)	-213	2071	4128	107
H(35B)	124	1611	4883	107
H(36A)	-1285	776	4863	174
H(36B)	-1617	1228	4104	174
H(37A)	-1476	47	3396	174
H(37B)	-1177	-414	4160	174
H(38A)	30	41	2972	80
H(38B)	346	-370	3762	80
H(39A)	5069	6827	3177	235
H(39B)	4253	6817	3843	235
H(39C)	4203	6013	3179	235
H(40A)	4836	5515	4277	109
H(40B)	5601	6401	4422	109
H(41A)	5714	5050	3168	105
H(41B)	6441	5964	3242	105
H(42A)	6332	4675	4359	93
H(42B)	7063	5581	4423	93
H(43A)	8837	4155	3998	101
H(43B)	8564	4962	4571	101
H(44A)	7308	3982	5114	119
H(44B)	7629	3179	4561	119
H(45A)	8783	4122	5812	132
H(45B)	9184	3386	5227	132
H(46A)	6629	3412	3551	102
H(46B)	6616	3941	2783	102
H(47A)	7675	3061	6342	185
H(47B)	8729	2712	6346	185
H(47C)	7919	2311	5693	185
H(48A)	8165	2979	3182	122
H(48B)	8103	3475	2396	122
H(49A)	6825	1961	2791	179
H(49B)	6643	2487	2046	179
H(50A)	8669	4900	2853	100
H(50B)	7676	5267	2619	100
H(51A)	8038	6449	3611	109
H(51B)	9069	6099	3763	109

H(52A)	7895	1965	1411	311
H(52B)	7257	1137	1769	311
H(52C)	8274	1573	2183	311
H(53A)	9620	6446	2570	159
H(53B)	8558	6629	2292	159
H(54A)	8711	7951	2957	233
H(54B)	9719	7889	2500	233
H(54C)	9670	7754	3418	233

7. DFT Calculations

B3LYP hybrid[7] and B97D empirically corrected[8] density functional studies were carried out in the G09 suite of electronic structure codes.[9] Geometries were optimized for each complex starting from the X-ray coordinates for CK/Cl (starting guess C-H distances adjusted to 1.07 Å and 1.09Å for Csp^2-H and Csp^3-H distances, respectively). The LANL2 basis sets and effective core potentials were used for P and Cl, supplemented by double zeta d functions with exponents of 0.93,0.34 for P, and 1.5, 0.375 for Cl. A LANL08[10] basis set and effective core potentials was used for Rh, an f exponent of 1.35 was added as well. H, C, and N, and F were described with a 6-31g* model.[11]

---

[7] Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652

[8] Grimme, S. *J. Comp. Chem.* **2006**, 27, 1787-99

[9] Frisch, M. J.; et. al. *Gaussian 09, Revision A.1*, Gaussian, Inc.: Wallingford CT, 2009

[10] Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299-310. Roy, L. E.; Hay, P. J.; Martin, R. L. *J. Chem. Theory Comput.* **2008**, *4*, 1029–1031.

[11] (a) Binkley, J. S.; Pople, J. A.; Hehre, W. J. *J. Am. Chem. Soc.* **1980**, *102*, 939-947; (b) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724-728; (c) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. *J. Chem. Phys.* **1982**, *77*, 3654-3665; (d) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257-2261.

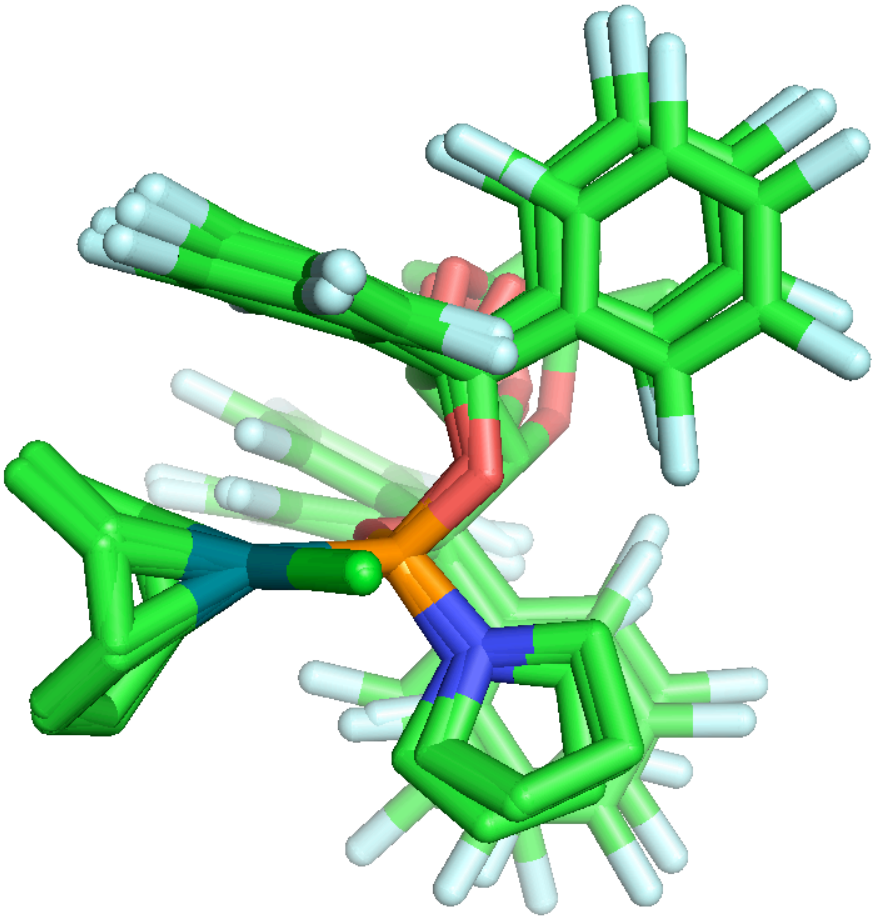


Figure 1. Overlay of Rh(cod)Cl/CKphos structures.

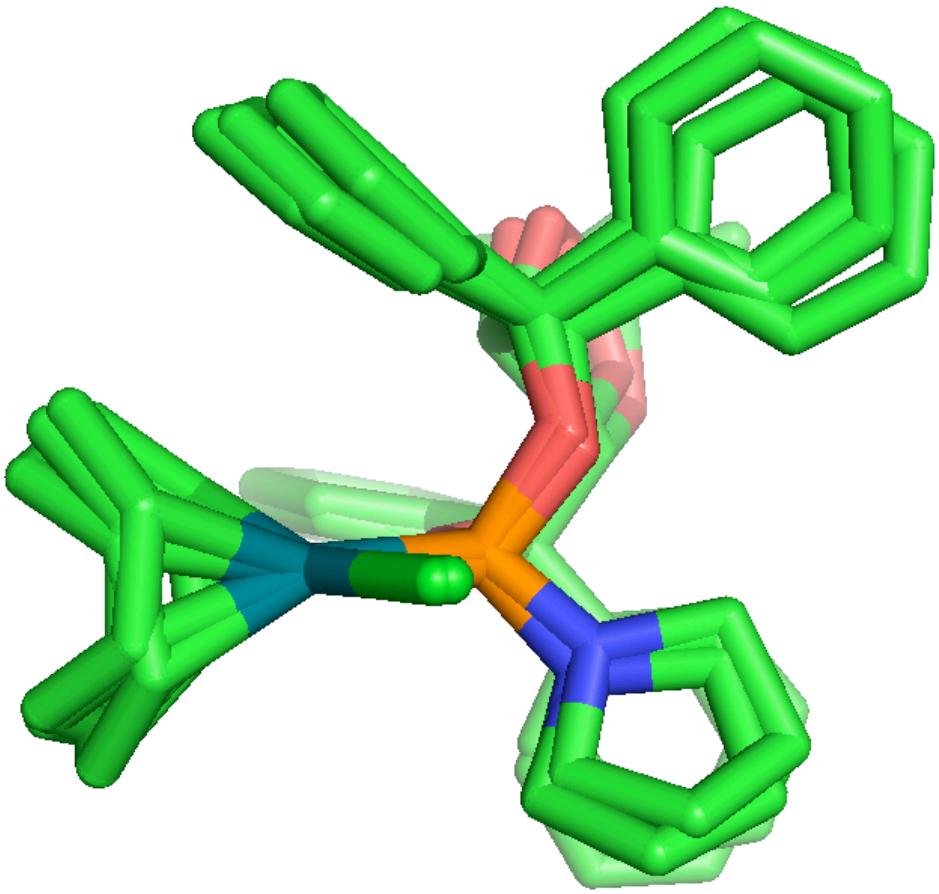


Figure 2. Overlay of Rh(cod)Cl/**T4** structures.

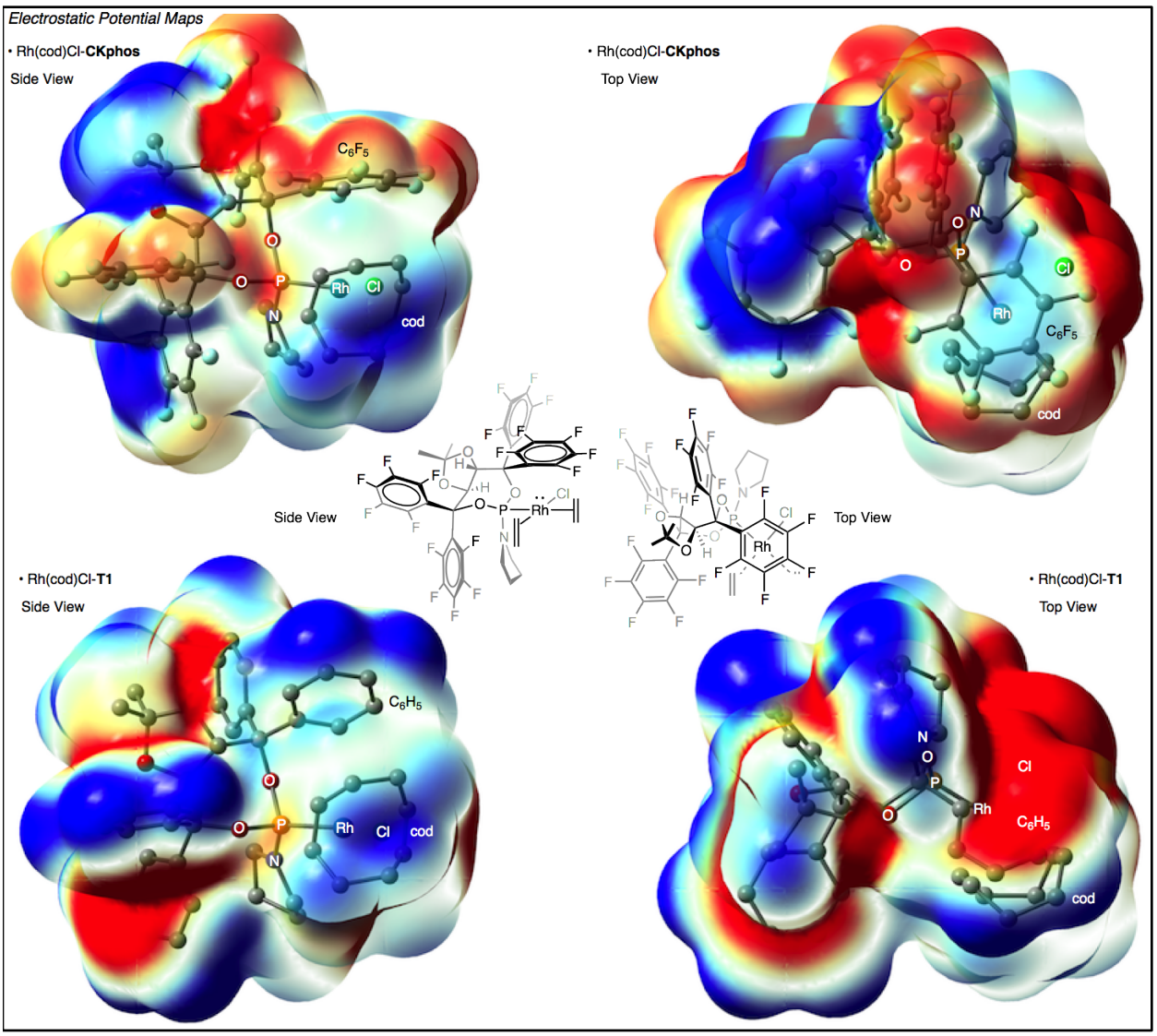


Figure 3. Electrostatic potential maps of Rh(cod)Cl/CKphos and Rh(cod)Cl/**T4**

Table 21. Select Computed bonded and non-bonded distances (Å).

	X-ray CK/Cl	B3LYP	B97D	X-ray **T4**	B3LYP	B97D
Rh-P	2.242	2.331	2.248	2.255	2.324	2.247
C=C	1.365	1.365	1.390	1.378	1.382	1.387
Rh-Aryl	3.728	3.790	3.492	4.039	4.257	4.008
Cl-Aryl	3.958	4.006	3.941	4.694	4.847	4.837

T4 B3LYP E(RB3LYP) = -2154.19845891 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.045794	-0.709029	0.140118
2	1	0	5.336739	-0.897483	-0.890895
3	6	0	4.807421	0.605102	0.495239
4	1	0	4.948817	1.357311	-0.277288
5	6	0	2.686513	-1.721306	1.411558
6	1	0	1.757228	-2.276254	1.296129
7	6	0	2.584396	-0.433934	1.985098
8	1	0	1.582829	-0.084244	2.225122
9	6	0	3.694430	0.255759	2.779176
10	1	0	3.236624	0.891212	3.545737
11	1	0	4.279995	-0.494036	3.323700
12	6	0	4.617718	1.134068	1.901613
13	1	0	4.175549	2.131541	1.816657
14	1	0	5.594076	1.268373	2.394256
15	6	0	5.235246	-1.850895	1.125124
16	1	0	5.970666	-2.553937	0.716869
17	1	0	5.667329	-1.467898	2.055215
18	6	0	3.919081	-2.608556	1.415063
19	1	0	3.773446	-3.372981	0.641854
20	1	0	3.999097	-3.154609	2.369428
21	6	0	-1.734299	-1.410808	0.503108
22	6	0	-2.442742	-0.044209	0.210475
23	1	0	-2.519655	0.079088	-0.873974
24	6	0	-1.688559	1.144135	0.824942
25	1	0	-1.036926	0.802030	1.634772
26	6	0	-0.802083	1.906523	-0.224642
27	6	0	-3.958440	1.286684	1.400703
28	6	0	-4.374543	1.061863	2.851649
29	1	0	-5.304315	0.485905	2.895005
30	1	0	-4.534514	2.024315	3.348145
31	1	0	-3.596024	0.509371	3.383672
32	6	0	-4.986077	2.081039	0.598513
33	1	0	-4.646951	2.203518	-0.433215
34	1	0	-5.125665	3.073199	1.038859
35	1	0	-5.947587	1.557341	0.600582
36	6	0	0.315631	2.717633	0.440180
37	6	0	1.423565	3.114129	-0.323265

38	6	0	2.404814	3.935004	0.231253
39	6	0	2.294719	4.375539	1.553249
40	6	0	1.197183	3.982347	2.319463
41	6	0	0.211943	3.158432	1.766926
42	6	0	-1.664020	2.828667	-1.107827
43	6	0	-2.110850	2.426231	-2.372022
44	6	0	-2.917677	3.264568	-3.147391
45	6	0	-3.291403	4.519927	-2.671714
46	6	0	-2.847727	4.931874	-1.412847
47	6	0	-2.042436	4.096881	-0.640697
48	6	0	1.289440	-2.322988	-2.626843
49	1	0	0.932213	-3.293018	-2.252054
50	1	0	2.292583	-2.137259	-2.233653
51	6	0	1.234916	-2.274912	-4.156764
52	1	0	1.913784	-1.494519	-4.517307
53	1	0	1.520660	-3.227563	-4.614239
54	6	0	-0.225680	-1.886324	-4.425745
55	1	0	-0.878905	-2.758610	-4.304353
56	1	0	-0.390226	-1.475417	-5.427009
57	6	0	-0.525409	-0.850447	-3.329283
58	1	0	-0.273554	0.161131	-3.665425
59	1	0	-1.578730	-0.869191	-3.029517
60	6	0	-2.160216	-2.520456	-0.467044
61	6	0	-1.397033	-3.696341	-0.531678
62	6	0	-1.772277	-4.745189	-1.367316
63	6	0	-2.928063	-4.643293	-2.148789
64	6	0	-3.704488	-3.488471	-2.075763
65	6	0	-3.325567	-2.433022	-1.238273
66	6	0	-1.983692	-1.872110	1.950117
67	6	0	-1.019570	-1.712593	2.951887
68	6	0	-1.275971	-2.124796	4.263496
69	6	0	-2.499677	-2.703366	4.593969
70	6	0	-3.466411	-2.871981	3.599109
71	6	0	-3.210591	-2.463582	2.291915
72	17	0	3.235279	0.630037	-2.359627
73	1	0	1.527846	2.767942	-1.345574
74	1	0	3.256628	4.229213	-0.375759
75	1	0	3.055914	5.023616	1.980179
76	1	0	1.096920	4.321783	3.347194
77	1	0	-0.652666	2.892676	2.367180
78	1	0	-1.812235	1.464186	-2.764335
79	1	0	-3.244104	2.932024	-4.129416
80	1	0	-3.914333	5.174201	-3.275821

81	1	0	-3.124794	5.910460	-1.029587
82	1	0	-1.703451	4.436304	0.331066
83	1	0	-3.962400	-1.556875	-1.170227
84	1	0	-4.613099	-3.402569	-2.665861
85	1	0	-3.223319	-5.462304	-2.799083
86	1	0	-1.165752	-5.646271	-1.406006
87	1	0	-0.503614	-3.783111	0.079121
88	1	0	-3.969514	-2.606280	1.531312
89	1	0	-4.423357	-3.327811	3.839476
90	1	0	-2.698163	-3.026663	5.612391
91	1	0	-0.508884	-1.995281	5.022651
92	1	0	-0.056944	-1.284688	2.706817
93	7	0	0.362900	-1.243757	-2.211946
94	8	0	-0.298403	-1.170734	0.392596
95	8	0	-0.245104	0.906648	-1.125698
96	8	0	-3.739492	0.012869	0.777360
97	8	0	-2.700728	1.975838	1.365456
98	15	0	0.599230	-0.446159	-0.782343
99	45	0	2.826405	-0.261857	-0.146318

T4 B97D: E(RB97D) = -2153.08504790 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.956396	-0.887400	0.305762
2	1	0	5.249127	-1.324622	-0.651965
3	6	0	4.790200	0.487867	0.372315
4	1	0	4.988892	1.069276	-0.531311
5	6	0	2.487499	-1.467614	1.667796
6	1	0	1.535772	-2.003651	1.660811
7	6	0	2.428335	-0.069237	1.931855
8	1	0	1.434312	0.369948	2.053548
9	6	0	3.548296	0.713713	2.628155
10	1	0	3.098967	1.560847	3.168542
11	1	0	4.015408	0.062185	3.384816
12	6	0	4.634923	1.275267	1.663485
13	1	0	4.362327	2.301300	1.392650
14	1	0	5.607193	1.325884	2.190234
15	6	0	5.046418	-1.768775	1.544429
16	1	0	5.766544	-2.581756	1.360105
17	1	0	5.442616	-1.176064	2.382851

18	6	0	3.675908	-2.384410	1.931722
19	1	0	3.517337	-3.295436	1.331924
20	1	0	3.689109	-2.702662	2.993361
21	6	0	-1.752942	-1.267428	0.670186
22	6	0	-2.385772	0.104504	0.236021
23	1	0	-2.468931	0.114590	-0.860318
24	6	0	-1.524404	1.282622	0.724240
25	1	0	-0.848219	0.970103	1.532355
26	6	0	-0.634649	1.854152	-0.451081
27	6	0	-3.776660	1.675892	1.252687
28	6	0	-4.301872	1.659542	2.688431
29	1	0	-5.307248	1.212831	2.713043
30	1	0	-4.357721	2.687296	3.077756
31	1	0	-3.626544	1.060072	3.314353
32	6	0	-4.648975	2.473789	0.279822
33	1	0	-4.227566	2.420752	-0.732726
34	1	0	-4.684848	3.528359	0.590354
35	1	0	-5.671152	2.064572	0.277440
36	6	0	0.582914	2.625037	0.061138
37	6	0	1.712916	2.753466	-0.770435
38	6	0	2.792337	3.551866	-0.372518
39	6	0	2.761244	4.223752	0.861202
40	6	0	1.650051	4.075096	1.705323
41	6	0	0.562697	3.279090	1.306642
42	6	0	-1.499583	2.723042	-1.375526
43	6	0	-2.112380	2.186011	-2.523521
44	6	0	-2.975855	2.971554	-3.304276
45	6	0	-3.239548	4.302208	-2.948080
46	6	0	-2.625351	4.844783	-1.807805
47	6	0	-1.762891	4.062201	-1.029451
48	6	0	1.090580	-2.756988	-2.355767
49	1	0	0.746966	-3.632346	-1.774605
50	1	0	2.141391	-2.542637	-2.118081
51	6	0	0.844479	-2.972176	-3.857734
52	1	0	1.485958	-2.282170	-4.427341
53	1	0	1.055177	-4.005226	-4.172549
54	6	0	-0.639057	-2.578829	-4.011073
55	1	0	-1.286703	-3.380458	-3.624014
56	1	0	-0.928822	-2.357682	-5.049374
57	6	0	-0.764317	-1.336933	-3.106322
58	1	0	-0.514224	-0.413234	-3.652639
59	1	0	-1.772752	-1.236480	-2.677896
60	6	0	-2.233724	-2.442495	-0.184789

61	6	0	-1.482150	-3.632721	-0.188871
62	6	0	-1.899447	-4.737622	-0.939507
63	6	0	-3.086564	-4.672241	-1.691168
64	6	0	-3.851470	-3.497320	-1.674953
65	6	0	-3.428958	-2.386511	-0.923370
66	6	0	-2.026886	-1.520929	2.159531
67	6	0	-1.089120	-1.177701	3.150388
68	6	0	-1.396793	-1.345572	4.510732
69	6	0	-2.644509	-1.855368	4.897366
70	6	0	-3.582186	-2.205955	3.911363
71	6	0	-3.274963	-2.041529	2.554857
72	17	0	3.307157	-0.034999	-2.503759
73	1	0	1.747592	2.226541	-1.721970
74	1	0	3.661233	3.638233	-1.027390
75	1	0	3.601662	4.851015	1.166758
76	1	0	1.619262	4.586755	2.669768
77	1	0	-0.310629	3.195616	1.954291
78	1	0	-1.904432	1.159107	-2.814351
79	1	0	-3.437357	2.539338	-4.194876
80	1	0	-3.910778	4.912716	-3.555707
81	1	0	-2.817047	5.881178	-1.521944
82	1	0	-1.291984	4.489742	-0.145755
83	1	0	-4.042712	-1.485537	-0.900477
84	1	0	-4.780432	-3.438915	-2.246000
85	1	0	-3.413491	-5.533018	-2.278067
86	1	0	-1.298701	-5.649530	-0.940537
87	1	0	-0.558284	-3.675768	0.388121
88	1	0	-4.006955	-2.312084	1.794798
89	1	0	-4.555823	-2.608843	4.198439
90	1	0	-2.883395	-1.985235	5.955090
91	1	0	-0.653467	-1.078604	5.265204
92	1	0	-0.111961	-0.798765	2.861785
93	7	0	0.245766	-1.580086	-2.047943
94	8	0	-0.302867	-1.126036	0.540667
95	8	0	-0.202966	0.724374	-1.268392
96	8	0	-3.666882	0.310775	0.806555
97	8	0	-2.440881	2.226899	1.253138
98	15	0	0.586977	-0.613944	-0.754030
99	45	0	2.744943	-0.392646	-0.166655

CKphos/Cl B3LYP: E(RB3LYP) = -4138.68423078 A.U.

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.138142	-4.333540	-1.008653
2	1	0	3.249506	-4.286784	-2.089635
3	6	0	3.944889	-3.503100	-0.253178
4	1	0	4.652744	-2.877230	-0.791624
5	6	0	0.746546	-3.726187	0.450013
6	1	0	-0.275829	-3.358995	0.403084
7	6	0	1.608280	-3.071726	1.353959
8	1	0	1.187880	-2.233351	1.898756
9	6	0	2.812329	-3.722384	2.038470
10	1	0	2.950899	-3.252239	3.018078
11	1	0	2.588145	-4.776453	2.239962
12	6	0	4.137818	-3.597698	1.245515
13	1	0	4.672871	-2.703210	1.575835
14	1	0	4.799680	-4.444418	1.485734
15	6	0	2.359705	-5.511055	-0.445626
16	1	0	2.350917	-6.319428	-1.185764
17	1	0	2.879675	-5.907524	0.432564
18	6	0	0.904220	-5.138688	-0.083338
19	1	0	0.281746	-5.220223	-0.982863
20	1	0	0.494835	-5.867396	0.635032
21	6	0	-2.040450	-0.090862	0.328078
22	6	0	-1.510469	1.374011	0.594175
23	1	0	-1.462938	1.901331	-0.356206
24	6	0	-0.126832	1.358268	1.281644
25	1	0	0.023150	0.423703	1.817059
26	6	0	1.029890	1.556966	0.233876
27	6	0	-1.541313	2.754401	2.489186
28	6	0	-1.907439	2.221277	3.872639
29	1	0	-2.969621	2.390726	4.075248
30	1	0	-1.317377	2.732058	4.639653
31	1	0	-1.703459	1.148731	3.935202
32	6	0	-1.736151	4.261263	2.364410
33	1	0	-1.505760	4.586108	1.346162
34	1	0	-1.078304	4.786795	3.063541
35	1	0	-2.773329	4.526675	2.589970
36	6	0	2.429401	1.071629	0.655880
37	6	0	3.472629	1.232509	-0.270238
38	6	0	4.762798	0.769626	-0.039635
39	6	0	5.050039	0.120415	1.155878
40	6	0	4.048761	-0.038339	2.104788
41	6	0	2.764159	0.435667	1.855116

42	6	0	1.096842	3.054296	-0.147612
43	6	0	0.471044	3.633601	-1.257693
44	6	0	0.562074	4.997365	-1.542869
45	6	0	1.280052	5.840963	-0.705802
46	6	0	1.896944	5.305711	0.420160
47	6	0	1.794028	3.944220	0.685215
48	6	0	-0.341160	-2.163163	-3.238947
49	1	0	-1.342858	-2.607923	-3.152002
50	1	0	0.382327	-2.861452	-2.806401
51	6	0	-0.018682	-1.793185	-4.688307
52	1	0	1.067000	-1.706826	-4.800665
53	1	0	-0.392560	-2.534744	-5.401342
54	6	0	-0.684350	-0.418533	-4.835878
55	1	0	-1.764947	-0.535158	-4.986868
56	1	0	-0.291746	0.166205	-5.673279
57	6	0	-0.404974	0.267969	-3.488847
58	1	0	0.534539	0.825608	-3.513227
59	1	0	-1.202719	0.956947	-3.201764
60	6	0	-2.979898	-0.239400	-0.890263
61	6	0	-3.267028	-1.529046	-1.360912
62	6	0	-4.080339	-1.765259	-2.463142
63	6	0	-4.678959	-0.695643	-3.122761
64	6	0	-4.449474	0.595443	-2.662726
65	6	0	-3.620896	0.808604	-1.560380
66	6	0	-2.776931	-0.621385	1.580847
67	6	0	-2.226596	-1.484386	2.537049
68	6	0	-2.949703	-1.939170	3.642502
69	6	0	-4.257519	-1.520563	3.845626
70	6	0	-4.829601	-0.638823	2.934561
71	6	0	-4.092853	-0.201034	1.839125
72	17	0	3.120787	-1.349076	-2.532842
73	9	0	3.245876	1.849786	-1.434102
74	9	0	5.713764	0.928322	-0.959688
75	9	0	6.267558	-0.378687	1.381819
76	9	0	4.310603	-0.689992	3.246882
77	9	0	1.865378	0.230485	2.836488
78	9	0	-0.281437	2.924591	-2.113991
79	9	0	-0.050992	5.490590	-2.623538
80	9	0	1.368887	7.144729	-0.970762
81	9	0	2.580293	6.100481	1.249907
82	9	0	2.406636	3.510400	1.796017
83	9	0	-3.497993	2.081671	-1.157465
84	9	0	-5.035123	1.634095	-3.266205

85	9	0	-5.463505	-0.908274	-4.179741
86	9	0	-4.275020	-3.015969	-2.896040
87	9	0	-2.739376	-2.610110	-0.764342
88	9	0	-4.712648	0.662047	1.022085
89	9	0	-6.081313	-0.206416	3.116715
90	9	0	-4.951144	-1.948538	4.900604
91	9	0	-2.372529	-2.774170	4.512358
92	9	0	-0.961011	-1.919965	2.474115
93	7	0	-0.296850	-0.860575	-2.523593
94	8	0	-0.882517	-0.925307	0.105867
95	8	0	0.663921	0.811684	-0.950220
96	8	0	-2.336064	2.085882	1.494559
97	8	0	-0.177296	2.442528	2.185358
98	15	0	0.346705	-0.801541	-0.999944
99	45	0	2.019538	-2.386673	-0.652613

CKphos/Cl B97D: E(RB97D) = -4136.65357295 A.U.

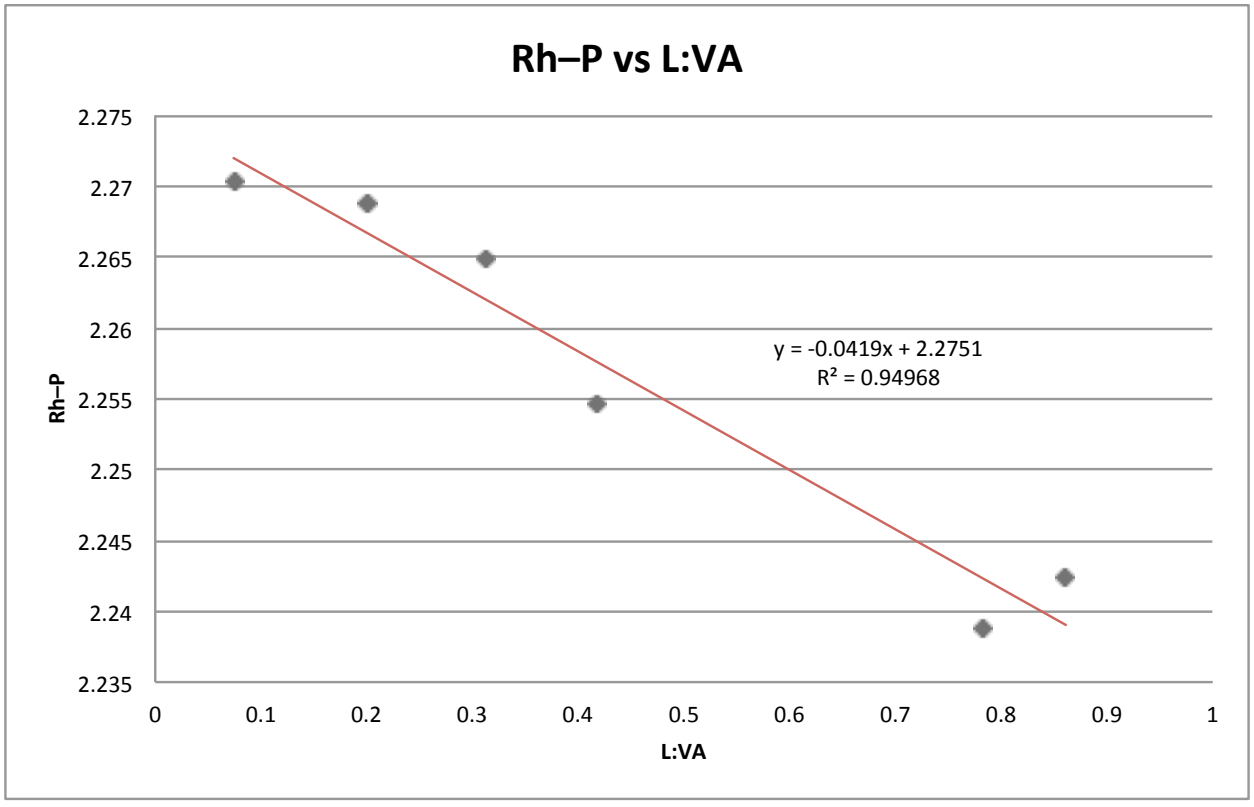
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.520765	-3.992548	-0.562303
2	1	0	3.606790	-4.049169	-1.650094
3	6	0	4.269639	-3.028025	0.101449
4	1	0	4.929404	-2.395416	-0.498419
5	6	0	1.096158	-3.413004	0.885738
6	1	0	0.036522	-3.156893	0.837581
7	6	0	1.914886	-2.585392	1.699561
8	1	0	1.430415	-1.730064	2.169431
9	6	0	3.164952	-3.089198	2.433311
10	1	0	3.294330	-2.496593	3.349555
11	1	0	2.985823	-4.129666	2.749159
12	6	0	4.483903	-3.008890	1.606193
13	1	0	5.022874	-2.092114	1.866719
14	1	0	5.147492	-3.846475	1.893453
15	6	0	2.851728	-5.158694	0.153341
16	1	0	2.895345	-6.051171	-0.490330
17	1	0	3.418186	-5.395757	1.066631
18	6	0	1.370208	-4.862613	0.507863
19	1	0	0.744945	-5.088913	-0.370925
20	1	0	1.031306	-5.538921	1.317412
21	6	0	-2.027373	-0.289585	0.323250
22	6	0	-1.662807	1.252386	0.399313

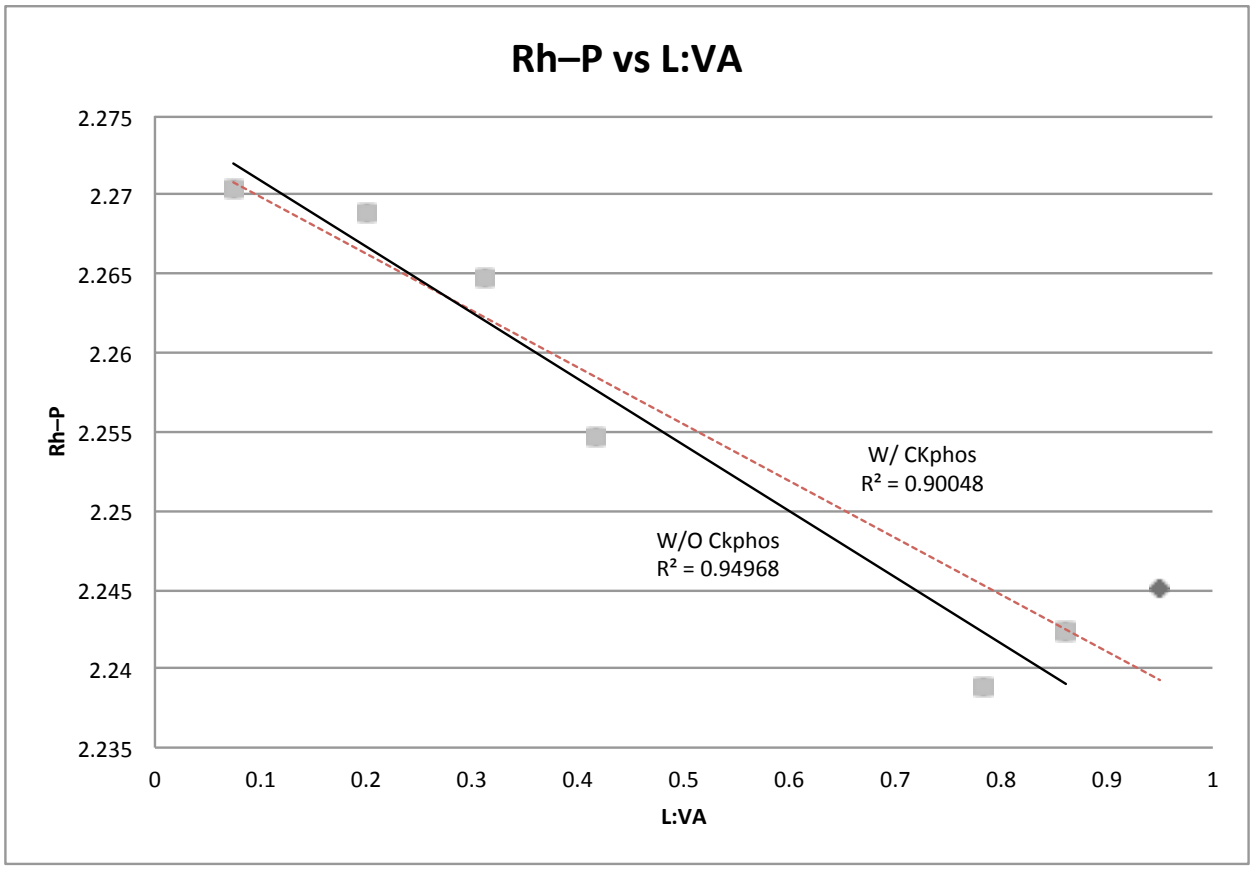
23	1	0	-1.583965	1.644367	-0.615780
24	6	0	-0.327753	1.435264	1.165619
25	1	0	-0.100517	0.555687	1.767468
26	6	0	0.839591	1.651079	0.107579
27	6	0	-1.928433	2.928294	1.995223
28	6	0	-2.510549	2.787674	3.401764
29	1	0	-3.583136	3.032443	3.387797
30	1	0	-1.994683	3.470978	4.092064
31	1	0	-2.378721	1.752698	3.748197
32	6	0	-2.040788	4.343303	1.421562
33	1	0	-1.653302	4.358301	0.394090
34	1	0	-1.455799	5.043154	2.036654
35	1	0	-3.093663	4.662118	1.414244
36	6	0	2.271054	1.296280	0.549965
37	6	0	3.287355	1.411727	-0.423569
38	6	0	4.599865	0.986130	-0.195858
39	6	0	4.939868	0.460236	1.055215
40	6	0	3.969279	0.373920	2.056998
41	6	0	2.656221	0.787258	1.800689
42	6	0	0.772784	3.113348	-0.377137
43	6	0	0.136316	3.557833	-1.551686
44	6	0	0.049894	4.920876	-1.884309
45	6	0	0.596899	5.888708	-1.034945
46	6	0	1.232269	5.480812	0.144242
47	6	0	1.312353	4.117761	0.454053
48	6	0	-0.103425	-2.542293	-2.928710
49	1	0	-1.032591	-3.109340	-2.743092
50	1	0	0.736664	-3.076704	-2.460719
51	6	0	0.112641	-2.297760	-4.429435
52	1	0	1.176814	-2.076844	-4.599080
53	1	0	-0.186655	-3.161525	-5.041414
54	6	0	-0.738917	-1.040260	-4.688770
55	1	0	-1.807565	-1.306202	-4.737948
56	1	0	-0.469247	-0.514857	-5.616546
57	6	0	-0.461843	-0.169870	-3.448639
58	1	0	0.436148	0.448082	-3.587219
59	1	0	-1.302461	0.488271	-3.193995
60	6	0	-2.859147	-0.733903	-0.899138
61	6	0	-2.985373	-2.117466	-1.139677
62	6	0	-3.596066	-2.630349	-2.287503
63	6	0	-4.148471	-1.752705	-3.229336
64	6	0	-4.103478	-0.375806	-2.988961
65	6	0	-3.480919	0.115150	-1.830254

66	6	0	-2.746822	-0.690238	1.629758
67	6	0	-2.123562	-1.256566	2.758253
68	6	0	-2.826880	-1.535767	3.943506
69	6	0	-4.187664	-1.228648	4.043420
70	6	0	-4.835231	-0.641022	2.949528
71	6	0	-4.115686	-0.376013	1.778203
72	17	0	3.201273	-1.287940	-2.453236
73	9	0	3.011198	1.929843	-1.631107
74	9	0	5.525196	1.073552	-1.158359
75	9	0	6.186733	0.017307	1.287660
76	9	0	4.295875	-0.128396	3.264323
77	9	0	1.789097	0.673098	2.831480
78	9	0	-0.445501	2.715786	-2.429050
79	9	0	-0.558025	5.296811	-3.021502
80	9	0	0.511500	7.189895	-1.344712
81	9	0	1.751192	6.397266	0.978106
82	9	0	1.936690	3.800945	1.604942
83	9	0	-3.512826	1.453460	-1.665730
84	9	0	-4.643852	0.476489	-3.875417
85	9	0	-4.695470	-2.227100	-4.358075
86	9	0	-3.609248	-3.955961	-2.514005
87	9	0	-2.457740	-3.016250	-0.282348
88	9	0	-4.800089	0.219477	0.782308
89	9	0	-6.137242	-0.320875	3.033157
90	9	0	-4.862698	-1.490235	5.171197
91	9	0	-2.190122	-2.095718	4.985590
92	9	0	-0.811801	-1.562089	2.787600
93	7	0	-0.224040	-1.168372	-2.368119
94	8	0	-0.768309	-1.013652	0.256829
95	8	0	0.546005	0.782281	-1.021314
96	8	0	-2.610584	1.997301	1.136449
97	8	0	-0.537137	2.539663	2.021862
98	15	0	0.435596	-0.857150	-0.878393
99	45	0	2.243371	-2.096171	-0.377433

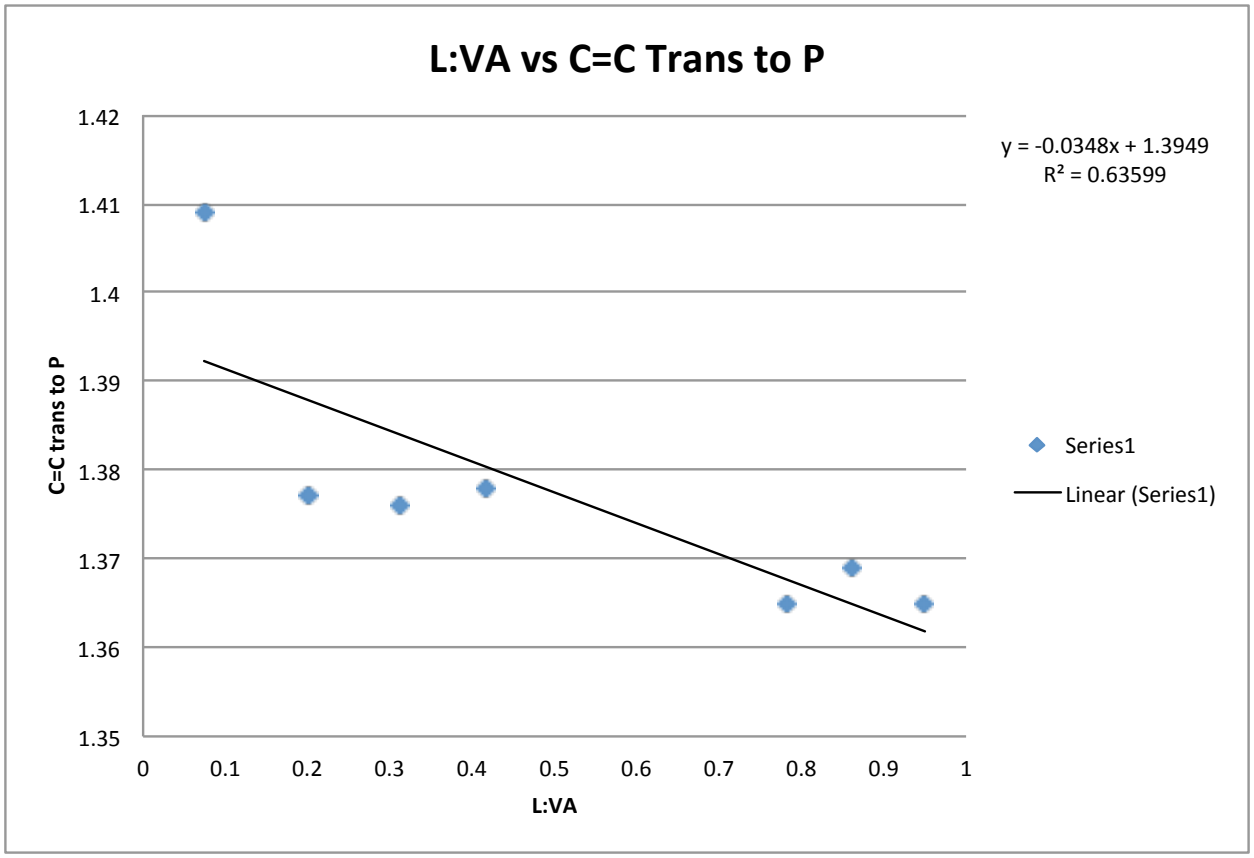
8. Structure-Function Relationships of Phosphoramidites and Product Selectivity

	L/VA	Rh–P
Xypip (**T2**)	0.07407	2.2703
Xypyr [Ref 21 **T8**]	0.2	2.2688
PhNMe2 [Ref 21 **T1**]	0.3125	2.2648
Phpyr [**T4**]	0.41667	2.2547
Guiphos [Ref 21 **B1**]	0.782608696	2.2388
tBu (**B1**)	0.861111111	2.2423
CK	0.95	2.2451




Rh–P vs L:VA
2.275
2.27
2.265
2.26
2.255
2.25
2.245
2.24
2.235
Rh–P
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
L:VA
W/ CKphos
R² = 0.90048
W/O Ckphos
R² = 0.94968

	L/VA	C=C trans to P
Xypip (T2)	0.07407	1.409
Xypyr [Ref 21 T8]	0.2	1.377
PhNMe2 [Ref 21 T1]	0.3125	1.376
Phpyr [T4]	0.41667	1.378
Guiphos [Ref 21 B1]	0.782608696	1.365
tBu (B1)	0.861111111	1.369
CK	0.95	1.365



	L/VA	Rh–Centroid
Xypip (T2)	0.07407	4.025
Xypyr [Ref 21 T8]	0.2	4.022
PhNMe2 [Ref 21 T1]	0.3125	4.059
Phpyr [T4]	0.41667	4.039
CK	0.95	3.728