Mechanistic Studies on C-C Reductive Elimination of Five-Coordinate Rh(III) Complexes

Shanshan Chen[a,c], Yan Su[b], Keli Han,[b] Xingwei Li[a,b]*

[a] Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371

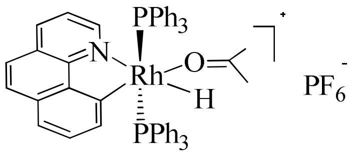
[b]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

[c]Department of Applied Chemistry, School of Sciences, Anhui Agricultural University, Hefei 230036, China.

Contents

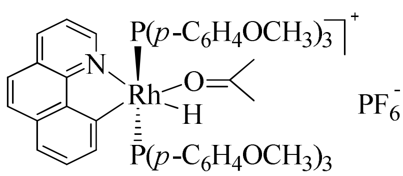
General Consideration. All manipulations were performed using standard Schlenk techniques and in glove box. All chemicals were used as received without any further purification unless otherwise mentioned. All solvent were degassed and dried by standard techniques. NMR spectra were obtained on a Bruker DPX 300, AMX 400 or 500 spectrometers. The sample temperature in VT NMR analysis was calibrated by 4 % methanol in methanol-d_4. The chemical shift is given as dimensionless δ values and is frequency referenced relative to Me_4Si for ^1H and ^{13}C NMR spectroscopy. Elemental analyses were performed in the Division of Chemistry and Biological Chemistry, Nanyang Technological University. X-ray crystallographic analyses were performed on a Bruker X8 APEX diffractometer. IR spectra were recorded on a Shimadzu IRPESTIGE-21 FTIR spectrometer from 4000 to 600 cm-1 with 4 cm^{-1} resolution.

General Method for the Synthesis of Rhodium Hydride 1. To a suspension of $[Rh(NBD)(PAr_3)_2]^+$， PF_6^- (Ar = Ph, *p*-$C_6H_4OCH_3$, *p*-C_6H_4F) (0.50 mmol) in acetone (8 mL) was bubbled H_2 for 15min at 0 °C, during which time the colour of the solution changed from red to pale yellow. *tert*-Butylethylene (1.2 ml) and benzo(*h*)quinoline, 2-phenylpridine or dibenzo[*f*,*h*]quinoline (0.60 mmol) were added to the solution and were reflux under 65 °C for 5 h. The solvent was concentrated to 0.5 ml under reduced pressure. The residue was put into the glove box and washed with diethyl ether 3 × 10 ml to give white powder Rhodium hydride complexes.



1a

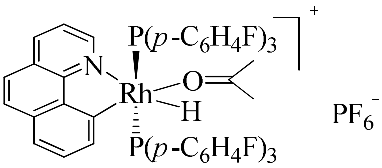
Yield: 454 mg (0.45 mmol, 92%). ^1H NMR (δ, 300 MHz, CD_3COCD_3, 295 K): -12.29 (dt, $^1J_{RhH}$ = 16.6 Hz, $^2J_{PH}$ =11.0 Hz, 1H, Rh*H*), 2.06 (s, 6H, C*H*$_3$COC*H*$_3$), 6.96 (t, ^3J =7.7 Hz, 1H), 7.05-7.38 [m, 32H, 2H ($C_{13}H_8N$) + 30H (P*Ph*$_3$)], 7.43 (d, ^3J =7.7 Hz, 1H), 7.57 (d, ^3J =8.8 Hz, 1H), 7.78 (dd, ^3J =8.0 Hz, ^3J =5.0 Hz, 1H), 8.16 (d, ^3J =7.9 Hz, 1H), 9.79 (d, ^3J =4.9 Hz, 1H); ^{31}P {^1H} NMR (δ, 121 MHz, CD_3COCD_3, 295 K): -143.56 (m, $^1J_{FP}$ = 704.0 Hz, *P*F$_6$), 39.91 (d, $^1J_{RhP}$ = 114.3 Hz, *P*Ph$_3$); ^{13}C {^1H} NMR (δ, 100 MHz, CD_3COCD_3, 295 K): 29.8 (s, *C*H$_3$), 120.52 (s), 122.44 (s), 122.83 (s), 126.83 (s), 127.31 (s), 128.08 (t, J_{PC} = 4.7 Hz, P*Ph*$_3$), 128.60 (t, $^1J_{PC}$ = 23.0 Hz, *ipso*-P*Ph*$_3$), 130.30 (s, *p*-P*Ph*$_3$), 133.36 (t, J_{PC} = 5.6 Hz, P*Ph*$_3$), 134.73 (s), 135.73 (s), 138.44 (s), 139.65 (s), 148.19 (s), 150.71 (s), 153.08 (dt, $^1J_{RhC}$ = 31.0 Hz, $^2J_{PC}$ = 11.2 Hz, *C*Rh), 205.26 (*C*O). Anal. Calcd. For $C_{54}H_{45}F_6NOP_3Rh$ (1009.74): C, 61.85; H, 4.49; N, 1.39. Found: C, 61.54; H, 4.95; N, 1.43.



1b

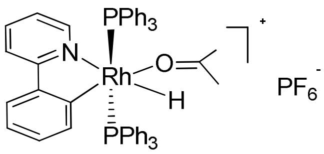
Yield: 530 mg (0.45 mmol, 89%). ^1H NMR (δ, 300 MHz, CD_3COCD_3, 295 K): -12.49 (dt, $^1J_{RhH}$ = 17.6 Hz, $^2J_{PH}$ =10.9 Hz, 1H, Rh*H*), 3.75 (s, 18H, PC$_6$H$_4$OC*H*$_3$), 6.69 (d, ^3J = 8.5 Hz, 12H, PC$_6$*H*$_4$OCH$_3$), 6.93-6.99 (m, 12H, PC$_6$*H*$_4$OCH$_3$), 7.06 (m, 1H), 7.29 (d, ^3J = 7.3 Hz, 1H), 7.39-7.45 (m, 2H), 7.60 (d, ^3J = 8.8 Hz, 1H), 7.78 (dd, ^3J = 7.9 Hz, ^3J = 5.1 Hz, 1H), 8.20 (d, ^3J = 7.8 Hz, 1H), 9.76 (d, ^3J = 4.8 Hz, 1H); ^{31}P {^1H} NMR (δ, 121 MHz, CD_3COCD_3, 295 K): -143.54 (m, $^1J_{FP}$ = 704.8 Hz, *P*F$_6$), 36.32 (d, $^1J_{RhP}$ = 112.8 Hz, *P*C$_6$H$_4$OCH$_3$); ^{13}C {^1H} NMR (δ, 75 MHz, CD_3COCD_3, 295 K): 26.17 (*C*D$_3$CO*C*D$_3$), 55.67 (PC$_6$H$_4$OC*H*$_3$), 114.34 (t, J_{PC} = 5.2 Hz,

$PC_6H_4OCH_3$), 120.99 (t, $^1J_{PC}$ = 25.4 Hz, *ipso*-$PC_6H_4OCH_3$), 121.52 (s), 122.44 (s), 124.81 (s), 127.99 (s), 128.44 (s), 129.51 (s), 135.45 (s), 135.63 (t, J_{PC} = 6.4 Hz, $PC_6H_4OCH_3$), 136.39 (s), 139.08 (s), 140.73 (s), 148.97 (s), 151.97 (s), 156.01 (dt, $^1J_{RhC}$ = 31.8 Hz, $^2J_{PC}$ = 11.1 Hz, *C*Rh), 161.96 (s, *p*-$PC_6H_4OCH_3$), 206.20 (*C*O). Anal. Calcd. For $C_{58}H_{57}F_6NO_7P_3Rh$ (1189.89): C, 58.54; H, 4.83; N, 1.18. Found: C, 58.12; H, 4.97; N, 1.61.



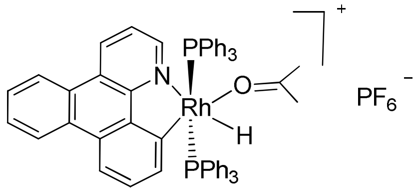
1c

Yield: 475 mg (0.43 mmol, 85%). ^{1}H NMR (δ, 300 MHz, CD_3COCD_3, 295 K): -12.36 (dt, $^1J_{RhH}$ = 16.5 Hz, $^2J_{PH}$ =11.0 Hz, 1H, Rh*H*), 2.09 (s, 6H, CH_3COCH_3), 6.97 (m, 12H, PC_6H_4F), 7.04 (t, ^3J = 8.0 Hz, 1H), 7.11-7.18 (m, 12H, PC_6H_4F), 7.31 (d, ^3J = 7.4 Hz, 1H), 7.46-7.51 (m, 2H), 7. 64 (d, ^3J = 8.8, 1H), 7.85 (dd, ^3J = 8.0 Hz, ^3J = 5.1 Hz, 1H), 8.28 (d, ^3J = 7.9 Hz, 1H), 9.83 (d, ^3J = 4.8 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_3COCD_3, 295 K): -143.50 (m, $^1J_{FP}$ = 705.4 Hz, PF_6), 38.47 (d, $^1J_{RhP}$ = 115.5 Hz, PC_6H_4F); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2Cl_2, 295K): -109.11 (s, PC_6H_4F), -72.69 (d, J_{P-F} = 709.9 Hz, PF_6); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_3COCD_3, 295 K): 116.28 (dt, J_{FC} = 21.5 Hz, J_{PC} = 5.4 Hz, PC_6H_4F), 122.35 (s), 123.24 (s), 125.03 (td, $^1J_{PC}$ = 24.4 Hz, $^4J_{FC}$ = 3.4 Hz, *ipso*-PC_6H_4F), 125.03 (s), 128.10 (s), 129.02 (s), 129.02 (s), 135.68 (s), 136.62 (dt, J_{FC} = 8.4 Hz, J_{PC} = 6.7 Hz, PC_6H_4F), 136.99 (s), 139.23 (s), 140.29 (s), 149.40 (s), 151.24 (s), 153.51(dt, $^1J_{RhC}$ = 31.6 Hz, $^2J_{PC}$ = 12.5 Hz, *C*Rh), 163.86 (d, $^1J_{FC}$ = 249.8 Hz, *p*-PC_6H_4F), 206.11 (*C*O). Anal. Calcd. For $C_{52}H_{39}F_{12}NOP_3Rh$ (1117.11): C, 55.88; H, 3.52; N, 1.25. Found: C, 56.04; H, 3.23; N, 1.21.



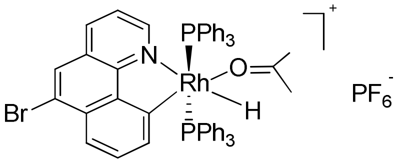
1d

Yield: 428 mg (0.44 mmol, 87%). ^{1}H NMR (δ, 300 MHz, CD_3CN, 295 K): -12.26 (dt, $^1J_{RhH}$ = 15.6 Hz, $^2J_{PH}$ =10.9 Hz, 1H, Rh*H*), 2.06 (s, 6H, CH_3COCH_3), 6.50 (t, ^3J = 6.7 Hz, 1H), 6.87 (t, ^3J = 7.6 Hz, 1H), 7.03 (d, ^3J = 7.7 Hz, 1H), 7.12-7.42 [m, 33H, 3H ($C_{13}H_8N$) + 30H (PPh_3)], 7.62 (t, ^3J = 6.8 Hz, 1H), 9.46 (d, ^3J = 5.5 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_3CN, 295 K): -143.58 (m, $^1J_{FP}$ = 705.1 Hz, PF_6), 39.91 (d, $^1J_{RhP}$ = 115.8 Hz, PPh_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_3CN, 295 K): 119.31 (s), 121.99 (s), 122.22 (s), 124.64 (s), 128.54 (s), 128.16 (t, J_{PC} = 4.9 Hz, PPh_3), 129.93 (t, $^1J_{PC}$ = 23.4 Hz, *ipso*-PPh_3), 130.30 (s, *p*-PPh_3), 133.39 (t, J_{P-C} = 5.8 Hz, PPh_3), 136.85 (s), 142.10 (s), 144.03 (s), 149.33 (s), 161.69 (s), 159.56 (dt, $^1J_{RhC}$ = 28.4 Hz, $^2J_{PC}$ = 10.3 Hz, *C*Rh), 206.45 (*C*O). Anal. Calcd. For $C_{50}H_{45}F_6NOP_3Rh$ (985.72): C, 60.92; H, 4.60; N, 1.42. Found: C, 60.52; H, 4.96; N, 1.51.



1e

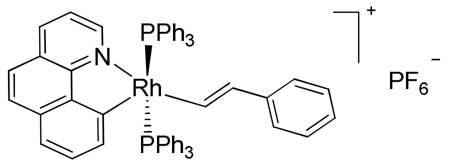
Yield: 440 mg (0.42 mmol, 83%). ^{1}H NMR (δ, 400 MHz, CD_3CN, 295 K): -12.28 (dt, $^{1}J_{RhH}$ = 14.1 Hz, $^{2}J_{PH}$ = 9.6 Hz, 1H, Rh*H*), 2.05 (s, 6H, CH_3COCH_3), 6.81 (t, ^{3}J = 7.7 Hz, 1H), 7.04-7.18 [m, 31H, 30H (P*Ph*$_3$) + 1H ($C_{17}H_{10}N$)], 7.40 (dd, ^{3}J = 8.0 Hz, ^{3}J = 5.2 Hz, 1H), 7.64 (m, 2H), 7.94 (d, ^{3}J = 8.0 Hz, 1H), 8.38 (d, ^{3}J = 7.9 Hz, 1H), 8.48 (d, ^{3}J = 7.9 Hz, 1H), 8.63 (d, ^{3}J = 8.2 Hz, 1H), 8.82 (d, ^{3}J = 4.8 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_3CN, 295 K): -144.62 (m, $^{1}J_{FP}$ = 706.3 Hz, *P*F$_6$), 40.18 (d, $^{1}J_{RhP}$ = 111.9 Hz, *P*Ph$_3$); ^{13}C {^{1}H} NMR (δ, 100 MHz, CD_3CN, 295K): 29.90 (CH_3COCH_3), 116.20 (s), 121.68 (s), 123.12 (s), 123.43 (s), 125.68 (s), 127.21 (s), 127.76 (s), 127.92 (t, J_{PC} = 4.9 Hz, P*Ph*$_3$), 128.31 (s), 129.60 (t, $^{1}J_{PC}$ = 24.0 Hz, *ipso*-P*Ph*$_3$), 130.01 (s, *p*-P*Ph*$_3$), 130.55 (s), 130.91 (s), 132.03 (s), 133.15 (t, $J_{P\text{-}C}$ = 5.8 Hz, P*Ph*$_3$), 138.61 (s), 140.45 (s), 148.51 (s), 151.78 (s), 157.46 (dt, $^{1}J_{RhC}$ = 27.9 Hz, $^{2}J_{PC}$ = 11.4 Hz, *C*Rh), 206.49 (*C*O). Anal. Calcd. For $C_{56}H_{47}F_6NOP_3Rh$ (1059.80): C, 63.46; H, 4.47; N, 1.32. Found: C, 63.06; H, 4.45; N, 1.56.



1f

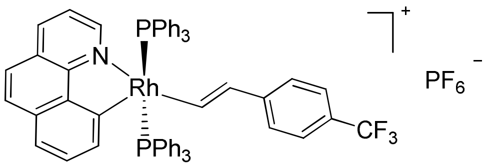
Yield: 463 mg (0.43 mmol, 85%). ^{1}H NMR (δ, 300 MHz, CD_3COCD_3, 295 K): -12.13 (dt, $^{1}J_{RhH}$ = 16.1 Hz, $^{2}J_{PH}$ =10.7 Hz, 1H, Rh*H*), 2.11 (s, 6H, CH_3COCH_3), 7.10-7.22 [m, 25H, 24H (P*Ph*$_3$) + 1H ($C_{13}H_7N$)], 7.31-7.36 (m, 6H, P*Ph*$_3$), 7.42 (d, ^{3}J = 7.4 Hz, 1H), 7.69 (d, ^{3}J = 8.0 Hz, 1H), 7.80 (s, 1H), 7.86 (dd, ^{3}J = 7.9 Hz, ^{3}J = 5.1 Hz, 1H), 8.19 (d, ^{3}J = 7.9 Hz, 1H), 9.89 (d, ^{3}J = 4.1 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_3COCD_3, 295 K): -143.48 (m, $^{1}J_{FP}$ = 705.2 Hz, *P*F$_6$), 40.05 (d, $^{1}J_{RhP}$ = 113.1 Hz, *P*Ph$_3$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_3COCD_3, 295 K): 120.52 (s), 122.44 (s), 122.82 (s), 126.83 (s), 127.31 (s), 128.08 (t, $J_{P\text{-}C}$ = 4.7 Hz, P*Ph*$_3$), 128.33 (t, $^{1}J_{PC}$ = 23.1 Hz, *ipso*-P*Ph*$_3$), 128.40 (s), 128.75 (s), 130.42 (s, *p*-P*Ph*$_3$), 132.90 (s), 133.34 (t, $J_{P\text{-}C}$ = 5.7 Hz, P*Ph*$_3$), 135.12 (s), 139.55 (s), 148.90 (s), 150.02 (s), 154.48 (dt, $^{1}J_{RhC}$ = 31.9 Hz, $^{2}J_{PC}$ = 11.3 Hz, *C*Rh), 205.32 (*C*O). Anal. Calcd. For $C_{52}H_{44}BrF_6NOP_3Rh$ (1089.63): C, 57.37; H, 4.07; N, 1.29. Found: C, 56.99; H, 3.65; N, 1.71.

General method for the synthesis of the five-coordinate Rhodium complexes 2. To a solution of the Rhodium hydride complexes (0.1 mmol) in dichloromethane (3 ml) was dropped terminal alkynes (0.2 mmol) and then the solution was stirred for 2 h at -20 ^{o}C. Then the solvent was removed under reduced pressure at -20 ^{o}C and the residue was transferred into glove box and washed with diethyl ether 3 × 6 ml to give an orange powder. The five-coordinate complexes in solution are unstable and easily turn to C-C coupling rhodium complexes at room temperature, so the NMR is performed at -20 ^{o}C.



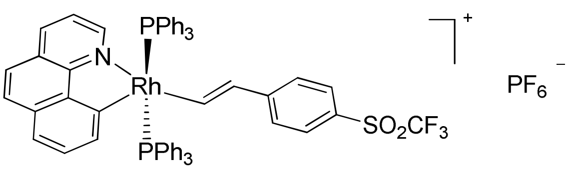
2aa

Yield: 95 mg (0.090 mmol, 90%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.10 (d, $^3J_{CH=CH}$ = 17.0 Hz, 1H, CH=CHC$_6$H$_5$), 6.52 (d, ^3J = 7.1 Hz, 2H, CHC$_6$$H_5$), 6.90-6.98 (m, 12H, P$Ph_3$), 7.02-7.20 [m, 15H, 12H (PPh_3) + 1H (C$_{13}$$H_8$N) + 2H (CHC$_6$$H_5$)], 7.30-7.41 [m, 8H, 6H (PPh_3) + 2H (C$_{13}$$H_8$N)], 7.55 (t, ^3J = 7.7 Hz, 1H), 7.66-7.70 (m, 2H), 7.92-7.96 (m, 2H), 8.13 (dt, $^3J_{CH=CH}$ = 17.0 Hz, $^3J_{PH}$ = 5.9 Hz, 1H, RhCH=CH), 8.71 (d, ^3J = 4.9 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.88 (m, $^1J_{FP}$ = 707.6 Hz, PF$_6$), 23.23 (d, $^1J_{RhP}$ = 112.5 Hz, PPh$_3$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 122.41 (s), 123.24 (s), 124.58 (s), 124.78 (s), 124.96 (s), 126.12 (t, $^1J_{PC}$ = 24.0 Hz, *ipso*-PPh_3), 127.10 (s), 127.97 (s), 128.11 (s), 128.22 (s), 128.71 (t, J_{PC} = 4.9 Hz, PPh_3), 131.33 (s, *p*-PPh_3), 131.49 (s), 132.07 (s), 133.00 (t, J_{PC} = 5.5Hz, PPh_3), 134.13 (s), 136.32 (s), 136.44 (s), 138.00 (s), 144.95 (dt, $^1J_{RhC}$ = 42.0 Hz, $^2J_{PC}$ = 9.4 Hz, CRh), 147.76 (dt, $^1J_{RhC}$ = 31.0 Hz, $^2J_{PC}$ = 11.3 Hz, RhCH=CH), 147.82 (s), 148.53 (s). Anal. Calcd. For $C_{57}H_{45}F_6NP_3Rh{\bullet}1.5CH_2Cl_2$ (1181.19): C, 59.48; H, 4.10; N, 1.19. Found: C, 59.11; H, 4.02; N, 1.23.



2ab

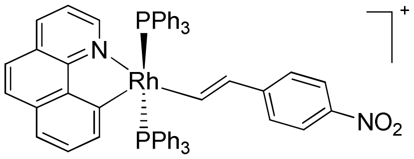
Yield: 101 mg (0.090 mmol, 90%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.13 (d, $^3J_{CH=CH}$ = 17.0 Hz, 1H, CH=CHC$_6$H$_4$CF$_3$), 6.59 (d, ^3J = 8.1, 2H, C$_6$$H_4CF_3$), 6.83-7.04 [m, 13H, 12H (PPh_3)+1H (C$_{13}$$H_8$N)], 7.18 (m, 12H, P$Ph_3$), 7.32-7.42 [m, 9H, 6H (PPh_3) + 3H (C$_{13}$$H_8$N)], 7.57 (t, ^3J = 7.7 Hz, 1H), 7.67-7.70 (m, 2H), 7.95 (d, ^3J = 7.9, 2H, C$_6$$H_4CF_3$), 8.36 (dt, $^3J_{CH=CH}$ = 17.0 Hz, $^3J_{PH}$ = 5.5 Hz, 1H, RhCH=CH), 8.56 (d, ^3J = 4.1, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.85 (m, $^1J_{FP}$ = 710.6 Hz, PF$_6$), 23.38 (d, $^1J_{RhP}$ = 112.1 Hz, PPh$_3$); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2Cl_2, 255 K): -73.20 (d, $^1J_{PF}$ = 710.3 Hz, 6F, PF_6), -62.48 (s, CF_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 122.85 (s), 123.69 (s), 124.83 (q, $^1J_{FC}$ = 271.1 Hz, CF$_3$), 124.94 (s), 125.24 (s), 125.44 (q, $^3J_{FC}$ = 3.8 Hz, C_6H$_4$CF$_3$), 126.25 (t, $^1J_{PC}$ = 24.0 Hz, *ipso*-PPh_3), 127.05 (q, $^2J_{FC}$ = 31.7 Hz, C_6H$_4$CF$_3$), 127.47 (s), 128.97 (s), 129.11 (t, $J_{P\text{-}C}$ = 4.8 Hz, PPh_3), 131.74 (s, *p*-PPh_3), 133.25 (t, $J_{P\text{-}C}$ = 5.4 Hz, PPh_3), 134.48 (s), 136.73 (s), 141.49 (s), 145.08 (dt, $^1J_{RhC}$ = 42.9 Hz, $^2J_{PC}$ = 9.2 Hz, CRh), 148.08 (s), 148.95 (s), 153.65 (dt, $^1J_{RhC}$ = 32.2 Hz, $^2J_{PC}$ = 10.7 Hz, RhCH=CH). Anal. Calcd. For $C_{58}H_{44}F_9NP_3Rh$ (1121.79): C, 62.10; H, 3.95, N, 1.25. Found: C, 61.94; H, 4.30; N, 1.15.



2ac

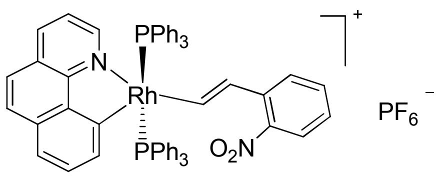
Yield: 113 mg (0.092 mmol, 92%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.27 (d, $^3J_{CH=CH}$ = 17.2

Hz, 1H, CH=C*H*$C_6H_4SO_2CF_3$), 6.74 (d, ^3J = 8.2 Hz, 2H, $CHC_6H_4SO_2CF_3$), 6.90 (m, ^3J = 5.4 Hz, 12H, P*Ph*$_3$), 7.18 (t, ^3J = 7.1 Hz, 12H, P*Ph*$_3$), 7.36-7.41 [m, 8H, 6H (P*Ph*$_3$) + 2H ($C_{13}H_8N$)], 7.59 (t, ^3J = 7.7 Hz, 1H), 7.69 (d, ^3J = 7.1 Hz, 2H), 7.75 (d, ^3J = 8.2 Hz, 2H, $CHC_6H_4SO_2CF_3$), 7.96 (d, ^3J = 7.8 Hz, 2H), 8.72-8.78 [m, 2H, 1H (RhC*H*=CH)+1H ($C_{13}H_8N$)]; ^{31}P {^1H} NMR (*δ*, 121 MHz, CD_2Cl_2, 255 K): -143.81 (m, $^1J_{FP}$ = 708.3 Hz, *P*F_6), 23.45 (d, $^1J_{RhP}$ = 110.6 Hz, *P*Ph_3); ^{19}F {^1H} NMR (*δ*, 282 MHz, CD_2Cl_2, 255 K): -73.11 (d, $^1J_{PF}$ = 710.3 Hz, 6F, P*F*$_6$), -79.24 (s, SO_2CF_3); ^{13}C {^1H} NMR (*δ*, 75 MHz, CD_2Cl_2, 255 K): 119.74 (q, $^1J_{F\text{-}C}$ = 320.3 Hz, *C*F_3), 122.69 (s), 123.53 (s), 124.67 (s), 125.75 (s), 125.75 (t, $^1J_{PC}$ = 23.7 Hz, *ipso*-P*Ph*$_3$), 127.20 (s), 128.68 (s), 128.87 (t, J_{PC} = 4.9 Hz, P*Ph*$_3$), 131.04 (s), 131.15 (s), 131.36 (s), 131.52 (s, *p*-P*Ph*$_3$), 132.91 (t, J_{PC} = 5.4 Hz, P*Ph*$_3$), 133.53 (s), 134.23 (s), 136.43 (s), 136.54 (s), 144.80 (dt, $^1J_{RhC}$ = 43.5 Hz, $^2J_{PC}$ = 9.0 Hz, *C*Rh), 145.45 (s), 147.80 (s), 148.74 (s), 161.61 (dt, $^1J_{RhC}$ = 31.3 Hz, $^2J_{PC}$ = 11.0 Hz, Rh*C*H=CH). Anal. Calcd. For $C_{58}H_{44}F_9NO_2P_3RhS$•0.5$CH_2Cl_2$ (1228.32): C, 57.20; H, 3.69; N, 1.18; S, 2.61. Found: C, 57.15; H, 3.53; N, 1.40; S, 2.38.



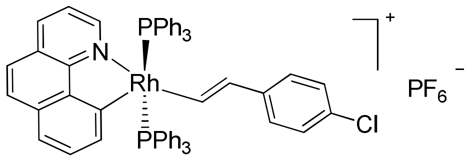
2ad

Yield: 108 mg (0.095 mmol, 95%). ^1H NMR (*δ*, 300 MHz, CD_2Cl_2, 255 K): 5.25 (d, $^3J_{CH=CH}$ = 17.0 Hz, 1H, CH=C*H*$C_6H_4NO_2$), 6.62 (d, ^3J = 8.6 Hz, 2H, $CHC_6H_4NO_2$), 6.91 (m, 12H, P*Ph*$_3$), 7.16 (t, ^3J = 7.5 Hz, 12H, P*Ph*$_3$), 7.36-7.42 [m, 8H, 6H (P*Ph*$_3$) + 2H ($C_{13}H_8N$)], 7.60 (t, ^3J = 7.7 Hz, 1H), 7.69 (d, ^3J = 8.5 Hz, 2H, $C_6H_4NO_2$), 7.97 (m, 4H), 8.65 (dt, $^3J_{CH=CH}$ = 17.1 Hz, $^3J_{PH}$ = 5.5 Hz, 1H, RhC*H*=CH), 8.73 (d, ^3J = 4.9 Hz, 1H); ^{31}P {^1H} NMR (*δ*, 121 MHz, CD_2Cl_2, 255 K): -143.81 (m, $^1J_{FP}$ = 708.8 Hz, *P*F_6), 23.42 (d, $^1J_{RhP}$ = 110.7 Hz, *P*Ph_3); ^{13}C {^1H} NMR (*δ*, 75 MHz, CD_2Cl_2, 255 K): 122.64 (s), 123.50 (s), 123.64 (s), 123.91 (s), 124.65 (s), 125.49 (t, $^1J_{PC}$ = 24.1 Hz, *ipso*-P*Ph*$_3$), 127.19 (s), 128.67 (s), 128.84 (t, J_{PC} = 4.9 Hz, P*Ph*$_3$), 131.31(s), 131.49 (s, *p*-P*Ph*$_3$), 132.92 (t, J_{PC} = 5.5 Hz, P*Ph*$_3$), 134.22 (s), 136.38 (s), 136.52 (s), 143.72 (s), 144.77 (dt, $^1J_{RhC}$ = 42.7 Hz, $^2J_{PC}$ = 9.2 Hz, *C*Rh), 145.05 (s), 147.77 (s), 148.75 (s), 159.38 (dt, $^1J_{RhC}$ = 31.3 Hz, $^2J_{PC}$ = 11.4 Hz, Rh*C*H=CH). Anal. Calcd. For $C_{57}H_{44}F_6N_2O_2P_3Rh$•0.5$CH_2Cl_2$ (1141.25): C, 60.51; H, 3.97; N, 2.45. Found: C, 60.70; H, 3.71; N, 2.88.



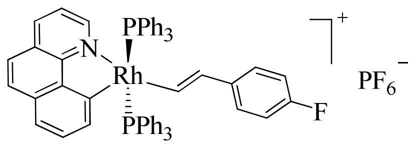
2ai

Yield: 100 mg (0.088 mmol, 88%). ^1H NMR (*δ*, 300 MHz, CD_2Cl_2, 255 K): 5.97 (d, $^3J_{CH=CH}$ = 16.9 Hz, 1H, CH=C*H*$C_6H_4NO_2$), 6.83 (d, ^3J = 7.8 Hz, 1H), 6.89-6.99 (m, 12H, P*Ph*$_3$), 7.13-7.21 [m, 13H, 12H (P*Ph*$_3$) + 1H ($C_{13}H_8N$)], 7.16-7.38 [m, 9H, 6H (P*Ph*$_3$) + 3H ($C_{13}H_8N$)], 7.57-7.69 (m, 4H), 7.93-7.99 (m, 2H), 8.41(dt, $^3J_{CH=CH}$ = 16.8 Hz, $^3J_{PH}$ = 6.0 Hz, 1H, RhC*H*=CH), 8.65 (d, ^3J = 4.8 Hz, 1H); ^{31}P {^1H} NMR (*δ*, 121 MHz, CD_2Cl_2, 255 K): -143.88 (m, $^1J_{FP}$ = 707.7 Hz, *P*F_6), 22.78 (d, $^1J_{RhP}$ = 111.2 Hz, *P*Ph_3); ^{13}C {^1H} NMR (*δ*, 75 MHz, CD_2Cl_2, 255 K): 122.47 (s), 123.39 (s), 123.99 (s), 124.61 (s), 124.77 (s), 125.90 (t, $^1J_{PC}$ = 24.0 Hz, *ipso*-P*Ph*$_3$), 126.09 (s), 126.77 (s), 127.11 (s), 127.26 (s), 128.72 (t, J_{PC} = 4.8 Hz, P*Ph*$_3$), 131.39 (s, *p*-P*Ph*$_3$), 131.63 (s), 132.58 (s), 132.96 (t, $J_{P\text{-}C}$ = 5.5 Hz, P*Ph*$_3$), 134.23 (s), 136.52 (s), 145.10 (dt, $^1J_{RhC}$ = 42.2 Hz, $^2J_{PC}$ = 8.6 Hz, *C*Rh), 145.92 (s), 147.89 (s), 148.44 (s), 157.80 (dt, $^1J_{RhC}$ = 31.7 Hz, $^2J_{PC}$ = 10.7 Hz, Rh*C*H=CH). Anal. Calcd. For $C_{57}H_{44}F_6N_2O_2P_3Rh$•$0.5CH_2Cl_2$ (1141.25): C, 60.51; H, 3.97; N, 2.45. Found: C, 60.73; H, 3.82; N, 2.80.



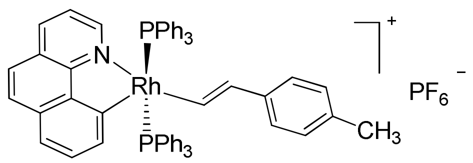
2ae

Yield: 102 mg (0.090 mmol, 90%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.12 (d, $^3J_{CH=CH}$ = 16.9 Hz, 1H, CH=C*H*C_6H_4Cl), 6.48 (d, ^3J = 8.4 Hz, 2H, CHC_6*H*$_4$Cl), 6.91-7.02 (m, 12H, P*Ph*$_3$), 7.08-7.25 [m, 14H, 12H (P*Ph*$_3$) + 2H (C_{13}*H*$_8$N)], 7.34-7.39 [m, 8H, 6H (P*Ph*$_3$) + 2H (C_{13}*H*$_8$N)], 7.47 (t, ^3J = 8.4 Hz, 1H), 7.56 (d, ^3J = 7.7 Hz, 2H, CHC_6*H*$_4$Cl), 7.90-7.94 (m, 2H), 8.14 (dt, $^3J_{CH=CH}$ = 17.1 Hz, $^3J_{PH}$ = 5.7 Hz, 1H, RhC*H*=CH), 8.74 (d, ^3J = 4.8 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.84 (m, $^1J_{FP}$ = 708.9 Hz, *P*F_6), 23.10 (d, $^1J_{RhP}$ = 112.3 Hz, *P*Ph_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 122.79 (s), 123.56 (s), 124.88 (s), 126.43 (t, $^1J_{PC}$ = 24.3 Hz, *ipso*-P*Ph*$_3$), 127.40 (s), 128.52 (s), 129.01 (t, J_{PC} = 4.8 Hz, P*Ph*$_3$), 131.15(s), 131.61 (s, *p*-P*Ph*$_3$), 131.95 (s); 133.30 (t, $J_{P\text{-}C}$ = 5.4 Hz, P*Ph*$_3$), 133.69 (s), 133.77 (s), 133.83 (s), 134.43 (s), 136.64 (s), 136.95 (s), 145.53 (dt, $^1J_{RhC}$ = 40.2 Hz, $^2J_{PC}$ = 9.6 Hz, *C*Rh), 148.26 (s), 148.92 (s), 149.69 (dt, $^1J_{RhC}$ = 31.0 Hz, $^2J_{PC}$ = 10.9 Hz, Rh*C*H=CH). Anal. Calcd. For $C_{57}H_{44}ClF_6NP_3Rh$•$2CH_2Cl_2$ (1130.70): C, 61.08; H, 4.01; N, 1.24. Found: C, 61.26; H, 4.61; N, 1.39.



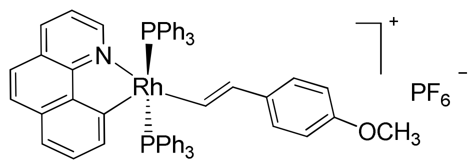
2af

Yield: 100 mg (0.09 mmol, 93%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.15 (d, $^3J_{CH=CH}$ = 16.9 Hz, 1H, CH=C*H*C_6H_4F), 6.45-6.50 (m, 2H, CHC_6*H*$_4$F), 6.77-6.93 [m, 15H, 12H (P*Ph*$_3$) + 3H (C_{13}*H*$_8$N)], 7.11 (t, ^3J = 8.0 Hz, 12H, P*Ph*$_3$), 7.29-7.34 [m, 7H, 6H (P*Ph*$_3$) + 1H (C_{13}*H*$_8$N)], 7.49 (t, ^3J = 7.7 Hz, 1H), 7.61-7.64 (m, 2H), 7.84-7.89 (m, 2H), 7.95 (dt, $^3J_{CH=CH}$ = 17.2 Hz, $^3J_{PH}$ = 5.6 Hz, 1H, RhC*H*=CH), 8.70 (d, ^3J = 4.9 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.87 (m, $^1J_{FP}$ = 709.0 Hz, *P*F_6), 22.91 (d, $^1J_{RhP}$ = 112.4 Hz, *P*Ph_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 115.22 (d, $^2J_{FC}$ = 21.7 Hz, *C*$_6$H$_4$F), 122.72 (s), 123.47 (s), 124.83 (s), 126.57 (t, $^1J_{PC}$ = 23.7 Hz, *ipso*-P*Ph*$_3$), 127.57 (d, $^3J_{FC}$ = 7.4 Hz, *C*$_6$H$_4$F), 127.37 (s), 128.41 (s), 128.54 (s), 129.98 (t, J_{PC} = 4.9 Hz, P*Ph*$_3$), 131.57 (s, *p*-P*Ph*$_3$), 132.16 (s), 132.35 (s), 133.38 (t, J_{PC} = 5.4 Hz, P*Ph*$_3$), 134.43 (s), 134.96 (s), 136.62 (s), 137.17 (s), 145.82 (dt, $^1J_{RhC}$ = 41.3 Hz, $^2J_{PC}$ = 12.4 Hz, *C*Rh), 147.39 (dt, $^1J_{RhC}$ = 41.3 Hz, $^2J_{PC}$ = 12.4 Hz, Rh*C*H=CH), 148.43 (s), 148.87 (s). Anal. Calcd. For $C_{57}H_{44}F_7NP_3Rh$ (1071.78): C, 63.88; H, 4.14; N, 1.31. Found: C, 63.56; H, 3.95; N, 1.35.



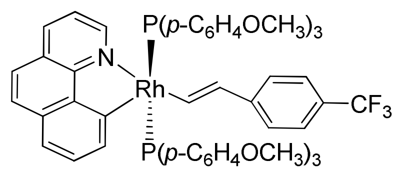
2ag

Yield: 102 mg (0.095 mmol, 95%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 2.22 (s, 3H, PhCH_3), 5.02 (d, $^{3}J_{CH=CH}$ = 16.6 Hz, 1H, CH=C$H$$C_6H_5$), 6.40 (d, ^{3}J = 7.2 Hz, 2H, CH$C_6$$H_4$$CH_3$), 6.89-7.65 [m, 37H, 30H (PPh_3) + 5H ($C_{13}$$H_8$N) + 2H ($C_6$$H_4$$CH_3$)], 7.92 (m, 1H), 8.01 (dt, $^{3}J_{CH=CH}$ = 17.1 Hz, $^{3}J_{PH}$ = 6.3 Hz, 1H, RhCH=CH), 8.68 (d, ^{3}J = 3.8 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.88 (m, $^{1}J_{FP}$ = 708.2 Hz, PF_6), 23.17 (d, $^{1}J_{RhP}$ = 113.1 Hz, PPh_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 20.86 (s, CH_3), 122.38 (s), 123.20 (s), 124.57 (s), 124.84 (s), 126.17 (t, $^{1}J_{PC}$ = 23.9 Hz, *ipso*-PPh_3), 127.08 (s), 128.69 (t, J_{PC} = 4.6 Hz, PPh_3), 128.87 (s), 131.30 (s, *p*-PPh_3), 131.53 (s), 132.47 (s), 133.00 (t, J_{PC} = 5.2 Hz, PPh_3), 134.12 (s), 135.27 (s), 135.56 (s), 136.28 (s), 136.40 (s), 144.97 (dt, $^{1}J_{RhC}$ = 42.1 Hz, $^{2}J_{PC}$ = 8.8 Hz, *C*Rh), 145.91 (dt, $^{1}J_{RhC}$ = 30.2 Hz, $^{2}J_{PC}$ = 10.3 Hz, Rh*C*H=CH), 147.84 (s), 148.50 (s). Anal. Calcd. For $C_{58}H_{47}F_6NP_3Rh$ (1067.82): C, 65.24; H, 4.44; N, 1.31. Found: C, 64.73; H, 4.27; N, 1.16.



2ah

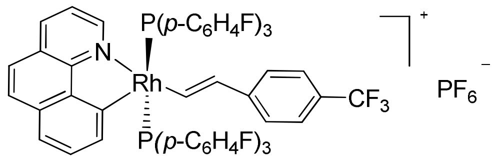
Yield: 102 mg (0.094 mmol, 94%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 3.74 (s, 3H, PhOCH_3), 5.02 (d, $^{3}J_{CH=CH}$ = 18.0 Hz, 1H, CH=C$H$$C_6H_4OCH_3$), 6.45 (d, ^{3}J = 8.4 Hz, 2H, CH$C_6$$H_4$$OCH_3$), 6.66 (d, ^{3}J = 8.4 Hz, 2H, CH$C_6$$H_4$$OCH_3$), 6.93 (d, 12H, P$Ph_3$), 7.17 (m, 12H, P$Ph_3$), 7.30-7.40 [m, 8H, 6H (PPh_3) + 2H ($C_{13}$$H_8$N)], 7.54 (s, 1H), 7.65-7.69 (m, 2H), 7.87 (dt, $^{3}J_{CH=CH}$ = 18.0 Hz, $^{3}J_{PH}$ = 6.0 Hz, 1H, RhCH=CH), 7.92 (d, ^{3}J = 7.7 Hz, 2H), 8.71 (d, ^{3}J = 5.1 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.88 (m, $^{1}J_{FP}$ = 707.5 Hz, PF_6), 23.09 (d, $^{1}J_{RhP}$ = 114.0 Hz, PPh_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 55.55 (s, OCH_3), 113.66 (s), 122.71 (s), 123.49 (s), 124.89 (s), 125.11 (s), 126.32 (s), 126.57 (t, $^{1}J_{PC}$ = 23.8 Hz, *ipso*-PPh_3), 127.41 (s), 128.27 (s), 128.40 (s), 129.00 (t, J_{PC} = 4.9 Hz, PPh_3), 131.49 (s), 131.61 (s, *p*-PPh_3), 131.97 (s), 132.34 (*s*), 133.36 (t, J_{PC} = 5.5 Hz, PPh_3), 134.45 (s), 136.60 (s), 136.84 (s), 144.48 (dt, $^{1}J_{RhC}$ = 30.6 Hz, $^{2}J_{PC}$ = 10.7 Hz, Rh*C*H=CH), 145.46 (dt, $^{1}J_{RhC}$ = 42.1 Hz, $^{2}J_{PC}$ = 9.5 Hz, *C*Rh), 148.23 (s), 148.85 (s). Anal. Calcd. For $C_{58}H_{47}F_6NOP_3Rh\bullet CH_2Cl_2$ (1168.75): C, 60.63; H, 4.23; N, 1.20. Found: C, 60.20; H, 4.17; N, 1.21.



2bb

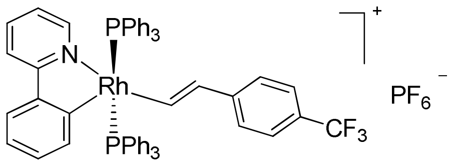
Yield: 110 mg (0.084 mmol, 84%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 3.56 (s, 18H, OCH_3), 5.36 (d, $^{3}J_{CH=CH}$ = 16.8 Hz, 1H, CH=C$H$$C_6H_4CF_3$), 6.64 (d, 12H, P$C_6$$H_4$$OCH_3$), 6.72-6.79 [m, 14H, 12 (P$C_6$$H_4$$OCH_3$) + 2H ($C_6$$H_4$$CF_3$)], 7.39-7.45 [m, 4H, 2H ($C_{13}$$H_8$N) + 2H ($C_6$$H_4$$CF_3$)], 7.56 (t, ^{3}J = 7.7 Hz, 1H), 7.69 (m, 2H), 7.93 (d, ^{3}J = 7.6 Hz, 1H), 8.00 (d, ^{3}J = 7.9 Hz, 1H), 8.44 (dt, 1H, $^{3}J_{CH=CH}$ = 17.1 Hz, $^{3}J_{PH}$ = 5.6 Hz, RhCH=CH), 8.71 (d, ^{3}J = 4.7 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.88 (m, $^{1}J_{FP}$ = 708.9 Hz, PF_6), 21.03 (d, $^{1}J_{RhP}$ = 110.4 Hz, PPh_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2Cl_2, 255 K): -72.99 (d, $^{1}J_{PF}$ = 710.3 Hz, 6F, PF_6), -62.18 (s, CF_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 55.56 (s, OCH_3), 114.14 (t, J_{PC} = 5.3 Hz, PPh_3), 117.30 (t, $^{1}J_{PC}$ = 26.5 Hz, *ipso*-P$C_6H_4OCH_3$), 122.56 (s), 122.99 (s), 124.30 (s), 124.61 (q, $^{1}J_{FC}$ =

269.6 Hz, *C*F_3), 124.96 (s), 125.11 (q, $^3J_{FC}$ = 3.8 Hz, $C_6H_4CF_3$), 126.55 (q, $^2J_{FC}$ = 31.7 Hz, $C_6H_4CF_3$), 127.05 (s), 128.50 (s), 128.77 (s), 131.06 (s), 131.33 (s), 134.12 (s), 134.36 (t, J_{PC} = 6.1 Hz, P$C_6H_4OCH_3$), 136.01 (s), 136.71 (s), 141.51 (s), 145.91 (dt, $^1J_{RhC}$ = 43.1 Hz, $^2J_{PC}$ = 9.5 Hz, *C*Rh), 147.98 (s), 148.77 (s), 155.87 (dt, $^1J_{RhC}$ = 32.4 Hz, $^2J_{PC}$ = 11.1 Hz, Rh*C*H=CH), 161.56 (s, *p*-P$C_6H_4OCH_3$). Anal. Calcd. For $C_{64}H_{56}F_9NO_6P_3Rh$ (1301.95): C, 59.04; H, 4.34; N, 1.08. Found: C, 58.80; H, 3.66; N, 1.44.



2cb

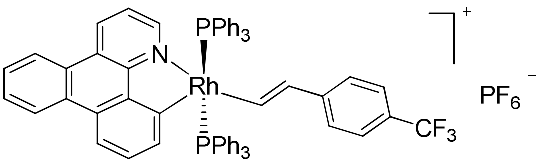
Yield: 113 mg (0.092 mmol, 92%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.20 (d, 1H, $^3J_{CH=CH}$ = 17.1 Hz, CH=C*H*$C_6H_4CF_3$), 6.89-6.91 [m, 25H, 24H (PC_6H_4F) + 1H ($C_{13}H_8N$)], 6.47-7.64 [m, 5H, 2H ($C_6H_4CF_3$) + 3H ($C_{13}H_8N$)], 7.72-7.79 [m, 3H, 1 H ($C_{13}H_8N$) + 2H ($C_6H_4CF_3$)], 8.04 (d, ^3J = 7.9 Hz, 1H), 8.33 (dt, 1H, $^3J_{CH=CH}$ = 17.0 Hz, $^3J_{PH}$ = 5.1 Hz, RhC*H*=CH), 9.04 (d, ^3J = 4.9 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.65 (m, $^1J_{FP}$ = 709.1 Hz, *P*F_6), 22.58 (d, $^1J_{RhP}$ = 113.2 Hz, *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2Cl_2, 255 K): -106.93 (s, Ph*F*), -72.44 (d, 6F, $^1J_{PF}$ = 710.3 Hz, PF_6), -62.54 (s, CF_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 116.57 (dt, $^2J_{F\text{-}C}$ = 21.4 Hz, $^3J_{P\text{-}C}$ = 5.2 Hz, PC_6H_4F), 121.94 (td, $^1J_{PC}$ = 25.1 Hz, $^4J_{FC}$ = 3.1 Hz, *ipso*-PC_6H_4F), 123.65 (s), 124.00 (s), 124.82 (q, $^1J_{FC}$ = 269.8 Hz, *C*F_3), 124.96 (s), 125.20 (s), 125.83 (q, $^3J_{FC}$ = 3.8 Hz, $C_6H_4CF_3$), 127.27 (s), 127.51(q, $^2J_{FC}$ = 36.5 Hz, $C_6H_4CF_3$), 129.10 (s), 129.27 (s), 132.33 (s), 132.73 (s), 134.47 (s), 135.60 (dt, $^3J_{FC}$ = 8.2 Hz, $^2J_{PC}$ = 6.5 Hz, PC_6H_4F), 136.70 (s), 137.32 (s), 140.91 (s), 145.25 (dt, $^1J_{RhC}$ = 41.9 Hz, $^2J_{PC}$ = 11.0 Hz, *C*Rh), 148.16 (s), 149.84 (s), 151.60 (dt, $^1J_{RhC}$ = 31.7 Hz, $^2J_{PC}$ = 12.8 Hz, Rh*C*H=CH), 164.58 (d, $^1J_{CF}$ = 252. 7 Hz, P*C*6H4F). Anal. Calcd. For $C_{58}H_{38}F_{15}NP_3Rh$ (1229.73): C, 56.65; H, 3.11; N, 1.14. Found: C, 57.02; H, 3.29; N, 1.08.



2db

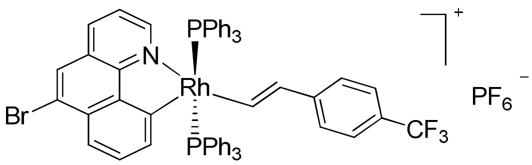
Yield: 98 mg (0.089 mmol, 89%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.07 (d, 1H, $^3J_{CH=CH}$ = 17.2 Hz, CH=C*H*$C_6H_4CF_3$), 6.50 (d, ^3J = 7.8 Hz, 2H, $C_6H_4CF_3$), 6.99-7.03 [m, 13H, 12H (PPh_3) + 1H ($C_{11}H_8N$)], 7.13-7.17 (m, 3H), 7.26-7.37 [m, 15H, 12H (PPh_3) + 3H ($C_{11}H_8N$)], 7.44-7.53 [m, 7H, 6H (PPh_3) +1H ($C_{11}H_8N$)], 7.60 (m, 1H), 8.03 [dt, $^3J_{CH=CH}$ = 17.2 Hz, $^2J_{PH}$ = 5.4 Hz, 1H, RhC*H*=CH), 8.34 (d, $^2J_{PH}$ = 5.0 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.96 (m, $^1J_{FP}$ = 708.8 Hz, *P*F_6), 23.68 (d, $^1J_{RhP}$ = 112.9 Hz, *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2Cl_2, 255 K): -72.95 (d, $^1J_{PF}$ = 710.4 Hz, 6F, PF_6), -62.12 (s, 3F, CF_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 120.33 (s), 123.35 (s), 124.53 (q, $^1J_{FC}$ = 269.7 Hz, *C*F_3), 124.91 (s), 125.00 (s), 125.08 (q, $^3J_{FC}$ = 3.6 Hz, $C_6H_4CF_3$), 125.33 (s), 126.13 (t, $^1J_{PC}$ = 23.9 Hz, *ipso*-PPh_3), 126.59 (q, $^2J_{FC}$ = 31.5 Hz, $C_6H_4CF_3$), 129.07 (t, J_{PC} = 4.8 Hz, PPh_3), 130.19(s), 131.51 (s, *p*-PPh_3), 132.35 (s), 133.28 (t, J_{PC} = 5.3 Hz, PPh_3), 134.49 (s), 138.21 (s), 141.25 (s), 141.35 (s), 148.92 (s), 149.20 (dt, $^1J_{RhC}$ = 40.7 Hz, $^2J_{PC}$ = 8.7 Hz, *C*Rh), 149.85 (s), 154.22 (dt, $^1J_{RhC}$ = 31.1 Hz, $^2J_{PC}$ = 10.5 Hz, Rh*C*H=CH). Anal. Calcd. For $C_{56}H_{44}F_9NP_3Rh{\bullet}CH_2Cl_2$ (1182.70): C, 57.89; H, 3.92; N, 1.18.

Found: C, 58.28; H, 3.94; N, 1.37.



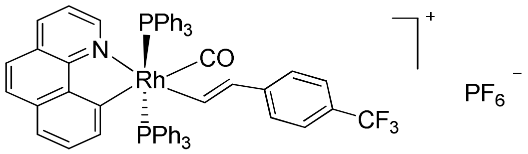
2eb

Yield: 103 mg (0.088 mmol, 88%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 295 K): 5.17 (d, $^{3}J_{CH=CH}$ = 16.8 Hz, 1H, CH=C*H*C_6*H*$_4CF_3$), 6.62 (d, ^{3}J = 7.9 Hz, 2H, C_6*H*$_4CF_3$), 6.95 (m, 12H, P*Ph*$_3$), 7.13 [m, 13H, 12H (P*Ph*$_3$) + 1H (C_{17}*H*$_{10}$N)], 7.37-7.29 [7H, 6H (P*Ph*$_3$) + 1H (C_{17}*H*$_{10}$N)], 7.54 (t, ^{3}J = 8.9 Hz, 1H), 7.84-7.73 (m, 3H), 8.38-8.22 (m, 3H), 8.67-8.54 (m, 3H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_3CN, 295K): -143.69 (m, $^{1}J_{FP}$ = 707.6 Hz, *P*F_6), 23.66 (d, $^{1}J_{RhP}$ = 112.4 Hz, *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_3CN, 255 K): -72.76 (d, 6F, $^{1}J_{PF}$ = 710.6 Hz, P*F*$_6$), -62.06 (s, 3F, C*F*$_3$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 118.70 (s), 122.87 (s), 123.40 (s), 123.92 (s), 124.57 (q, $^{1}J_{FC}$ = 269.3 Hz, *C*F_3), 124.95 (s), 125.19 (q, $^{3}J_{FC}$ = 3.0 Hz, *C*$_6H_4CF_3$), 125.93 (t, $^{1}J_{PC}$ = 24.0 Hz, *ipso*-P*Ph*$_3$), 126.61 (q, $^{2}J_{FC}$ = 33.0 Hz, *C*$_6H_4CF_3$), 127.29 (s), 128.28 (s), 128.79 (t, J_{PC} = 4.6 Hz, P*Ph*$_3$), 129.12 (s), 129.58 (s), 131.38 (s, *p*-P*Ph*$_3$), 131.73 (s), 131.94 (s), 132.32 (s), 132.63 (s), 133.09 (t, J_{PC} = 5.4 Hz, P*Ph*$_3$), 135.56 (s), 141.24 (s), 147.26 (dt, $^{1}J_{RhC}$ = 39.3 Hz, $^{2}J_{PC}$ = 9.3 Hz, *C*Rh), 148.38 (s), 148.60 (s), 153.76 (dt, $^{1}J_{RhC}$ = 30.5 Hz, $^{2}J_{PC}$ = 11.4 Hz, Rh*C*H=CH). Anal. Calcd. For $C_{62}H_{46}F_9NP_3Rh$ (1171.85): C, 63.55; H, 3.96; N, 1.20. Found: C, 63.15; H, 4.32; N, 1.35.



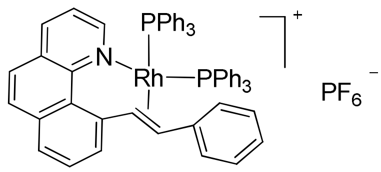
2fb

Yield: 100 mg (0.083 mmol, 83%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 255 K): 5.18 (d, $^{3}J_{CH=CH}$ = 17.1 Hz, 1H, CH=C*H*$C_6H_4CF_3$), 6.62 (d, ^{3}J = 7.1 Hz, 2H, C_6*H*$_4CF_3$), 6.85 [m, 14 H 12H (P*Ph*$_3$) + 1 H (C_{13}*H*$_7$N)], 7.11-7.16 [m, 13H, 12H (P*Ph*$_3$) + 1H (C_{13}*H*$_7$N)], 7.32-7.37 [m, 8H, 6H (P*Ph*$_3$) + 2H (C_{13}*H*$_7$N)], 7.60 (t, ^{3}J = 7.1 Hz, 1H), 7.71 (s, 1H), 7.76 (d, ^{3}J = 10.3 Hz, 1H), 7.90 (t, ^{3}J = 10.3 Hz, 1H), 8.27 (dt, $^{3}J_{CH=CH}$ = 16.1 Hz, $^{3}J_{PH}$ = 6.1 Hz, 1H, RhC*H*=CH), 8.54 (d, ^{3}J = 4.5 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 255 K): -143.84 (m, $^{1}J_{FP}$ = 708.0 Hz, *P*F_6), 23.11 (d, $^{1}J_{RhP}$ = 110.7 Hz, *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2Cl_2, 255 K): -72.79 (d, $^{1}J_{PF}$ = 710.4 Hz, 6F, P*F*$_6$), -62.22 (s, C*F*$_3$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 123.07 (s), 124.54 (q, $^{1}J_{FC}$ = 268.5 Hz, *C*F_3), 124.97 (s), 125.19 (q, $^{3}J_{FC}$ = 2.3 Hz, *C*$_6H_4CF_3$), 125.83 (t, $^{1}J_{PC}$ = 24.8 Hz, *ipso*-P*Ph*$_3$), 126.68 (q, $^{2}J_{FC}$ = 30.0 Hz, *C*$_6H_4CF_3$), 126.73 (s), 127.59 (s), 128.26 (s), 128.79 (t, J_{PC} = 5.3 Hz, P*Ph*$_3$), 129.21 (s), 131.43 (s, p-P*Ph*$_3$), 131.97 (s), 132.55 (s), 132.97 (t, J_{PC} = 6.8 Hz, P*Ph*$_3$), 135.49 (s), 136.98 (s), 141.08 (s), 145.65 (dt, $^{1}J_{RhC}$ = 41.3 Hz, $^{2}J_{PC}$ = 9.8 Hz, *C*Rh), 147.41 (s), 149.18 (s), 152.61 (dt, $^{1}J_{RhC}$ = 32.3 Hz, $^{2}J_{PC}$ = 9.0 Hz, Rh*C*H=CH). Anal. Calcd. For $C_{58}H_{43}BrF_9NP_3Rh$ (1200.69): C, 58.02; H, 3.61; N, 1.17. Found: C, 58.45; H, 3.84; N, 1.30.



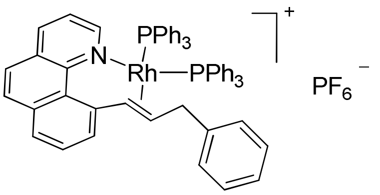
4

To the solution of the five coordinate intermediate in CD_2Cl_2 in NMR tube was bubbled CO at 0 °C for 15 min, during which time the color of the solution turn from orange to yellow, and then obtained the six coordinate complexes. Yield: 103 mg (0.09 mmol, 90%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 6.47 (d, 1H, $^3J_{CH=CH}$ = 16.3 Hz, CH=C*H*$C_6H_4CF_3$), 6.82-6.86 (m, 12H, P*Ph*$_3$), 7.02-7.11 [m, 14H, 12H (P*Ph*$_3$) + 2H ($C_6H_4CF_3$)], 7.25-7.33 [m, 8H, 6H (P*Ph*$_3$) + 2H ($C_{13}H_8N$)], 7.41-7.49 [m, 2H, 1H ($C_{13}H_8N$) + 1H (C*H*=CH$C_6H_4CF_3$)], 7.55-7.58 [m, 3H, 1H ($C_{13}H_8N$) + 2H ($C_6H_4CF_3$)], 7.73 (d, ^3J = 8.8 Hz, 1H), 7.78 (d, ^3J = 7.6 Hz, 1H), 7.95 (d, ^3J = 7.9 Hz, 1H), 9.01 (d, ^3J = 4.9 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -144.27 (m, $^1J_{FP}$ = 709.8 Hz, *P*F_6), 19.00 (d, $^1J_{RhP}$ = 99.2 Hz, *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2Cl_2, 295 K): -73.18 (d, $^1J_{PF}$ = 709.7 Hz, 6F, P*F*$_6$), -62.50 (s, C*F*$_3$); ^{13}C {^{1}H} NMR (δ, 100 MHz, CD_2Cl_2, 295 K): 123.13 (s), 124.34 (s), 124.61 (s), 125.17 (s), 125.56 (q, $^3J_{CF}$ = 3.9 Hz, *C*$_6H_4CF_3$), 126.32 (s), 127.75 (s), 127.80 (t, $^1J_{P\text{-}C}$ = 25.2 Hz, *ipso*-P*Ph*$_3$), 127.86 (s), 128.05 (t, $^4J_{P\text{-}C}$ = 3.0 Hz, P*Ph*$_3$), 129.42 (s), 129.49 (s), 131.04 (s, *p*-P*Ph*$_3$), 133.45 (t, J_{PC} = 5.0Hz, P*Ph*$_3$), 134.63 (s), 135.60 (s), 137.08 (s), 140.90 (s), 141.76 (s), 142.00 (s), 142.24 (dt, $^1J_{RhC}$ = 25.9 Hz, $^2J_{PC}$ = 9.3 Hz, Rh*C*H=CH), 150.77 (s), 151.71 (s), 159.01 (dt, $^1J_{RhC}$ = 22.2 Hz, $^2J_{PC}$ = 11.1 Hz, *C*Rh), 188.90 (dt, $^1J_{RhC}$ = 44.4 Hz, $^2J_{PC}$ = 9.2 Hz, Rh*C*O). Anal. Calcd. For $C_{59}H_{44}F_9NOP_3Rh$ (1149.80): C, 61.63; H, 3.86; N, 1.22. Found: C, 61.40; H, 3.49; N, 1.96.



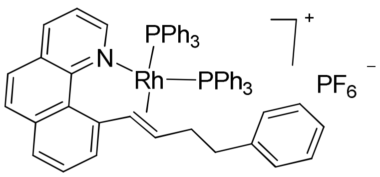
3aa

To a solution of the Rhodium hydride complexes (0.1 mmol) in dichloromethane (3 ml) was dropped terminal alkynes (0.2 mmol) and then the solution was stirred for 5 h at 0 °C. Then the solvent was removed under reduced pressure at room temperature and the residue was transferred into the glove box and washed with diethyl ether 3 × 6 ml to give a red powder. Yield: 96 mg (0.091 mmol, 91%). ^{1}H NMR (δ, 500 MHz, CD_2Cl_2, 295 K): 5.50 (dd, $^3J_{CH=CH}$ = 13.8 Hz, $^3J_{RhH}$ = 6.7 Hz, 1H, CH=C*H*-Ph), 6.48 (dd, $^3J_{CH=CH}$ = 14.0 Hz, $^3J_{RhH}$ = 2.9 Hz, 1H, C*H*=CH-Ph), 6.61 (d, ^3J = 7.2 Hz, 2H, CH-C_6H_5), 6.77 (m, 2H), 6.83 (t, ^3J = 7.0 Hz, 1H), 6.94 (m, 6H, P*Ph*$_3$), 7.01 (t, ^3J = 7.9 Hz, 6H, P*Ph*$_3$), 7.15-7.17 [m, 10H, 9H (P*Ph*$_3$) + 1H ($C_{13}H_8N$)], 7.25 (t, ^3J = 8.5 Hz, 6H, P*Ph*$_3$), 7.35 [m, 4H, 3H (P*Ph*$_3$) + 1H ($C_{13}H_8N$)], 7.60 (dd, ^3J = 7.9 Hz, ^3J = 5.4 Hz, 1H), 7.79 (d, ^3J = 8.6 Hz, 1H), 7.96 (t, ^3J = 7.3 Hz, 1H), 8.01 (m, 2H), 8.17 (d, ^3J = 7.0 Hz, 1H), 9.48 (m, 1H); ^{31}P {^{1}H} NMR (δ, 202 MHz, CD_2Cl_2, 298 K): -144.35 (m, $^1J_{FP}$ = 708.4 Hz, *P*F_6), 30.95 (dd, $^1J_{RhP}$ = 169.4 Hz, $^2J_{PP}$ = 44.5 Hz, *P*Ph_3), 36.21 (dd, $^1J_{RhP}$ = 155.6 Hz, $^2J_{PP}$ = 43.0 Hz, *P*Ph_3); ^{13}C {^{1}H} NMR (δ, 125 MHz, CD_2Cl_2, 295 K): 78.62 (dd, $^1J_{RhC}$ = 19.9 Hz, $^2J_{PC}$ = 6.2 Hz, CH=*C*H-Ph), 85.00 (d, $^1J_{RhC}$ = 12.1 Hz, *C*H=CH-Ph), 123.75 (s), 124.93 (s), 126.29 (s), 126.34 (s), 127.93 (s), 127.98 (d, J_{PC} = 10.1 Hz, P*Ph*$_3$), 128.05 (d, J_{PC} = 9.8 Hz, P*Ph*$_3$), 128.30 (s), 129.10 (s), 129.7 (s), 130.08 (s), 130.29 (s, *p*-P*Ph*$_3$), 130.62 (d, $^1J_{PC}$ = 45.8 Hz, *ipso*-P*Ph*$_3$), 130.81 (s), 130.86 (d, $^1J_{PC}$ = 41.4 Hz, *ipso*-P*Ph*$_3$), 132.84 (d, J_{PC} = 12.2 Hz, P*Ph*$_3$), 134.72 (d, J_{PC} = 10.4 Hz, P*Ph*$_3$), 136.37 (s), 136.67 (s), 137.64 (s), 137.74 (s), 143.22 (s), 147.83 (s). Anal. Calcd. For $C_{57}H_{45}F_6NP_3Rh•1.5CH_2Cl_2$ (1181.19): C, 59.48; H, 4.10; N, 1.19. Found: C, 59.11; H, 4.02; N, 1.23.



3aj

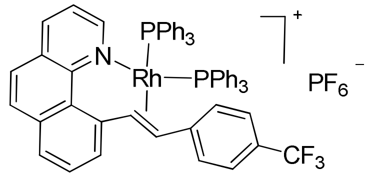
Complex was synthesized by following the procedure of the above method. Yield: 98 mg (0.092 mmol, 92%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 2.10-2.17 (t, ^3J = 10.9 Hz, 1H, CH_2), 3.24 (dt, ^3J = 13.8 Hz, ^2J =3.9 Hz, 1H, CH_2), 4.15-4.23 (m, 1H, CH=C*H*-CH$_2$-Ph), 5.82 (dd, ^3J = 13.2 Hz, $^3J_{PH}$ = 4.4 Hz, 1H, C*H*=CH-CH$_2$Ph), 6.42 (d, ^3J = 7.7 Hz, 2H, C_6H_5), 6.90-7.02 [m, 15H, 12H (P*Ph*$_3$) + 2H (C_6H_5) + 1H ($C_{13}H_8N$)], 7.17 (m, 3H, P*Ph*$_3$), 7.26-7.33 [m, 7H, 6H (P*Ph*$_3$) + 1H ($C_{13}H_8N$)], 7.43-7.46 [m, 4H, 3H (P*Ph*$_3$) + 1H ($C_{13}H_8N$)], 7.50 (dd, ^3J = 8.2 Hz, ^3J = 5. 2Hz, 1H, $C_{13}H_8N$), 7.60 (m, 6H, P*Ph*$_3$), 7.69 (d, ^3J = 8.8 Hz, 1H), 7.84-7.94 (m, 4H, $C_{13}H_8N$), 9.35 (m, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -143.75 (m, $^1J_{FP}$ = 707.7 Hz, *P*F$_6$), 29.32 (dd, $^1J_{RhP}$ = 160.9 Hz, $^2J_{PP}$ = 41.4 Hz, *P*Ph$_3$), 36.98 (dd, $^1J_{RhP}$ = 155.9 Hz, $^2J_{PP}$ = 41.9 Hz, *P*Ph$_3$); ^{13}C {^{1}H} NMR (δ, 100 MHz, CD_2Cl_2, 295 K): 40.27 (s, *C*H$_2$), 76.10 (dd, $^1J_{RhC}$ = 22.7 Hz, $^2J_{PC}$ = 7.5 Hz, CH=*C*H-CH$_2$Ph), 91.99 (d, $^1J_{RhC}$ = 12.0 Hz, CH=*C*H-CH$_2$Ph), 123.75 (s), 125.08 (s), 126.32 (s), 126.41 (s), 128.09 (s), 128.41 (d, J_{PC} = 10.2 Hz, P*Ph*$_3$), 128.66 (s, CH$_2$*C*$_6$H$_5$), 128.93 (d, J = 9.8 Hz, P*Ph*$_3$), 129.38 (s), 129.92 (s), 131.02 (s), 130.45 (s), 131.16 (d, $^4J_{PC}$ = 2.0 Hz, *p*-P*Ph*$_3$), 131.29 (d, $^1J_{PC}$ = 40.2 Hz, *ipso*-P*Ph*$_3$), 131.78 (dd, $^1J_{PC}$ = 45.0 Hz, $^2J_{RhC}$ = 2.0 Hz, P*Ph*$_3$), 133.25 (d, J_{PC} = 12.4 Hz, P*Ph*$_3$), 135.08 (d, J_{PC} = 10.4 Hz, P*Ph*$_3$), 136.97 (s), 137.21 (s), 137.89 (s), 141.42 (s), 143.32 (s), 148.11 (s). Anal. Calcd. For $C_{58}H_{47}F_6NP_3Rh$ (1067.82): C, 65.24; H, 4.44; N, 1.31. Found: C, 65.07; H, 4.42; N, 1.52.



3ak

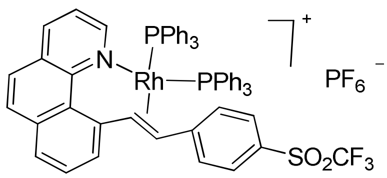
Complex was synthesized by following the procedure of the above method. Yield: 95 mg (0.089 mmol, 89%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 295 K): 1.01-1.17 (m, 1H, C*H*$_2$CH$_2$Ph), 1.90-2.00 (m, 1H, C*H*$_2$CH$_2$Ph), 2.35-2.43 (m, 2H, CH$_2$C*H*$_2$Ph), 3.89-3.99 (m, 1H, CH=C*H*-CH$_2$CH$_2$Ph), 5.21 (dd, $^3J_{CH=CH}$ = 13.2 Hz, $^2J_{RhH}$ = 4.8 Hz, 1H, C*H*=CH-CH$_2$-Ph), 6.19 (d, ^3J = 7.2 Hz, 2H, CH$_2$-C$_6$*H*$_5$), 6.81-7.03 [m, 15H, 12H (P*Ph*$_3$) + 3H ($C_{13}H_8N$)], 7.11-7.16 (m, 3H, P*Ph*$_3$), 7.24-7.35 [m, 8H, 6H (P*Ph*$_3$) + 2H ($C_{13}H_8N$)], 7.41-7.54 [m, 10H, 6H (P*Ph*$_3$) + 3H (P*Ph*$_3$) + 1H ($C_{13}H_8N$)], 7.70-7.75 (m, 2H, $C_{13}H_8N$), 7. 90 (d, ^3J = 7.7 Hz, 1H), 7.97 (d, ^3J = 7.9 Hz, 1H), 9.30-9.32 (m, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 295 K): -143.36 (m, $^1J_{FP}$ = 710.3 Hz, *P*F$_6$), 28.87 (dd, $^1J_{RhP}$ = 161.5 Hz, $^2J_{PP}$ = 41.4 Hz, *P*Ph$_3$), 39.22 (dd, $^1J_{RhP}$ = 156.3 Hz, $^2J_{PP}$ = 41.4 Hz, *P*Ph$_3$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 295 K): 35.92 (s, CH$_2$*C*H$_2$Ph), 37.42 (d, $^2J_{RhC}$ = 6.0 Hz, *C*H$_2$CH$_2$Ph), 75.65 (dd, $^1J_{RhC}$ = 22.8 Hz, $^2J_{PC}$ = 7.5 Hz, CH=*C*H-CH$_2$CH$_2$Ph), 93.30 (d, $^1J_{RhC}$ = 12.1 Hz, CH=*C*H-CH$_2$Ph), 123.62 (s), 124.83 (s), 125.81 (s), 126.47 (s), 126.77 (s), 127.98 (s), 128.33 (d, J_{PC} = 10.0 Hz, P*Ph*$_3$), 128.47 (s, CH_2-*C*$_6H_5$), 128.85 (d, J_{PC} = 9.8 Hz, P*Ph*$_3$), 129.08 (s), 129.37 (s), 130.00 (s), 130.33 (d, J_{PC} = 2.2 Hz, p-P*Ph*$_3$), 130.87 (s), 131.00 (d, J_{PC} = 2.2 Hz, *p*-P*Ph*$_3$), 131.50 (d, $^1J_{PC}$ = 40.2 Hz, *ipso*-P*Ph*$_3$), 131.78 (dd, $^1J_{PC}$ = 45.1 Hz, *ipso*-P*Ph*$_3$), 132.71 (d, J_{PC} = 12.4 Hz, P*Ph*$_3$), 135.09 (d, J_{PC} = 10.4 Hz, P*Ph*$_3$), 136.74 (s), 137.19 (s), 137.80 (s), 140.66 (s), 143.29 (s), 147.95 (s). Anal. Calcd. For $C_{59}H_{49}F_6NP_3Rh$ (1081.84): C, 65.50; H, 4.57; N, 1.29. Found: C, 65.05; H, 4.37; N, 1.56.

The following C-C coupling products were obtained by slowly converting from five coordinate intermediate at room temperature for several hours.



3ab

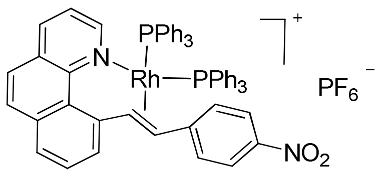
Yield: 94 mg (0.084 mmol, 93%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 5.32 (dd, $^3J_{CH=CH}$ = 13.5 Hz, $^2J_{Rh\text{-}H}$ = 6.9 Hz, 1H, CH=C*H*–$C_6H_4CF_3$), 6.46 (dd, $^3J_{CH=CH}$ = 13.5 Hz, $^2J_{Rh\text{-}H}$ = 4.8 Hz, 1H, CH=C*H*–$C_6H_4CF_3$), 6.72 (d, ^3J = 6.0 Hz, 2H, C_6*H*$_4CF_3$), 6.91-7.00 [m, 14H, 12H (P*Ph*$_3$) + 2H (C_{13}*H*$_8$N)], 7.14-7.26 [m, 15H, 12H (P*Ph*$_3$) + 3H (P*Ph*$_3$)], 7.32-7.38 [m, 4H, 3H (P*Ph*$_3$) +1H (C_{13}*H*$_8$N)], 7.67 (dd, ^3J = 8.0 Hz, ^3J = 5.2 Hz, 1H), 7.77 (d, ^3J = 8.8 Hz, 1H), 7.95 (t, ^3J = 7.2 Hz, 1H), 8.01-8.04 (m, 2H), 8.20 (d, ^3J = 6.8 Hz, 1H), 9.53 (m, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -143.53 (m, $^1J_{F\text{-}P}$ = 707.6 Hz, *P*F_6), 31.07 (dd, $^1J_{Rh\text{-}P}$ = 166.8 Hz, $^2J_{P\text{-}P}$ = 43.0 Hz, *P*Ph_3), 35.81 (dd, $^1J_{Rh\text{-}P}$ = 153.7 Hz, $^2J_{P\text{-}P}$ = 42.8 Hz, *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2CL_2, 295 K): -72.73 (d, $^1J_{PF}$ = 710.6 Hz, P*F*$_6$), 62.27 (s, C*F*$_3$); ^{13}C {^{1}H} NMR (δ, 100 MHz, CD_2Cl_2, 295 K): 74.05 (dd, $^1J_{Rh\text{-}C}$ = 21.8 Hz, $^2J_{P\text{-}C}$ = 6.3 Hz, CH=*C*H-$C_6H_4CF_3$), 84.05 (d, $^1J_{Rh\text{-}C}$ = 12.6 Hz, *C*H=CH-$C_6H_4CF_3$), 124.42 (s), 124.60 (q, $^1J_{F\text{-}C}$ = 270.1 Hz, *C*F_3), 125.14 (s), 125.38 (q, $^3J_{F\text{-}C}$ = 3.6 Hz, *C*$_6H_4CF_3$), 126.87 (s), 126.92 (s), 127.53 (q, $^2J_{F\text{-}C}$ = 33.1 Hz, *C*$_6H_4CF_3$), 128.31 (s), 128.48 (d, $J_{P\text{-}C}$ = 10.4 Hz, P*Ph*$_3$), 128.59 (d, $J_{P\text{-}C}$ = 10.1 Hz, P*Ph*$_3$), 128.68 (s), 129.63 (s), 130.05 (s), 130.66 (d, $^1J_{P\text{-}C}$ = 46.1 Hz, *ipso*-P*Ph*$_3$), 130.57 (d, $^4J_{P\text{-}C}$ = 2.1 Hz, *p*-P*Ph*$_3$), 130.89 (d, $^4J_{P\text{-}C}$ = 1.9 Hz, *p*-P*Ph*$_3$), 131.00 (d, $^1J_{P\text{-}C}$ = 42.6 Hz, *ipso*-P*Ph*$_3$), 133.22 (d, $J_{P\text{-}C}$ = 12.10 Hz, P*Ph*$_3$), 134.99 (d, $J_{P\text{-}C}$ = 10.4 Hz, P*Ph*$_3$), 136.60 (s), 137.11 (s), 138.22 (s), 142.84 (s), 143.23 (s), 148.28 (s). Anal. Calcd. For $C_{58}H_{44}F_9NP_3Rh$ (1121.79): C, 62.10; H, 3.95, N, 1.25. Found: C, 61.94; H, 4.30; N, 1.15.



3ac

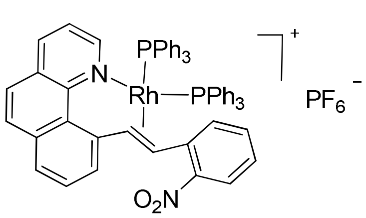
Yield: 108 mg (0.088 mmol, 96%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 295 K): 5.26 (dd, $^3J_{CH=CH}$ = 13.5 Hz, $^2J_{RhH}$ = 7.5 Hz, 1H, CH=C*H*$C_6H_4SO_2CF_3$), 6.48 (dd, $^3J_{CH=CH}$ = 13.5 Hz, $^2J_{RhH}$ = 4.5 Hz, 1H, *C*H=C*H*$C_6H_4SO_2CF_3$), 6.78-6.80 (m, 2H, CH-C_6*H*$_4SO_2CF_3$), 6.94-6.97 (m, 12H, P*Ph*$_3$), 7.20-7.40 [m, 21 H, 12H (P*Ph*$_3$) + 6H (P*Ph*$_3$) + 2H ($C_6H_4SO_2CF_3$) + 1H (C_{13}*H*$_8$N)], 7.74-7.80 (m, 2H), 7.97 (t, ^3J = 7.5 Hz, 1H), 8.07 (m, 2H), 8.26 (d, ^3J = 6.9 Hz, 1H), 9.59 (m, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 295 K): -143.56 (m, $^1J_{FP}$ = 708.7 Hz, *P*F_6), 31.71 (dd, $^1J_{RhP}$ = 167.1

Hz, $^{2}J_{PP}$ = 43.1 Hz, *P*Ph$_3$), 34.43 (dd, $^{1}J_{RhP}$ = 153.1 Hz, $^{2}J_{PP}$ = 43.0 Hz, *P*Ph$_3$); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2CL_2, 295 K): -79.23 (s, SO_2CF_3), -72.92 (d, $^{1}J_{PF}$ = 710.1 Hz, P*F*$_6$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 298 K): 69.90 (dd, $^{1}J_{RhC}$ = 23.2 Hz, $^{2}J_{PC}$ = 6.8 Hz, CH=*C*H-PhSO$_2$CF$_3$), 82.03 (d, $^{1}J_{RhC}$ = 13.3 Hz, *C*H=CH-PhSO$_2$CF$_3$), 119.50 (q, $^{1}J_{FC}$ = 323.85 Hz, *C*F$_3$), 124.30 (s), 124.62 (s), 126.16 (s), 126.56 (s), 126.73 (s), 128.16 (d, J_{PC} = 10.3 Hz, P*Ph*$_3$), 128.34 (d, J_{PC} = 9.9 Hz, P*Ph*$_3$), 128.53 (s), 128.63 (s), 129.42 (s), 129.58 (dd, $^{1}J_{PC}$ = 46.1 Hz, $^{3}J_{RhC}$ = 2.6 Hz, *ipso*-P*Ph*$_3$), 129.42 (s), 129.68 (s), 130.28 (d, $^{1}J_{PC}$ = 42.5Hz, *ipso*-P*Ph*$_3$), 130.34 (d, $^{4}J_{PC}$ = 2.2 Hz, *p*-P*Ph*$_3$), 130.43 (s), 130.87 (s, *p*-P*Ph*$_3$), 132.75 (d, J_{PC} = 12.0 Hz, P*Ph*$_3$), 134.65 (d, J_{PC} = 10.4 Hz, P*Ph*$_3$), 136.05 (s), 136.79 (s), 138.03 (s), 142.47 (s), 147.69 (s), 148.59 (s). Anal. Calcd. For $C_{58}H_{44}F_9NO_2P_3RhS{\bullet}0.5CH_2Cl_2$ (1228.32): C, 57.20; H, 3.69; N, 1.18; S, 2.61. Found: C, 57.15; H, 3.53; N, 1.40; S, 2.38.



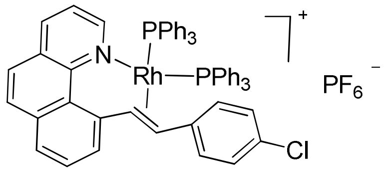
3ad

Yield: 102 mg (0.090 mmol, 95%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 295 K): 5.29 (dd, $^{3}J_{CH=CH}$ = 13.5 Hz, $^{2}J_{RhH}$ = 7.2 Hz, 1H, CH=C*H*-C$_6$*H*$_4$NO$_2$), 6.51 (dd, $^{3}J_{CH=CH}$ = 13.5 Hz, $^{2}J_{RhH}$ = 4.8 Hz, 1H, C*H*=CH-C$_6$*H*$_4$NO$_2$), 6.72 (d, ^{3}J = 7.6 Hz, 2H, CH-C$_6$*H*$_4$NO$_2$), 6.94-6.98 (m, 12H, P*Ph*$_3$), 7.16-7,28 (m, 15H, P*Ph*$_3$), 7.35-7.41 [m, 4H, 3H (P*Ph*$_3$) + 1H (C$_{13}$*H*$_8$N)], 7.53 (d, ^{3}J = 8.8 Hz, 2H, CH-C$_6$*H*$_4$NO$_2$), 7.75-7.80 (m, 2H), 8.01 (t, ^{3}J = 6.8 Hz, 1H), 8.10 (m, 2H), 8.29 (d, ^{3}J = 6.7 Hz, 1H), 9.61 (m, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 295 K): -143.55 (m, $^{1}J_{FP}$ = 708.7 Hz, *P*F$_6$), 31.40 (dd, $^{1}J_{RhP}$ = 167.4 Hz, $^{2}J_{PP}$ = 42.6 Hz, *P*Ph$_3$), 34.96 (dd, $^{1}J_{RhP}$ = 153.1 Hz, $^{2}J_{PP}$ = 42.5 Hz, *P*Ph$_3$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 295 K): 68.49 (dd, $^{1}J_{RhC}$ = 22.8 Hz, $^{2}J_{PC}$ = 6.9 Hz, CH=*C*H-C$_6$H$_4$NO$_2$), 82.56 (d, $^{1}J_{RhC}$ = 12.9 Hz, CH=*C*H-C$_6$H$_4$NO$_2$), 123.27 (s), 124.16 (s), 124.61 (s), 124.96 (s), 126.56 (s), 126.65 (s), 128.12 (d, J_{PC} = 10.2 Hz, P*Ph*$_3$), 128.33 (d, J_{PC} = 9.92 Hz, P*Ph*$_3$), 128.50 (s), 129.35 (s), 129.67 (s), 129.91 (d, $^{1}J_{PC}$ = 45.8 Hz, *ipso*-P*Ph*$_3$), 130.42 (d, $^{1}J_{PC}$ = 41.5 Hz, *ipso*-P*Ph*$_3$), 130.84 (s), 132.77 (d, J_{PC} = 11.6 Hz, P*Ph*$_3$), 134.58 (d, J_{PC} = 10.4 Hz, P*Ph*$_3$), 136.18 (s), 136.75 (s), 137.95 (s), 142.89 (s), 144.77 (s), 146.41 (s), 146.47 (s), 147.77 (s). Anal. Calcd. For $C_{57}H_{44}F_6N_2O_2P_3Rh{\bullet}0.5CH_2Cl_2$ (1141.25): C, 60.51; H, 3.97; N, 2.45. Found: C, 60.90; H, 3.71; N, 2.88.



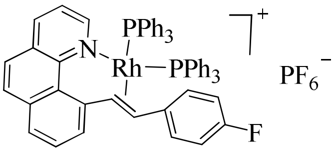
3ai

Yield: 90 mg (0.079 mmol, 90%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 5.69 (dd, $^{3}J_{CH=CH}$ = 13.3 Hz, $^{2}J_{RhH}$ = 6.9 Hz, 1H, CH=C*H*-C$_6$*H*$_4$NO$_2$), 5.95 (d, ^{3}J = 7.9 Hz, 1H, C$_6$*H*$_4$NO$_2$), 6.54 (dd, $^{3}J_{CH=CH}$ = 13.2 Hz, $^{2}J_{RhH}$ = 5.1 Hz, 1H, C*H*=CH-C$_6$*H*$_4$NO$_2$), 6.72 (t, ^{3}J = 7.6 Hz, 1H, C$_6$*H*$_4$NO$_2$), 6.94-6.97 (m, 12H, P*Ph*$_3$), 7.01 (t, ^{3}J = 7.7 Hz, 1H, C$_6$*H*$_4$NO$_2$), 7.14-7.21 (m, 9H, P*Ph*$_3$), 7.27 (t, ^{3}J = 7.7 Hz, 6H, P*Ph*$_3$), 7.35-7.41 [m, 4H, 3H (P*Ph*$_3$) + 1H (C$_6$*H*$_4$NO$_2$)], 7.59 (q, ^{3}J = 8.0 Hz, ^{3}J = 5.4 Hz, 1H), 7.81 (t, ^{3}J = 8.6 Hz, 2H), 7.98 (t, ^{3}J = 7.4 Hz, 1H), 8.03-8.08 (m, 2H), 8.21 (d, ^{3}J = 7.1 Hz, 1H), 9.56 (m, ^{3}J = 3.9 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 298 K): -144.42 (m, $^{1}J_{FP}$ = 710.3 Hz, PF_6), 29.78 (dd, $^{1}J_{RhP}$ = 165.6 Hz, $^{2}J_{PP}$ = 43.6 Hz, PPh_3), 35.44 (dd, $^{1}J_{RhP}$ = 153.9 Hz, $^{2}J_{PP}$ = 43.7 Hz, PPh_3); ^{13}C {^{1}H} NMR (δ, 100 MHz, CD_2Cl_2, 295 K): 68.33 (dd, $^{1}J_{RhC}$ = 23.0 Hz, $^{2}J_{PC}$ = 7.0 Hz, CH=*C*H-$C_6H_4NO_2$), 81.34 (d, $^{1}J_{RhC}$ = 13.0 Hz, CH=*C*H-$C_6H_4NO_2$), 122.77 (s), 124.71 (s), 125.85 (s), 126.31 (s), 126.35 (s), 126.65 (s), 126.97 (s), 126.99 (s), 128.09 (d, J_{PC} = 10.1 Hz, PPh_3), 128.31 (d, J_{PC} = 9.90 Hz, P*Ph*$_3$), 128.51 (s), 129.08 (s), 129.58 (s), 130.30 (d, $^{4}J_{PC}$= 2.0 Hz, *p*-P*Ph*$_3$), 130.31 (d, $^{1}J_{PC}$ = 42.0 Hz, *ipso*-P*Ph*$_3$), 130.42 (dd, $^{1}J_{PC}$ = 47.0 Hz, *ipso*-P*Ph*$_3$), 130.65 (d, $^{4}J_{PC}$= 3.0 Hz, *p*-P*Ph*$_3$), 130.80 (s), 132.91 (d, J_{PC} = 12.0 Hz, P*Ph*$_3$), 133.83 (s), 134.42 (d, J_{PC} = 10.0 Hz, P*Ph*$_3$), 135.03 (d, J_{PC} = 5 Hz, P*Ph*$_3$), 136.40 (s), 136.85 (s), 138.01 (s). Anal. Calcd. For $C_{57}H_{44}F_6N_2O_2P_3Rh{\bullet}0.5CH_2Cl_2$ (1141.25): C, 60.51; H, 3.97; N, 2.45. Found: C, 60.73; H, 3.82; N, 2.80.



3ae

Yield: 98 mg (0.086 mmol, 96%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 5.36 (dd, $^{3}J_{CH=CH}$ = 13.6 Hz, $^{2}J_{RhH}$ = 6.8 Hz，1H, CH=C*H*-C$_6$*H*$_4$Cl), 6.41 (dd, $^{3}J_{CH=CH}$ = 13.6 Hz, $^{2}J_{RhH}$ = 4.8 Hz, 1H, C*H*=CH-C$_6$*H*$_4$Cl), 6.56(d, ^{3}J = 7.8 Hz, 2H, CH-C$_6$*H*$_4$Cl), 6.71 (d, ^{3}J = 8.0 Hz, 2H, CH-C$_6$*H*$_4$Cl), 6.92-7.01 (m, 12H, P*Ph*$_3$), 7.15-7.21 (m, 9H, P*Ph*$_3$), 7.24-7.29 (m, 6H, P*Ph*$_3$), 7.35-7.38 [m, 4H, 3H (P*Ph*$_3$) + 1H (C$_{13}$*H*$_8$N)], 7.63 (dd, ^{3}J = 8 Hz, ^{3}J = 5.6 Hz, 1H), 7.79 (d, ^{3}J = 8.8 Hz, 1H), 7.93-8.03 (m, 3H, C$_{13}$*H*$_8$N), 8.17 (d, ^{3}J = 7.2 Hz, 1H), 9.49 (m, ^{3}J = 6.8 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -144.29 (m, $^{1}J_{FP}$ = 711.5 Hz, PF_6), 30.47 (dd, $^{1}J_{RhP}$ = 172.3 Hz, $^{2}J_{PP}$ = 44.8 Hz, PPh_3), 35.77 (dd, $^{1}J_{RhP}$ = 160.3 Hz, $^{2}J_{PP}$ = 45.5 Hz, PPh_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 295 K): 76.03 (dd, $^{1}J_{RhC}$ = 21.4 Hz, $^{2}J_{PC}$ = 6.2 Hz, CH=*C*H-C_6H_5Cl), 84.70 (d, $^{1}J_{RhC}$ = 12.9 Hz, *C*H=CH-Ph), 124.33 (s), 125.23 (s), 126.76 (s), 126.84 (s), 128.44 (d, J_{PC} = 10.0 Hz, P*Ph*$_3$), 128.50 (d, J_{PC} = 9.8 Hz, P*Ph*$_3$), 128.77 (s), 128.93 (s), 129.53 (s), 130.04 (s), 130.52 (s), 130.83 (d, J_{PC} = 2.3 Hz, *p*-P*Ph*$_3$), 130.92 (d, $^{1}J_{PC}$ = 46.4 Hz, *ipso*-P*Ph*$_3$), 131.17 (d, $^{1}J_{PC}$ = 41.7 Hz, *ipso*-P*Ph*$_3$), 131.21 (s), 131.85 (s), 132.12 (s), 133.36 (d, J_{PC} = 12.2 Hz, P*Ph*$_3$), 135.07 (d, J_{PC} = 10.4 Hz, P*Ph*$_3$), 136.63 (s), 137.07 (s), 137.23 (s), 138.13 (s), 143.40 (s), 148.38 (s). Anal. Calcd. For $C_{57}H_{44}ClF_6NP_3Rh{\bullet}2CH_2Cl_2$ (1130.70): C, 61.08; H, 4.01; N, 1.24. Found: C, 61.26; H, 4.61; N, 1.39.

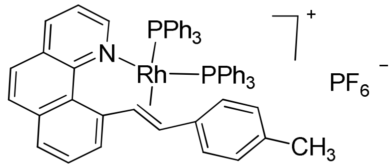


3af

Yield: 84 mg (0.080 mmol, 90%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295K): 5.44 (dd, $^{3}J_{CH=CH}$ = 13.0 Hz, $^{2}J_{RhH}$ = 6.9Hz, 1H, CH=C*H*- C$_6$*H*$_4$F), 6.40-6.49 [m, 3H, 1H (C*H*=CH-C$_6$*H*$_4$F) + 2H (C$_6$*H*$_4$F)], 6.60-6.62 (m, 2H, CH-C$_6$*H*$_4$F), 6.92-7.02 (m, 12H, P*Ph*$_3$), 7.18-7.20 (m, 9H, P*Ph*$_3$), 7.25-7.28 (m, 6H, P*Ph*$_3$), 7.35-7.38 [m, 4H, 3H (P*Ph*$_3$) + 1H (C$_{13}$*H*$_8$N)], 7.60 (m, 1H), 7.80 (d, ^{3}J = 8.6 Hz, 1H), 7.94-8.03 (m, 3H), 8.17 (d, ^{3}J = 7.0 Hz, 1H), 9.47 (m, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -144.38 (m, $^{1}J_{FP}$ = 711.2 Hz, PF_6), 30.60 (dd, $^{1}J_{RhC}$ = 168.6 Hz, $^{2}J_{PC}$ = 44.2 Hz,

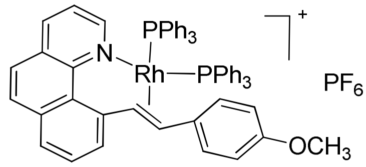
PPh_3), 36.11 (dd, $^1J_{RhC}$ = 155.7 Hz, $^2J_{PC}$ = 43.0 Hz, PPh_3). No ^{13}C NMR spectra could be obtained with acceptable signal to noise ratio. Anal. Calcd. For $C_{57}H_{44}F_7NP_3Rh•2CH_2Cl_2$ (1241.65): C, 57.07; H, 3.90; N, 1.13. Found: C, 57.09; H, 3.37; N, 1.35

3ag



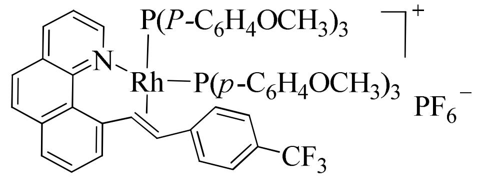
Yield: 95 mg (0.088 mmol, 93%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 5.55 (dd, $^3J_{CH=CH}$ = 13.9 Hz, $^3J_{RhH}$ = 6.2 Hz, 1H, CH=CH-C$_6H_4$CH$_3$), 6.41 (dd, $^3J_{CH=CH}$ = 14.0 Hz, $^2J_{RhH}$ = 4.8 Hz, 1H, CH=CH-C$_6H_4$CH$_3$), 6.53 (d, 2H, CH-C$_6H_4$CH$_3$), 6.59 (d, ^3J = 7.9 Hz, 2H, CH-C$_6H_4$CH$_3$), 6.93(t, 6H, PPh_3), 7.01 (m, 6H, PPh_3), 7.13-7.18 (m, 9H, PPh_3), 7.25 (m, 6H, PPh_3), 7.31-7.36 [m, 4H, 3H (PPh_3) + 1H ($C_{13}H_8$N)], 7.55 (dd, ^3J = 7.6 Hz, ^3J = 5.2 Hz, 1H), 7.79 (d, ^3J = 8.8 Hz, 1H), 7.93-8.01 (m, 3H, CHN), 8.12 (d, ^3J = 7.2 Hz, 1H), 9.44 (m, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -144.35 (m, $^1J_{F\text{-}P}$ = 709.5 Hz, PF_6), 31.12 (dd, $^1J_{Rh\text{-}P}$ = 169.5 Hz, $^2J_{P\text{-}P}$ = 43.7 Hz, PPh_3), 36.44 (dd, $^1J_{Rh\text{-}P}$ = 156.9 Hz, $^2J_{P\text{-}P}$ = 44.7 Hz PPh_3); ^{13}C {^{1}H} NMR (δ, 100 MHz, CD_2Cl_2, 295 K): 20.74 (s, CH$_3$), 80.64 (dd, $^1J_{Rh\text{-}C}$ = 18.8 Hz, $^2J_{P\text{-}C}$ = 6.0 Hz, CH=CH-C$_6$H$_4$CH$_3$), 85.38 (d, $^1J_{Rh\text{-}C}$ = 12.0 Hz, CH=CH-C$_6$H$_4$CH$_3$), 123.68 (s), 125.00 (s), 126.25 (s), 127.68 (s), 127.80 (s), 127.94 (d, $J_{P\text{-}C}$ = 9.7 Hz, PPh_3), 127.97 (d, $J_{P\text{-}C}$ = 10.1 Hz, PPh_3), 129.01 (s), 129.66 (s), 130.03 (d, $^4J_{P\text{-}C}$ = 1.8 Hz, p-PPh_3), 130.14 (d, $J_{P\text{-}C}$ = 1.7 Hz, p-PPh_3), 130.77 (s), 130.89 (dd, $^1J_{P\text{-}C}$ = 45.9 Hz, *ipso*-PPh_3), 130.93 (d, $^1J_{P\text{-}C}$ = 41.2 Hz, *ipso*-PPh_3), 132.88 (d, $J_{P\text{-}C}$ = 12.2 Hz, PPh_3), 134.70 (d, $J_{P\text{-}C}$ = 10.4 Hz, PPh_3), 136.25 (s), 136.63 (s), 136.70 (s), 137.57 (s), 143.37 (s), 148.06 (s). Anal. Calcd. For $C_{58}H_{47}F_6NP_3Rh$ (1067.82): C, 65.24; H, 4.44; N, 1.31. Found: C, 64.73; H, 4.27; N, 1.16.

3ah



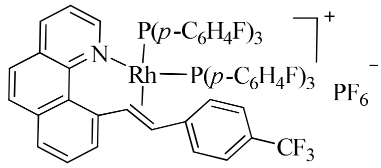
Yield: 93 mg (0.086 mmol, 91%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 295 K): 5.59 (dd, $^3J_{CH=CH}$ = 14.1 Hz, $^2J_{Rh\text{-}H}$ = 6.3 Hz, 1H, CH=CH-C$_6H_4$OCH$_3$), 6.32 [m, 3H, 2H (CH-C$_6H_4$OCH$_3$) + 1H (CH=CH-C$_6H_4$OCH$_3$)], 6.36 (dd, $^3J_{CH=CH}$ = 15.3 Hz, $^2J_{Rh\text{-}H}$ = 4.8 Hz, 1H, CH=CH-C$_6H_4$CH$_3$), 6.58 (d, ^3J = 8.0 Hz, 2H, CH-C$_6H_4$CH$_3$), 6.90-7.05(m, 12H, PPh_3), 7.14-7.19 (m, 9H, PPh_3), 7.25-7.36 [m, 10H, 9H (PPh_3) + 1H ($C_{13}H_8$N)], 7.56 (dd, ^3J = 8 Hz, ^3J = 5.2 Hz, 1H), 7.78 (d, ^3J = 8.8 Hz, 1H), 7.92-7.99 (m, 3H, CHN), 8.11 (d, ^3J = 6.8 Hz, 1H), 9.47 (m, 1H); ^{31}P {^{1}H} NMR (δ, 121 MHz, CD_2Cl_2, 295 K): -143.66 (m, $^1J_{F\text{-}P}$ = 708.3 Hz, PF_6), 31.79 (dd, $^1J_{Rh\text{-}P}$ = 169.5 Hz, $^2J_{P\text{-}P}$ = 44.3 Hz, PPh_3), 37.40 (dd, $^1J_{Rh\text{-}P}$ = 157.7 Hz, $^2J_{P\text{-}P}$ = 44.4 Hz, PPh_3); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 295 K): 55.17 (s, OCH$_3$), 81.15 (dd, $^1J_{Rh\text{-}C}$ = 18.5 Hz, $^2J_{P\text{-}C}$ = 5.9 Hz, CH=CH-C$_6$H$_4$OCH$_3$), 85.60 (d, $^1J_{Rh\text{-}C}$ = 9.8 Hz, CH=CH- C$_6$H$_4$OCH$_3$), 113.81 (s), 123.74 (s), 124.99 (s), 126.17 (s), 126.22 (s), 127.70 (s), 127.95 (d, $J_{P\text{-}C}$ = 10.1 Hz, PPh_3), 127.97 (d, $J_{P\text{-}C}$ = 9.8 Hz, PPh_3), 128.94 (s), 129.15 (s), 129.60 (s), 129.92 (s), 129.99 (d, $^4J_{P\text{-}C}$ = 2.2 Hz, p-PPh_3), 130.16 (d, $^4J_{P\text{-}C}$ = 2.2 Hz, p-PPh_3), 130.96 (dd, $^1J_{P\text{-}C}$ = 44.3 Hz, *ipso*-PPh_3), 131.02 (d, $^1J_{P\text{-}C}$ = 40.1

Hz, *ipso*-PPh_3), 132.88 (d, $J_{P\text{-}C}$ = 12.2 Hz, PPh_3), 134.74 (d, $J_{P\text{-}C}$ = 10.4 Hz, PPh_3), 136.20 (s), 136.58 (s), 137.52 (s), 143.36 (s), 148.26 (s), 158.54 (s). Anal. Calcd. For $C_{58}H_{47}F_6NOP_3Rh{\bullet}CH_2Cl_2$ (1168.75): C, 60.63; H, 4.23; N, 1.20. Found: C, 60.20; H, 4.17; N, 1.21.



3bb

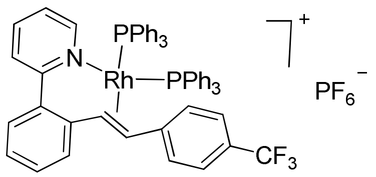
Yield: 105 mg (0.080 mmol, 95%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 3.74 (s, 9H, OCH_3), 3.83 (s, 9H, OCH_3), 5.20 (dd, $^3J_{CH=CH}$ = 12.0 Hz, $^2J_{RhH}$ = 4.4 Hz, 1H, CH=C*H*-$C_6H_4CF_3$), 6.45-6.47 (m, 6H, $PC_6H_4OCH_3$), 6.63-6.73 [m, 9H, 6H ($PC_6\textit{H}_4OCH_3$) + 1H (C*H*=$CHC_6\textit{H}_4CF_3$) + 2H ($C_6\textit{H}_4CF_3$)], 6.87 (m, 6H, $PC_6\textit{H}_4OCH_3$), 7.00 (d, ^3J = 6.8 Hz, 2H, $C_6\textit{H}_4CF_3$), 7.16 (m, 6H, $PC_6\textit{H}_4OCH_3$), 7.42(d, ^3J = 8.0 Hz, 1H), 7. 67 (m, 1H), 7.78 (d, ^3J = 8.0 Hz, 1H), 7.95-7.99 (m, 2H), 8.09 (d, ^3J = 7.2 Hz, 1H), 8.23 (d, ^3J = 5.6 Hz, 1H), 9.48 (m, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -144.19 (m, $^1J_{FP}$ = 711.2 Hz, *P*F_6), 27.50 (dd, $^1J_{RhP}$ = 169.2 Hz, $^2J_{PP}$ = 43.4 Hz, *P*Ph_3), 31.74 (dd, $^1J_{RhP}$ = 155.2 Hz, $^2J_{PP}$ = 43.1 Hz, *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2CL_2, 295 K): -73.10 (d, $^1J_{PF}$ = 710.6 Hz, P*F*$_6$), 62.84 (s, C*F*$_3$);^{13}C {^{1}H} NMR (δ, 100 MHz, CD_2Cl_2, 295 K): 55.75 (s, O*C*H_3), 55.78 (s, O*C*H_3), 72.39 (dd, $^1J_{RhC}$ = 22.3 Hz, $^2J_{PC}$ = 6.5 Hz, CH=*C*H-$C_6H_4CF_3$), 82.76 (d, $^1J_{RhC}$ = 12.7 Hz, *C*H=CH-$C_6H_4CF_3$), 113.54 (d, J_{PC} = 11.1 Hz, P*C*$_6H_4OCH_3$), 113.59 (d, J_{PC} = 10.9 Hz, $PC_6\textit{H}_4OCH_3$), 121.86 (d, $^1J_{PC}$ = 49.9 Hz, *ipso*-P*C*$_6H_4OCH_3$), 124.35 ($^1J_{PC}$ = 46.9 Hz, *ipso*-P-*C*$_6H_4OCH_3$), 123.56 (s), 124.35 (q, $^1J_{FC}$ = 270.0 Hz, *C*F_3), 124.86 (q, $^3J_{FC}$ = 3.6 Hz, *C*$_6H_4CF_3$), 126.12 (s), 126.30 (s), 126.72 (q, $^2J_{FC}$ = 31.0 Hz, *C*$_6H_4CF_3$), 127.74 (s), 127.86 (s), 129.22 (s), 129.49 (s), 130.83 (s), 134.09 (d, J_{PC} = 13.4 Hz, P*C*$_6H_4OCH_3$), 135.89 (d, J_{PC} = 11.7 Hz, $PC_6H_4OCH_3$), 136.65 (s), 136.69 (s), 137.53 (s), 143.09 (s), 143.16 (s), 147.76 (s), 160.88 (d, $^4J_{PC}$ = 1.8 Hz, *p*-P*C*$_6H_4OCH_3$), 161.15 (d, $^4J_{PC}$ = 1.9 Hz, *p*-P*C*$_6H_4OCH_3$). Anal. Calcd. For $C_{64}H_{56}F_9NO_6P_3Rh$ (1301.95): C, 59.04; H, 4.34; N, 1.08. Found: C, 58.80; H, 3.66; N, 1.44.



3cb

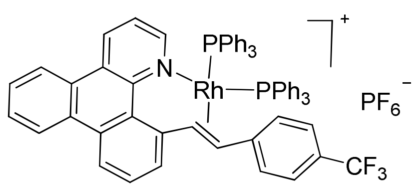
Yield: 106 mg (0.086 mmol, 94%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 5.48 (dd, $^3J_{CH=CH}$ = 14.0 Hz, $^2J_{RhH}$ = 6.8 Hz, 1H, CH=C*H*-$C_6\textit{H}_4CF_3$), 6.42 (dd, $^3J_{CH=CH}$ = 13.2 Hz, $^2J_{RhH}$ = 2.4 Hz, 1H, C*H*=CH-$C_6\textit{H}_4CF_3$), 6.74 (m, 6H, $PC_6\textit{H}_4F$), 6.86 (m, 2H, $C_6\textit{H}_4CF_3$), 6.89-7.07 [m, 14H, 12H ($PC_6\textit{H}_4F$) + 2H ($C_6\textit{H}_4CF_3$)], 7.18-7.24 (m, 6H, $PC_6\textit{H}_4F$), 7.49 (d, ^3J = 8.4 Hz, 1H), 7.82-7.86 (m, 2H), 8.00 (t, ^3J = 7.2 Hz, 1H), 8.07 (d, ^3J = 8.0 Hz, 1H), 8.12 (d, ^3J = 6.8 Hz, 1H), 8.21 (d, ^3J = 6.9 Hz, 1H), 9.67 (m, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -143.99 (m, $^1J_{FP}$ = 711.2 Hz, *P*F_6), 28.28 (dd, $^1J_{RhP}$ = 170.0 Hz, $^2J_{PP}$ = 43.6 Hz, *P*C_6H_4F), 34.55 (dd, $^1J_{RhP}$ = 156.4Hz, $^2J_{PP}$ = 43.6 Hz, *P*C_6H_4F); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2CL_2, 295 K): -108.21(s, Ph*F*), -108.40 (s, Ph*F*), -72.44 (d, $^1J_{PF}$ = 710.6 Hz, P*F*$_6$), 63.04 (s, C*F*$_3$); ^{13}C {^{1}H} NMR (δ, 100 MHz, CD_2Cl_2, 295

K): 75.46 (dd, $^1J_{RhC}$ = 21.7 Hz, $^2J_{PC}$ = 6.6 Hz, CH=*C*H-$C_6H_4CF_3$), 85.20 (d, $^1J_{RhC}$ = 12.5 Hz, *C*H=CH-$C_6H_4CF_3$), 115.69 (dd, J_{FC} = 21.9 Hz, J_{PC} = 11.4 Hz, PC_6H_4F), 115.90 (dd, J_{FC} = 21.9 Hz, J_{PC} = 11.0 Hz, PC_6H_4F), 124.06 (q, $^1J_{FC}$ = 270.0 Hz, *C*F_3), 124.66 (s), 124.76 (s), 125.15 (q, $^3J_{FC}$ = 3.5 Hz, $C_6H_4CF_3$), 126.01 (d, $^1J_{PC}$ = 47.9Hz, *ipso*-PC_6H_4F), 126.18 (d, $^1J_{PC}$ = 40.5 Hz, *ipso*-PC_6H_4F), 126.38 (s), 126.74 (s), 128.02 (s), 125.15 (q, $^4J_{FC}$ = 3.5 Hz, $C_6H_4CF_3$), 127.86 (q, $^2J_{FC}$ = 32.7 Hz, $C_6H_4CF_3$), 128.01 (s), 128.67 (s), 129.32 (s), 129.63 (s), 131.09 (s), 134.74 (dd, J_{FC} = 11.9 Hz, J_{PC} = 8.6 Hz, PC_6H_4F), 136.68 (s), 137.97 (s), 142.03 (s), 142.57 (s), 148.68 (s), 163.83 (d, $^1J_{FC}$ = 252.4 Hz, *p*-PC_6H_4F), 164.07 (d, $^1J_{FC}$ = 252.4 Hz, *p*-PC_6H_4F). Anal. Calcd. For $C_{58}H_{38}F_{15}NP_3Rh$ (1229.73): C, 56.65; H, 3.11; N, 1.14. Found: C, 57.02; H, 3.29; N, 1.08.



3db

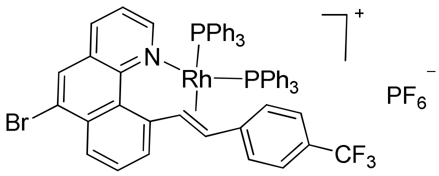
Yield: 89 mg (0.081 mmol, 91%). ^{1}H NMR (δ, 300 MHz, CD_2Cl_2, 295 K): 4.78 (d, $^3J_{CH=CH}$ = 14.0 Hz, 1H, CH=C*H*-$C_6H_4CF_3$), 6.02 (d, $^3J_{CH=CH}$ = 14.2 Hz, 1H, C*H*=CH-$C_6H_4CF_3$), 6.68 (d, $^3J_{CH=CH}$ = 7.2 Hz, 2H, $C_6H_4CF_3$), 6.94 (d, ^3J = 7.6 Hz, 1H), 7.02-7.12 [m, 25H, 24 H (P*Ph*$_3$) + 1H ($C_{11}H_8N$)], 7.32 [m, 7H, 6H (P*Ph*$_3$) + 1H ($C_{11}H_8N$)], 7.43-7.55 [m, 4H, 2H ($C_6H_4CF_3$) + 2H ($C_{11}H_8N$)], 7.75-7.82 (m, 2H), 9.00 (d, ^3J = 4.7 Hz, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -144.31 (m, $^1J_{FP}$ = 711.6 Hz, *P*F_6), 30.91 (dd, $^1J_{RhP}$ = 171.3 Hz, $^2J_{PP}$ = 41.2Hz, *P*Ph_3), 35.48 (dd, $^1J_{RhP}$ = 156.2 Hz, $^2J_{PP}$ = 41.8 Hz *P*Ph_3); ^{19}F {^{1}H} NMR (δ, 282 MHz, CD_2CL_2, 295 K): -73.24 (d, $^1J_{PF}$ = 707.8 Hz, P*F*$_6$), 63.07 (s, C*F*$_3$); ^{13}C {^{1}H} NMR (δ, 75 MHz, CD_2Cl_2, 255 K): 81.90 (dd, $^1J_{RhC}$ = 18.1 Hz, $^2J_{PC}$ = 5.8 Hz, CH=*C*H-$C_6H_4CF_3$), 87.67 (d, $^1J_{RhC}$ = 10.1 Hz, *C*H=CH-$C_6H_4CF_3$), 124.40 (q, $^1J_{FC}$ = 270.2 Hz, CF_3), 125.53 (q, $^3J_{FC}$ = 3.5 Hz, $C_6H_4CF_3$), 125.72 (s), 125.80 (s), 127.89 (q, $^2J_{FC}$ = 32.0 Hz, $C_6H_4CF_3$), 128.03 (s), 128.12 (s), 128.35 (d, J_{PC} = 9.8 Hz, P*Ph*$_3$), 128.70 (d, J_{PC} = 10.3 Hz, P*Ph*$_3$), 128.93 (s), 129.10 (s), 130.69 (s, *p*-P*Ph*$_3$), 130.81 (d, $^1J_{PC}$ = 44.3 Hz, *ipso*-P*Ph*$_3$), 131.13 (d, $^1J_{PC}$ = 43.7 Hz, *ipso*-P*Ph*$_3$), 132.14 (s), 132.29 (s), 133.30 (s), 133.64 (d, J_{PC} = 12.0 Hz, P*Ph*$_3$), 134.65 (s), 134.86 (d, J_{PC} = 10.4 Hz, P*Ph*$_3$), 135.98 (s), 139.39 (s), 141.94 (s), 149.88 (s), 156.28 (s), 162.65 (s). Anal. Calcd. For $C_{56}H_{44}F_9NP_3Rh{\cdot}CH_2Cl_2$ (1182.70): C, 57.89; H, 3.92; N, 1.18. Found: C, 58.28; H, 3.94; N, 1.37.



3eb

Yield: 92 mg (0.079 mmol, 90%). ^{1}H NMR (δ, 400 MHz, CD_2Cl_2, 295 K): 5.25 (dd, $^3J_{CH=CH}$ = 13.7 Hz, $^2J_{RhH}$ = 6.9 Hz, 1H, CH=C*H*-$C_6H_4CF_3$), 6.41 (d, ^3J = 13.6 Hz, 1H, C*H*=CH-$C_6H_4CF_3$), 6.72 (d, ^3J = 6.5 Hz, 2H, $C_6H_4CF_3$), 6.87-6.90 (m, 6H, P*Ph*$_3$), 6.94-6.97 [m, 10H, 9H (P*Ph*$_3$) + 1H ($C_{17}H_8N$)], 7.10-7.25 [m, 13H, 12H (P*Ph*$_3$) + 1H ($C_{17}H_{10}N$)], 7.33-7.37 (m, 3H, P*Ph*$_3$), 7.71 (t, ^3J = 7.3 Hz, 1H), 7.76-7.81 [m, 3H, 2H ($C_6H_4CF_3$) + 1H ($C_{17}H_{10}N$)], 8.04 (t, ^3J = 7.9 Hz, 1H), 8.15 (d, ^3J = 7.3 Hz, 1H), 8.33 (d, ^3J = 7.2 Hz, 1H), 8.59 (d, ^3J = 8.2 Hz, 1H), 8.74 (d, ^3J = 8.2 Hz, 1H), 9.55 (m, 1H); ^{31}P {^{1}H} NMR (δ, 162 MHz, CD_2Cl_2, 295 K): -144.23 (m, $^1J_{FP}$ = 709.9 Hz,

PF_6), 30.88 (dd, $^1J_{RhP}$ = 169.7 Hz, $^2J_{PP}$ = 43.0Hz, PPh_3), 35.71(dd, $^1J_{RhP}$ = 156.2Hz, $^2J_{PP}$ = 44.0 Hz, PPh_3); ^{13}C {^1H} NMR (δ, 75 MHz, CD_2Cl_2, 295 K): 75.33 (dd, $^1J_{RhC}$ = 21.9 Hz, $^2J_{PC}$ = 6.3 Hz, CH=CH-$C_6H_4CF_3$), 84.53 (d, $^2J_{RhC}$ = 12.0 Hz, CH=CH-$C_6H_4CF_3$), 122.41 (s), 122.94 (s), 123.75 (s), 124.49 (s), 125.06 (q, $^3J_{FC}$ = 3.7 Hz, $C_6H_4CF_3$), 125.07 (d, $^1J_{FC}$ = 134.3 Hz, CF_3), 126.80 (s), 127.31 (q, $^2J_{FC}$ = 31.1 Hz, $C_6H_4CF_3$), 127.85 (s), 127.91 (s), 128.06 (d, J_{PC} = 9.7 Hz, PPh_3), 128.18 (d, J_{PC} = 9.0 Hz, PPh_3), 128.40 (s), 128.73 (s), 129.49 (s), 129.61 (s), 130.00 (d, $^4J_{PC}$ = 2.2 Hz, *p*-PPh_3), 130.18 (dd, $^1J_{PC}$ = 45.8 Hz, *ipso*-PPh_3), 130.32 (s), 130.49 (d, $^4J_{PC}$ = 2.0 Hz, *p*-PPh_3), 130.60 (d, $^1J_{PC}$ = 42.1 Hz, *ipso*-PPh_3), 131.46 (s), 132.39 (s), 132.83 (d, J_{PC} = 12.1 Hz, PPh_3), 134.57 (d, J_{PC} = 10.5 Hz, PPh_3), 135.29 (s), 136.28 (s), 142.24 (s), 143.38 (s), 147.12 (s). Anal. Calcd. For $C_{62}H_{46}F_9NP_3Rh$ (1171.85): C, 63.55; H, 3.96; N, 1.20. Found: C, 63.15; H, 4.32; N, 1.35.

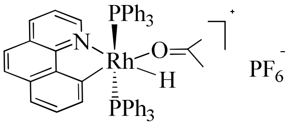


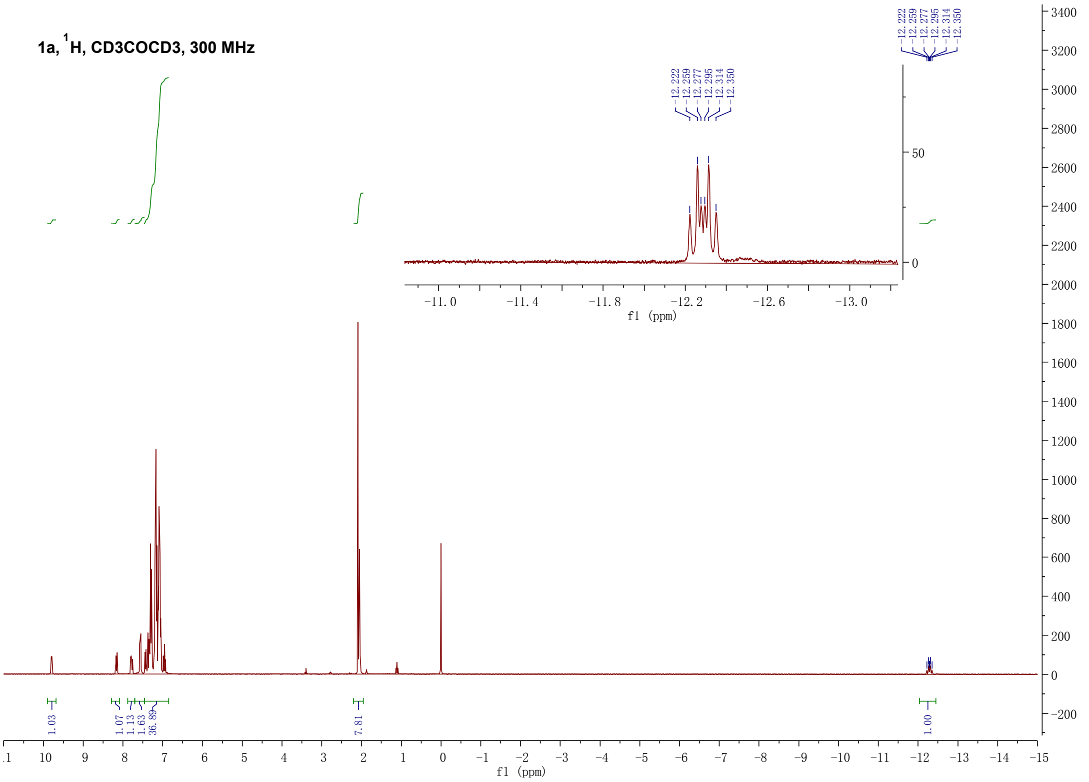
3fb

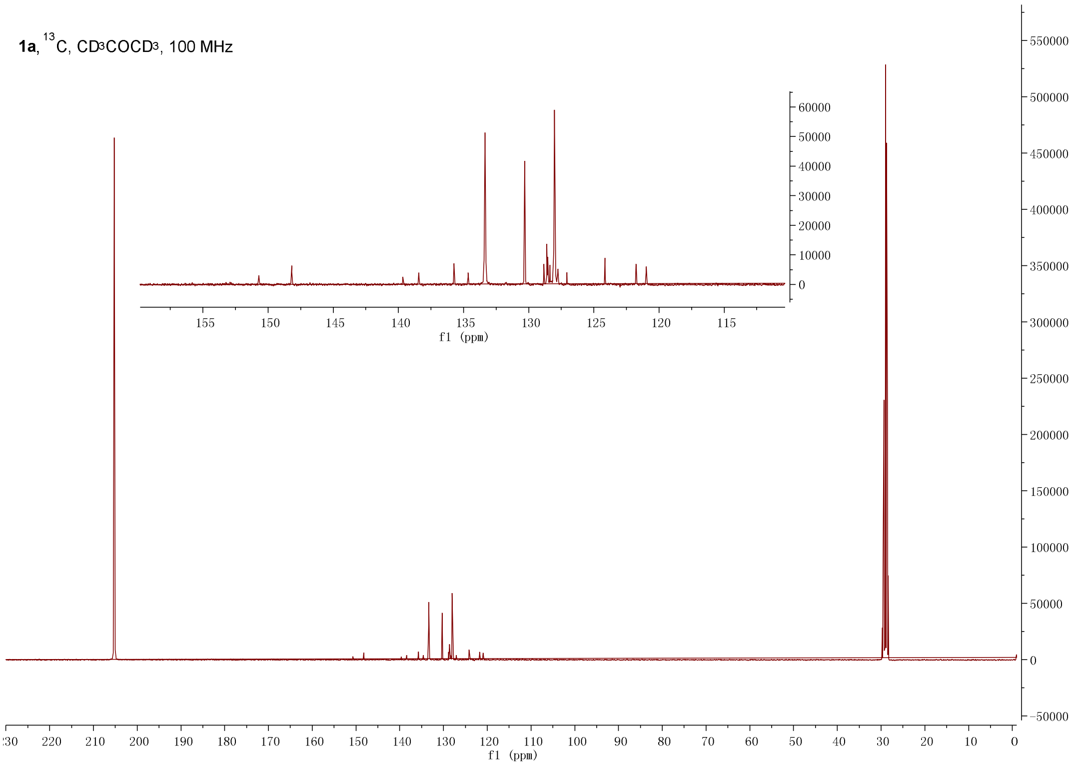
Yield: 93 mg (0.077 mmol, 93%). ^1H NMR (δ, 500 MHz, CD_2Cl_2, 295 K): 5.28 (dd, $^3J_{CH=CH}$ = 14.0 Hz, $^2J_{Rh\text{-}H}$ = 7.4 Hz, 1H, CH=CH-$C_6H_4CF_3$), 6.48 (d, $^3J_{CH=CH}$ = 12.7 Hz, 1H, CH=CH-$C_6H_4CF_3$), 6.87-6.90 (m, 2H, $C_6H_4CF_3$), 6.95-6.97 (m, 6H, PPh_3), 6.95-6.97 [m, 14H, 12H (PPh_3) + 2H ($C_6H_4CF_3$)], 7.19-7.24 (m, 15H, PPh_3), 7.34-7.37 (m, 3H, PPh_3), 7.73-7.77 (m, 2H), 7.98 (d, ^3J = 7.9 Hz, 1H), 8.06 (t, ^3J = 7.6 Hz, 1H), 8.28 (d, ^3J = 7.2 Hz, 1H), 8.49 (d, ^3J = 8.2 Hz, 1H), 9.60 (m, 1H); ^{31}P {^1H} NMR (δ, 202 MHz, CD_2Cl_2, 295 K): -144.19 (m, $^1J_{FP}$ = 709.4 Hz, PF_6), 30.39 (dd, $^1J_{RhP}$ = 167.9 Hz, $^2J_{PP}$ = 43.1 Hz, PPh_3), 34.82 (dd, $^1J_{RhP}$ = 154.0 Hz, $^2J_{PP}$ = 42.8 Hz, PPh_3); ^{19}F {^1H} NMR (δ, 282 MHz, CD_2CL_2, 295 K): -72.95 (d, $^1J_{PF}$ = 710.6 Hz, PF_6), 62.97 (s, CF_3); ^{13}C {^1H} NMR (δ, 125 MHz, CD_2Cl_2, 295 K): 73.85 (dd, $^1J_{RhC}$ = 20.8 Hz, $^2J_{PC}$ = 6.5 Hz, CH=CH-$C_6H_4CF_3$), 82.90 (d, $^1J_{RhC}$ = 12.6 Hz, CH=CH-$C_6H_4CF_3$), 124.18 (q, $^1J_{FC}$ = 270.1 Hz, CF_3), 124.35 (s), 124.77 (s), 125.03 (q, $^3J_{FC}$ = 3.1 Hz, $C_6H_4CF_3$), 125.83 (s), 127.23 (q, $^2J_{FC}$ = 33.0 Hz, $C_6H_4CF_3$), 127.11 (s), 127.41 (s), 127.98 (s), 128.18 (d, J_{PC} = 12.4 Hz, PPh_3), 128.27 (d, J_{PC} = 10.3 Hz, PPh_3), 129.05 (s), 129.89 (s), 130.19 (d, $^1J_{PC}$ = 48.5 Hz, *ipso*-PPh_3), 130.22 (s), 130.59 (s, *p*-PPh_3), 130.55 (d, $^1J_{PC}$ = 42.1 Hz, *ipso*-PPh_3), 131.67 (s), 132.81 (d, J_{PC} = 12.0 Hz, PPh_3), 134.54 (d, J_{PC} = 10.3 Hz, PPh_3), 135.07 (s), 136.53 (s), 136.87 (s), 142.16 (s), 148.34 (s). Anal. Calcd. For $C_{58}H_{43}BrF_9NP_3Rh$ (1200.69): C, 58.02; H, 3.61; N, 1.17. Found: C, 58.45; H, 3.84; N, 1.30.

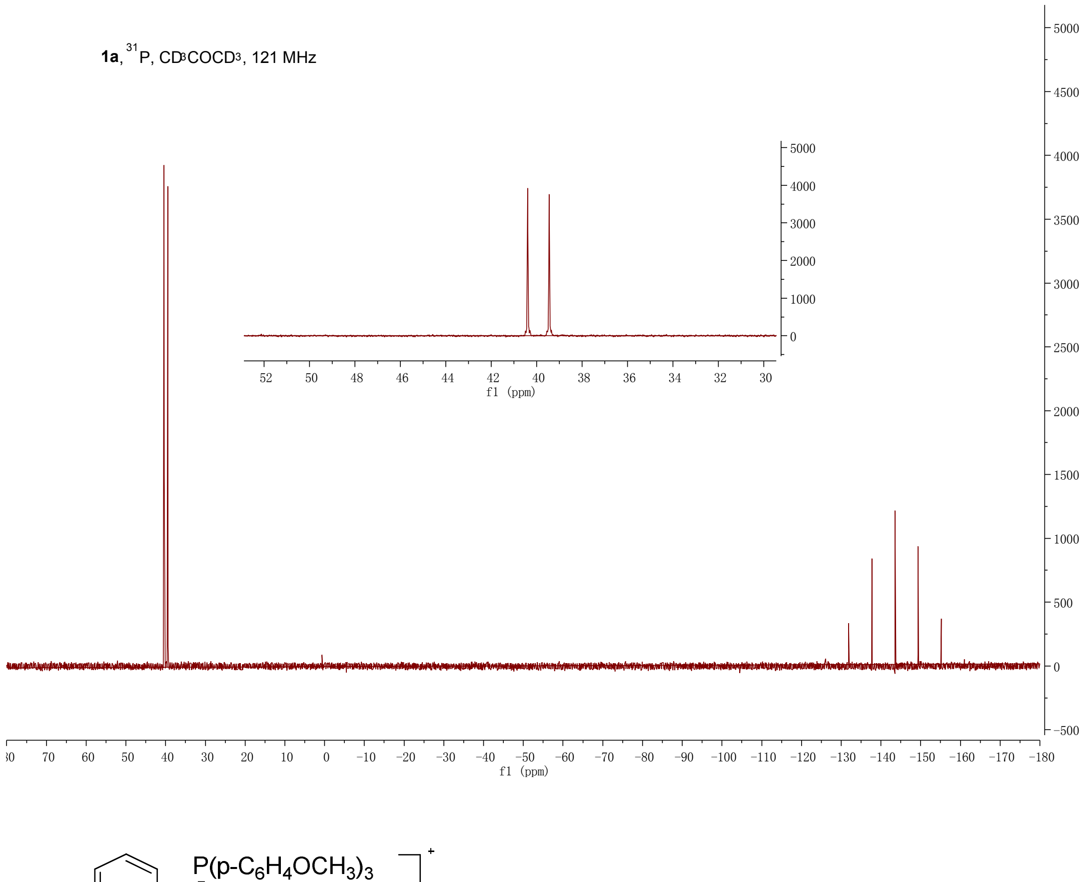
NMR Spectra of Rhodium Hydrides 1, Intermediates 2 and Coupling products 3

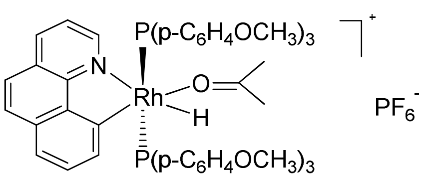
1a



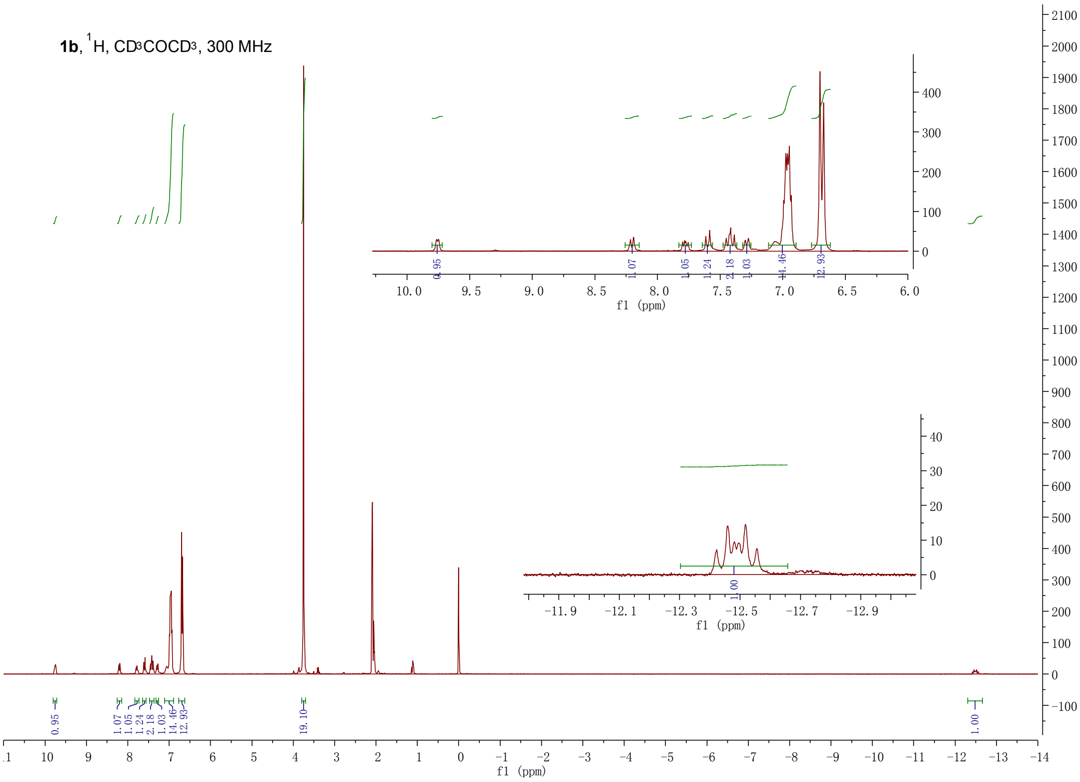


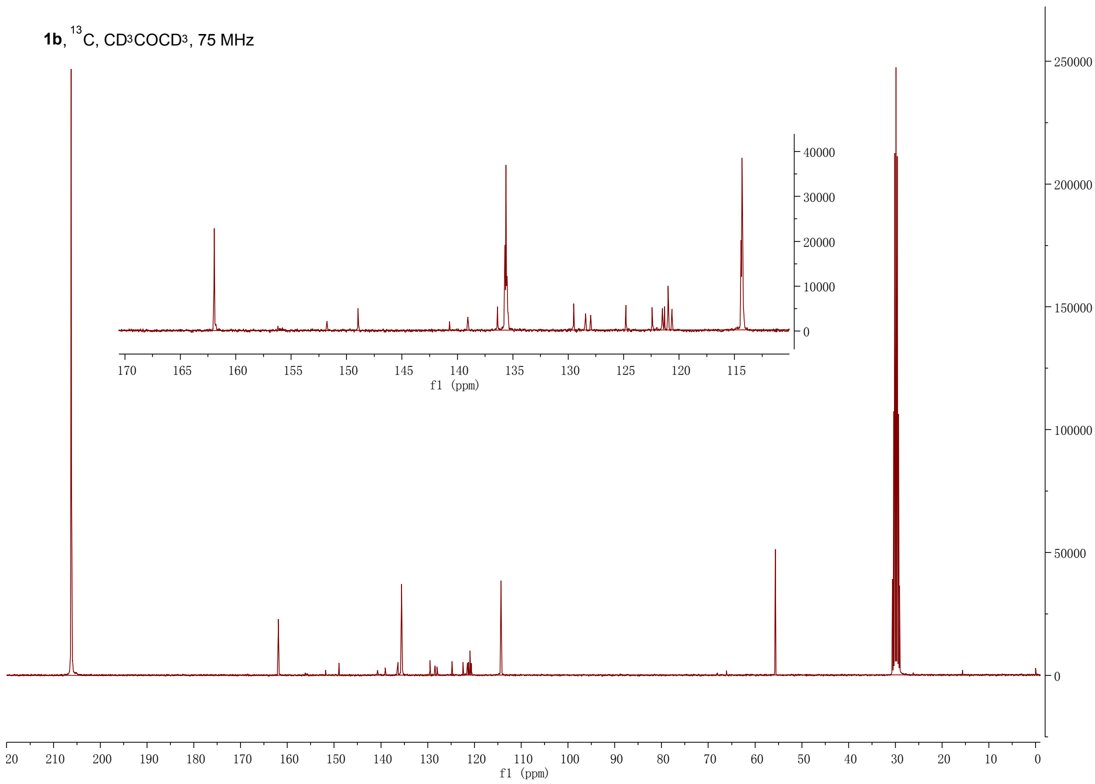

1a, 13C, CD3COCD3, 100 MHz
f1 (ppm)

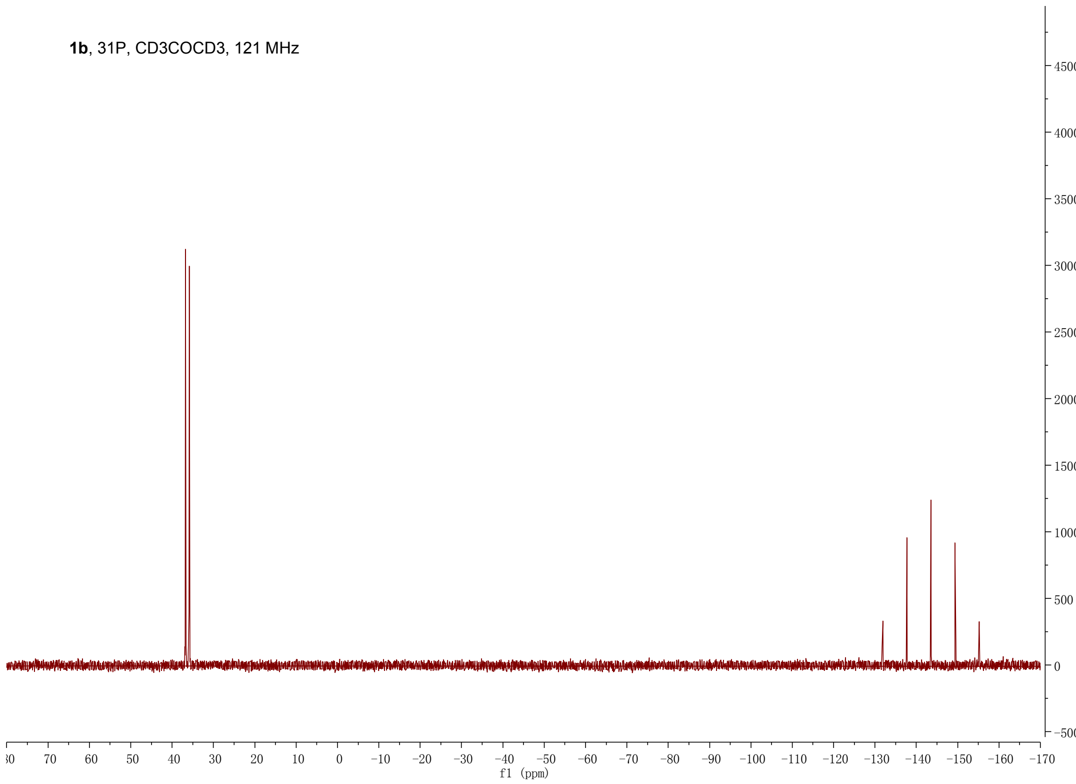

1a, 31P, CD3COCD3, 121 MHz
f1 (ppm)

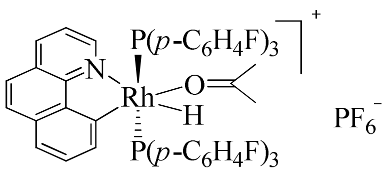

P(p-C6H4OCH3)3
N
Rh
O
H
P(p-C6H4OCH3)3
PF6-

1b

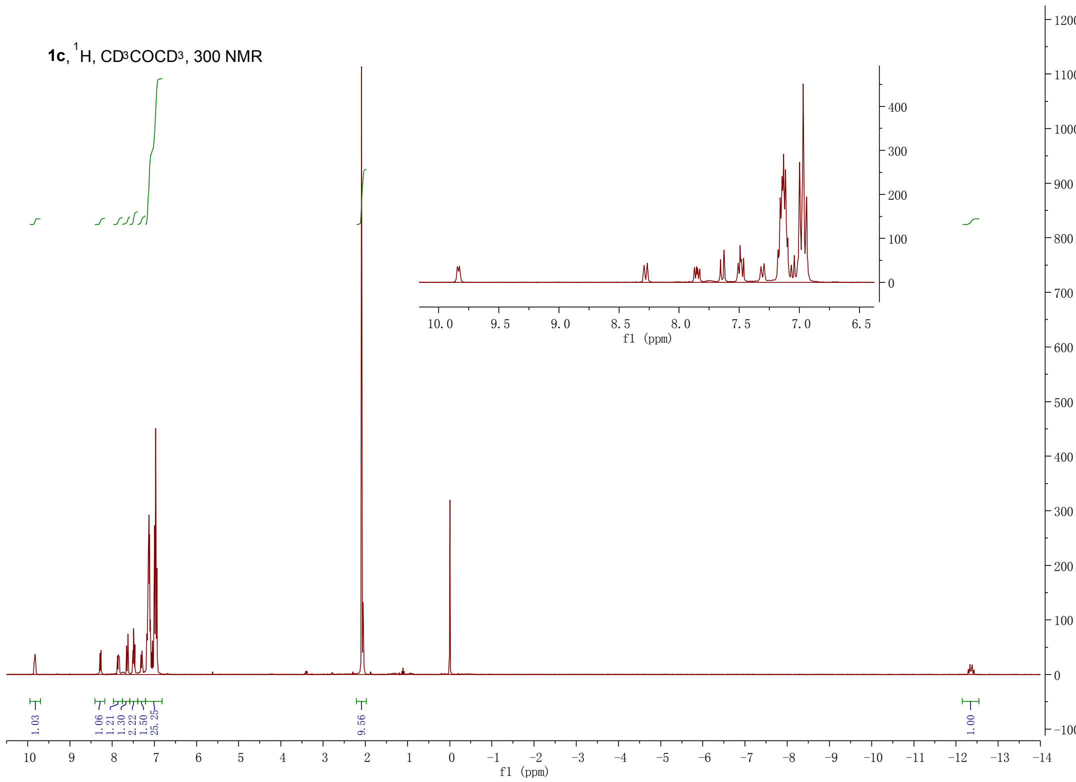

1b, 1H, CD3COCD3, 300 MHz
f1 (ppm)

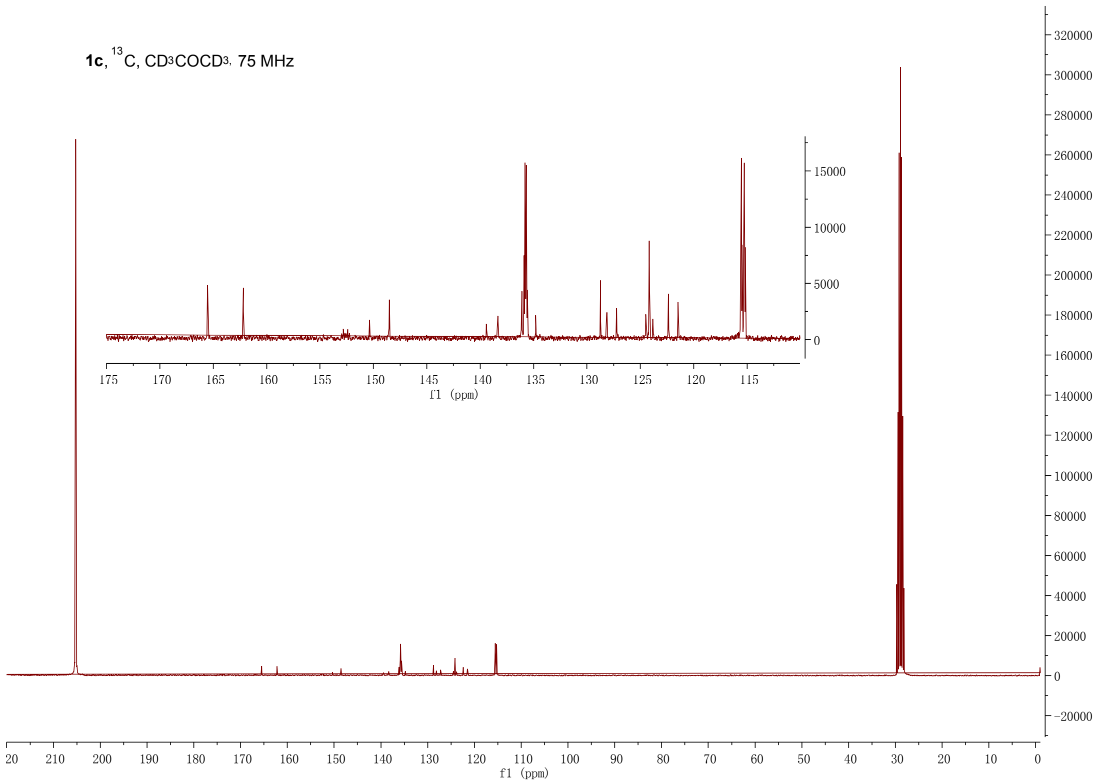

1b, 13C, CD3COCD3, 75 MHz
f1 (ppm)

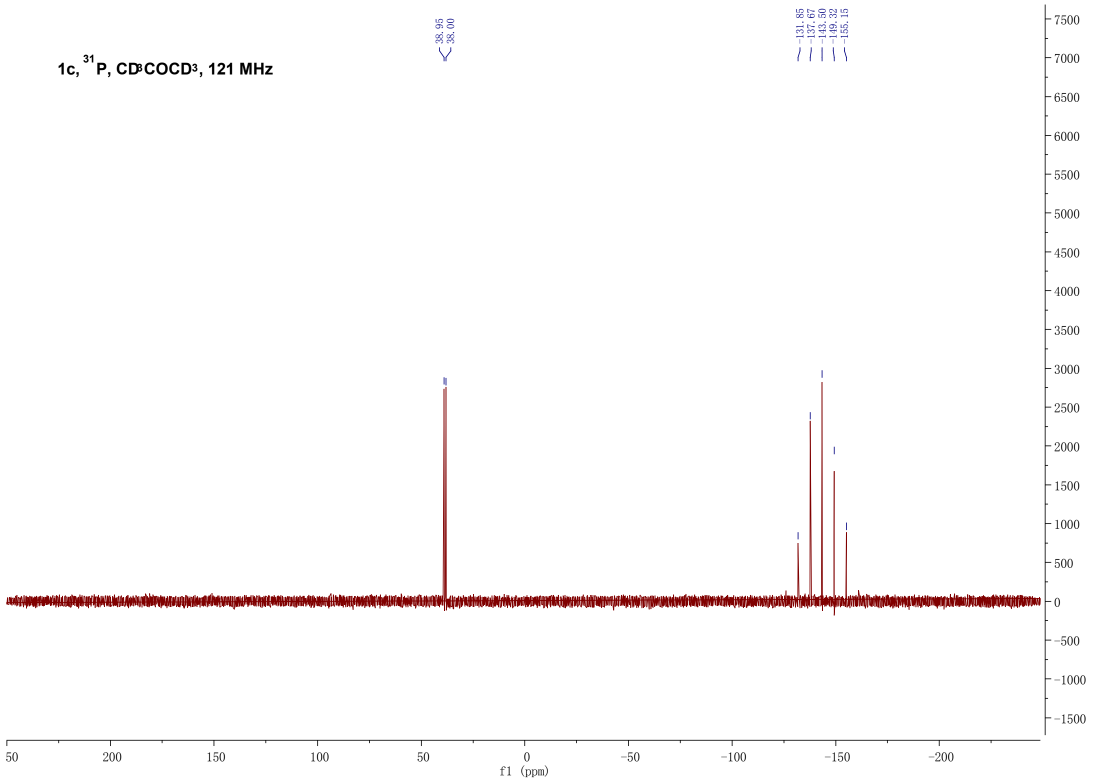

1b, 31P, CD3COCD3, 121 MHz
f1 (ppm)


P(p-C6H4F)3
Rh
O
H
N
P(p-C6H4F)3
+
PF6-

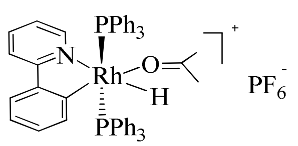
1c


1c, 1H, CD3COCD3, 300 NMR
1.03
1.06
1.21
1.30
2.22
1.50
25.25
9.56
1.00
f1 (ppm)

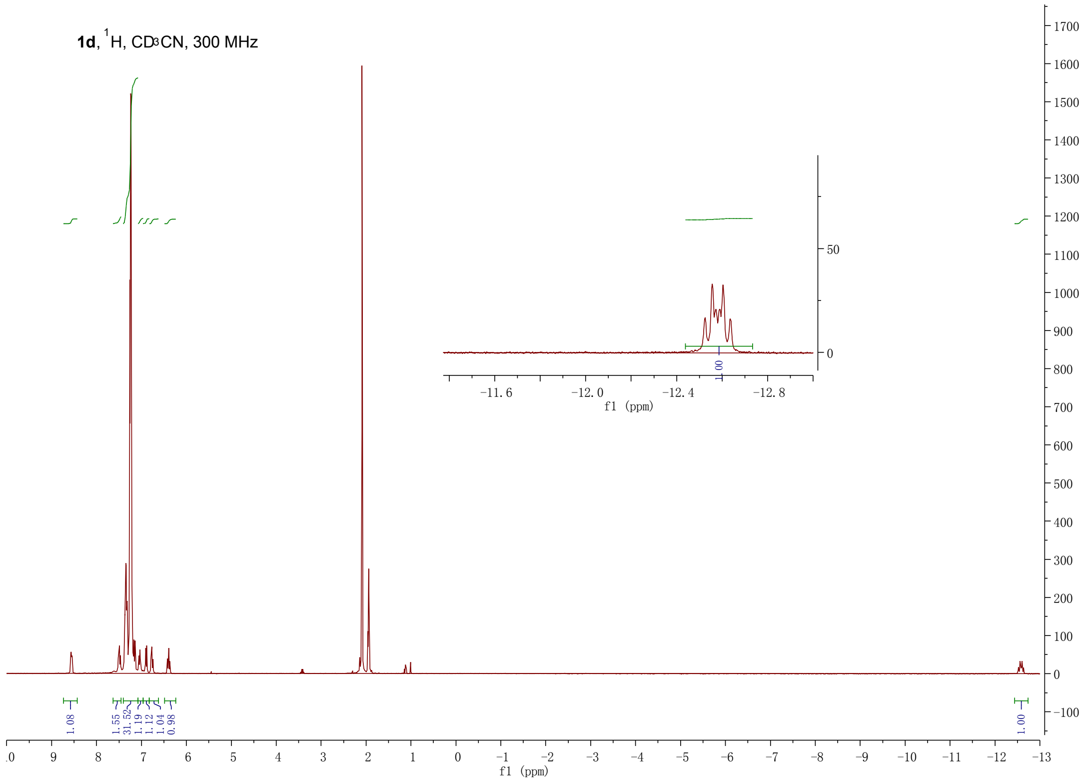

1c, 13C, CD3COCD3, 75 MHz
f1 (ppm)


1c, 31P, CD3COCD3, 121 MHz
38.95
38.00
-131.85
-137.67
-143.50
-149.32
-155.15
f1 (ppm)

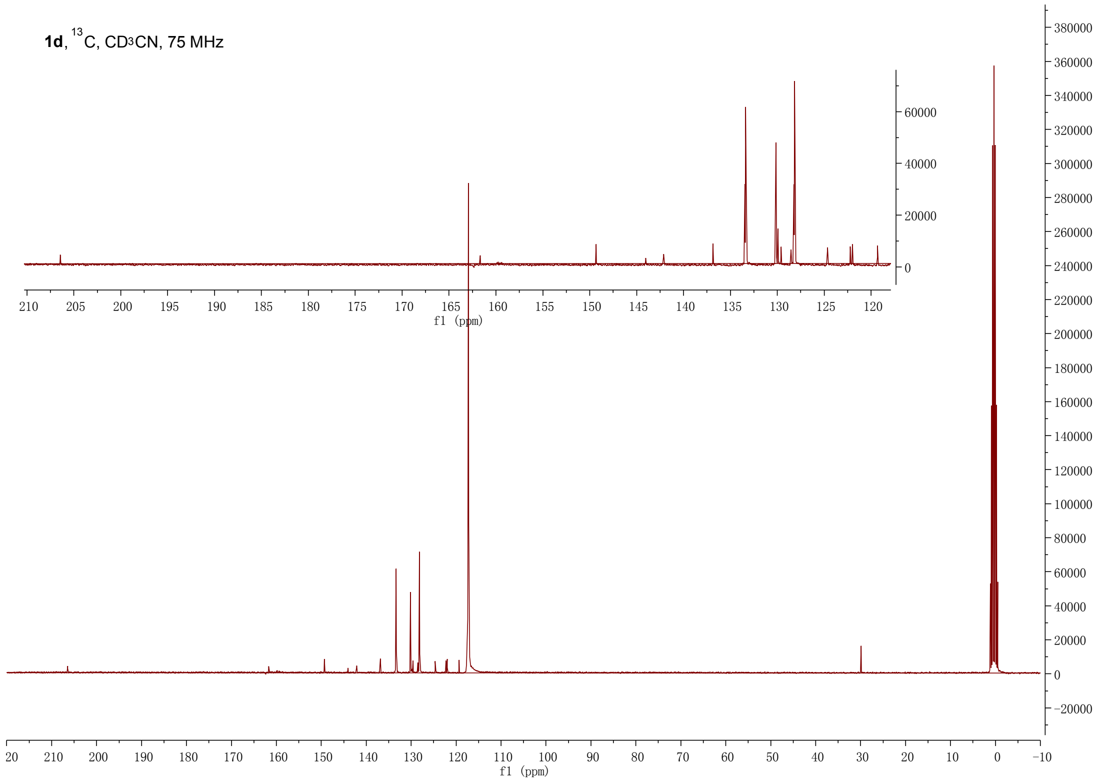
1d

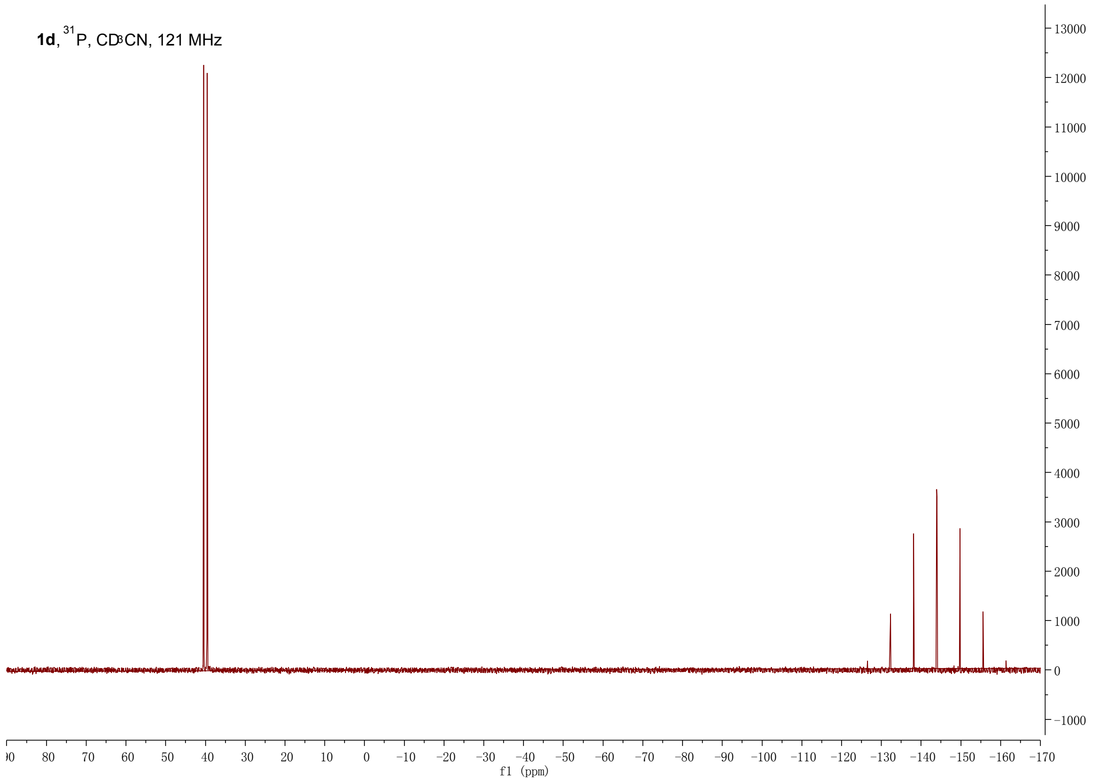

PPh3
N
Rh
O
H
PPh3
PF6

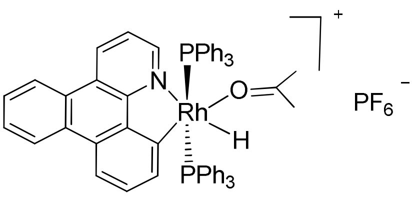
1d, ^{1}H, CD_3CN, 300 MHz



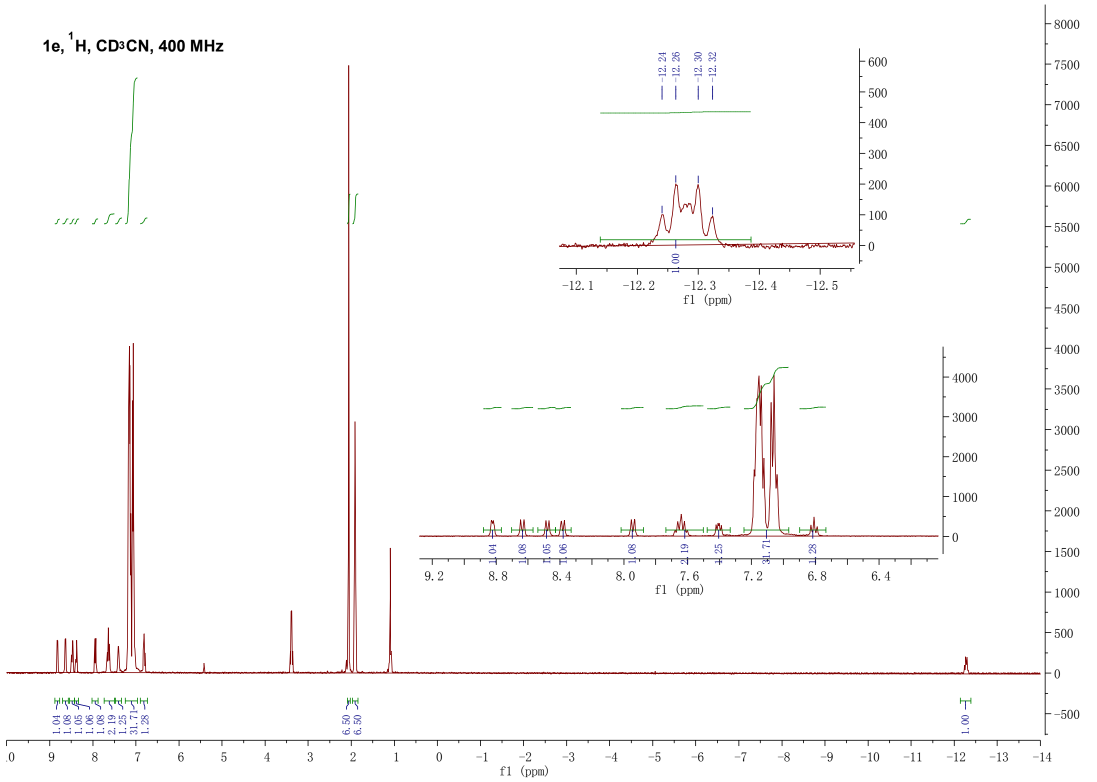
1d, ^{13}C, CD_3CN, 75 MHz

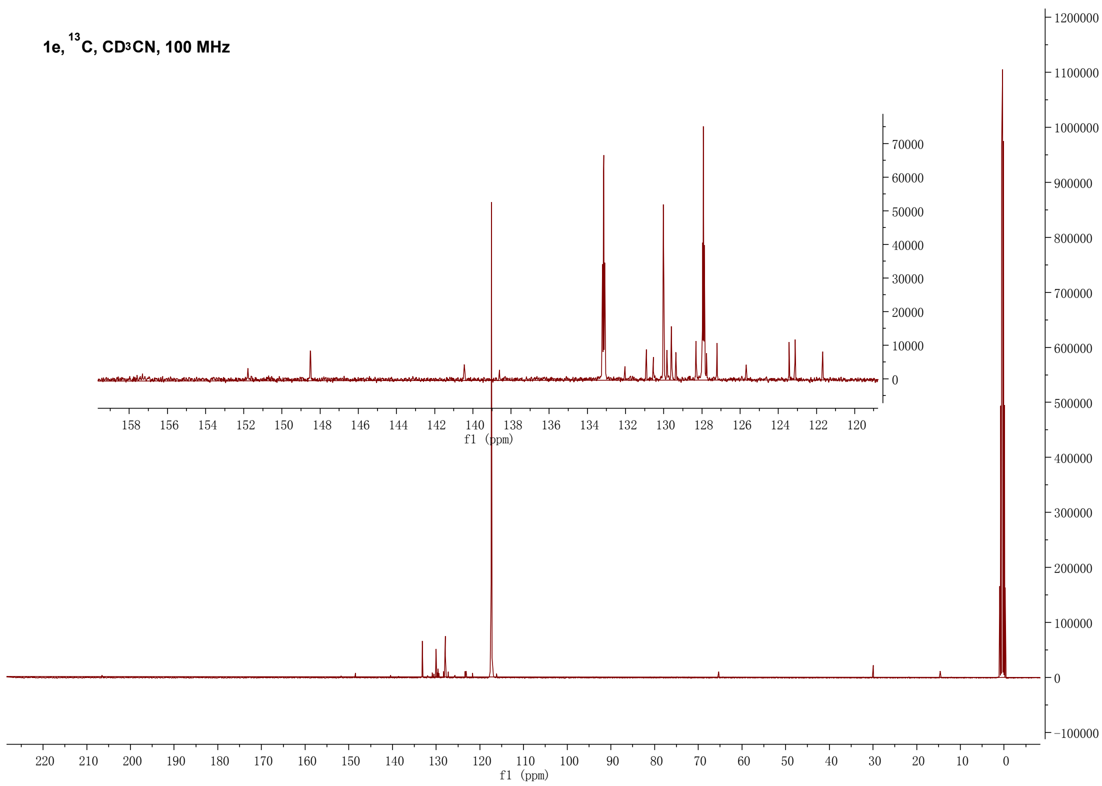


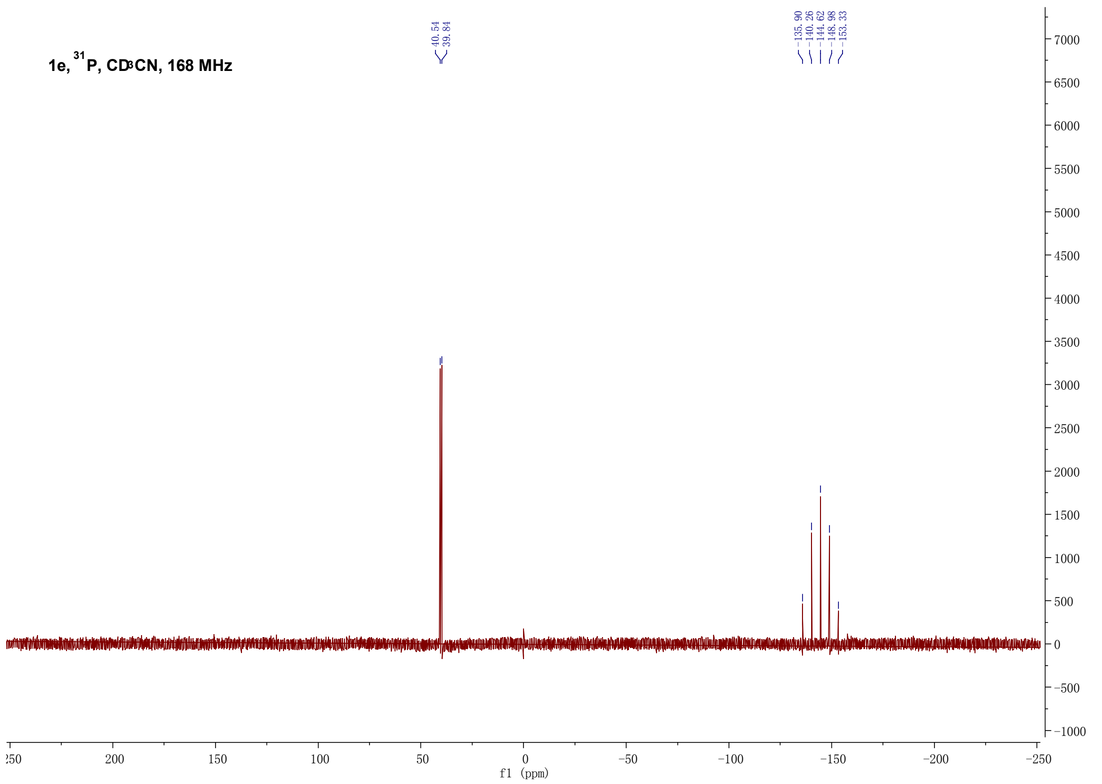

1d, 31P, CD3CN, 121 MHz
f1 (ppm)

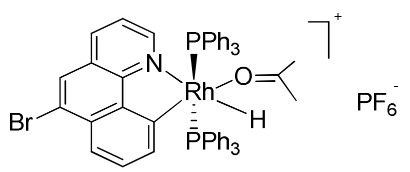

PPh3
N
Rh
O
H
PPh3
+
PF6
−

1e


1e, 1H, CD3CN, 400 MHz
f1 (ppm)

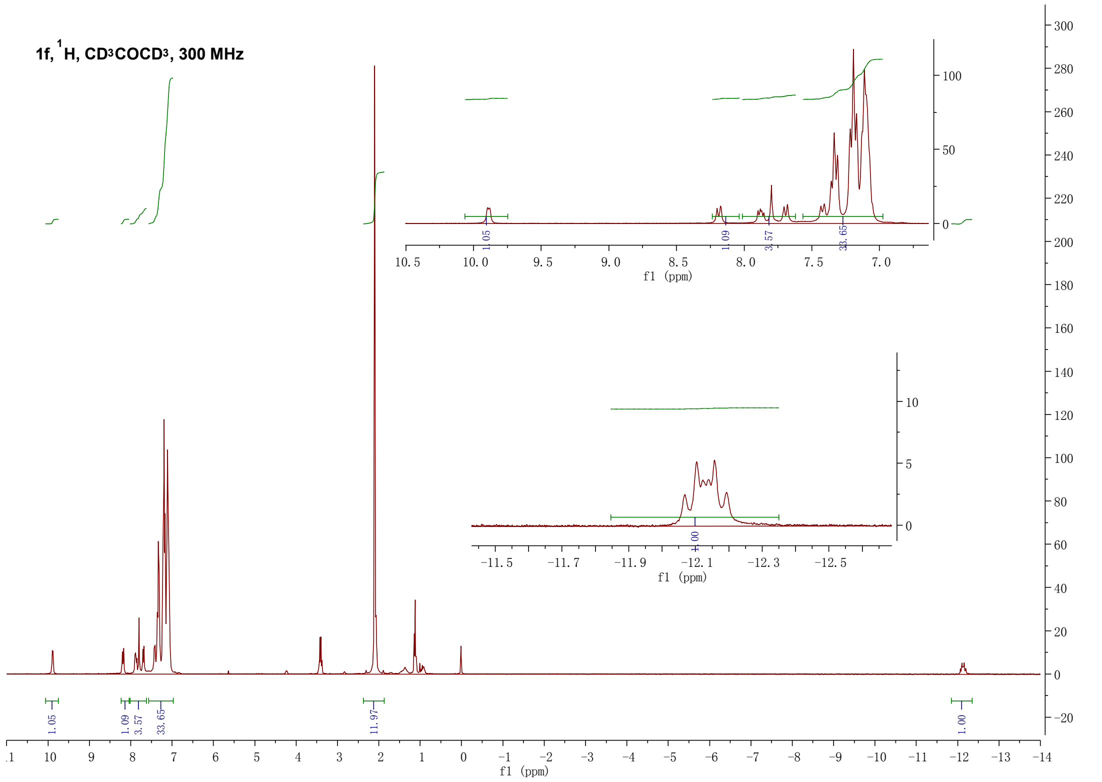

1e, 13C, CD3CN, 100 MHz
f1 (ppm)


1e, 31P, CD3CN, 168 MHz
40.54
39.84
-135.90
-140.26
-144.62
-148.98
-153.33
f1 (ppm)

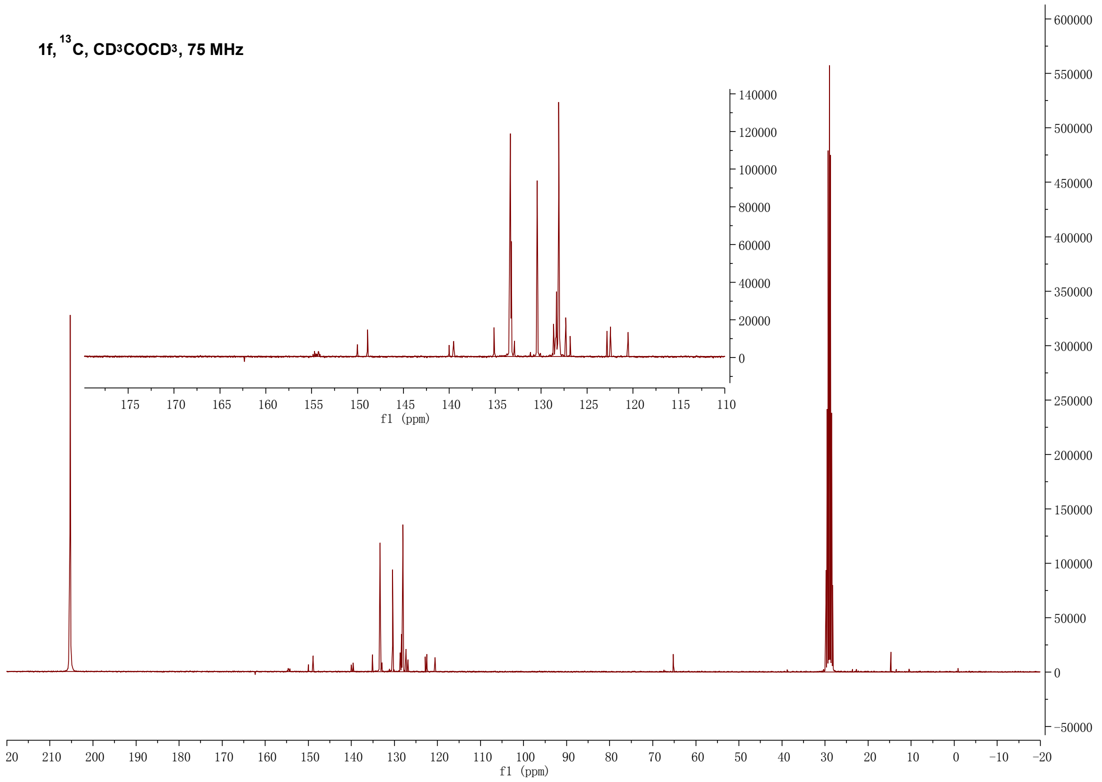

PPh3
N
Rh
O
H
Br
PPh3
PF6-
+

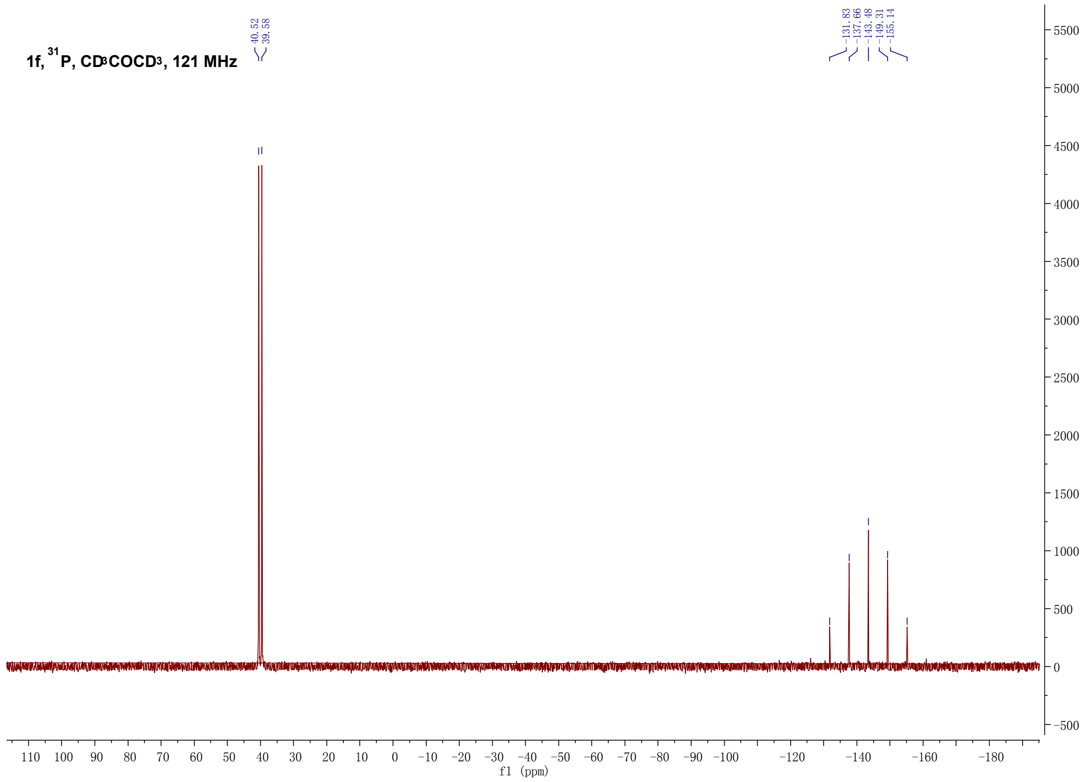
1f

1f, ^{1}H, CD_3COCD_3, 300 MHz

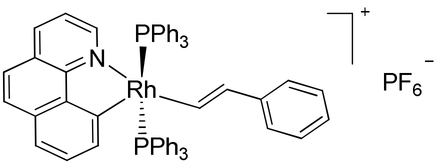


1f, ^{13}C, CD_3COCD_3, 75 MHz



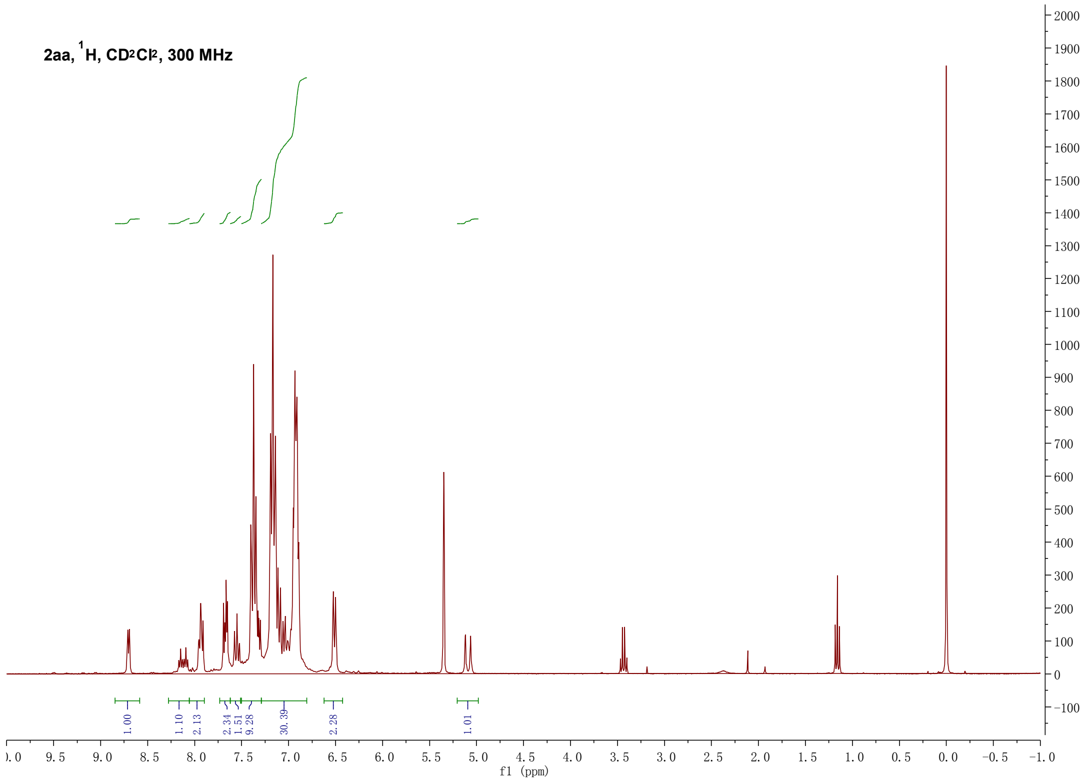


Five-coordinate Intermediate 2

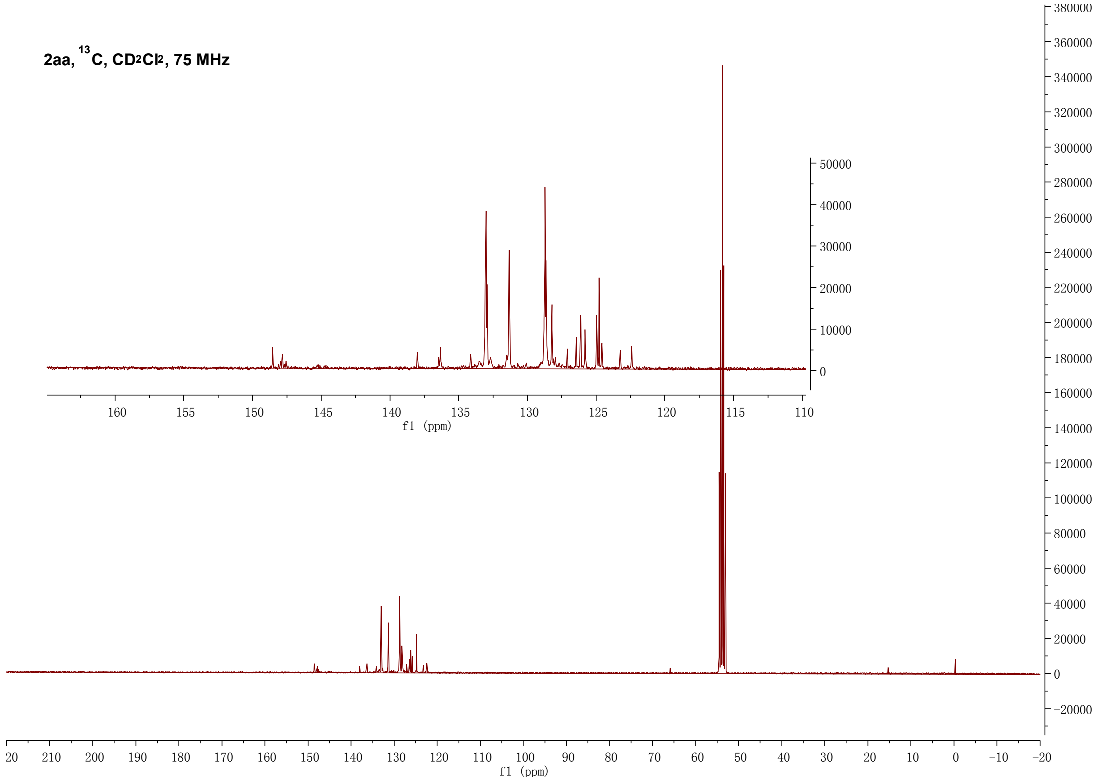


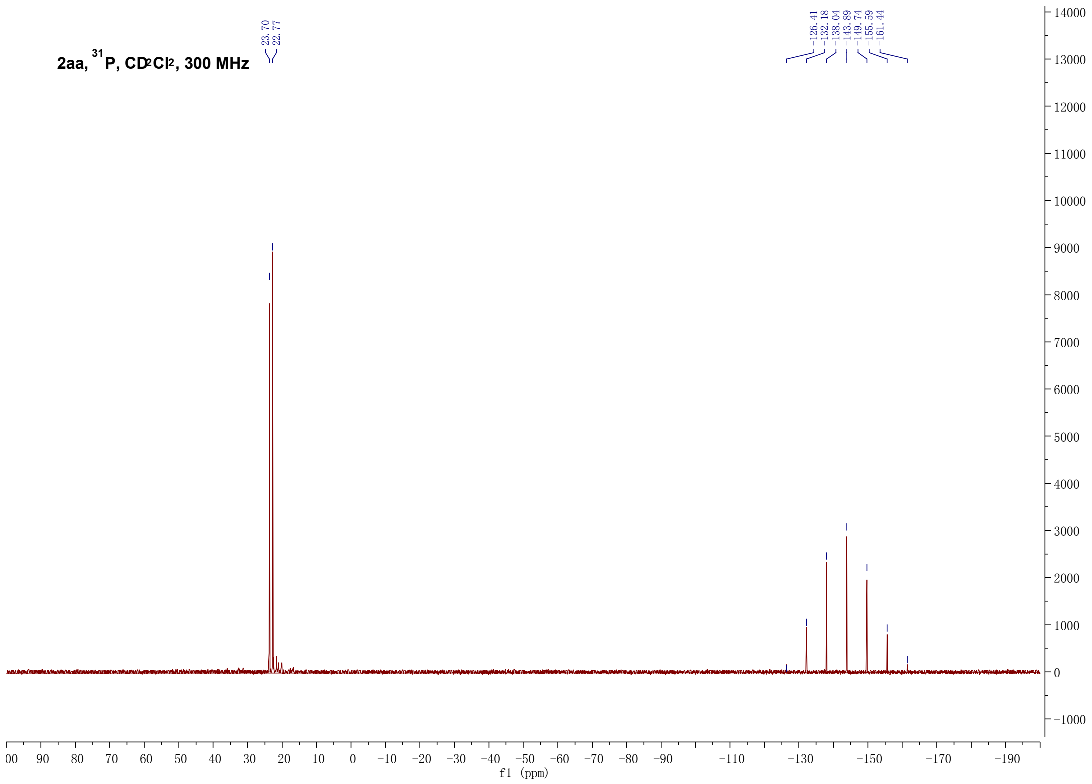
2aa

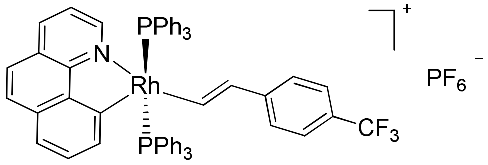
2aa, ^{1}H, CD_2Cl_2, 300 MHz



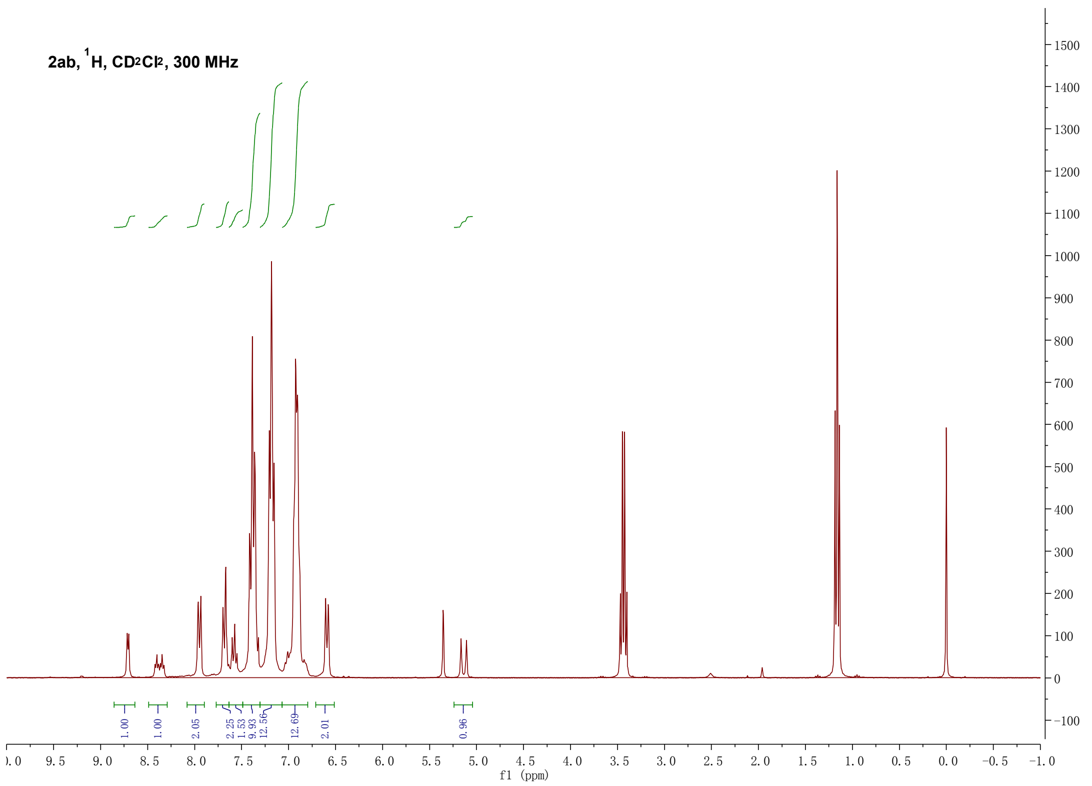
2aa, ^{13}C, CD_2Cl_2, 75 MHz

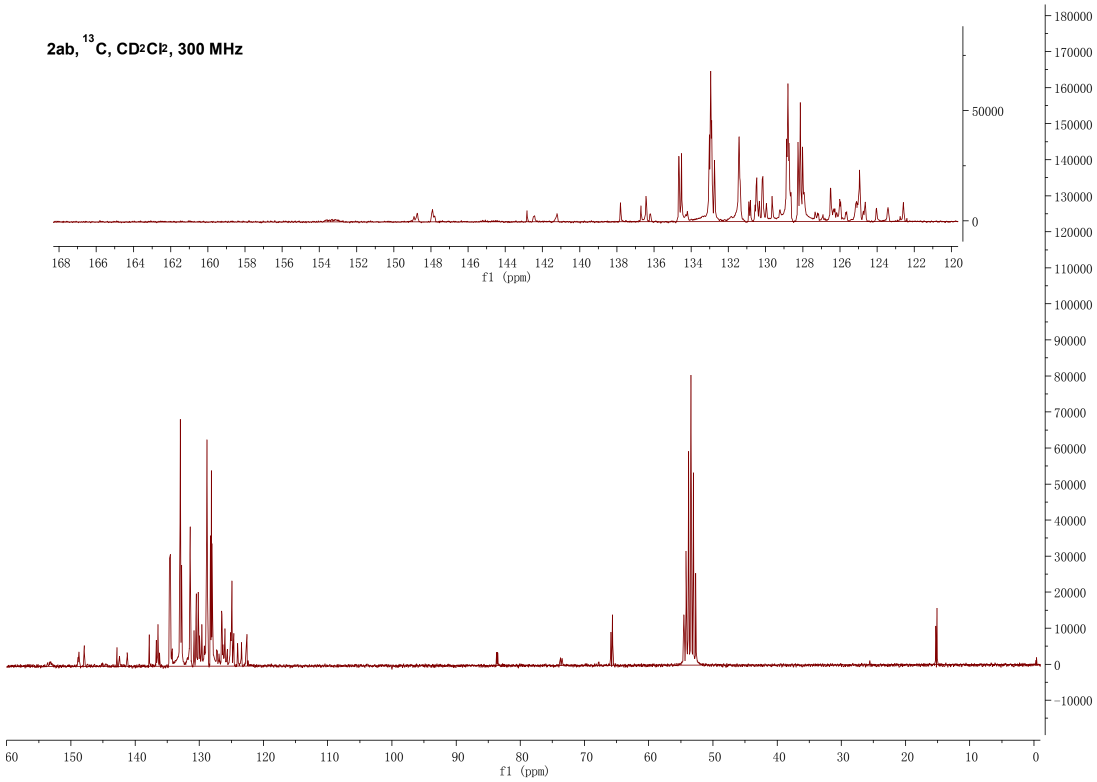


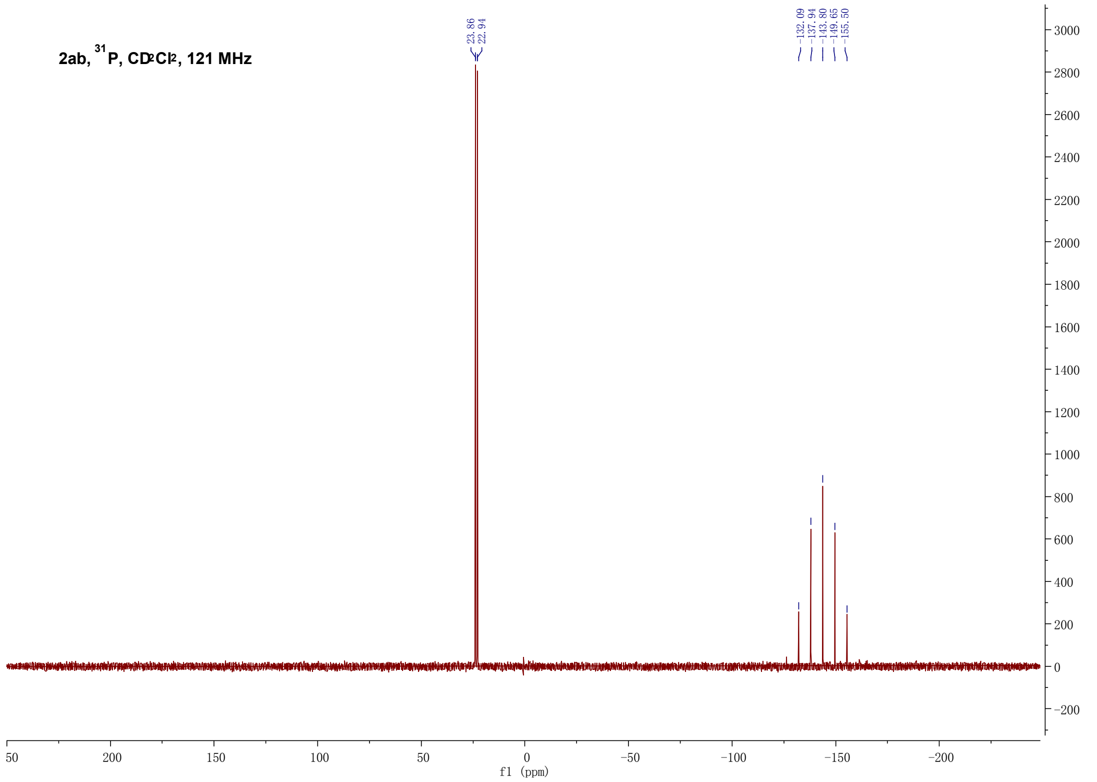

2aa, ³¹P, CD2Cl2, 300 MHz
23.70
22.77
-126.41
-132.18
-138.04
-143.89
-149.74
-155.59
-161.44
f1 (ppm)

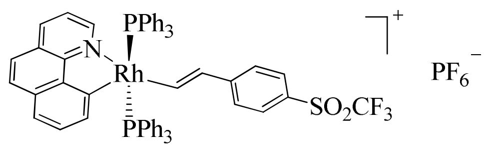

PPh3
N
Rh
PPh3
CF3
+
PF6
–

2ab

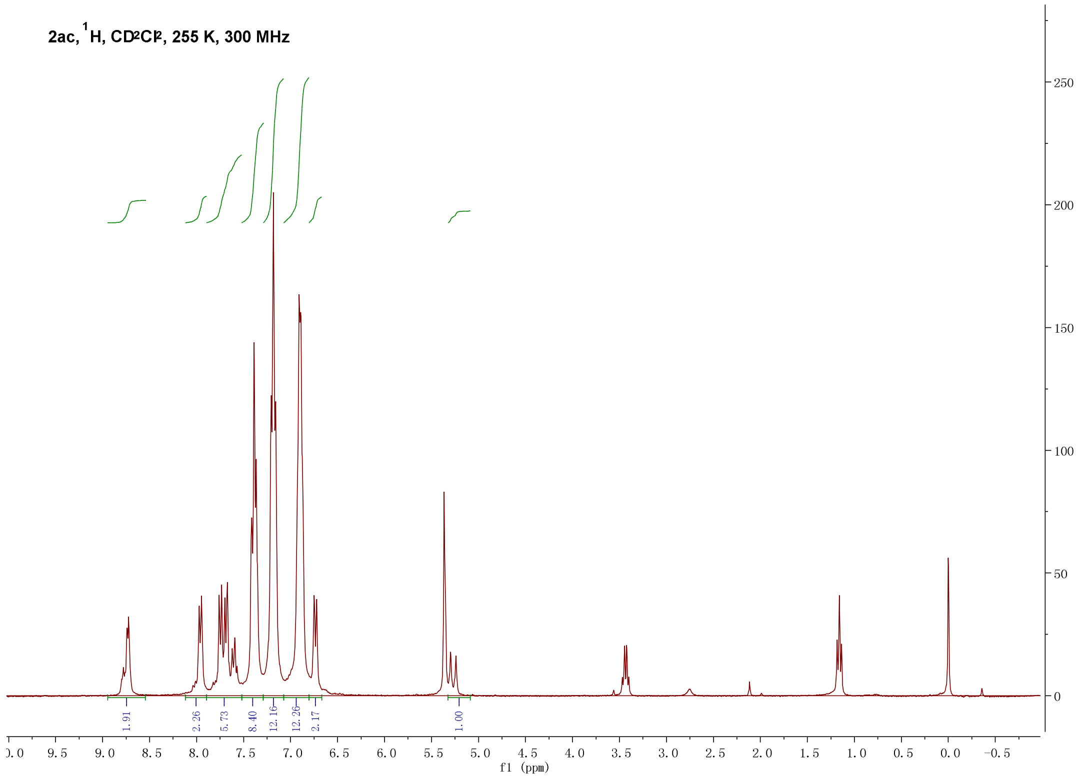

2ab, ¹H, CD2Cl2, 300 MHz
1.00
1.00
2.05
2.25
1.53
9.93
12.56
12.69
2.01
0.96
f1 (ppm)


2ab, 13C, CD2Cl2, 300 MHz
f1 (ppm)
f1 (ppm)

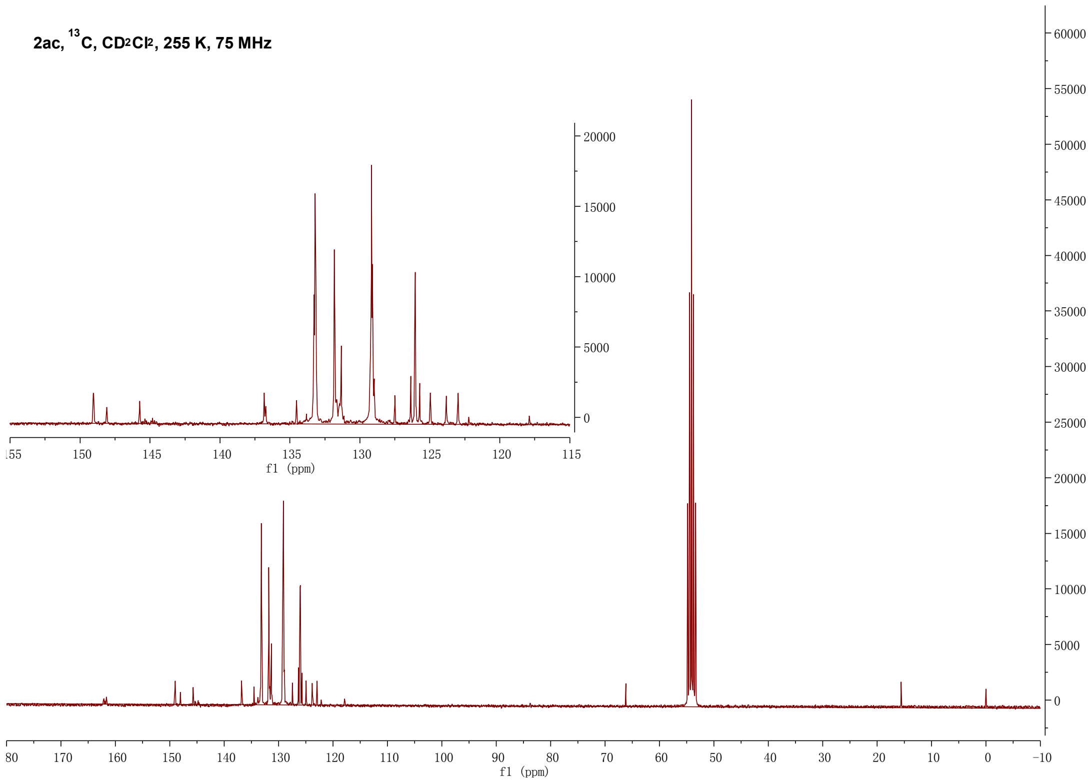

2ab, 31P, CD2Cl2, 121 MHz
23.86
22.94
-132.09
-137.94
-143.80
-149.65
-155.50
f1 (ppm)



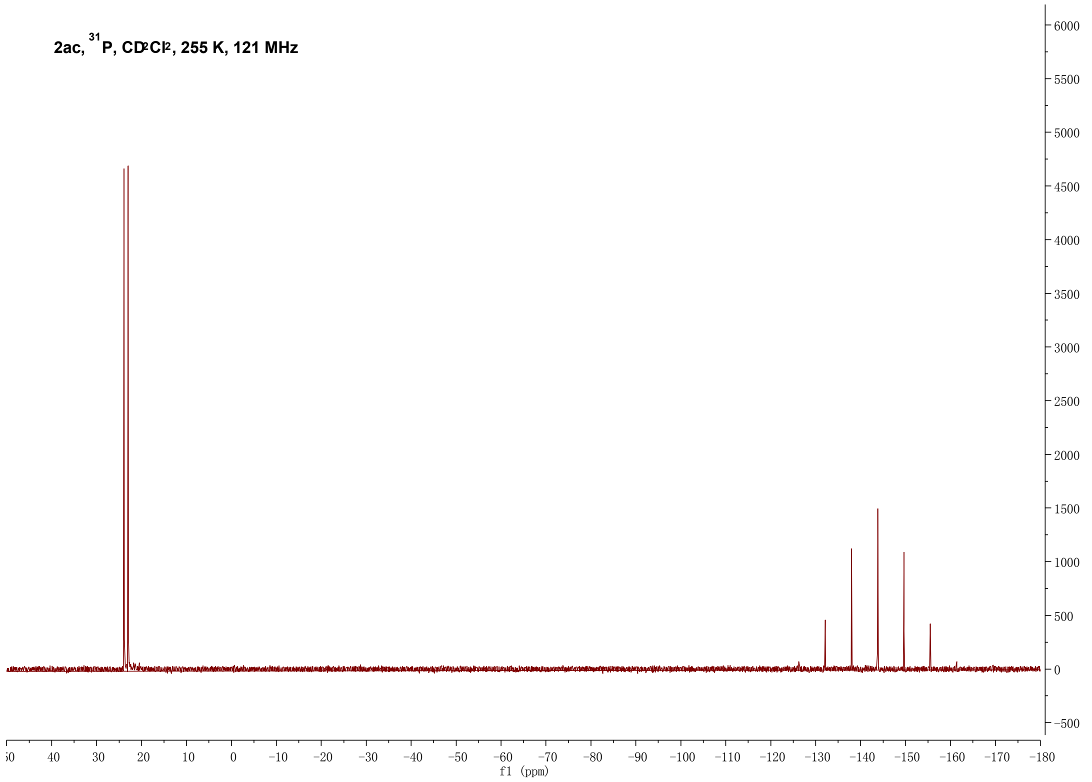
2ac

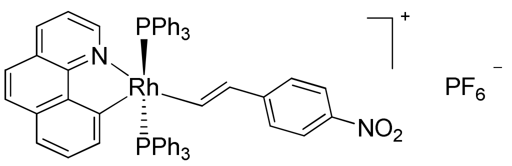


2ac, ¹H, CD2Cl2, 255 K, 300 MHz
f1 (ppm)

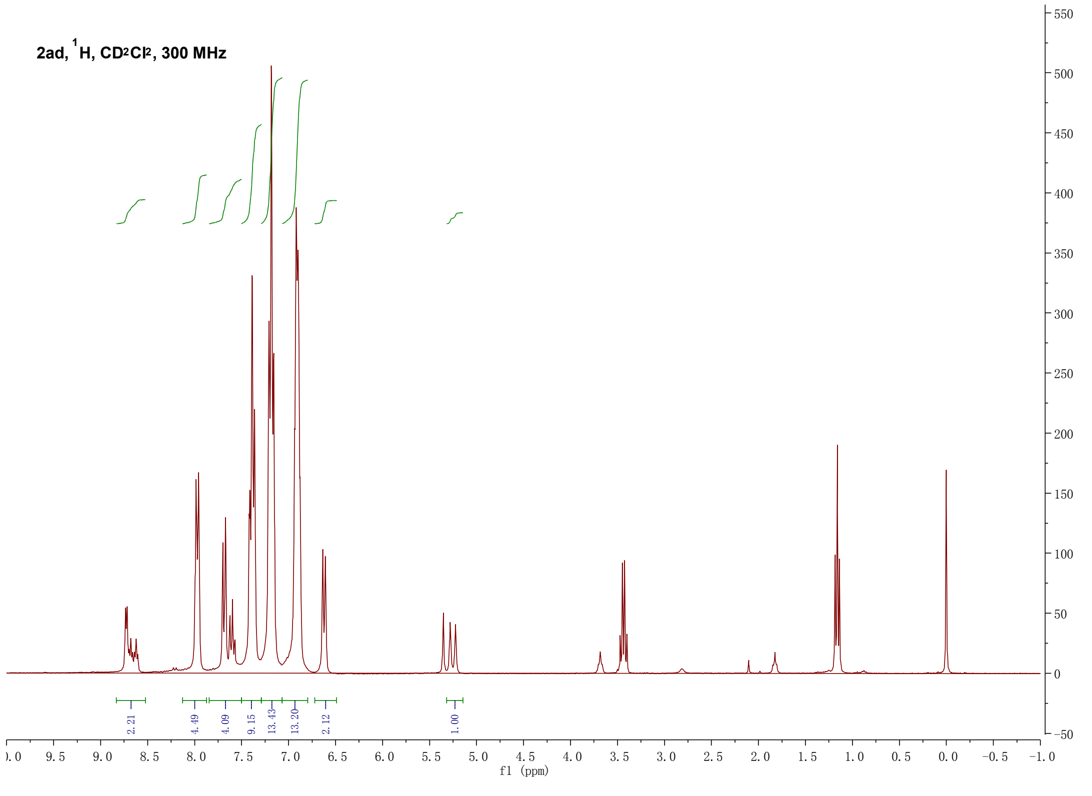


2ac, ¹³C, CD2Cl2, 255 K, 75 MHz
f1 (ppm)

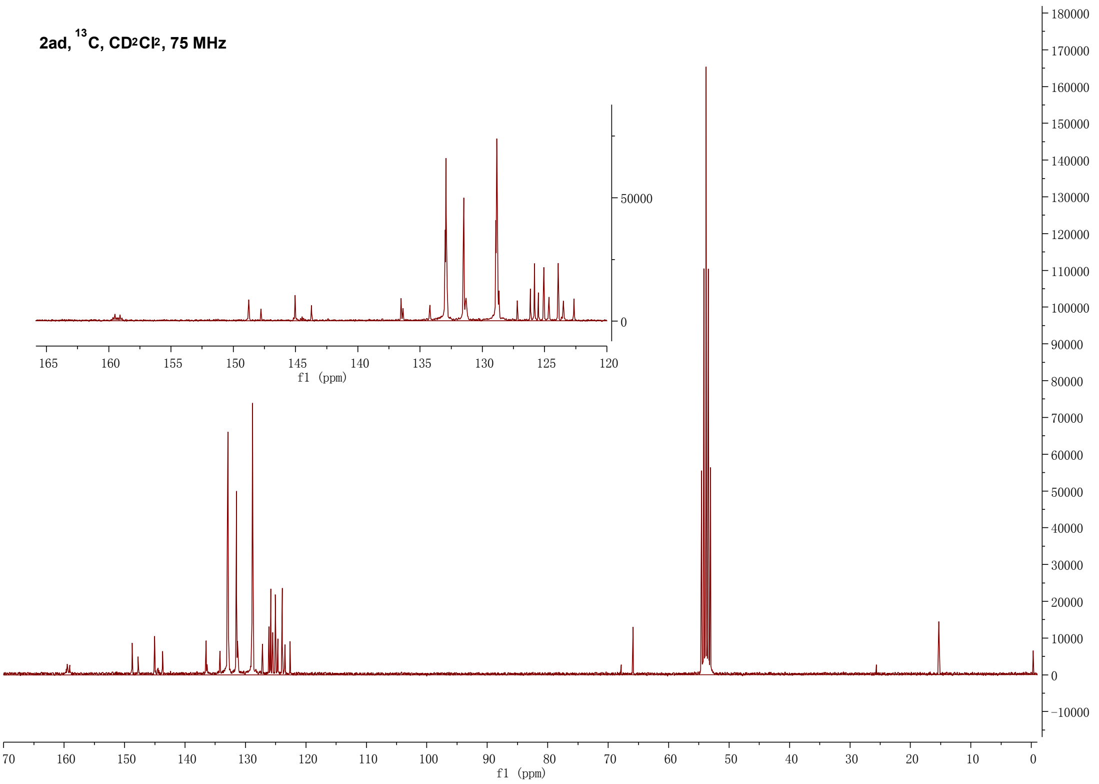




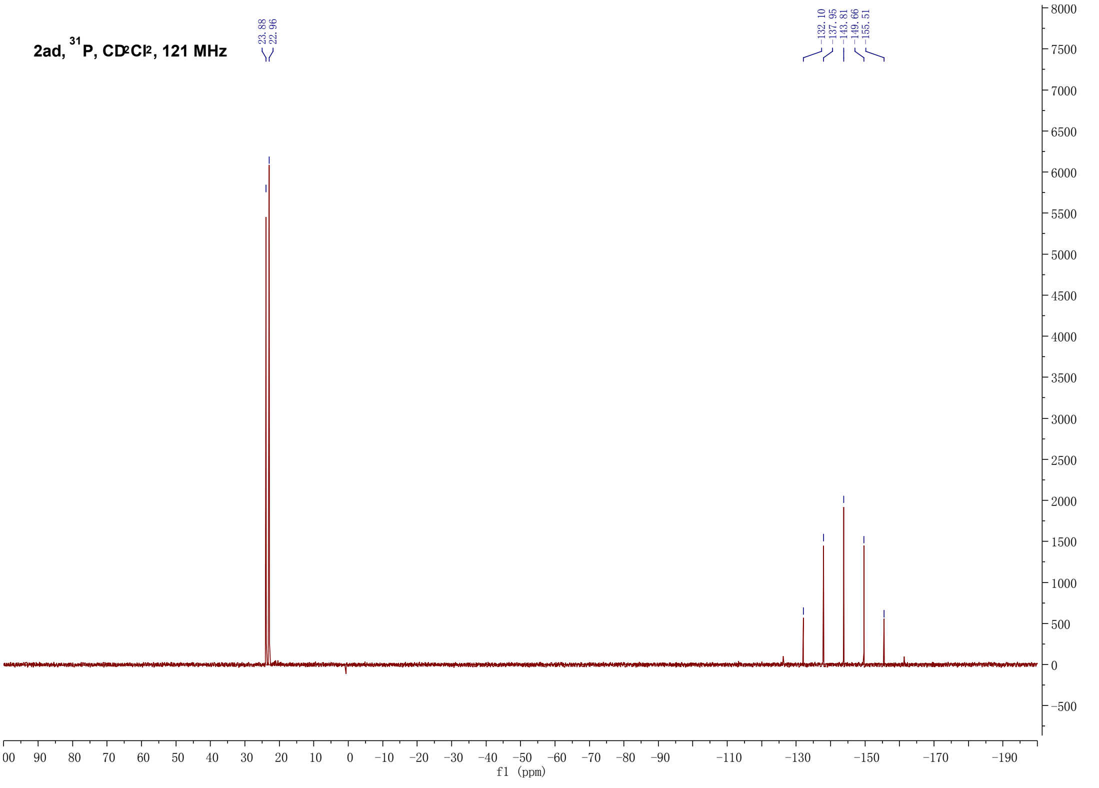
2ad



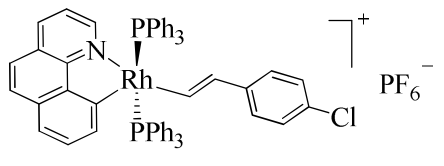
2ad, ^{13}C, CD_2Cl_2, 75 MHz



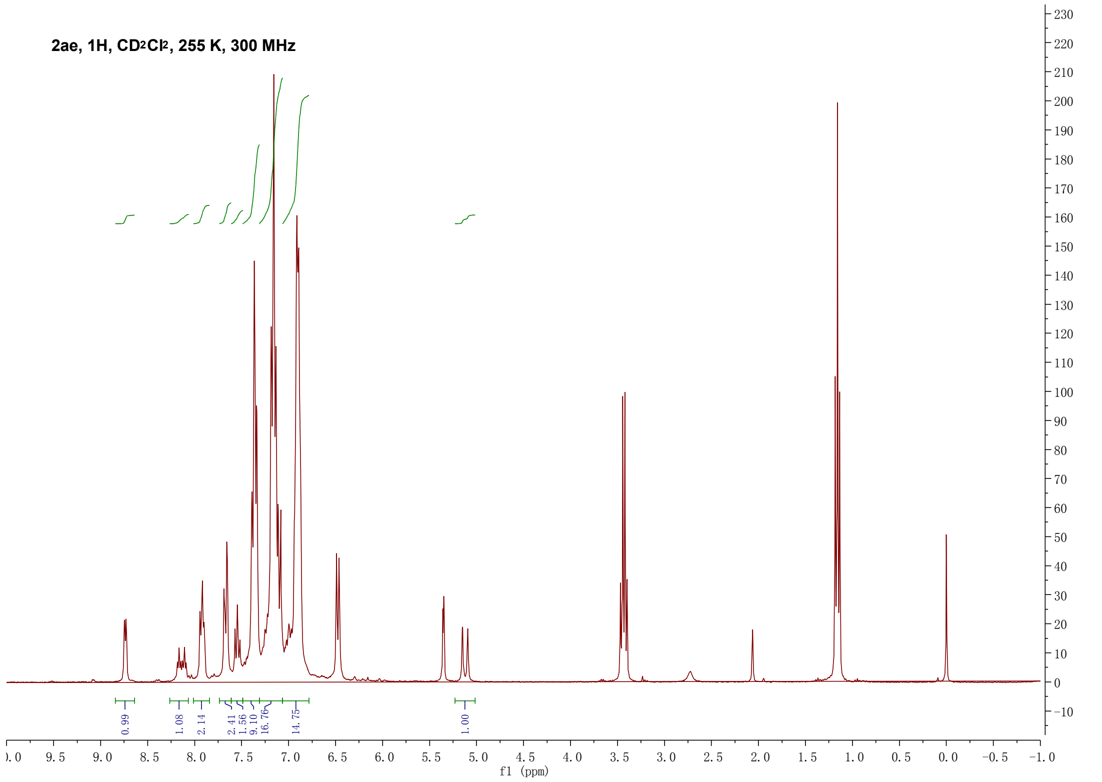
2ad, ^{31}P, CD_2Cl_2, 121 MHz



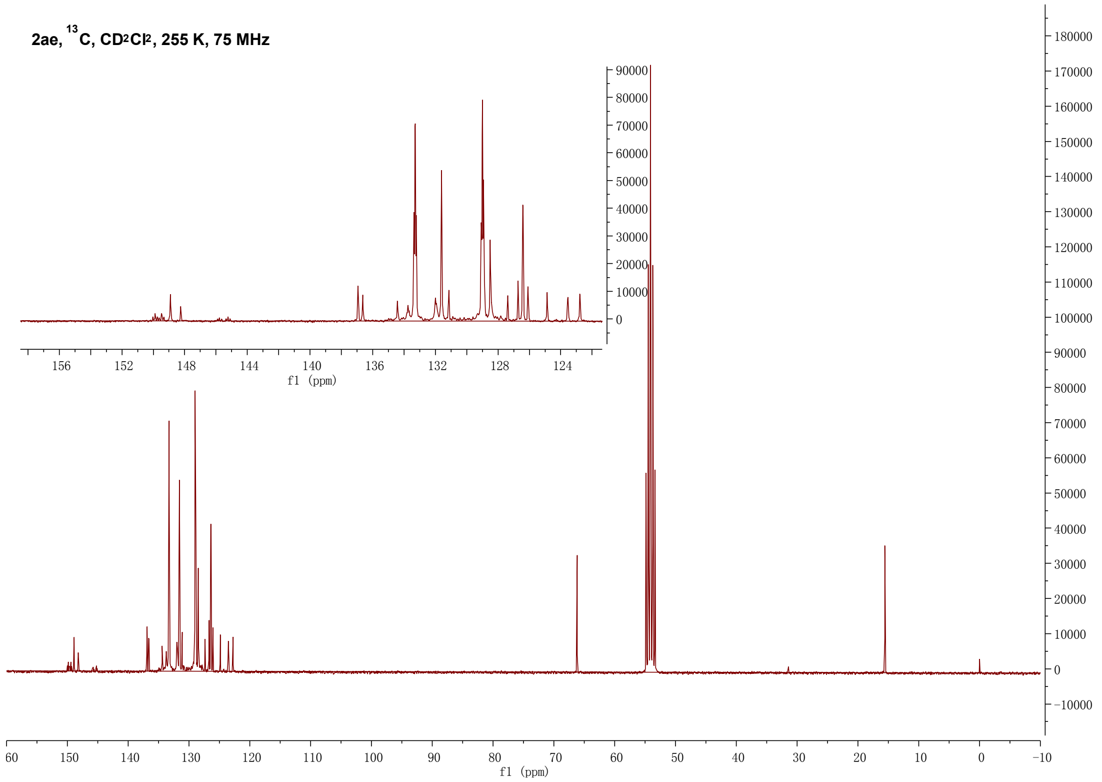
2ae

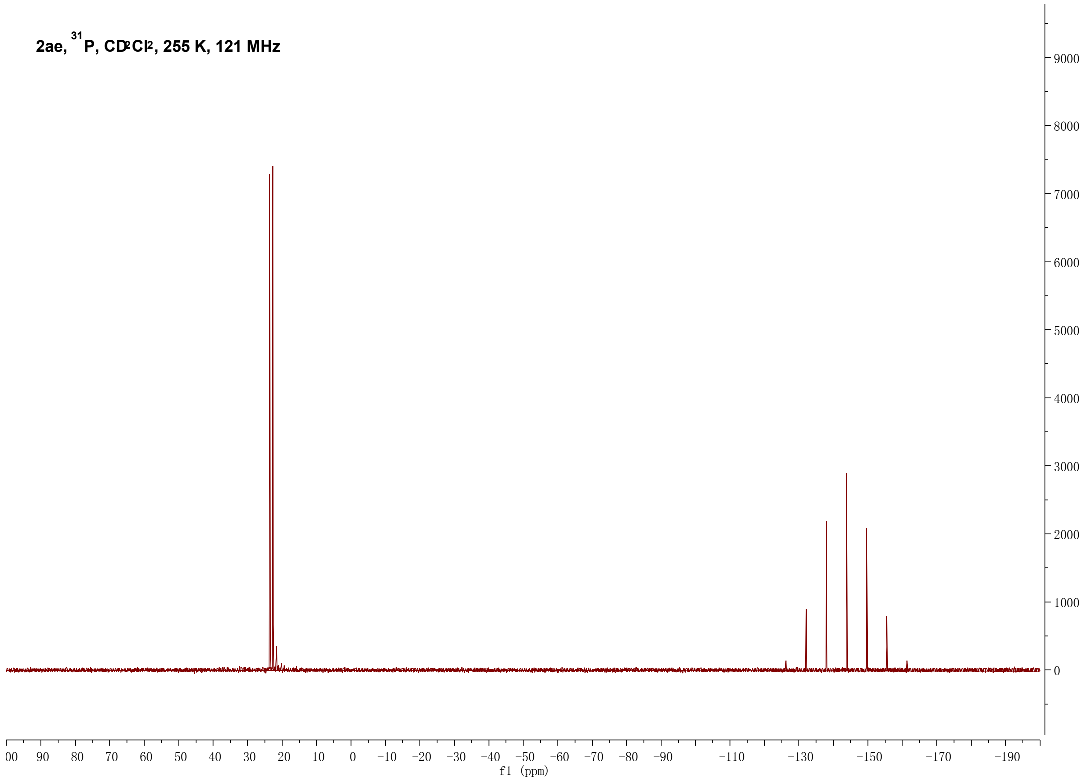


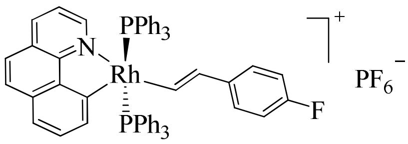
2ae, 1H, CD2Cl2, 255 K, 300 MHz



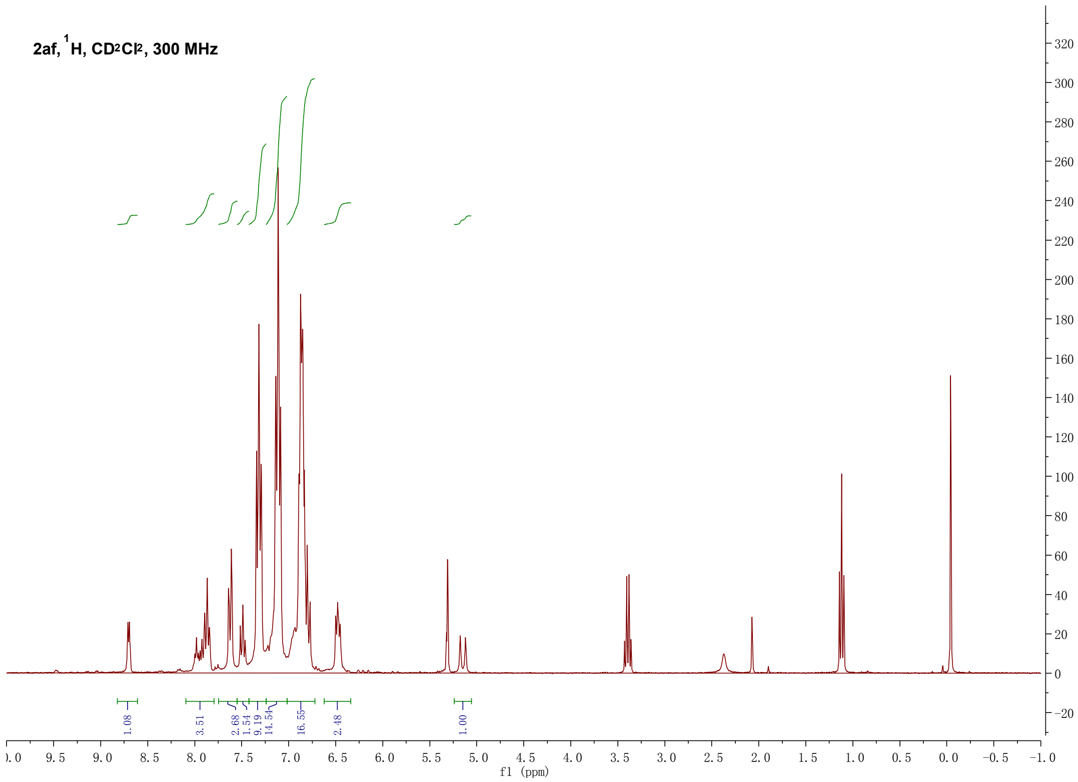
2ae, 13C, CD2Cl2, 255 K, 75 MHz

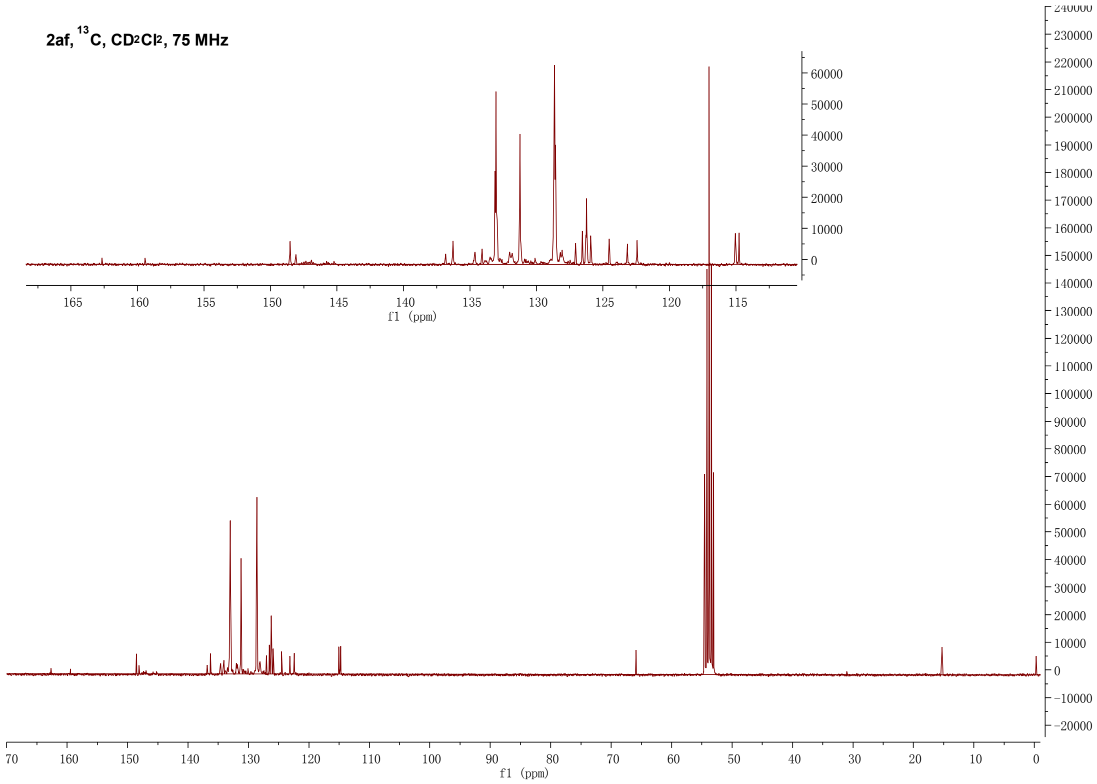


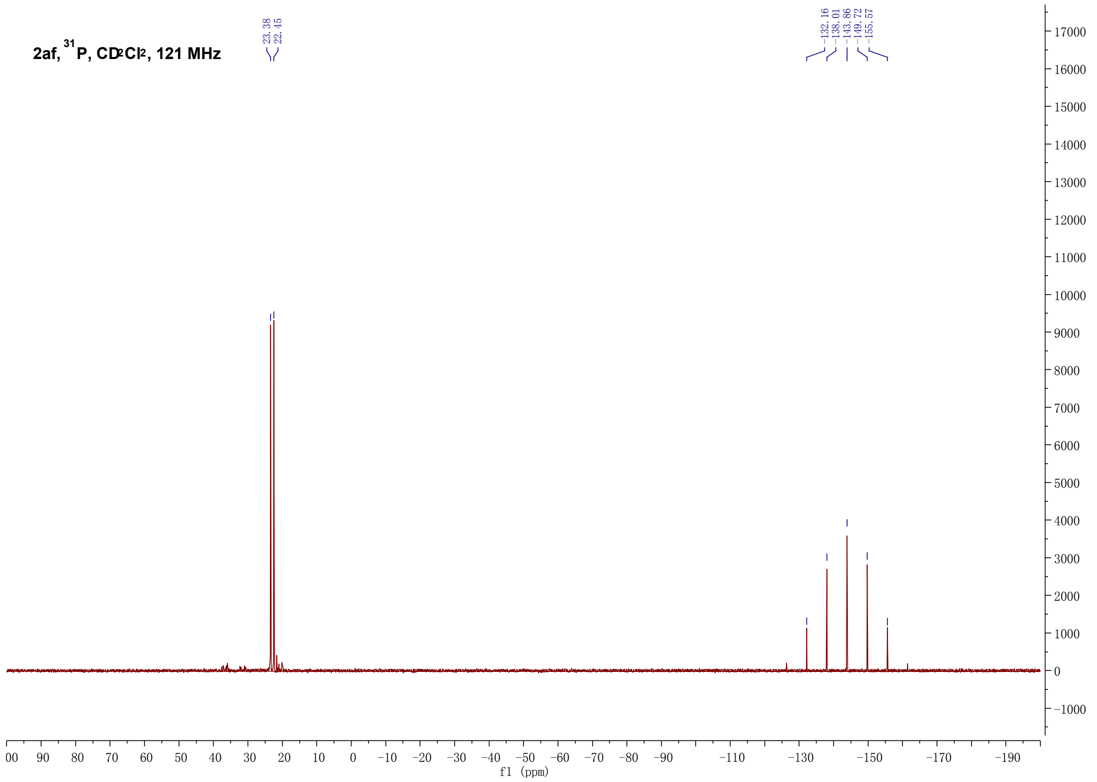

2ae, 31P, CD2Cl2, 255 K, 121 MHz
f1 (ppm)

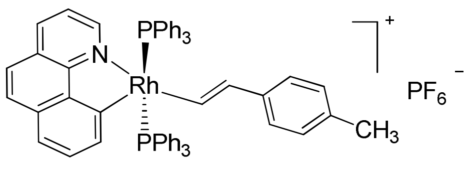

PPh3
N
Rh
PPh3
F
+
PF6
−

2af


2af, 1H, CD2Cl2, 300 MHz
1.08
3.51
2.68
1.54
9.19
14.54
16.55
2.48
1.00
f1 (ppm)

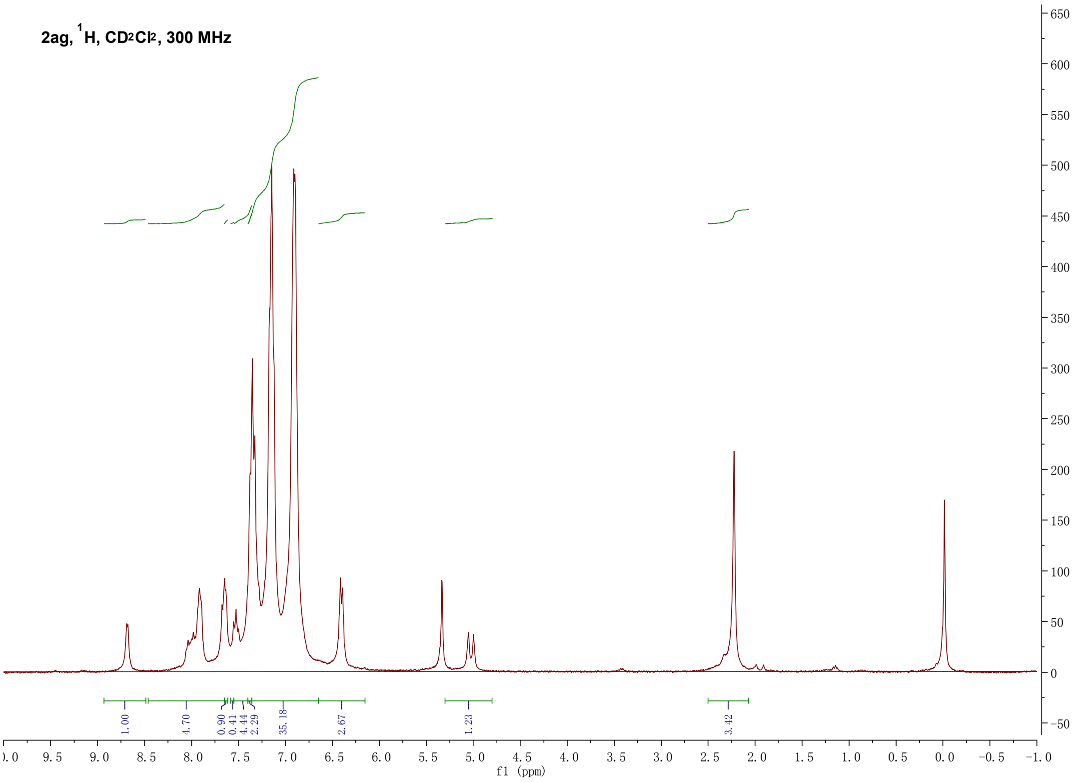

2af, 13C, CD2Cl2, 75 MHz
f1 (ppm)


2af, 31P, CD2Cl2, 121 MHz
23.38
22.45
-132.16
-138.01
-143.86
-149.72
-155.57
f1 (ppm)

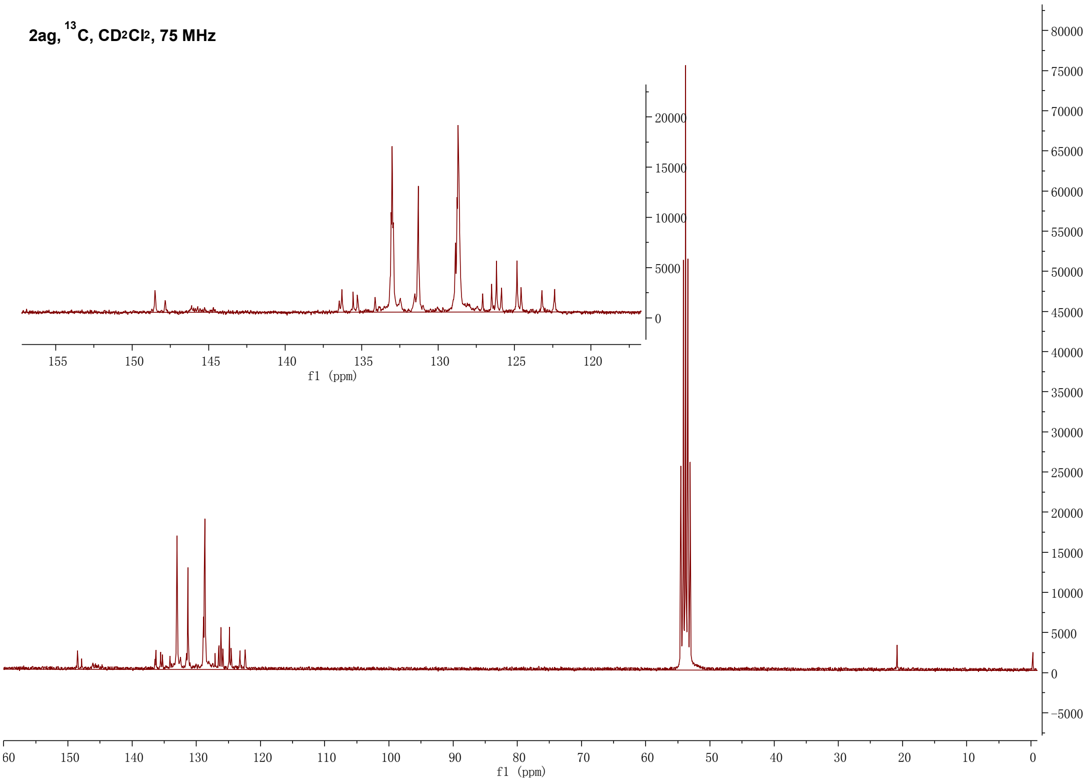

PPh3
N
Rh
PPh3
CH3
PF6

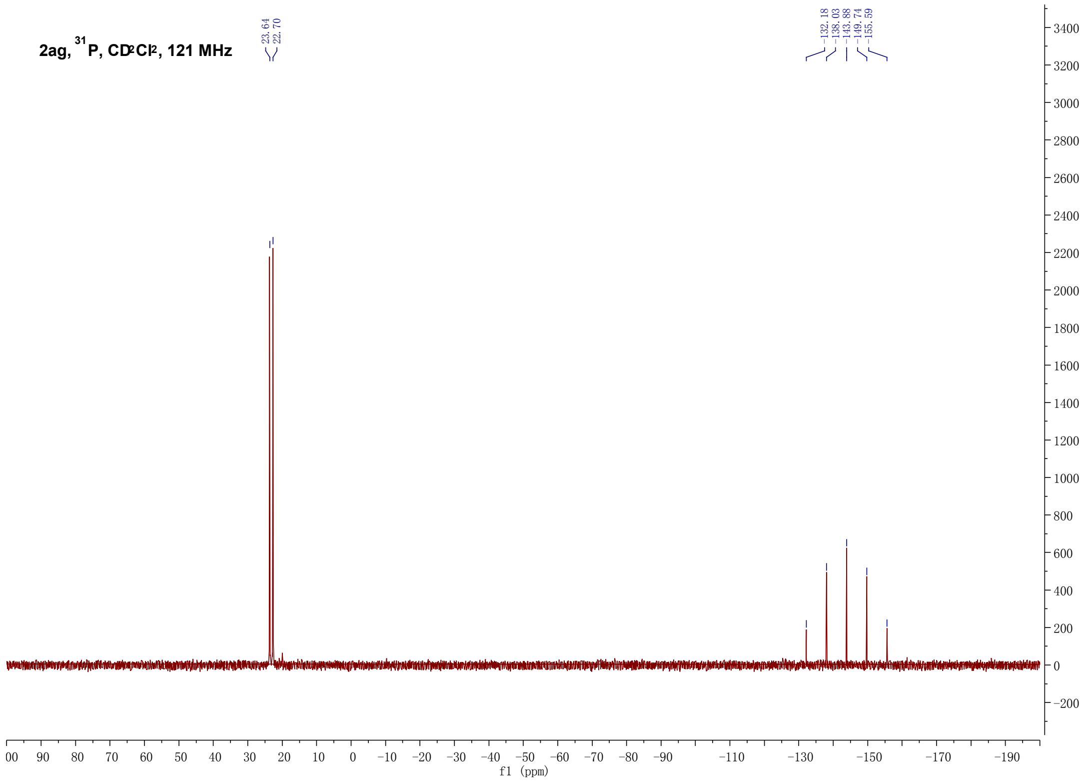
2ag

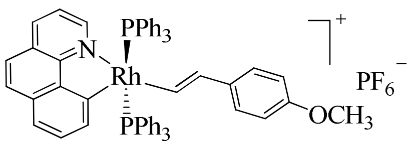
2ag, ^{1}H, CD_2Cl_2, 300 MHz



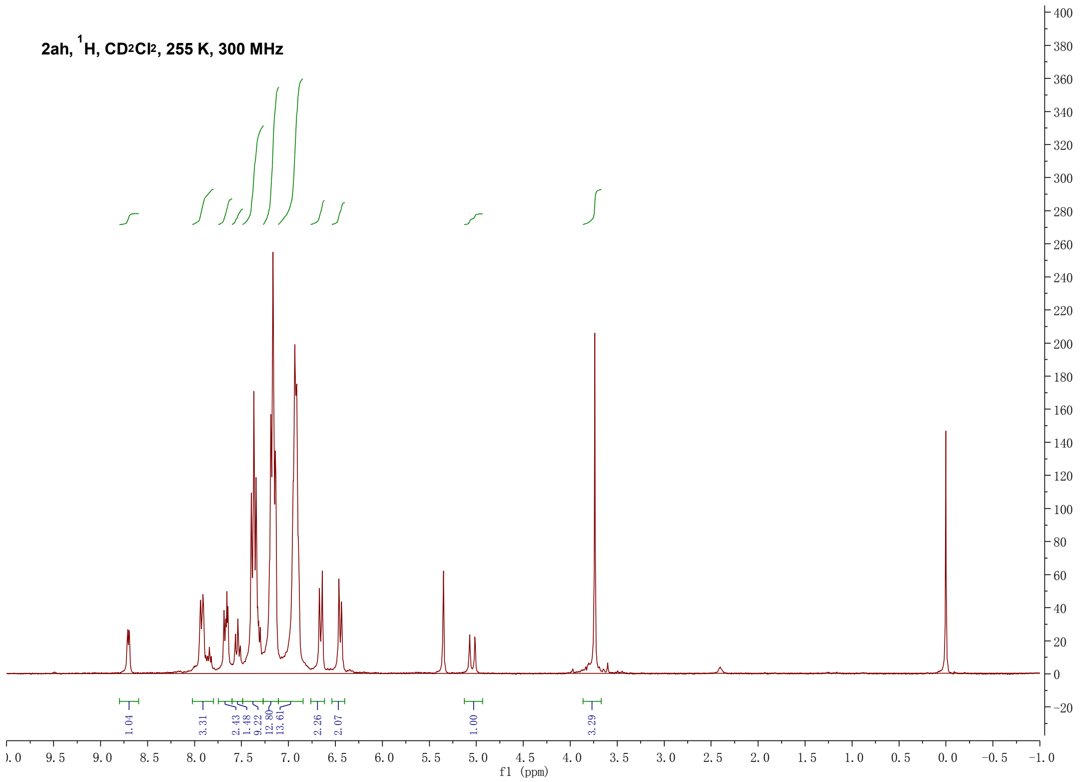
2ag, ^{13}C, CD_2Cl_2, 75 MHz

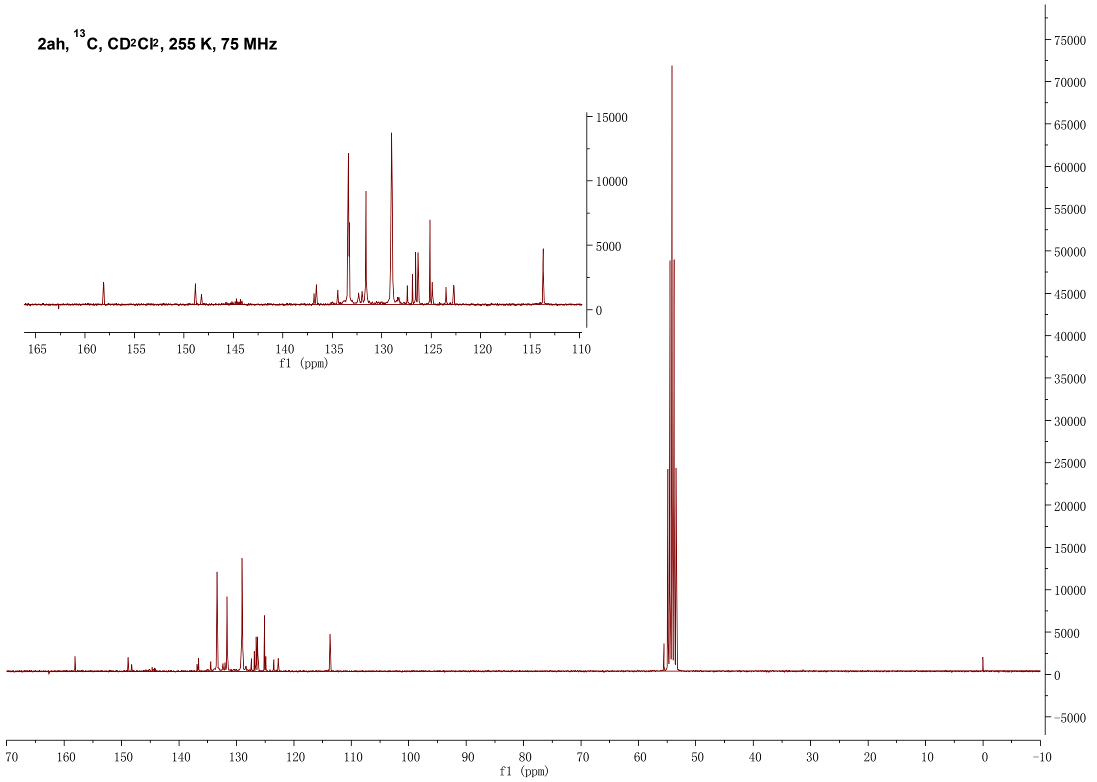


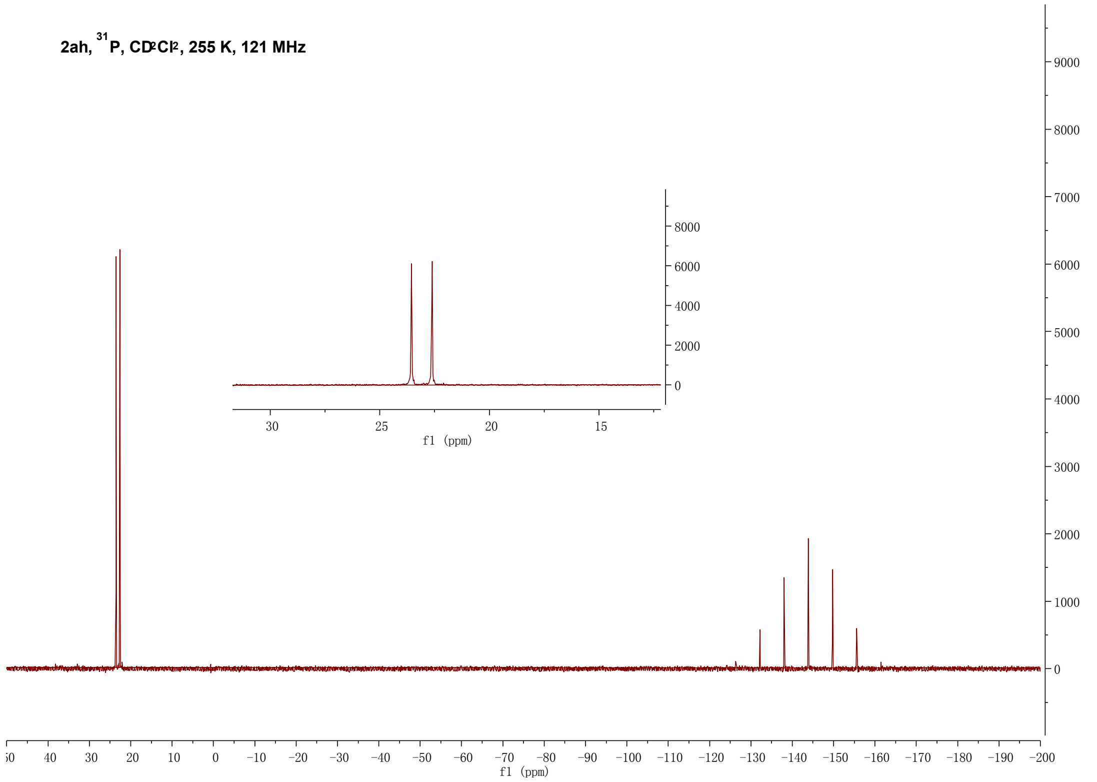

2ag, 31P, CD2Cl2, 121 MHz
23.64
22.70
-132.18
-138.03
-143.88
-149.74
-155.59
f1 (ppm)

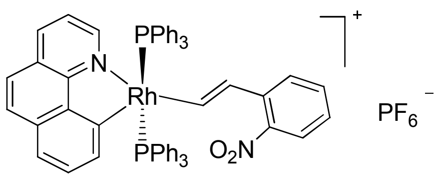

PPh3
N
Rh
PPh3
OCH3
PF6
+
−

2ah

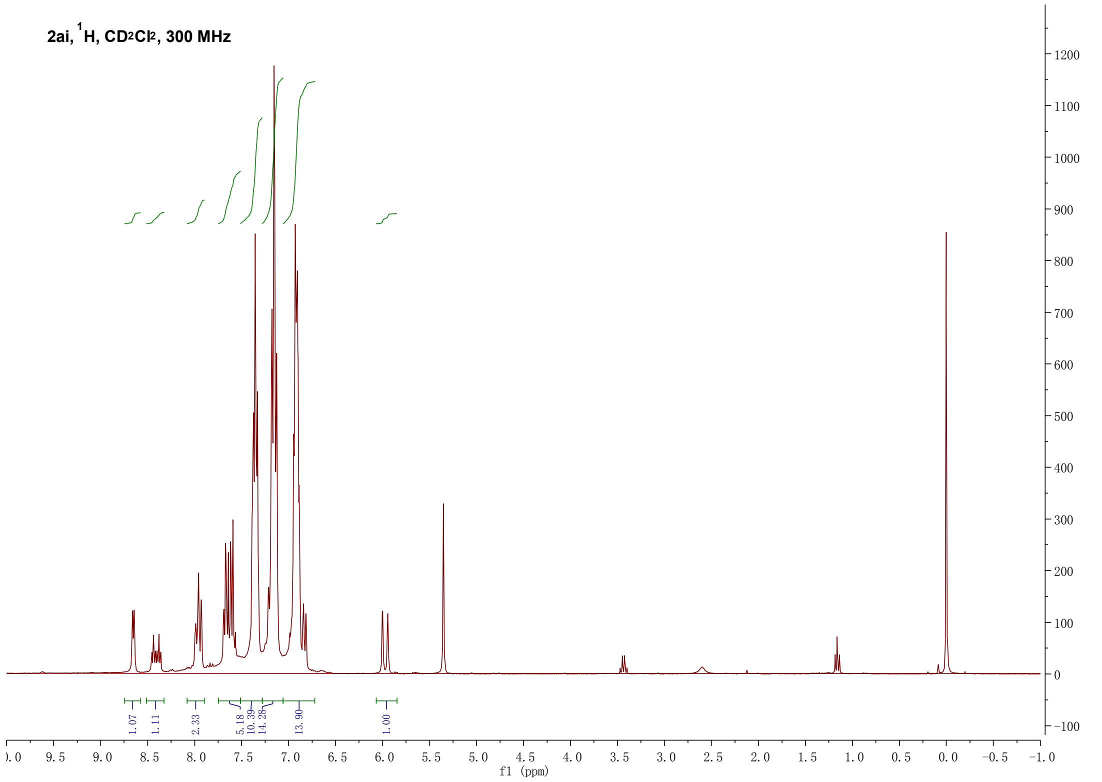

2ah, 1H, CD2Cl2, 255 K, 300 MHz
1.04
3.31
2.43
1.48
9.22
12.80
13.61
2.26
2.07
1.00
3.29
f1 (ppm)

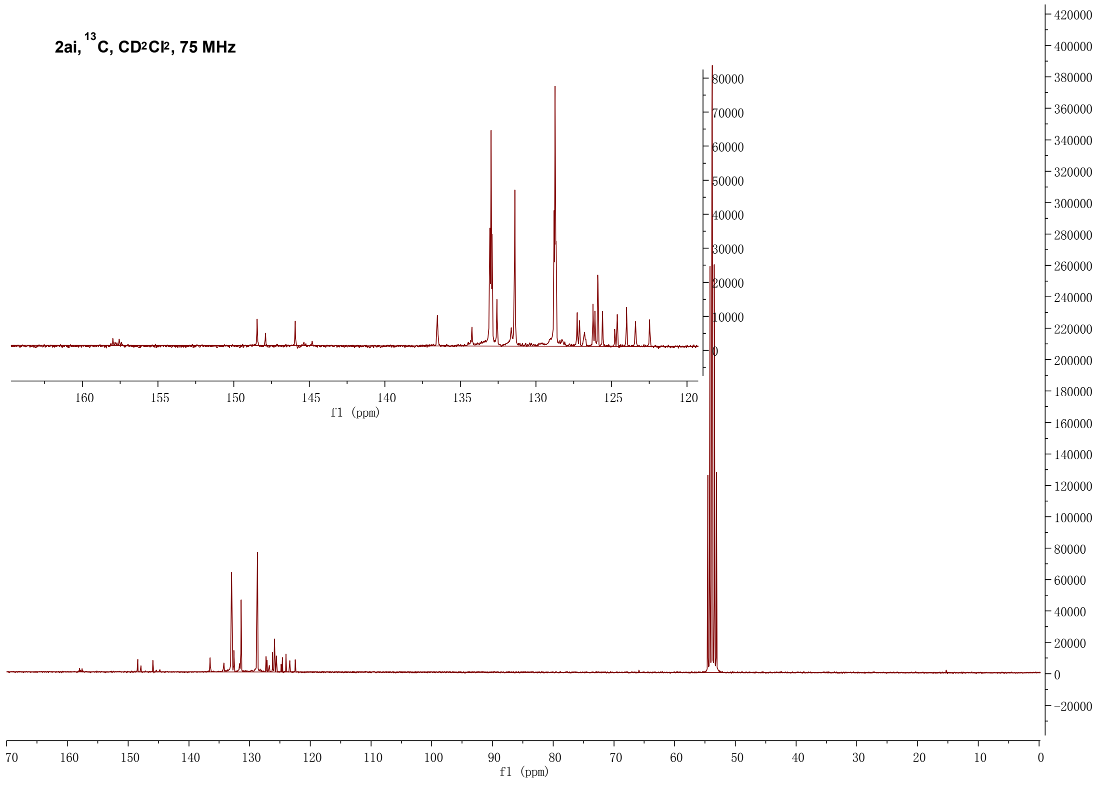

2ah, 13C, CD2Cl2, 255 K, 75 MHz
f1 (ppm)

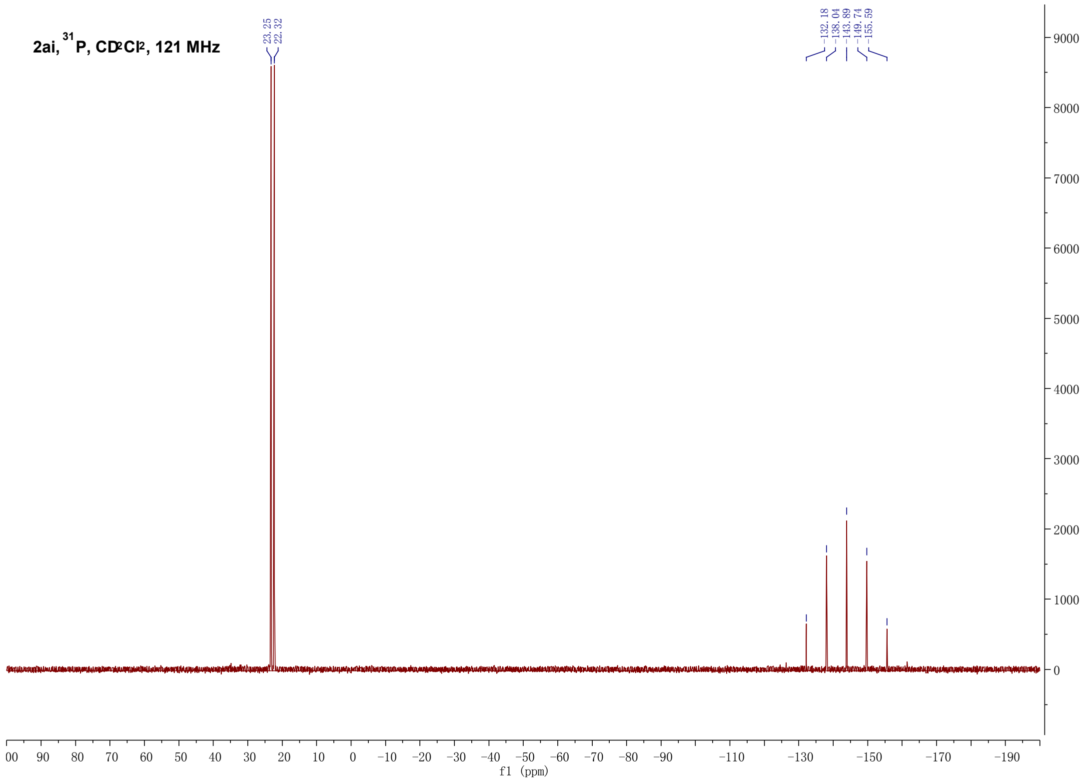

2ah, 31P, CD2Cl2, 255 K, 121 MHz
f1 (ppm)

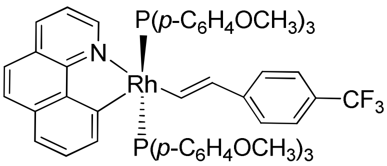

PPh3
N
Rh
PPh3
O2N
PF6

2ai

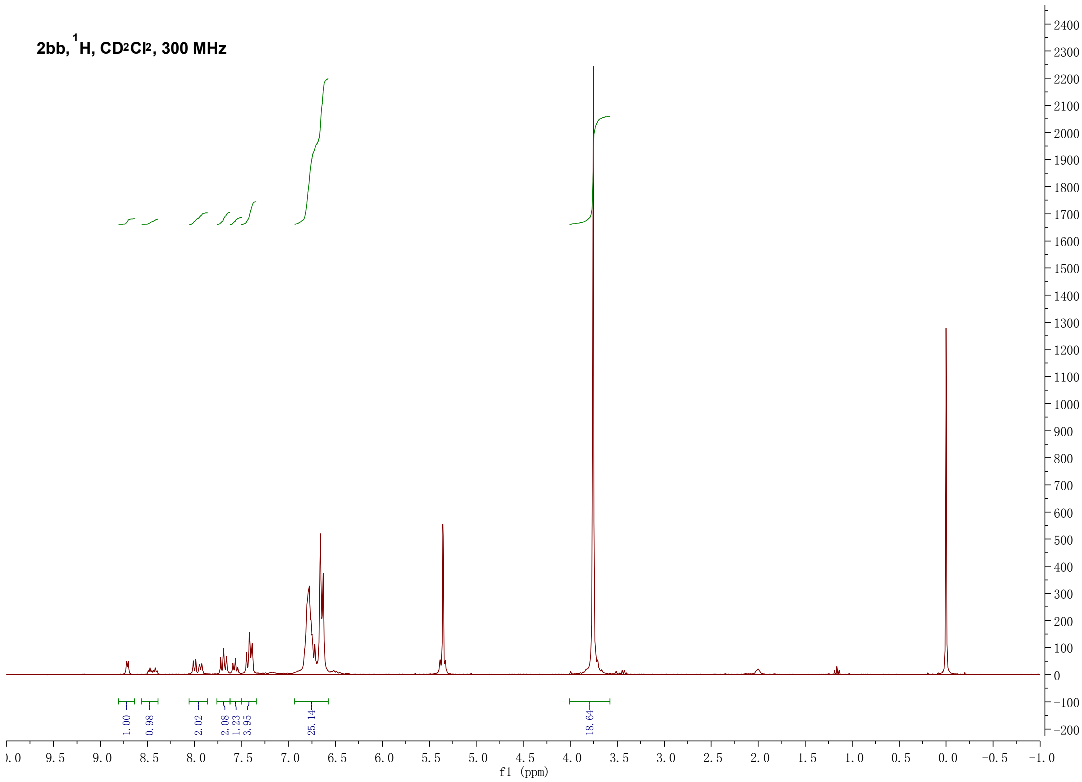

2ai, 1H, CD2Cl2, 300 MHz
f1 (ppm)

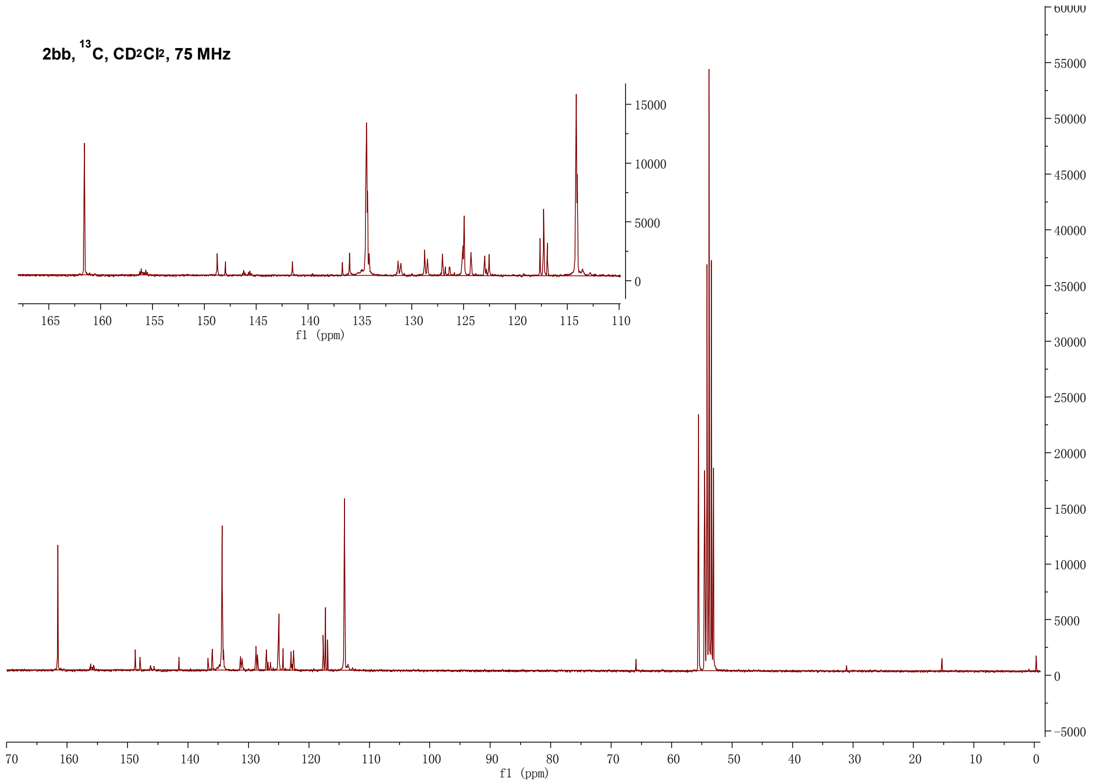

2ai, 13C, CD2Cl2, 75 MHz
f1 (ppm)

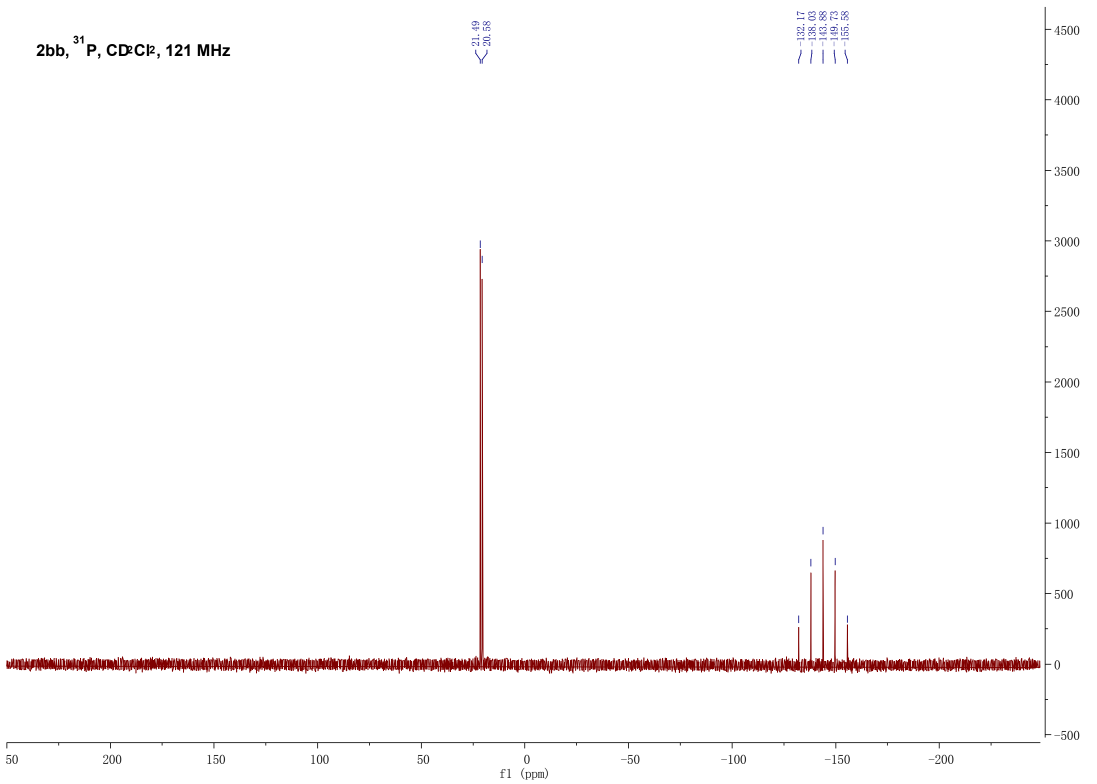

2ai, 31P, CD2Cl2, 121 MHz
23.25
22.32
-132.18
-138.04
-143.89
-149.74
-155.59
f1 (ppm)

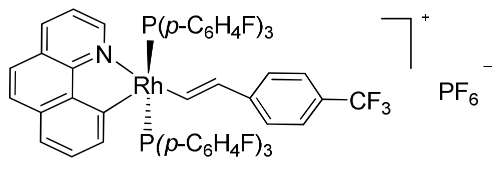

P(p-C6H4OCH3)3
N
Rh
CF3
P(p-C6H4OCH3)3

2bb

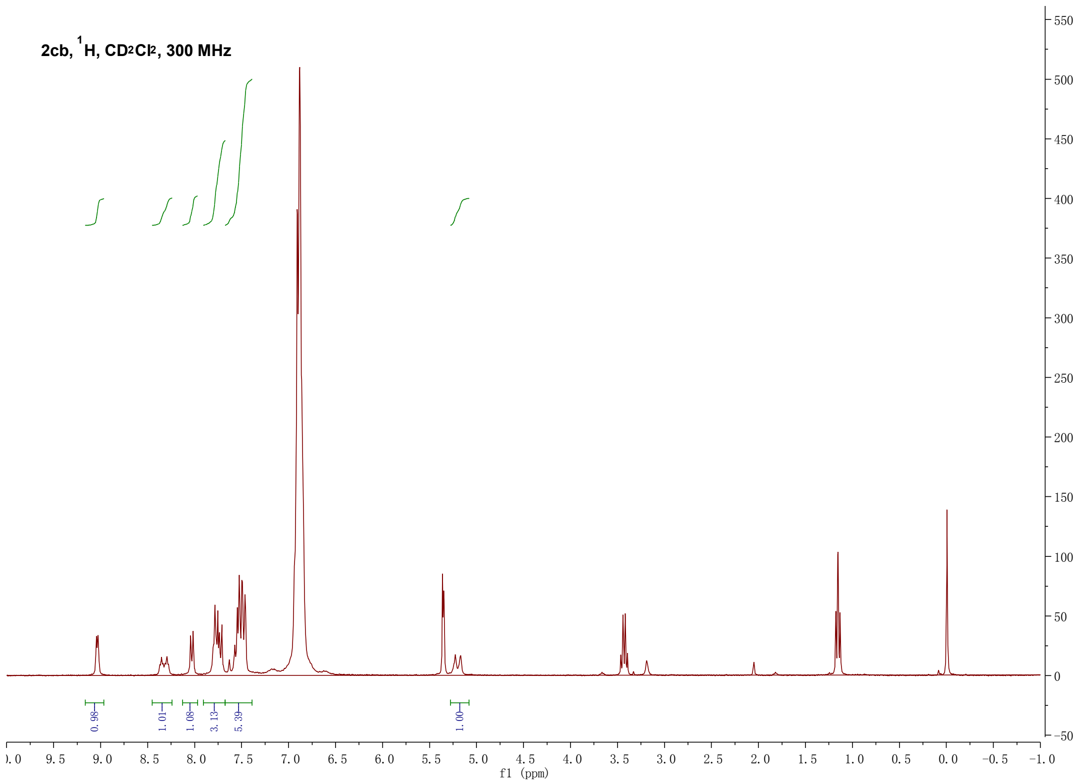

2bb, 1H, CD2Cl2, 300 MHz
1.00
0.98
2.02
2.08
1.23
3.95
25.14
18.64
f1 (ppm)

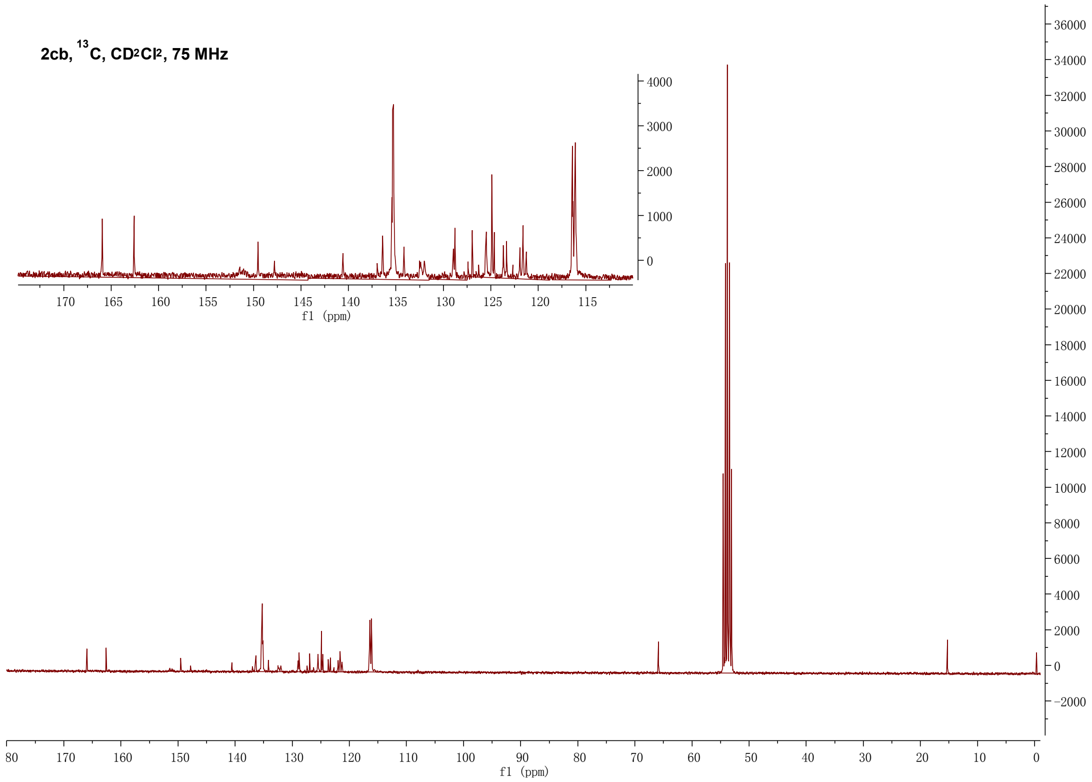

2bb, 13C, CD2Cl2, 75 MHz
f1 (ppm)

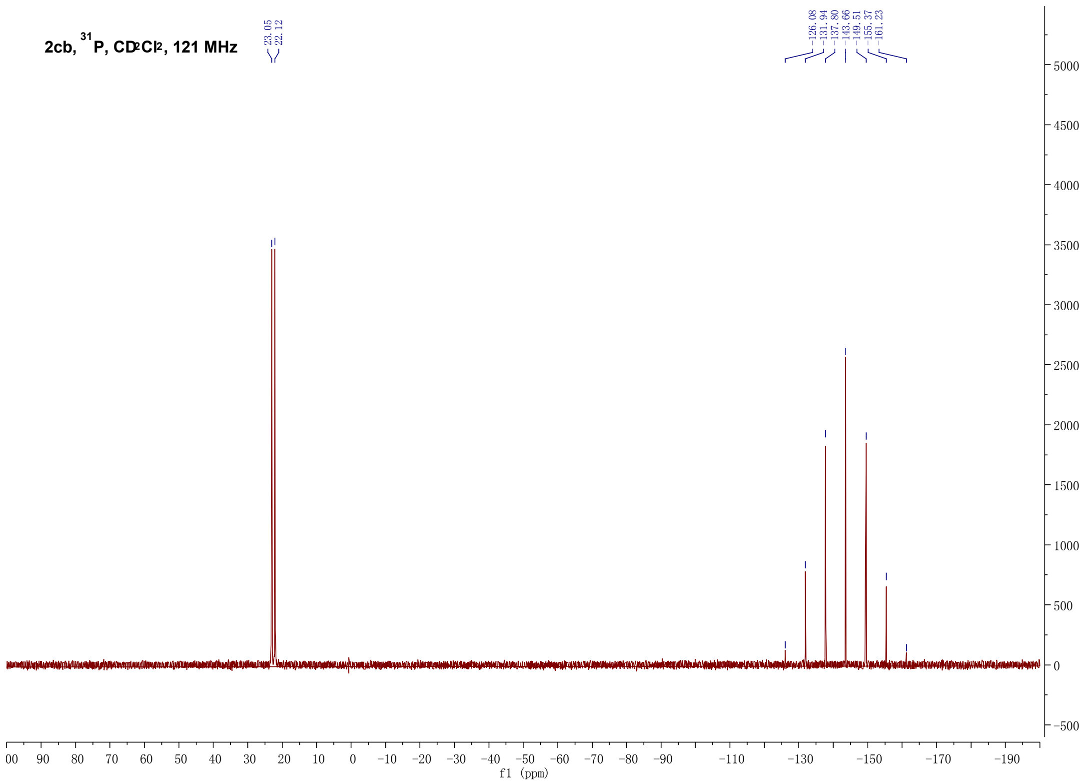

2bb, 31P, CD2Cl2, 121 MHz
21.49
20.58
-132.17
-138.03
-143.88
-149.73
-155.58
f1 (ppm)


P(p-C6H4F)3
N
Rh
CF3
PF6
P(p-C6H4F)3

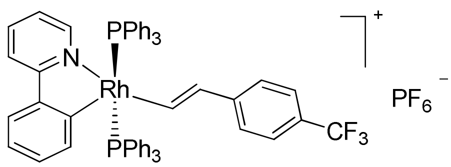
2cb

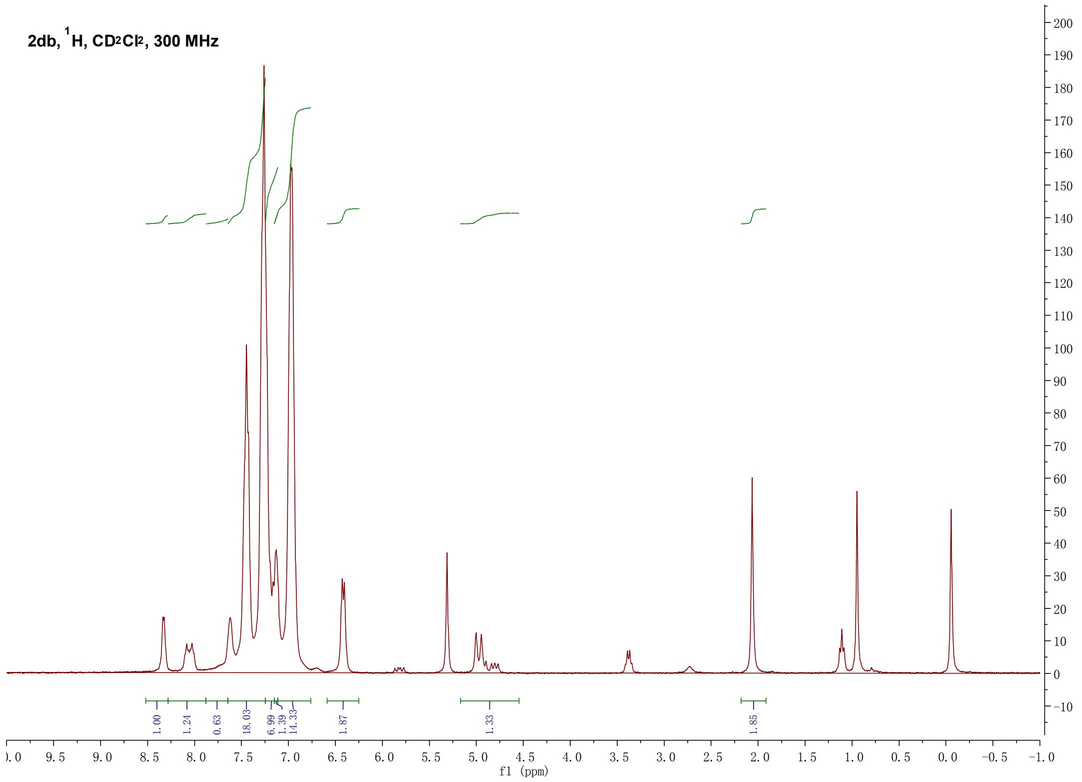

2cb, 1H, CD2Cl2, 300 MHz
f1 (ppm)

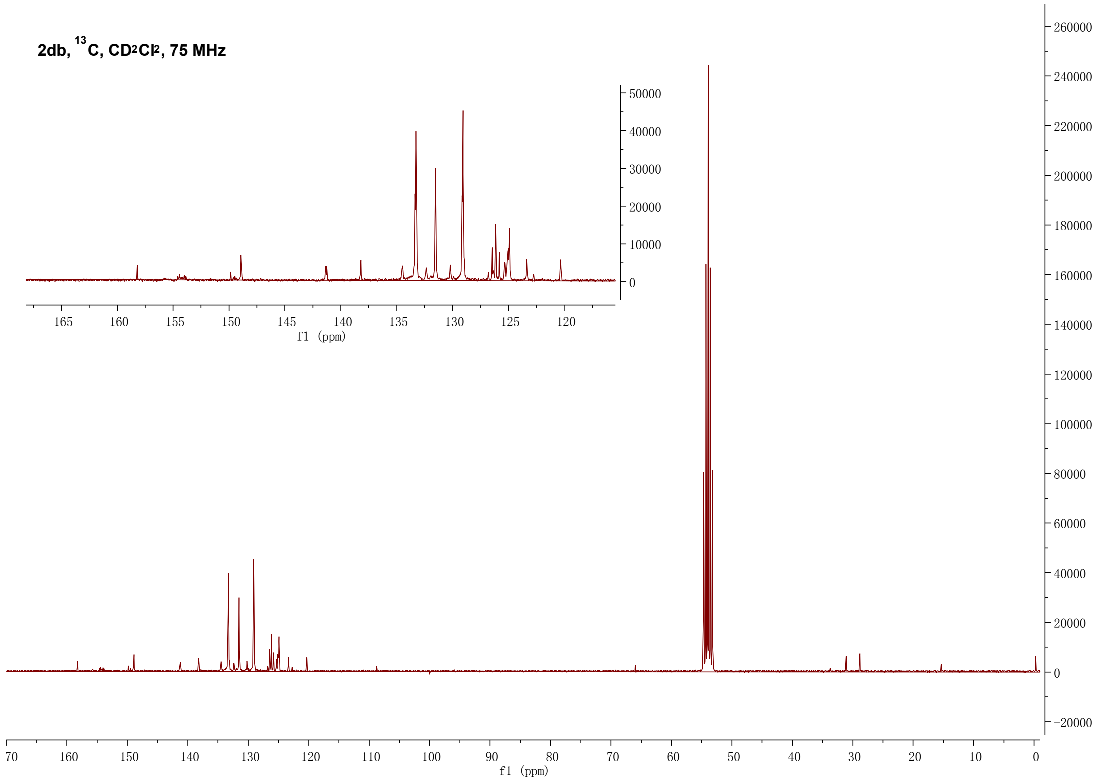

2cb, 13C, CD2Cl2, 75 MHz
f1 (ppm)

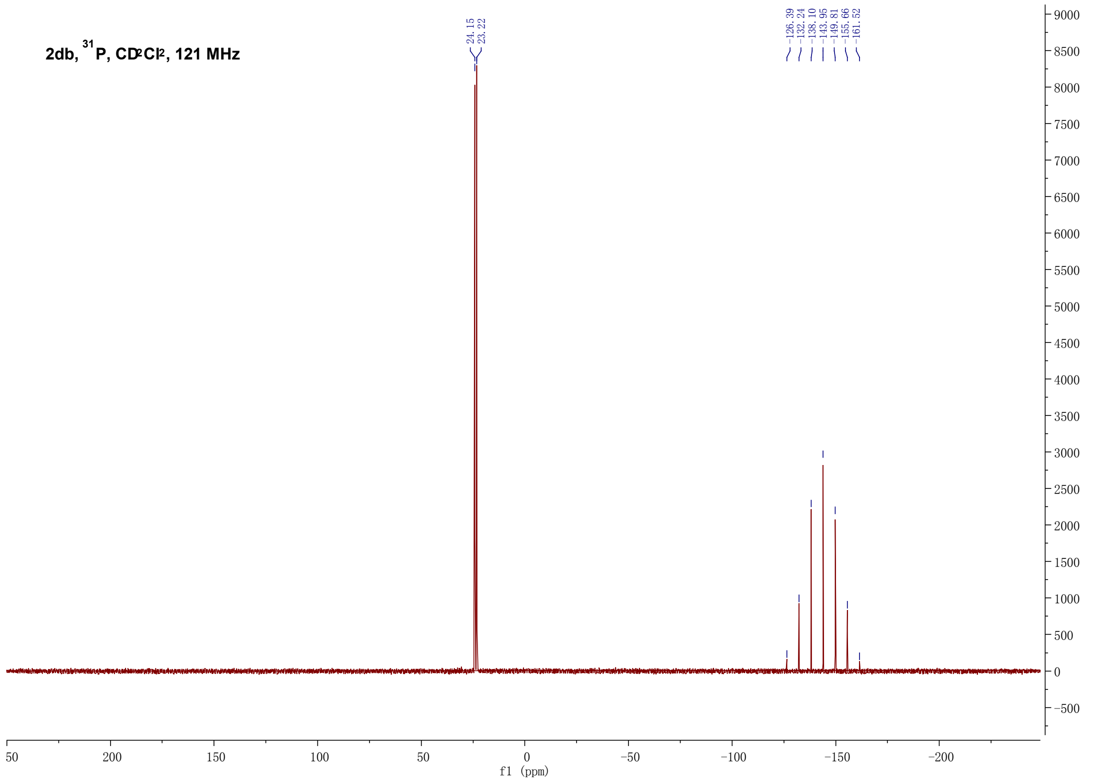

2cb, ³¹P, CD2Cl2, 121 MHz
23.05
22.12
-126.08
-131.94
-137.80
-143.66
-149.51
-155.37
-161.23
f1 (ppm)

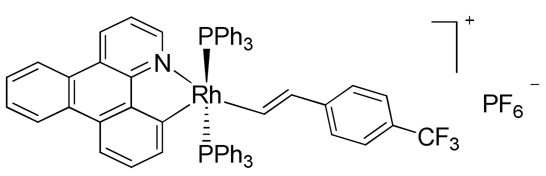
2db


PPh3
N
Rh
PPh3
CF3
+
PF6
−

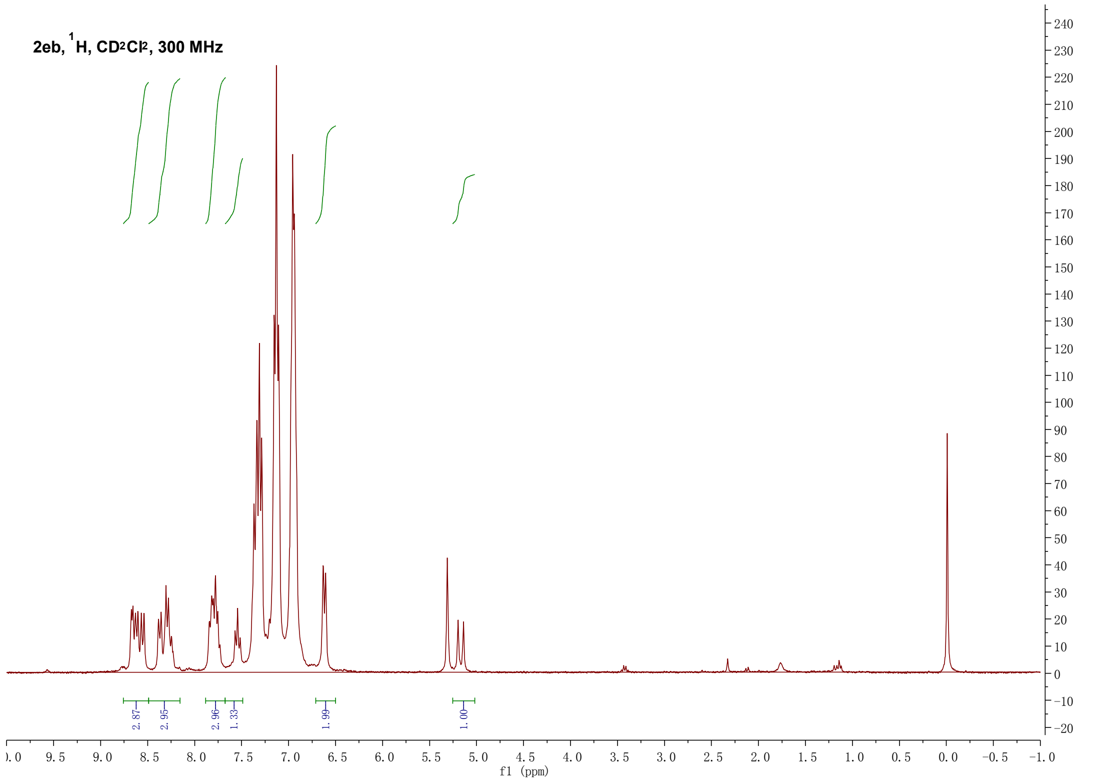

2db, ¹H, CD2Cl2, 300 MHz
1.00
1.24
0.63
18.03
6.99
1.39
14.33
1.87
1.33
1.85
f1 (ppm)

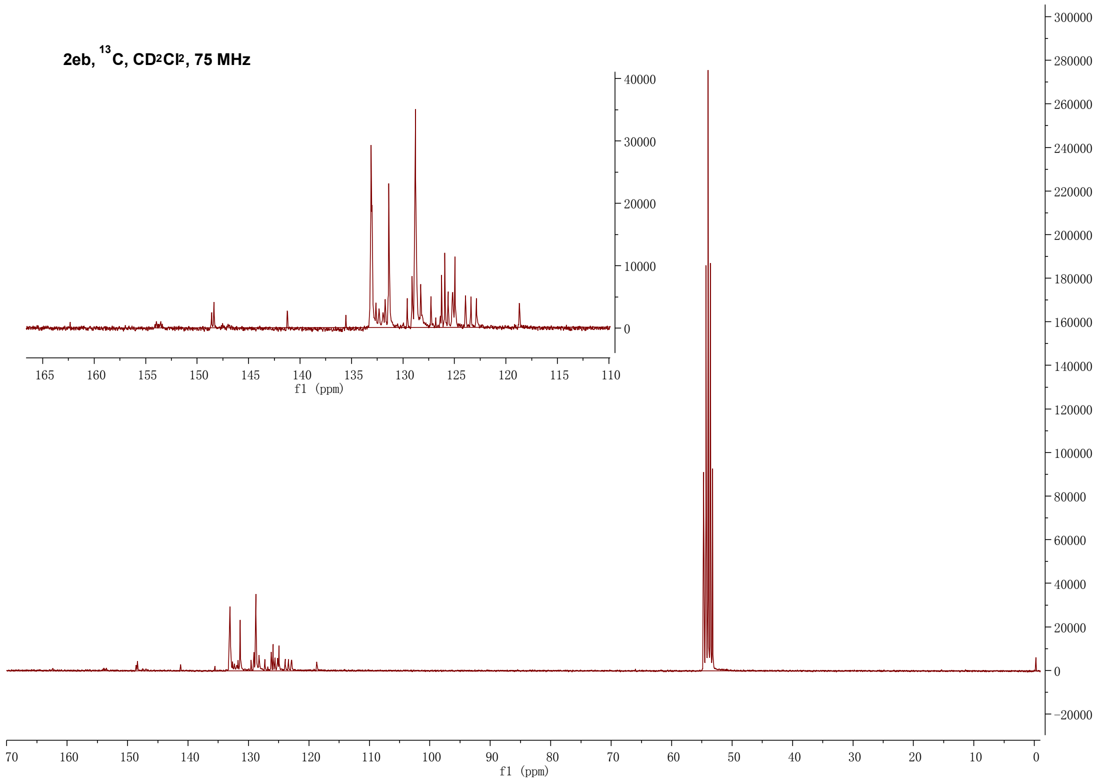

2db, 13C, CD2Cl2, 75 MHz
f1 (ppm)

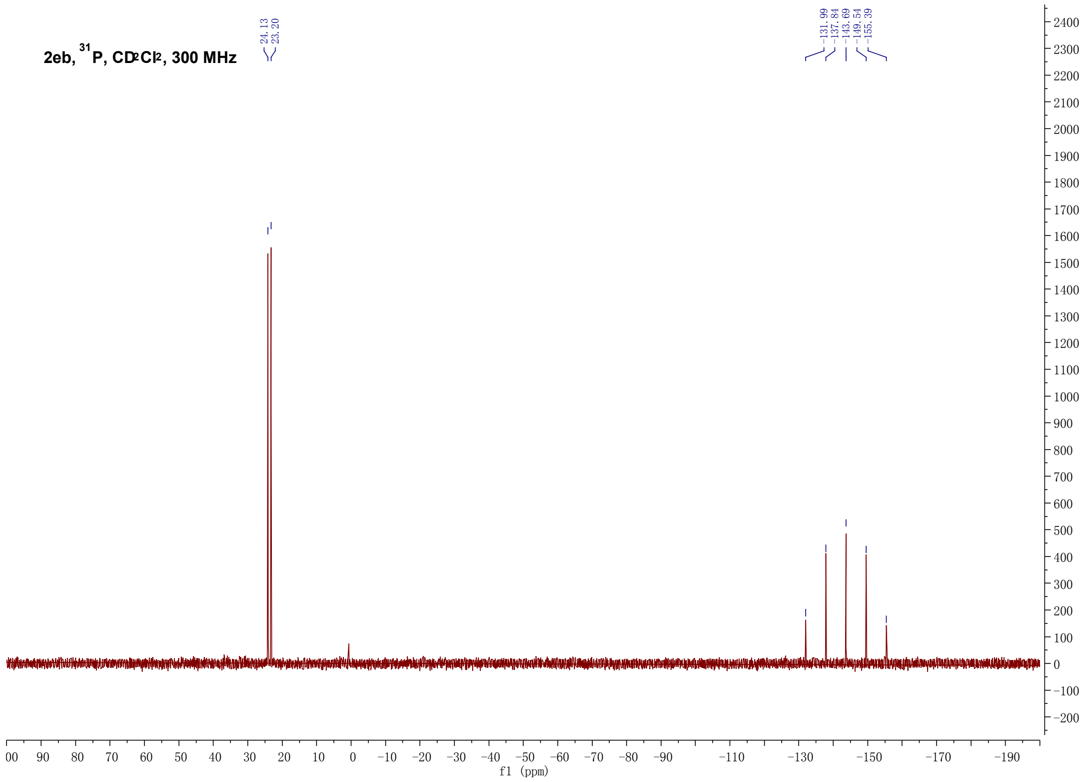

2db, 31P, CD2Cl2, 121 MHz
24.15
23.22
-126.39
-132.24
-138.10
-143.95
-149.81
-155.66
-161.52
f1 (ppm)

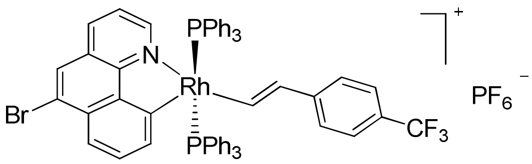

PPh3
N
Rh
PPh3
CF3
PF6

2eb

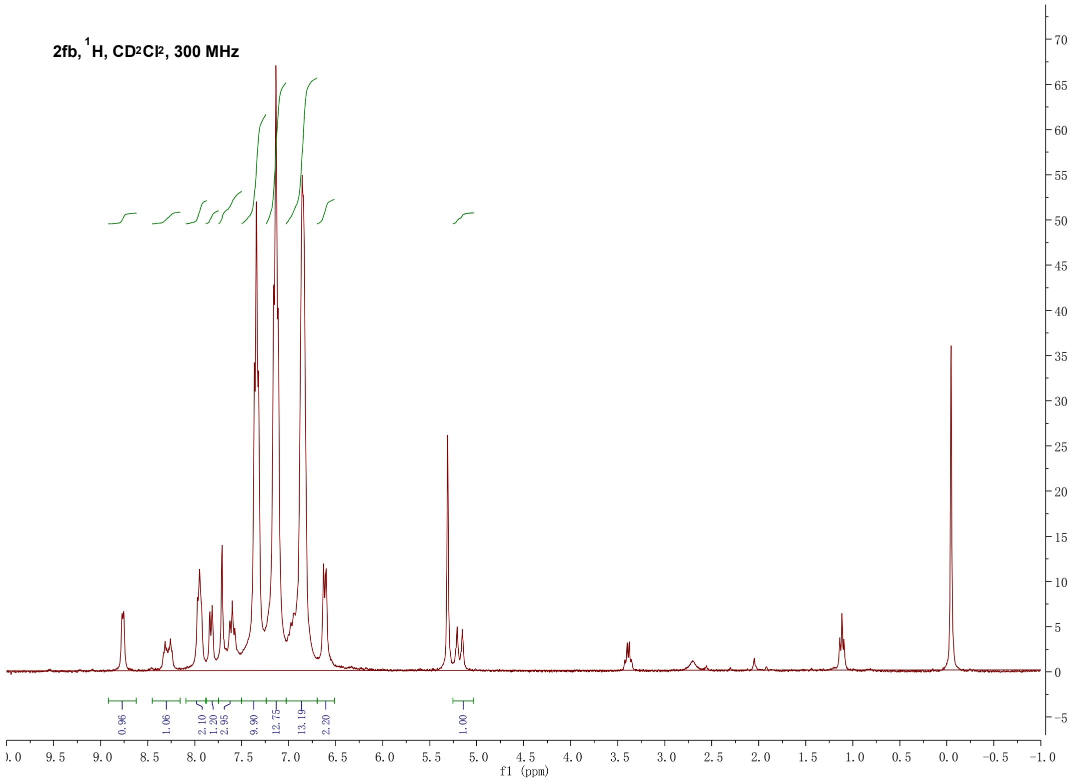

2eb, 1H, CD2Cl2, 300 MHz
2.87
2.95
2.96
1.33
1.99
1.00
f1 (ppm)

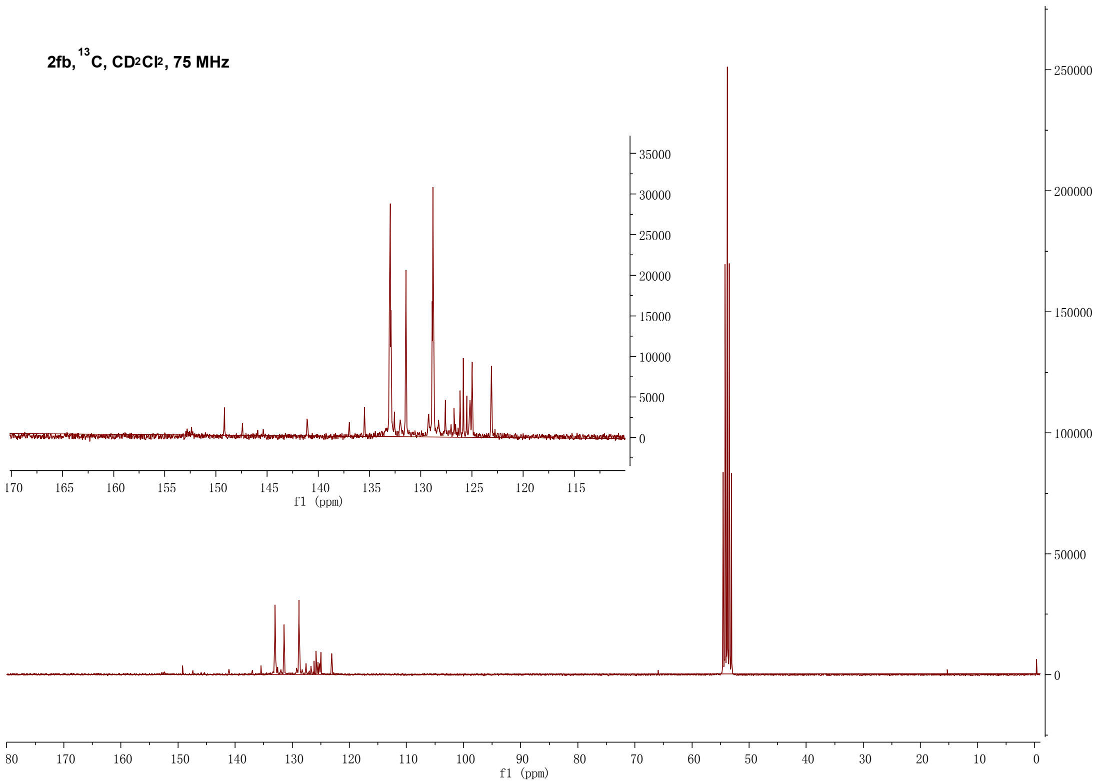

2eb, 13C, CD2Cl2, 75 MHz
f1 (ppm)
f1 (ppm)

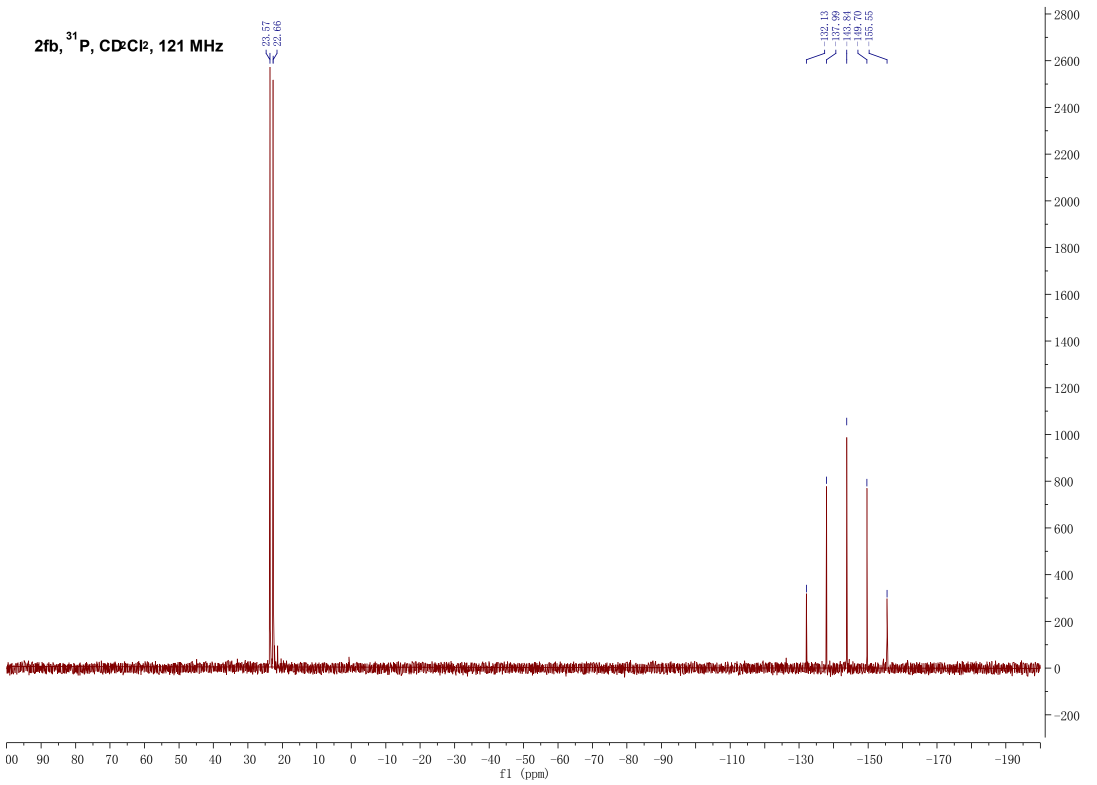

2eb, 31P, CD2Cl2, 300 MHz
24.13
23.20
-131.99
-137.84
-143.69
-149.54
-155.39
f1 (ppm)


PPh3
N
Rh
Br
PPh3
CF3
PF6
+
−

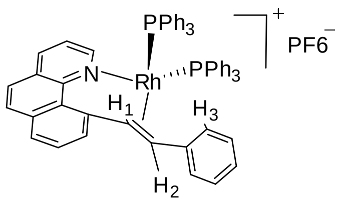
2fb


2fb, 1H, CD2Cl2, 300 MHz
0.96
1.06
2.10
1.20
2.95
9.90
12.75
13.19
2.20
1.00
f1 (ppm)

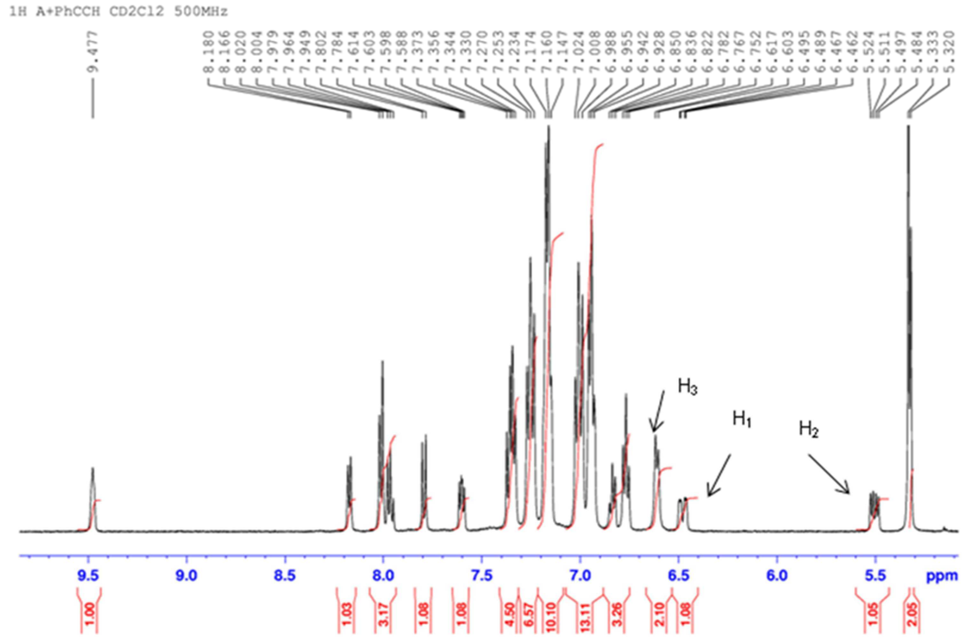


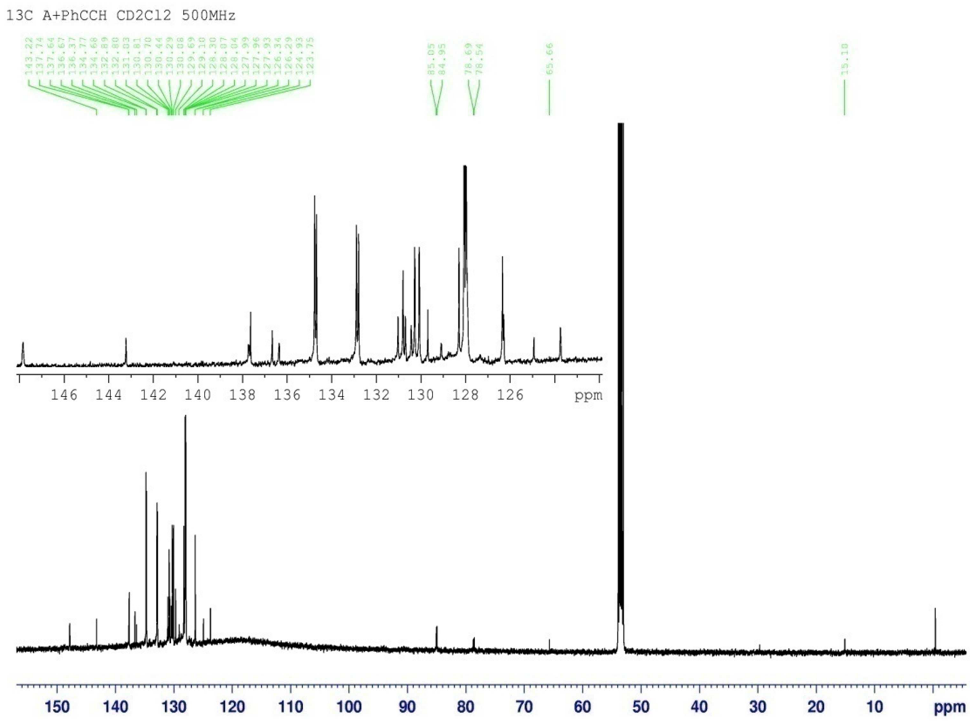


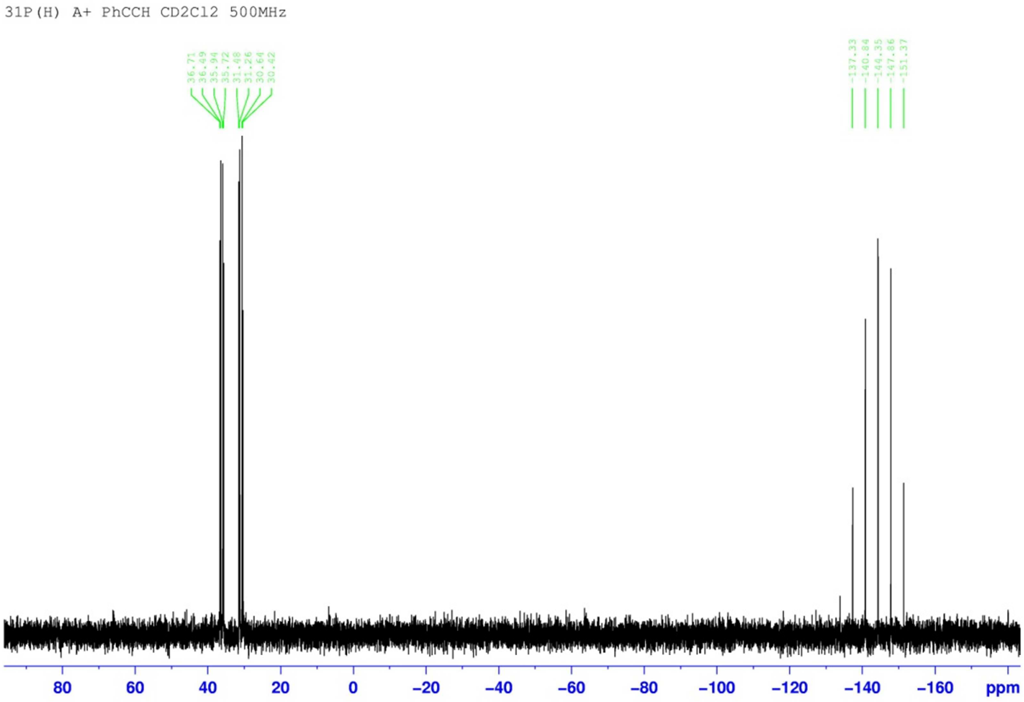
NMR Spectra of Coupling product 3


PPh3
PF6
N
Rh
PPh3
H1
H3
H2

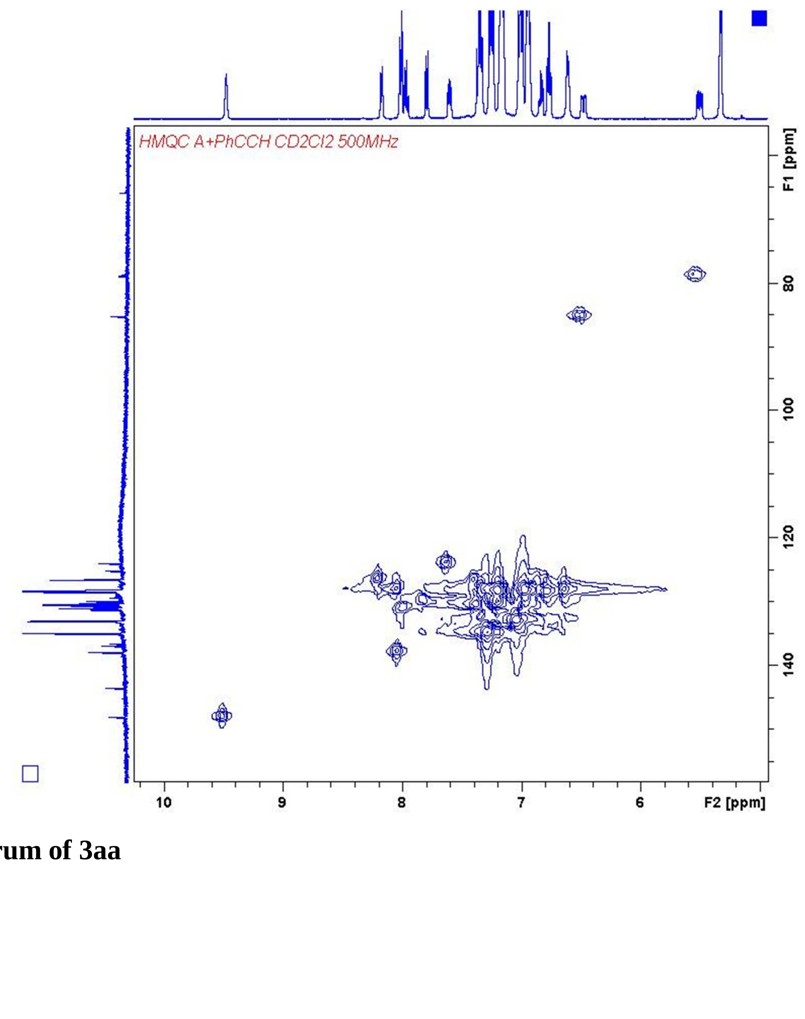
3aa


1H A+PhCCH CD2Cl2 500MHz
H3
H1
H2
ppm

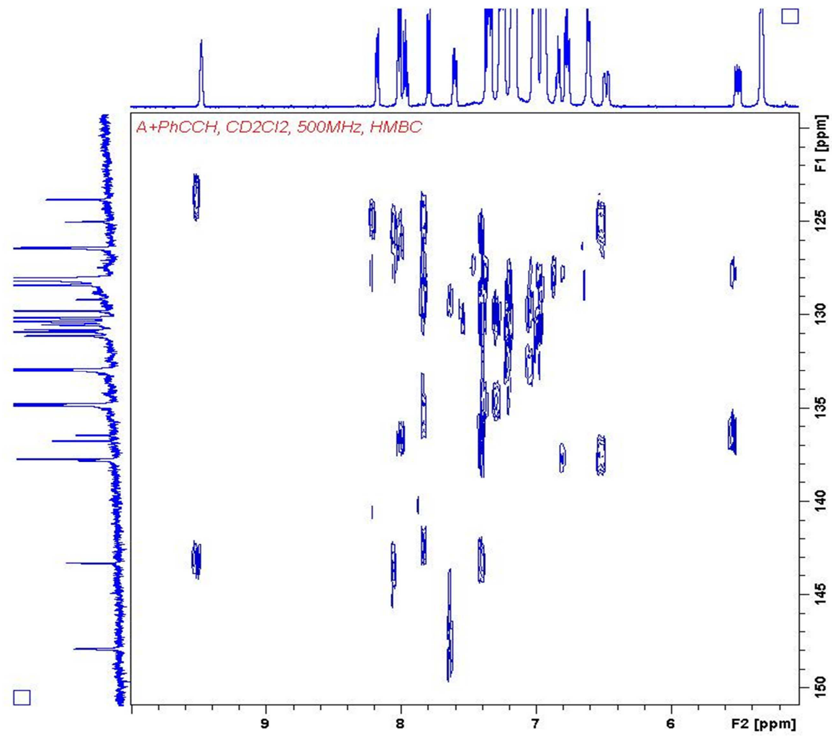

13C A+PhCCH CD2Cl2 500MHz
ppm

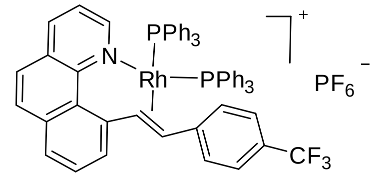


HMQC Spectrum of 3aa

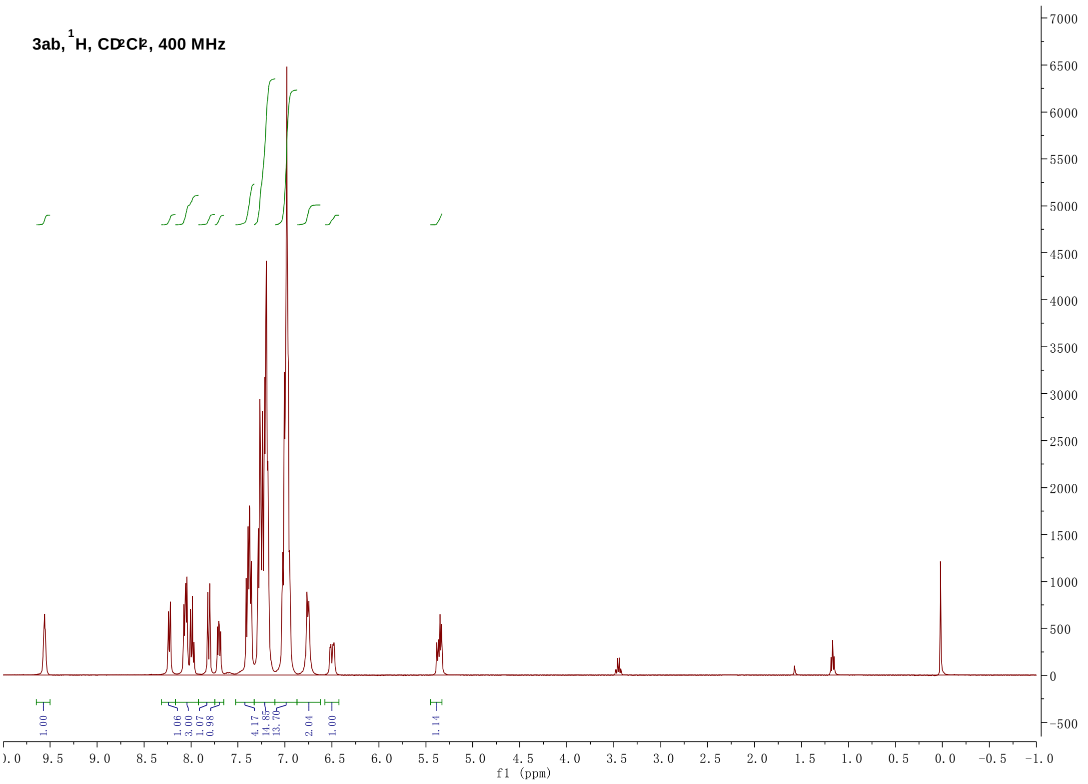


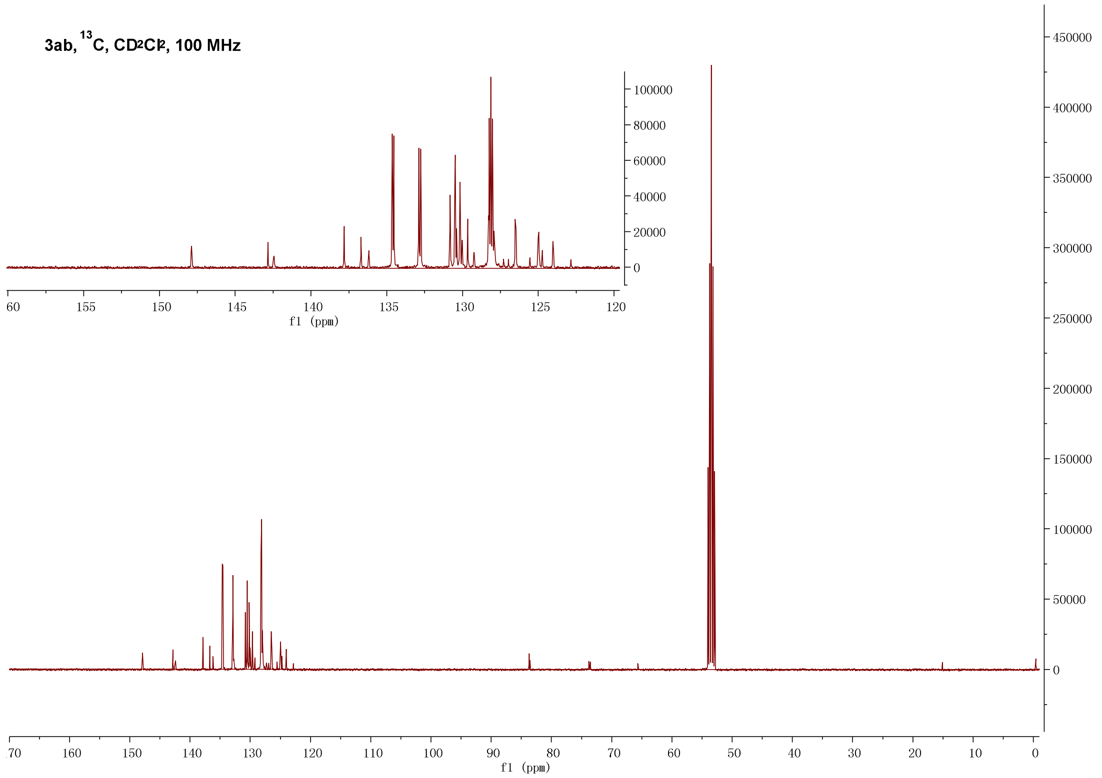
HMBC Spectrum of 3aa

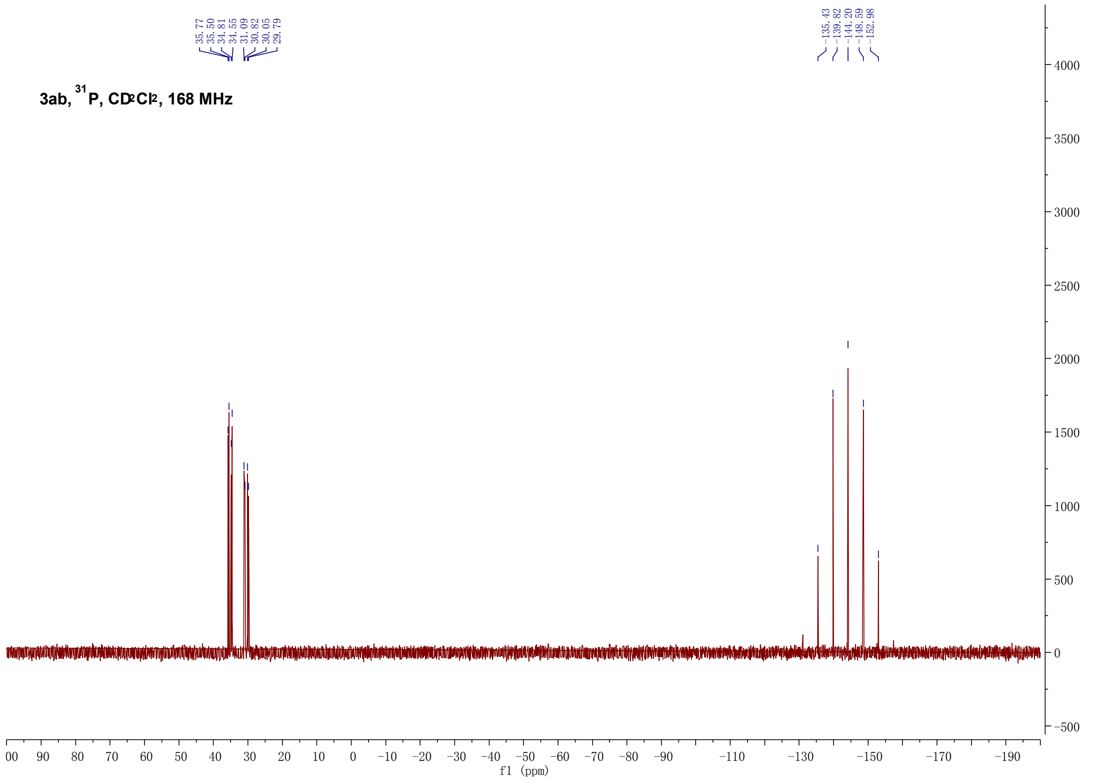

A+PhCCH, CD2Cl2, 500MHz, HMBC
F1 [ppm]
F2 [ppm]

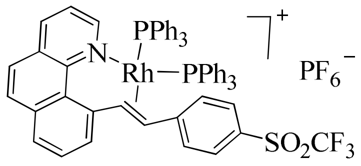

PPh3
N
Rh
PPh3
PF6
CF3

3ab

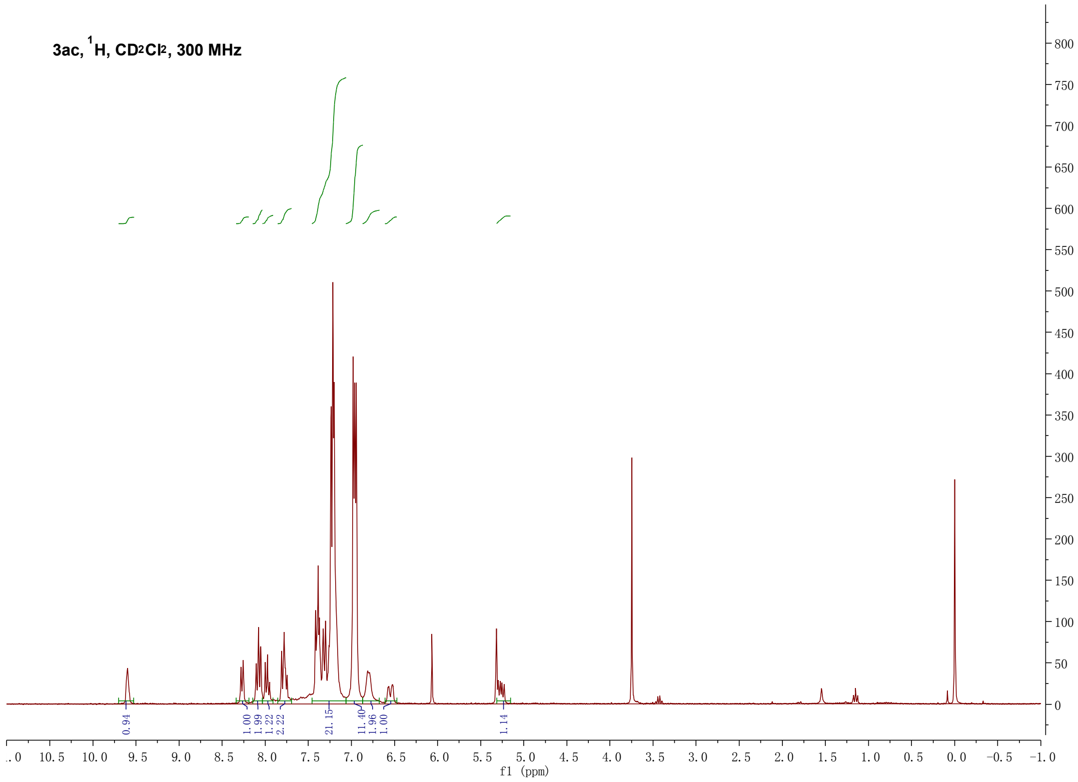

3ab, 1H, CD2Cl2, 400 MHz
f1 (ppm)

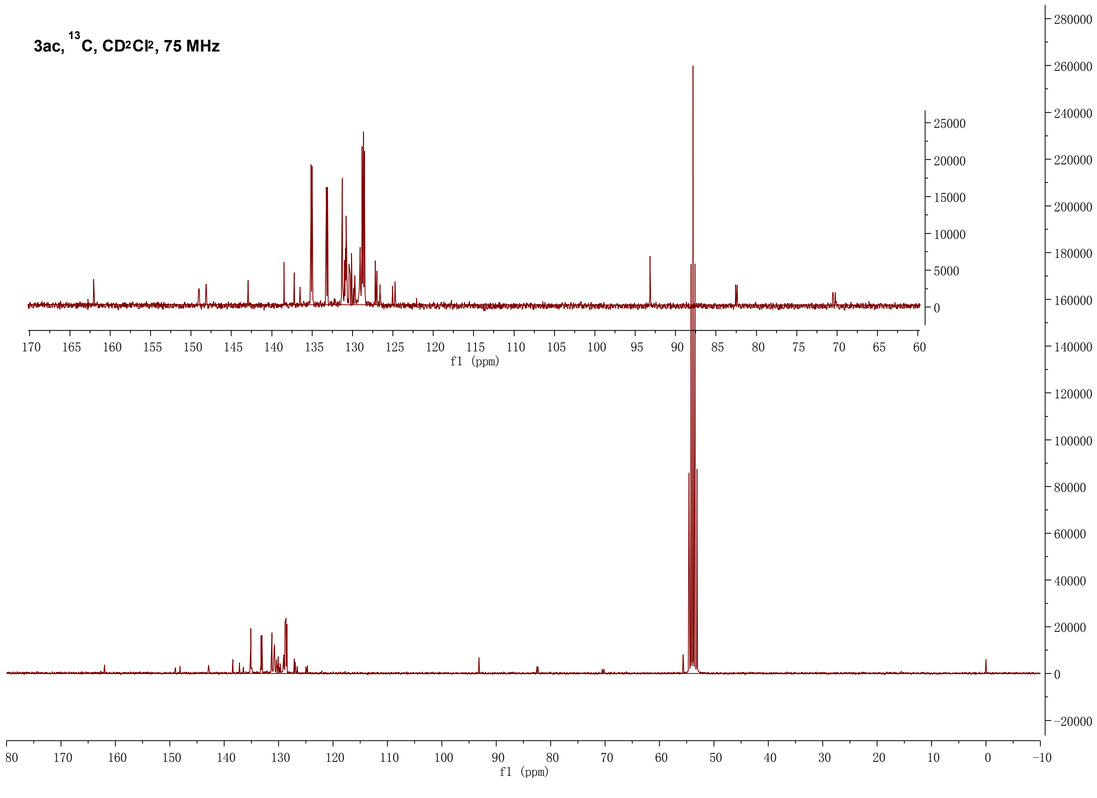

3ab, 13C, CD2Cl2, 100 MHz
f1 (ppm)

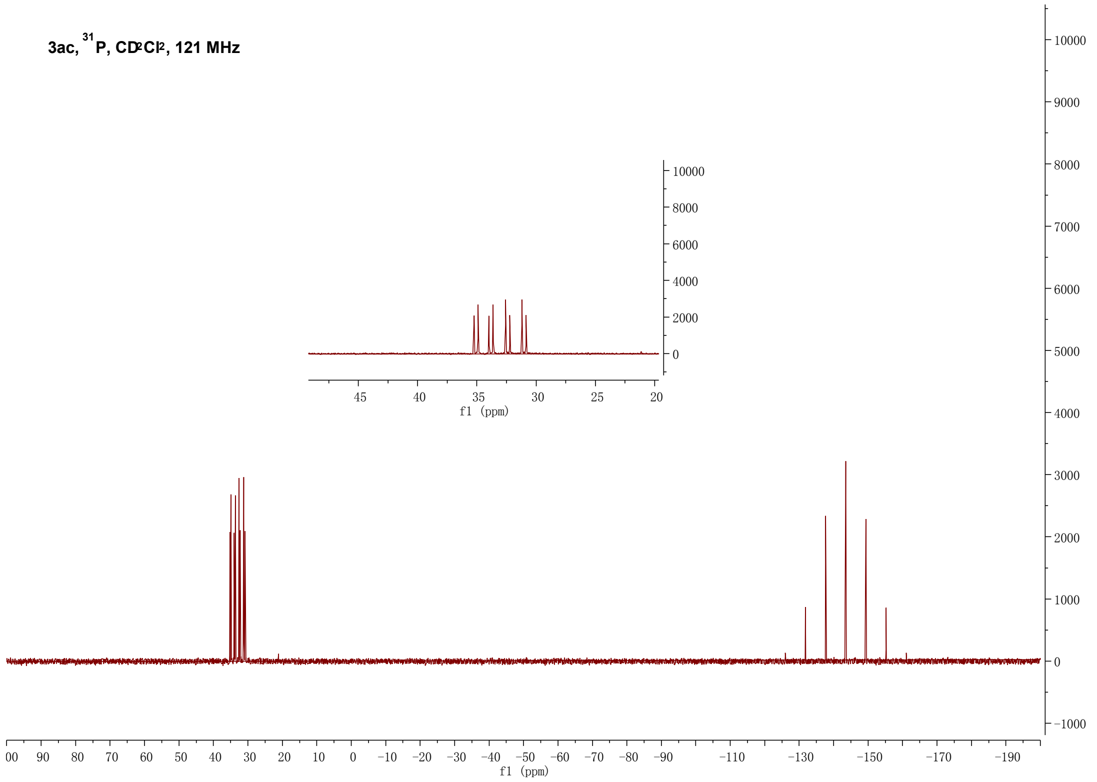

3ab, 31P, CD2Cl2, 168 MHz
35.77
35.50
34.81
34.55
31.09
30.82
30.05
29.79
-135.43
-139.82
-144.20
-148.59
-152.98
f1 (ppm)

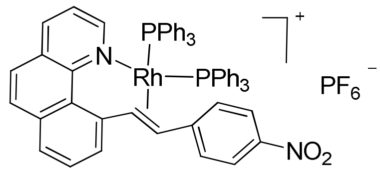

PPh3
N
Rh
PPh3
+
PF6
−
SO2CF3

3ac

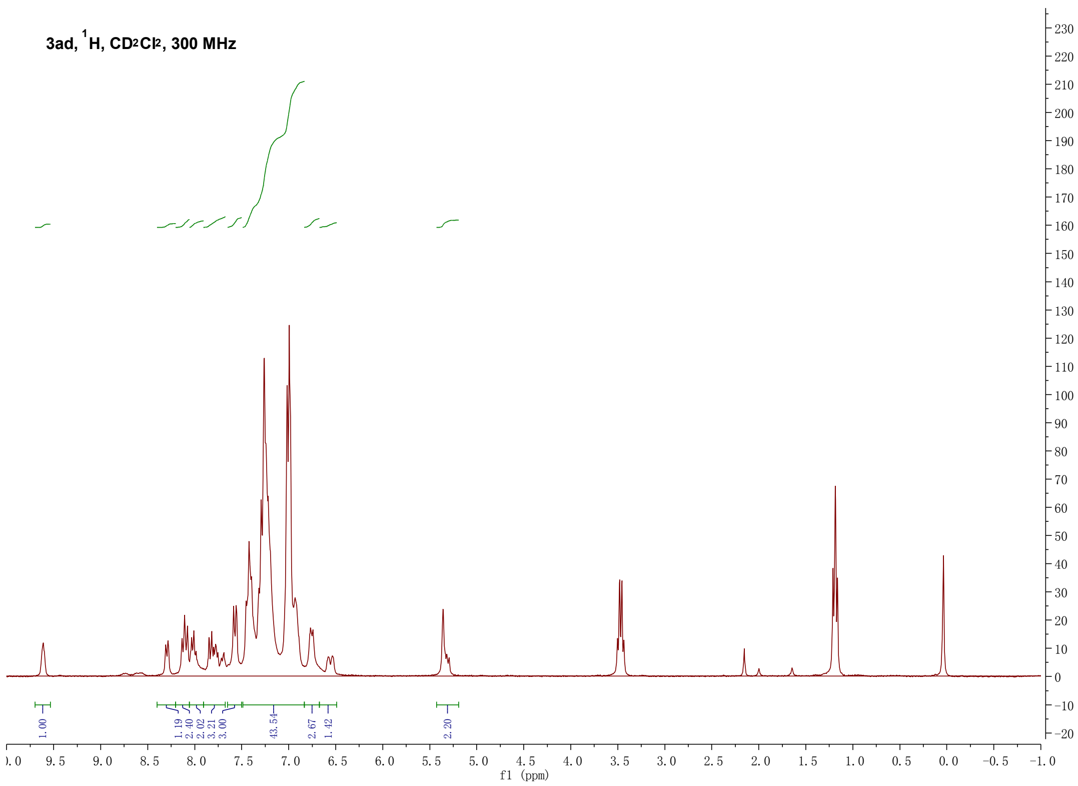

3ac, 1H, CD2Cl2, 300 MHz
f1 (ppm)

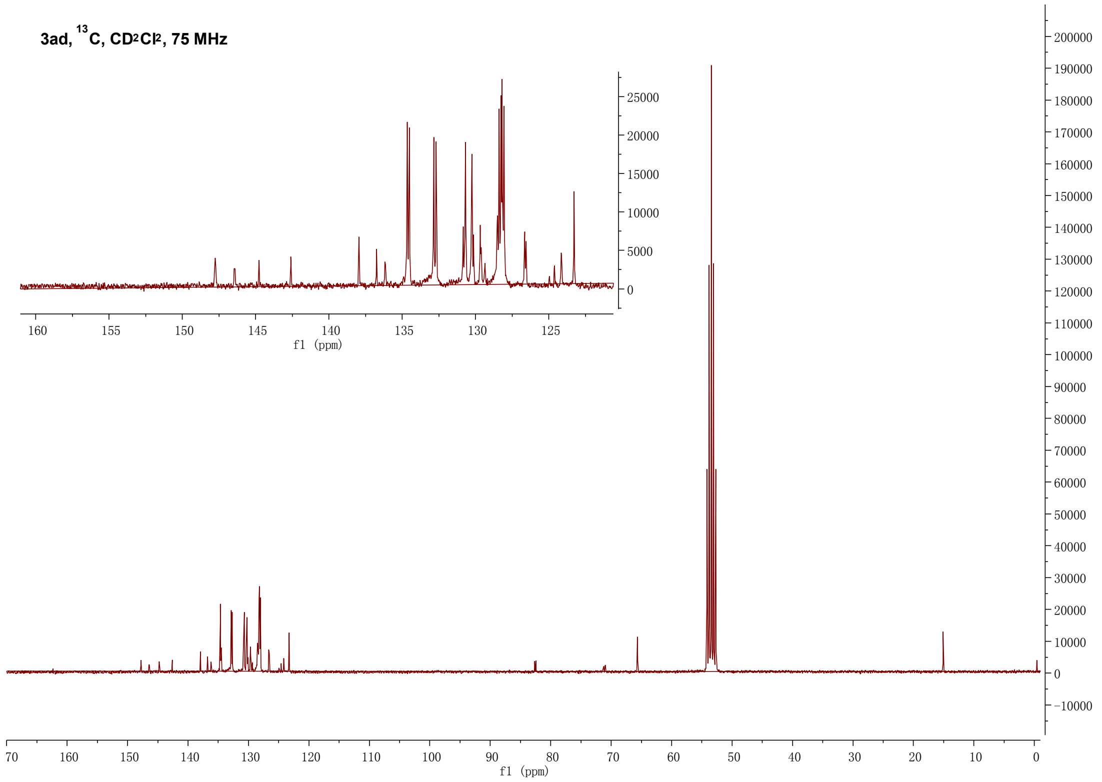

3ac, 13C, CD2Cl2, 75 MHz
f1 (ppm)

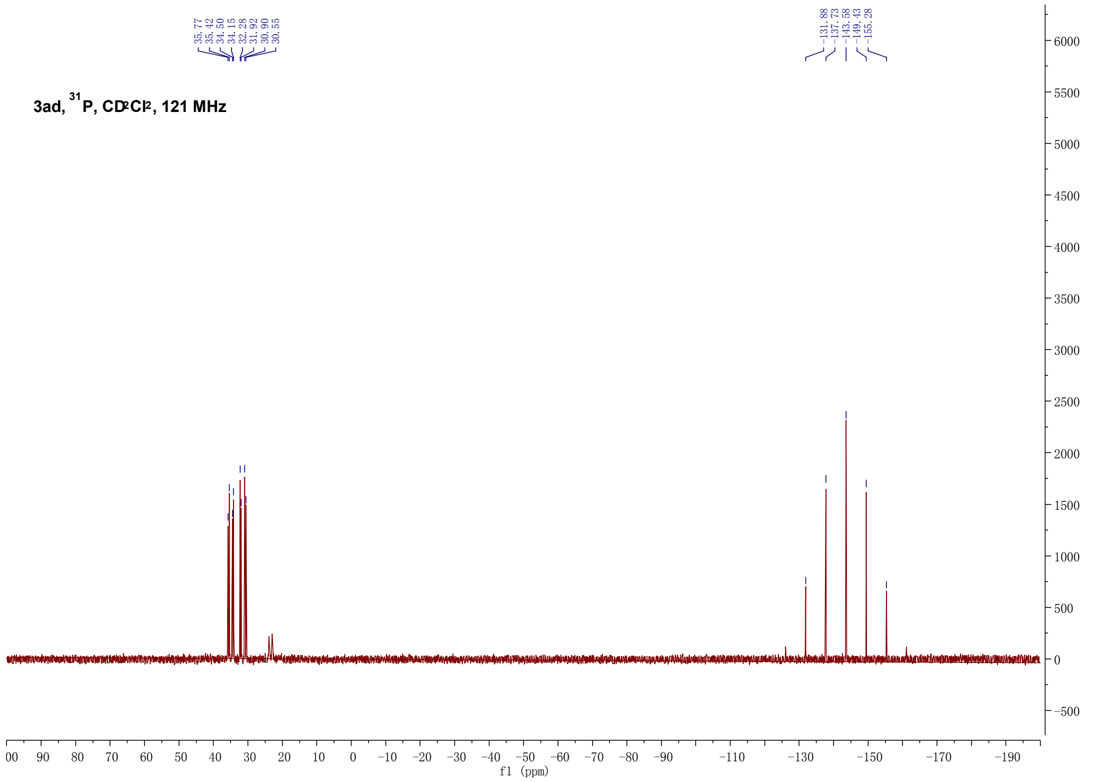

3ac, 31P, CD2Cl2, 121 MHz
f1 (ppm)

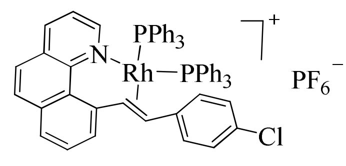

PPh3
N
Rh
PPh3
+
PF6
−
NO2

3ad

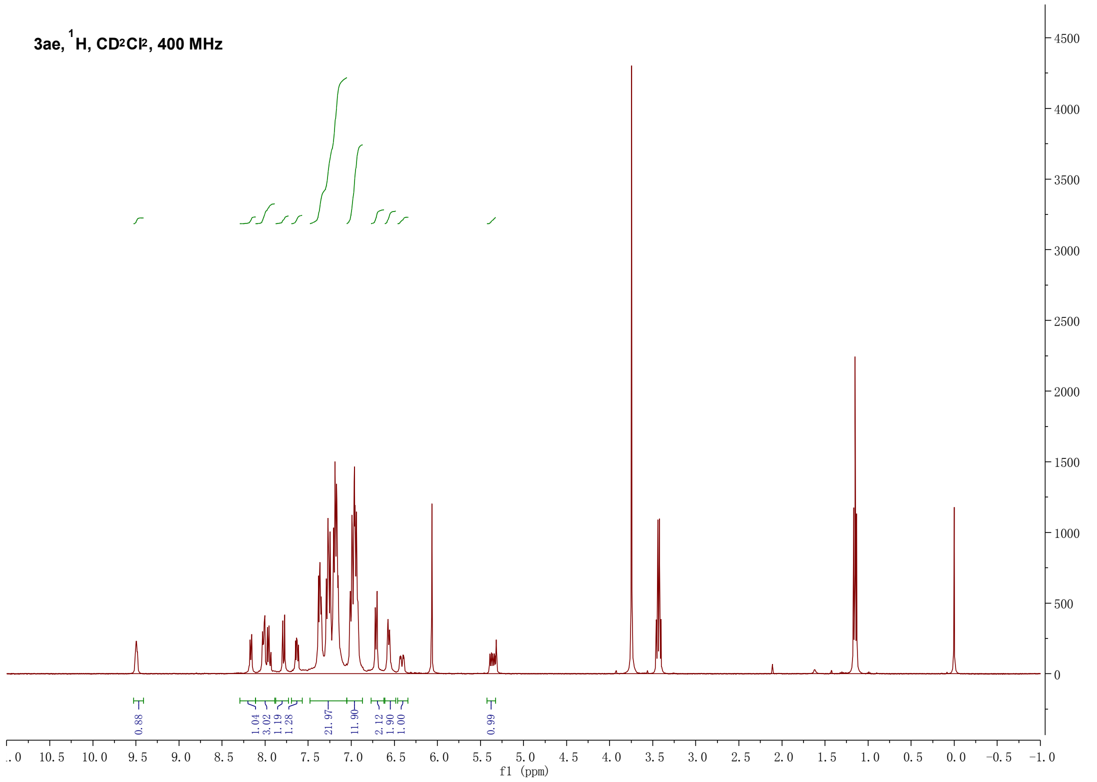

3ad, 1H, CD2Cl2, 300 MHz
1.00
1.19
2.40
2.02
3.21
3.00
43.54
2.67
1.42
2.20
f1 (ppm)

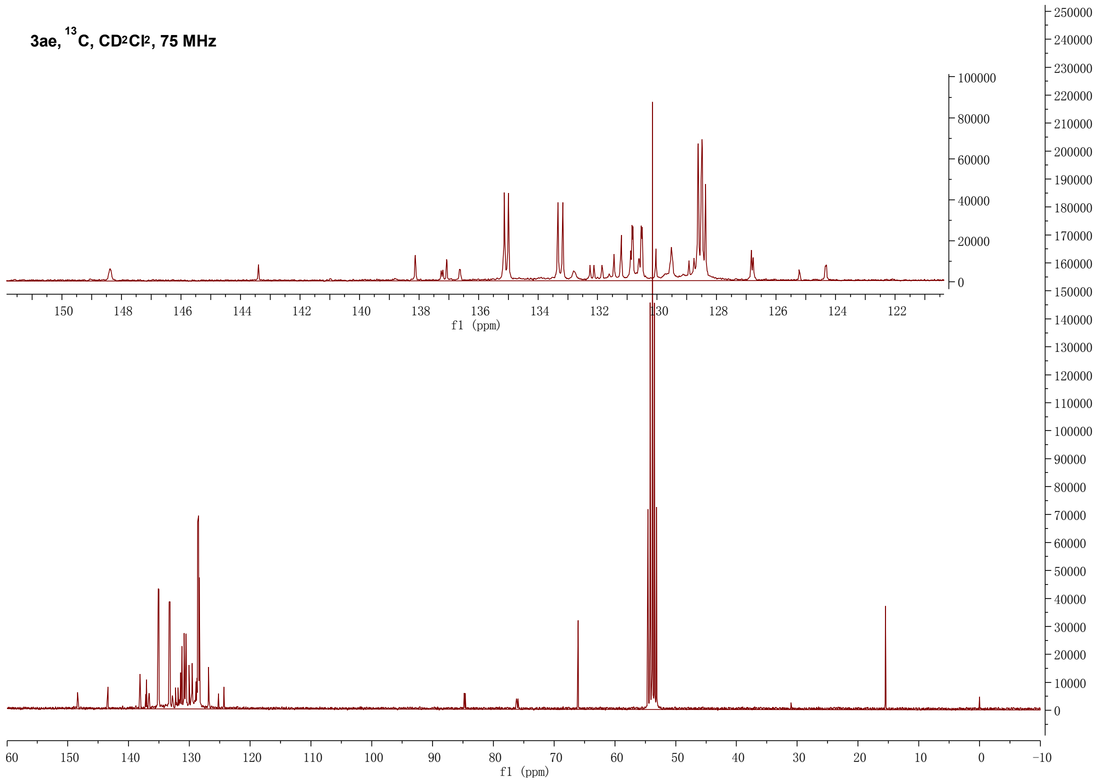

3ad, ^{13}C, CD_2Cl_2, 75 MHz

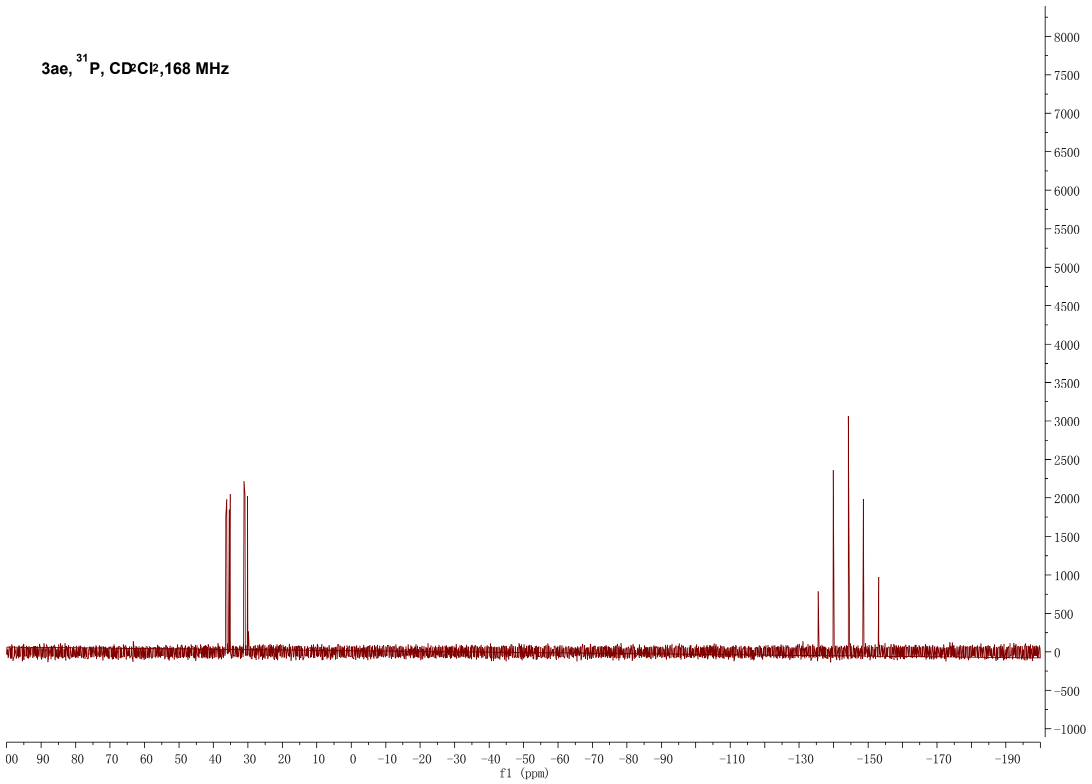

3ad, ^{31}P, CD_2Cl_2, 121 MHz
35.77
35.42
34.50
34.15
32.28
31.92
30.90
30.55
−131.88
−137.73
−143.58
−149.43
−155.28

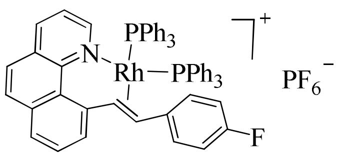


3ae

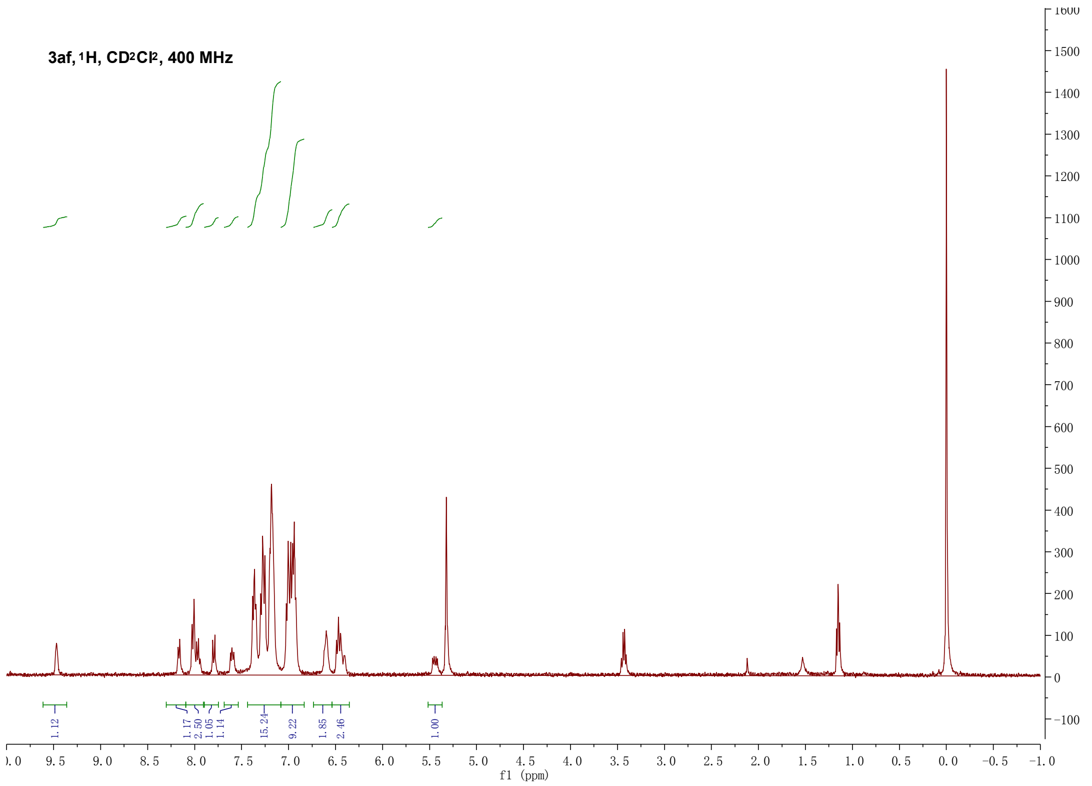

3ae, 1H, CD2Cl2, 400 MHz
f1 (ppm)


3ae, 13C, CD2Cl2, 75 MHz
f1 (ppm)

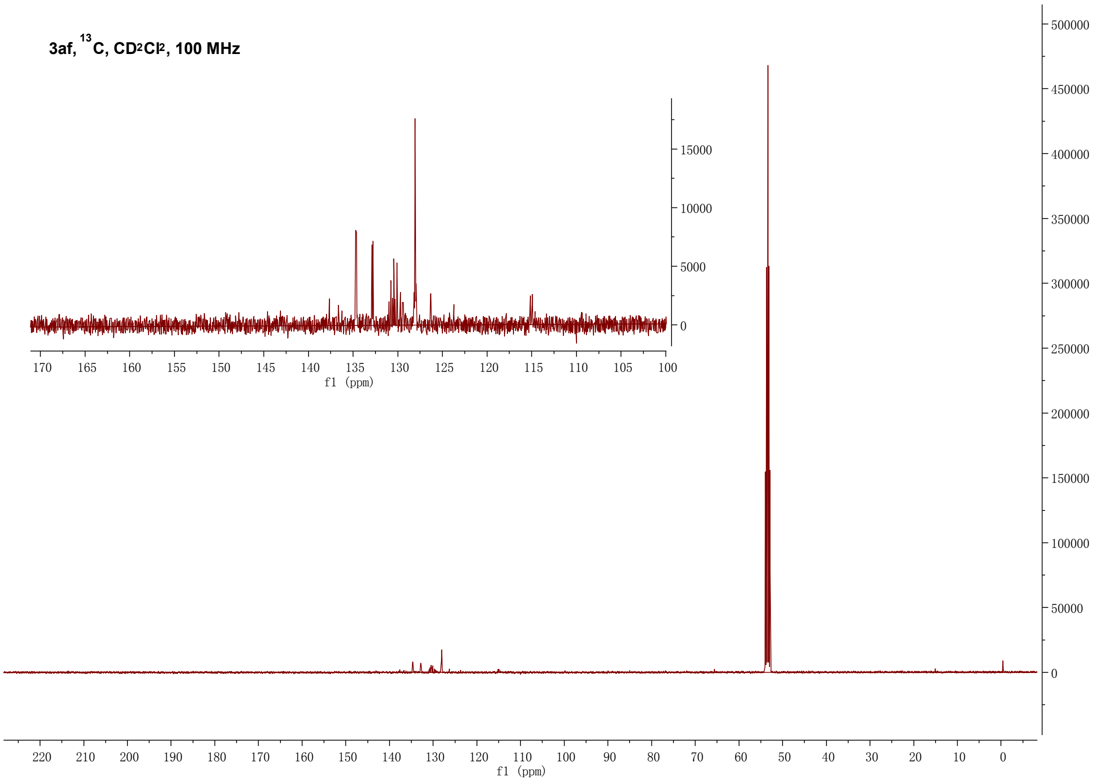

3ae, 31P, CD2Cl2,168 MHz
f1 (ppm)


PPh3
N
Rh
PPh3
PF6−
F

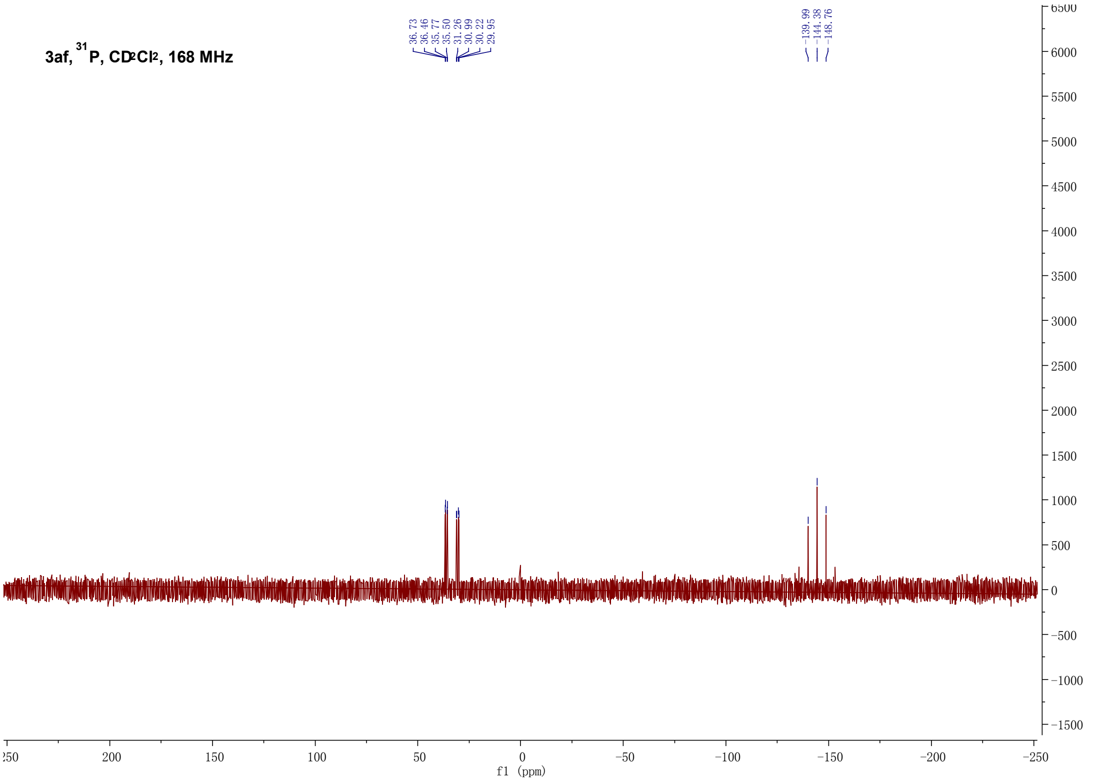
3af

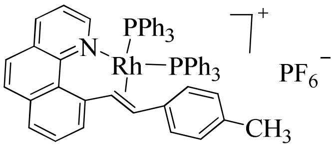

3af, 1H, CD2Cl2, 400 MHz
f1 (ppm)

3af, ^{13}C, CD_2Cl_2, 100 MHz

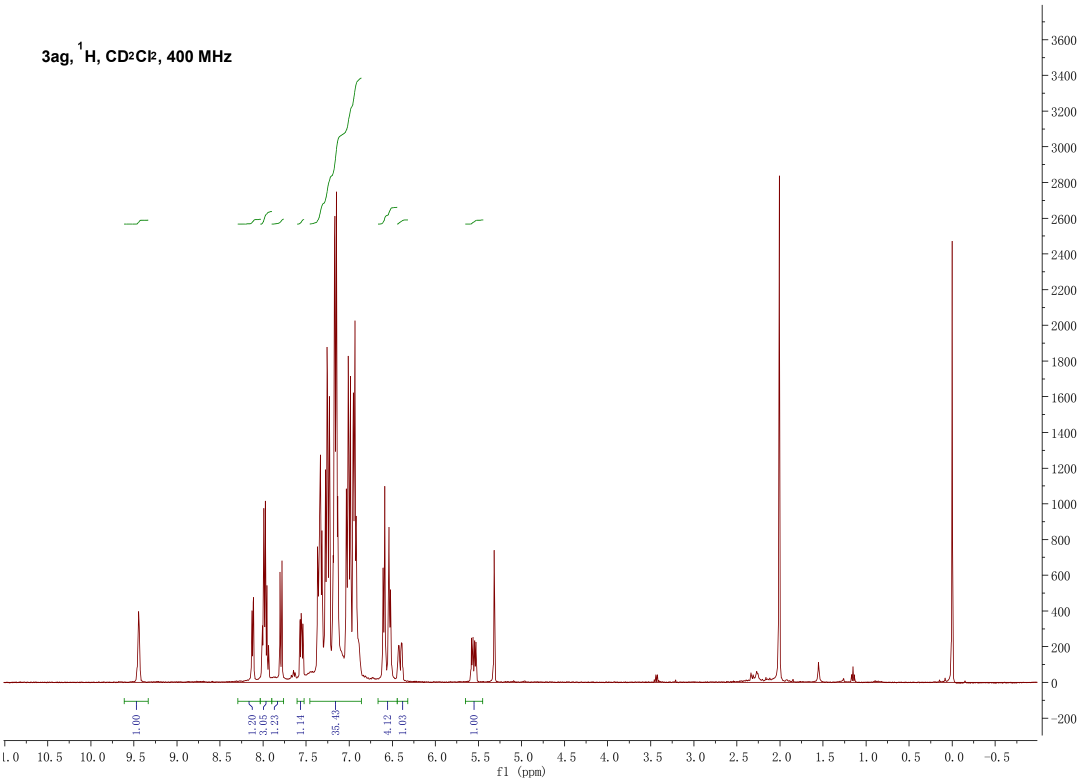


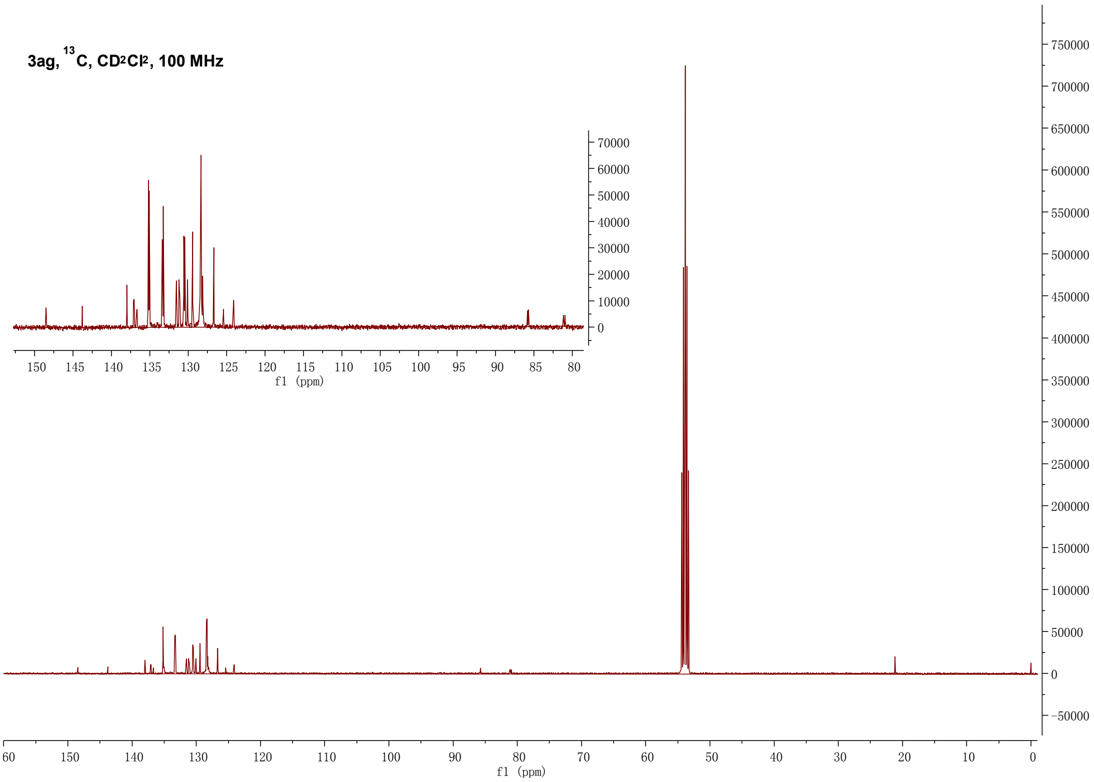
3af, ^{31}P, CD_2Cl_2, 168 MHz

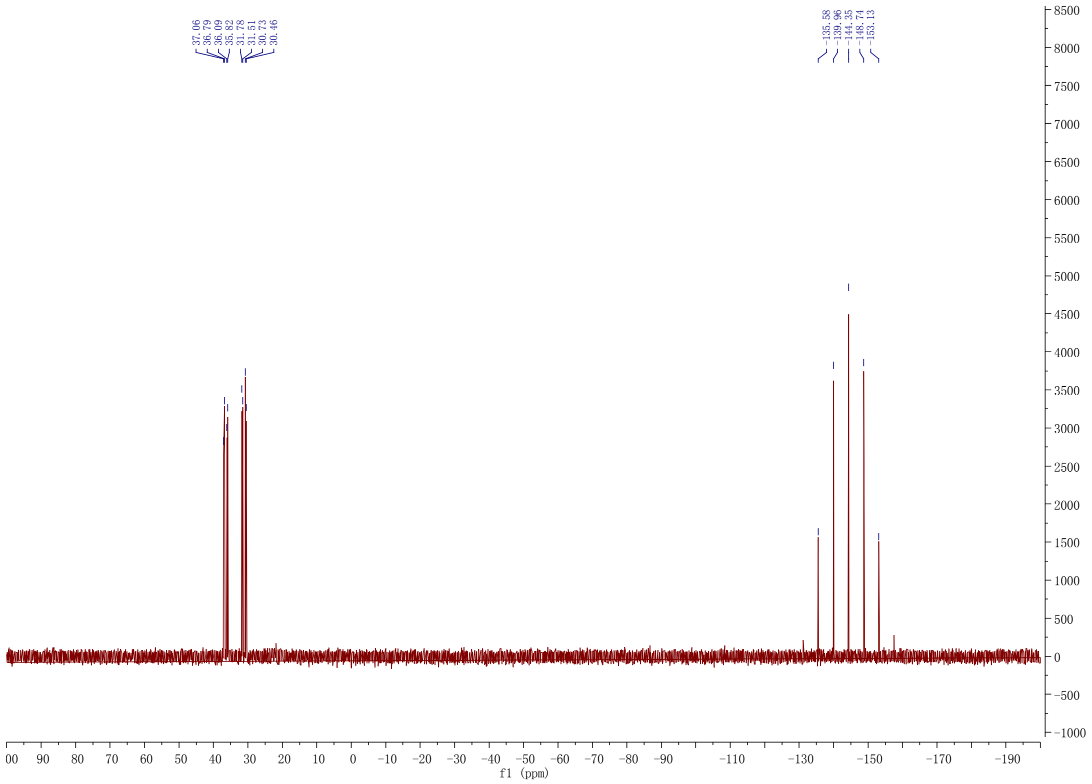


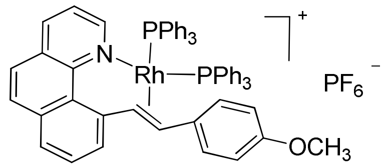

PPh3
N
Rh
PPh3
+
PF6
−
CH3

3ag

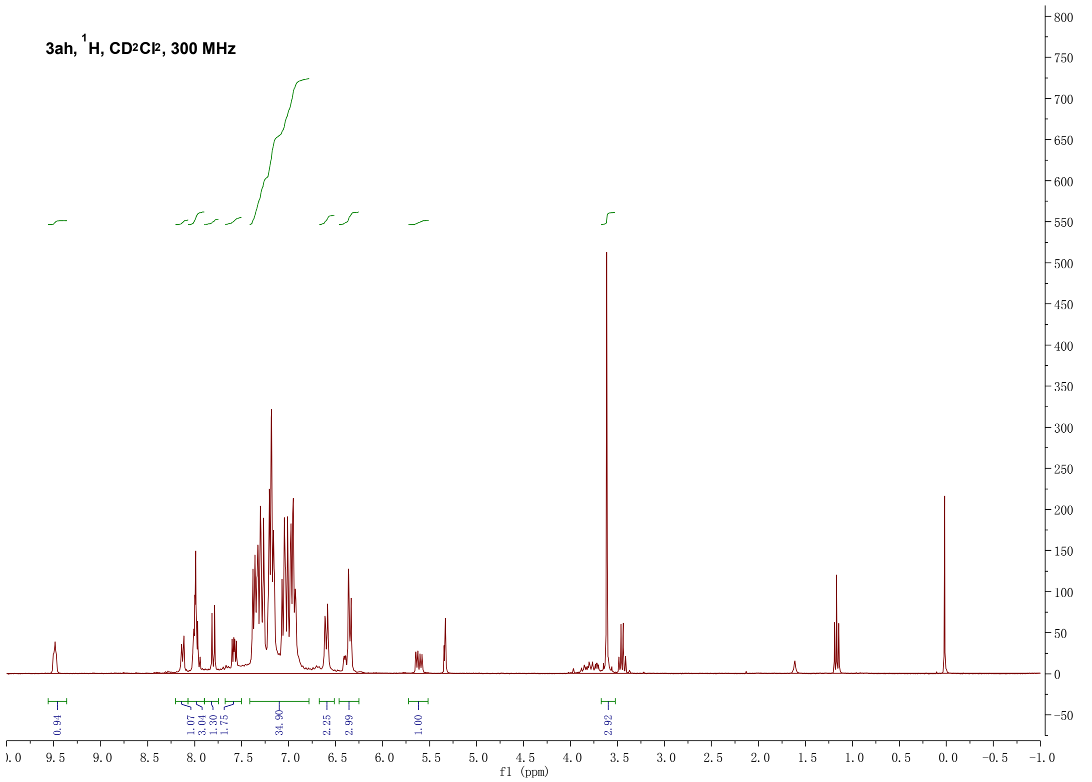

3ag, 1H, CD2Cl2, 400 MHz
1.00
1.20
3.05
1.23
1.14
35.43
4.12
1.03
1.00
f1 (ppm)

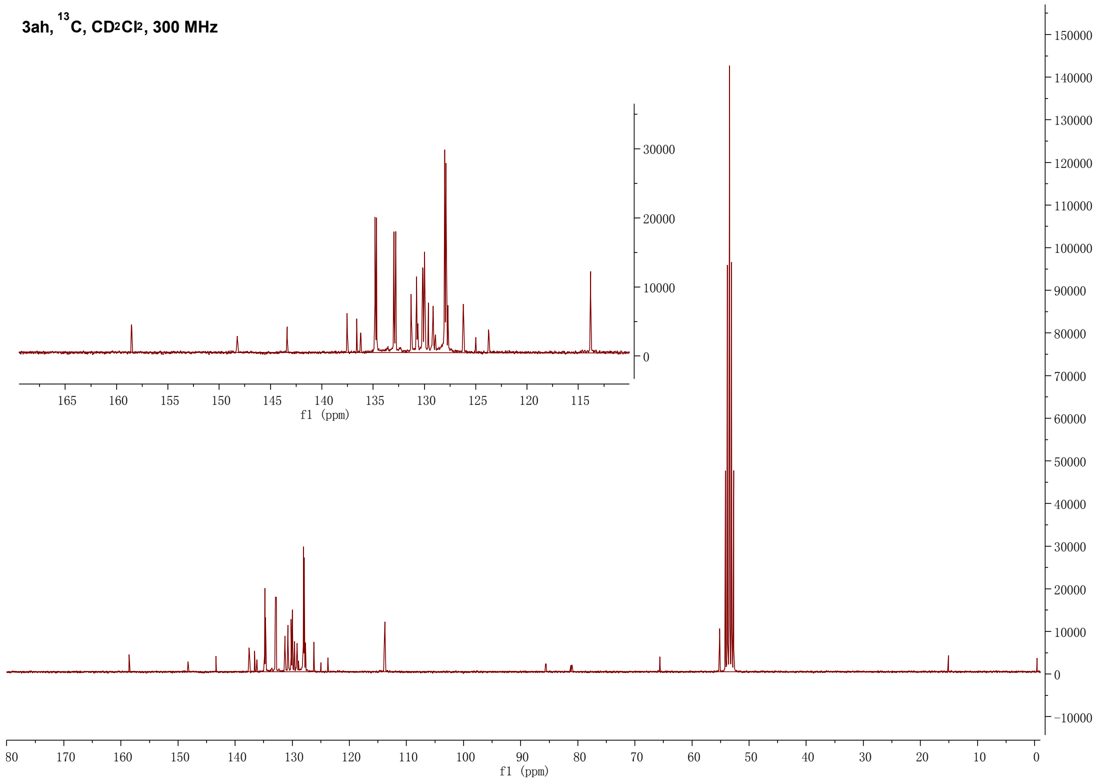

3ag, 13C, CD2Cl2, 100 MHz
f1 (ppm)
f1 (ppm)

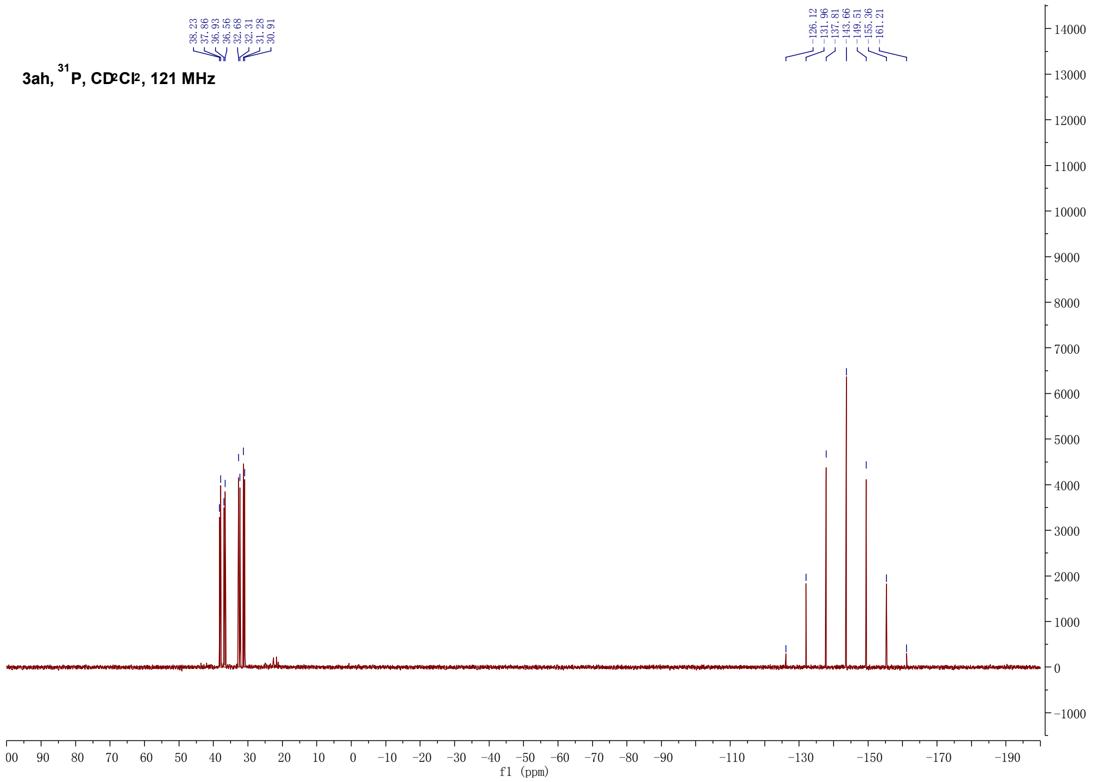

37.06
36.79
36.09
35.82
31.78
31.51
30.73
30.46
-135.58
-139.96
-144.35
-148.74
-153.13
f1 (ppm)

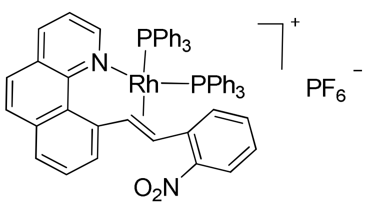

PPh3
N
Rh
PPh3
PF6
OCH3

3ah


3ah, 1H, CD2Cl2, 300 MHz
0.94
1.07
3.04
1.30
1.75
34.90
2.25
2.99
1.00
2.92
f1 (ppm)

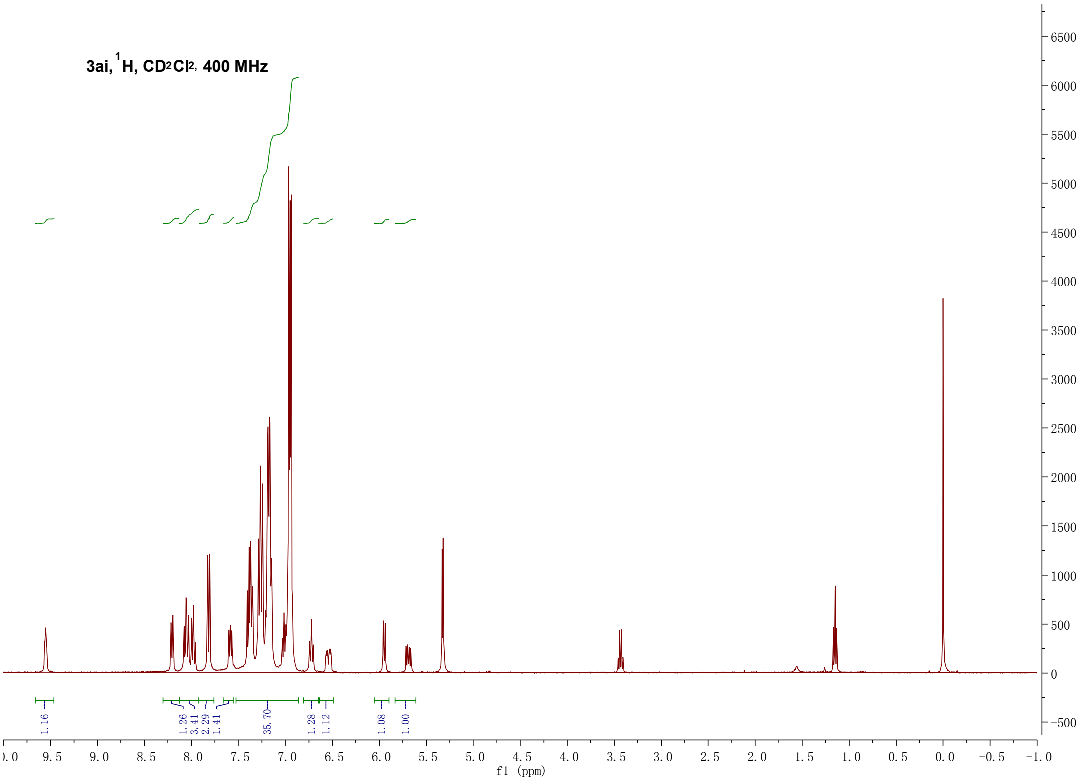

3ah, 13C, CD2Cl2, 300 MHz
f1 (ppm)


38.23
37.86
36.93
36.56
32.68
32.31
31.28
30.91
-126.12
-131.96
-137.81
-143.66
-149.51
-155.36
-161.21
3ah, 31P, CD2Cl2, 121 MHz
f1 (ppm)

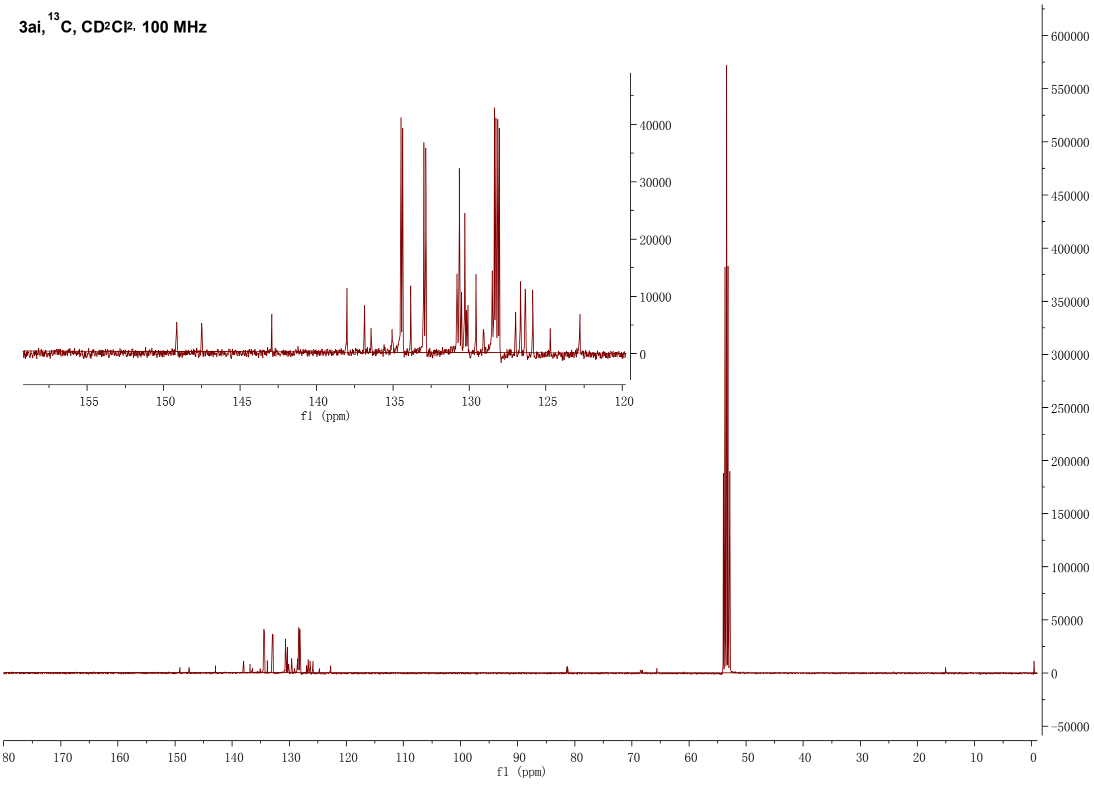

PPh3
N
Rh
PPh3
PF6
O2N

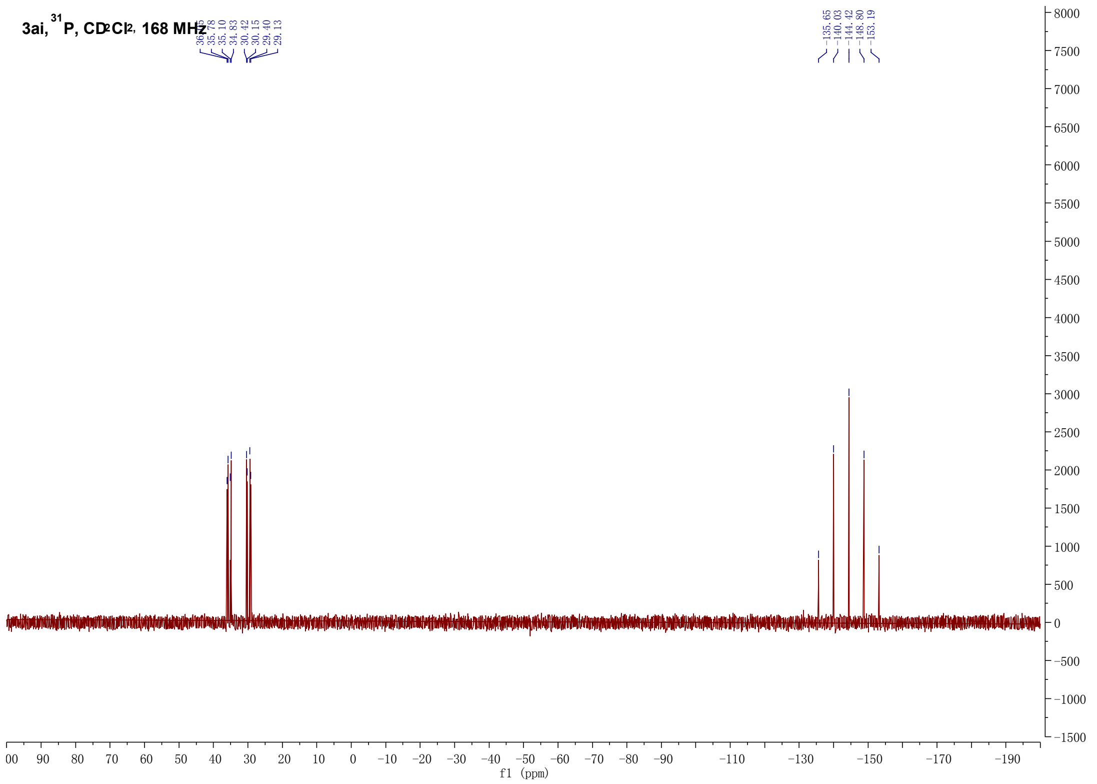
3ai

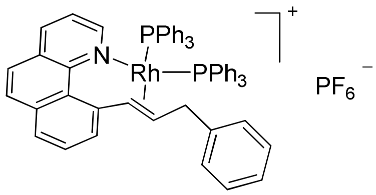
3ai, ^{1}H, CD_2Cl_2, 400 MHz



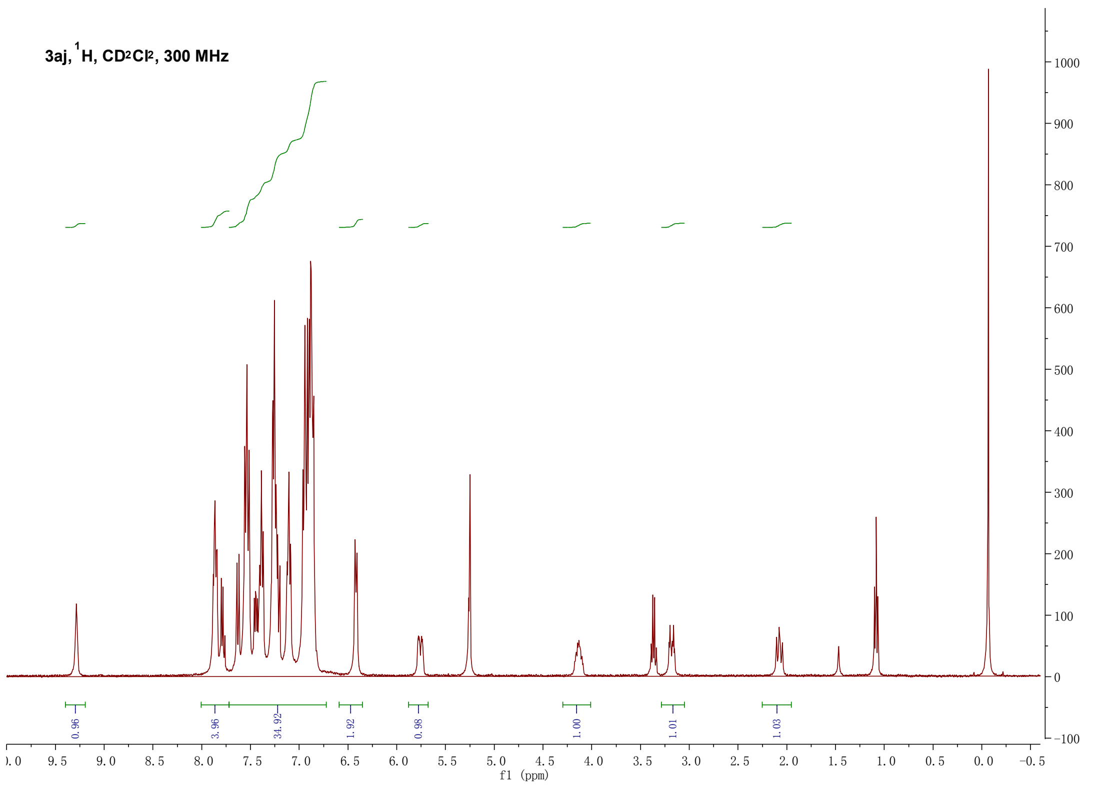
3ai, ^{13}C, CD_2Cl_2, 100 MHz

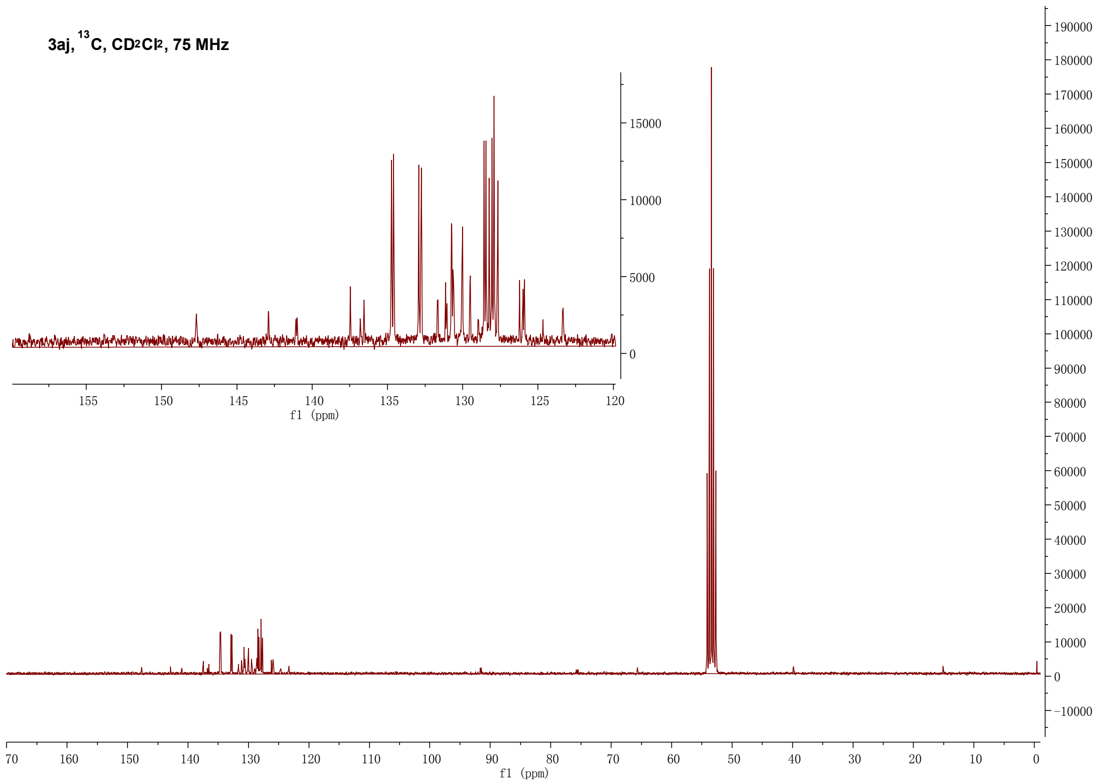


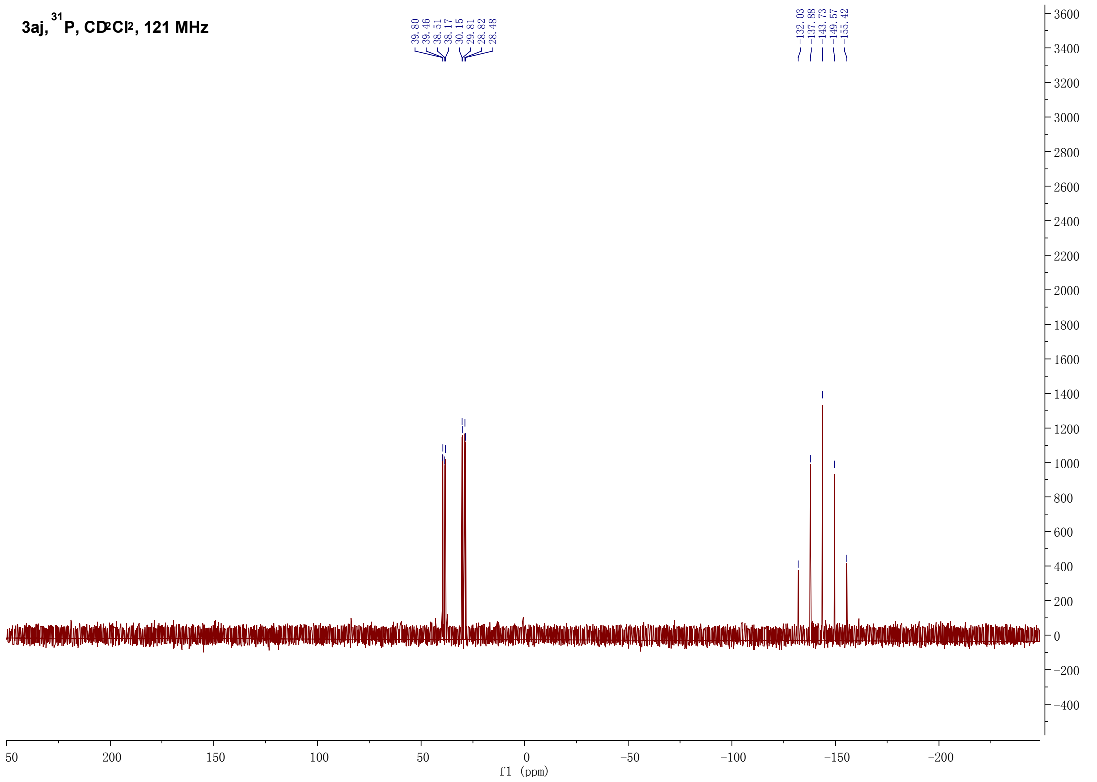

3ai, 31P, CD2Cl2, 168 MHz
36.05
35.78
35.10
34.83
30.42
30.15
29.40
29.13
-135.65
-140.03
-144.42
-148.80
-153.19
f1 (ppm)

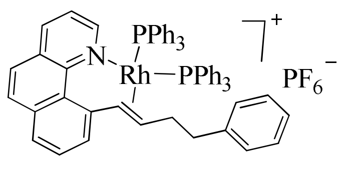

PPh3
N
Rh
PPh3
+
PF6
−

3aj

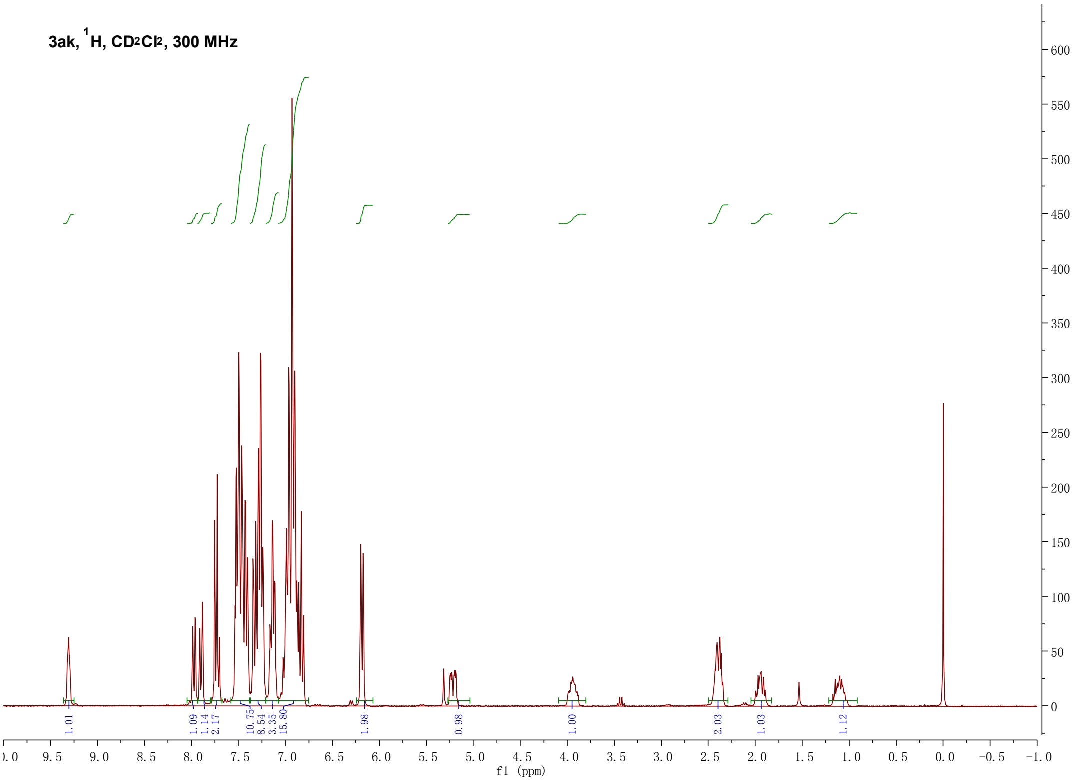

3aj, 1H, CD2Cl2, 300 MHz
0.96
3.96
34.92
1.92
0.98
1.00
1.01
1.03
f1 (ppm)

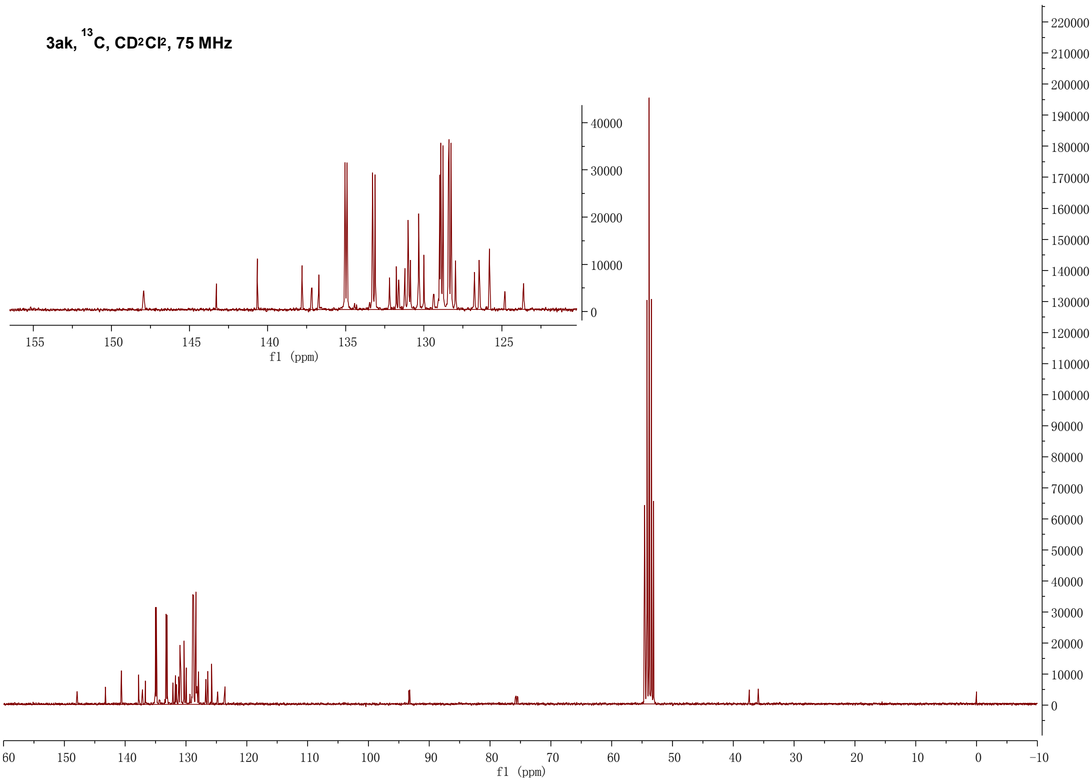

3aj, 13C, CD2Cl2, 75 MHz
f1 (ppm)

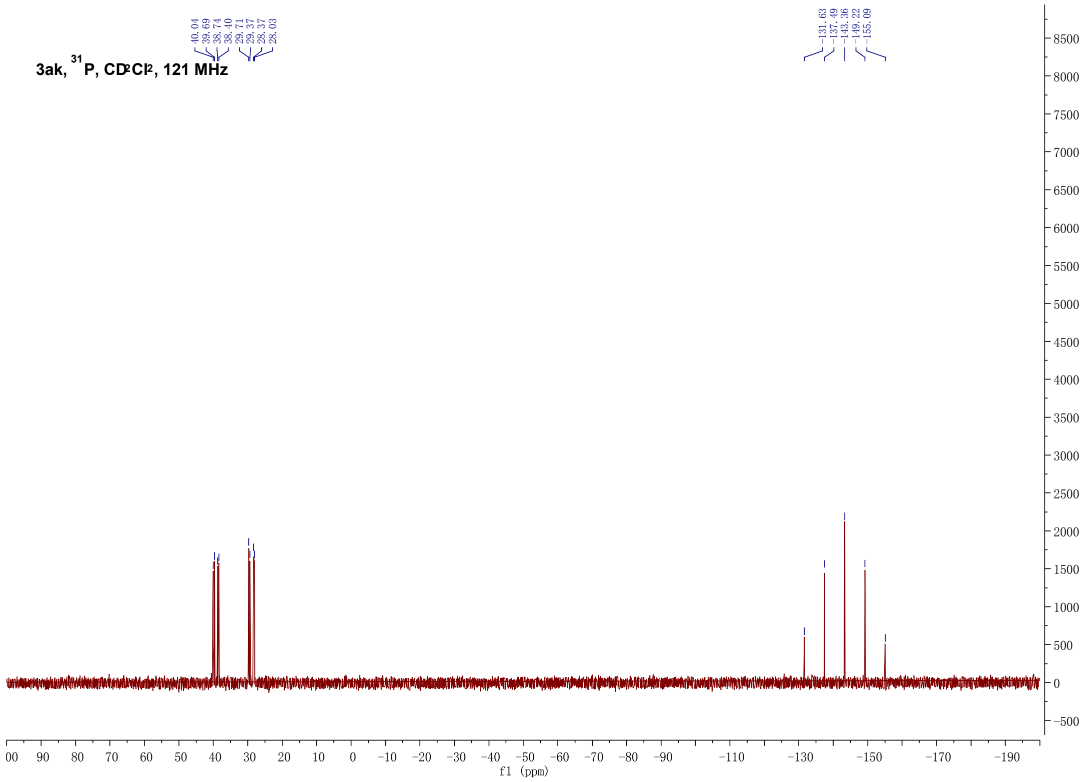

3aj, 31P, CD2Cl2, 121 MHz
39.80
39.46
38.51
38.17
30.15
29.81
28.82
28.48
-132.03
-137.88
-143.73
-149.57
-155.42
f1 (ppm)

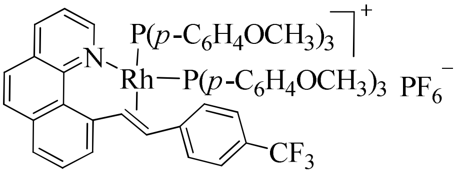

N
PPh3
Rh
PPh3
PF6
+
−

3ak

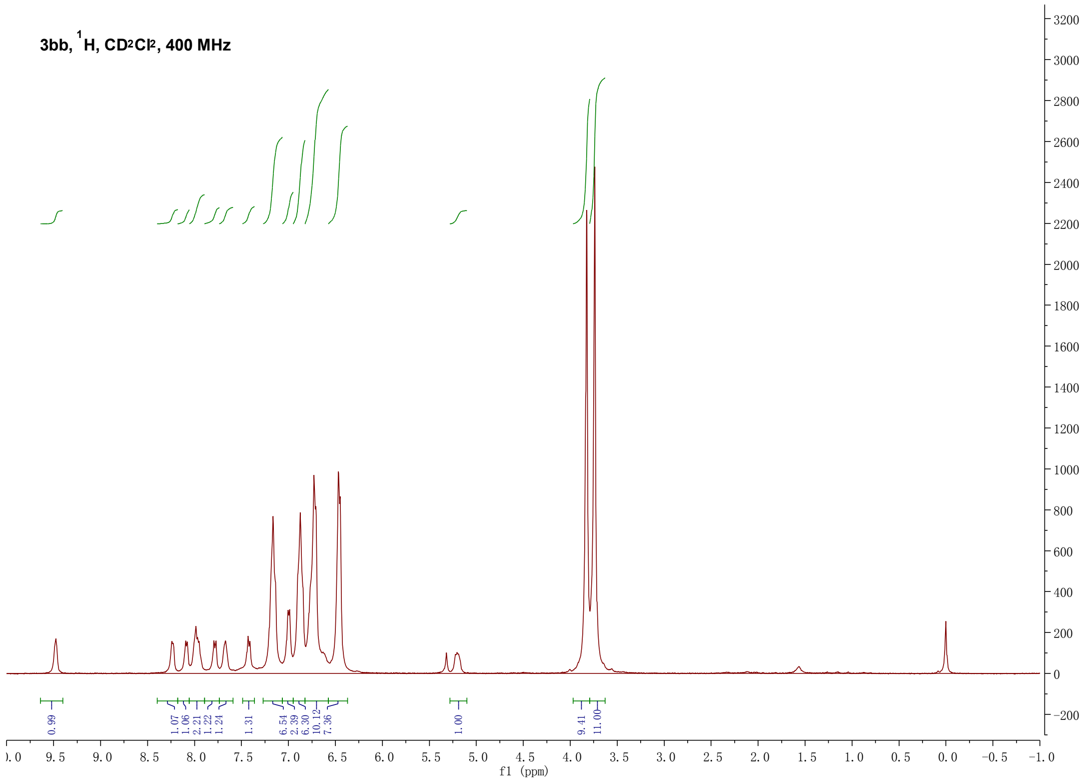

3ak, ^{1}H, CD_2Cl_2, 300 MHz

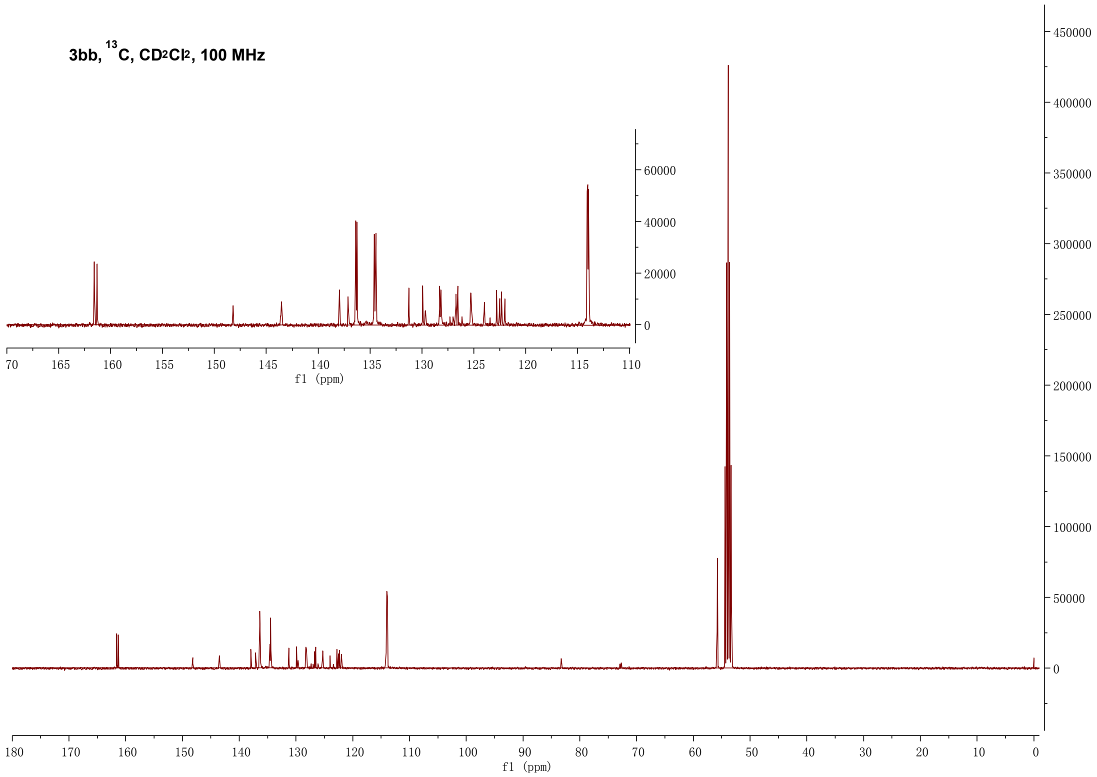

3ak, ^{13}C, CD_2Cl_2, 75 MHz

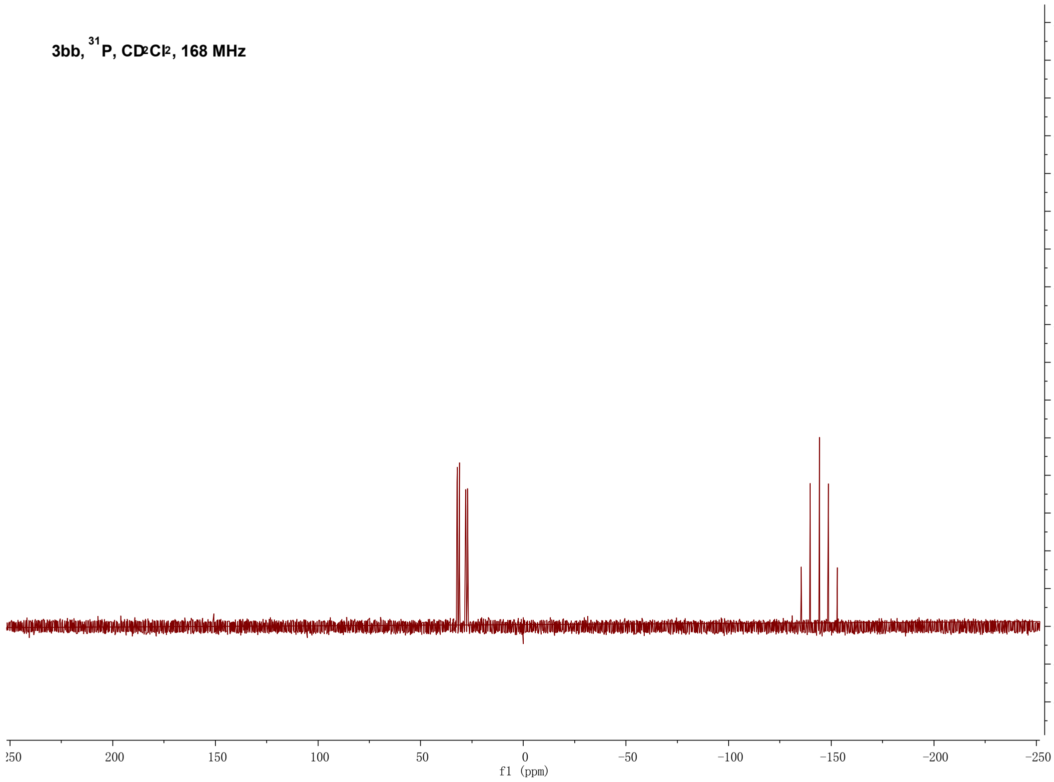


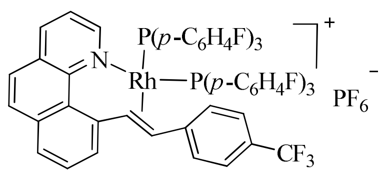


3bb

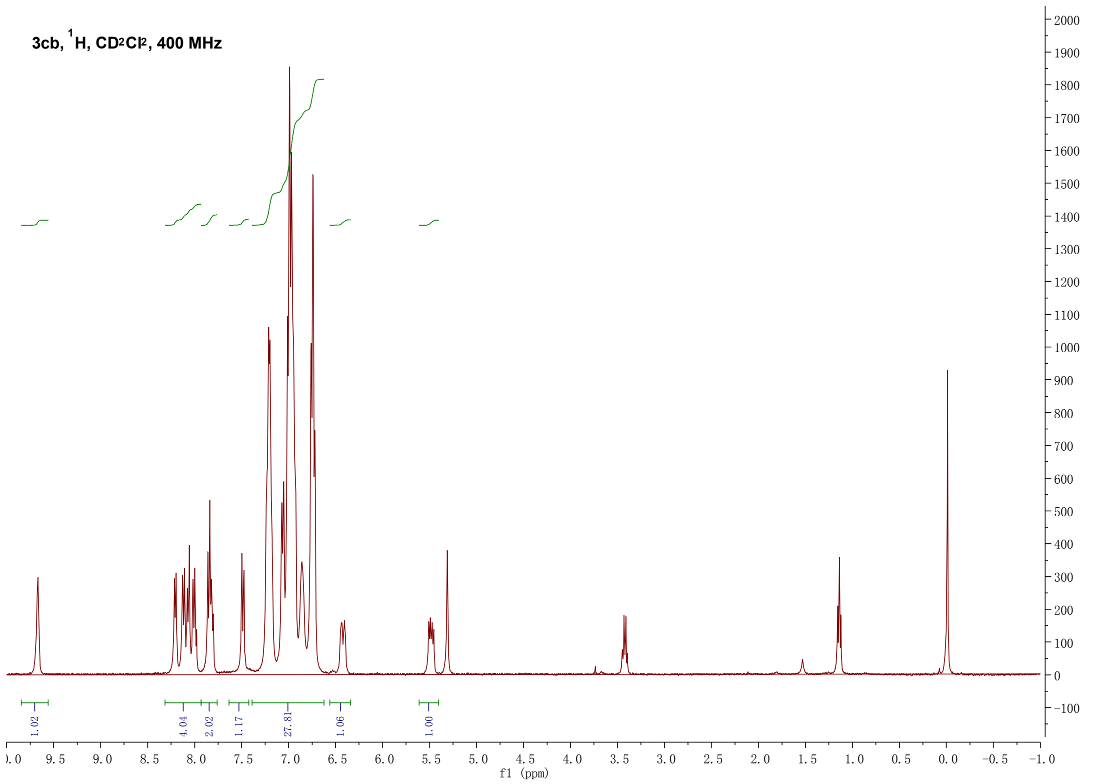


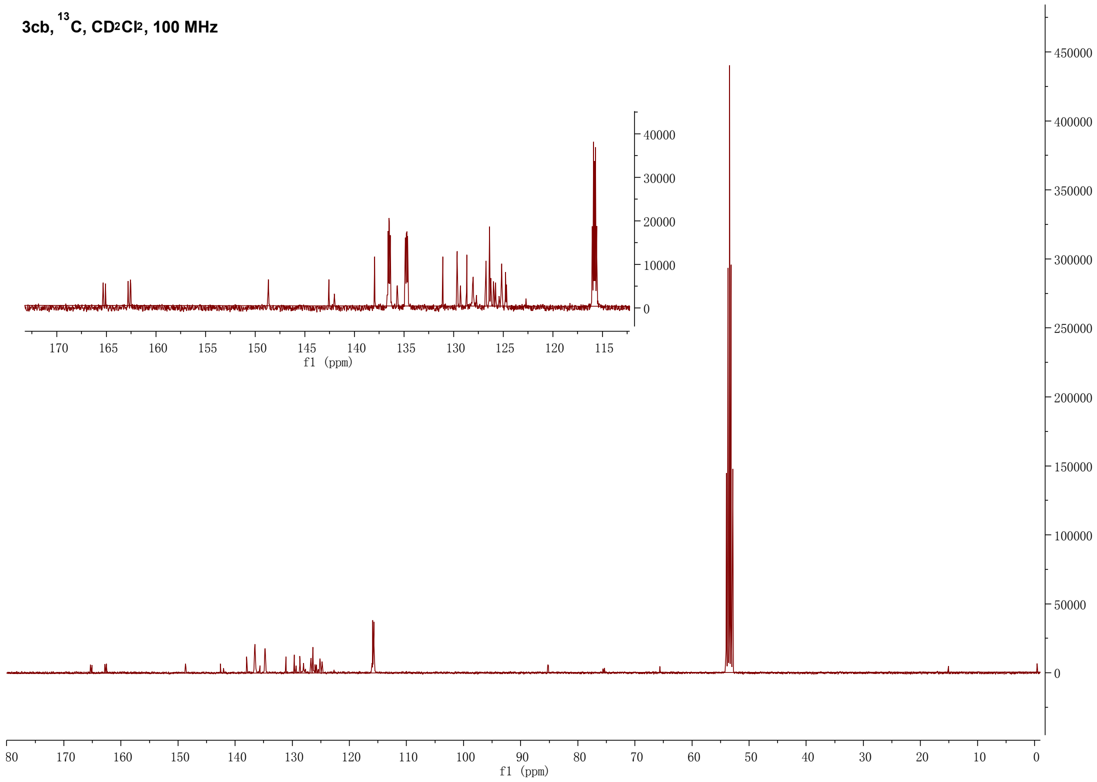

3bb, 13C, CD2Cl2, 100 MHz
f1 (ppm)

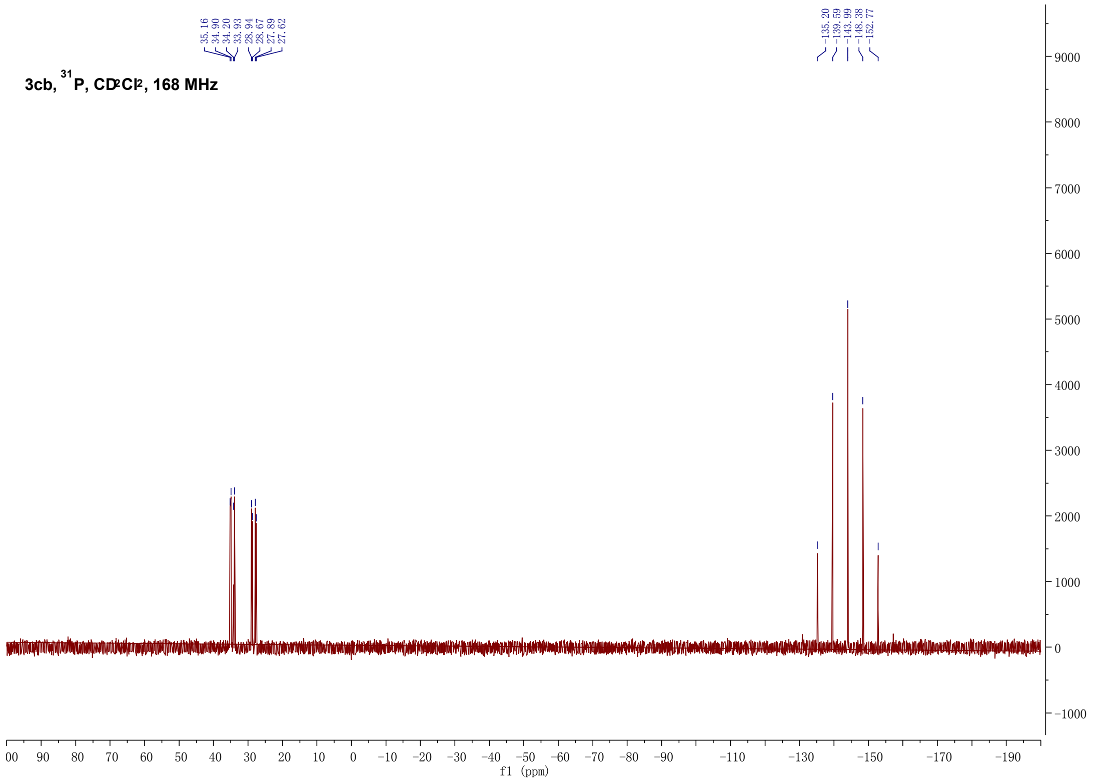

3bb, 31P, CD2Cl2, 168 MHz
f1 (ppm)

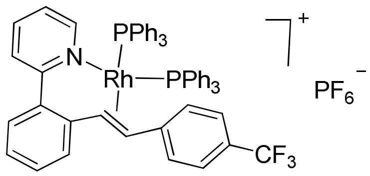

N
Rh
P(p-C6H4F)3
P(p-C6H4F)3
PF6
CF3

3cb

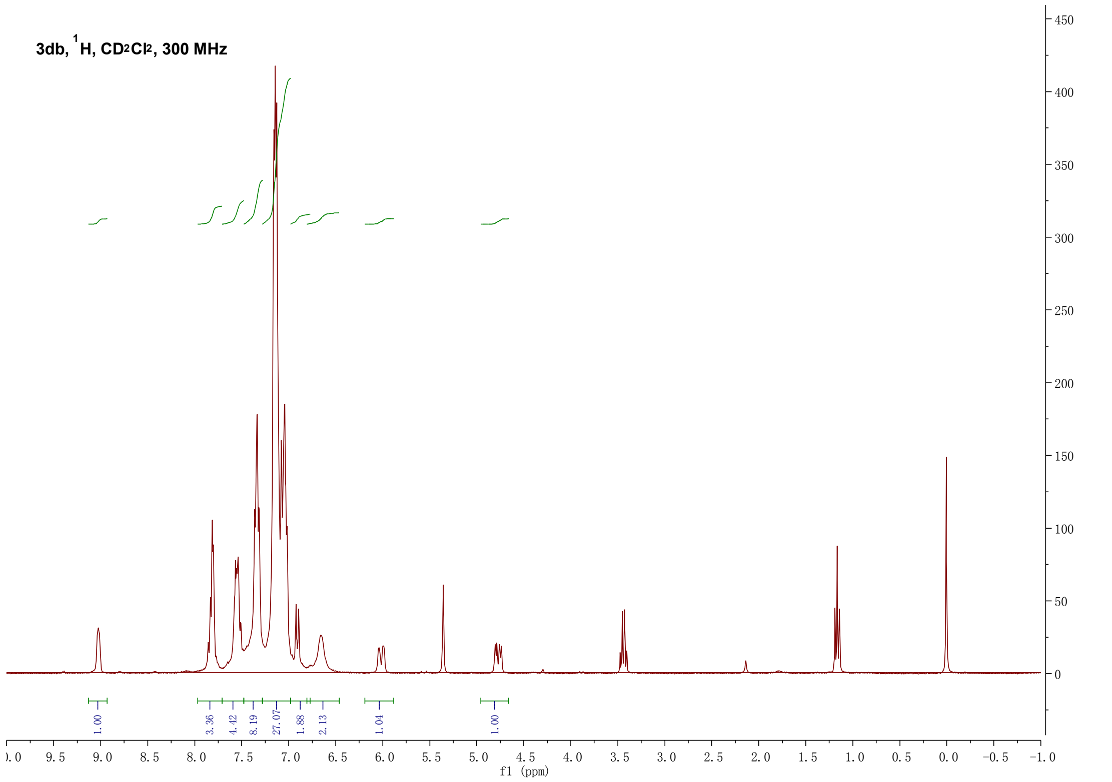

3cb, ^{1}H, CD_2Cl_2, 400 MHz
f1 (ppm)

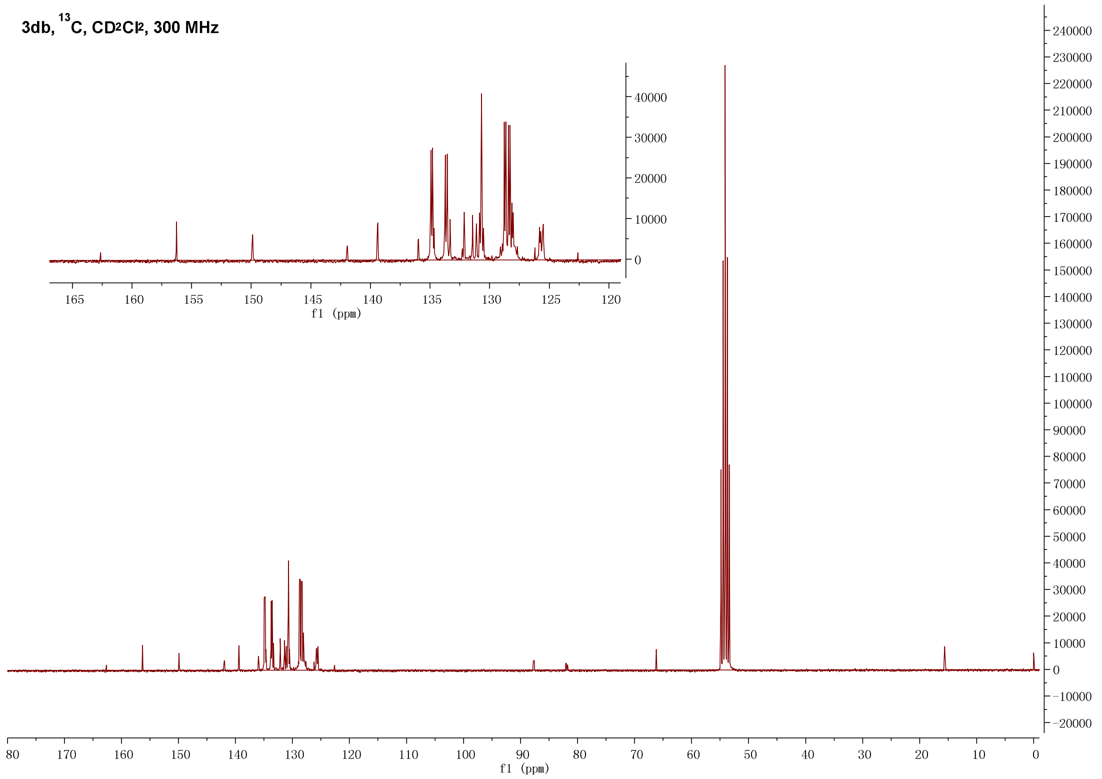

3cb, ^{13}C, CD_2Cl_2, 100 MHz
f1 (ppm)

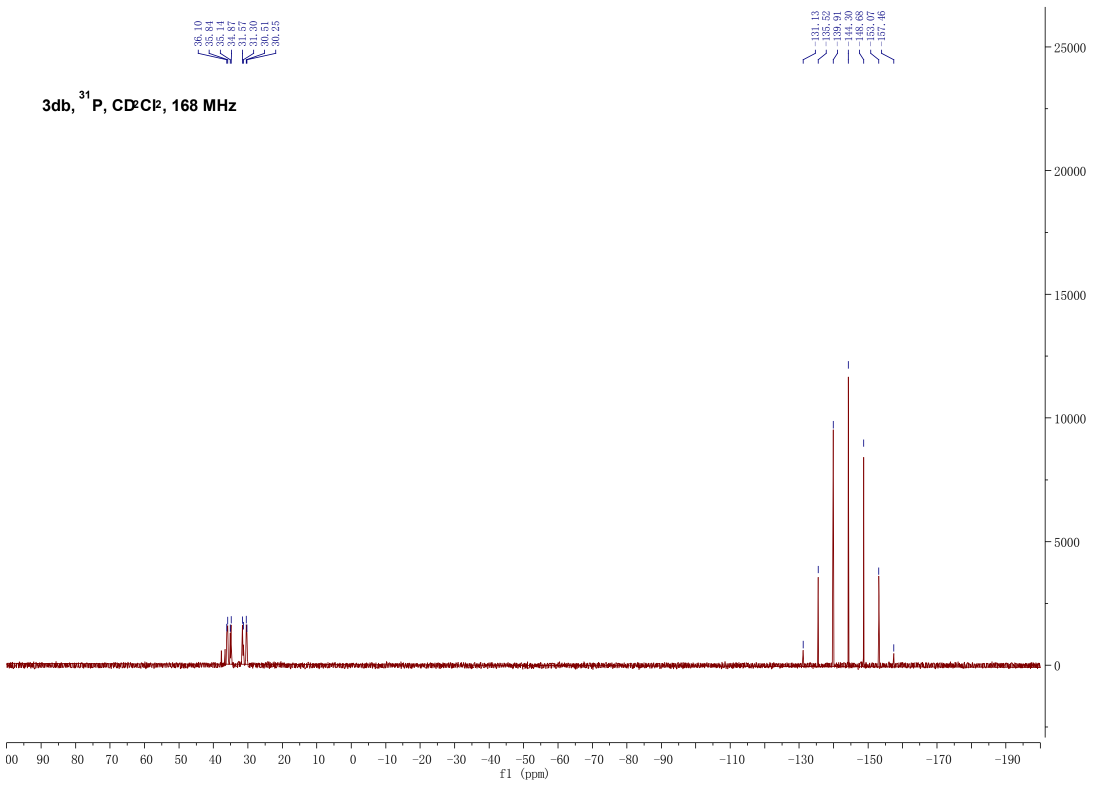

3cb, 31P, CD2Cl2, 168 MHz
35.16
34.90
34.20
33.93
28.94
28.67
27.89
27.62
-135.20
-139.59
-143.99
-148.38
-152.77
f1 (ppm)

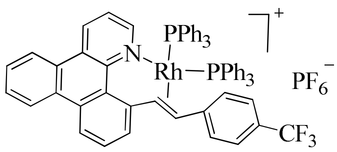

PPh3
N
Rh
PPh3
+
PF6
−
CF3

3db

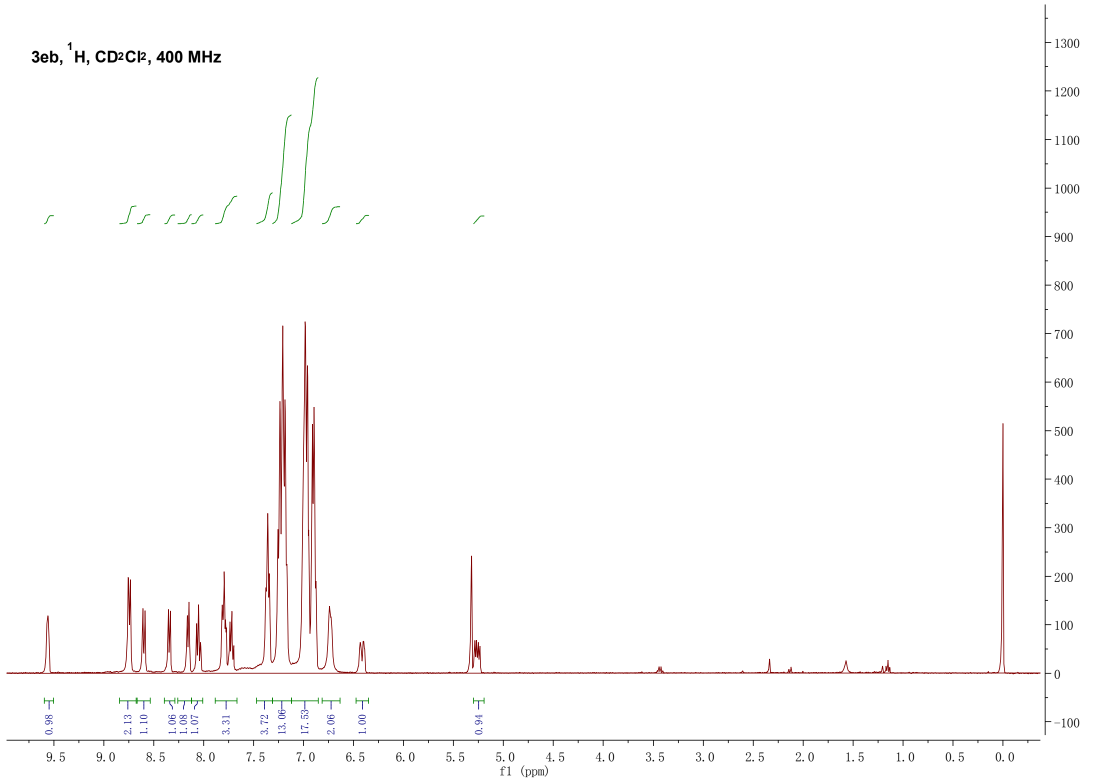

3db, 1H, CD2Cl2, 300 MHz
1.00
3.36
4.42
8.19
27.07
1.88
2.13
1.04
1.00
f1 (ppm)

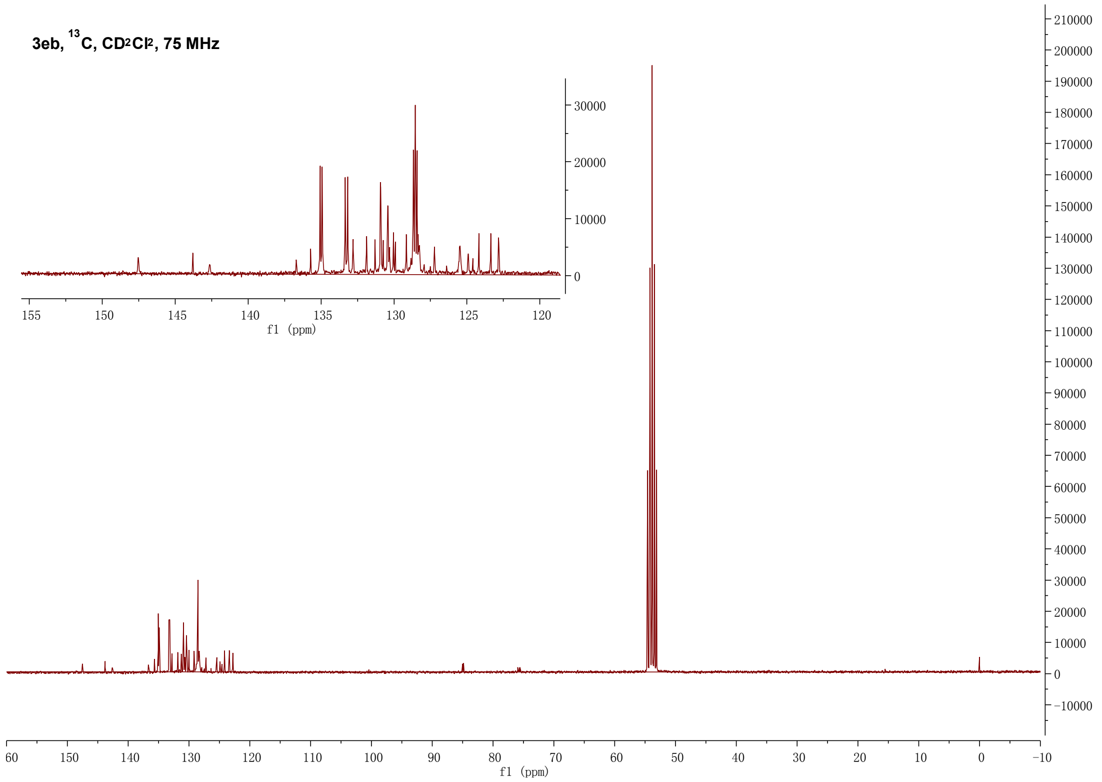

3db, 13C, CD2Cl2, 300 MHz
f1 (ppm)

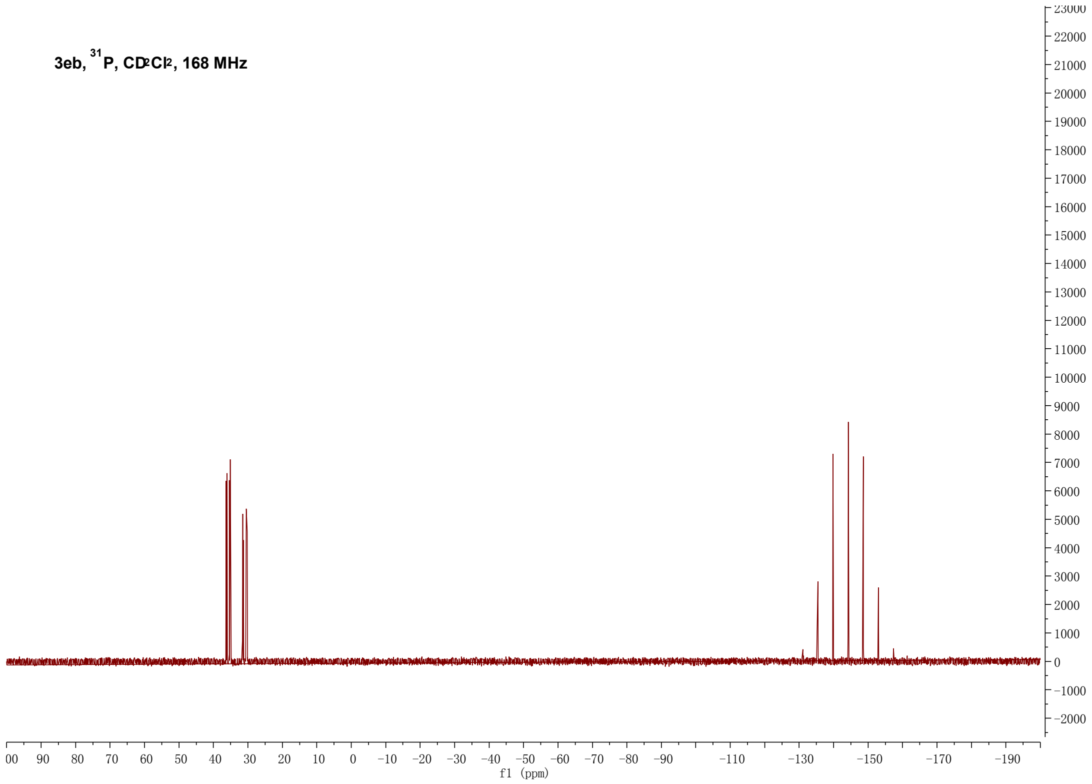

3db, 31P, CD2Cl2, 168 MHz
36.10
35.84
35.14
34.87
31.57
31.30
30.51
30.25
-131.13
-135.52
-139.91
-144.30
-148.68
-153.07
-157.46
f1 (ppm)

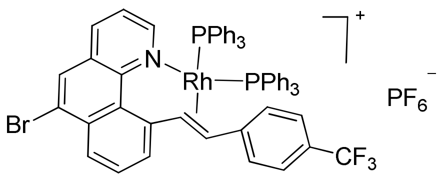

N
PPh3
Rh
PPh3
PF6−
CF3
+

3eb

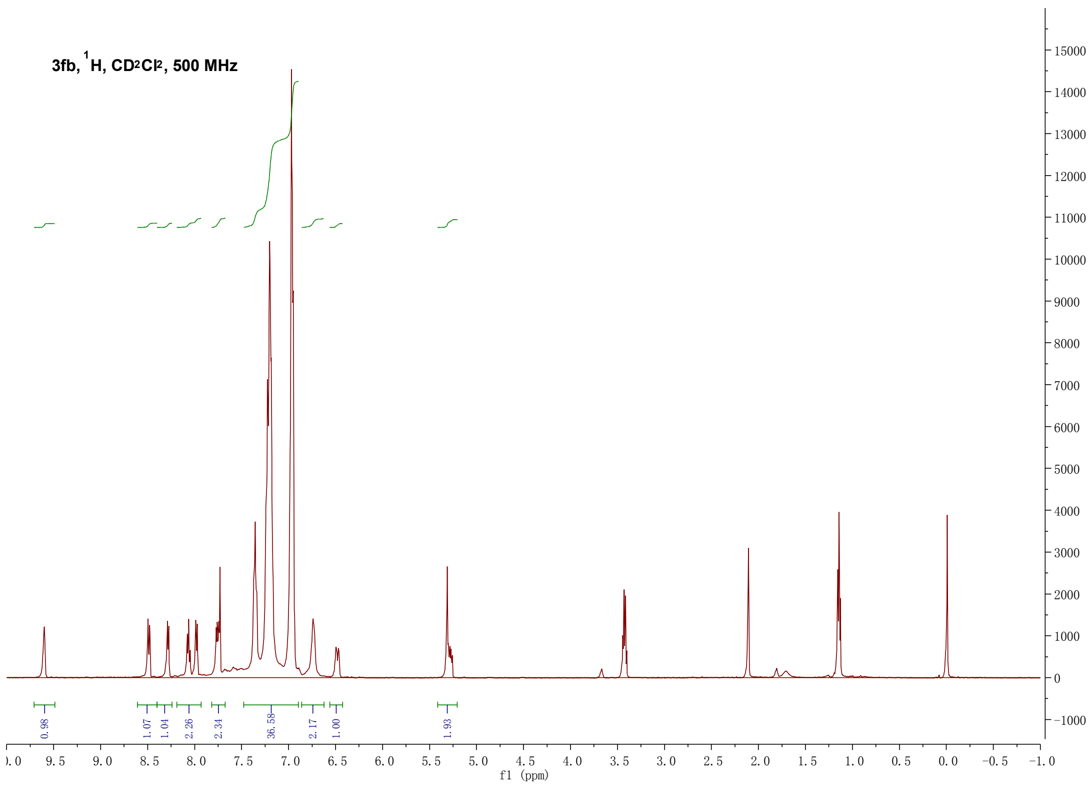

3eb, 1H, CD2Cl2, 400 MHz
f1 (ppm)

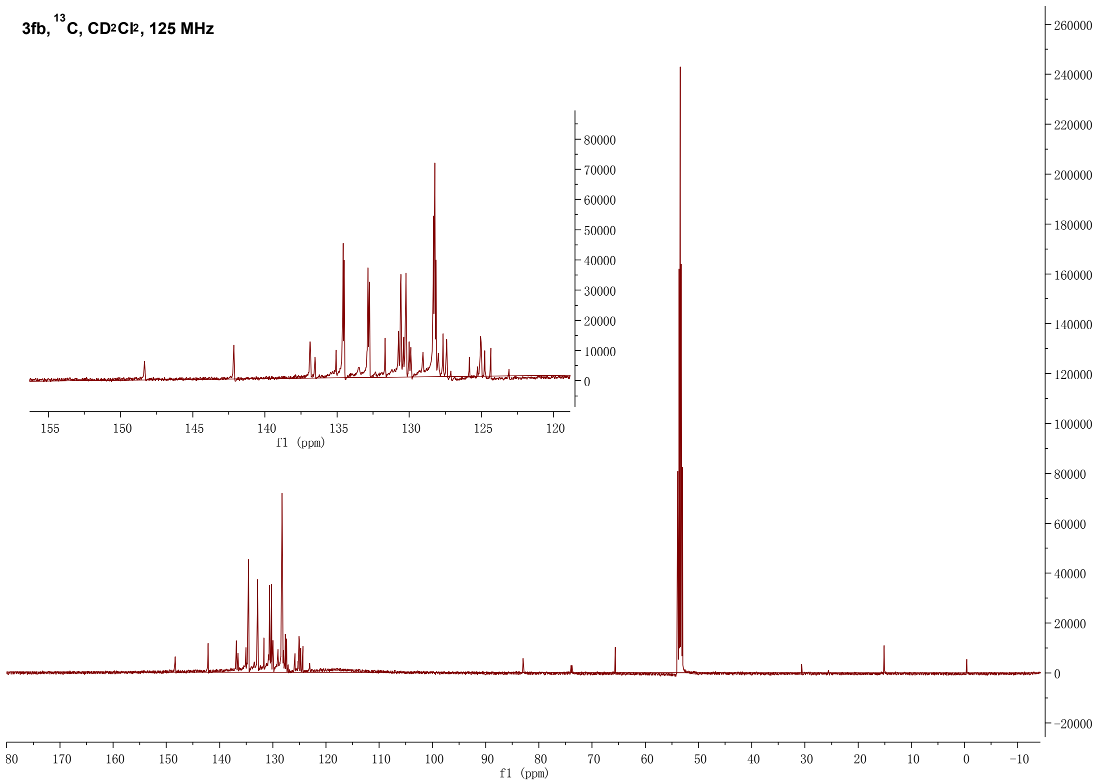

3eb, 13C, CD2Cl2, 75 MHz
f1 (ppm)

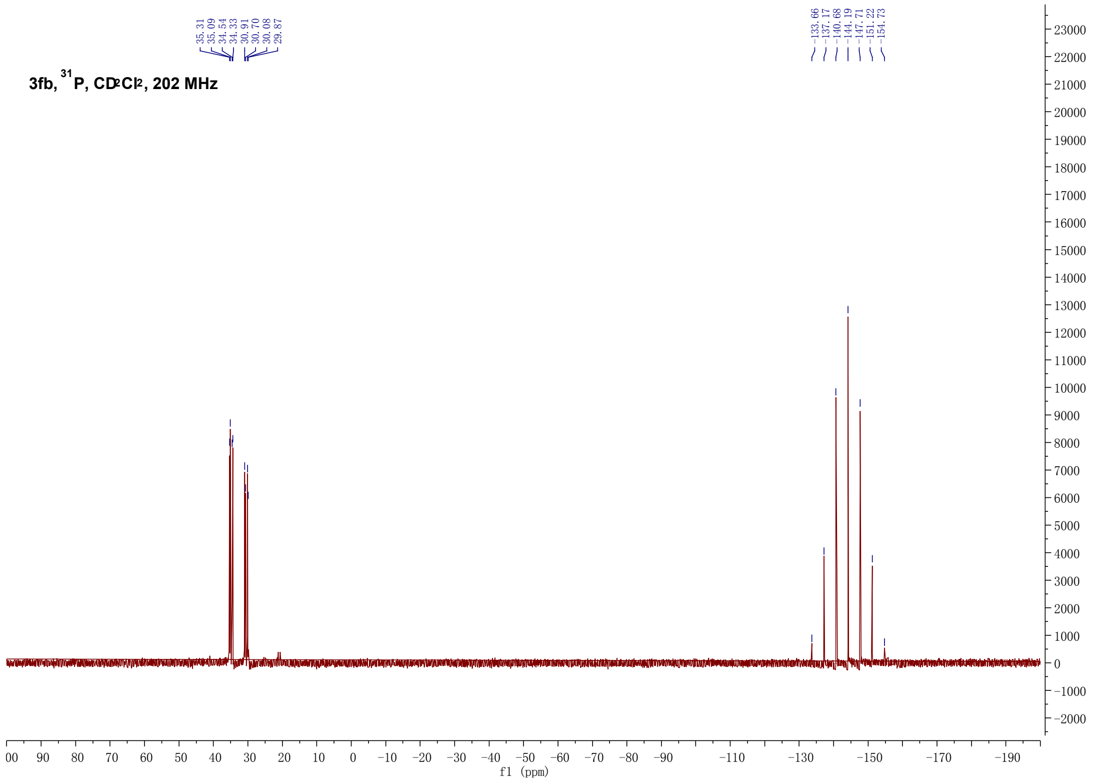

3eb, 31P, CD2Cl2, 168 MHz
f1 (ppm)

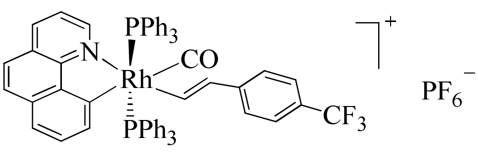

PPh3
N
Rh
PPh3
Br
CF3
PF6
+
−

3fb


3fb, 1H, CD2Cl2, 500 MHz
f1 (ppm)

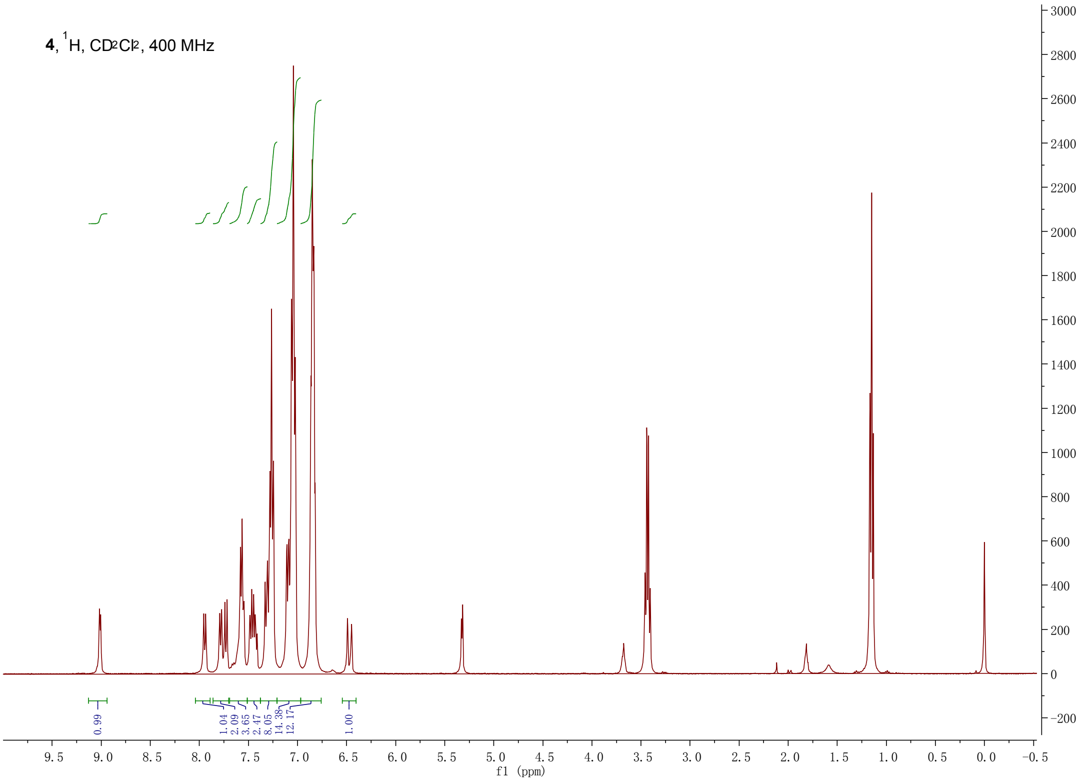

3fb, 13C, CD2Cl2, 125 MHz
f1 (ppm)


3fb, 31P, CD2Cl2, 202 MHz
35.31
35.09
34.54
34.33
30.91
30.70
30.08
29.87
-133.66
-137.17
-140.68
-144.19
-147.71
-151.22
-154.73
f1 (ppm)

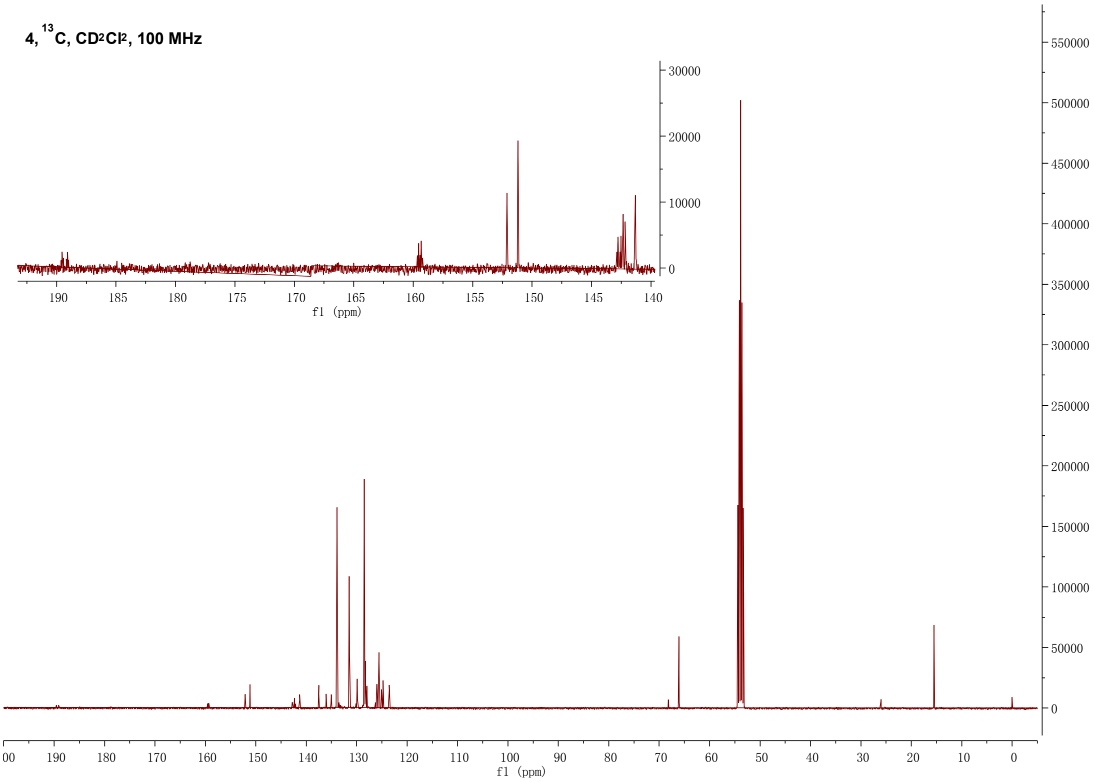

PPh3
CO
Rh
N
PPh3
CF3
PF6

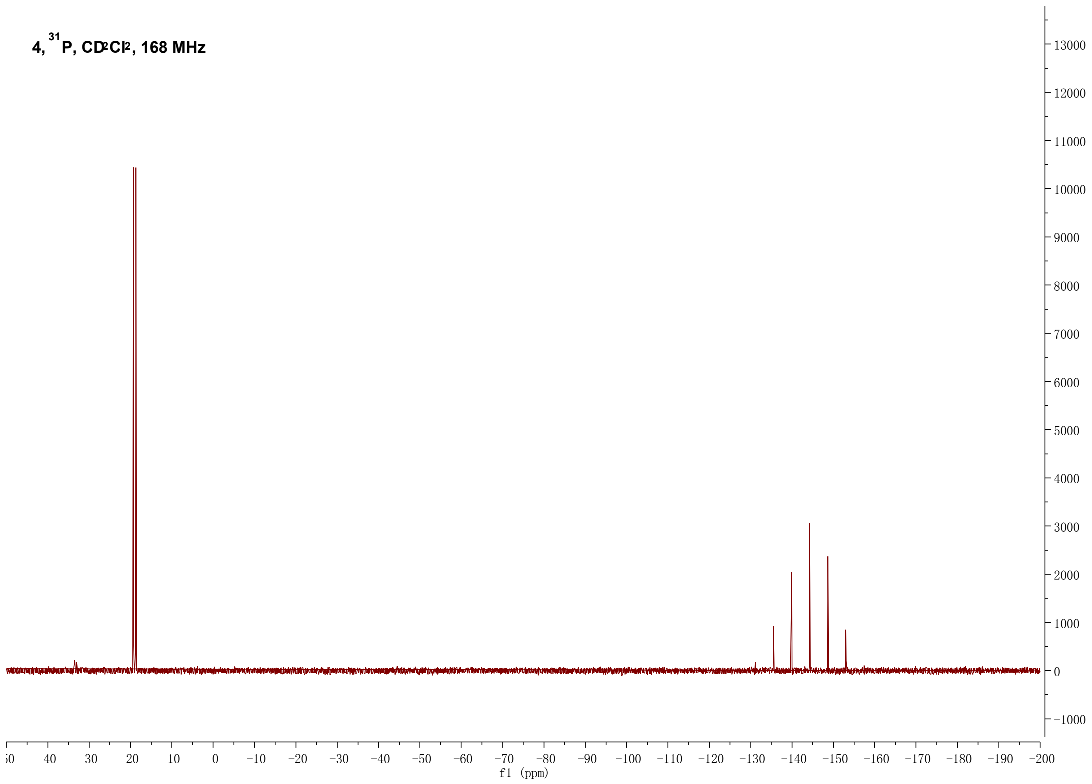
4

4, ^{1}H, CD_2Cl_2, 400 MHz



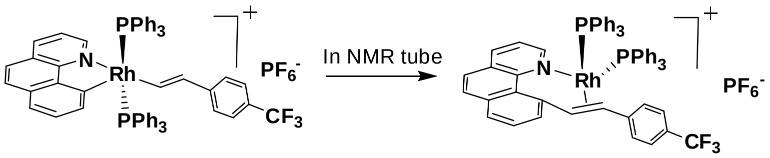
4, ^{13}C, CD_2Cl_2, 100 MHz




4, 31P, CD2Cl2, 168 MHz
f1 (ppm)

Kinetics Data of C-C Reductive Elimination From Rare five-Coordinate Rh(III) Complexes by NMR Spectroscopy.

1. Kinetic studies of the decay of 2ab.



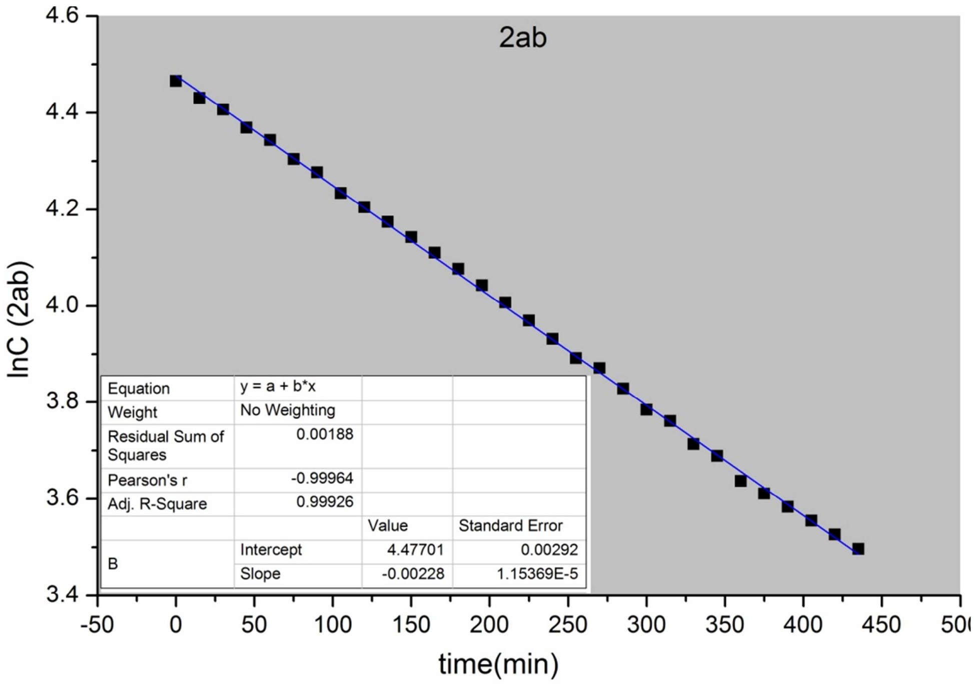


Chart 1. Ln [2ab] – times plot. based on ^{19}F NMR analysis at 287.67 K in CD_2Cl_2.

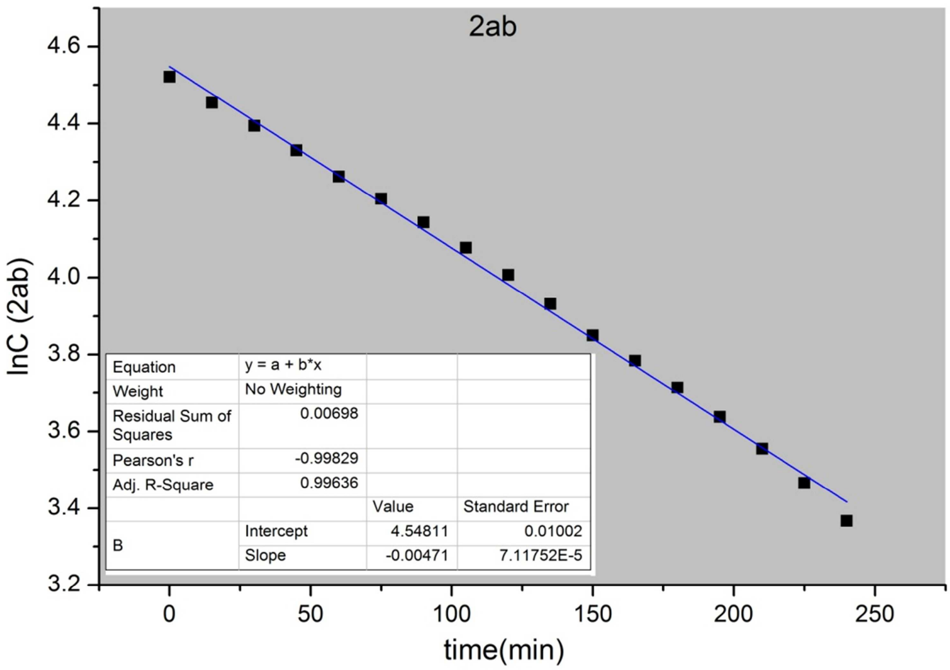


Chart 2. **Ln [2ab] – times plot. based on ^{19}F NMR analysis at 293.58 K in CD_2Cl_2.**

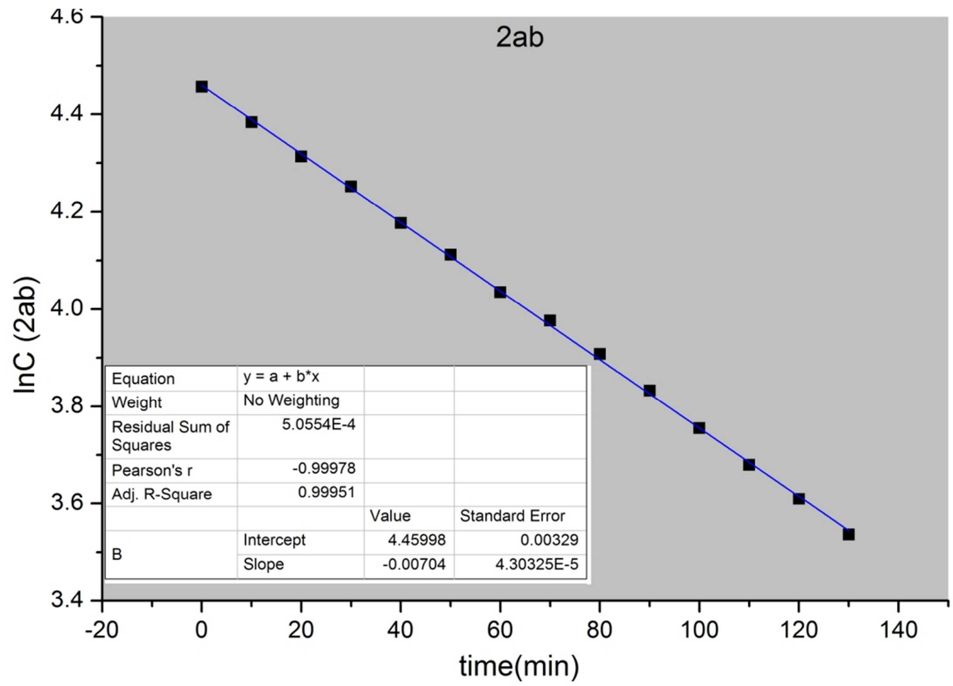


Chart 3. **Ln [2ab] – times plot. based on ^{19}F NMR analysis at 296.96 K in CD_2Cl_2.**

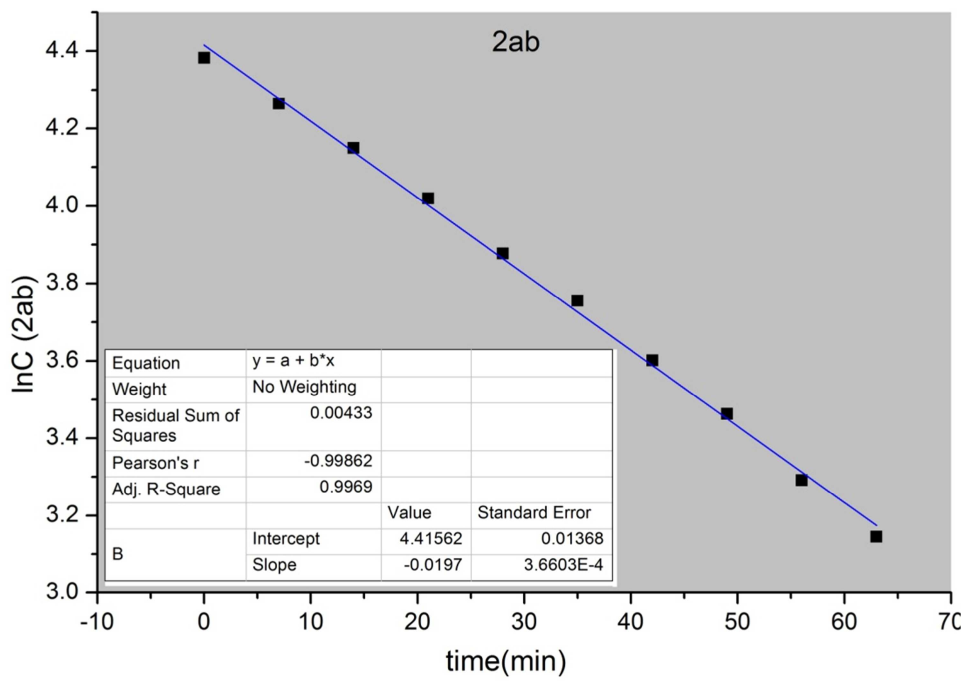


Chart 4. Ln [2ab] – times plot. based on[19]F NMR analysis at 305.3 K in CD_2Cl_2.

Table 1. Temperature-Dependent Kinetics for the Decay of 2ab

T **(K)**	**1/*T***	**ln(*k*/*T*)**	***k*** **(min-1)**
287.67	0.003476	-11.766	0.00228(1)
293.58	0.003406	-11.0392	0.00471(7)
296.96	0.003367	-10.65	0.00704(4)
305.3	0.003275	-9.6486	0.0197(1)

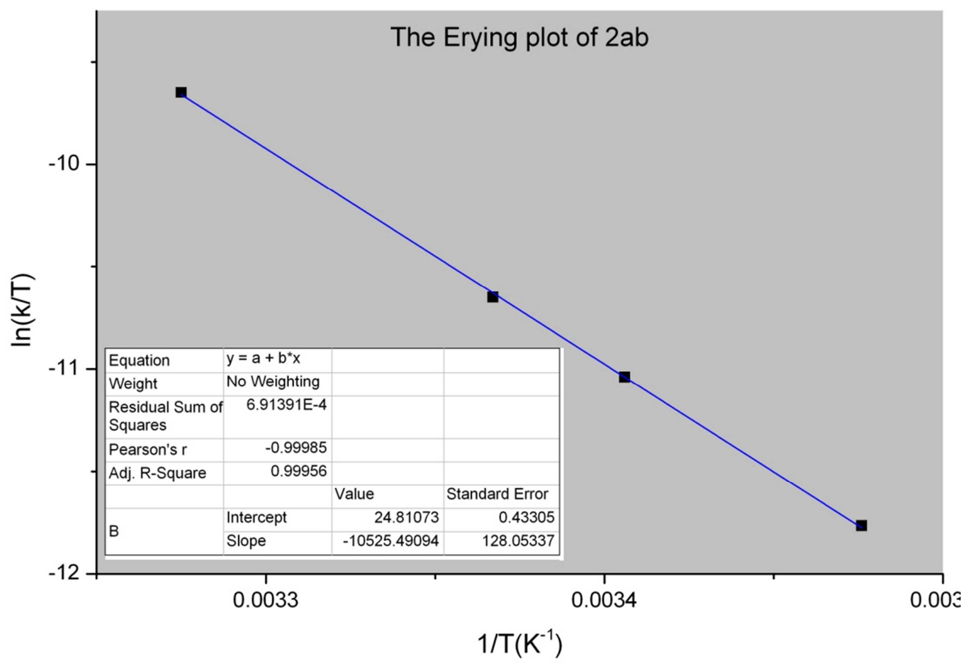
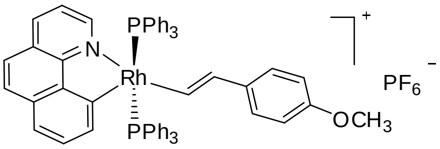


Chart 5. The Erying Plot for the kinetic studies of the decay of 2ab.

$$k = \frac{k_B T}{h} \exp\left(\frac{\Delta^{\ddagger} S^{\circ}}{R}\right) \exp\left(-\frac{\Delta^{\ddagger} H^{\circ}}{RT}\right) \qquad \textbf{(3)}$$

$\Delta H^{\neq}$ = 20.9 kcal/mol; $\Delta S^{\neq}$ = -6.1 eu

2. Electronic Effects of Reacting and Ancillary Ligands.



2ag

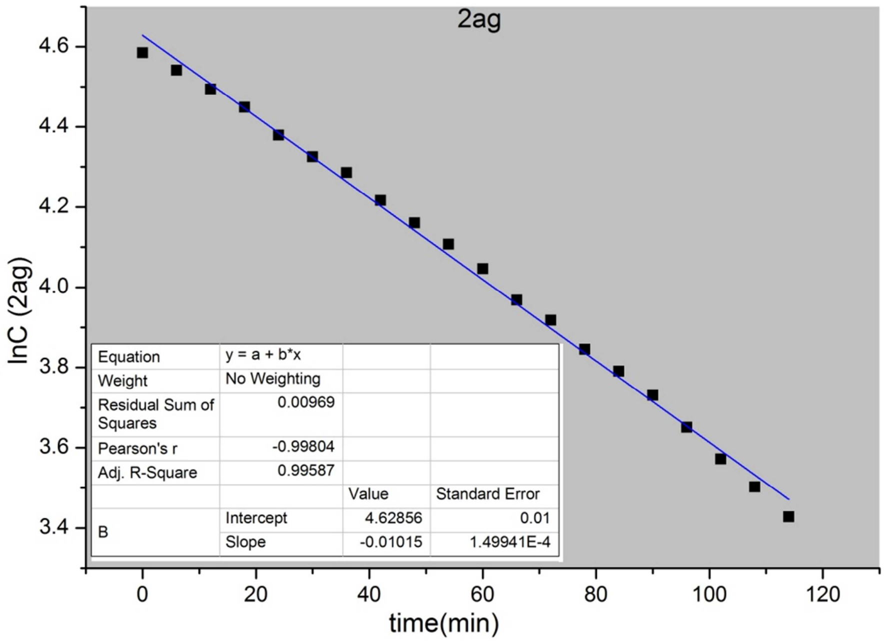
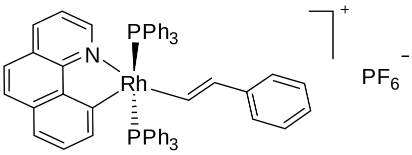


Chart 6. Ln [2ag] – times plot. based on [1]H NMR analysis at 293 K in CD_2Cl_2.



2aa

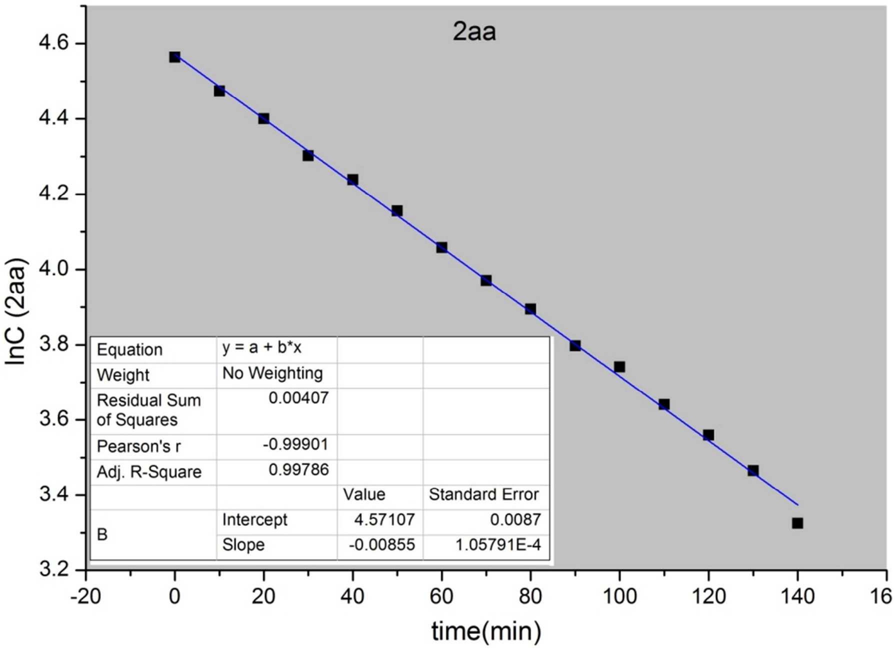
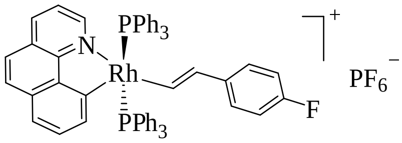


Chart 7. Ln [2aa] – times plot. based on ^{1}H NMR analysis at 293 K in CD_2Cl_2.



2af

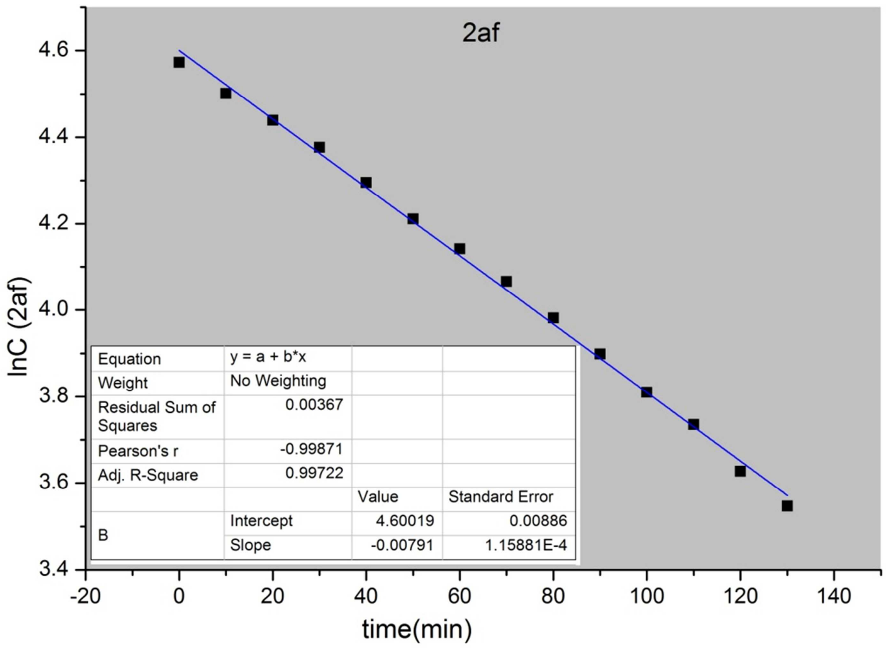
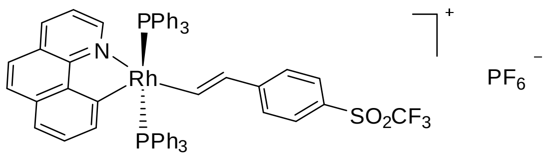


Chart 8. Ln [2af] – times plot. based on ^{1}H NMR analysis at 293 K in CD_2Cl_2.



2ac

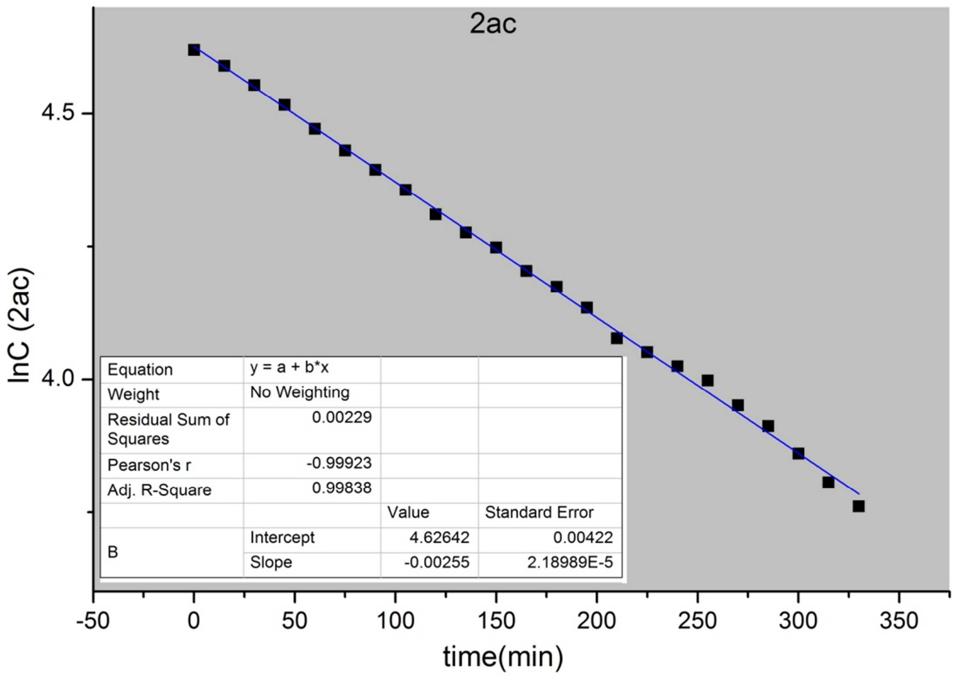
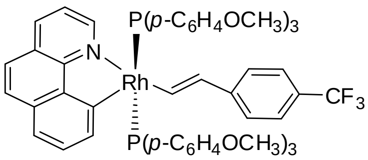


Chart 9. Ln [2ac] – times plot. based on ^{1}H NMR analysis at 293 K in CD_2Cl_2.

2bb



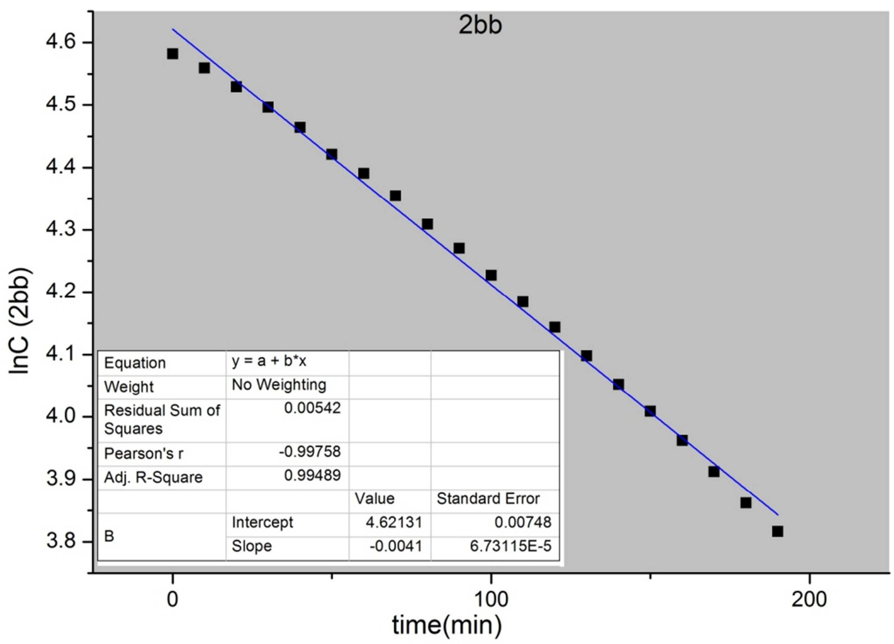
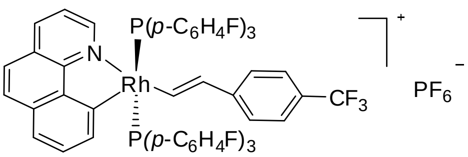


Chart 10. Ln [2bb] – times plot. based on ^{19}F NMR analysis at 293 K in CD_2Cl_2.

2cb



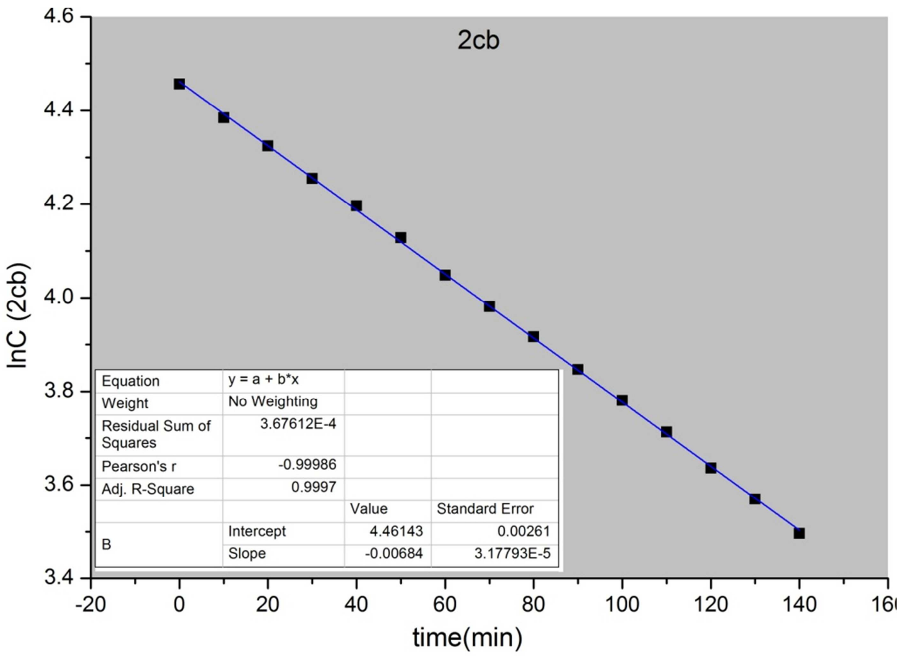
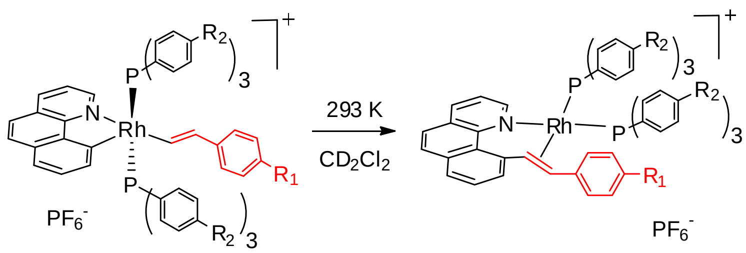


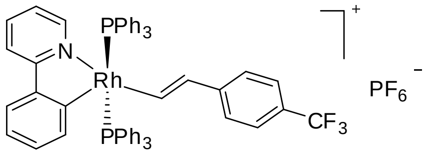
Chart 11. **Ln [2cb] – times plot. based on [19]F NMR analysis at 293 K in CD_2Cl_2**

Table 2. Electronic Effects of Reacting and Ancillary Ligands.



entry	R_1	R_2	σ_p (R_1)	*k* (min-1)
1	OMe	H	-0.27	0.0101(1)
2	H	H	0	0.0086(1)
3	F	H	0.06	0.0079(1)
4	CF_3	H	0.65	0.00471(7)
5	SO_2CF_3	H	0.93	0.00255(5)
6	CF_3	OMe		0.00410(7)
7	CF_3	F		0.00684(3)

3. Effects of the Cyclometalated Aryl Ligands on the Rate of C–C Reductive Elimination (297K, CD_2Cl_2)

2db 

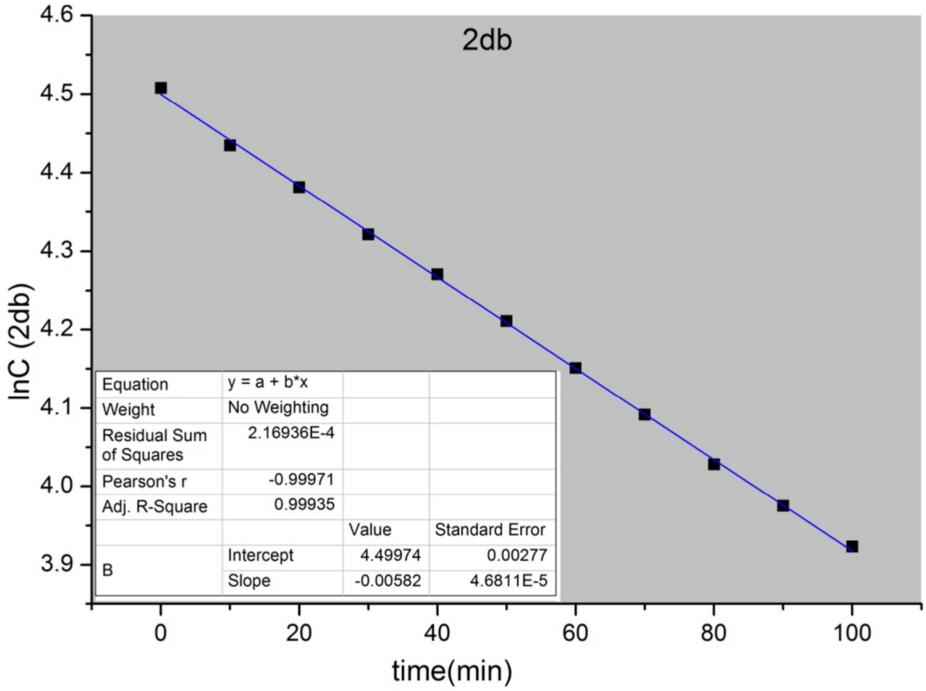
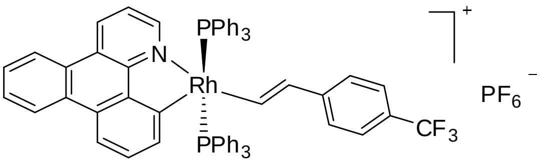


Chart 12. Ln [2db] – times plot. based on ^{19}F NMR analysis at 297 K in CD_2Cl_2.

2eb 

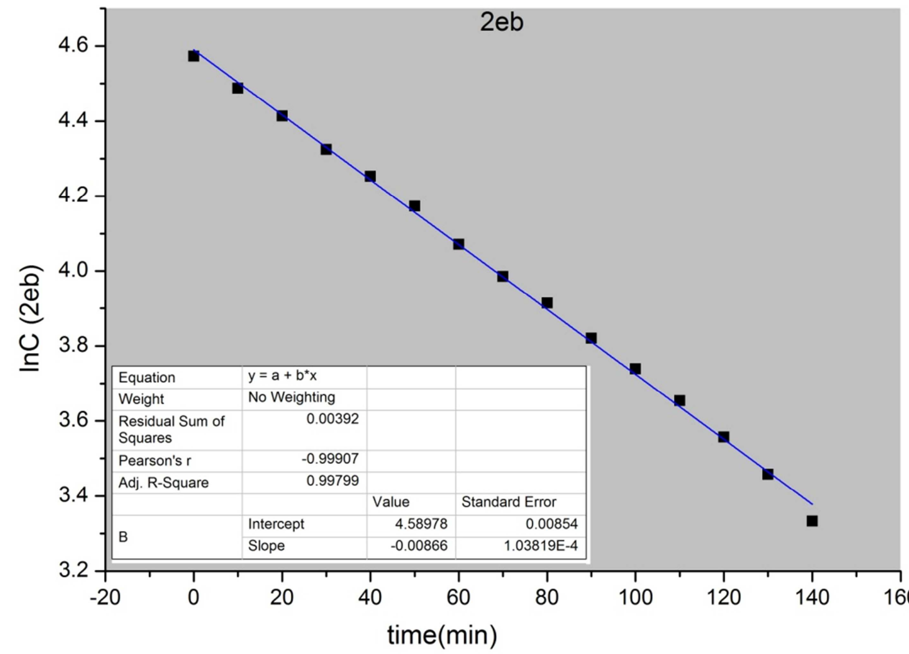


Chart 13. Ln [2eb] – times plot. based on ^{19}F NMR analysis at 297 K in CD_2Cl_2.

4. Solvent Effects for the Coupling of 2ab at 281 K

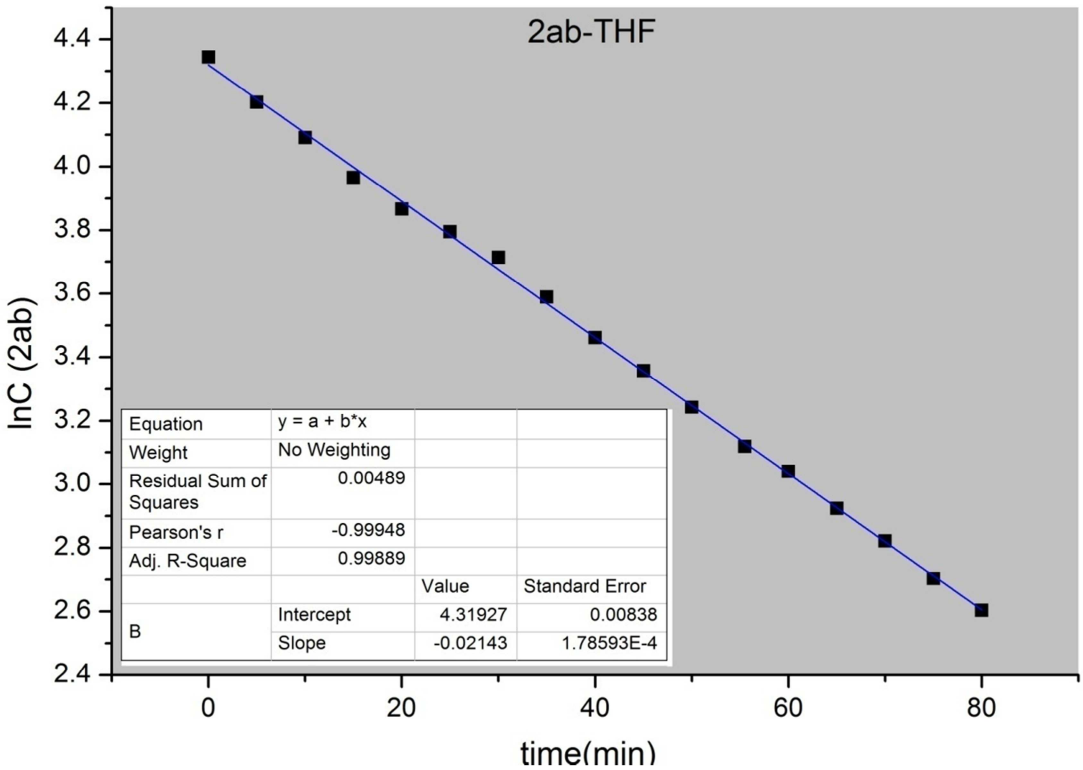


Chart 14. Ln [2ab] – times plot. based on ^{19}F NMR analysis at 281 K in THF-d_8.

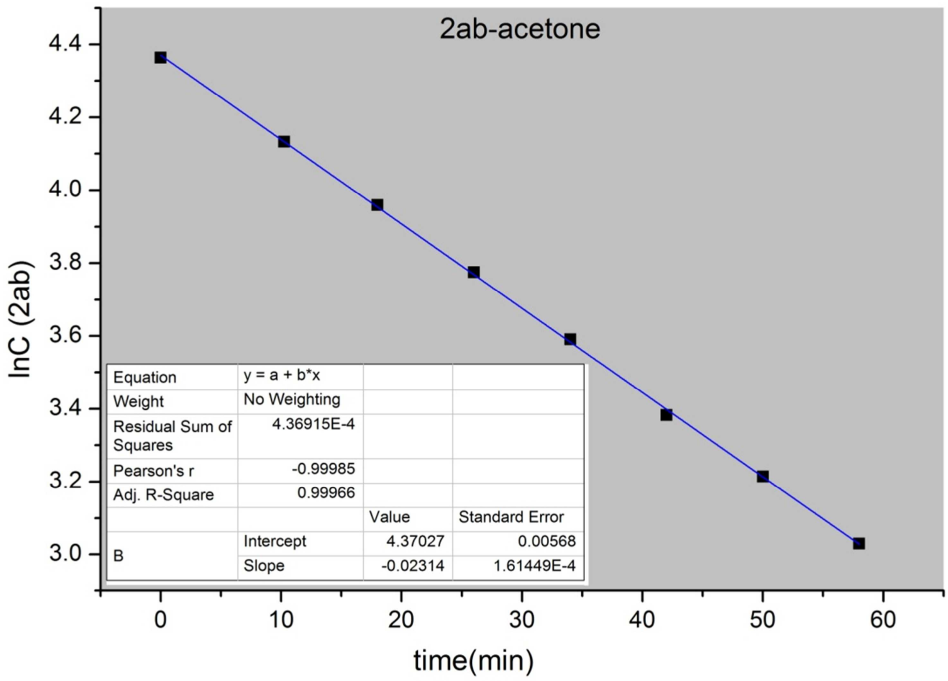


Chart 15. Ln [2ab] – times plot. based on ^{19}F NMR analysis at 281 K in acetone-d_6.

Table 3. Solvent Effects for the Coupling of 2ab at 281 K

entry	solvent	dielectric constant (F/m)	*k* (min^{-1})
1	CD_2Cl_2	9.1	0.000958 (extrapolated)
2	THF-d_8	7.5	0.0214(2)
3	acetone-d_6	21	0.0231(2)

5. The Effects of Added Phosphine

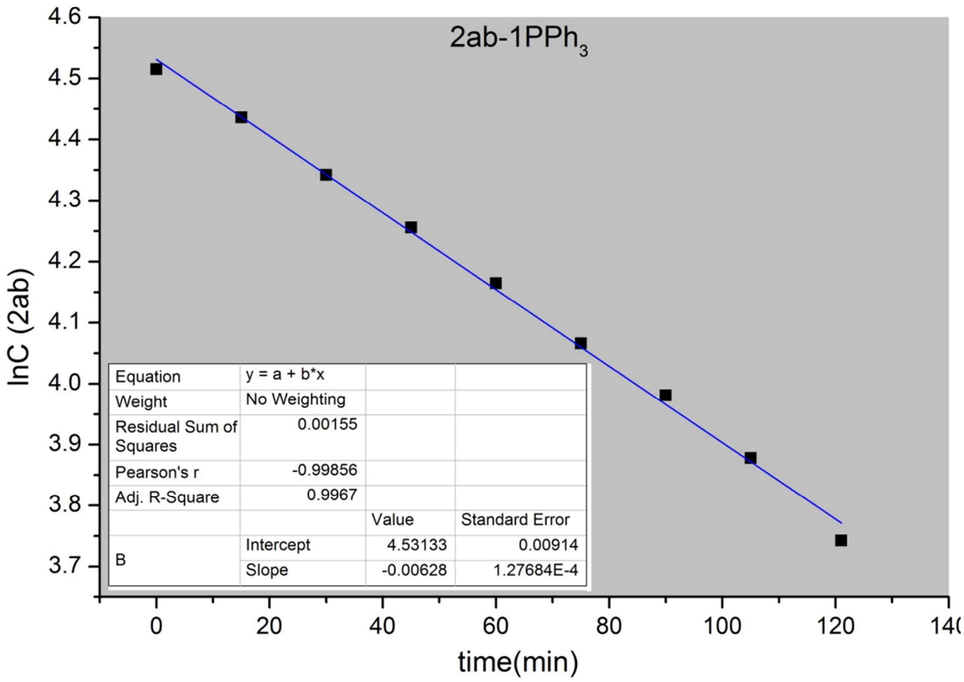


Chart 16. Ln [2ab] – times plot. based on [19]F NMR analysis at 297 K in CD_2Cl_2 with one equiv of PPh_3 .

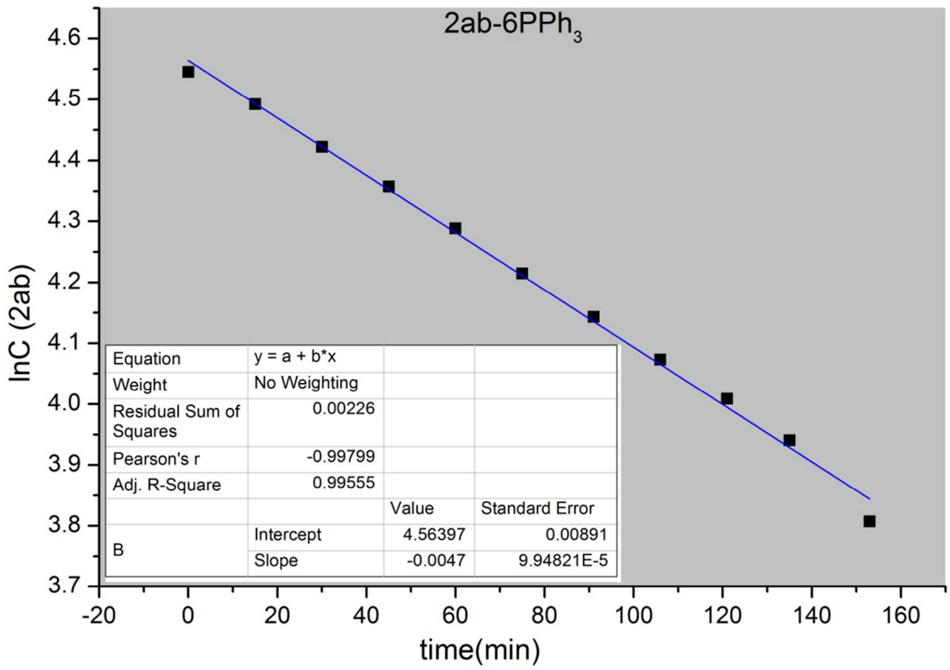


Chart 17. Ln [2ab] – times plot. based on ^{19}F NMR analysis at 297 K in CD_2Cl_2 with 6 equiv of PPh_3 .

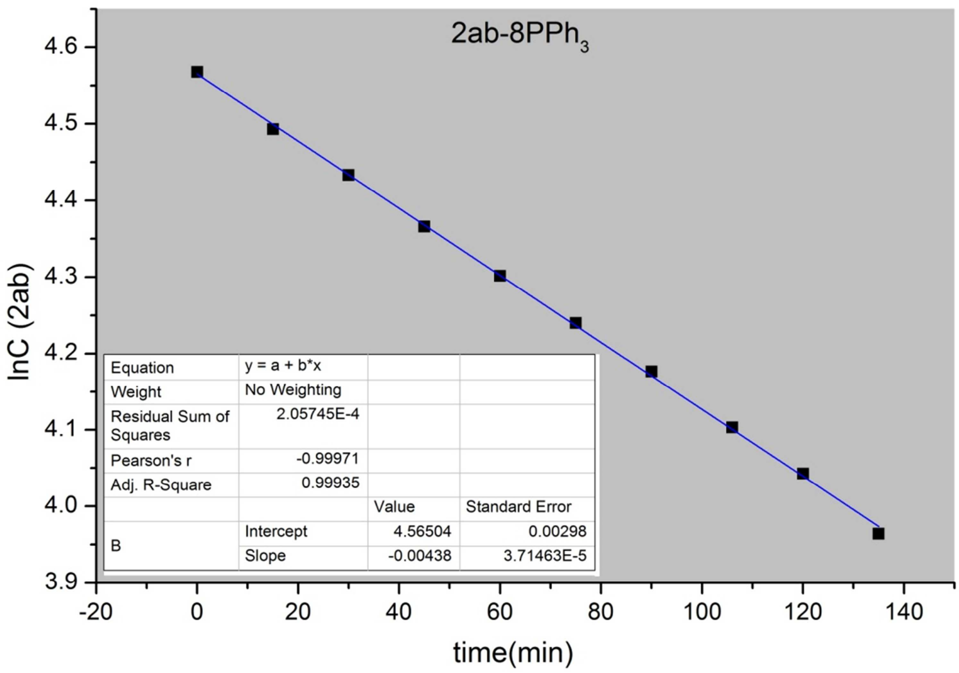


Chart 18. Ln [2ab] – times plot. based on ^{19}F NMR analysis at 297 K in CD_2Cl_2 with 8 equiv. PPh_3 .

Table 4. Phosphine Concentration-Dependent Kinetics for the Decay of Complex 2ab (297 K, CD_2Cl_2)

entry	$[PPh_3]$ (M)	k_{obs} ($M^{-1}min^{-1}$)
1	0	0.00704(4)

2	0.00936 (1 equiv)	0.00628(13)
3	0.0562 (6 equiv)	0.0047(1)
4	0.0749 (8 equiv)	0.00438(4)

Crystallographic Data

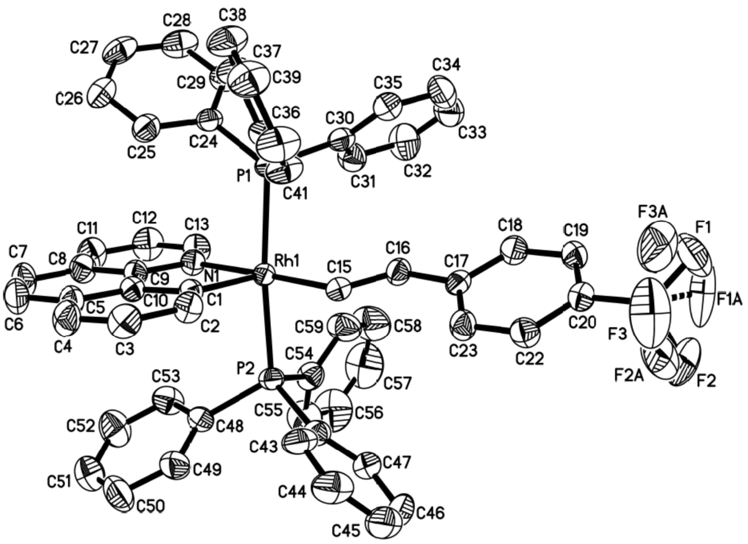


Table 1. Crystal data and structure refinement for **2ab**

Identification code	lxw50 (**2ab**)
Empirical formula	C59 H46 Cl2 F9 N P3 Rh

Formula weight	1206.69	
Temperature	223(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 13.6534(3) Å	α= 90°.
	b = 25.7008(6) Å	β= 93°.
	c = 15.5862(7) Å	γ = 90°.
Volume	5461.29(19) $Å^3$	
Z	4	
Density (calculated)	1.468 Mg/m^3	
Absorption coefficient	0.569 mm^{-1}	
F(000)	2448	
Crystal size	0.30 x 0.28x 0.26 mm^3	
Theta range for data collection	1.53 to 28.00°.	
Index ranges	-17<=h<=18, -33<=k<=33, -20<=l<=20	
Reflections collected	57442	
Independent reflections	13106 [R(int) = 0.0523]	
Completeness to theta = 28.00°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8662and 0.8479	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13106 / 259 /741	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0764, wR2 = 0.1829	
R indices (all data)	R1 = 0.0533, wR2 = 0.1514	
Largest diff. peak and hole	0.931 and -0.658 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}x 10^3) for **2ab** (lwx50). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	1686(1)	8476(1)	2300(1)	25(1)
C(1)	459(2)	8065(1)	2122(2)	29(1)
C(2)	336(3)	7535(1)	2028(3)	35(1)
C(3)	-611(3)	7328(2)	1881(3)	43(1)
C(4)	-1429(3)	7634(2)	1844(3)	45(1)
C(5)	-1336(3)	8178(2)	1955(3)	38(1)
C(6)	-2161(3)	8525(2)	1941(3)	48(1)
C(7)	-2051(3)	9044(2)	2058(3)	49(1)
C(8)	-1098(3)	9269(2)	2190(3)	39(1)
C(9)	-281(3)	8936(1)	2202(2)	31(1)
C(10)	-390(3)	8386(1)	2083(2)	30(1)
C(11)	-916(3)	9801(2)	2310(3)	49(1)
C(12)	40(3)	9970(2)	2447(3)	50(1)
C(13)	807(3)	9617(1)	2452(3)	39(1)
C(15)	2690(3)	7902(1)	2228(2)	30(1)
C(16)	3640(3)	7964(1)	2460(2)	32(1)
C(17)	4420(3)	7573(1)	2400(2)	31(1)
C(18)	5325(3)	7660(2)	2831(3)	36(1)
C(19)	6069(3)	7297(2)	2830(3)	36(1)
C(20)	5915(3)	6833(2)	2382(3)	34(1)
C(21)	6699(3)	6431(2)	2400(3)	47(1)
C(22)	5029(3)	6743(2)	1940(3)	36(1)
C(23)	4284(3)	7108(2)	1940(3)	37(1)
C(24)	936(3)	8795(1)	4380(2)	31(1)
C(25)	-68(3)	8717(2)	4241(3)	41(1)
C(26)	-723(3)	8996(2)	4699(3)	46(1)
C(27)	-382(4)	9361(2)	5293(3)	47(1)
C(28)	596(4)	9448(2)	5419(3)	47(1)
C(29)	1265(3)	9164(2)	4966(3)	39(1)
C(30)	2982(3)	8578(2)	4180(2)	34(1)
C(31)	3300(3)	9064(2)	3906(3)	42(1)
C(32)	4241(4)	9229(2)	4131(4)	58(1)
C(33)	4870(3)	8918(2)	4618(3)	58(1)

C(34)	4560(3)	8434(2)	4885(3)	56(1)
C(35)	3617(3)	8262(2)	4664(3)	43(1)
C(36)	1540(3)	7739(1)	4276(2)	32(1)
C(37)	1137(3)	7700(2)	5073(3)	42(1)
C(38)	949(4)	7218(2)	5436(3)	52(1)
C(39)	1150(4)	6774(2)	4983(3)	53(1)
C(40)	1550(4)	6803(2)	4202(3)	53(1)
C(41)	1746(3)	7279(2)	3856(3)	42(1)
C(42)	2354(3)	8065(2)	222(2)	36(1)
C(43)	1956(3)	7565(2)	270(3)	45(1)
C(44)	2321(4)	7167(2)	-199(3)	56(1)
C(45)	3102(4)	7254(2)	-703(3)	64(2)
C(46)	3535(3)	7733(2)	-732(3)	61(1)
C(47)	3161(3)	8148(2)	-263(3)	47(1)
C(48)	660(3)	8740(2)	194(2)	34(1)
C(49)	183(3)	8379(2)	-347(3)	49(1)
C(50)	-695(4)	8502(2)	-789(4)	68(2)
C(51)	-1112(4)	8987(2)	-683(4)	65(1)
C(52)	-660(4)	9336(2)	-142(4)	59(1)
C(53)	210(3)	9221(2)	308(3)	44(1)
C(54)	2569(3)	9158(2)	700(3)	39(1)
C(55)	2544(4)	9472(2)	-10(4)	61(1)
C(56)	3149(5)	9905(2)	-31(5)	81(2)
C(57)	3763(5)	10029(2)	636(5)	86(2)
C(58)	3789(5)	9725(2)	1358(4)	75(2)
C(59)	3191(4)	9291(2)	1397(3)	55(1)
C(60)	8855(5)	5459(3)	1641(5)	103(3)
Cl(1)	8254(2)	4963(1)	1068(2)	131(1)
Cl(2)	8794(2)	5383(1)	2759(2)	129(1)
F(1)	7386(5)	6501(3)	2993(4)	87(3)
F(2)	7226(4)	6477(2)	1656(4)	72(2)
F(3)	6405(4)	5965(2)	2371(7)	90(3)
F(1A)	7574(7)	6582(5)	2526(13)	87(6)
F(2A)	6615(11)	6077(6)	1826(9)	105(7)
F(3A)	6607(11)	6119(6)	3148(9)	91(5)
F(4)	2735(6)	998(3)	4142(5)	193(3)
F(5)	3316(6)	811(2)	2259(3)	159(3)
F(6)	3908(10)	1285(4)	3462(8)	145(5)

F(7)	2536(9)	1399(5)	2780(8)	156(6)
F(8)	2179(10)	573(6)	2959(10)	171(6)
F(9)	3646(8)	454(4)	3570(7)	117(4)
F(6A)	2995(12)	1478(3)	2984(8)	149(7)
F(7A)	1870(6)	905(6)	3106(11)	130(5)
F(8A)	2936(14)	291(3)	3324(10)	151(6)
F(9A)	4097(6)	882(8)	3366(11)	163(7)
N(1)	660(2)	9106(1)	2336(2)	31(1)
P(1)	1754(1)	8375(1)	3801(1)	28(1)
P(2)	1791(1)	8588(1)	815(1)	29(1)
P(3)	3024(1)	906(1)	3207(1)	53(1)

Table 3. Bond lengths and angles for **2ab** (lwx50).

Rh(1)-C(1)	1.987(3)
Rh(1)-C(15)	2.019(3)
Rh(1)-N(1)	2.145(3)
Rh(1)-P(2)	2.3448(10)
Rh(1)-P(1)	2.3503(9)
C(1)-C(2)	1.381(5)
C(1)-C(10)	1.421(5)
C(2)-C(3)	1.406(5)
C(3)-C(4)	1.364(6)
C(4)-C(5)	1.414(6)
C(5)-C(10)	1.403(5)
C(5)-C(6)	1.436(6)
C(6)-C(7)	1.353(6)
C(7)-C(8)	1.428(6)
C(8)-C(11)	1.402(6)
C(8)-C(9)	1.405(5)
C(9)-N(1)	1.363(5)
C(9)-C(10)	1.432(5)
C(11)-C(12)	1.381(6)
C(12)-C(13)	1.385(6)
C(13)-N(1)	1.338(5)
C(15)-C(16)	1.337(5)
C(16)-C(17)	1.471(5)
C(17)-C(18)	1.393(5)
C(17)-C(23)	1.401(5)
C(18)-C(19)	1.380(5)
C(19)-C(20)	1.391(5)
C(20)-C(22)	1.379(5)
C(20)-C(21)	1.489(5)
C(21)-F(1A)	1.262(10)
C(21)-F(3)	1.262(6)
C(21)-F(2A)	1.276(9)
C(21)-F(1)	1.293(6)
C(21)-F(2)	1.402(6)
C(21)-F(3A)	1.426(9)
C(22)-C(23)	1.384(5)

C(24)-C(29)	1.376(5)
C(24)-C(25)	1.390(5)
C(24)-P(1)	1.827(4)
C(25)-C(26)	1.376(6)
C(26)-C(27)	1.380(7)
C(27)-C(28)	1.358(7)
C(28)-C(29)	1.391(6)
C(30)-C(35)	1.382(6)
C(30)-C(31)	1.398(6)
C(30)-P(1)	1.823(4)
C(31)-C(32)	1.379(6)
C(32)-C(33)	1.372(7)
C(33)-C(34)	1.383(7)
C(34)-C(35)	1.387(6)
C(36)-C(41)	1.387(5)
C(36)-C(37)	1.389(5)
C(36)-P(1)	1.824(4)
C(37)-C(38)	1.393(6)
C(38)-C(39)	1.379(6)
C(39)-C(40)	1.362(7)
C(40)-C(41)	1.370(6)
C(42)-C(47)	1.387(6)
C(42)-C(43)	1.398(6)
C(42)-P(2)	1.824(4)
C(43)-C(44)	1.368(6)
C(44)-C(45)	1.377(8)
C(45)-C(46)	1.368(8)
C(46)-C(47)	1.404(7)
C(48)-C(49)	1.393(6)
C(48)-C(53)	1.395(6)
C(48)-P(2)	1.821(4)
C(49)-C(50)	1.387(7)
C(50)-C(51)	1.384(8)
C(51)-C(52)	1.358(8)
C(52)-C(53)	1.379(6)
C(54)-C(55)	1.367(6)
C(54)-C(59)	1.385(6)
C(54)-P(2)	1.824(4)

C(55)-C(56)	1.387(7)
C(56)-C(57)	1.338(9)
C(57)-C(58)	1.369(9)
C(58)-C(59)	1.385(7)
C(60)-Cl(1)	1.737(9)
C(60)-Cl(2)	1.761(8)
F(4)-P(3)	1.549(6)
F(5)-P(3)	1.569(5)
F(6)-P(3)	1.585(7)
F(7)-P(3)	1.563(9)
F(8)-P(3)	1.471(7)
F(9)-P(3)	1.529(7)
F(6A)-P(3)	1.510(8)
F(7A)-P(3)	1.576(8)
F(8A)-P(3)	1.597(8)
F(9A)-P(3)	1.473(8)
C(1)-Rh(1)-C(15)	100.04(14)
C(1)-Rh(1)-N(1)	81.82(13)
C(15)-Rh(1)-N(1)	177.27(13)
C(1)-Rh(1)-P(2)	91.35(11)
C(15)-Rh(1)-P(2)	87.56(10)
N(1)-Rh(1)-P(2)	90.41(9)
C(1)-Rh(1)-P(1)	93.90(11)
C(15)-Rh(1)-P(1)	89.10(10)
N(1)-Rh(1)-P(1)	92.77(9)
P(2)-Rh(1)-P(1)	174.20(3)
C(2)-C(1)-C(10)	118.3(3)
C(2)-C(1)-Rh(1)	129.5(3)
C(10)-C(1)-Rh(1)	112.2(2)
C(1)-C(2)-C(3)	119.8(3)
C(4)-C(3)-C(2)	122.1(4)
C(3)-C(4)-C(5)	119.8(4)
C(10)-C(5)-C(4)	118.1(3)
C(10)-C(5)-C(6)	118.7(4)
C(4)-C(5)-C(6)	123.2(4)
C(7)-C(6)-C(5)	122.0(4)
C(6)-C(7)-C(8)	120.8(4)

C(11)-C(8)-C(9)	117.2(4)
C(11)-C(8)-C(7)	124.6(4)
C(9)-C(8)-C(7)	118.2(4)
N(1)-C(9)-C(8)	123.2(3)
N(1)-C(9)-C(10)	115.3(3)
C(8)-C(9)-C(10)	121.4(3)
C(5)-C(10)-C(1)	121.8(3)
C(5)-C(10)-C(9)	119.0(3)
C(1)-C(10)-C(9)	119.2(3)
C(12)-C(11)-C(8)	119.1(4)
C(11)-C(12)-C(13)	120.3(4)
N(1)-C(13)-C(12)	122.2(4)
C(16)-C(15)-Rh(1)	123.4(3)
C(15)-C(16)-C(17)	126.7(3)
C(18)-C(17)-C(23)	118.3(3)
C(18)-C(17)-C(16)	119.0(3)
C(23)-C(17)-C(16)	122.6(3)
C(19)-C(18)-C(17)	121.6(4)
C(18)-C(19)-C(20)	119.3(4)
C(22)-C(20)-C(19)	120.0(3)
C(22)-C(20)-C(21)	120.2(3)
C(19)-C(20)-C(21)	119.8(3)
F(1A)-C(21)-F(3)	126.5(8)
F(1A)-C(21)-F(2A)	112.1(9)
F(3)-C(21)-F(2A)	44.3(8)
F(1A)-C(21)-F(1)	37.0(8)
F(3)-C(21)-F(1)	112.1(6)
F(2A)-C(21)-F(1)	129.5(7)
F(1A)-C(21)-F(2)	65.1(9)
F(3)-C(21)-F(2)	103.2(5)
F(2A)-C(21)-F(2)	60.7(9)
F(1)-C(21)-F(2)	101.2(5)
F(1A)-C(21)-F(3A)	99.9(8)
F(3)-C(21)-F(3A)	57.0(7)
F(2A)-C(21)-F(3A)	99.5(9)
F(1)-C(21)-F(3A)	65.6(7)
F(2)-C(21)-F(3A)	142.8(5)
F(1A)-C(21)-C(20)	117.6(7)

F(3)-C(21)-C(20)	115.5(4)
F(2A)-C(21)-C(20)	116.4(6)
F(1)-C(21)-C(20)	114.1(4)
F(2)-C(21)-C(20)	109.0(4)
F(3A)-C(21)-C(20)	108.1(5)
C(20)-C(22)-C(23)	120.7(4)
C(22)-C(23)-C(17)	120.1(4)
C(29)-C(24)-C(25)	119.1(3)
C(29)-C(24)-P(1)	123.3(3)
C(25)-C(24)-P(1)	117.5(3)
C(26)-C(25)-C(24)	120.5(4)
C(25)-C(26)-C(27)	119.8(4)
C(28)-C(27)-C(26)	120.2(4)
C(27)-C(28)-C(29)	120.5(4)
C(24)-C(29)-C(28)	119.9(4)
C(35)-C(30)-C(31)	119.7(4)
C(35)-C(30)-P(1)	123.2(3)
C(31)-C(30)-P(1)	116.9(3)
C(32)-C(31)-C(30)	119.8(4)
C(33)-C(32)-C(31)	120.6(4)
C(32)-C(33)-C(34)	119.7(4)
C(33)-C(34)-C(35)	120.5(5)
C(30)-C(35)-C(34)	119.7(4)
C(41)-C(36)-C(37)	117.5(4)
C(41)-C(36)-P(1)	122.0(3)
C(37)-C(36)-P(1)	120.4(3)
C(36)-C(37)-C(38)	121.2(4)
C(39)-C(38)-C(37)	118.9(4)
C(40)-C(39)-C(38)	120.8(4)
C(39)-C(40)-C(41)	119.9(4)
C(40)-C(41)-C(36)	121.7(4)
C(47)-C(42)-C(43)	119.5(4)
C(47)-C(42)-P(2)	122.1(3)
C(43)-C(42)-P(2)	118.4(3)
C(44)-C(43)-C(42)	120.4(4)
C(43)-C(44)-C(45)	119.9(5)
C(46)-C(45)-C(44)	121.0(4)
C(45)-C(46)-C(47)	119.8(4)

C(42)-C(47)-C(46)	119.3(5)
C(49)-C(48)-C(53)	118.3(4)
C(49)-C(48)-P(2)	122.3(3)
C(53)-C(48)-P(2)	119.3(3)
C(50)-C(49)-C(48)	120.8(4)
C(51)-C(50)-C(49)	119.8(5)
C(52)-C(51)-C(50)	119.6(5)
C(51)-C(52)-C(53)	121.6(5)
C(52)-C(53)-C(48)	119.9(4)
C(55)-C(54)-C(59)	118.5(4)
C(55)-C(54)-P(2)	124.3(4)
C(59)-C(54)-P(2)	117.1(3)
C(54)-C(55)-C(56)	120.2(6)
C(57)-C(56)-C(55)	121.5(6)
C(56)-C(57)-C(58)	119.3(5)
C(57)-C(58)-C(59)	120.5(6)
C(54)-C(59)-C(58)	120.1(5)
Cl(1)-C(60)-Cl(2)	112.3(4)
C(13)-N(1)-C(9)	118.0(3)
C(13)-N(1)-Rh(1)	130.6(3)
C(9)-N(1)-Rh(1)	111.4(2)
C(30)-P(1)-C(36)	106.84(18)
C(30)-P(1)-C(24)	104.27(17)
C(36)-P(1)-C(24)	102.32(16)
C(30)-P(1)-Rh(1)	106.09(12)
C(36)-P(1)-Rh(1)	120.28(12)
C(24)-P(1)-Rh(1)	115.74(12)
C(48)-P(2)-C(42)	104.90(18)
C(48)-P(2)-C(54)	104.88(19)
C(42)-P(2)-C(54)	106.17(18)
C(48)-P(2)-Rh(1)	117.15(13)
C(42)-P(2)-Rh(1)	117.32(13)
C(54)-P(2)-Rh(1)	105.28(14)
F(8)-P(3)-F(9A)	141.1(7)
F(8)-P(3)-F(6A)	119.7(7)
F(9A)-P(3)-F(6A)	95.3(6)
F(8)-P(3)-F(9)	93.8(6)
F(9A)-P(3)-F(9)	51.7(6)

F(6A)-P(3)-F(9)	146.3(6)
F(8)-P(3)-F(4)	95.7(7)
F(9A)-P(3)-F(4)	98.6(7)
F(6A)-P(3)-F(4)	93.6(5)
F(9)-P(3)-F(4)	86.1(6)
F(8)-P(3)-F(7)	92.8(6)
F(9A)-P(3)-F(7)	120.2(8)
F(6A)-P(3)-F(7)	26.9(7)
F(9)-P(3)-F(7)	171.3(6)
F(4)-P(3)-F(7)	98.8(5)
F(8)-P(3)-F(5)	84.1(7)
F(9A)-P(3)-F(5)	81.5(7)
F(6A)-P(3)-F(5)	86.5(5)
F(9)-P(3)-F(5)	93.8(5)
F(4)-P(3)-F(5)	179.8(4)
F(7)-P(3)-F(5)	81.3(5)
F(8)-P(3)-F(7A)	37.5(6)
F(9A)-P(3)-F(7A)	175.3(9)
F(6A)-P(3)-F(7A)	87.9(6)
F(9)-P(3)-F(7A)	124.6(6)
F(4)-P(3)-F(7A)	77.8(7)
F(7)-P(3)-F(7A)	63.7(6)
F(5)-P(3)-F(7A)	102.1(7)
F(8)-P(3)-F(6)	177.6(6)
F(9A)-P(3)-F(6)	41.1(6)
F(6A)-P(3)-F(6)	58.0(6)
F(9)-P(3)-F(6)	88.5(5)
F(4)-P(3)-F(6)	84.2(6)
F(7)-P(3)-F(6)	84.9(5)
F(5)-P(3)-F(6)	95.9(6)
F(7A)-P(3)-F(6)	140.3(7)
F(8)-P(3)-F(8A)	52.5(6)
F(9A)-P(3)-F(8A)	91.2(6)
F(6A)-P(3)-F(8A)	171.3(7)
F(9)-P(3)-F(8A)	41.3(5)
F(4)-P(3)-F(8A)	91.1(6)
F(7)-P(3)-F(8A)	144.8(7)
F(5)-P(3)-F(8A)	88.7(6)

F(7A)-P(3)-F(8A)	85.9(6)
F(6)-P(3)-F(8A)	129.9(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (^{2}x 10^3)for **2ab** (lwx50).The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	23(1)	28(1)	25(1)	-3(1)	2(1)	-1(1)
C(1)	26(2)	30(2)	30(2)	-3(1)	3(1)	-4(1)
C(2)	35(2)	26(2)	43(2)	-5(2)	5(2)	-2(1)
C(3)	46(2)	31(2)	52(3)	-8(2)	8(2)	-12(2)
C(4)	34(2)	45(2)	56(3)	-6(2)	5(2)	-13(2)
C(5)	30(2)	41(2)	43(2)	-8(2)	2(2)	-4(2)
C(6)	27(2)	56(3)	60(3)	-5(2)	0(2)	0(2)
C(7)	29(2)	53(3)	64(3)	-8(2)	0(2)	10(2)
C(8)	36(2)	38(2)	43(2)	-3(2)	1(2)	9(2)
C(9)	28(2)	32(2)	34(2)	-5(2)	1(1)	0(1)
C(10)	28(2)	32(2)	30(2)	-2(1)	1(1)	-1(1)
C(11)	47(2)	37(2)	62(3)	-8(2)	3(2)	13(2)
C(12)	55(3)	29(2)	66(3)	-15(2)	4(2)	5(2)
C(13)	39(2)	29(2)	49(2)	-9(2)	0(2)	-3(2)
C(15)	30(2)	35(2)	25(2)	-2(1)	4(1)	1(1)
C(16)	29(2)	32(2)	34(2)	-2(2)	4(2)	4(1)
C(17)	28(2)	36(2)	28(2)	-3(2)	7(1)	0(1)
C(18)	33(2)	35(2)	39(2)	-6(2)	1(2)	-1(2)
C(19)	27(2)	43(2)	36(2)	-6(2)	-2(2)	0(2)
C(20)	31(2)	36(2)	35(2)	-2(2)	2(2)	5(1)
C(21)	38(2)	41(2)	62(3)	-14(2)	-8(2)	11(2)
C(22)	37(2)	32(2)	39(2)	-7(2)	-3(2)	0(2)
C(23)	27(2)	39(2)	44(2)	-9(2)	0(2)	-3(2)
C(24)	35(2)	33(2)	24(2)	1(1)	4(1)	3(1)
C(25)	37(2)	47(2)	38(2)	-7(2)	6(2)	-3(2)
C(26)	41(2)	52(2)	46(2)	-1(2)	15(2)	2(2)
C(27)	63(3)	38(2)	41(2)	4(2)	22(2)	14(2)
C(28)	71(3)	30(2)	40(2)	-9(2)	10(2)	6(2)
C(29)	46(2)	34(2)	37(2)	-3(2)	1(2)	-1(2)
C(30)	35(2)	42(2)	26(2)	-4(2)	5(2)	-2(2)
C(31)	40(2)	43(2)	44(2)	0(2)	0(2)	-6(2)
C(32)	48(3)	55(3)	72(4)	-1(3)	2(2)	-17(2)
C(33)	37(2)	82(4)	55(3)	2(3)	-2(2)	-17(2)

C(34)	38(2)	77(3)	51(3)	13(2)	-6(2)	2(2)
C(35)	38(2)	53(2)	38(2)	4(2)	5(2)	0(2)
C(36)	32(2)	36(2)	28(2)	1(2)	0(1)	0(1)
C(37)	56(3)	41(2)	31(2)	1(2)	9(2)	4(2)
C(38)	69(3)	51(3)	37(2)	10(2)	14(2)	5(2)
C(39)	71(3)	40(2)	49(3)	16(2)	10(2)	5(2)
C(40)	77(3)	35(2)	48(3)	3(2)	10(2)	9(2)
C(41)	58(3)	36(2)	32(2)	0(2)	10(2)	6(2)
C(42)	40(2)	40(2)	29(2)	1(2)	1(2)	9(2)
C(43)	58(3)	48(2)	29(2)	-2(2)	6(2)	8(2)
C(44)	82(4)	39(2)	47(3)	-4(2)	-3(3)	21(2)
C(45)	73(3)	69(3)	48(3)	-13(3)	-9(3)	43(3)
C(46)	40(2)	97(4)	48(3)	-1(3)	10(2)	22(3)
C(47)	40(2)	67(3)	35(2)	-4(2)	2(2)	10(2)
C(48)	34(2)	39(2)	29(2)	3(2)	-1(2)	3(2)
C(49)	45(2)	57(3)	44(3)	-16(2)	-4(2)	5(2)
C(50)	44(3)	86(4)	73(4)	-27(3)	-19(3)	4(2)
C(51)	46(3)	89(4)	60(3)	2(3)	-8(2)	13(3)
C(52)	54(3)	49(3)	72(3)	5(2)	-10(2)	14(2)
C(53)	53(2)	37(2)	42(2)	0(2)	-4(2)	7(2)
C(54)	38(2)	37(2)	43(2)	-1(2)	8(2)	-6(2)
C(55)	63(3)	60(3)	60(3)	15(2)	5(3)	-19(2)
C(56)	86(4)	60(3)	99(5)	29(3)	17(4)	-20(3)
C(57)	75(4)	56(3)	126(6)	3(4)	13(4)	-32(3)
C(58)	77(4)	75(4)	73(4)	-12(3)	-4(3)	-33(3)
C(59)	57(3)	64(3)	44(3)	-2(2)	0(2)	-20(2)
C(60)	84(5)	98(5)	130(7)	45(5)	40(5)	25(4)
Cl(1)	111(2)	105(2)	177(3)	20(2)	5(2)	25(1)
Cl(2)	79(1)	145(2)	163(2)	41(2)	9(1)	21(1)
F(1)	80(5)	99(6)	76(4)	-35(4)	-46(4)	50(4)
F(2)	62(3)	60(3)	95(4)	-5(3)	27(3)	26(2)
F(3)	65(3)	24(2)	180(10)	15(4)	3(5)	0(2)
F(1A)	27(5)	35(5)	201(19)	0(10)	16(9)	3(4)
F(2A)	103(12)	106(13)	100(11)	-65(9)	-52(9)	81(10)
F(3A)	98(9)	89(9)	90(9)	40(7)	27(7)	63(8)
F(4)	204(6)	215(7)	172(6)	-105(5)	109(5)	-64(5)
F(5)	270(8)	129(4)	82(3)	0(3)	36(4)	36(4)
F(6)	165(11)	106(8)	156(9)	21(7)	-71(8)	-77(7)

F(7)	113(9)	156(11)	201(12)	47(9)	14(8)	85(8)
F(8)	130(10)	174(13)	203(12)	-42(11)	-50(9)	-95(9)
F(9)	119(8)	91(7)	139(8)	56(6)	-21(6)	21(5)
F(6A)	152(13)	41(5)	262(17)	14(7)	105(13)	-11(6)
F(7A)	56(5)	156(12)	179(12)	39(10)	23(6)	-17(6)
F(8A)	238(17)	38(5)	170(12)	16(6)	-43(12)	18(7)
F(9A)	35(5)	242(18)	210(13)	-42(14)	-7(6)	24(8)
N(1)	30(2)	28(1)	35(2)	-7(1)	3(1)	-1(1)
P(1)	30(1)	32(1)	22(1)	-3(1)	2(1)	-1(1)
P(2)	32(1)	32(1)	24(1)	-1(1)	3(1)	0(1)
P(3)	47(1)	47(1)	64(1)	-12(1)	-5(1)	6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2}x 10^3)
For **2ab** (lxw50).

	x	y	z	U(eq)
H(2)	884	7313	2061	42
H(3)	-683	6966	1806	51
H(4)	-2052	7483	1745	54
H(6)	-2796	8388	1848	57
H(7)	-2608	9259	2053	58
H(11)	-1437	10040	2297	58
H(12)	171	10325	2537	60
H(13)	1453	9740	2540	47
H(15)	2478	7575	2021	36
H(16)	3829	8290	2684	38
H(18)	5432	7975	3130	43
H(19)	6673	7362	3128	43
H(22)	4931	6430	1635	43
H(23)	3686	7044	1630	44
H(25)	-301	8473	3831	49
H(26)	-1400	8939	4609	55
H(27)	-828	9549	5611	56
H(28)	823	9702	5816	56
H(29)	1942	9224	5060	47
H(31)	2874	9279	3570	51
H(32)	4452	9557	3949	70
H(33)	5510	9033	4770	70
H(34)	4991	8221	5218	67
H(35)	3412	7932	4842	52
H(37)	990	8005	5373	51
H(38)	690	7196	5982	62
H(39)	1008	6446	5215	64
H(40)	1691	6497	3902	64
H(41)	2027	7295	3319	50
H(43)	1435	7503	626	54
H(44)	2038	6834	-177	68
H(45)	3342	6980	-1032	77

H(46)	4081	7785	-1064	74
H(47)	3455	8479	-278	56
H(49)	460	8047	-413	59
H(50)	-1006	8256	-1159	82
H(51)	-1705	9074	-985	78
H(52)	-947	9665	-72	70
H(53)	500	9466	691	53
H(55)	2115	9394	-484	73
H(56)	3127	10116	-524	98
H(57)	4172	10322	609	103
H(58)	4215	9811	1830	90
H(59)	3208	9086	1897	66
H(60A)	8560	5794	1469	123
H(60B)	9544	5466	1496	123

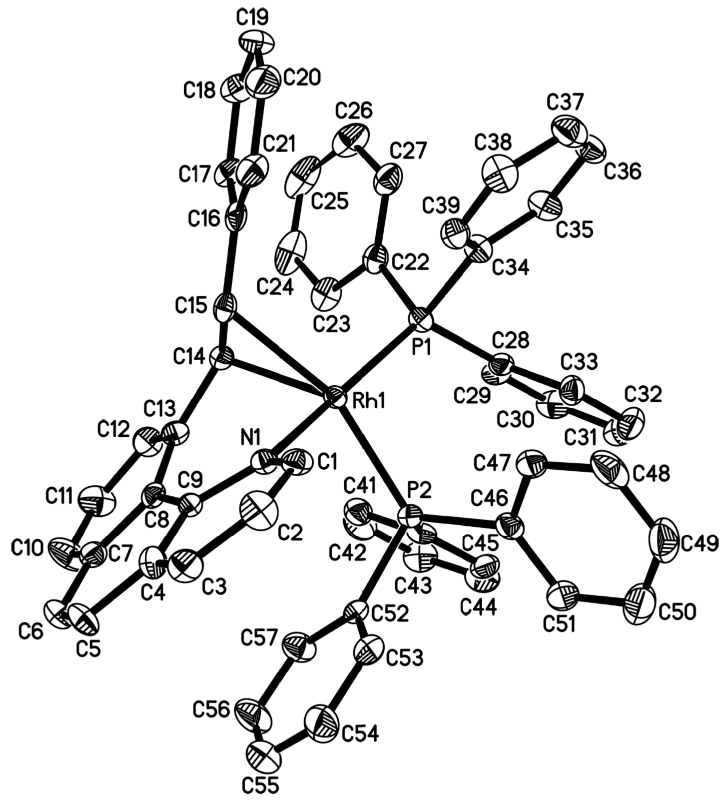


Table 1. Crystal data and structure refinement for **3aa** (lxw10).

Identification code	lxw10	
Empirical formula	C57 H45 F6 N P3 Rh · 2CH2Cl2	
Formula weight	1223.61	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.3535(5) Å	α= 90°.
	b = 28.8354(12) Å	β= 99.472(2)°.
	c = 15.2713(6) Å	γ = 90°.
Volume	5365.7(4) Å^3	
Z	4	
Density (calculated)	1.515 Mg/m^3	
Absorption coefficient	0.669 mm^{-1}	
F(000)	2488	
Crystal size	0.20 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.41 to 26.00°.	
Index ranges	-15<=h<=10, -35<=k<=35,	
-18<=l<=18		

Reflections collected	43515
Independent reflections	10441 [R(int) = 0.0619]
Completeness to theta = 26.00°	99.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9361 and 0.8779
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10441 / 0 / 667
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0648, wR2 = 0.1762
R indices (all data)	R1 = 0.0830, wR2 = 0.2067
Largest diff. peak and hole	2.216 and -0.833 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3aa** (lxw10). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	7511(1)	6418(1)	2982(1)	14(1)
N(1)	7739(3)	6054(1)	1841(3)	16(1)
P(1)	6928(1)	6756(1)	4191(1)	16(1)
P(2)	8487(1)	5833(1)	3805(1)	17(1)
C(1)	6993(4)	5731(2)	1581(3)	21(1)
C(2)	7037(4)	5430(2)	870(4)	28(1)
C(3)	7940(4)	5448(2)	446(3)	25(1)
C(4)	8741(4)	5792(2)	715(3)	20(1)
C(5)	9726(4)	5813(2)	328(3)	26(1)
C(6)	10491(4)	6142(2)	604(4)	27(1)
C(7)	10319(4)	6487(2)	1229(4)	21(1)
C(8)	9315(4)	6507(2)	1578(3)	18(1)
C(9)	8578(4)	6118(2)	1373(3)	17(1)
C(10)	11148(5)	6820(2)	1517(4)	37(1)
C(11)	10990(5)	7164(2)	2101(4)	33(1)
C(12)	9970(4)	7202(2)	2379(4)	25(1)
C(13)	9111(4)	6897(2)	2106(3)	19(1)
C(14)	8048(4)	7032(2)	2369(3)	19(1)
C(15)	6976(4)	6954(2)	1881(3)	18(1)
C(16)	6037(4)	7267(2)	1903(3)	20(1)
C(17)	6124(4)	7713(2)	2265(3)	23(1)
C(18)	5203(5)	7995(2)	2252(4)	32(1)
C(19)	4184(5)	7831(2)	1885(4)	35(1)
C(20)	4076(5)	7395(2)	1499(4)	35(1)
C(21)	4997(4)	7121(2)	1510(4)	27(1)
C(22)	7084(4)	7388(2)	4325(3)	22(1)
C(23)	8126(5)	7583(2)	4330(3)	27(1)
C(24)	8272(6)	8059(2)	4372(4)	40(2)
C(25)	7389(6)	8342(2)	4425(4)	41(2)
C(26)	6359(6)	8153(2)	4433(4)	39(2)
C(27)	6214(5)	7683(2)	4390(4)	29(1)
C(28)	7418(4)	6555(2)	5335(3)	19(1)
C(29)	8159(4)	6806(2)	5943(3)	23(1)

C(30)	8503(5)	6642(2)	6791(4)	33(1)
C(31)	8119(5)	6213(2)	7049(4)	36(1)
C(32)	7375(5)	5961(2)	6456(4)	33(1)
C(33)	7019(4)	6126(2)	5611(3)	24(1)
C(34)	5454(4)	6646(2)	4106(3)	20(1)
C(35)	4895(4)	6730(2)	4822(3)	24(1)
C(36)	3782(4)	6643(2)	4730(4)	26(1)
C(37)	3204(5)	6480(2)	3929(4)	31(1)
C(38)	3742(5)	6403(2)	3226(4)	28(1)
C(39)	4858(4)	6481(2)	3312(3)	23(1)
C(40)	9494(4)	6067(2)	4711(3)	20(1)
C(41)	9992(4)	6483(2)	4514(4)	25(1)
C(42)	10799(4)	6688(2)	5135(4)	33(1)
C(43)	11125(5)	6477(2)	5945(4)	31(1)
C(44)	10621(5)	6067(2)	6151(4)	32(1)
C(45)	9817(4)	5866(2)	5543(3)	24(1)
C(46)	7672(4)	5371(2)	4195(3)	21(1)
C(47)	6539(4)	5380(2)	3896(4)	24(1)
C(48)	5875(5)	5027(2)	4115(4)	36(1)
C(49)	6318(6)	4655(2)	4604(4)	41(2)
C(50)	7453(6)	4633(2)	4899(4)	38(1)
C(51)	8121(5)	4988(2)	4686(4)	27(1)
C(52)	9376(4)	5501(2)	3175(3)	21(1)
C(53)	8991(5)	5094(2)	2730(4)	29(1)
C(54)	9645(6)	4863(2)	2219(4)	37(1)
C(55)	10679(5)	5025(2)	2141(4)	39(2)
C(56)	11065(5)	5429(2)	2567(4)	42(2)
C(57)	10420(4)	5658(2)	3086(4)	27(1)
C(58)	4521(6)	5512(2)	8220(5)	44(2)
C(59)	2547(8)	6718(3)	8973(6)	68(3)
Cl(1)	3422(2)	5816(1)	7577(2)	66(1)
Cl(2)	5789(2)	5725(1)	8064(2)	81(1)
Cl(3)	2854(2)	7303(1)	9088(2)	82(1)
Cl(4)	1215(2)	6603(1)	8421(2)	69(1)
F(1)	2820(3)	5425(1)	1176(3)	47(1)
F(2)	4486(3)	5719(2)	1736(2)	46(1)
F(3)	4619(3)	5999(1)	380(3)	53(1)
F(4)	4294(3)	5239(1)	551(2)	38(1)

F(5)	2953(3)	5698(1)	-167(2)	40(1)
F(6)	3159(3)	6185(1)	1001(3)	47(1)
P(3)	3722(1)	5709(1)	783(1)	24(1)

Table 3. Bond lengths [Å] and angles [°] for **3aa** (lxw10).

Rh(1)-N(1)	2.093(4)
Rh(1)-C(14)	2.158(5)
Rh(1)-C(15)	2.300(5)
Rh(1)-P(1)	2.3042(12)
Rh(1)-P(2)	2.3192(13)
N(1)-C(1)	1.323(6)
N(1)-C(9)	1.366(6)
P(1)-C(34)	1.831(5)
P(1)-C(22)	1.842(5)
P(1)-C(28)	1.846(5)
P(2)-C(46)	1.827(5)
P(2)-C(40)	1.830(5)
P(2)-C(52)	1.844(5)
C(1)-C(2)	1.397(7)
C(2)-C(3)	1.381(8)
C(3)-C(4)	1.413(7)
C(4)-C(9)	1.414(7)
C(4)-C(5)	1.439(7)
C(5)-C(6)	1.357(8)
C(6)-C(7)	1.420(7)
C(7)-C(10)	1.420(8)
C(7)-C(8)	1.429(7)
C(8)-C(13)	1.431(7)
C(8)-C(9)	1.445(7)
C(10)-C(11)	1.369(8)
C(11)-C(12)	1.398(8)
C(12)-C(13)	1.389(7)
C(13)-C(14)	1.488(7)
C(14)-C(15)	1.427(7)
C(15)-C(16)	1.474(7)
C(16)-C(21)	1.391(7)
C(16)-C(17)	1.396(7)
C(17)-C(18)	1.395(7)
C(18)-C(19)	1.375(9)
C(19)-C(20)	1.388(9)
C(20)-C(21)	1.382(8)

C(22)-C(27)	1.387(8)
C(22)-C(23)	1.403(8)
C(23)-C(24)	1.384(8)
C(24)-C(25)	1.375(10)
C(25)-C(26)	1.386(10)
C(26)-C(27)	1.368(8)
C(28)-C(29)	1.395(7)
C(28)-C(33)	1.421(7)
C(29)-C(30)	1.378(8)
C(30)-C(31)	1.404(9)
C(31)-C(32)	1.384(9)
C(32)-C(33)	1.378(8)
C(34)-C(39)	1.395(7)
C(34)-C(35)	1.407(7)
C(35)-C(36)	1.382(7)
C(36)-C(37)	1.393(8)
C(37)-C(38)	1.371(8)
C(38)-C(39)	1.382(8)
C(40)-C(45)	1.393(7)
C(40)-C(41)	1.403(7)
C(41)-C(42)	1.390(8)
C(42)-C(43)	1.376(8)
C(43)-C(44)	1.398(8)
C(44)-C(45)	1.370(8)
C(46)-C(51)	1.397(7)
C(46)-C(47)	1.400(7)
C(47)-C(48)	1.383(8)
C(48)-C(49)	1.368(9)
C(49)-C(50)	1.401(10)
C(50)-C(51)	1.387(8)
C(52)-C(57)	1.394(7)
C(52)-C(53)	1.400(8)
C(53)-C(54)	1.384(8)
C(54)-C(55)	1.383(9)
C(55)-C(56)	1.380(10)
C(56)-C(57)	1.382(8)
C(58)-Cl(2)	1.736(7)
C(58)-Cl(1)	1.772(8)

C(59)-Cl(3)	1.732(9)
C(59)-Cl(4)	1.753(9)
F(1)-P(3)	1.581(4)
F(2)-P(3)	1.600(3)
F(3)-P(3)	1.590(4)
F(4)-P(3)	1.595(3)
F(5)-P(3)	1.597(4)
F(6)-P(3)	1.598(4)
N(1)-Rh(1)-C(14)	87.63(17)
N(1)-Rh(1)-C(15)	77.94(16)
C(14)-Rh(1)-C(15)	37.16(18)
N(1)-Rh(1)-P(1)	168.90(11)
C(14)-Rh(1)-P(1)	99.18(13)
C(15)-Rh(1)-P(1)	102.22(12)
N(1)-Rh(1)-P(2)	87.51(11)
C(14)-Rh(1)-P(2)	131.52(13)
C(15)-Rh(1)-P(2)	161.16(13)
P(1)-Rh(1)-P(2)	94.37(5)
C(1)-N(1)-C(9)	119.3(4)
C(1)-N(1)-Rh(1)	114.9(3)
C(9)-N(1)-Rh(1)	125.8(3)
C(34)-P(1)-C(22)	105.3(2)
C(34)-P(1)-C(28)	100.3(2)
C(22)-P(1)-C(28)	101.2(2)
C(34)-P(1)-Rh(1)	107.99(16)
C(22)-P(1)-Rh(1)	117.79(16)
C(28)-P(1)-Rh(1)	121.94(16)
C(46)-P(2)-C(40)	111.3(2)
C(46)-P(2)-C(52)	101.4(2)
C(40)-P(2)-C(52)	101.3(2)
C(46)-P(2)-Rh(1)	116.25(17)
C(40)-P(2)-Rh(1)	111.70(16)
C(52)-P(2)-Rh(1)	113.37(16)
N(1)-C(1)-C(2)	123.7(5)
C(3)-C(2)-C(1)	118.7(5)
C(2)-C(3)-C(4)	118.1(5)
C(3)-C(4)-C(9)	119.9(4)

C(3)-C(4)-C(5)	120.5(5)
C(9)-C(4)-C(5)	119.6(4)
C(6)-C(5)-C(4)	119.6(5)
C(5)-C(6)-C(7)	121.7(5)
C(10)-C(7)-C(6)	120.1(5)
C(10)-C(7)-C(8)	119.0(5)
C(6)-C(7)-C(8)	120.8(5)
C(7)-C(8)-C(13)	119.0(4)
C(7)-C(8)-C(9)	116.4(4)
C(13)-C(8)-C(9)	124.6(4)
N(1)-C(9)-C(4)	119.4(4)
N(1)-C(9)-C(8)	119.9(4)
C(4)-C(9)-C(8)	120.7(4)
C(11)-C(10)-C(7)	121.2(5)
C(10)-C(11)-C(12)	119.2(5)
C(13)-C(12)-C(11)	122.8(5)
C(12)-C(13)-C(8)	118.1(4)
C(12)-C(13)-C(14)	114.7(4)
C(8)-C(13)-C(14)	127.2(4)
C(15)-C(14)-C(13)	127.0(5)
C(15)-C(14)-Rh(1)	76.9(3)
C(13)-C(14)-Rh(1)	104.4(3)
C(14)-C(15)-C(16)	123.9(4)
C(14)-C(15)-Rh(1)	66.0(3)
C(16)-C(15)-Rh(1)	121.8(3)
C(21)-C(16)-C(17)	117.1(5)
C(21)-C(16)-C(15)	118.6(5)
C(17)-C(16)-C(15)	124.2(5)
C(16)-C(17)-C(18)	121.4(5)
C(19)-C(18)-C(17)	119.8(5)
C(18)-C(19)-C(20)	120.1(5)
C(21)-C(20)-C(19)	119.5(5)
C(20)-C(21)-C(16)	122.1(5)
C(27)-C(22)-C(23)	118.4(5)
C(27)-C(22)-P(1)	123.1(4)
C(23)-C(22)-P(1)	118.5(4)
C(24)-C(23)-C(22)	120.6(6)
C(25)-C(24)-C(23)	119.5(6)

C(24)-C(25)-C(26)	120.3(6)
C(27)-C(26)-C(25)	120.2(6)
C(26)-C(27)-C(22)	120.9(6)
C(29)-C(28)-C(33)	118.5(5)
C(29)-C(28)-P(1)	123.0(4)
C(33)-C(28)-P(1)	118.6(4)
C(30)-C(29)-C(28)	120.9(5)
C(29)-C(30)-C(31)	120.0(6)
C(32)-C(31)-C(30)	119.7(5)
C(33)-C(32)-C(31)	120.6(5)
C(32)-C(33)-C(28)	120.3(5)
C(39)-C(34)-C(35)	118.6(5)
C(39)-C(34)-P(1)	119.8(4)
C(35)-C(34)-P(1)	121.7(4)
C(36)-C(35)-C(34)	119.8(5)
C(35)-C(36)-C(37)	120.6(5)
C(38)-C(37)-C(36)	119.8(5)
C(37)-C(38)-C(39)	120.3(5)
C(38)-C(39)-C(34)	120.9(5)
C(45)-C(40)-C(41)	118.7(5)
C(45)-C(40)-P(2)	126.5(4)
C(41)-C(40)-P(2)	114.8(4)
C(42)-C(41)-C(40)	120.5(5)
C(43)-C(42)-C(41)	119.8(6)
C(42)-C(43)-C(44)	120.0(5)
C(45)-C(44)-C(43)	120.3(5)
C(44)-C(45)-C(40)	120.7(5)
C(51)-C(46)-C(47)	118.5(5)
C(51)-C(46)-P(2)	124.0(4)
C(47)-C(46)-P(2)	117.1(4)
C(48)-C(47)-C(46)	120.6(5)
C(49)-C(48)-C(47)	120.6(6)
C(48)-C(49)-C(50)	120.0(6)
C(51)-C(50)-C(49)	119.6(6)
C(50)-C(51)-C(46)	120.6(5)
C(57)-C(52)-C(53)	118.1(5)
C(57)-C(52)-P(2)	121.5(4)
C(53)-C(52)-P(2)	120.3(4)

C(54)-C(53)-C(52)	119.6(5)
C(55)-C(54)-C(53)	121.3(6)
C(56)-C(55)-C(54)	119.8(5)
C(55)-C(56)-C(57)	119.2(6)
C(56)-C(57)-C(52)	122.0(5)
Cl(2)-C(58)-Cl(1)	112.0(3)
Cl(3)-C(59)-Cl(4)	114.0(4)
F(1)-P(3)-F(3)	179.4(3)
F(1)-P(3)-F(4)	90.5(2)
F(3)-P(3)-F(4)	89.9(2)
F(1)-P(3)-F(5)	89.1(2)
F(3)-P(3)-F(5)	90.5(2)
F(4)-P(3)-F(5)	90.02(19)
F(1)-P(3)-F(6)	90.5(2)
F(3)-P(3)-F(6)	89.1(2)
F(4)-P(3)-F(6)	178.9(2)
F(5)-P(3)-F(6)	89.6(2)
F(1)-P(3)-F(2)	90.6(2)
F(3)-P(3)-F(2)	89.9(2)
F(4)-P(3)-F(2)	90.0(2)
F(5)-P(3)-F(2)	179.6(3)
F(6)-P(3)-F(2)	90.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3) for **3aa** (lxw10). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	14(1)	14(1)	14(1)	-1(1)	3(1)	0(1)
N(1)	18(2)	15(2)	16(2)	-2(2)	2(2)	1(2)
P(1)	17(1)	17(1)	15(1)	-3(1)	3(1)	-1(1)
P(2)	16(1)	16(1)	19(1)	1(1)	3(1)	2(1)
C(1)	17(2)	15(2)	31(3)	0(2)	5(2)	0(2)
C(2)	26(3)	27(3)	29(3)	-8(2)	2(2)	-9(2)
C(3)	35(3)	19(3)	20(3)	-7(2)	3(2)	1(2)
C(4)	23(3)	24(3)	13(2)	-2(2)	1(2)	-2(2)
C(5)	27(3)	32(3)	22(3)	-7(2)	12(2)	2(2)
C(6)	22(3)	32(3)	31(3)	3(2)	14(2)	5(2)
C(7)	19(2)	18(2)	26(3)	4(2)	5(2)	1(2)
C(8)	17(2)	19(2)	15(2)	4(2)	1(2)	1(2)
C(9)	16(2)	20(2)	15(2)	4(2)	3(2)	5(2)
C(10)	19(3)	38(3)	56(4)	-11(3)	16(3)	-6(2)
C(11)	22(3)	27(3)	51(4)	-3(3)	7(2)	-5(2)
C(12)	27(3)	18(2)	30(3)	-3(2)	7(2)	-4(2)
C(13)	17(2)	19(2)	20(2)	1(2)	0(2)	2(2)
C(14)	17(2)	18(2)	21(2)	4(2)	5(2)	1(2)
C(15)	24(3)	16(2)	13(2)	0(2)	2(2)	-4(2)
C(16)	23(2)	26(3)	9(2)	4(2)	2(2)	-1(2)
C(17)	28(3)	21(3)	20(2)	3(2)	0(2)	3(2)
C(18)	43(3)	33(3)	19(3)	-3(2)	4(2)	17(3)
C(19)	28(3)	43(4)	35(3)	7(3)	11(2)	18(3)
C(20)	22(3)	40(3)	42(3)	13(3)	2(2)	-1(2)
C(21)	25(3)	24(3)	29(3)	6(2)	-1(2)	-3(2)
C(22)	27(3)	24(3)	14(2)	-1(2)	2(2)	-2(2)
C(23)	36(3)	21(3)	22(3)	-5(2)	-1(2)	-7(2)
C(24)	53(4)	35(3)	28(3)	3(3)	-8(3)	-23(3)
C(25)	77(5)	17(3)	26(3)	-4(2)	-4(3)	-6(3)
C(26)	65(4)	26(3)	25(3)	-5(2)	5(3)	14(3)
C(27)	44(3)	22(3)	21(3)	0(2)	7(2)	4(2)
C(28)	21(2)	18(2)	17(2)	0(2)	5(2)	5(2)
C(29)	23(3)	20(3)	27(3)	-1(2)	2(2)	4(2)

C(30)	34(3)	38(3)	24(3)	-5(2)	-1(2)	9(3)
C(31)	53(4)	37(3)	18(3)	2(2)	6(2)	16(3)
C(32)	44(3)	29(3)	29(3)	10(2)	12(3)	6(3)
C(33)	30(3)	23(3)	20(3)	1(2)	9(2)	0(2)
C(34)	18(2)	23(3)	19(2)	-3(2)	2(2)	-2(2)
C(35)	23(3)	27(3)	22(3)	-10(2)	3(2)	0(2)
C(36)	24(3)	29(3)	29(3)	-3(2)	11(2)	4(2)
C(37)	22(3)	32(3)	40(3)	-2(3)	8(2)	-1(2)
C(38)	26(3)	34(3)	23(3)	-6(2)	-1(2)	-6(2)
C(39)	27(3)	25(3)	17(2)	-2(2)	5(2)	3(2)
C(40)	18(2)	19(2)	22(2)	-4(2)	3(2)	4(2)
C(41)	21(3)	25(3)	30(3)	0(2)	7(2)	0(2)
C(42)	21(3)	40(3)	38(3)	-5(3)	4(2)	-7(2)
C(43)	27(3)	34(3)	28(3)	-6(2)	-5(2)	-2(2)
C(44)	26(3)	40(3)	26(3)	-4(2)	-2(2)	4(2)
C(45)	29(3)	20(3)	23(3)	2(2)	4(2)	7(2)
C(46)	21(2)	17(2)	26(3)	-4(2)	9(2)	-1(2)
C(47)	26(3)	18(2)	28(3)	-1(2)	8(2)	2(2)
C(48)	23(3)	37(3)	52(4)	-8(3)	17(3)	-7(2)
C(49)	49(4)	32(3)	46(4)	3(3)	23(3)	-11(3)
C(50)	50(4)	33(3)	34(3)	6(3)	12(3)	-2(3)
C(51)	31(3)	20(3)	31(3)	-1(2)	8(2)	1(2)
C(52)	22(3)	22(3)	20(2)	9(2)	6(2)	9(2)
C(53)	35(3)	19(3)	34(3)	6(2)	12(2)	4(2)
C(54)	53(4)	29(3)	32(3)	-4(3)	18(3)	2(3)
C(55)	45(4)	39(4)	38(3)	3(3)	21(3)	12(3)
C(56)	23(3)	57(4)	48(4)	6(3)	16(3)	8(3)
C(57)	21(3)	28(3)	34(3)	-4(2)	6(2)	-1(2)
C(58)	57(4)	23(3)	58(4)	8(3)	23(3)	-6(3)
C(59)	80(6)	44(4)	68(6)	-8(4)	-22(4)	19(4)
Cl(1)	67(1)	63(1)	66(1)	-4(1)	3(1)	7(1)
Cl(2)	58(1)	64(1)	128(2)	20(1)	36(1)	-12(1)
Cl(3)	96(2)	56(1)	84(2)	2(1)	-11(1)	-10(1)
Cl(4)	66(1)	73(1)	63(1)	5(1)	-7(1)	-4(1)
F(1)	36(2)	59(2)	48(2)	-5(2)	18(2)	-10(2)
F(2)	29(2)	73(3)	33(2)	-26(2)	-10(1)	8(2)
F(3)	41(2)	42(2)	81(3)	-1(2)	24(2)	-11(2)
F(4)	36(2)	35(2)	41(2)	-13(2)	5(2)	10(2)

F(5)	40(2)	46(2)	31(2)	-8(2)	-5(2)	6(2)
F(6)	35(2)	43(2)	59(3)	-28(2)	-1(2)	11(2)
P(3)	19(1)	27(1)	26(1)	-11(1)	2(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)
For **3aa** (lxw10).

	x	y	z	U(eq)
H(1)	6394	5702	1896	25
H(2)	6457	5218	683	33
H(3)	8021	5235	-14	30
H(5)	9840	5597	-119	31
H(6)	11160	6141	373	33
H(10)	11825	6804	1300	44
H(11)	11565	7374	2314	40
H(12)	9861	7447	2771	30
H(14)	8099	7313	2758	22
H(15)	6993	6827	1274	21
H(17)	6825	7827	2526	28
H(18)	5281	8298	2496	38
H(19)	3552	8018	1895	41
H(20)	3376	7285	1229	42
H(21)	4917	6823	1241	32
H(23)	8737	7387	4304	32
H(24)	8977	8189	4366	48
H(25)	7485	8669	4455	50
H(26)	5752	8351	4469	47
H(27)	5507	7556	4406	35
H(29)	8430	7094	5771	28
H(30)	9000	6819	7200	39
H(31)	8369	6096	7629	43
H(32)	7108	5673	6634	40
H(33)	6505	5951	5210	29
H(35)	5282	6846	5367	29
H(36)	3408	6696	5217	32
H(37)	2438	6422	3871	37
H(38)	3346	6296	2677	34
H(39)	5225	6421	2823	27
H(41)	9776	6625	3952	30
H(42)	11124	6972	5001	40

H(43)	11693	6612	6363	37
H(44)	10838	5926	6715	38
H(45)	9477	5588	5691	29
H(47)	6223	5631	3540	28
H(48)	5104	5043	3925	43
H(49)	5857	4412	4742	49
H(50)	7762	4377	5242	46
H(51)	8892	4971	4877	32
H(53)	8284	4977	2779	34
H(54)	9379	4587	1915	44
H(55)	11122	4858	1796	47
H(56)	11765	5547	2504	50
H(57)	10696	5932	3390	33
H(58A)	4456	5537	8856	53
H(58B)	4470	5179	8057	53
H(59A)	2640	6575	9570	81
H(59B)	3079	6569	8643	81

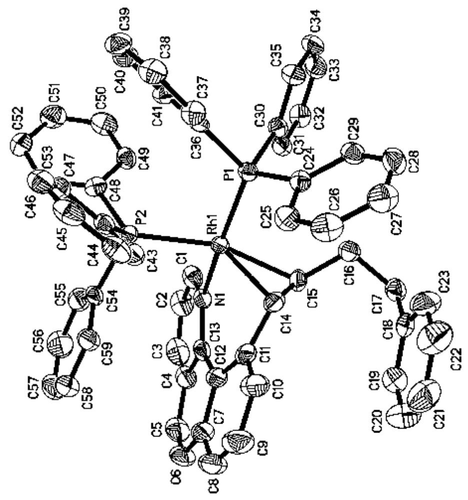


Table 1. Crystal data and structure refinement for **3ak (**lxw43).

Identification code	lxw43	
Empirical formula	C65 H61 F6 N O2 P3 Rh	
Formula weight	1197.97	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.8319(4) Å	α= 75.156(2)?
	b = 13.2288(4) Å	β= 79.856(2)?
	c = 22.0889(8) Å	γ = 69.201(2)?
Volume	2847.44(17) $Å^3$	
Z	2	
Density (calculated)	1.397 Mg/m^3	
Absorption coefficient	0.449 mm^{-1}	
F(000)	1236	
Crystal size	0.30 x 0.15 x 0.12 mm^3	
Theta range for data collection	0.96 to 25.50°.	
Index ranges	-13<=h<=13, -16<=k<=15, -26<=l<=26	
Reflections collected	66048	
Independent reflections	10559 [R(int) = 0.0443]	

Completeness to theta = 25.50	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9480 and 0.8770
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10559 / 117 / 742
Goodness-of-fit on F^2	1.130
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1606
R indices (all data)	R1 = 0.0711, wR2 = 0.1810
Largest diff. peak and hole	1.233 and -1.349 e.$^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}x 10^3) for **3ak (**lxw43). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Rh(1)	9660(1)	6639(1)	7321(1)	23(1)
C(1)	10771(5)	4282(4)	7828(2)	35(1)
C(2)	11156(5)	3233(4)	8222(3)	43(1)
C(3)	10700(6)	3136(5)	8840(3)	49(1)
C(4)	9917(5)	4077(5)	9075(2)	41(1)
C(5)	9317(6)	4001(5)	9711(3)	49(1)
C(6)	8497(6)	4906(6)	9910(2)	51(2)
C(7)	8295(5)	5989(5)	9524(2)	41(1)
C(8)	7502(6)	6936(6)	9766(3)	52(2)
C(9)	7378(6)	7977(6)	9425(3)	54(2)
C(10)	8085(5)	8108(5)	8829(2)	45(1)
C(11)	8900(5)	7221(4)	8567(2)	33(1)
C(12)	8960(5)	6130(4)	8902(2)	34(1)
C(13)	9665(4)	5130(4)	8663(2)	31(1)
C(14)	9752(5)	7502(4)	7993(2)	32(1)
C(15)	11079(5)	6912(4)	7827(2)	29(1)
C(16)	12085(5)	7478(4)	7516(2)	35(1)
C(17)	12725(5)	7704(5)	8021(2)	38(1)
C(18)	11756(5)	8588(5)	8355(2)	42(1)
C(19)	11294(7)	8343(6)	8980(3)	58(2)
C(20)	10389(9)	9152(8)	9282(3)	77(2)
C(21)	9934(8)	10230(7)	8959(4)	72(2)
C(22)	10381(8)	10483(7)	8339(3)	68(2)
C(23)	11271(6)	9693(6)	8038(3)	56(2)
C(24)	9552(4)	9376(3)	6560(2)	26(1)
C(25)	8435(5)	9913(4)	6923(2)	35(1)
C(26)	8223(6)	10978(4)	7004(3)	43(1)
C(27)	9169(6)	11497(4)	6739(3)	46(1)
C(28)	10289(5)	10964(4)	6387(2)	39(1)
C(29)	10480(5)	9917(4)	6292(2)	32(1)
C(30)	11268(4)	7514(4)	5972(2)	27(1)
C(31)	12197(5)	6513(4)	6217(2)	30(1)
C(32)	13380(5)	6077(4)	5869(2)	34(1)

C(33)	13658(5)	6654(4)	5271(2)	39(1)
C(34)	12740(5)	7649(4)	5017(2)	37(1)
C(35)	11550(5)	8072(4)	5364(2)	33(1)
C(36)	8521(4)	8400(4)	5844(2)	25(1)
C(37)	7534(4)	9435(4)	5719(2)	31(1)
C(38)	6711(5)	9678(4)	5247(2)	36(1)
C(39)	6834(5)	8897(5)	4909(2)	38(1)
C(40)	7794(5)	7863(4)	5035(2)	36(1)
C(41)	8641(5)	7621(4)	5490(2)	30(1)
C(42)	6411(4)	7420(4)	6901(2)	27(1)
C(43)	6130(5)	8285(4)	7217(2)	32(1)
C(44)	5038(5)	9224(4)	7095(2)	39(1)
C(45)	4213(5)	9325(4)	6657(2)	41(1)
C(46)	4483(5)	8491(4)	6335(2)	39(1)
C(47)	5586(4)	7539(4)	6450(2)	30(1)
C(48)	8182(4)	5328(4)	6541(2)	28(1)
C(49)	9459(5)	4982(4)	6237(2)	31(1)
C(50)	9734(5)	4321(4)	5796(3)	42(1)
C(51)	8748(6)	4009(5)	5659(3)	46(1)
C(52)	7484(6)	4318(5)	5971(2)	42(1)
C(53)	7211(5)	4956(4)	6417(2)	33(1)
C(54)	7242(4)	5391(4)	7825(2)	32(1)
C(55)	7734(5)	4229(4)	7938(2)	41(1)
C(56)	7362(6)	3618(5)	8501(3)	52(2)
C(57)	6496(6)	4126(5)	8950(3)	51(2)
C(58)	5996(6)	5271(5)	8840(3)	48(1)
C(59)	6377(5)	5897(5)	8284(2)	39(1)
C(60)	5634(7)	5551(7)	2307(3)	63(2)
C(61)	6006(6)	6160(6)	1675(3)	51(1)
C(62)	5445(8)	7398(6)	1533(4)	71(2)
C(63)	3730(40)	8660(20)	9840(20)	128(16)
C(64)	4061(19)	9580(20)	9394(12)	122(10)
C(65)	4210(40)	9760(40)	8701(15)	172(18)
O(2)	4240(20)	10271(18)	9612(13)	182(13)
C(63A)	3580(30)	8797(18)	9951(17)	109(11)
C(64A)	3423(13)	9753(13)	9416(8)	73(5)
C(65A)	4150(20)	9630(20)	8802(9)	88(7)
O(2A)	2679(17)	10641(10)	9497(7)	133(7)

F(1)	3493(5)	3355(4)	5769(2)	78(1)
F(2)	2723(4)	2146(4)	6500(2)	79(1)
F(3)	4252(6)	1940(4)	7129(2)	87(1)
F(4)	4867(4)	1661(3)	6144(2)	71(1)
F(5)	5024(3)	3171(3)	6381(2)	64(1)
F(6)	2877(4)	3644(4)	6755(2)	81(1)
N(1)	10044(4)	5205(3)	8036(2)	26(1)
O(1)	6766(5)	5654(5)	1290(2)	76(1)
P(1)	9683(1)	8013(1)	6446(1)	24(1)
P(2)	7882(1)	6215(1)	7104(1)	24(1)
P(3)	3877(1)	2652(1)	6453(1)	41(1)

Table 3. Bond lengths and angles for **3ak (**lxw43).

Rh(1)-N(1)	2.098(3)
Rh(1)-C(14)	2.127(5)
Rh(1)-C(15)	2.224(4)
Rh(1)-P(1)	2.2925(11)
Rh(1)-P(2)	2.3420(11)
C(1)-N(1)	1.342(6)
C(1)-C(2)	1.398(7)
C(2)-C(3)	1.357(8)
C(3)-C(4)	1.401(9)
C(4)-C(13)	1.418(7)
C(4)-C(5)	1.435(8)
C(5)-C(6)	1.338(9)
C(6)-C(7)	1.431(8)
C(7)-C(8)	1.419(9)
C(7)-C(12)	1.433(7)
C(8)-C(9)	1.362(9)
C(9)-C(10)	1.403(8)
C(10)-C(11)	1.387(7)
C(11)-C(12)	1.428(7)
C(11)-C(14)	1.478(7)
C(12)-C(13)	1.453(7)
C(13)-N(1)	1.361(6)
C(14)-C(15)	1.405(7)
C(15)-C(16)	1.508(6)
C(16)-C(17)	1.548(7)
C(17)-C(18)	1.521(8)
C(18)-C(19)	1.381(8)
C(18)-C(23)	1.401(9)
C(19)-C(20)	1.394(11)
C(20)-C(21)	1.375(11)
C(21)-C(22)	1.366(10)
C(22)-C(23)	1.371(10)
C(24)-C(25)	1.397(6)
C(24)-C(29)	1.399(6)
C(24)-P(1)	1.837(4)
C(25)-C(26)	1.398(7)

C(26)-C(27)	1.396(8)
C(27)-C(28)	1.384(8)
C(28)-C(29)	1.392(7)
C(30)-C(31)	1.391(6)
C(30)-C(35)	1.397(6)
C(30)-P(1)	1.843(4)
C(31)-C(32)	1.387(7)
C(32)-C(33)	1.387(7)
C(33)-C(34)	1.387(8)
C(34)-C(35)	1.386(7)
C(36)-C(37)	1.402(6)
C(36)-C(41)	1.404(7)
C(36)-P(1)	1.843(4)
C(37)-C(38)	1.391(7)
C(38)-C(39)	1.381(8)
C(39)-C(40)	1.388(7)
C(40)-C(41)	1.379(7)
C(42)-C(47)	1.395(6)
C(42)-C(43)	1.406(7)
C(42)-P(2)	1.834(4)
C(43)-C(44)	1.383(7)
C(44)-C(45)	1.381(8)
C(45)-C(46)	1.380(8)
C(46)-C(47)	1.398(7)
C(48)-C(49)	1.398(6)
C(48)-C(53)	1.400(7)
C(48)-P(2)	1.834(4)
C(49)-C(50)	1.395(7)
C(50)-C(51)	1.377(8)
C(51)-C(52)	1.390(8)
C(52)-C(53)	1.384(7)
C(54)-C(59)	1.386(7)
C(54)-C(55)	1.406(7)
C(54)-P(2)	1.861(5)
C(55)-C(56)	1.380(8)
C(56)-C(57)	1.372(9)
C(57)-C(58)	1.387(9)
C(58)-C(59)	1.382(7)

C(60)-C(61)	1.487(9)
C(61)-O(1)	1.227(8)
C(61)-C(62)	1.499(10)
C(63)-C(64)	1.471(17)
C(64)-O(2)	1.22(2)
C(64)-C(65)	1.478(17)
C(63A)-C(64A)	1.475(17)
C(64A)-O(2A)	1.202(16)
C(64A)-C(65A)	1.462(15)
F(1)-P(3)	1.596(4)
F(2)-P(3)	1.592(4)
F(3)-P(3)	1.581(4)
F(4)-P(3)	1.592(4)
F(5)-P(3)	1.587(4)
F(6)-P(3)	1.590(4)

N(1)-Rh(1)-C(14)	87.42(17)
N(1)-Rh(1)-C(15)	79.50(15)
C(14)-Rh(1)-C(15)	37.59(17)
N(1)-Rh(1)-P(1)	167.70(11)
C(14)-Rh(1)-P(1)	97.29(14)
C(15)-Rh(1)-P(1)	97.30(12)
N(1)-Rh(1)-P(2)	88.21(10)
C(14)-Rh(1)-P(2)	130.15(13)
C(15)-Rh(1)-P(2)	162.41(13)
P(1)-Rh(1)-P(2)	97.26(4)
N(1)-C(1)-C(2)	123.4(5)
C(3)-C(2)-C(1)	118.2(5)
C(2)-C(3)-C(4)	120.2(5)
C(3)-C(4)-C(13)	118.9(5)
C(3)-C(4)-C(5)	121.9(5)
C(13)-C(4)-C(5)	119.1(5)
C(6)-C(5)-C(4)	120.7(5)
C(5)-C(6)-C(7)	121.6(5)
C(8)-C(7)-C(6)	120.3(5)
C(8)-C(7)-C(12)	119.4(5)
C(6)-C(7)-C(12)	120.3(5)
C(9)-C(8)-C(7)	121.3(5)

C(8)-C(9)-C(10)	119.0(6)
C(11)-C(10)-C(9)	122.9(6)
C(10)-C(11)-C(12)	118.4(5)
C(10)-C(11)-C(14)	115.4(5)
C(12)-C(11)-C(14)	125.8(4)
C(11)-C(12)-C(7)	118.7(5)
C(11)-C(12)-C(13)	124.8(4)
C(7)-C(12)-C(13)	116.5(5)
N(1)-C(13)-C(4)	119.9(5)
N(1)-C(13)-C(12)	119.6(4)
C(4)-C(13)-C(12)	120.4(4)
C(15)-C(14)-C(11)	127.8(5)
C(15)-C(14)-Rh(1)	75.0(3)
C(11)-C(14)-Rh(1)	108.3(3)
C(14)-C(15)-C(16)	122.4(4)
C(14)-C(15)-Rh(1)	67.4(3)
C(16)-C(15)-Rh(1)	124.6(3)
C(15)-C(16)-C(17)	110.2(4)
C(18)-C(17)-C(16)	112.3(4)
C(19)-C(18)-C(23)	116.7(6)
C(19)-C(18)-C(17)	121.9(6)
C(23)-C(18)-C(17)	121.4(5)
C(18)-C(19)-C(20)	121.8(7)
C(21)-C(20)-C(19)	120.2(7)
C(22)-C(21)-C(20)	118.6(7)
C(21)-C(22)-C(23)	121.7(7)
C(22)-C(23)-C(18)	121.1(6)
C(25)-C(24)-C(29)	118.5(4)
C(25)-C(24)-P(1)	117.5(3)
C(29)-C(24)-P(1)	124.0(3)
C(24)-C(25)-C(26)	121.1(5)
C(27)-C(26)-C(25)	119.5(5)
C(28)-C(27)-C(26)	119.7(5)
C(27)-C(28)-C(29)	120.7(5)
C(28)-C(29)-C(24)	120.4(5)
C(31)-C(30)-C(35)	118.5(4)
C(31)-C(30)-P(1)	118.8(3)
C(35)-C(30)-P(1)	122.6(3)

C(32)-C(31)-C(30)	121.1(4)
C(31)-C(32)-C(33)	119.7(5)
C(34)-C(33)-C(32)	120.1(5)
C(35)-C(34)-C(33)	119.9(5)
C(34)-C(35)-C(30)	120.7(4)
C(37)-C(36)-C(41)	118.5(4)
C(37)-C(36)-P(1)	123.2(4)
C(41)-C(36)-P(1)	118.3(3)
C(38)-C(37)-C(36)	120.0(4)
C(39)-C(38)-C(37)	120.6(4)
C(38)-C(39)-C(40)	119.9(4)
C(41)-C(40)-C(39)	120.2(5)
C(40)-C(41)-C(36)	120.8(4)
C(47)-C(42)-C(43)	118.7(4)
C(47)-C(42)-P(2)	124.6(4)
C(43)-C(42)-P(2)	116.7(3)
C(44)-C(43)-C(42)	120.7(5)
C(45)-C(44)-C(43)	120.1(5)
C(46)-C(45)-C(44)	120.1(5)
C(45)-C(46)-C(47)	120.6(5)
C(42)-C(47)-C(46)	119.8(5)
C(49)-C(48)-C(53)	118.7(4)
C(49)-C(48)-P(2)	117.9(4)
C(53)-C(48)-P(2)	123.3(4)
C(50)-C(49)-C(48)	120.2(5)
C(51)-C(50)-C(49)	120.1(5)
C(50)-C(51)-C(52)	120.4(5)
C(53)-C(52)-C(51)	119.7(5)
C(52)-C(53)-C(48)	120.7(5)
C(59)-C(54)-C(55)	118.8(5)
C(59)-C(54)-P(2)	121.2(4)
C(55)-C(54)-P(2)	119.7(4)
C(56)-C(55)-C(54)	119.8(5)
C(57)-C(56)-C(55)	121.0(6)
C(56)-C(57)-C(58)	119.7(5)
C(59)-C(58)-C(57)	120.1(6)
C(58)-C(59)-C(54)	120.7(5)
O(1)-C(61)-C(60)	120.3(7)

O(1)-C(61)-C(62)	121.6(6)
C(60)-C(61)-C(62)	118.1(6)
O(2)-C(64)-C(63)	117.8(17)
O(2)-C(64)-C(65)	116.3(18)
C(63)-C(64)-C(65)	126(3)
O(2A)-C(64A)-C(65A)	120.5(14)
O(2A)-C(64A)-C(63A)	118.4(15)
C(65A)-C(64A)-C(63A)	121(2)
C(1)-N(1)-C(13)	118.9(4)
C(1)-N(1)-Rh(1)	113.5(3)
C(13)-N(1)-Rh(1)	127.6(3)
C(24)-P(1)-C(30)	107.0(2)
C(24)-P(1)-C(36)	101.4(2)
C(30)-P(1)-C(36)	99.9(2)
C(24)-P(1)-Rh(1)	118.14(15)
C(30)-P(1)-Rh(1)	106.74(15)
C(36)-P(1)-Rh(1)	121.57(14)
C(48)-P(2)-C(42)	107.9(2)
C(48)-P(2)-C(54)	101.0(2)
C(42)-P(2)-C(54)	102.5(2)
C(48)-P(2)-Rh(1)	119.03(15)
C(42)-P(2)-Rh(1)	114.39(15)
C(54)-P(2)-Rh(1)	109.96(14)
F(3)-P(3)-F(5)	91.9(3)
F(3)-P(3)-F(6)	90.5(3)
F(5)-P(3)-F(6)	89.9(2)
F(3)-P(3)-F(4)	90.0(3)
F(5)-P(3)-F(4)	90.5(2)
F(6)-P(3)-F(4)	179.3(3)
F(3)-P(3)-F(2)	90.1(3)
F(5)-P(3)-F(2)	178.0(3)
F(6)-P(3)-F(2)	90.6(2)
F(4)-P(3)-F(2)	89.0(2)
F(3)-P(3)-F(1)	179.1(3)
F(5)-P(3)-F(1)	88.9(2)
F(6)-P(3)-F(1)	90.0(3)
F(4)-P(3)-F(1)	89.5(2)
F(2)-P(3)-F(1)	89.2(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (^{2}x 10^3) for **3ak (**lxw43). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Rh(1)	19(1)	30(1)	20(1)	-2(1)	-4(1)	-8(1)
C(1)	25(2)	35(3)	40(3)	0(2)	-7(2)	-8(2)
C(2)	33(3)	34(3)	54(3)	-1(2)	-10(2)	-4(2)
C(3)	43(3)	41(3)	54(4)	14(3)	-18(3)	-15(3)
C(4)	35(3)	55(3)	33(3)	10(2)	-14(2)	-21(2)
C(5)	54(3)	58(4)	35(3)	17(3)	-14(3)	-30(3)
C(6)	50(3)	82(4)	22(3)	7(3)	-5(2)	-34(3)
C(7)	36(3)	66(4)	25(2)	-4(2)	-7(2)	-22(3)
C(8)	42(3)	87(5)	28(3)	-11(3)	4(2)	-26(3)
C(9)	39(3)	79(4)	41(3)	-25(3)	5(2)	-10(3)
C(10)	35(3)	63(4)	32(3)	-13(2)	-3(2)	-11(3)
C(11)	25(2)	50(3)	26(2)	-8(2)	-8(2)	-12(2)
C(12)	24(2)	54(3)	23(2)	-2(2)	-8(2)	-14(2)
C(13)	23(2)	40(3)	29(2)	4(2)	-8(2)	-17(2)
C(14)	28(2)	44(3)	28(2)	-13(2)	-3(2)	-13(2)
C(15)	30(2)	30(2)	33(2)	-7(2)	-5(2)	-15(2)
C(16)	29(2)	48(3)	29(2)	-2(2)	-5(2)	-15(2)
C(17)	31(3)	51(3)	35(3)	0(2)	-8(2)	-21(2)
C(18)	45(3)	64(4)	35(3)	-9(2)	-8(2)	-36(3)
C(19)	77(5)	74(4)	42(3)	-10(3)	1(3)	-50(4)
C(20)	97(6)	108(7)	45(4)	-33(4)	16(4)	-53(5)
C(21)	82(5)	81(5)	68(5)	-40(4)	1(4)	-32(4)
C(22)	70(5)	77(5)	61(4)	-20(4)	-15(4)	-20(4)
C(23)	57(4)	82(5)	32(3)	-8(3)	-10(3)	-27(3)
C(24)	26(2)	24(2)	27(2)	-4(2)	-5(2)	-7(2)
C(25)	30(2)	35(3)	37(3)	-9(2)	-1(2)	-8(2)
C(26)	43(3)	35(3)	43(3)	-13(2)	-2(2)	-2(2)
C(27)	62(4)	31(3)	42(3)	-8(2)	-6(3)	-13(3)
C(28)	45(3)	34(3)	41(3)	1(2)	-8(2)	-21(2)
C(29)	28(2)	37(2)	28(2)	2(2)	-4(2)	-10(2)
C(30)	21(2)	33(2)	26(2)	-6(2)	0(2)	-10(2)
C(31)	29(2)	33(2)	28(2)	-2(2)	-3(2)	-13(2)
C(32)	28(2)	30(2)	42(3)	-11(2)	-2(2)	-5(2)

C(33)	30(3)	51(3)	39(3)	-18(2)	8(2)	-16(2)
C(34)	42(3)	45(3)	28(2)	-10(2)	9(2)	-23(2)
C(35)	34(3)	32(2)	29(2)	-2(2)	-1(2)	-10(2)
C(36)	21(2)	30(2)	20(2)	2(2)	1(2)	-10(2)
C(37)	25(2)	30(2)	33(2)	-6(2)	-4(2)	-4(2)
C(38)	25(2)	37(3)	35(3)	0(2)	-5(2)	0(2)
C(39)	27(2)	56(3)	25(2)	-3(2)	-7(2)	-8(2)
C(40)	35(3)	48(3)	25(2)	-7(2)	-1(2)	-13(2)
C(41)	28(2)	34(2)	22(2)	-2(2)	-3(2)	-6(2)
C(42)	19(2)	32(2)	26(2)	-2(2)	0(2)	-7(2)
C(43)	27(2)	35(2)	31(2)	-6(2)	1(2)	-11(2)
C(44)	33(3)	35(3)	41(3)	-7(2)	8(2)	-9(2)
C(45)	26(2)	40(3)	37(3)	6(2)	3(2)	-1(2)
C(46)	28(2)	47(3)	31(3)	5(2)	-6(2)	-8(2)
C(47)	27(2)	34(2)	27(2)	0(2)	-4(2)	-13(2)
C(48)	27(2)	26(2)	26(2)	-6(2)	-5(2)	-2(2)
C(49)	25(2)	32(2)	34(2)	-2(2)	-4(2)	-9(2)
C(50)	38(3)	37(3)	42(3)	-11(2)	7(2)	-4(2)
C(51)	58(4)	45(3)	40(3)	-18(2)	1(3)	-19(3)
C(52)	48(3)	49(3)	39(3)	-13(2)	-5(2)	-24(3)
C(53)	32(2)	37(3)	32(2)	-6(2)	-4(2)	-15(2)
C(54)	22(2)	51(3)	23(2)	5(2)	-6(2)	-19(2)
C(55)	38(3)	46(3)	37(3)	1(2)	-12(2)	-16(2)
C(56)	52(4)	52(3)	47(3)	10(3)	-16(3)	-18(3)
C(57)	55(4)	62(4)	38(3)	13(3)	-11(3)	-35(3)
C(58)	44(3)	73(4)	32(3)	-8(3)	2(2)	-29(3)
C(59)	32(3)	54(3)	29(2)	-1(2)	-3(2)	-18(2)
C(60)	52(4)	95(5)	43(3)	-6(3)	-3(3)	-33(4)
C(61)	48(3)	72(4)	43(3)	-10(3)	-7(3)	-30(3)
C(62)	82(5)	75(5)	63(4)	-4(4)	-19(4)	-36(4)
C(63)	74(19)	170(30)	100(20)	30(20)	-17(17)	-19(19)
C(64)	88(18)	160(20)	87(15)	-52(14)	13(15)	4(16)
C(65)	140(30)	230(30)	80(20)	-50(20)	-10(19)	20(20)
O(2)	130(20)	151(19)	300(30)	-140(20)	-15(18)	-31(15)
C(63A)	83(18)	113(17)	130(20)	22(15)	-34(16)	-52(15)
C(64A)	69(11)	76(9)	82(10)	-33(8)	-4(9)	-22(8)
C(65A)	91(13)	126(15)	73(13)	4(11)	-32(10)	-74(13)
O(2A)	164(17)	87(9)	128(12)	-48(8)	-30(10)	8(9)

F(1)	92(3)	80(3)	64(3)	-2(2)	-22(2)	-33(2)
F(2)	65(3)	85(3)	105(3)	-34(3)	12(2)	-47(2)
F(3)	144(4)	75(3)	49(2)	-1(2)	-24(3)	-44(3)
F(4)	76(3)	55(2)	82(3)	-37(2)	19(2)	-18(2)
F(5)	42(2)	60(2)	100(3)	-27(2)	1(2)	-24(2)
F(6)	64(3)	75(3)	103(3)	-51(3)	33(2)	-20(2)
N(1)	23(2)	27(2)	26(2)	3(2)	-7(2)	-9(2)
O(1)	72(3)	104(4)	54(3)	-23(3)	11(3)	-34(3)
P(1)	20(1)	27(1)	22(1)	-2(1)	-2(1)	-7(1)
P(2)	20(1)	28(1)	22(1)	-3(1)	-4(1)	-7(1)
P(3)	35(1)	43(1)	46(1)	-16(1)	5(1)	-15(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2}x 10^3)
For **3ak (**lxw43).

	x	y	z	U(eq)
H(1)	11039	4344	7391	42
H(2)	11720	2606	8062	51
H(3)	10912	2428	9114	58
H(5)	9504	3302	9993	59
H(6)	8038	4826	10318	61
H(8)	7048	6843	10175	63
H(9)	6822	8604	9587	65
H(10)	8001	8836	8595	53
H(14)	9525	8317	7825	39
H(15)	11451	6257	8166	35
H(16A)	11647	8186	7234	42
H(16B)	12782	7005	7259	42
H(17A)	13053	7009	8335	46
H(17B)	13496	7941	7817	46
H(19)	11601	7602	9211	70
H(20)	10087	8958	9713	93
H(21)	9321	10788	9162	86
H(22)	10066	11225	8111	82
H(23)	11564	9899	7607	67
H(25)	7808	9548	7118	42
H(26)	7441	11345	7238	51
H(27)	9044	12214	6799	55
H(28)	10936	11316	6210	47
H(29)	11246	9567	6043	39
H(31)	12017	6121	6629	36
H(32)	13998	5386	6039	41
H(33)	14478	6368	5035	46
H(34)	12926	8041	4606	44
H(35)	10919	8749	5186	40
H(37)	7426	9971	5957	37
H(38)	6060	10387	5157	44
H(39)	6261	9066	4591	46

H(40)	7869	7321	4808	44
H(41)	9312	6920	5564	36
H(43)	6695	8223	7517	38
H(44)	4855	9802	7313	46
H(45)	3459	9968	6577	49
H(46)	3915	8565	6033	46
H(47)	5774	6974	6222	35
H(49)	10141	5197	6330	37
H(50)	10603	4086	5591	50
H(51)	8933	3579	5349	55
H(52)	6809	4092	5879	51
H(53)	6357	5144	6641	39
H(55)	8321	3867	7627	49
H(56)	7711	2833	8579	63
H(57)	6240	3696	9334	61
H(58)	5390	5627	9149	57
H(59)	6042	6681	8215	46
H(60A)	5930	4759	2310	94
H(60B)	4669	5819	2401	94
H(60C)	6060	5674	2625	94
H(62A)	5812	7691	1115	107
H(62B)	5679	7686	1849	107
H(62C)	4478	7626	1544	107
H(63A)	4137	8493	10228	191
H(63B)	4060	8002	9650	191
H(63C)	2762	8858	9929	191
H(65A)	3353	9882	8553	257
H(65B)	4870	9105	8571	257
H(65C)	4493	10407	8519	257
H(63D)	3931	8931	10292	163
H(63E)	4195	8130	9815	163
H(63F)	2715	8696	10101	163
H(65D)	3564	10065	8470	131
H(65E)	4468	8849	8776	131
H(65F)	4911	9894	8747	131

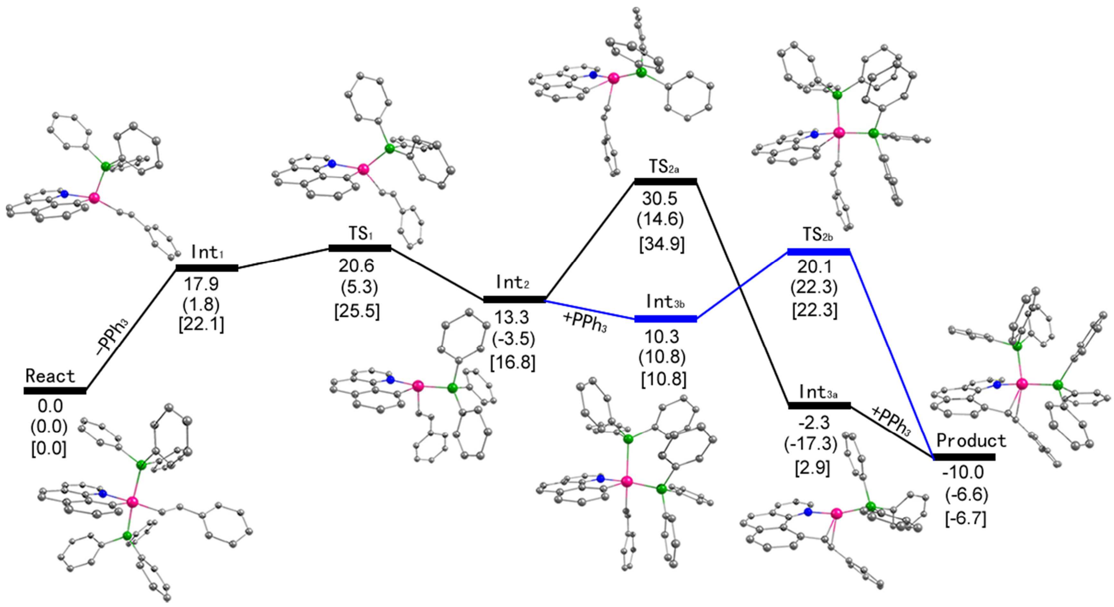


Figure 3. Energy profiles for C-C coupling reaction of R=PPh_3. (a) Values (ΔE) without any parentheses are total energy changes with correction of the zero-point energy. (b) Values (ΔG^0) in parentheses are Gibbs free energy where translation, rotation, and vibration movements are taken into consideration to estimate the thermal entropy and free energy. (c) Values (ΔG_v^0) in square brackets are Gibbs free energy where only vibration movements are taken into consideration to estimate the thermal entropy and free energy.

DFT Data

React

Rh	2.27446700	21.76065500	3.48409600
C	0.58641400	20.69918300	3.33014100
C	0.46549500	19.32069000	3.23465300
H	1.33986700	18.68103300	3.25551500
C	-0.81209700	18.72695500	3.11795300
H	-0.88200700	17.64489300	3.04387500
C	-1.96454600	19.49281500	3.10208500
H	-2.93934800	19.02178100	3.01146800
C	-1.87848700	20.89687900	3.21934000
C	-3.03738300	21.74937500	3.24473600
H	-4.01612800	21.28743900	3.14444400
C	-2.93265400	23.10071200	3.39887600
H	-3.82187800	23.72459500	3.42283000
C	-1.64900400	23.72735700	3.54284800
C	-0.49015000	22.91076200	3.50042100
C	-0.59098200	21.49193400	3.33584000
C	-1.46239200	25.10991000	3.73980500

H	-2.32543200	25.76932700	3.78142600
C	-0.18036100	25.61361100	3.88702900
H	-0.00441100	26.67198300	4.04752600
C	0.90836500	24.72999500	3.82922600
H	1.92573200	25.09710700	3.93432800
C	3.64219300	20.27975400	3.24561900
H	3.33873500	19.44173200	2.61682000
C	4.91633000	20.31640200	3.68357900
H	5.23557500	21.12759600	4.33955900
C	5.98443900	19.33546900	3.40099500
C	7.15952400	19.37582000	4.17369700
H	7.25390600	20.12987800	4.95244400
C	8.19223800	18.46245600	3.96631500
H	9.08817400	18.51191100	4.57939300
C	8.07567000	17.48871400	2.97299800
C	6.91956600	17.44317500	2.18780300
H	6.82645000	16.69684900	1.40310100
C	5.88844400	18.35625900	2.39398800
H	5.01043400	18.32033300	1.75535000
C	1.05038900	22.46926200	6.81391400
C	-0.27113700	21.98861600	6.78846600
H	-0.50706300	21.06742000	6.26426300
C	-1.28515700	22.67636900	7.45315300
H	-2.29971500	22.28874900	7.43172400
C	-0.99742300	23.85477000	8.14750000
H	-1.78777700	24.38693400	8.66923600
C	0.31064100	24.33807600	8.17736300
H	0.54509100	25.24606300	8.72595200
C	1.33139900	23.65048400	7.51545600
H	2.34650800	24.02965200	7.56495200
C	3.94705400	22.26044900	6.43180700
C	4.33994000	23.47976700	5.84979800
H	3.68279900	23.98199800	5.14309200
C	5.56246200	24.06547900	6.17927900
H	5.84803900	25.01148000	5.72777900
C	6.41531300	23.43378200	7.08791700
H	7.36942500	23.88537400	7.34358500
C	6.03663600	22.22099700	7.66660100
H	6.69545700	21.72647200	8.37461000
C	4.81077800	21.63479600	7.34231500
H	4.53211000	20.69007300	7.79650400
C	2.27329300	19.86647800	6.73175100
C	1.86629200	19.76651000	8.07532500
H	1.56036600	20.65189000	8.62248100

C	1.84982400	18.52847000	8.71725200
H	1.53451400	18.46703700	9.75491900
C	2.23420900	17.37513900	8.02973200
H	2.21794700	16.41159000	8.53110200
C	2.64175600	17.46604800	6.69837900
H	2.94833200	16.57443500	6.15888900
C	2.66256900	18.70288700	6.05162700
H	3.00345600	18.77054300	5.02667300
C	3.03864200	20.68210900	0.05530100
C	2.33188900	19.46770500	0.12137900
H	1.46226800	19.37701200	0.76507500
C	2.73821800	18.37084300	-0.63921600
H	2.17824300	17.44141200	-0.58449800
C	3.86211800	18.46625200	-1.46391500
H	4.17999400	17.61098000	-2.05323100
C	4.57476000	19.66395800	-1.52577900
H	5.45173600	19.74504100	-2.16141200
C	4.16733000	20.76742900	-0.77284100
H	4.73302600	21.69052000	-0.83457300
C	0.97940800	22.75250500	0.17312800
C	0.23606900	21.94508000	-0.70121500
H	0.55262500	20.93096400	-0.91513800
C	-0.90927200	22.44334300	-1.32597900
H	-1.46756800	21.80442800	-2.00422500
C	-1.32657500	23.75331800	-1.09270000
H	-2.21385000	24.14043900	-1.58538600
C	-0.59025000	24.56790900	-0.22936200
H	-0.89977100	25.59341100	-0.04829000
C	0.54924600	24.07180300	0.40193100
H	1.11472400	24.72347000	1.05916300
C	3.74654800	23.42006800	0.81178700
C	3.71511200	24.30214500	-0.28176400
H	2.91403900	24.23882100	-1.01061800
C	4.71313200	25.26448800	-0.43986300
H	4.67814100	25.93839600	-1.29109300
C	5.75377200	25.35918700	0.48728800
H	6.52880600	26.10962700	0.36048900
C	5.80031500	24.47969300	1.57021900
H	6.61573200	24.53569900	2.28584100
C	4.80435600	23.51482400	1.73205800
H	4.87395800	22.80997700	2.55506000
N	0.76361800	23.41972400	3.63790700
P	2.34567600	21.51447000	5.91249300
P	2.46966100	22.11570900	1.05945400

H	8.87938600	16.77727600	2.80568500

PPh$_3$

P	10.43563900	16.55129500	3.91477700
C	11.51670600	17.32622900	5.20676000
C	12.08572100	18.57272600	4.89331900
H	11.88600300	19.02491600	3.92434300
C	12.89851500	19.23956500	5.80914800
H	13.33339400	20.20044700	5.54621000
C	13.14101800	18.68007300	7.06582100
H	13.76598400	19.20285800	7.78511800
C	12.56984700	17.45043500	7.39561400
H	12.75047700	17.01082000	8.37342300
C	11.76598200	16.77637200	6.47317400
H	11.32893300	15.81984500	6.74292100
C	9.60839400	15.17670500	4.84381200
C	8.37001900	15.46906300	5.43989600
H	7.95046800	16.46767200	5.34075000
C	7.66941300	14.49462700	6.15075100
H	6.71445500	14.74091700	6.60780400
C	8.18804800	13.20293800	6.26207100
H	7.63926200	12.43915100	6.80683400
C	9.41095700	12.89530100	5.66337800
H	9.81839800	11.89045900	5.74232300
C	10.11741200	13.87429900	4.96162300
H	11.06734300	13.62189300	4.50018600
C	11.66212500	15.64714400	2.85827600
C	11.23666000	15.26946500	1.57359400
H	10.22726000	15.51378700	1.25031400
C	12.09308600	14.59202700	0.70579200
H	11.74455100	14.30541900	-0.28310500
C	13.39872600	14.29563300	1.10246100
H	14.07105700	13.77659600	0.42434200
C	13.83873800	14.67688600	2.37111900
H	14.85539000	14.45336600	2.68486200
C	12.97750700	15.34578300	3.24357600
H	13.33230300	15.63878700	4.22720600

Int$_1$

Rh	2.22648700	21.60835500	4.14057400
C	0.53084500	20.60420000	3.86442600
C	0.31432200	19.24492500	4.02283200

H	1.08042300	18.60125700	4.44079600
C	-0.92081500	18.67844900	3.63308100
H	-1.06857500	17.60846000	3.75010000
C	-1.93362000	19.45908300	3.10514400
H	-2.87508200	19.00841100	2.80387300
C	-1.75708000	20.85426100	2.96414900
C	-2.78051400	21.72200800	2.44536300
H	-3.71962700	21.27658200	2.12827400
C	-2.59608500	23.07023700	2.34637100
H	-3.38139200	23.70749000	1.94985600
C	-1.36523800	23.67754000	2.76861100
C	-0.33826100	22.84370700	3.27613700
C	-0.51686600	21.42373200	3.36411500
C	-1.10692300	25.06375600	2.71188400
H	-1.86784300	25.73712900	2.32636200
C	0.11338800	25.55242800	3.14575100
H	0.34081000	26.61241300	3.11272600
C	1.07084700	24.65153200	3.63861400
H	2.03775900	25.00606500	3.98493900
C	3.49154800	20.10796500	3.82060500
H	3.09574100	19.12714900	3.55783500
C	4.80588300	20.39187900	3.68669700
H	5.16810800	21.36063500	4.04369200
C	5.86244200	19.55325800	3.09720700
C	7.18442300	20.03529700	3.09695400
H	7.39299600	21.01251300	3.52691400
C	8.22500900	19.28177700	2.55688400
H	9.23812200	19.67372300	2.56766800
C	7.96346800	18.02828200	2.00143000
C	6.65365300	17.53633100	1.98999200
H	6.44321300	16.56381500	1.55374700
C	5.61480600	18.28833100	2.52911300
H	4.60277200	17.89451900	2.50068200
C	1.04382600	22.44248800	7.23092200
C	-0.31514400	22.32144100	6.89260900
H	-0.62428600	21.63706500	6.10946300
C	-1.27471300	23.07558400	7.56623200
H	-2.32265100	22.97251600	7.30024700
C	-0.89012400	23.96120400	8.57674600
H	-1.63932200	24.55025100	9.09765800
C	0.45734800	24.08490200	8.91819800
H	0.76080600	24.76698900	9.70696300
C	1.42384100	23.32891700	8.25235900
H	2.46629300	23.42785900	8.53481000

C	3.92356100	22.11022900	6.79515100
C	4.23702100	23.37672200	6.26398600
H	3.49179500	23.92841200	5.69518500
C	5.48851700	23.94798700	6.49295700
H	5.71921600	24.92699700	6.08334900
C	6.43823100	23.26240100	7.25468300
H	7.41269800	23.70638000	7.43528900
C	6.13111800	22.00961400	7.78994800
H	6.86475300	21.47925800	8.38976900
C	4.88181100	21.43017600	7.56129500
H	4.65753000	20.45545600	7.98027800
C	2.16980400	19.73986400	7.15481700
C	1.25055600	19.49692100	8.18915000
H	0.58598800	20.28171900	8.53123300
C	1.18674400	18.23757400	8.78801400
H	0.47109000	18.06090800	9.58545400
C	2.03726600	17.21436700	8.36853500
H	1.98469500	16.23609900	8.83742000
C	2.95782000	17.45070800	7.34380600
H	3.62531300	16.65938000	7.01543400
C	3.02234800	18.70250300	6.73378900
H	3.73461900	18.87689300	5.93463500
N	0.85622400	23.33857600	3.70937800
P	2.28772300	21.39649400	6.38593500
H	8.77102900	17.43889600	1.57703100

TS_1

Rh	-0.25482600	0.27513200	-0.75346300
C	-1.44890200	0.62685500	0.80327200
C	-1.24306300	1.52880100	1.83506100
H	-0.38293800	2.18956800	1.83821600
C	-2.15905700	1.59916500	2.91056000
H	-1.97768800	2.31274900	3.70950300
C	-3.27085000	0.77983100	2.95756400
H	-3.96750300	0.84353900	3.78869700
C	-3.50880200	-0.15612300	1.92485200
C	-4.64247700	-1.04155500	1.93093400
H	-5.33943300	-0.97680900	2.76211500
C	-4.85148700	-1.94844400	0.93380800
H	-5.71201100	-2.61080300	0.95974500
C	-3.93603400	-2.05057300	-0.16696600
C	-2.81554600	-1.18405200	-0.20037500
C	-2.58774800	-0.22647100	0.84320600

C	-4.07577900	-2.97189300	-1.22733200
H	-4.92204200	-3.65381100	-1.23627200
C	-3.13504200	-3.00488300	-2.24259100
H	-3.21729000	-3.70578300	-3.06611200
C	-2.05478000	-2.10983500	-2.19431000
H	-1.29533400	-2.11029400	-2.97150400
C	1.45610000	0.22545800	0.25241900
H	1.34062700	0.27344300	1.33428400
C	2.61853200	-0.07789900	-0.35263800
H	2.67730800	-0.01950300	-1.44130800
C	3.87625300	-0.50264900	0.29091800
C	5.02331100	-0.64904700	-0.50980800
H	4.95431300	-0.45251900	-1.57746000
C	6.24250400	-1.03574500	0.04477700
H	7.11575300	-1.14218700	-0.59275800
C	6.33877100	-1.28805900	1.41396900
C	5.20506600	-1.15304700	2.22218500
H	5.27043900	-1.35676200	3.28740600
C	3.98742400	-0.76788500	1.66907600
H	3.11437100	-0.68596700	2.31041100
N	-1.90078500	-1.22474200	-1.21024300
P	0.17145200	2.42006400	-1.35207400
H	7.28608300	-1.59299500	1.84898100
C	-1.31781000	3.06996200	-2.20331500
C	-2.58818700	2.90247000	-1.62515200
C	-1.19921400	3.77526800	-3.41402200
C	-3.71806100	3.43118100	-2.24959400
H	-2.69364400	2.36554700	-0.68841600
C	-2.33446100	4.29931800	-4.03282400
H	-0.22659700	3.91923300	-3.87266600
C	-3.59381800	4.12677200	-3.45426900
H	-4.69503700	3.29756900	-1.79438400
H	-2.23267200	4.84345200	-4.96718600
H	-4.47541900	4.53421300	-3.94046900
C	1.44589200	2.25306100	-2.65651200
C	2.67012300	2.93568100	-2.62311700
C	1.19238500	1.33940800	-3.69874700
C	3.62392900	2.70784700	-3.61720200
H	2.88062600	3.64426400	-1.82956800
C	2.15135100	1.11286800	-4.68558100
H	0.23340500	0.82831000	-3.75546000
C	3.36981800	1.79604100	-4.64393600
H	4.56621900	3.24690300	-3.58832900
H	1.94506500	0.41143800	-5.48863300

H	4.11571100	1.62272700	-5.41399900
C	0.70681700	3.71761200	-0.17751500
C	1.82861400	3.51248500	0.64810100
C	0.00704000	4.93351500	-0.09834800
C	2.24244000	4.51263100	1.52735800
H	2.37421300	2.57635800	0.60223800
C	0.42613400	5.92645400	0.78853100
H	-0.86057900	5.10979700	-0.72394400
C	1.54164200	5.71943600	1.60085700
H	3.11231000	4.34649100	2.15601600
H	-0.12233400	6.86224400	0.84161900
H	1.86471900	6.49460600	2.28958600

Int_2

Rh	2.12430100	21.88107600	3.09394600
C	0.66144500	20.52094900	3.05355300
C	0.71997500	19.17330000	2.73853800
H	1.64552500	18.70653900	2.42160100
C	-0.44898400	18.37738900	2.82076700
H	-0.37941600	17.32124100	2.57563500
C	-1.66510600	18.91580400	3.19881900
H	-2.55097700	18.28946300	3.25452500
C	-1.76605700	20.29291400	3.50352600
C	-2.99893600	20.93213200	3.88130500
H	-3.89450400	20.32059500	3.95056400
C	-3.06604100	22.27064000	4.14422300
H	-4.00910900	22.73095900	4.42433400
C	-1.89575500	23.09804200	4.05164300
C	-0.67373100	22.48276100	3.69423900
C	-0.59068200	21.08384000	3.42123800
C	-1.87063100	24.48969100	4.28916500
H	-2.78622300	25.00500200	4.56677400
C	-0.68154200	25.18860100	4.16203500
H	-0.63648200	26.25861200	4.33248500
C	0.48625500	24.49712300	3.79944000
H	1.43310300	25.01500800	3.67880800
C	1.97548000	22.39064300	1.18514700
H	1.02595600	22.10424100	0.73755800
C	2.89197100	23.15094600	0.56867600
H	3.83133800	23.37138900	1.07599200
C	2.78626500	23.73713900	-0.78401400
C	3.93278800	24.32127600	-1.35087900
H	4.86006500	24.33143500	-0.78237300

C	3.89752900	24.87787100	-2.62880600
H	4.79533500	25.32364800	-3.04789600
C	2.71223500	24.86411200	-3.36534200
C	1.56227800	24.29256800	-2.81136600
H	0.63343300	24.28619800	-3.37501100
C	1.59610500	23.73835200	-1.53481200
H	0.68788100	23.31521800	-1.11480400
C	4.41273300	19.80913100	4.52196500
C	3.36650600	19.31908000	5.32408800
H	2.34214000	19.34675100	4.96499200
C	3.63792400	18.77714300	6.58143700
H	2.82221700	18.40215200	7.19263500
C	4.95129100	18.71917200	7.05075800
H	5.16079900	18.30021500	8.03063900
C	5.99685400	19.20013400	6.25850000
H	7.02035700	19.15286800	6.61879200
C	5.73284000	19.74458900	5.00169100
H	6.55277700	20.11862500	4.39706200
C	4.13554700	19.14334200	1.65988600
C	4.67549000	17.89737800	2.01863300
H	5.03101900	17.72374200	3.02887100
C	4.75633500	16.87238000	1.07438200
H	5.17373300	15.91147800	1.36070800
C	4.30452200	17.08098900	-0.22977900
H	4.36942000	16.28122200	-0.96182000
C	3.76612300	18.31849700	-0.59233600
H	3.41206800	18.48439200	-1.60559600
C	3.67474200	19.34599300	0.34621500
H	3.24850200	20.30241700	0.06008800
C	5.41627200	21.66143900	2.51333500
C	6.24524500	21.52861000	1.39070300
H	6.12295700	20.68665500	0.71749400
C	7.23503300	22.48125100	1.13470000
H	7.87772400	22.36535200	0.26686900
C	7.40189500	23.57271000	1.98915000
H	8.17312700	24.30986800	1.78603900
C	6.58060600	23.71155100	3.11184400
H	6.71337300	24.55314800	3.78542000
C	5.59299000	22.76280700	3.37342300
H	4.97691900	22.86613500	4.26479100
N	0.48838400	23.18343900	3.57947700
P	4.02963500	20.51342600	2.86931700
H	2.68059300	25.29993900	-4.35966500

TS$_{2a}$

Rh	2.63854200	21.71392600	3.14143400
N	0.97412600	22.87929300	3.81622400
C	0.98064700	24.02968200	4.48925300
H	0.06235900	17.55704300	1.14432200
C	-1.22935700	18.96240100	2.11915700
H	-2.11742200	18.34524600	2.01834100
C	-2.55176400	20.72014000	3.31531900
H	-3.44802200	20.11531100	3.20733200
C	-1.32194300	20.21701100	2.76453300
C	-2.61393900	21.92333800	3.95708600
H	-3.55482400	22.28738000	4.35966500
C	-1.39745300	23.94214200	4.84018500
H	-2.31565000	24.35387100	5.25044600
C	-0.14947600	21.00663100	2.88361500
C	-1.43317600	22.71769600	4.13999400
C	-0.21008600	22.22979800	3.61489500
C	-0.19205800	24.60254500	5.00776900
H	-0.13506300	25.54525000	5.54101400
C	-0.01000900	18.52771200	1.62694300
H	1.94623400	24.50555100	4.62654100
C	1.52215400	22.96261800	0.69640500
H	2.57766900	21.14151500	0.50850700
C	1.55483200	23.41916800	-0.69392600
C	2.06604100	21.81628200	1.18714800
H	0.99479700	23.62671100	1.37640600
C	1.00300500	24.68059200	-0.99603100
H	0.56806900	25.27333300	-0.19455400
C	1.09146000	20.59660100	2.30404200
C	1.55899600	24.42050500	-3.33236500
H	0.57604500	26.15278100	-2.50386700
C	2.10574900	23.16301300	-3.05313600
H	2.52973800	22.56585100	-3.85568700
C	2.10593600	22.66802800	-1.75352200
H	2.52586700	21.68408500	-1.56422800
C	1.00665800	25.17714900	-2.29716600
H	2.06480600	18.97693400	1.26530400
C	1.14167800	19.33328000	1.71131800
H	1.56103100	24.80289500	-4.34886900
H	4.42930500	22.78975000	8.23134500
C	4.49519700	22.32316000	7.25294700
C	4.52561800	20.92582600	7.14708200
C	4.56410700	23.11209600	6.10741900
C	4.61155500	20.31134300	5.90071100

H	4.48483300	20.31507000	8.04430500
H	4.56747000	24.19547800	6.18664600
C	4.66583900	22.50701200	4.84683500
C	4.69722800	21.09485700	4.73477100
H	4.62759000	19.22860700	5.82914700
H	4.82076000	23.12775400	3.96456100
P	4.56291000	20.45428200	3.01985600
C	6.02248900	21.07664000	2.11487200
C	4.64630300	18.63104700	3.04789900
C	5.85426900	21.67277900	0.85538100
C	7.31115900	20.98417900	2.67141400
C	5.71358800	17.93134700	2.46203700
C	3.60022900	17.91198200	3.65593400
H	4.86224400	21.77434700	0.42707900
C	6.96123900	22.15826000	0.15658300
C	8.41186600	21.47362400	1.96967400
H	7.45335100	20.53636900	3.65114300
H	6.52073900	18.46917300	1.97661200
C	5.74097100	16.53636700	2.50076600
C	3.64074800	16.51922400	3.70034200
H	2.75284800	18.43966200	4.08334200
H	6.82302000	22.62038200	-0.81636400
C	8.23784900	22.05848000	0.71172800
H	9.40403600	21.40238100	2.40564000
H	6.57004500	16.00379100	2.04427500
C	4.71064900	15.82980900	3.12299500
H	2.83280300	15.97255600	4.17784000
H	9.09733400	22.44091900	0.16891100
H	4.73698400	14.74444100	3.15303200

Int_{3a}

Rh	8.67772800	18.85750600	3.08903100
N	9.36668900	17.46337000	1.65226500
P	8.08070600	19.97489800	5.01880700
C	8.61524300	16.35710400	1.62159500
H	7.76473200	16.33935700	2.29798200
C	8.88465800	15.26179100	0.79784600
H	8.23282900	14.39539400	0.81351100
C	10.01182300	15.31822300	0.00398200
H	10.29034900	14.48052600	-0.62936600
C	10.82858600	16.46635100	0.01640100
C	12.03642500	16.50258900	-0.74847800
H	12.29141200	15.64122300	-1.35871300
C	12.85965500	17.57804700	-0.66951500

H	13.80099300	17.59384900	-1.21124800
C	12.51057800	18.73129800	0.10855200
C	11.26427900	18.79374300	0.81283900
C	10.45615000	17.58185600	0.83243000
C	13.41923800	19.81275200	0.15375000
H	14.36043200	19.72568000	-0.38124900
C	13.11711600	20.95133700	0.86817500
H	13.81988300	21.77736800	0.91906600
C	11.86961900	21.05251700	1.49857800
H	11.61072900	21.97891100	2.00381500
C	10.91857800	20.03004600	1.45458500
C	9.59686900	20.39549900	2.02014600
H	9.65725200	21.29948600	2.62036700
C	8.33096400	20.13352700	1.40322600
H	8.32547900	19.46497200	0.54409600
C	7.15940000	21.03287300	1.43457000
C	7.16117900	22.29261400	2.06321000
H	8.05443600	22.65383500	2.56318900
C	6.02855800	23.10394800	2.03627100
H	6.05434200	24.07658100	2.51936700
C	4.86885200	22.67925300	1.38151300
H	3.99038400	23.31743500	1.35739600
C	4.85370800	21.43624700	0.74338800
H	3.96293400	21.10229500	0.21890100
C	5.98812400	20.62680000	0.76615600
H	5.97396000	19.66443900	0.25950000
C	8.78086400	18.52493900	5.90684800
C	8.23696100	17.27623200	5.52830900
C	9.88849400	18.55451600	6.76934400
C	8.79472600	16.08567900	6.00608800
H	7.32754300	17.23919200	4.92707600
C	10.42909100	17.36324000	7.25155700
H	10.31981300	19.50429600	7.06866200
C	9.89106900	16.12993500	6.86669000
H	8.35930800	15.13188100	5.72231200
H	11.27425700	17.39543100	7.93317100
H	10.32121400	15.20829200	7.24722300
C	6.34063400	20.09114400	5.57378400
C	6.01086100	19.94866100	6.93406000
C	5.32185000	20.30742000	4.63344700
C	4.68113000	20.03077000	7.34361300
H	6.78982100	19.76980700	7.67011100
C	3.99168500	20.38886800	5.05153800
H	5.56252200	20.41048500	3.58093300

C	3.67076000	20.25165800	6.40256400
H	4.43274900	19.91857800	8.39501600
H	3.20905600	20.55789200	4.31781800
H	2.63508500	20.31254300	6.72446200
C	8.94447500	21.48048600	5.59610300
C	10.32067100	21.61858400	5.33273900
C	8.26576200	22.51956100	6.25132600
C	11.00439000	22.76342500	5.74096800
H	10.85748700	20.82793100	4.81512800
C	8.95403000	23.66818900	6.64748600
H	7.20372400	22.43454500	6.45515200
C	10.32147000	23.79098400	6.39765700
H	12.06896900	22.85422900	5.54473300
H	8.41879700	24.46533000	7.15515400
H	10.85407600	24.68414400	6.71104500

Int_{3b}

Rh	2.06243200	21.80784100	3.43986300
C	0.71140600	20.35752100	3.12455600
C	0.91046800	19.02204700	2.81675200
H	1.90374200	18.61405400	2.67346900
C	-0.19996300	18.15796100	2.65298300
H	-0.01555700	17.11107900	2.42663200
C	-1.50000300	18.61963100	2.75267700
H	-2.33866400	17.94397900	2.61009400
C	-1.74020400	19.98836200	3.00577400
C	-3.05703500	20.56680600	3.05354300
H	-3.91236500	19.90935400	2.92228800
C	-3.24916500	21.90672700	3.23382600
H	-4.25250200	22.32308900	3.24493500
C	-2.13322800	22.79565600	3.39991100
C	-0.83395000	22.23458900	3.40151000
C	-0.62096000	20.84213700	3.19213600
C	-2.23197900	24.19555500	3.54351100
H	-3.20920900	24.67097000	3.53446900
C	-1.08123000	24.95187500	3.68846200
H	-1.12481200	26.02949900	3.80038300
C	0.16665800	24.30824400	3.70723500
H	1.08381800	24.87135600	3.84827100
C	1.97292300	22.07742700	1.43548500
H	1.84725300	21.18876800	0.82125100
C	2.07246300	23.29229700	0.87054200
H	2.19570900	24.17125800	1.50761800
C	2.08279100	23.60679100	-0.57285100

C	2.41290500	24.91160500	-0.98054300
H	2.64742300	25.65954500	-0.22582800
C	2.44742800	25.26067100	-2.32996100
H	2.70629700	26.27586200	-2.61823300
C	2.14771700	24.30931400	-3.30606700
C	1.81069100	23.00877100	-2.91769900
H	1.56444500	22.26461600	-3.67055100
C	1.77738900	22.66038900	-1.57000200
H	1.49669200	21.64942600	-1.28861700
C	1.40407500	23.52058000	6.80573400
C	0.00260500	23.57424500	6.90991900
H	-0.59475900	22.69963900	6.67002000
C	-0.63717000	24.73469800	7.34472700
H	-1.72005400	24.74847500	7.43241600
C	0.10858500	25.86934600	7.67219300
H	-0.38914800	26.77155700	8.01611800
C	1.49882200	25.83059200	7.56528300
H	2.09137500	26.70183500	7.83062100
C	2.14301900	24.66606600	7.13811600
H	3.22634600	24.65168100	7.09904100
C	3.87283700	21.98669100	6.95480900
C	4.83096600	22.86705300	6.42298800
H	4.58827700	23.48366700	5.56384900
C	6.10535400	22.96734300	6.98099200
H	6.82429800	23.66313400	6.55748700
C	6.45369200	22.16973400	8.07241800
H	7.44467700	22.24525000	8.51090300
C	5.52270100	21.26888100	8.58957900
H	5.78749800	20.63438100	9.43081500
C	4.24310900	21.17549100	8.03755200
H	3.53862000	20.46658000	8.45618400
C	1.25024100	20.69752500	7.17297400
C	1.00777900	20.89661100	8.54571500
H	1.36362500	21.79758700	9.03599000
C	0.30422100	19.94778500	9.28551700
H	0.12783200	20.11444500	10.34441800
C	-0.17873700	18.79080300	8.66662300
H	-0.73161000	18.05530800	9.24415100
C	0.04209800	18.59118900	7.30460200
H	-0.34311600	17.70282000	6.81193300
C	0.75216900	19.53903100	6.56196400
H	0.89772400	19.38277800	5.50026700
C	4.79745500	19.61680600	4.42681500
C	3.94960900	18.67840900	5.03936700

H	2.91243900	18.59765000	4.73322000
C	4.42750300	17.83389200	6.04167500
H	3.75762900	17.11178200	6.49969300
C	5.75734000	17.92407200	6.45658800
H	6.13139200	17.26773000	7.23711700
C	6.60113200	18.86734800	5.86943900
H	7.63370100	18.95331400	6.19523400
C	6.12816500	19.70840800	4.86041500
H	6.79925700	20.43768300	4.42210200
C	4.25933700	19.51883400	1.57300000
C	4.36419400	18.12531400	1.70701300
H	4.40347800	17.66975500	2.69057100
C	4.44374000	17.30936900	0.57576700
H	4.53081300	16.23344400	0.69772600
C	4.42545100	17.87212900	-0.70034300
H	4.49124800	17.23614500	-1.57842100
C	4.33528200	19.25880000	-0.84326700
H	4.33312100	19.70876500	-1.83190900
C	4.25346700	20.07859400	0.28182400
H	4.19777100	21.15357300	0.15032200
C	5.39876100	21.91790200	2.67286700
C	6.64276600	21.57744700	2.11428500
H	6.86866500	20.54164400	1.88025700
C	7.58956200	22.56493300	1.84043400
H	8.54688100	22.28635700	1.40966400
C	7.30457400	23.90613100	2.10731300
H	8.04056300	24.67359500	1.88608100
C	6.06626400	24.25929700	2.64577400
H	5.83197300	25.30203300	2.84026300
C	5.12245300	23.26954200	2.92381900
H	4.15470600	23.56459000	3.32419800
N	0.28582900	22.98999900	3.57047800
P	2.18737200	21.94803300	6.18767500
P	4.12918100	20.63592900	3.04146700
H	2.16975800	24.57774500	-4.35835200

TS_{2b}

Rh	2.29665600	22.01799100	3.82987100
N	0.52319500	23.22391000	3.81296000
P	2.35303200	22.32317200	6.37671600
P	4.41454700	20.88314700	3.65445000
C	0.40742400	24.53126600	4.04686500
C	-1.26852600	18.95208600	2.59487800
C	-2.81869300	20.88696800	2.99112800

C	-1.50310800	20.30988400	2.90594100
C	-3.00669300	22.21580200	3.24494300
C	-1.98123600	24.46674400	3.74541000
C	-0.38416600	21.15260100	3.12544100
C	-1.88932900	23.08248300	3.49426400
C	-0.59320500	22.50945700	3.48820500
C	-0.82916600	25.19441800	3.99501900
C	0.03331000	18.49094600	2.47850500
C	1.62012700	22.82750300	0.98943300
C	1.82267900	22.98496800	-0.45445000
C	2.08810400	21.81305700	1.76427000
C	1.47439500	24.21343600	-1.05106100
C	0.95605800	20.69852200	2.94467100
C	2.16988900	23.41519300	-3.22237300
C	2.50923700	22.18457300	-2.65016200
C	2.33909700	21.96943700	-1.28600300
C	1.64918700	24.42922100	-2.41589500
C	1.14035700	19.35168200	2.62824700
C	3.98089100	22.36386400	7.26078800
C	4.26573200	21.58855500	8.39456800
C	4.97167600	23.23972800	6.78404500
C	5.49325600	21.71264500	9.04879500
C	6.19465300	23.36833600	7.44305300
C	6.45684400	22.60791500	8.58381000
C	1.34879200	21.02895700	7.23150900
C	1.05496000	21.12874100	8.60510900
C	0.82449400	19.95017100	6.50772300
C	0.28156600	20.15595500	9.23666300
C	0.04274400	18.97967000	7.14092600
C	-0.22429300	19.07668200	8.50601000
C	1.52719100	23.87350600	7.00425500
C	2.24615800	25.05158500	7.26191600
C	0.13407400	23.88725000	7.19078200
C	1.59234700	26.20583300	7.69944900
C	-0.51570300	25.03872500	7.63717200
C	0.21020600	26.20350700	7.89200800
C	5.69966200	22.17719800	3.37424100
C	7.04378500	21.84530800	3.12651700
C	5.31914700	23.52619700	3.31881000
C	7.98513000	22.84371900	2.87714600
C	6.25965700	24.52558400	3.05875000
C	7.59640900	24.18572100	2.84733100
C	4.94291100	19.84901300	5.08915100
C	4.03643200	18.88307000	5.55928400

C	6.20504500	19.94064400	5.69270700
C	4.39386100	18.01203000	6.58907600
C	6.55763400	19.07111000	6.72640400
C	5.65924700	18.10073200	7.17179800
C	4.75093800	19.75805900	2.21213700
C	5.01893300	20.31914500	0.94979600
C	4.74584100	18.35954600	2.33694700
C	5.27159100	19.50261300	-0.15296400
C	4.99631900	17.54548600	1.22945800
C	5.25832900	18.11267100	-0.01761900
H	0.21353900	17.44766400	2.23291400
H	-2.10907000	18.28381900	2.43139400
H	-3.67581200	20.24076200	2.82136500
H	-4.00797600	22.63652500	3.27036300
H	-2.95315600	24.95311800	3.73992400
H	-0.86647900	26.26097400	4.18656700
H	1.31647200	25.06269400	4.30601500
H	2.66430300	21.03345000	1.28084100
H	1.04389000	23.62965400	1.44272100
H	1.06511200	25.00620700	-0.42868500
H	1.37543200	25.38627200	-2.85115500
H	2.89974800	21.38609600	-3.27541600
H	2.59134300	21.00077000	-0.86583000
H	2.13516700	18.96041000	2.44440200
H	2.30269300	23.57737200	-4.28813800
H	3.54055700	20.87700900	8.77025300
H	4.79923300	23.82544500	5.88731900
H	5.69261600	21.10449500	9.92668800
H	6.94102000	24.05815400	7.05914800
H	7.40717400	22.70678500	9.10071300
H	1.41924100	21.97422200	9.18034700
H	1.01122300	19.87826700	5.44250200
H	0.06660700	20.24563500	10.29773200
H	-0.36113500	18.15468400	6.56078800
H	-0.83216000	18.32336800	8.99917700
H	3.32462900	25.07241400	7.15524500
H	-0.45003000	22.99242300	7.00186300
H	2.17115400	27.10199000	7.90524300
H	-1.59144600	25.02101100	7.78885700
H	-0.29487000	27.09812200	8.24497000
H	7.35464900	20.80539500	3.10743900
H	4.27382300	23.79530500	3.45592500
H	9.02029100	22.57189300	2.69166000
H	5.94555300	25.56447200	3.01157900

H	8.33003800	24.96032200	2.64328300
H	3.04740300	18.80436000	5.11932800
H	6.91192300	20.69810600	5.37689600
H	3.68100000	17.26952100	6.93621200
H	7.53842800	19.15775800	7.18503700
H	5.93996600	17.42279300	7.97279300
H	5.04559100	21.39688900	0.82419100
H	4.56969200	17.89524800	3.30083700
H	5.48386500	19.95736200	-1.11638800
H	4.99709700	16.46582300	1.34967500
H	5.45896900	17.47786100	-0.87579700

Product

Rh	9.18516900	18.46398300	3.04421300
N	9.46141400	17.41634600	1.18973700
P	8.44042500	19.53459700	5.05478500
P	10.45129800	16.70818500	4.12714800
C	8.61623300	16.39838600	0.99973500
H	7.91493900	16.20767600	1.80571300
C	8.63474800	15.58480600	-0.13792100
H	7.91056600	14.78414100	-0.24215300
C	9.63308700	15.79309000	-1.06843400
H	9.73474300	15.14442100	-1.93427400
C	10.54786900	16.84938700	-0.89024300
C	11.65436200	17.03410600	-1.77892800
H	11.77076100	16.34891500	-2.61361300
C	12.56414200	18.01488000	-1.54238500
H	13.43782100	18.12221600	-2.17916900
C	12.37857700	18.96702800	-0.48416600
C	11.22302700	18.89849400	0.35371800
C	10.38189400	17.72310500	0.22807800
C	13.32950500	19.99692800	-0.30274500
H	14.21036200	20.01607600	-0.93807900
C	13.13149400	20.96563200	0.65928000
H	13.86430700	21.75315300	0.80823600
C	11.94123100	20.97059900	1.40137500
H	11.74693000	21.79729700	2.07936900
C	10.95544700	19.99132000	1.24249200
C	9.66721400	20.27925200	1.91578100
H	9.74587200	21.12244100	2.59442700
C	8.38239400	20.00856400	1.42315400
H	8.29387100	19.32546400	0.58509800
C	7.18242700	20.85079700	1.57905600
C	7.19409500	22.13290900	2.15753700

H	8.11741800	22.54646800	2.54748800
C	6.03376600	22.90379200	2.20626900
H	6.06974000	23.89421900	2.65149400
C	4.83751300	22.42119500	1.67083500
H	3.93829400	23.02956200	1.70338400
C	4.81316500	21.15954000	1.07120600
H	3.89408800	20.78121400	0.63227000
C	5.97179000	20.38941300	1.02395500
H	5.94906200	19.41318400	0.54336000
C	8.81271500	21.34450000	5.17359700
C	10.14571900	21.75746200	4.99909400
H	10.91310600	21.01946000	4.78260000
C	10.49902200	23.10271300	5.11658700
H	11.53582600	23.40245400	4.98972400
C	9.52188700	24.05999800	5.40087000
H	9.79414400	25.10762400	5.49127300
C	8.19509900	23.66184800	5.56761400
H	7.42832800	24.39978700	5.78637000
C	7.84055600	22.31488900	5.45395600
H	6.80185300	22.02950000	5.57311800
C	8.92591000	18.94878600	6.75680500
C	9.82418300	19.65370800	7.57110800
H	10.28592100	20.56816700	7.21885300
C	10.12260600	19.20206900	8.85863000
H	10.81419100	19.76947000	9.47499500
C	9.53131400	18.04070300	9.35493300
H	9.75804200	17.69707300	10.36032700
C	8.63721200	17.32916300	8.55285400
H	8.16093200	16.42786800	8.92876000
C	8.33574300	17.78029300	7.26828300
H	7.61650100	17.22669900	6.67651000
C	6.60281100	19.37539400	5.17858300
C	5.91221400	19.74707400	6.34751600
H	6.45626300	20.14430900	7.19882300
C	4.52945100	19.59255500	6.43240200
H	4.01024100	19.88758000	7.33987700
C	3.81541700	19.05062200	5.35969500
H	2.73856800	18.92591300	5.43069600
C	4.49050900	18.66753200	4.20145000
H	3.94215000	18.24671900	3.36341300
C	5.87525600	18.83096300	4.11140300
H	6.39736200	18.54181200	3.20485200
C	11.63080400	17.32891000	5.40538200
C	12.34035500	18.50526700	5.10364100

H	12.12989900	19.03819000	4.17943200
C	13.31812200	18.99042000	5.97264200
H	13.86756300	19.89261300	5.71745300
C	13.58692800	18.31943600	7.16737200
H	14.34657800	18.69599700	7.84644900
C	12.86797500	17.16775600	7.48762900
H	13.05944200	16.64813100	8.42215800
C	11.89831000	16.67168600	6.61329300
H	11.34492100	15.78237000	6.89048600
C	9.48430300	15.31609600	4.85355100
C	8.08304600	15.38606800	4.82993700
H	7.59957100	16.27425600	4.42994200
C	7.30475000	14.33453400	5.32062300
H	6.22103100	14.40683100	5.29477700
C	7.92105400	13.19676000	5.84259400
H	7.31923300	12.37791500	6.22638800
C	9.31589100	13.10744500	5.85909700
H	9.80014700	12.21798600	6.25203400
C	10.09267900	14.15274100	5.35968700
H	11.17344600	14.05163100	5.34535500
C	11.58904300	15.80113800	2.96492000
C	11.16370800	14.62149800	2.33099500
H	10.18414000	14.20822100	2.54533900
C	11.99999800	13.94866700	1.43857100
H	11.65524000	13.03039100	0.97084500
C	13.27464500	14.44286000	1.15931100
H	13.92903700	13.91370500	0.47239400
C	13.70582400	15.61690500	1.77839300
H	14.69968300	16.00712600	1.57771500
C	12.87149500	16.29151800	2.67084000
H	13.23962800	17.19024700	3.15209800