Supporting Information for

Synthesis and Energetics of Tp′Rh(P(OMe)$_3$)(R)H: A Systematic Investigation of Ligand Effects on C-H Activation at Rhodium

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Experimental Procedures

EXPERIMENTAL SECTION

General Procedure. All operations and routine manipulations were performed under a nitrogen atmosphere, either on a high-vacuum line using modified Schlenk techniques or in a Vacuum Atmospheres Corp. Dri-Lab. Benzene-d_6, THF-d_8 and cyclohexane-d_{12} were dried over CaH_2, and vacuum-distilled prior to use. All hydrocarbons used in reactions are either taken from an Innovative Technologies PS-MD-6 Solvent System or stirred over appropriate drying reagents, distilled, and transferred prior to use. Trimethylphosphite was purchased from Alfa Aesar and used without further purification. All ^1H, $^{13}C\{^1H\}$, $^{19}F\{^1H\}$ and $^{31}P\{^1H\}$ NMR spectra were recorded on Bruker Avance 400 or 500 MHz NMR spectrometers. All ^1H chemical shifts are reported in ppm (δ) relative to the chemical shift of residual solvent (benzene-d_6, δ 7.16; cyclohexane-d_{12}, δ 1.40; THF-d_8, δ 3.58) or $CDCl_3$ (δ 7.26). $^{13}C\{^1H\}$ were referenced to benzene-d_6 (δ 128.0), THF-d_8 (δ 67.4), cyclohexane-d_{12} (δ 27.2) or $CDCl_3$ (δ 77.2). ^{19}F NMR spectra were referenced to external $C_6F_5CF_3$ in cyclohexane-d_{12} (δ 0.0). $^{31}P\{^1H\}$ NMR spectra were referenced to external H_3PO_4 (δ 0.0). IR spectra were recorded in the solid state on a Nicolet 4700 FTIR spectrometer between 4000 and 600 cm^{-1}. All photolysis experiments were carried out using a water-filtered 200-W Hg-Xe lamp, which was fitted with a 270-370 nm band pass filter. Silica gel was heated overnight at 200 °C and then stored under nitrogen. A Bruker-AXS SMART platform diffractometer equipped with an APEX II CCD detector was used for X-ray crystal structure determination. Elemental analyses were performed by the University of Rochester using a Perkin-Elmer 2400 series II elemental analyzer in CHN mode. All kinetic plots and least-squares error analysis were done using Microsoft Excel.

For Tp'Rh[P(OMe)$_3$]Cl$_2$ (1). To a suspension of 100 mg (0.195 mmol) of Tp'Rh(CH_3CN)Cl_2 in 20 mL of C_6H_6 was added 34 uL (0.288 mmol) of trimethyl phosphite all at once. The reaction mixture was heated to reflux. A clear yellow-orange solution was observed within 10 min. After refluxing for 20 min, the solvent was evaporated and the crude product was washed with cold hexane to give light orange powders (100 mg, 86%). The product is air-stable and large orange crystals can be obtained from a CH_2Cl_2 solution layered with hexanes. ^1H NMR (400 MHz, C_6D_6): δ 2.11 (s, 6H, 2×pzCH_3), 2.13 (s, 3 H, pzCH_3), 2.79 (s, 6H, 2×pzCH_3), 3.22 (d, $^3J_{PH}$ = 11.4 Hz, 9H, P(OMe)$_3$), 3.25 (s, 3H, pzCH_3), 5.48 (s, 2H, 2×pzH), 5.55 (d, $^5J_{PC}$ = 3.1 Hz, 1H, pzH). $^{13}C\{^1H\}$ NMR (500 MHz, C_6D_6): δ 12.30 (s, pzCH_3), 12.96 (s, 2×pzCH_3), 15.40 (s, pzCH_3), 16.09 (s, 2×pzCH_3), 52.61 (d, $^2J_{PC}$ = 4.8 Hz, P(OCH_3)$_3$), 108.74 (d, $^4J_{PC}$ = 7.8 Hz, pzCH), 109.94 (s, 2×pzCH), 142.29 (d, $^3J_{PC}$ = 5.6 Hz, pzCq), 144.44 (s, 2×pzCq), 154.71 (d, $^3J_{PC}$ = 7.2 Hz, pzCq), 156.24 (s, 2×pzCq). $^{31}P\{^1H\}$ NMR (400 MHz, C_6D_6): δ 100.59 (d, $^1J_{RhP}$ = 161.9 Hz). Anal. Calcd for $C_{18}H_{31}BCl_2N_6O_3PRh$: C, 36.33; H, 5.25; N, 14.12. Found: C, 36.36; H, 5.28; N, 14.01.

For Tp'Rh[P(OMe)$_3$]H$_2$ (2). To a suspension of 100 mg (0.168 mmol) of **1** in 40 mL of C_6H_6 was added 56 mg (0.251 mmol) of Cp_2ZrH_2. The suspension was stirred for 1 h, giving a clear golden-brown solution. The product was purified by flash chromatography through silica gel in a frit funnel using 9:1 hexanes:THF as the eluent. Evaporation gave 88 mg (99%) of **2** as an white powder. ^1H NMR (400 MHz, C_6D_6): δ – 15.96 (dd, $^1J_{RhH}$ = 19.4 Hz, $^2J_{PH}$ = 26.2 Hz, 2H, RhH_2), 2.20 (s, 3H, pzCH_3), 2.33 (s, 6H, 2×pzCH_3), 2.40 (s, 6H, 2×pzCH_3), 2.44 (s, 3H, pzCH_3), 3.26 (d, $^3J_{PH}$ = 12.2 Hz, 9H, P(OMe)$_3$), 5.59 (s, 1H, pzH), 5.75 (s, 2H, 2×pzH). $^{13}C\{^1H\}$ NMR (500 MHz, C_6D_6): 12.69 (s, pzCH_3), 12.94 (s, 2×pzCH_3), 15.11 (s, 2×pzCH_3), 16.79 (s, pzCH_3), 50.76 (s, P(OCH_3)$_3$), 105.27 (d, $^4J_{PC}$ = 4.8 Hz, pzCH), 106.06 (s, 2×pzCH), 143.13 (d, $^3J_{PC}$ = 4.1 Hz, pzCq), 143.81 (s, 2×pzCq), 149.77 (d, $^3J_{PC}$ = 2.9 Hz, pzCq), 151.07 (s, 2×pzCq). $^{31}P\{^1H\}$ NMR (400 MHz, C_6D_6): δ 153.83 (d, $^1J_{RhP}$ = 228.8 Hz). IR (cm^{-1}): 2512 (B-H), 2060 (Rh-H). UV-Vis (C_6H_6), λ, nm (ε, M^{-1} cm^{-1}): 282 (1751) Anal. Calcd for $C_{18}H_{33}BN_6O_3PRh \cdot THF_{0.35}$: C, 42.26; H, 6.54; N, 15.24. Found: C, 42.26; H, 6.47; N, 15.41. (see NMR Fig.S-4 for THF).

For Tp'Rh[P(OMe)$_3$](CH$_3$)Cl (3). To a stirred solution of 80 mg (0.134 mmol) of **1** in 10 mL

THF was added dropwise 49 μL (0.147 mmol) of 3 M CH_3MgCl solution in THF. The color changed from orange to light yellow upon addition of the Grignard reagent. After stirring for 20 min, the reaction was quenched with a saturated solution of NH_4Cl (aq) until the reaction mixture was clear again. The volatiles were removed under vacuum. The solids were mixed with 5 mL of methylene chloride and filtered through celite to give a yellow solution, which was layered with hexane for recrystallization (73 mg, 94%). ^{1}H NMR (500 MHz, C_6D_6): δ 2.15 (s, 3H, pzCH_3), 2.16 (s, 3H, pzCH_3), 2.29 (s, 3H, pzCH_3), 2.34 (s, 3H, pzCH_3), 2.46 (t, $^2J_{RhH}$ = $^3J_{PH}$ = 2.0 Hz, 3H, CH_3), 2.82 (s, 3H, pzCH_3), 2.91 (s, 3H, pzCH_3), 3.15 (d, $^2J_{PH}$ = 11.0 Hz, 9H, PMe_3), 5.52 (s, 1H, pzH), 5.53 (d, $^5J_{PH}$ = 2.4 Hz, 1H, pzH), 5.72 (s, 1H, pzH). ^{13}C{^{1}H} NMR (500 MHz, C_6D_6): δ 0.26 (dd, $^1J_{RhC}$ = 10.5 Hz, $^2J_{PC}$ = 19.3 Hz, $RhCH_3$), 12.68 (s, pzCH_3), 12.82 (s, pzCH_3), 13.32 (s, pzCH_3), 14.33 (s, pzCH_3), 14.66 (s, pzCH_3), 15.05 (s, pzCH_3), 51.84 (d, $^2J_{PC}$ = 4.8 Hz, $P(OCH_3)_3$), 108.10 (s, pzCH), 108.36 (d, $^4J_{PC}$ = 6.1 Hz, pzCH), 109.02 (s, pzCH), 142.41 (d, $^3J_{PC}$ = 4.6 Hz, pzCq), 143.22 (s, pzCq), 144.23 (s, pzCq), 152.42 (d, $^3J_{PC}$ = 6.1 Hz, pzCq), 153.47 (s, pzCq), 153.89 (s, pzCq). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 116.05 (d, $^1J_{RhP}$ = 199.1 Hz). Anal. Calcd for $C_{19}H_{34}BClN_6O_3PRh$: C, 39.71; H, 5.96; N, 14.62. Found: C, 40.01; H, 6.08; N, 14.46.

For Tp'Rh[P(OMe)$_3$](CH$_3$)H (4). To a yellow solution of 10 mg (0.017 mmol) of **3** in 0.5 mL THF was added 6 mg (0. 027 mmol) of Cp_2ZrH_2. The suspension was stirred for 1 h and changed from light yellow to white. A white crystalline solid (79%, NMR yield) was then isolated from the zirconium complexes by flash chromatography through silica gel in a pipette with a glass wool plug using 5:1 hexanes:THF as the eluent. ^{1}H NMR (400 MHz, C_6D_6): δ – 16.31 (dd, $^1J_{RhH}$ = 22.3 Hz, $^2J_{PH}$ = 24.3 Hz, 1H, RhH), 1.15 (d, $^2J_{RhH}$ = 2.0 Hz, 3H, CH_3), 2.20 (s, 3H, pzCH_3), 2.27 (s, 3H, pzCH_3), 2.33 (s, 3H, pzCH_3), 2.34 (s, 3H, pzCH_3), 2.54 (s, 3H, pzCH_3), 2.57 (s, 3H, pzCH_3), 3.22 (d, $^3J_{PH}$ = 11.9 Hz, 9H, $P(OCH_3)_3$), 5.64 (s, 1H, pzH), 5.65 (s, 1H, pzH), 5.80 (s, 1H, pzH). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 146.00 (d, $^1J_{RhP}$ = 236.9 Hz). Other hydride resonances are attributable to Tp'Rh[P(OMe)$_3$](Cl)H (10%), Tp'Rh(P(OMe)$_3$)(furanyl)H (10%) and Tp'Rh[P(OMe)$_3$]H_2 (1%) (See SI for spectra). For Tp'Rh[P(OMe)$_3$](Cl)H (**5**). ^{1}H NMR (500 MHz, C_6D_6): δ -14.87 (dd, $^1J_{RhH}$ = 11.3 Hz, $^2J_{PH}$ = 23.4 Hz, 1H, RhH). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 124.84 (d, $^1J_{RhP}$ = 191.3 Hz).

Preparation of Tp'Rh[P(OMe)$_3$](R)H (6)-general procedure. 50 mg (0.087 mmol) of **3** was used for *in situ* preparation of **4**, which was then dissolved in 0.6 mL of corresponding RH and transferred to a resealable 5 mm NMR tube. After the reaction is complete at room temperature, the solvent was removed in vacuo and the resulting residue was dissolved in C_6D_6. For activation of fluoromethane, dimethyl ether, and 3,3-trifluoro-1-propyne, **4** was dissolved in 1 mL of pentane and transferred to a high pressure NMR tube, followed by pressurization with 50 psi of the corresponding gas. The yield is almost quantitative for each reaction. ^{1}H, ^{13}C{^{1}H}, ^{19}F and ^{31}P{^{1}H} NMR spectra were collected (See SI for spectra).

For Tp'Rh[P(OMe)$_3$](Ph)H (6a). Reaction was complete after standing overnight. The volatiles were removed to give white solids, which were dissolved in C_6D_6. **6a** can also be generated from photolysis of 10 mg of **2** in 0.6 mL of benzene at room temperature for 6 h. ^{1}H NMR (400 MHz, C_6D_6): δ – 14.88 (dd, $^1J_{RhH}$ = 20.5 Hz, $^2J_{PH}$ = 23.1 Hz, 1H, RhH), 1.78 (s, 3H, pzCH_3), 2.16 (s, 3H, pzCH_3), 2.27 (s, 3H, pzCH_3), 2.28 (s, 3H, pzCH_3), 2.33 (s, 3H, pzCH_3), 2.40 (s, 3H, pzCH_3), 3.16 (d, $^3J_{PH}$ = 11.3 Hz, 9H, $P(OCH_3)_3$), 5.51 (s, 1H, pzH), 5.66 (s, 1H, pzH), 5.90 (s, 1H, pzH), 6.84 (br, 1H, arylH), 7.00 (t, $^3J_{HH}$ = 7.1 Hz, 1H, arylH), 7.96(br, 1H, arylH), other two aryH's are missing due to overlapping with the benzene peak. ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 138.16 (d, $^1J_{RhP}$ = 235.3 Hz).

For Tp'Rh[P(OMe)$_3$](C_6D_5)D (6a-*d*$_6$). The resulting solution of **6a** from 10 mg of **3** was dissolved in C_6D_6 and heated at 70 °C for 17 h. The ^{1}H NMR spectrum was identical to that of **6a** except that the hydride signal had almost disappeared. A new set of resonances was observed for **6a-*d*$_6$** in the ^{31}P{^{1}H} NMR spectrum along with a small quantity of residual **6a** (16%). ^{31}P{^{1}H}

NMR (400 MHz, C_6D_6): δ 138.32 (d, $^1J_{RhP}$ = 235.7 Hz).

For Tp'Rh[P(OMe)$_3$][CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$]H (6b). Reaction was complete after 2 d. ^{1}H NMR (400 MHz, C_6D_6): δ – 16.18 (t, $^1J_{RhH}$ = $^2J_{PH}$ = 21.5 Hz, 1H, RhH), 2.20 (s, 3H, pzCH$_3$), 2.21 (s, 3H, pzCH$_3$), 2.27 (s, 6H, 2×arylCH$_3$), 2.28 (s, 3H, pzCH$_3$), 2.37 (s, 3H, pzCH$_3$), 2.68 (s, 3H, pzCH$_3$), 2.69 (s, 3H, pzCH$_3$), 3.08 (d, $^3J_{PH}$ = 11.7 Hz, 9H, P(OCH$_3$)$_3$), 3.42 (br d, 1H, $^2J_{HH}$ = 10.3 Hz, RhCH$_2$), 3.77 (dd, 1H, $^2J_{HH}$ = 10.3 Hz, $^2J_{RhH}$ = 3.0 Hz, RhCH$_2$), 5.59 (s, 1H, pzH), 5.61 (s, 1H, pzH), 5.84 (s, 1H, pzH), 6.70 (s, 1H, arylH), 7.22 (s, 2H, 2×arylH). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 144.12 (d, $^1J_{RhP}$ = 237.3 Hz).

For Tp'Rh[P(OMe)$_3$][CH=CHC(CH$_3$)$_3$]H (6c). Reaction of **3** and Cp_2ZrH_2 in *t*-butyl ethylene gave **4** as the initial product, which continued to react with the solvent to form **6c** after 2 d in this one-pot reaction. ^{1}H NMR (400 MHz, C_6D_6): δ – 15.43 (dd, $^1J_{RhH}$ = $^2J_{PH}$ = 22.5 Hz, 1H, RhH), 1.15 (s, 9H, t-Bu), 2.17 (s, 3H, pzCH$_3$), 2.25 (s, 3H, pzCH$_3$), 2.30 (s, 3H, pzCH$_3$), 2.33 (s, 3H, pzCH$_3$), 2.55 (s, 3H, pzCH$_3$), 2.57 (s, 3H, pzCH$_3$), 3.24 (d, $^3J_{PH}$ = 11.7 Hz, 9H, P(OCH$_3$)$_3$), 5.31 (d, $^3J_{HH}$ = 15.7 Hz, 1H, RhCHC<u>H</u>), 5.64 (s, 1H, pzH), 5.68 (s, 1H, pzH), 5.89 (s, 1H, pzH), 6.87 (dd, $^3J_{HH}$ = 15.7 Hz, $^2J_{RhH}$ = 7.2 Hz, 1H, RhCH). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 142.23 (d, $^1J_{RhP}$ = 234.3 Hz).

For Tp'Rh[P(OMe)$_3$][CH$_2$OC(CH$_3$)$_3$]H (6d). The synthesis of **6d** was identical to that of **6c** except that *t*-butyl methyl ether was used as the solvent. ^{1}H NMR (400 MHz, C_6D_6): δ – 16.10 (dd, $^1J_{RhH}$ = 21.3 Hz, $^2J_{PH}$ = 23.0 Hz, 1H, RhH), 1.24 (s, 9H, *t*Bu), 2.20 (s, 3H, pzCH$_3$), 2.25 (s, 3H, pzCH$_3$), 2.31 (s, 3H, pzCH$_3$), 2.32 (s, 3H, pzCH$_3$), 2.62(s, 3H, pzCH$_3$), 2.78 (s, 3H, pzCH$_3$), 3.39 (d, $^2J_{PH}$ = 11.9 Hz, 9H, P(OCH$_3$)$_3$), 4.49 (m, 1H, RhCH$_2$), 4.90 (m, 1H, RhCH$_2$), 5.64 (s, 1H, pzH), 5.71 (s, 1H, pzH), 5.78 (s, 1H, pzH). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 145.11 (d, $^1J_{RhP}$ = 245.3 Hz).

For Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)H (6e). The synthesis of **6e** was identical to that of **6c** except that 2-butyne was used as the solvent and the reaction was complete after 3 d. ^{1}H NMR (400 MHz, C_6D_6): δ – 15.95 (dd, $^1J_{RhH}$ = $^2J_{PH}$ = 21.1 Hz, 1H, RhH), 1.61 (br, 3H, CH$_3$), 2.18 (s, 3H, pzCH$_3$), 2.22 (s, 3H, pzCH$_3$), 2.30 (s, 6H, 2×pzCH$_3$), 2.41 (dt, $^1J_{HH}$ = 13.1 Hz, $^2J_{RhH}$ = $^3J_{PH}$ = 2.9 Hz, 2H, RhCH$_2$), 2.55 (s, 3H, pzCH$_3$), 2.85 (s, 3H, pzCH$_3$), 3.36 (d, $^3J_{PH}$ = 11.8 Hz, 9H, P(OCH$_3$)$_3$), 5.62 (s, 1H, pzH), 5.66 (s, 1H, pzH), 5.75 (s, 1H, pzH). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 142.41 (d, $^1J_{RhP}$ = 234.7 Hz).

For Tp'Rh[P(OMe)$_3$][CH$_2$C(O)CH$_3$]H (6f). The synthesis of **6f** was identical to that of **6c** except that acetone was used as the solvent and the reaction was complete after standing overnight. ^{1}H NMR (400 MHz, C_6D_6): δ – 15.77 (dd, $^1J_{RhH}$ = $^2J_{PH}$ = 20.4 Hz, 1H, RhH), 1.86 (s, 3H, CH$_3$), 2.15 (s, 3H, pzCH$_3$), 2.17 (s, 3H, pzCH$_3$), 2.19 (s, 3H, pzCH$_3$), 2.32 (s, 3H, pzCH$_3$), 2.58 (s, 3H, pzCH$_3$), 2.71 (s, 3H, pzCH$_3$), 2.79 (m, 1H, RhCH$_2$), 2.95 (m, 1H, RhCH$_2$), 3.22 (d, $^3J_{PH}$ = 11.8 Hz, 9H, P(OCH$_3$)$_3$), 5.54 (s, 1H, pzH), 5.62 (s, 1H, pzH), 5.84 (s, 1H, pzH). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 141.13 (d, $^1J_{RhP}$ = 226.4 Hz).

For Tp'Rh[P(OMe)$_3$](CH$_2$F)H (6g). Reaction was complete after two weeks. ^{1}H NMR (400 MHz, C_6D_6): δ – 15.83 (dt, $^1J_{RhH}$ = $^2J_{PH}$ = 22.4 Hz, $^3J_{FH}$ = 15.6 Hz, 1H, RhH), 2.17 (s, 3H, pzCH$_3$), 2.23 (s, 3H, pzCH$_3$), 2.27 (s, 3H, pzCH$_3$), 2.28 (s, 3H, pzCH$_3$), 2.49 (s, 3H, pzCH$_3$), 2.75 (s, 3H, pzCH$_3$), 3.30 (d, $^3J_{PH}$ = 12.0 Hz, 9H, P(OCH$_3$)$_3$), 5.62 (s, 1H, pzH), 5.66 (s, 1H, pzH), 5.71 (s, 1H, pzH), 6.32 (dq, $^2J_{RhH}$ = $^3J_{PH}$ = $^2J_{HH}$ = 3.1 Hz, $^2J_{FH}$ = 49.5 Hz, 1H, RhCH$_2$), 6.70 (ddt, $^2J_{RhH}$ = $^2J_{HH}$ = 2.9 Hz, $^3J_{PH}$ = 8.3 Hz, $^2J_{FH}$ = 49.8 Hz, 1H, RhCH$_2$). ^{19}F NMR (400 MHz, C_6D_6): -137.72 (m). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 144.29 (dd, $^1J_{RhP}$ = 238.5 Hz, $^3J_{FP}$ = 7.7 Hz). As the commercial CH_3F contains 16% impurity of dimethyl ether, a second hydride species was co-synthesized as Tp'Rh[P(OMe)$_3$](CH$_2$OMe)H **(6h) :** ^{1}H NMR (400 MHz, C_6D_6): δ –16.06 (t, $^1J_{RhH}$ = $^2J_{PH}$ = 22.1 Hz, 1H, RhH), ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 145.06 (d, $^1J_{RhP}$ = 243.1 Hz).

For Tp'Rh[P(OMe)$_3$][C≡CC(CH$_3$)$_3$]H (6i). Reaction was not complete after a week at ambient temperature. The solvent was removed and the residue was dissolved in 0.5 mL of C_6D_6. The solution was heated at 140 °C for 0.5 h. White crystals of **6h** were grown from 1:1 hexane: ether solution at room temperature. ^{1}H NMR (500 MHz, C_6D_6): δ –15.05 (dd, $^1J_{RhH}$ = 19.4 Hz, $^2J_{PH}$ = 24.7 Hz, 1H, RhH), 1.40 (s, 9H, C(CH$_3$)$_3$), 2.12 (s, 3H, pzCH$_3$), 2.23 (s, 3H, pzCH$_3$), 2.28 (s, 3H, pzCH$_3$), 2.32 (s, 3H, pzCH$_3$), 2.87 (s, 3H, pzCH$_3$), 2.88 (s, 3H, pzCH$_3$), 3.32 (d, $^3J_{PH}$ = 11.9 Hz, 9H, PMe$_3$), 5.54 (s, 1H, pzH), 5.60 (s, 1H, pzH), 5.79 (s, 1H, pzH). ^{13}C{^{1}H} NMR (500 MHz, C_6D_6): δ 12.61 (s, pzCH$_3$), 12.86 (s, pzCH$_3$), 12.89 (s, pzCH$_3$), 14.76 (s, pzCH$_3$), 15.58 (s, pzCH$_3$), 16.45 (s, pzCH$_3$), 29.83 (s, C(CH$_3$)$_3$), 33.01 (s, C(CH$_3$)$_3$), 51.41 (d, $^2J_{PC}$ = 2.1 Hz, P(OCH$_3$)$_3$), 74.57 (dd, $^1J_{RhC}$ = 30.0 Hz, $^2J_{PC}$ = 43.7 Hz, Rh-CC), 106.12 (d, $^4J_{PC}$ = 5.6 Hz, pzCH), 106.46 (s, pzCH), 107.12 (s, pzCH), 112.51 (d, $^2J_{RhC}$ = 9.8 Hz, Rh-CC), 142.88 (d, $^3J_{PC}$ = 4.4 Hz, pzCq), 143.48 (s, pzCq), 143.96 (s, pzCq), 151.26 (s, pzCq), 151.36 (d, $^3J_{PC}$ = 4.3 Hz, pzCq), 153.44 (s, pzCq). ^{31}P{^{1}H} NMR (400MHz, C_6D_6): δ 134.43 (d, $^1J_{RhP}$ = 202.2 Hz). IR (cm^{-1}): *ν* 1975, 2028, 2160 (C≡C). Anal. Calcd for $C_{24}H_{41}BN_6PRh$: C, 47.54; H, 6.82; N, 13.86. Found: C, 47.61; H, 6.70; N, 13.81.

For Tp'Rh[P(OMe)$_3$][C≡CSi(CH$_3$)$_3$]H (6j). The synthesis was identical to that of **6i** except that **4** was dissolved in 0.6 mL of ethynyltrimethylsilane. ^{1}H NMR (500MHz, C_6D_6): δ -14.69 (dd, $^1J_{RhH}$ = 19.5 Hz, $^2J_{PH}$ = 24.0 Hz, 1H, RhH), 0.33 (s, 9H, Si(CH$_3$)$_3$), 2.10 (s, 3H, pzCH$_3$), 2.21 (s, 3H, pzCH$_3$),2.25 (s, 3H, pzCH$_3$), 2.31 (s, 3H, pzCH$_3$), 2.86 (s, 6H, 2×pzCH$_3$), 3.31 (d, $^3J_{PH}$ = 11.9 Hz, 9H, P(OCH$_3$)$_3$), 5.50 (s, 1H, pzH), 5.58 (s, 1H, pzH), 5.76 (s, 1H, pzH). ^{13}C{^{1}H} NMR (500MHz, C_6D_6): δ 1.74 (s, Si(CH$_3$)$_3$) 12.60 (s, pzCH$_3$), 12.83 (s, pzCH$_3$), 12.87 (s, pzCH$_3$), 14.79 (s, pzCH$_3$), 15.52 (s, pzCH$_3$), 16.63 (s, pzCH$_3$), 51.63 (d, $^2J_{PC}$ = 2.6 Hz, P(OCH$_3$)$_3$), 106.25 (d, $^4J_{PC}$ = 5.5 Hz, pzCH), 106.55 (s, pzCH), 107.27 (pzCH), 111.31 (d, $^2J_{RhC}$ = 8.4 Hz, Rh-CC), 119.60 (dd, $^1J_{RhC}$ = 28.4 Hz, $^2J_{PC}$ = 41.4 Hz, Rh-CC), 143.01 (d, $^3J_{PC}$ = 4.5 Hz, pzCq), 143.61 (s, pzCq), 144.15 (s, pzCq), 151.37 (s, pzCq), 151.49 (d, $^3J_{PC}$ = 4.2 Hz, pzCq), 153.61 (s, pzCq). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 133.18 (d, $^1J_{RhP}$ = 200.4 Hz). IR (cm^{-1}): *ν* 1976, 2044, 2160 (C≡C). Anal. Calcd for $C_{23}H_{41}BN_6PRh$: C, 44.39; H, 6.64; N, 13.50. Found: C, 44.51; H, 6.72; N, 13.50.

For Tp'Rh[P(OMe)$_3$](C≡C*n*-hexyl)H (6k). The synthesis was identical to that of **6i** except that **4** was dissolved in 0.6 mL of 1-octyne. ^{1}H NMR (500 MHz, C_6D_6): δ -14.97 (dd, $^1J_{RhH}$ = 19.4 Hz, $^2J_{PH}$ = 24.5 Hz, 1H, RhH), 0.89 (t, 3H, CH$_2$(CH$_2$)$_4$CH$_3$), 1.29 (quintet, 4H, hexyl), 1.52 (m, 2H, hexyl), 1.64 (quintet, 2H, hexyl), 2.14 (s, 3H, pzCH$_3$), 2.23 (s, 3H, pzCH$_3$), 2.30 (s, 3H, pzCH$_3$), 2.33 (s, 3H, pzCH$_3$), 2.56 (t, 2H, CH$_2$(CH$_2$)$_4$CH$_3$), 2.90 (s, 6H, 2×pzCH$_3$), 3.34 (d, $^2J_{PH}$ = 11.9 Hz, 9H, PMe$_3$), 5.56 (s, 1H, pzH), 5.61 (s, 1H, pzH), 5.79 (s, 1H, pzH). ^{13}C{^{1}H} NMR (500 MHz, C_6D_6): δ 12.64 (s, pzCH$_3$), 12.86 (s, pzCH$_3$), 12.92 (s, pzCH$_3$), 14.42 (s, CH$_2$(CH$_2$)$_4$CH$_3$), 14.75 (s, pzCH$_3$), 15.59 (s, pzCH$_3$), 16.48 (s, pzCH$_3$), 22.50 (s, CH$_2$(CH$_2$)$_4$CH$_3$), 23.22 (s, hexyl), 29.23 (s, hexyl), 31.38 (s, hexyl), 32.18 (s, hexyl), 51.47 (d, $^3J_{PC}$ = 2.2 Hz, P(OCH$_3$)$_3$), 76.40 (dd, $^1J_{RhC}$ = 29.6 Hz, $^2J_{PC}$ = 43.8 Hz, Rh-CC), 103.25 (d, $^2J_{RhC}$ = 9.9 Hz, Rh-CC), 106.12 (d, $^4J_{PC}$ = 5.6 Hz, pzCH), 106.49 (s, pzCH), 107.11 (s, pzCH), 142.85 (d, $^3J_{PC}$ = 4.7 Hz, pzCq), 143.45 (s, pzCq), 144.05 (s, pzCq), 151.30 (d, $^3J_{PC}$ = 4.2 Hz, pzCq), 151.32 (s, pzCq), 153.35 (s, pzCq). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 134.77 (d, $^1J_{RhP}$ = 202.6 Hz). IR (cm^{-1}): *ν* 1977, 2026, 2159 (C≡C). Anal. Calcd for $C_{26}H_{45}BN_6O_3PRh$: C, 49.23; H, 7.15; N, 13.25. Found: C, 48.85; H, 7.13; N, 13.25.

For Tp'Rh[P(OMe)$_3$](C≡CCF$_3$)H (6l). The exchange reaction was almost complete after 2 d at ambient temperature. The volatiles were removed and the residue was dissolved in 0.5 mL of C_6D_6. The solution was heated at 140 °C for 2 h. Colorless crystals of **6l** were grown from 1:1 hexane: ether solution at room temperature. ^{1}H NMR (500 MHz, C_6D_6): δ -14.41 (dd, $^1J_{RhH}$ = 19.7 Hz, $^2J_{PH}$ = 23.7 Hz, 1 H, RhH), 2.09 (s, 3H, pzCH$_3$), 2.17 (s, 3H, 2×pzCH$_3$), 2.28 (s, 3H, pzCH$_3$), 2.72(s, 3H, pzCH$_3$), 2.73 (s, 3H, pzCH$_3$), 3.14 (d, $^3J_{PH}$ = 12.1 Hz, 9H, P(OCH$_3$)$_3$), 5.44 (s, 1 H, pzH), 5.54 (s, 1 H, pzH), 5.69 (s, 1 H, pzH). ^{19}F NMR (400 MHz, C_6D_6): δ 18.13 (s, 3F's).

$^{31}P\{^{1}H\}$ NMR (400 MHz, C_6D_6): δ 131.48 (d, $^{1}J_{RhP}$ = 192.2 Hz).

For Tp'Rh[P(OMe)$_3$](C≡CPh)H (6m). The synthesis was identical to that of **6i** except that **4** was dissolved in 0.6 mL of phenylacetylene. ^{1}H NMR (500 MHz, THF-d_8): δ -15.09 (dd, $^{1}J_{RhH}$ = 18.8 Hz, $^{2}J_{PH}$ = 24.1 Hz, 1 H, RhH), 2.17 (s, 3H, pzCH$_3$), 2.28 (s, 3H, pzCH$_3$), 2.37 (s, 3H, pzCH$_3$), 2.42 (s, 3H, pzCH$_3$), 2.53 (s, 3 H, pzCH$_3$), 2.62 (s, 3H, pzCH$_3$), 3.51 (d, $^{3}J_{PH}$ = 11.9 Hz, 9H, P(OCH$_3$)$_3$), 5.64 (s, 1H, pzH), 5.74 (s, 1H, pzH), 5.75 (s, 1H, pzH), 6.95 (t, *J* = 7.0 Hz, 1H, Ph-*p*), 7.07 (t, *J* = 7.3 Hz, 2 H, Ph-*m*), 7.16 (d, *J* = 7.2 Hz, 2 H, Ph-*o*). $^{13}C\{^{1}H\}$ NMR (500 MHz, THF-d_8): δ 12.65 (s, pzCH$_3$), 12.80 (s, pzCH$_3$), 12.87 (s, pzCH$_3$), 14.58 (s, pzCH$_3$), 15.51 (s, pzCH$_3$), 16.12 (s, pzCH$_3$), 51.93 (d, $^{2}J_{PC}$ = 2.3 Hz, P(OCH$_3$)$_3$), 97.76 (dd, $^{1}J_{RhC}$ = 29.7 Hz, $^{2}J_{PC}$ = 44.7 Hz, Rh-CC), 106.09 (d, $^{4}J_{PC}$ = 5.5 Hz, pzCH), 106.81 (s, pzCH),106.88 (d, $^{2}J_{RhC}$ = 10.5 Hz, Rh-CC), 107.29 (s, pzCH), 124.66 (s, Ph-*p*), 128.29 (s, 2 C's, Ph-*m*), 130.78 (s, *ipso* C of Ph), 131.39 (s, 2 C's, Ph-*o*), 143.54 (d, $^{3}J_{PC}$ = 4.5 Hz, pzCq), 144.11 (s, pzCq), 144.91 (s, pzCq), 151.40 (d, $^{3}J_{PC}$ = 4.2 Hz, pzCq), 151.78 (s, pzCq), 153.65 (s, pzCq). $^{31}P\{^{1}H\}$ NMR (400 MHz, C_6D_6): δ 133.25 (d, $^{1}J_{RhP}$ = 199.0 Hz). IR (cm^{-1}): *ν* 1976, 2029, 2160 (C≡C). Anal. Calcd for $C_{26}H_{37}BN_6O_3PRh$: C, 49.86; H, 5.95; N, 13.42. Found: C, 50.14; H, 5.89; N, 13.24.

For Tp'Rh[P(OMe)$_3$](C≡CC$_6$H$_4$-*p*-OMe)H (6n). The synthesis was identical to that of **6i** except that **4** was dissolved in 0.6 mL of 4-ethynylanisole. ^{1}H NMR (500 MHz, C_6D_6): δ -14.65 (dd, $^{1}J_{RhH}$ = 19.2 Hz, $^{2}J_{PH}$ = 24.3 Hz, 1H, RhH), 2.15 (s, 3H, pzCH$_3$), 2.24 (s, 3H, pzCH$_3$), 2.30 (s, 3H, pzCH$_3$), 2.34 (s, 3H, pzCH$_3$), 2.91 (s, 3H, pzCH$_3$), 2.91 (s, 3H, pzCH$_3$), 3.28 (s, 3H, OCH$_3$), 3.32 (d, $^{2}J_{PH}$ = 11.9 Hz, 9H, P(OCH$_3$)$_3$), 5.52 (s, 1H, pzH), 5.62 (s, 1H, pzH), 5.77 (s, 1H, pzH), 6.79 (d, *J* = 8.8 Hz, 2H, *p*-OMePh-*m*), 7.50 (d, *J* = 8.8 Hz, 2H, *p*-OMe*Ph*-*o*). ^{13}C NMR (500 MHz, C_6D_6): δ 12.63 (s, pzCH$_3$), 12.85 (s, pzCH$_3$), 12.92 (s, pzCH$_3$), 14.66 (s, pzCH$_3$), 15.59 (s, pzCH$_3$), 16.39 (s, pzCH$_3$), 51.62 (d, $^{2}J_{PC}$ = 2.5 Hz, P(OCH$_3$)$_3$), 54.79 (s, OCH$_3$), 93.37 (dd, $^{1}J_{RhC}$ = 30.1 Hz, $^{2}J_{PC}$ = 44.4 Hz, Rh-CC), 106.27 (d, $^{2}J_{RhC}$ = 9.0 Hz, Rh-CC), 106.29 (d, $^{4}J_{PC}$ = 6.2 Hz, pzCH), 106.60 (s, pzCH), 107.28 (s, pzCH), 114.04 (s, 2 C's, *p*-OMePh-*m*), 123.12 (s, *ipso* C of *p*-OMePh), 132.35 (s, 2 C's, *p*-OMePh-*o*), 142.99 (d, $^{3}J_{PC}$ = 4.6 Hz, pzCq), 143.60 (s, pzCq), 144.21 (s, pzCq), 151.45 (s, pzCq), 151.48 (d, $^{3}J_{PC}$ = 5.5 Hz, pzCq), 153.50 (s, pzCq), 157.66 (s, ipso COMe of Ph). ^{31}P NMR (400 MHz, C_6D_6): δ 133.46 (d, $^{1}J_{RhP}$ = 199.9 Hz). IR (cm^{-1}): *ν* 1977, 2026, 2159 (C≡C).

For Tp'Rh[P(OMe)$_3$](C≡CC$_6$H$_4$-*p*-CF$_3$)H (6o). The exchange reaction was almost complete after 2 d at ambient temperature. White crystals of **6o** were grown from 1:1 hexane:THF solution at room temperature. ^{1}H NMR (500 MHz, C_6D_6): δ -14.58 (dd, $^{1}J_{RhH}$ = 19.1 Hz, $^{2}J_{PH}$ = 24.1 Hz, 1 H, RhH), 2.14 (s, 3H, pzCH$_3$), 2.24 (s, 3H, pzCH$_3$), 2.27 (s, 3H, pzCH$_3$), 2.33 (s, 3H, pzCH$_3$), 2.80 (s, 3H, pzCH$_3$), 2.81 (s, 3H, pzCH$_3$), 3.26 (d, $^{2}J_{P\text{-}H}$ = 12.0 Hz, 9H, P(OMe)$_3$), 5.53 (s, 1H, pzH), 5.61 (s, 1H, pzH), 5.78 (s, 1H, pzH), 7.34 (s, 4H, aryl H's). $^{13}C\{^{1}H\}$ NMR (500 MHz, C_6D_6): δ 12.59 (s, pzCH$_3$), 12.82 (s, pzCH$_3$), 12.90 (s, pzCH$_3$), 14.54 (s, pzCH$_3$), 15.55 (s, pzCH$_3$), 16.28 (s, pzCH$_3$), 51.49 (d, $^{2}J_{PC}$ = 2.4 Hz, P(OCH$_3$)$_3$), 104.43 (dd, $^{1}J_{RhC}$ = 29.3 Hz, $^{2}J_{PC}$ = 44.8 Hz, Rh-CC), 106.33 (d, $^{4}J_{PC}$ = 5.5 Hz, pzCH), 106.47 (d, $^{2}J_{Rh\text{-}C}$ = 10.1 Hz, Rh-CC), 106.72 (s, pzCH), 107.34 (s, pzCH), 125.22 (q, $^{3}J_{F\text{-}C}$ = 3.8 Hz, 2C, *p*-CF$_3$-C$_6$H$_4$-*m*), 126.23 (q, $^{2}J_{FC}$ = 32.0 Hz, *ipso* CCF$_3$ of Ph), 131.33 (s, 2C, *p*-CF$_3$-C$_6$H$_4$-*o*), 133.74 (s, ipso C of *p*-CF$_3$Ph), 143.27 (d, $^{3}J_{PC}$ = 4.6 Hz, pzCq), 143.83 (s, pzCq), 144.42 (s, pzCq), 151.33 (d, $^{3}J_{PC}$ = 4.2 Hz, pzCq), 151.54 (s, pzCq), 153.36 (s, pzCq), resonances for CF$_3$ is not detected due to multiple couplings. ^{19}F NMR (400 MHz, C_6D_{12}): δ 1.34 (s). $^{31}P\{^{1}H\}$ NMR (400 MHz, C_6D_6): δ 133.15 (d, $^{1}J_{RhP}$ = 197.8 Hz). IR (cm^{-1}): *ν* 1975, 2024, 2160 (C≡C). Anal. Calcd for $C_{27}H_{36}BF_3N_6O_3PRh$: C, 46.71; H, 5.23; N, 12.10. Found: C, 47.19; H, 5.00; N, 11.95.

For Tp'Rh[P(OMe)$_3$](*n*-pentyl)H (6p). No reaction was observed after 2 h. Decomposition occurred after longer reaction times. **6p** was prepared from photolysis of Tp'Rh[P(OMe)$_3$]H$_2$ (**2**). A solution of **2** with pentane was irradiated for 10 min at 10 °C. The solvent was removed in

vacuo and the resulting pale yellow residue was dissolved in THF-d_8/C_6D_6 (NMR yield: 39%). ^{1}H NMR (400 MHz, THF-d_8/C_6D_6): δ -16.59 (t, $^1J_{RhH}$ = $^2J_{PH}$ = 22.9 Hz, 1H, RhH), 1.53 (m, 1H, pentyl), 1.70 (m, 2H, pentyl), 1.96 (m, 2H, pentyl)), 2.06 (s, 3H, pzCH$_3$), 2.13 (s, 3H, pzCH$_3$), 2.17 (s, 6H, 2×pzCH$_3$), 2.36 (s, 3H, pzCH$_3$), 2.38 (s, 3H, pzCH$_3$), 3.18 (d, $^3J_{PH}$ = 10.9 Hz, 9H, P(OMe)$_3$), 3.34 (m, 2H, RhCH$_2$), 5.53 (s, 1H, pzH), 5.61 (s, 1H, pzH), 5.73 (s, 1H, pzH), other pentyl resonances are overlapping with those of solvent residues. ^{31}P{^{1}H} NMR (400 MHz, THF-d_8/C_6D_6): δ 146.5 (d, $^1J_{RhP}$ = 241.9 Hz).

For Tp'Rh[P(OMe)$_3$][CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$]Br (7b). To the resulting solution of **6b** (0.087 mmol, ~50 mg) in mesitylene, 31 μL of CHBr$_3$ (0.35 mmol) was added. The mixture was stirred for 10 min at room temperature. The volatiles were removed under vacuum and the crude product was purified as orange solids (9.8 mg, 16%) by chromatography using 5:1 hexane-THF as the eluent. ^{1}H NMR (500 MHz, C_6D_6): δ 2.04 (s, 3H, pzCH$_3$), 2.05 (s, 6H, 2×arylCH$_3$), 2.24 (s, 3H, pzCH$_3$), 2.24 (s, 3H, pzCH$_3$), 2.28 (s, 3H, pzCH$_3$), 2.71 (s, 3H, pzCH$_3$), 2.85 (s, 3H, pzCH$_3$), 3.15 (d, $^2J_{PH}$ = 10.8 Hz, 9H, P(OMe)$_3$), 4.59 (ddd, $^2J_{HH}$ = 12.8 Hz, $^2J_{RhH}$ = 7.2 Hz, $^3J_{PH}$ = 1.5 Hz, 1H, RhCH$_2$), 5.43 (d, $^5J_{PH}$ = 1.9 Hz, 1H, pzH), 5.44 (s, 1H, pzH), 5.53 (dd, $^3J_{PH}$ = 2.5 Hz, $^2J_{HH}$ = 12.8 Hz, 1H, RhCH$_2$), 5.70 (s, 1H, pzH), 6.29 (s, 2H, arylH), 6.61 (s, 1H, arylH). ^{13}C{^{1}H} NMR (500 MHz, C_6D_6): δ 12.74 (s, pzCH$_3$), 13.02 (s, pzCH$_3$), 13.26 (s, pzCH$_3$), 15.39 (s, pzCH$_3$), 15.42 (s, pzCH$_3$), 15.64 (s, pzCH$_3$), 18.58 (dd, $^1J_{RhC}$ = 9.7 Hz, $^2J_{PC}$ = 20.0 Hz, RhCH$_2$), 21.46 (s, 2×arylCH$_3$), 52.56 (d, $^2J_{PC}$ = 6.0 Hz, P(OCH$_3$)$_3$), 108.36 (s, pzCH), 108.52 (d, $^4J_{PC}$ = 6.6 Hz, pzCH), 108.54 (s, pzCH), 125.42 (s, 2×arylCH), 135.48 (s, 2×arylCq), 142.66 (d, $^4J_{PC}$ = 4.6 Hz, pzCq), 143.66 (s, pzCq), 143.98 (s, pzCq), 148.74 (s, arylCq), 154.27 (s, pzCq), 154.37 (s, pzCq), 154.46 (d, $^3J_{PC}$ = 6.4 Hz, pzCq), one aryCq peak is missing probably overlapped with the residual peaks of C_6D_6. ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 112.62 (d, $^1J_{RhP}$ = 196.6 Hz).

For Tp'Rh[P(OMe)$_3$][CH=CHC(CH$_3$)$_3$]Br (7c). To the resulting solution of **6c** (0.052 mmol, ~30 mg) in *t*-butylethylene, 23 μL of CHBr$_3$ (0.26 mmol) was added. The mixture was stirred overnight at room temperature. Orange-yellow crystals (31.1 mg, 87.1%) were grown from THF/hexane. ^{1}H NMR (400 MHz, C_6D_6): δ 1.17 (s, 9H, *t*Bu), 2.14 (s, 3H, pzCH$_3$), 2.14 (s, 3H, pzCH$_3$), 2.27 (s, 3H, pzCH$_3$), 2.40 (s, 3H, pzCH$_3$), 2.86 (s, 3H, pzCH$_3$), 2.90 (s, 3H, pzCH$_3$), 3.16 (d, $^3J_{PH}$ = 10.7 Hz, 9H, P(OCH$_3$)$_3$), 5.03 (d, $^3J_{HH}$ = 14.6 Hz, 1H, RhCHC<u>H</u>), 5.62 (s, 1H, pzH), 5.69 (s, 2H, 2×pzH), 7.60 (ddd, $^3J_{HH}$ = 14.5 Hz, $^2J_{RhH}$ = 2.3 Hz, $^3J_{PH}$ = 7.9 Hz, 1H, RhCH). ^{13}C{^{1}H} NMR (500 MHz, C_6D_6): δ12.80 (s, pzCH$_3$), 12.89 (s, pzCH$_3$), 13.32 (s, pzCH$_3$), 15.29 (s, pzCH$_3$), 16.78 (s, pzCH$_3$), 17.41 (s, pzCH$_3$), 30.43 (s, C(<u>C</u>H$_3$)$_3$), 35.47 (s, <u>C</u>(CH$_3$)$_3$), 52.67 (d, $^2J_{PC}$ = 6.4 Hz, P(OCH$_3$)$_3$), 108.21 (s, pzCH), 108.28 (d, $^4J_{PC}$ = 6.5 Hz, pzCH), 108.71 (s, pzCH), 126.83 (dd, $^1J_{RhC}$ = 13.6 Hz, $^2J_{PC}$ = 24.0 Hz, Rh<u>C</u>HCH), 142.47 (d, $^3J_{PC}$ = 4.8 Hz, pzCq), 143.54 (s, pzCq), 143.97 (s, pzCq), 144.85 (s, RhCH<u>C</u>H), 152.93 (s, pzCq), 153.32 (d, $^3J_{PC}$ = 6.3 Hz, pzCq), 154.38 (s, pzCq). ^{31}P{^{1}H} NMR (400 MHz, C_6D_6): δ 110.90 (d, $^1J_{RhP}$ = 195.8 Hz). Anal. Calcd for $C_{24}H_{42}BBrN_6O_3PRh$: C, 41.95; H, 6.16; N, 12.23. Found: C, 41.44; H, 6.06; N, 12.09.

For Tp'Rh[P(OMe)$_3$][CH$_2$OC(CH$_3$)$_3$]Br (7d). To the resulting solution of **6d** (0.087 mmol, ~50 mg) in *t*-butyl methyl ether, 0.2 ml of CHBr$_3$ (2.3 mmol) was added. The mixture was stirred for 10 min at room temperature. Most volatiles were removed under vacuum and the crude product was purified as yellow solids (12.6 mg, 21%) by chromatography with 3:1 hexane-THF as the eluent. ^{1}H NMR (400 MHz, C_6D_6): δ 1.29 (s, 9H, *t*Bu), 2.12 (s, 3H, pzCH$_3$), 2.16 (s, 3H, pzCH$_3$), 2.28 (s, 3H, pzCH$_3$), 2.59 (s, 3H, pzCH$_3$), 2.89 (s, 3H, pzCH$_3$), 3.03 (s, 3H, pzCH$_3$), 3.16 (d, $^3J_{PH}$ = 11.0 Hz, 9H, P(OCH$_3$)$_3$), 5.52 (s, 1H, pzH), 5.56 (d, $^2J_{RhH}$ = 3.1 Hz, 1H, RhCH$_2$), 5.63 (s, 1H, pzH), 5.71 (s, 1H, pzH), 6.40 (d, $^2J_{RhH}$ = 3.0 Hz, 1H, RhCH$_2$). ^{13}C{^{1}H} NMR (500 MHz, C_6D_6): δ 12.73 (s, pzCH$_3$), 12.95 (s, pzCH$_3$), 13.46 (s, pzCH$_3$), 15.10 (s, pzCH$_3$), 15.53 (s, pzCH$_3$), 15.97 (s, pzCH$_3$), 28.15 (s, C(<u>C</u>H$_3$)$_3$), 52.03 (d, $^2J_{PC}$ = 5.4 Hz, P(OCH$_3$)$_3$), 54.98 (dd, $^1J_{RhC}$ = 7.1 Hz, $^2J_{PC}$ = 20.1 Hz, RhCH$_2$), 73.91 (s, <u>C</u>(CH$_3$)$_3$), 108.02 (s, pzCH), 108.75 (d, $^4J_{PC}$ = 5.9 Hz, pzCH), 108.83 (s, pzCH), 142.63 (s, pzCq), 142.67 (d, $^3J_{PC}$ = 4.6 Hz, pzCq), 144.70 (s, pzCq), 152.72 (d,

$^{3}J_{PC}$ = 6.5 Hz, pzCq), 153.70 (s, pzCq), 154.49 (s, pzCq). $^{31}P\{^{1}H\}$ NMR (400 MHz, C_6D_6): δ 112.64 (d, $^{1}J_{RhP}$ = 205.6 Hz). Anal. Calcd for $C_{23}H_{42}BBrN_6O_4PRh\cdot THF_{0.5}$: C, 41.29; H, 6.38; N, 11.56. Found: C, 41.37; H, 6.31; N, 11.56. (see NMR Fig.S-58 for THF).

For Tp'Rh(P(OMe)$_3$)(CH$_2$C≡CCH$_3$)Br (7e). To the resulting solution of **6e** (0.087 mmol, ~50 mg) in *t*-butyl methyl ether, 0.1 mL of $CHBr_3$ (1.1 mmol) was added. The mixture was stirred for 1 d at room temperature. Most volatiles were removed under vacuum and the crude product was purified as orange-yellow solids (14.5 mg, 25%) by chromatography with 5:1 hexane-THF as the eluent. ^{1}H NMR (500 MHz, C_6D_6): δ 1.06 (t, J = 2.6 Hz, 3H, CH_3), 2.17 (s, 3H, pzCH_3), 2.17 (s, 3H, pzCH_3), 2.28 (s, 3H, pzCH_3), 2.60 (s, 3H, pzCH_3), 2.79 (s, 3H, pzCH_3), 3.06 (d, $^{3}J_{PH}$ = 10.9 Hz, 9H, P(OCH_3)$_3$), 3.16 (s, 3H, pzCH_3), 3.61 (m, 1H, RhCH_2), 4.60 (quintet of d, $^{2}J_{RhH}$ = 13.5 Hz, J_2 = 2.8 Hz, 1H, RhCH_2), 5.63 (d, $^{4}J_{RhH}$ = 2.0 Hz, 1H, pzH), 5.67 (s, 1H, pzH), 5.69 (s, 1H, pzH). $^{13}C\{^{1}H\}$ NMR (500 MHz, C_6D_6): δ –1.98 (dd, $^{1}J_{RhC}$ = 10.5 Hz, $^{2}J_{PC}$ = 19.1 Hz, RhCH_2), 4.60 (s, CH_3), 12.92 (s, pzCH_3), 12.94 (s, pzCH_3), 13.38 (s, pzCH_3), 14.98 (s, pzCH_3), 15.45 (s, pzCH_3), 15.50 (s, pzCH_3), 52.17 (d, $^{2}J_{PC}$ = 5.3 Hz, P(OCH_3)$_3$), 75.44 (s, RhCH_2C<u>C</u>), 88.60 (s, RhCH_2<u>C</u>C), 108.09 (d, $^{4}J_{PC}$ = 6.3 Hz, pzCH), 108.46 (s, pzCH), 108.62 (s, pzCH), 142.10 (d, $^{3}J_{PC}$ = 4.4 Hz, pzCq), 143.56 (s, 2×pzCq), 153.71 (s, pzCq), 153.74 (d, $^{3}J_{PC}$ = 6.9 Hz, pzCq), 154.62 (s, pzCq). $^{31}P\{^{1}H\}$ NMR (400 MHz, C_6D_6): δ 115.12 (d, $^{1}J_{RhP}$ = 192.4 Hz).

For Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)Br (7f). To the resulting solution of **6c** (0.052 mmol, ~30 mg) in *t*-butylethylene, 4.6 μL of $CHBr_3$ (0.052 mmol) was added. The mixture was stirred overnight at room temperature. Yellow crystals (30.5 mg, 89%) were grown from THF/hexane. ^{1}H NMR (400 MHz, C_6D_6): δ 1.72 (s, 3H, pzCH_3), 2.11 (s, 3H, pzCH_3), 2.12 (s, 3H, pzCH_3), 2.20 (s, 3H, pzCH_3), 2.47 (s, 3H, CH_3), 2.76 (s, 3H, pzCH_3), 2.94 (s, 3H, pzCH_3), 3.08 (d, $^{3}J_{PH}$ = 10.7 Hz, 9H, P(OCH_3)$_3$), 4.06 (m, 1H, RhCH_2), 4.36 (dd, $^{2}J_{HH}$ = 9.7 Hz, $^{2}J_{RhH}$ =1.5 Hz, 1H, RhCH_2), 5.50 (s, 1H, pzH), 5.58 (s, 1H, pzH), 5.61 (s, 1H, pzH). $^{13}C\{^{1}H\}$ NMR (500 MHz, C_6D_6): δ 12.79 (s, pzCH_3), 12.93 (s, pzCH_3), 13.27 (s, pzCH_3), 15.41 (s, pzCH_3), 16.04 (s, pzCH_3), 16.20 (s, pzCH_3), 21.94 (dd, $^{1}J_{RhC}$ = 10.1 Hz, $^{2}J_{PC}$ = 21.0 Hz, RhCH_2), 29.60 (s, CH_3), 53.07 (d, $^{1}J_{PC}$ = 7.2 Hz, P(OCH_3)$_3$), 108.64 (s, pzCH), 109.33 (d, $^{4}J_{PC}$ = 4.7 Hz, pzCH), 109.35 (s, pzCH), 143.09 (d, $^{3}J_{PC}$ = 4.5 Hz, pzCq), 143.86 (s, pzCq), 144.55 (s, pzCq), 153.82 (d, $^{3}J_{PC}$ = 6.9 Hz, pzCq), 154.15 (s, pzCq), 154.69 (s, pzCq), 215.23 (s, C(O)). $^{31}P\{^{1}H\}$ NMR (400 MHz, C_6D_6): δ 105.84 (d, $^{1}J_{RhP}$ = 190.6 Hz). Anal. Calcd for $C_{21}H_{36}BBrN_6O_4PRh\cdot THF_{0.5}$: C, 39.62; H, 5.78; N, 12.05. Found: C, 39.63; H, 5.44; N, 11.35. (see NMR Fig.S-64 for THF).

For Tp'Rh[P(OMe)$_3$](*n*-pentyl)Cl (7p). Pentylmagnesiumchloride (0.100 mL of a 2 M solution in THF, 0.200 mmol) was added dropwise to 100 mg (0.168 mmol) of Tp'Rh[P(OMe)$_3$]Cl_2 in 15 mL of THF. During addition of the Grignard reagent, the color of the solution changed from orange to yellow. The reaction mixture was stirred for an extra 20 min. 1.5 mL of saturated NH_4Cl (aq) solution was added to quench the reaction. The volatiles were removed under vacuum and 5 mL of methylene chloride was added to give a yellow slurry. This mixture was filtered through celite and layered with hexanes for recrystallization. Light yellow crystal clusters were collected (78.8 mg, 74%) and dissolved in C_6D_6. ^{1}H NMR (500 MHz, C_6D_6): δ 0.84 (t, $^{3}J_{HH}$ = 7.2 Hz, 3H, pentyl), 1.30 (sextet, $^{3}J_{H\text{-}H}$ = 7.3 Hz, 2H, pentyl), 1.47 (m, 2H, pentyl), 1.59 (m, 2H, pentyl), 2.13 (s, 3H, pzCH_3), 2.15 (s, 3H, pzCH_3), 2.27 (s, 3H, pzCH_3), 2.42 (s, 3H, pzCH_3), 2.76 (s, 3H, pzCH_3), 2.92 (s, 3H, pzCH_3), 3.15 (d, $^{2}J_{PH}$ = 10.8 Hz, 9H, P(OCH_3)$_3$), 3.27 (m, 1H, RhCH_2), 4.02 (m, 1H, RhCH_2), 5.59 (s, 1H, pzH), 5.66 (s, 1H, pzH), 5.69 (s, 1H, pzH). $^{13}C\{^{1}H\}$ NMR (500 MHz, C_6D_6): δ 12.82 (s, pzCH_3), 12.87 (s, pzCH_3), 13.47 (s, pzCH_3), 14.61 (s, 2C's, pzCH_3 and pentyl-CH_3), 14.70 (s, pzCH_3), 14.74 (s, pzCH_3), 23.19 (s, pentyl-CH_2), 32.51 (s, pentyl-CH_2), 35.32 (s, pentyl-CH_2), 52.02 (d, $^{1}J_{PC}$ = 5.2 Hz, P(OCH)$_3$)$_3$), 20.43 (dd, $^{1}J_{RhC}$ = 8.9 Hz, $^{2}J_{PC}$ = 19.6 Hz, RhCH_2), 108.01 (s, pzCH), 108.21 (d, $^{4}J_{PC}$ = 5.9 Hz, pzCH), 108.71 (s, pzCH), 142.68 (d, $^{4}J_{PC}$ = 4.4 Hz, pzCq), 143.29 (s, pzCq), 144.27 (s, pzCq), 152.68 (d, $^{3}J_{PC}$ = 6.4 Hz, pzCq), 153.23 (s, pzCq), 153.96 (s, pzCq). $^{31}P\{^{1}H\}$ NMR (400 MHz, C_6D_6): δ 114.22 (d,

$^{1}J_{RhP}$ = 201.7 Hz). Anal. Calcd for $C_{23}H_{42}BClN_6O_3PRh \cdot hexane_{0.25}$: C, 45.11; H, 7.03; N, 12.88. Found: C, 45.07; H, 6.98; N, 12.84. (see NMR Fig.S-67 for hexane).

Table S-1. Crystallographic Data for Tp'Rh[P(OMe)$_3$]Cl$_2$ (**1**)

formula	C18 H31 B Cl2 N6 O3 P Rh
formula weight	595.08
crystal system	Monoclinic
space group	$P2_1/n$
Z	4
a, Å	10.677(3)
b, Å	12.392(3)
c, Å	18.636(4)
b, deg	90.104(5)
V, Å^3	2465.8(10)
crystal dimensions, mm	0.32 x 0.20 x 0.08
T, K	100.0(1)
theta range for data collection, deg	1.09 to 37.78
reflections collected	73278
absorption coefficient, mm^{-1}	1.006
max. and min. transmission	0.9238 and 0.7389
R_1/R_2	0.0445/ 0.0836
goodness of fit	1.071
largest diff. peak and hole, e.Å^{-3}	1.279 and -1.653

Table S-2. Crystallographic Data for Tp'Rh[P(OMe)$_3$](CH$_3$)Cl (**3**)

formula	C19 H34 B Cl N6 O3 P Rh
formula weight	574.66
crystal system	Monoclinic
space group	$P2_1/n$
Z	8
a, Å	19.0753(11)
b, Å	8.1941(5)
c, Å	33.2922(19)
V, Å^3	5002.7(5)
crystal dimensions, mm	0.32 x 0.12 x 0.08
T, K	100.0(1)
theta range for data collection, deg	1.93 to 34.97
reflections collected	138012
absorption coefficient, mm^{-1}	0.886
max. and min. transmission	0.9166 and 0.7895
R_1/R_2	0.0614/ 0.1272
goodness of fit	1.048
largest diff. peak and hole, e.Å^{-3}	1.037 and -1.172

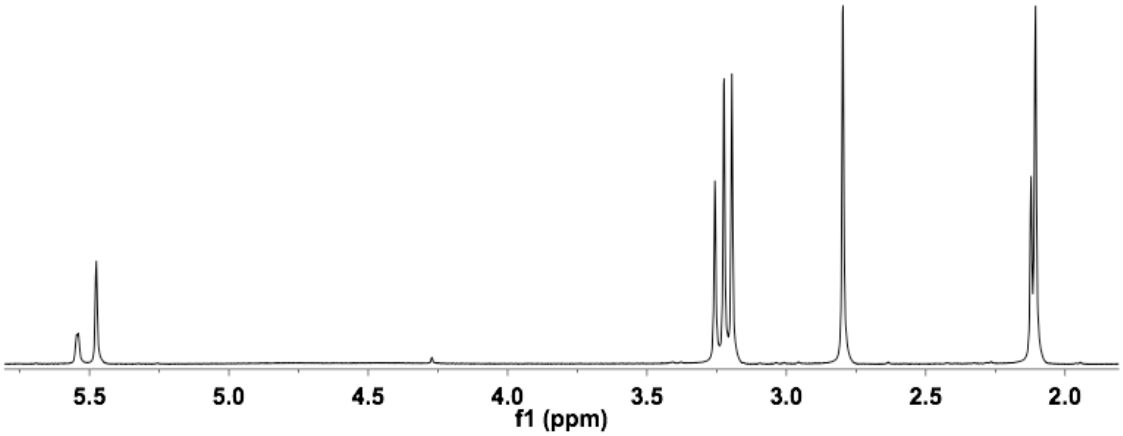


Figure S-1. ^{1}H NMR for Tp'Rh[P(OMe)$_3$]Cl$_2$ **(1)** in C_6D_6.

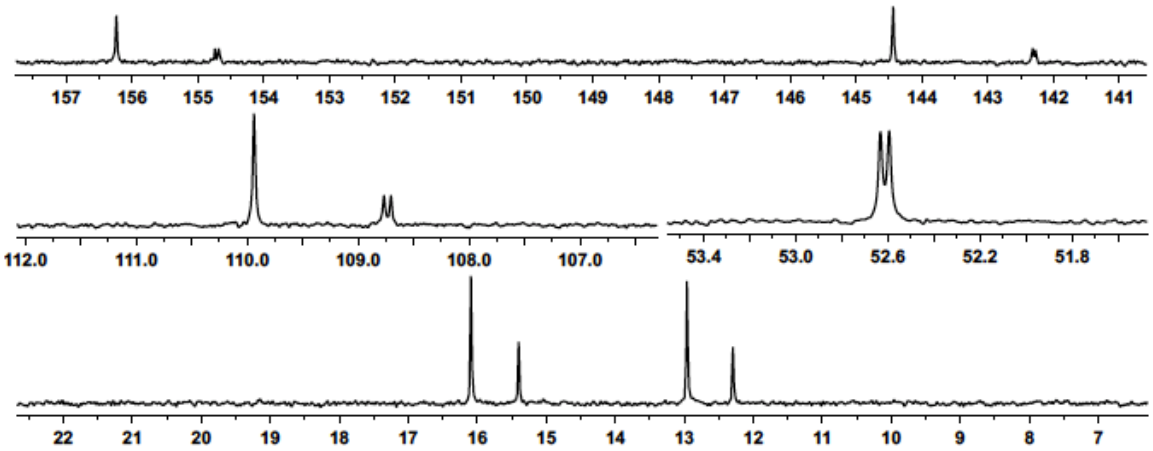


Figure S-2. $^{13}C\{^{1}H\}$ NMR for Tp'Rh(P(OMe)$_3$)Cl$_2$ **(1)** in C_6D_6.

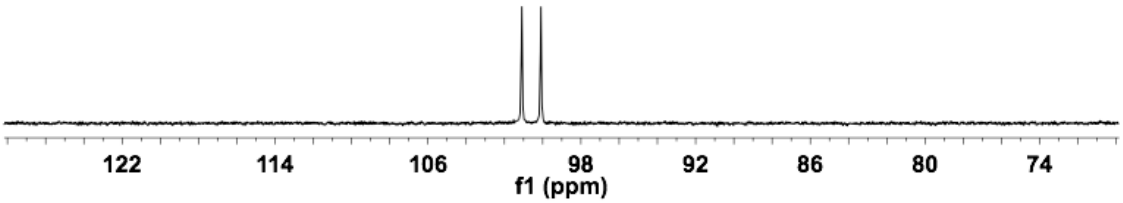


Figure S-3. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$]Cl$_2$ **(1)** in C_6D_6.

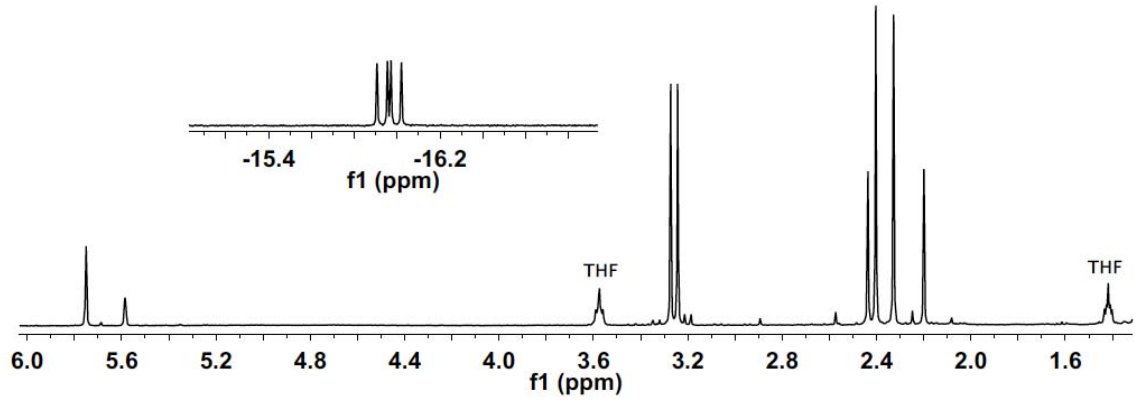


Figure S-4. ^{1}H NMR for Tp'Rh[P(OMe)$_3$]H$_2$ **(2)** in C_6D_6.

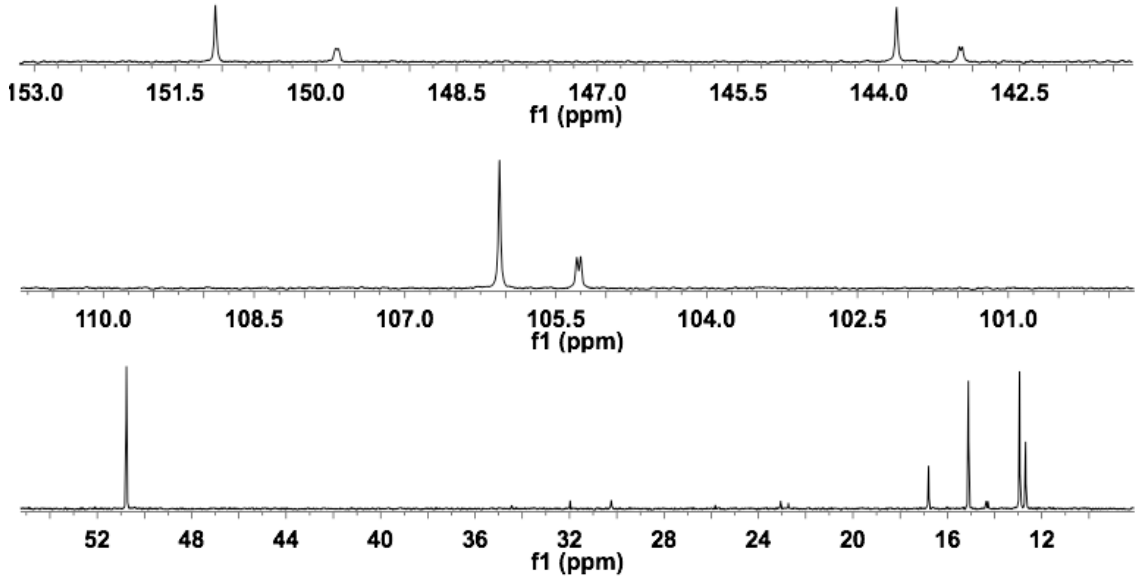


Figure S-5. $^{13}C\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$]H$_2$ **(2)** in C_6D_6.

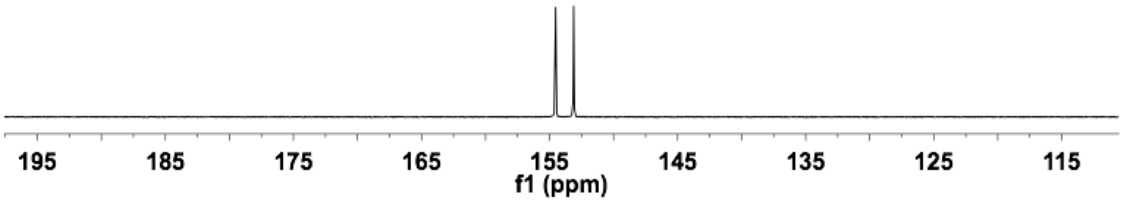


Figure S-6. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$]H$_2$ **(2)** in C_6D_6.

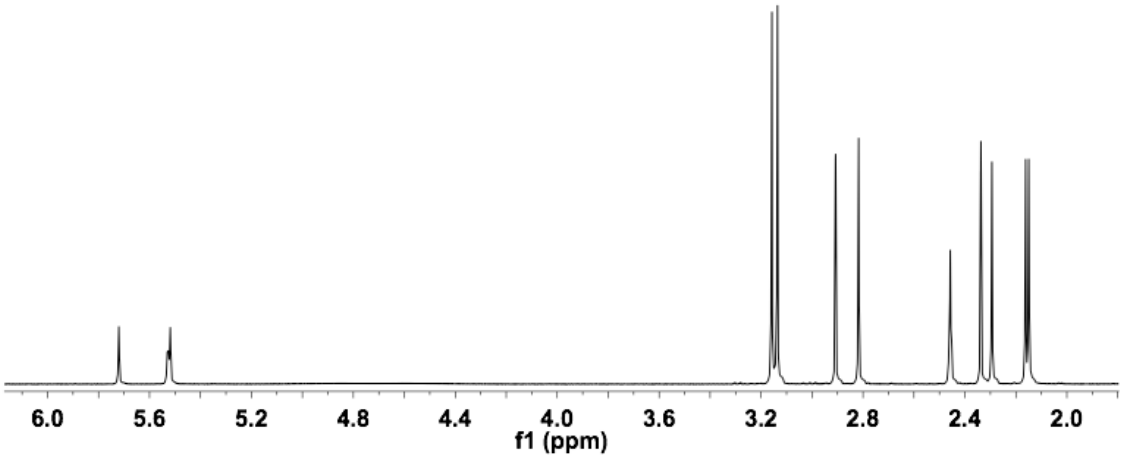


Figure S-7. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_3$)Cl **(3)** in C$_6$D$_6$.

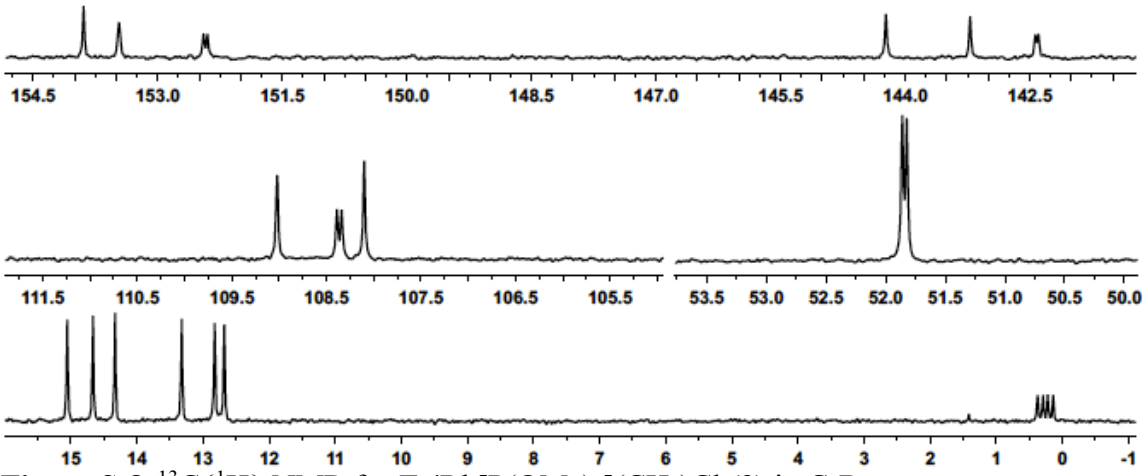


Figure S-8. ^{13}C{^{1}H} NMR for Tp'Rh[P(OMe)$_3$](CH$_3$)Cl **(3)** in C$_6$D$_6$.

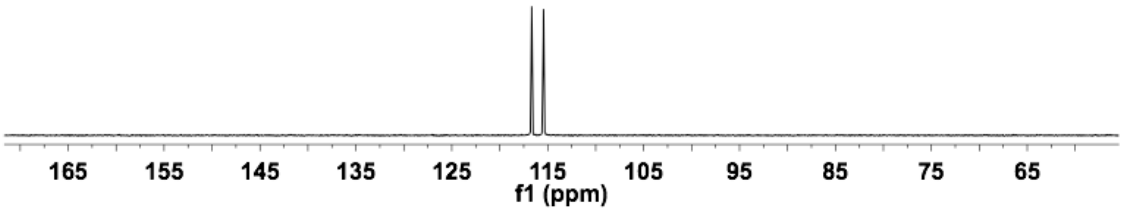


Figure S-9. ^{31}P{^{1}H} NMR for Tp'Rh[P(OMe)$_3$](CH$_3$)Cl **(3)** in C$_6$D$_6$.

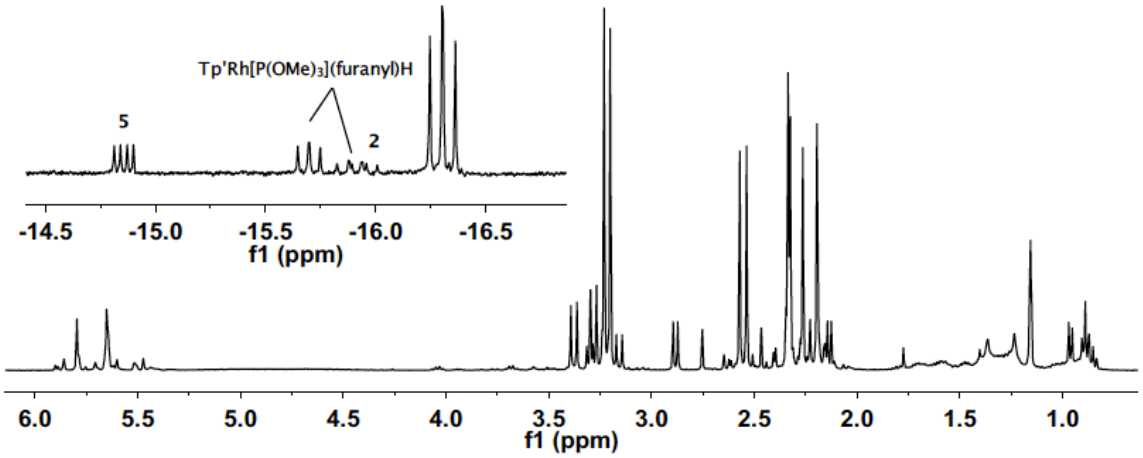


Figure S-10. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_3$)H **(4)** in C$_6$D$_6$.

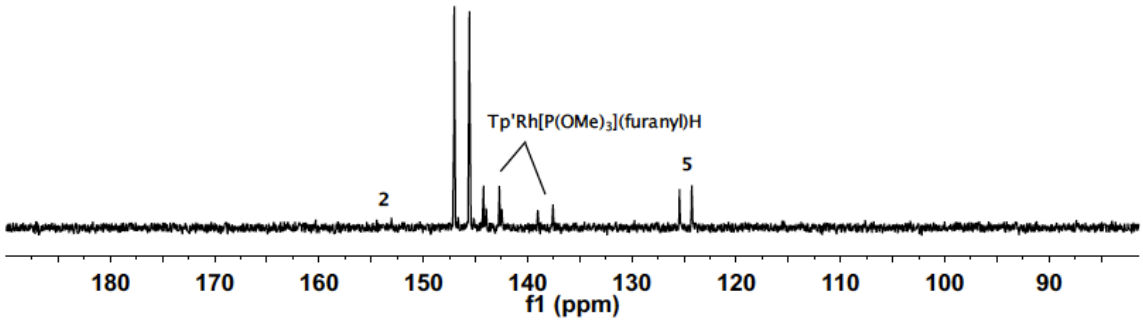


Figure S-11. ^{31}P{^{1}H} NMR for Tp'Rh[P(OMe)$_3$](CH$_3$)H **(4)** in C$_6$D$_6$.

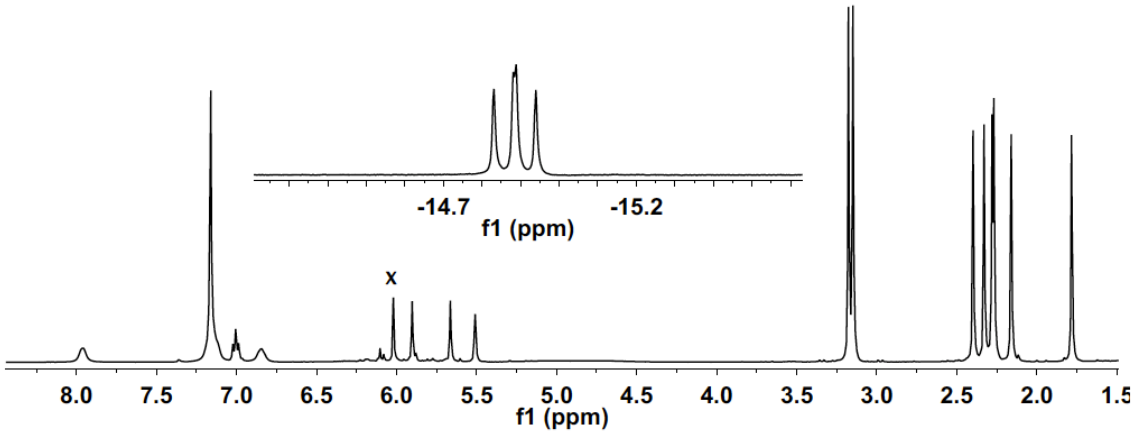


Figure S-12. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](Ph)H **(6a)** in C$_6$D$_6$. **X** denotes Cp$_2$ZrHCl.

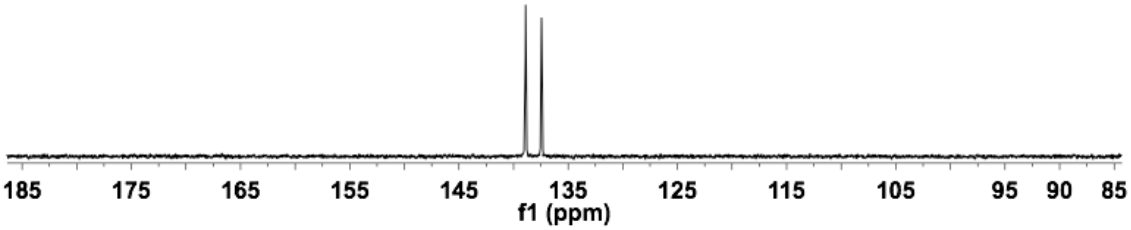


Figure S-13. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](Ph)H **(6a)** in C_6D_6.

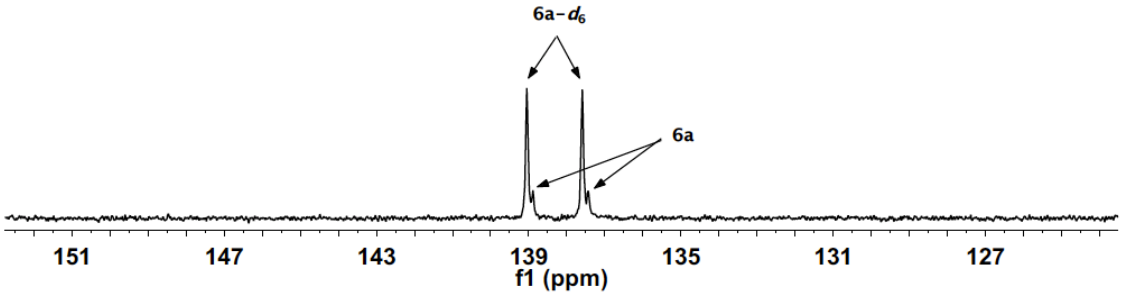


Figure S-14. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](C_6D_5)D **(6a-d$_6$)** in C_6D_6.

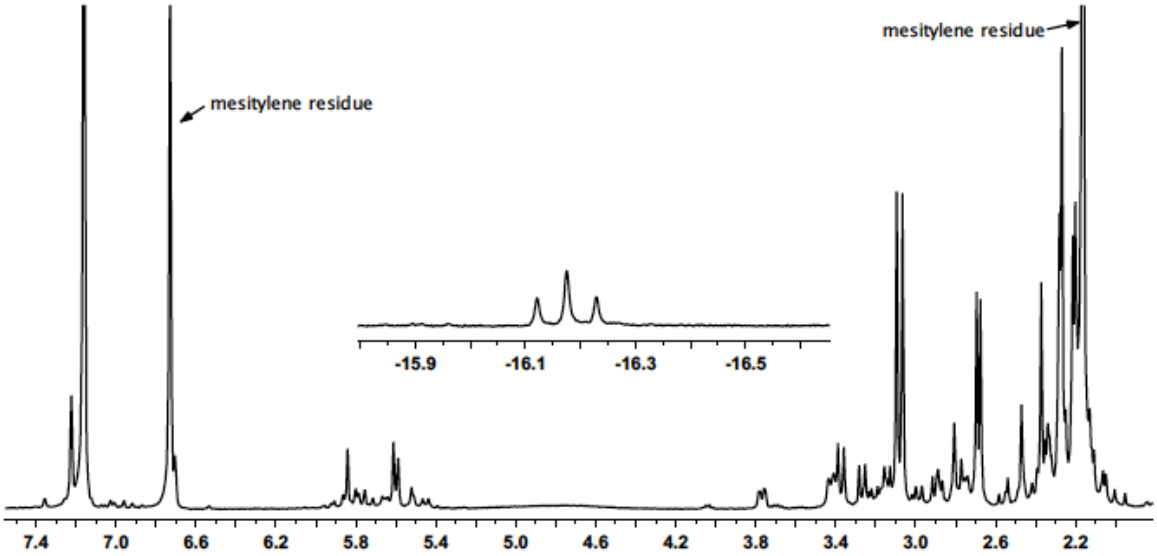


Figure S-15. ^{1}H NMR for Tp'Rh[P(OMe)$_3$]($CH_2C_6H_3$-3,5-(CH_3)$_2$)H **(6b)** in C_6D_6.

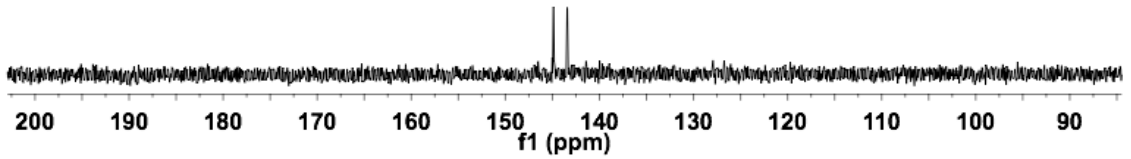


Figure S-16. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$]($CH_2C_6H_3$-3,5-(CH_3)$_2$)H **(6b)** in C_6D_6.

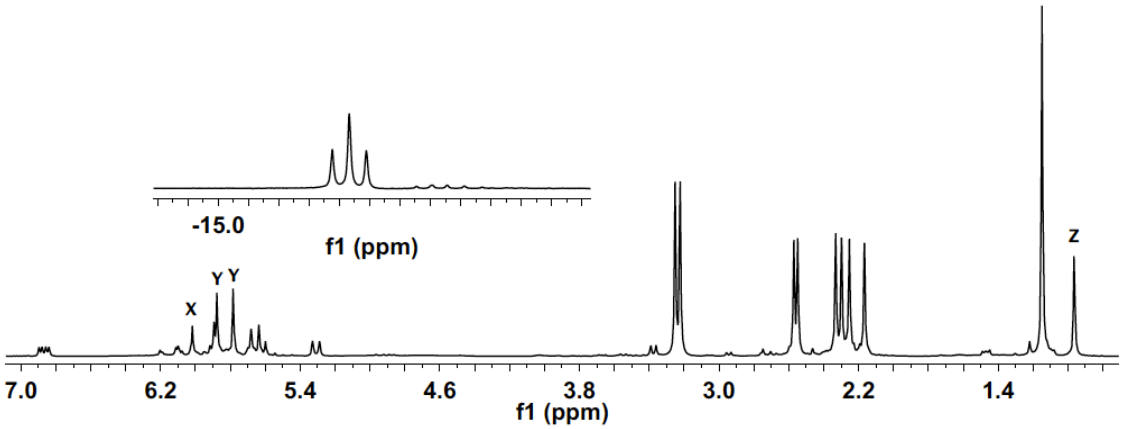


Figure S-17. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)H **(6c)** in C_6D_6. **X** denotes Cp_2ZrHCl; **Y** denotes Cp_2ZrCl_2 and presumable cyclopentadienyl resonances; **Z** denotes 3,3-dimethyl-1-butene.

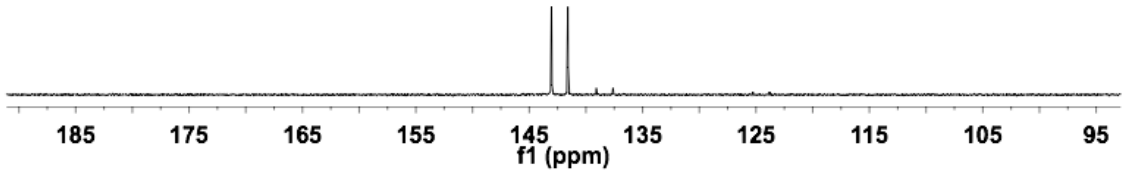


Figure S-18. ^{31}P{^{1}H} NMR for Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)H **(6c)** in C_6D_6.

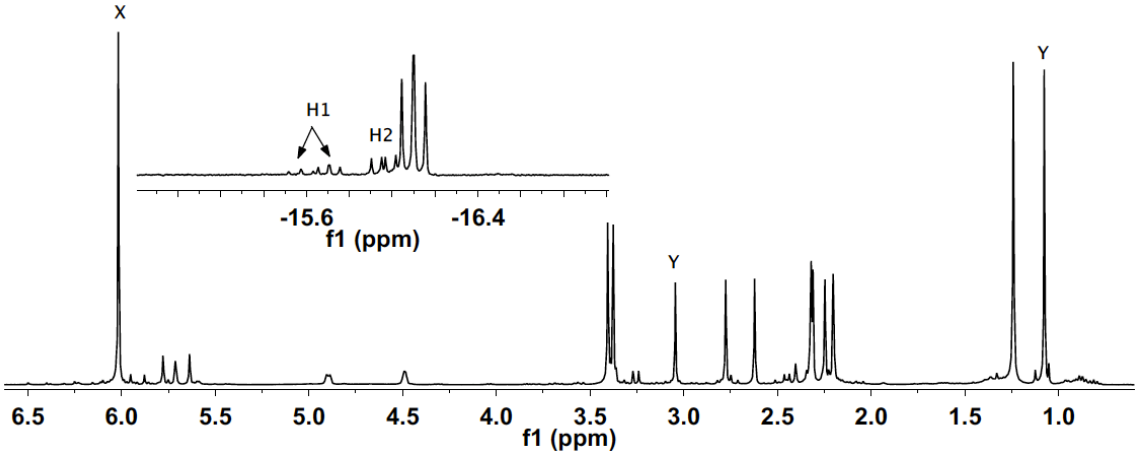


Figure S-19. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)H **(6d)** in C_6D_6. **X** denotes Cp_2ZrHCl; **Y** denotes 2-methoxy-2-methylpropane; **H1** denotes two isomers of Tp'Rh[P(OMe)$_3$](H$_4$furanyl)H; **H2** denotes Tp'Rh[P(OMe)$_3$]H$_2$ **(2)**.

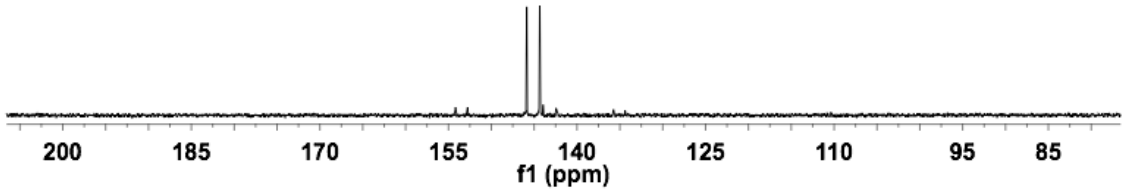


Figure S-20. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)H **(6d)** in C$_6$D$_6$.

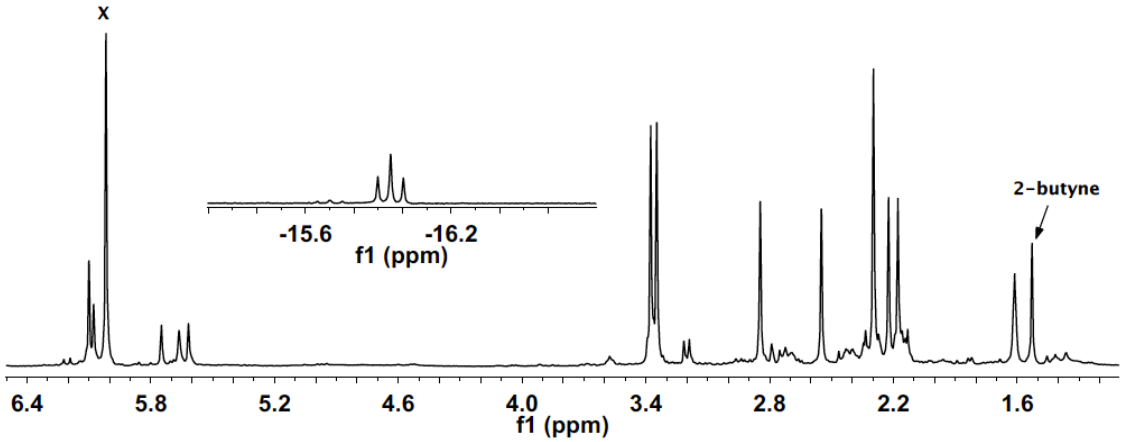


Figure S-21. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C≡C≡≡CH$_3$)H **(6e)** in C$_6$D$_6$. **X** denotes Cp$_2$ZrHCl.

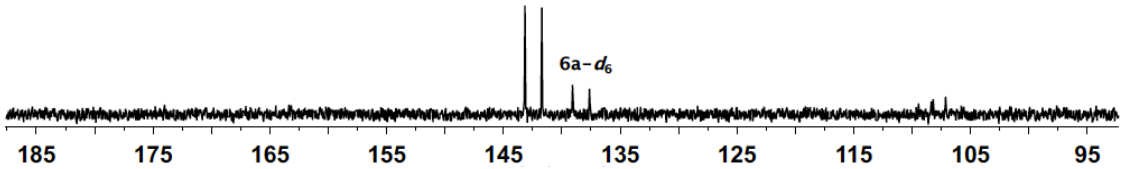


Figure S-22. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)H **(6e)** in C$_6$D$_6$**.**

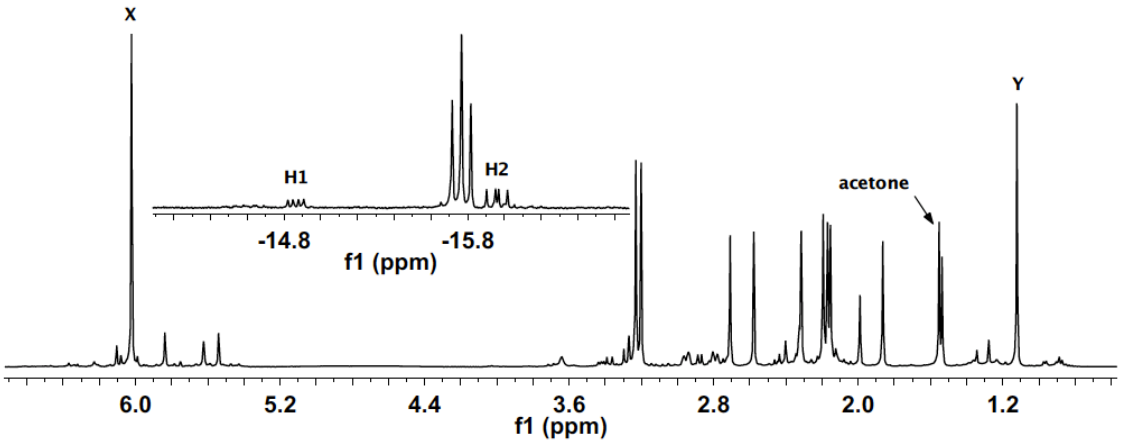


Figure S-23. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)H **(6f)** in C$_6$D$_6$. **X** denotes Cp$_2$ZrHCl; **Y** denotes impurity in acetone as shown in the ^{1}H NMR spectrum of Tp'Rh[PMe$_3$](CH$_2$C(O)CH$_3$)H in ref 25; **H1** denotes Tp'Rh[P(OMe)$_3$](Cl)H (**5**); **H2** denotes Tp'Rh[P(OMe)$_3$]H$_2$ (**2**).

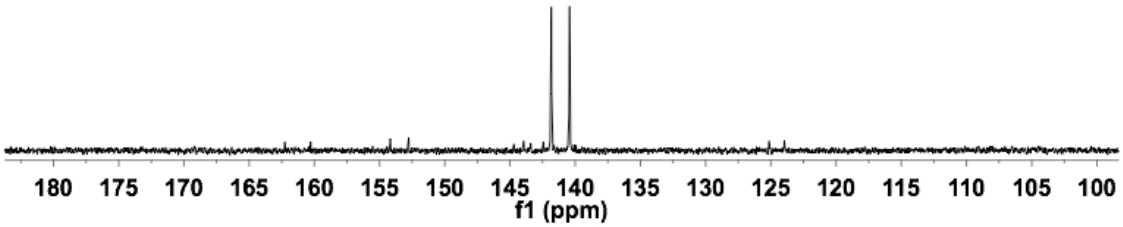


Figure S-24. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)H **(6f)** in C_6D_6.

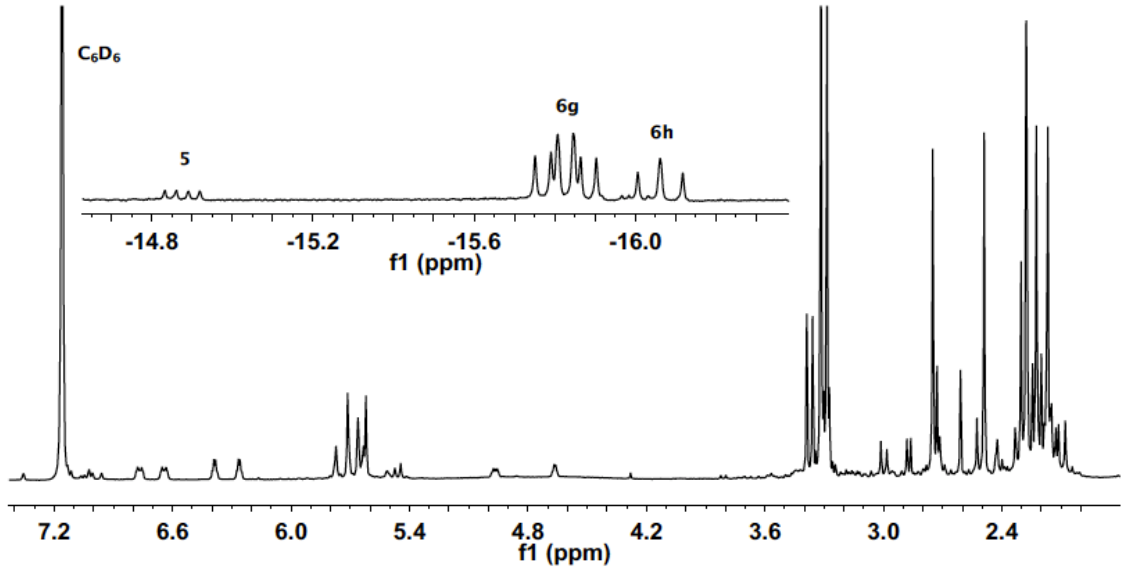


Figure S-25. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$F)H **(6g)** and Tp'Rh[P(OMe)$_3$](CH$_2$OMe)H **(6h)** in C_6D_6.

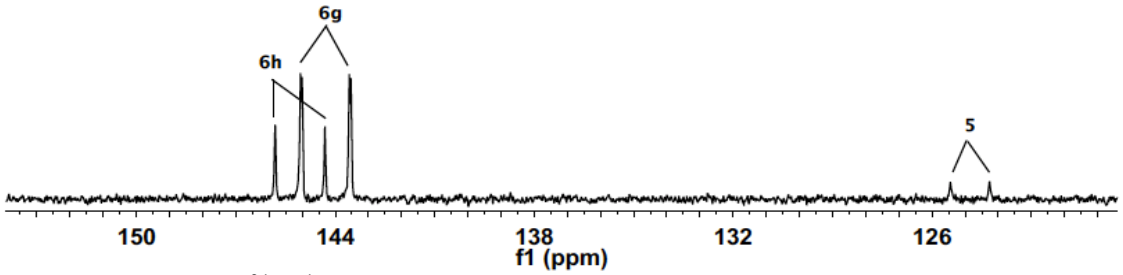


Figure S-26. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$F)H **(6g)** and Tp'Rh[P(OMe)$_3$](CH$_2$OMe)H **(6h)** in C_6D_6.

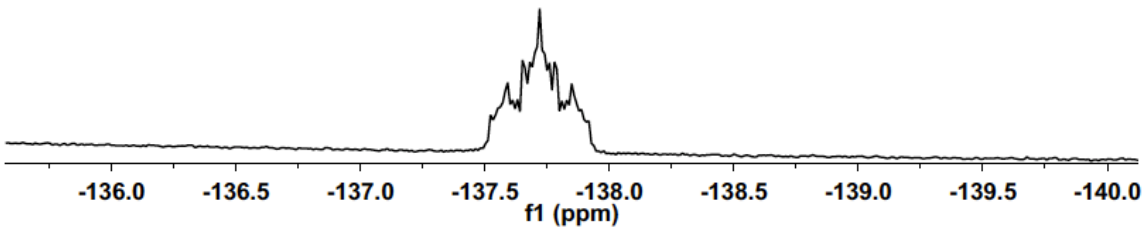


Figure S-27. ^{19}F NMR for Tp'Rh[P(OMe)$_3$](CH$_2$F)H **(6g)** in C_6D_6.

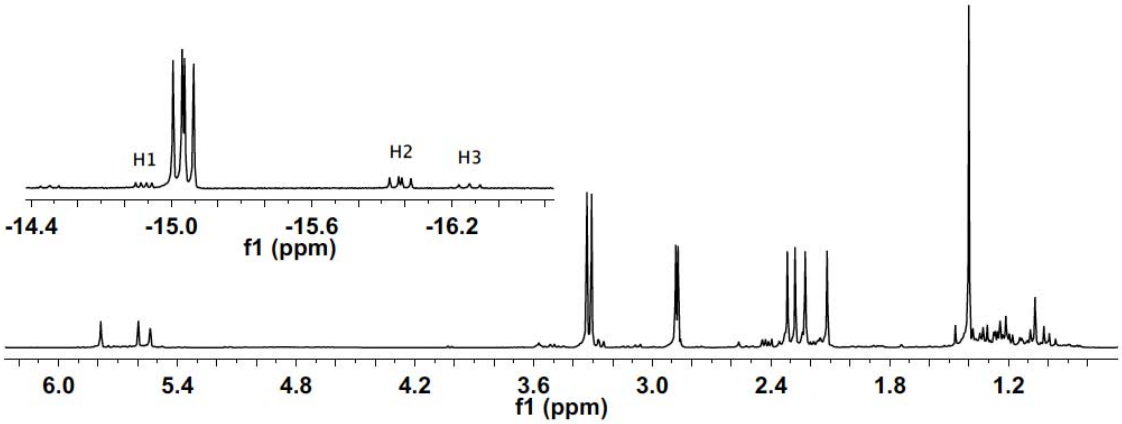


Figure S-28. ^{1}H NMR of Tp'Rh[P(OMe)$_3$](C≡CC(CH$_3$)$_3$)H **(6i)** in C$_6$D$_6$**. H1** denotes Tp'Rh[P(OMe)$_3$](Cl)H **(5)**; **H2** denotes Tp'Rh[(P(OMe)$_3$]H$_2$ **(2); H3** denotes Tp'Rh[P(OMe)$_3$](CH$_3$)H **(4)**.

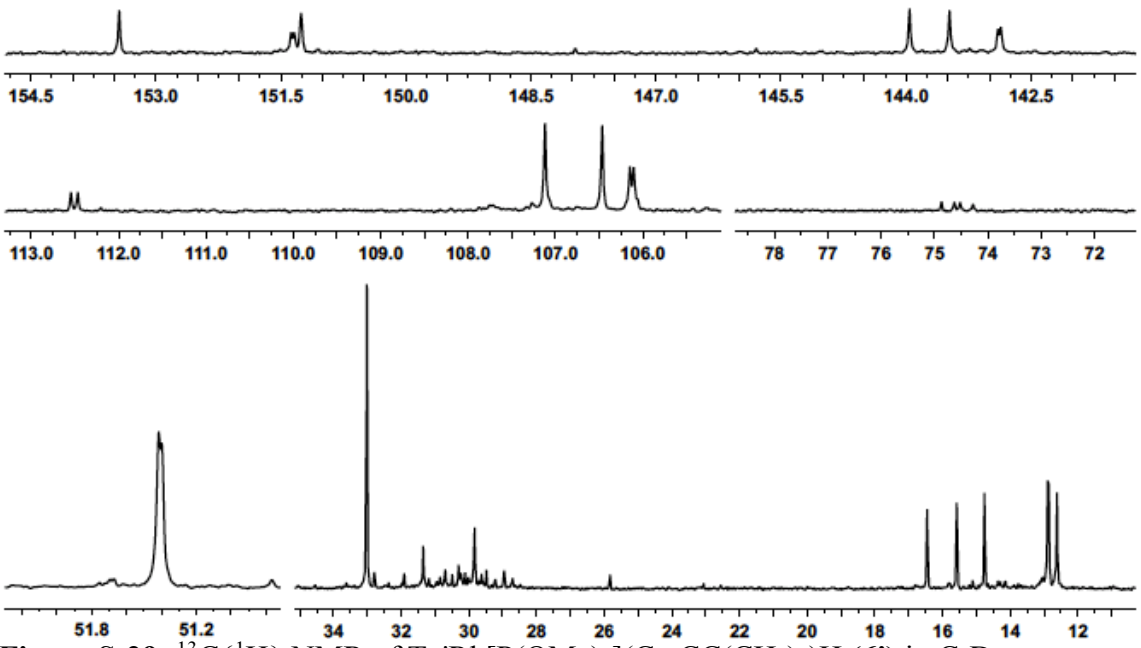


Figure S-29. ^{13}C{^{1}H} NMR of Tp'Rh[P(OMe)$_3$](C≡CC(CH$_3$)$_3$)H **(6i)** in C$_6$D$_6$**.**

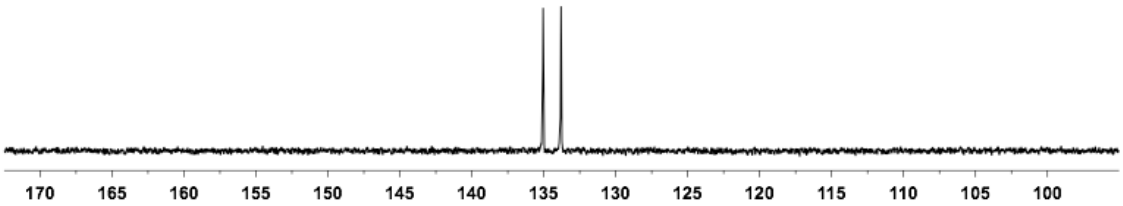


Figure S-30. ^{31}P{^{1}H} NMR of Tp'Rh[P(OMe)$_3$](C=CC(CH$_3$)$_3$)H **(6i)** in C$_6$D$_6$**.**

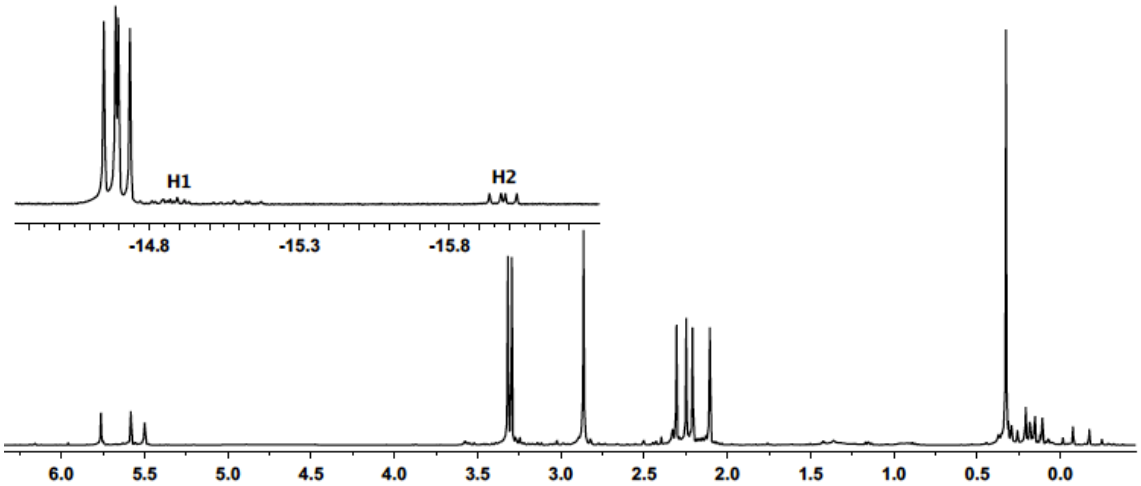


Figure S-31. ^{1}H NMR of Tp'Rh[P(OMe)$_3$](C≡CSi(CH$_3$)$_3$)H **(6j)** in C_6D_6**. H1** denotes Tp'Rh[P(OMe)$_3$](Cl)H **(5)**; **H2** denotes Tp'Rh[P(OMe)$_3$]H$_2$ **(2).**

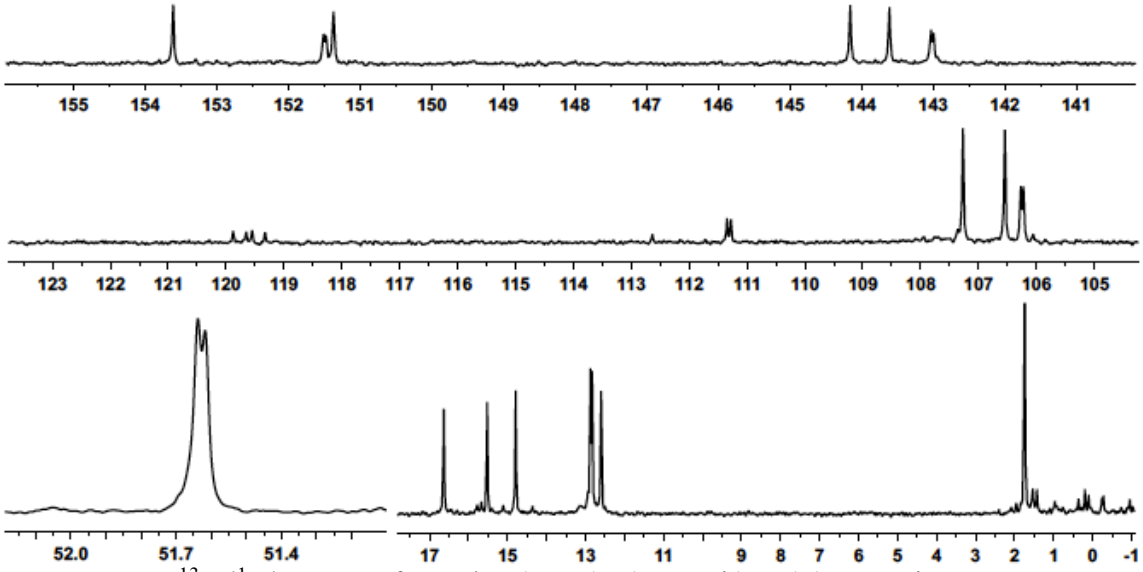


Figure S-32. ^{13}C{^{1}H} NMR of Tp'Rh[P(OMe)$_3$](C≡CSi(CH$_3$)$_3$)H **(6j)** in C_6D_6**.**

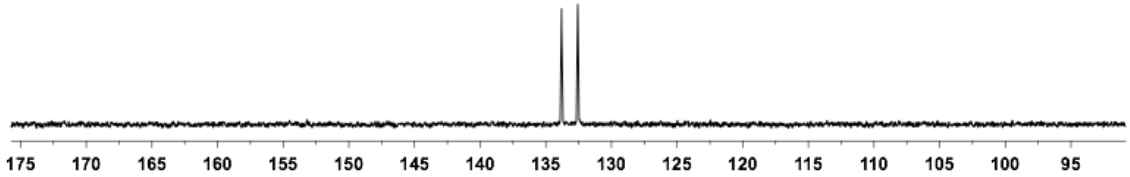


Figure S-33. ^{31}P{^{1}H} NMR of Tp'Rh[P(OMe)$_3$](C≡CSi(CH$_3$)$_3$)H **(6j)** in C_6D_6**.**

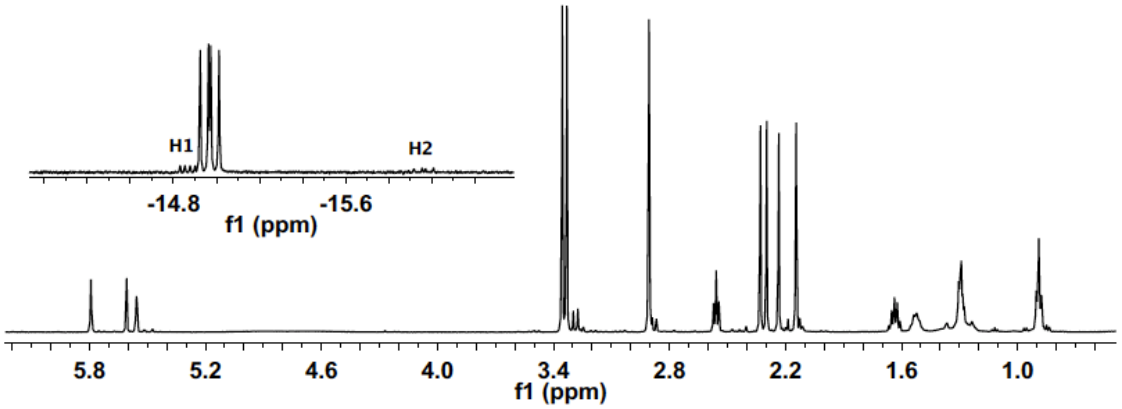


Figure S-34. ^{1}H NMR of Tp'Rh[P(OMe)$_3$](C≡C*n*-hexyl)H **(6k)** in C_6D_6. **H1** denotes Tp'Rh[P(OMe)$_3$](Cl)H **(5); H2** denotes Tp'Rh[P(OMe)$_3$]H$_2$ **(2).**

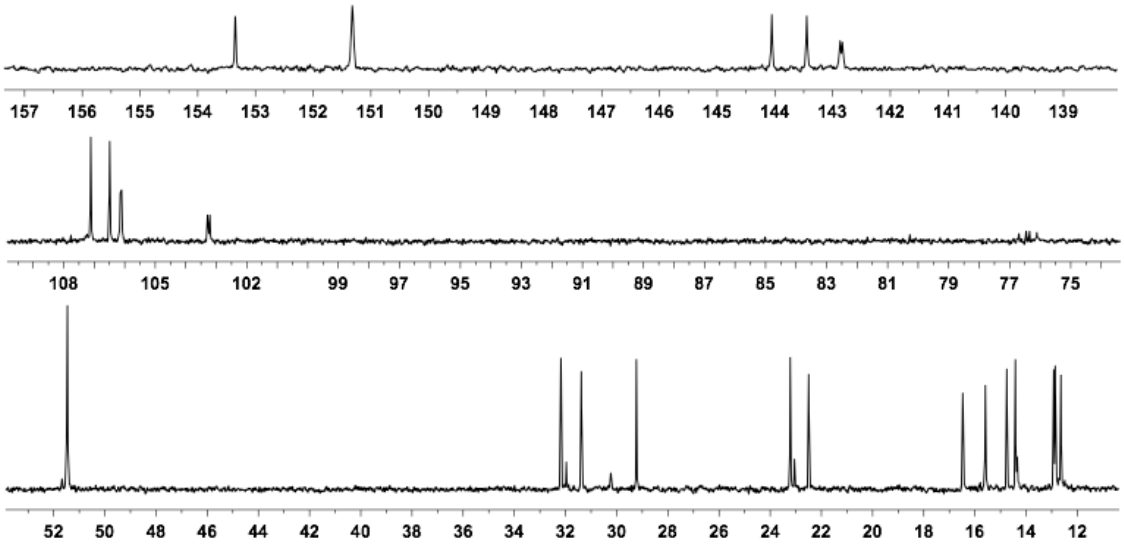


Figure S-35. ^{13}C{^{1}H} NMR of Tp'Rh[P(OMe)$_3$](C≡C*n*-hexyl)H **(6k)** in C_6D_6.

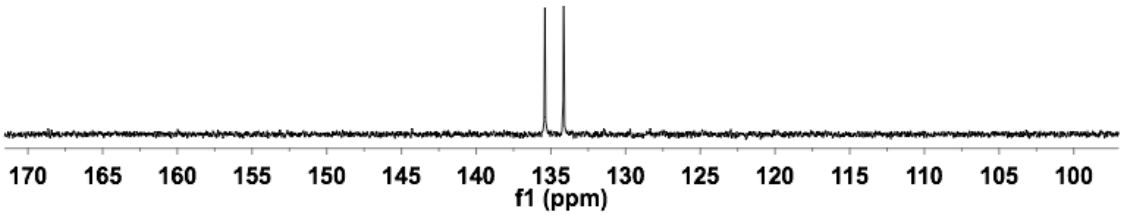


Figure S-36. ^{31}P{^{1}H} NMR of Tp'Rh[P(OMe)$_3$](C≡C*n*-hexyl)H **(6k)** in C_6D_6.

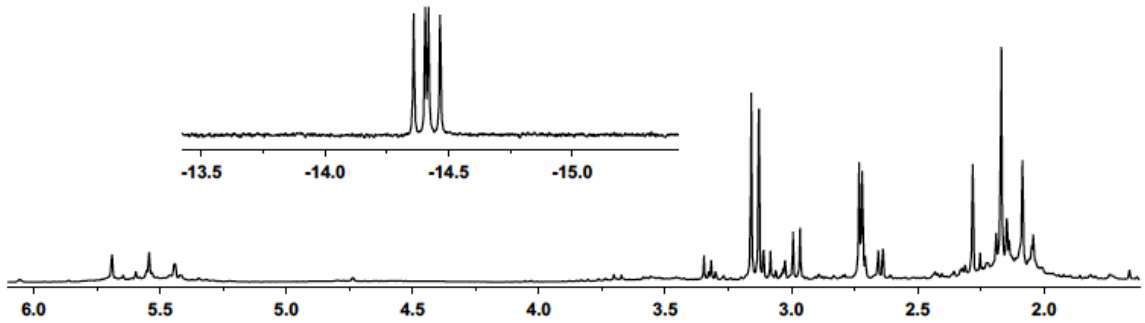


Figure S-37. ^{1}H NMR of Tp'Rh[P(OMe)$_3$](C≡CCF$_3$)H **(6l)** in C$_6$D$_6$.

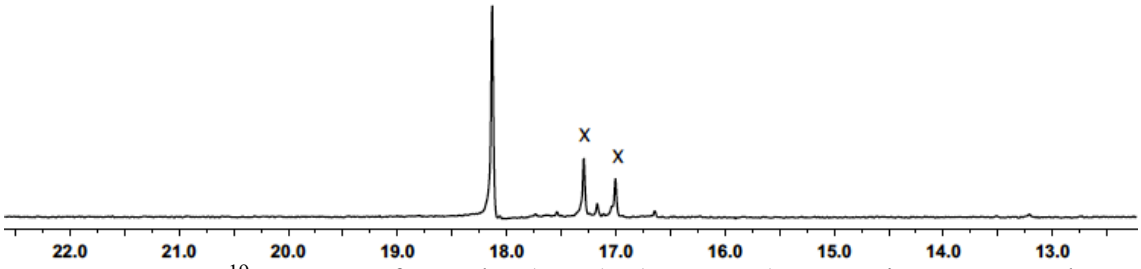


Figure S-38. ^{19}F NMR of Tp'Rh[P(OMe)$_3$](C≡CCF$_3$)H **(6l)** in C$_6$D$_6$. **X** denotes impurities.

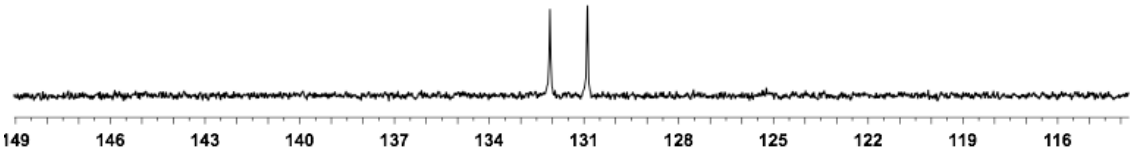


Figure S-39. ^{31}P{^{1}H} NMR of Tp'Rh[P(OMe)$_3$](C≡CCF$_3$)H **(6l)** in C$_6$D$_6$.

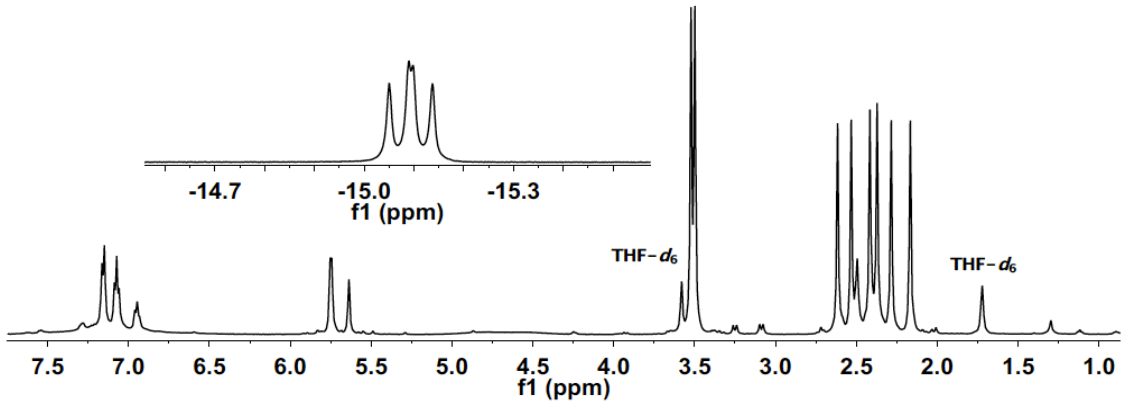


Figure S-40. ^{1}H NMR of Tp'Rh[P(OMe)$_3$](C≡CPh) **(6m)** in C$_6$D$_6$**.**

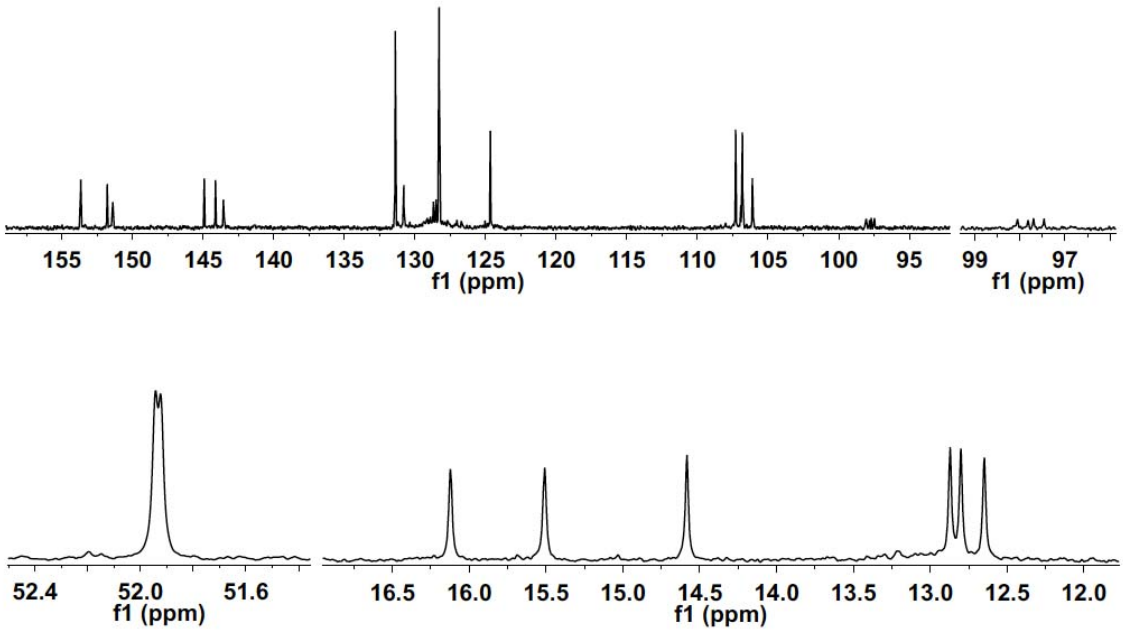


Figure S-41. $^{13}C\{^{1}H\}$ NMR of Tp'Rh[P(OMe)$_3$](C≡CPh) **(6m)** in C_6D_6.

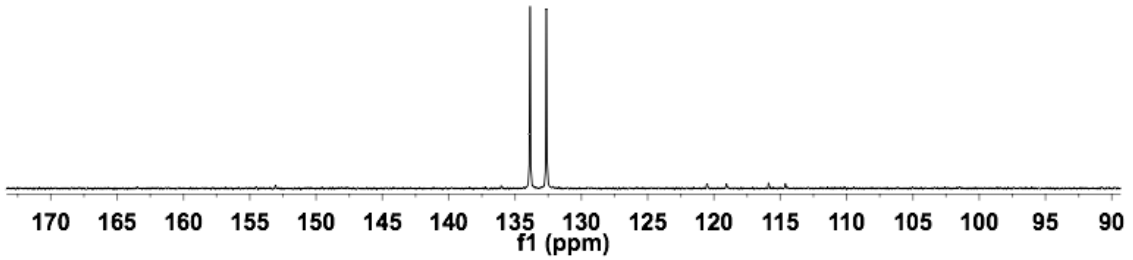


Figure S-42. $^{31}P\{^{1}H\}$ NMR of Tp'Rh[P(OMe)$_3$](C≡CPh) **(6m)** in C_6D_6.

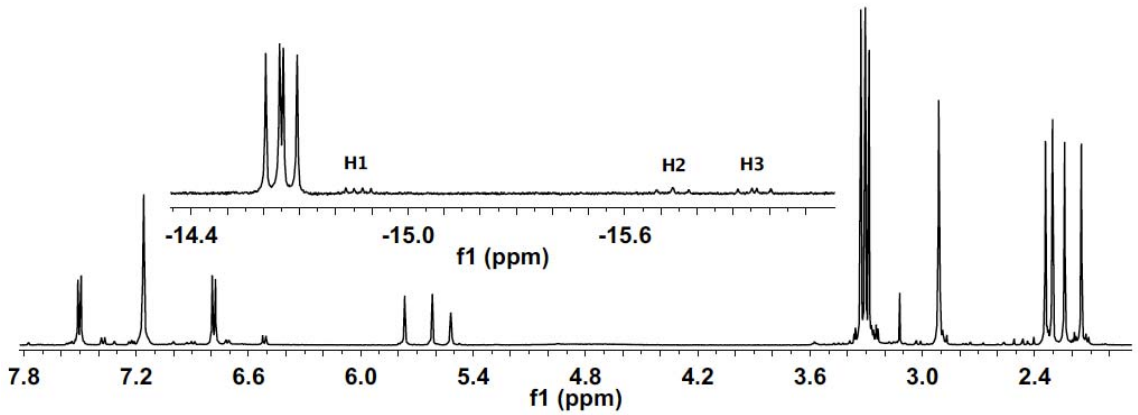


Figure S-43. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OMe)H **(6n)** in C_6D_6. **H1** denotes Tp'Rh[P(OMe)$_3$](Cl)H **(5)**; **H2** denotes Tp'Rh[P(OMe)$_3$](furanyl)H; **H3** denotes Tp'Rh[P(OMe)$_3$]H_2 **(2).**

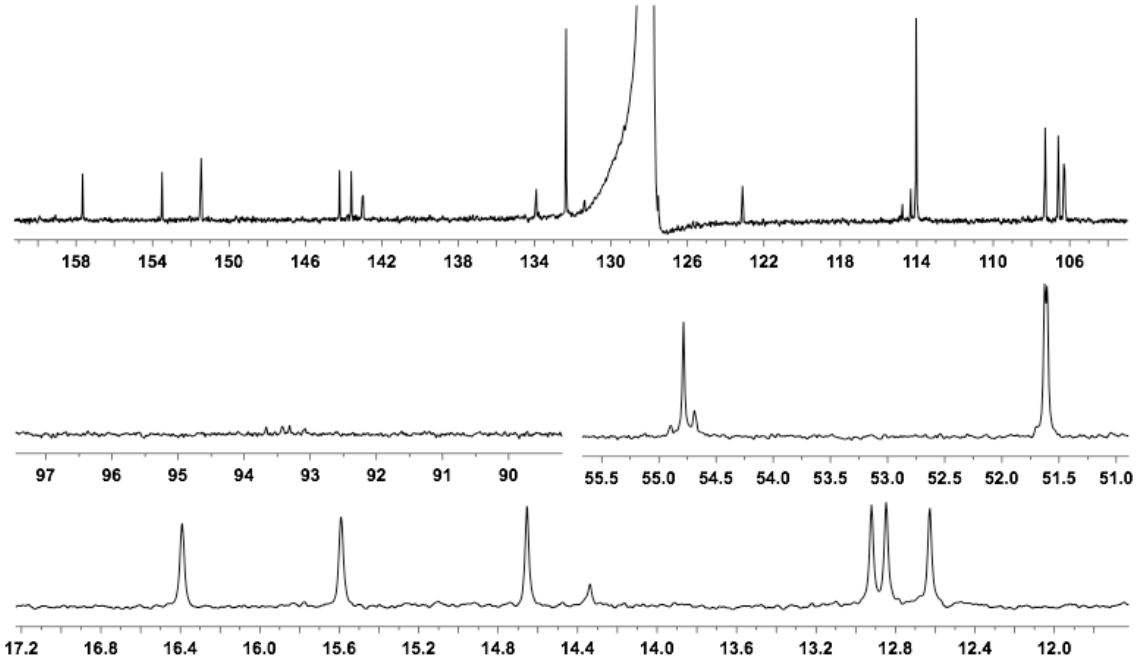


Figure S-44. $^{13}C\{^{1}H\}$ NMR of Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OMe)H **(6n)** in C_6D_6.

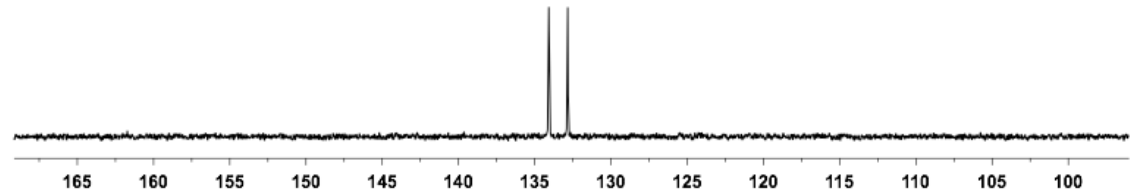


Figure S-45. $^{31}P\{^{1}H\}$ NMR of Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OMe)H **(6n)** in C_6D_6.

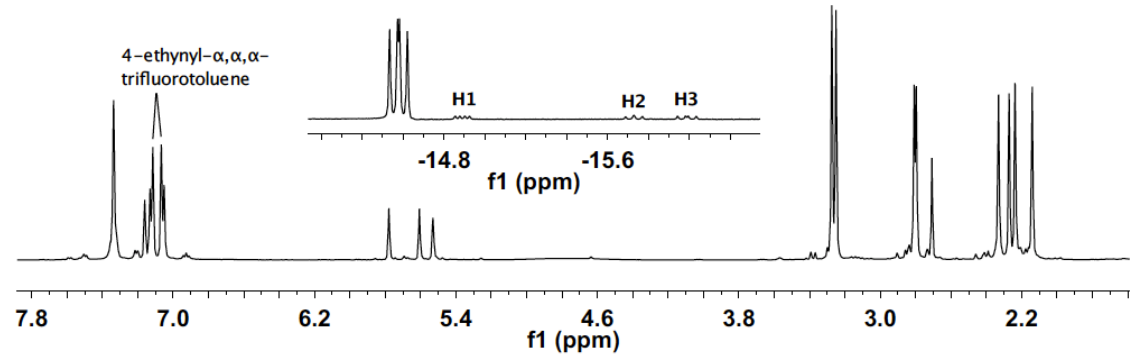


Figure S-46. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-CF_3)H **(6o)** in C_6D_6. **H1** denotes Tp'Rh[P(OMe)$_3$](Cl)H **(5)**; **H2** denotes Tp'Rh[P(OMe)$_3$](furanyl)H; **H3** denotes Tp'Rh[P(OMe)$_3$]H_2 **(2).**

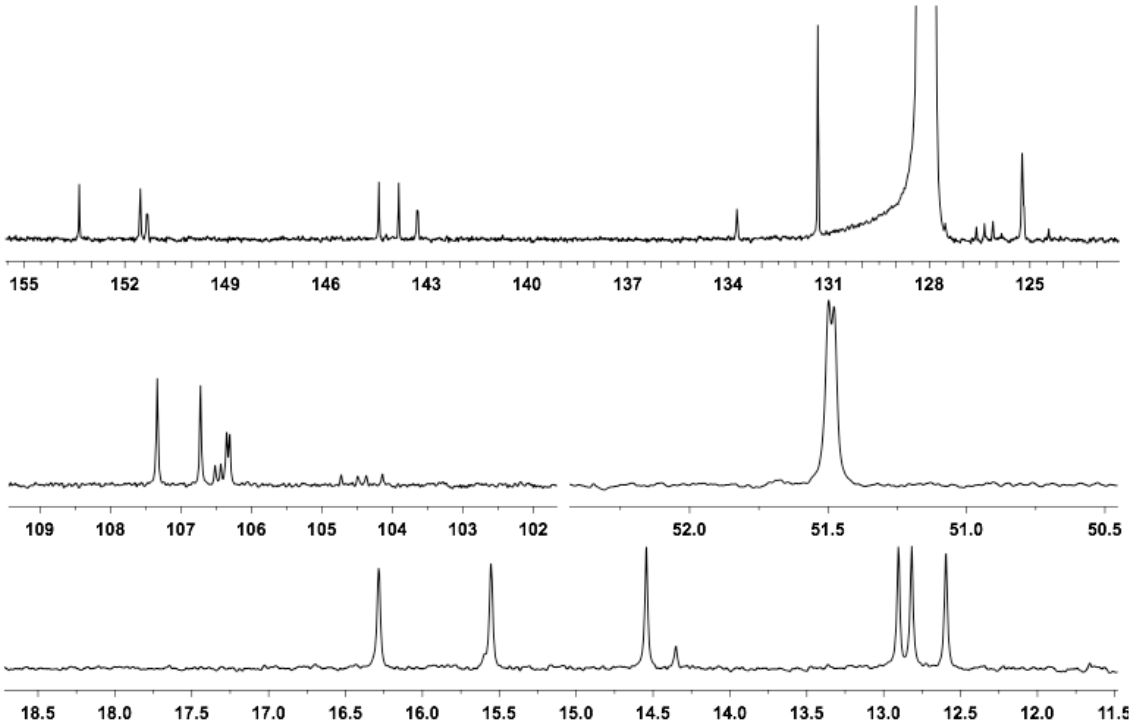


Figure S-47. $^{13}C\{^{1}H\}$ NMR of Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OCF_3)H **(6o)** in C_6D_6.

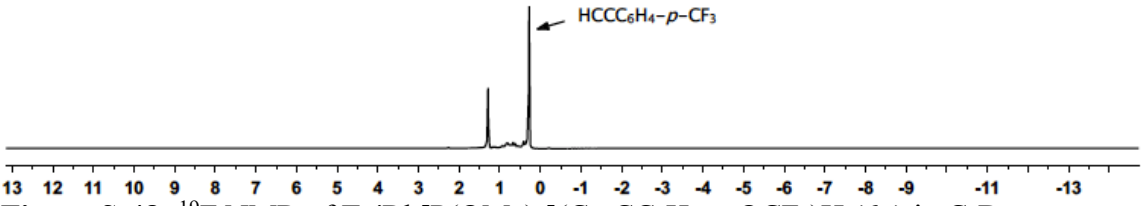


Figure S-48. ^{19}F NMR of Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OCF_3)H **(6o)** in C_6D_6.

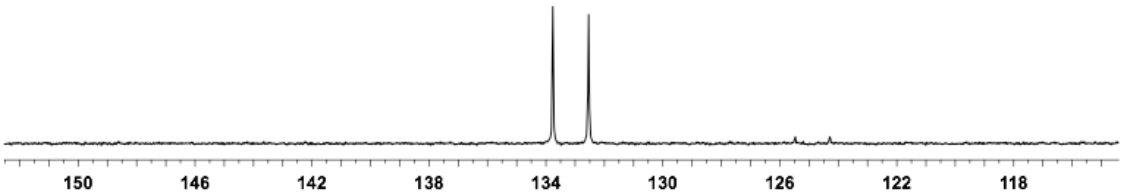


Figure S-49. $^{31}P\{^{1}H\}$ NMR of Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OCF_3)H **(6o)** in C_6D_6.

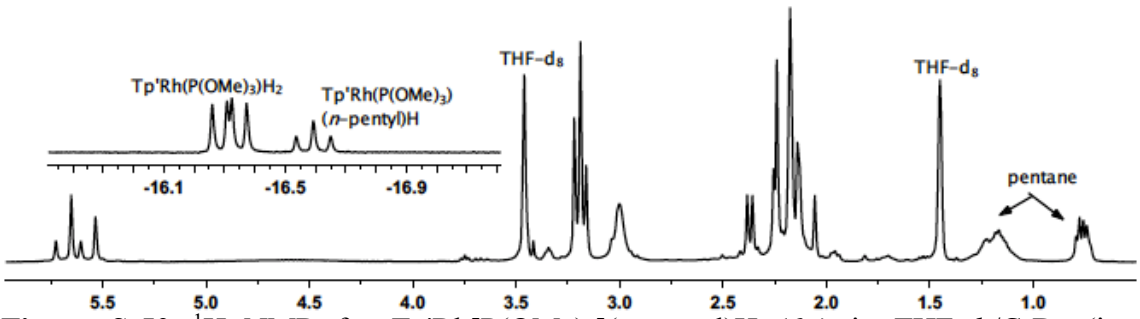


Figure S-50. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](n-pentyl)H **(6p)** in THF-d_8/C_6D_6 (in a

mixture with Tp'Rh[P(OMe)$_3$]H$_2$ **(2)**).

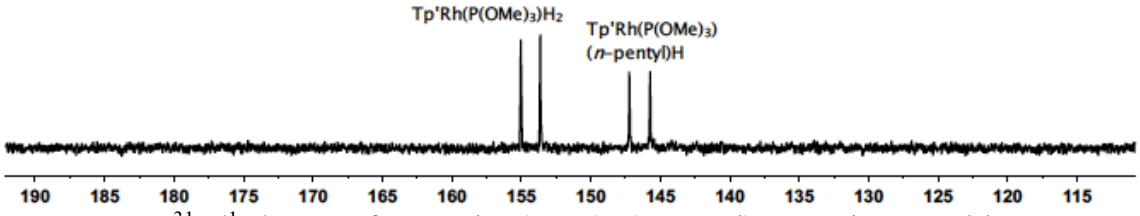


Figure S-51. $^{31}P\{^1H\}$ NMR for Tp'Rh[P(OMe)$_3$](*n*-pentyl)H **(6p)** in THF-d_8/C_6D_6**.**

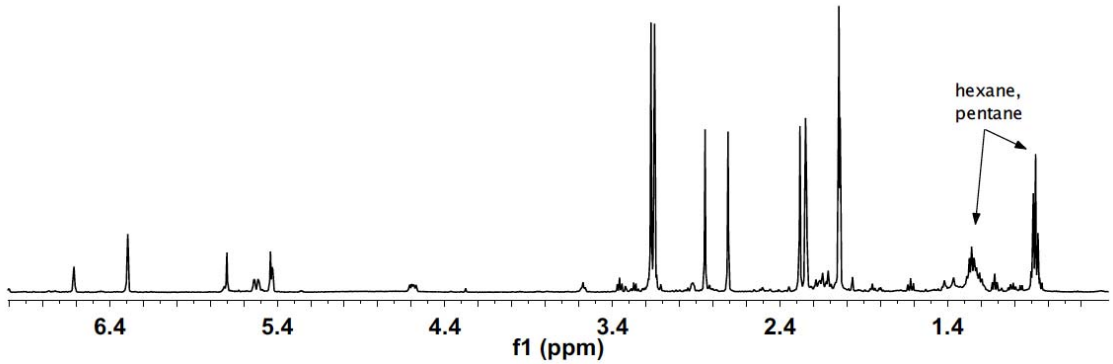


Figure S-52. ^1H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$)Br **(7b)** in C_6D_6.

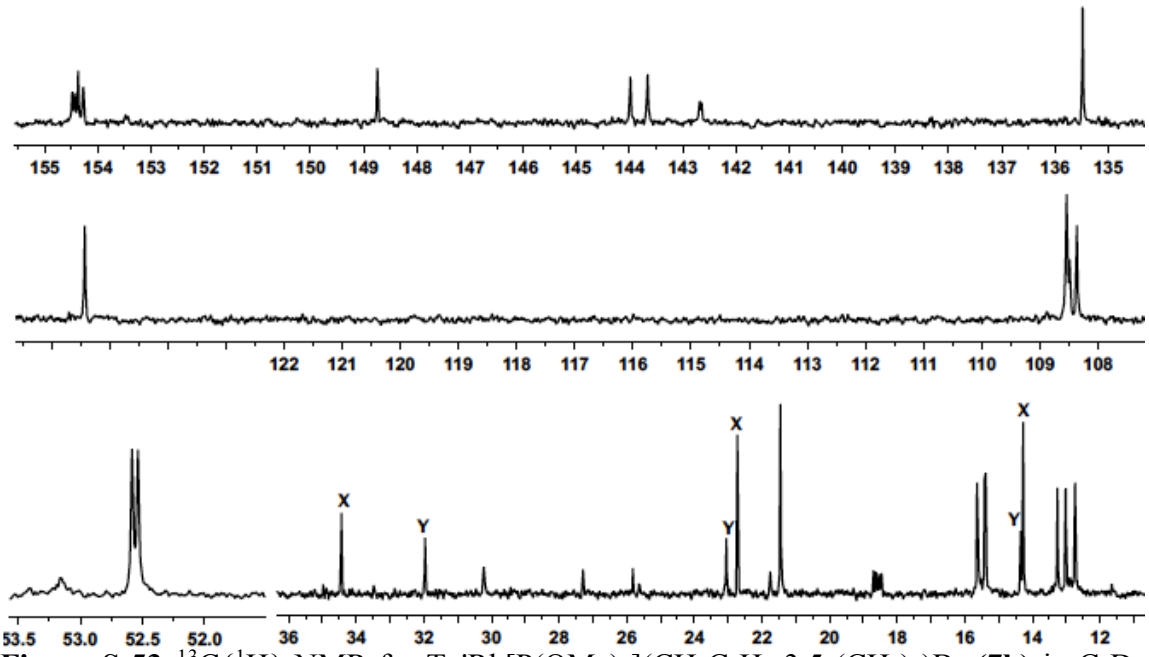


Figure S-53. $^{13}C\{^1H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$)Br **(7b)** in C_6D_6. **X** denotes *n*-pentane; **Y** denotes *n*-hexane.

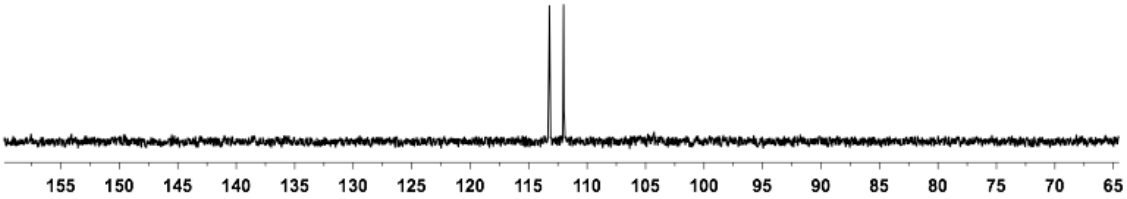


Figure S-54. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$)Br **(7b)** in C$_6$D$_6$.

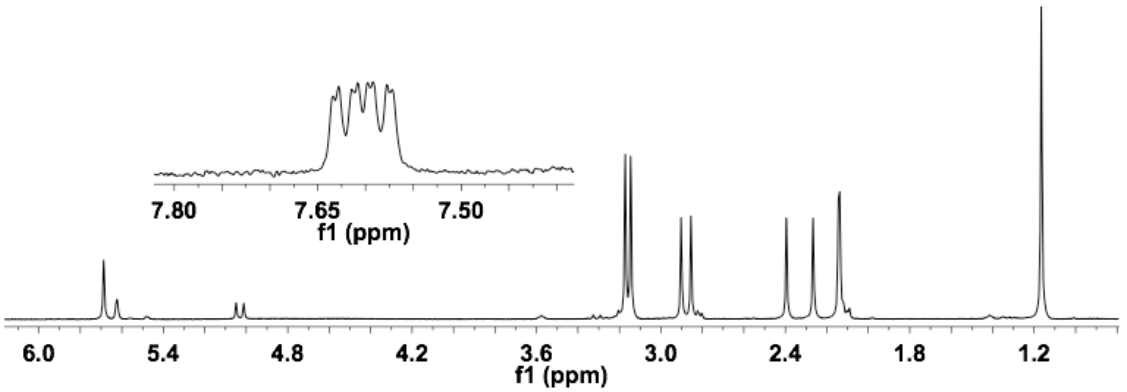


Figure S-55. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)Br **(7c)** in C$_6$D$_6$.

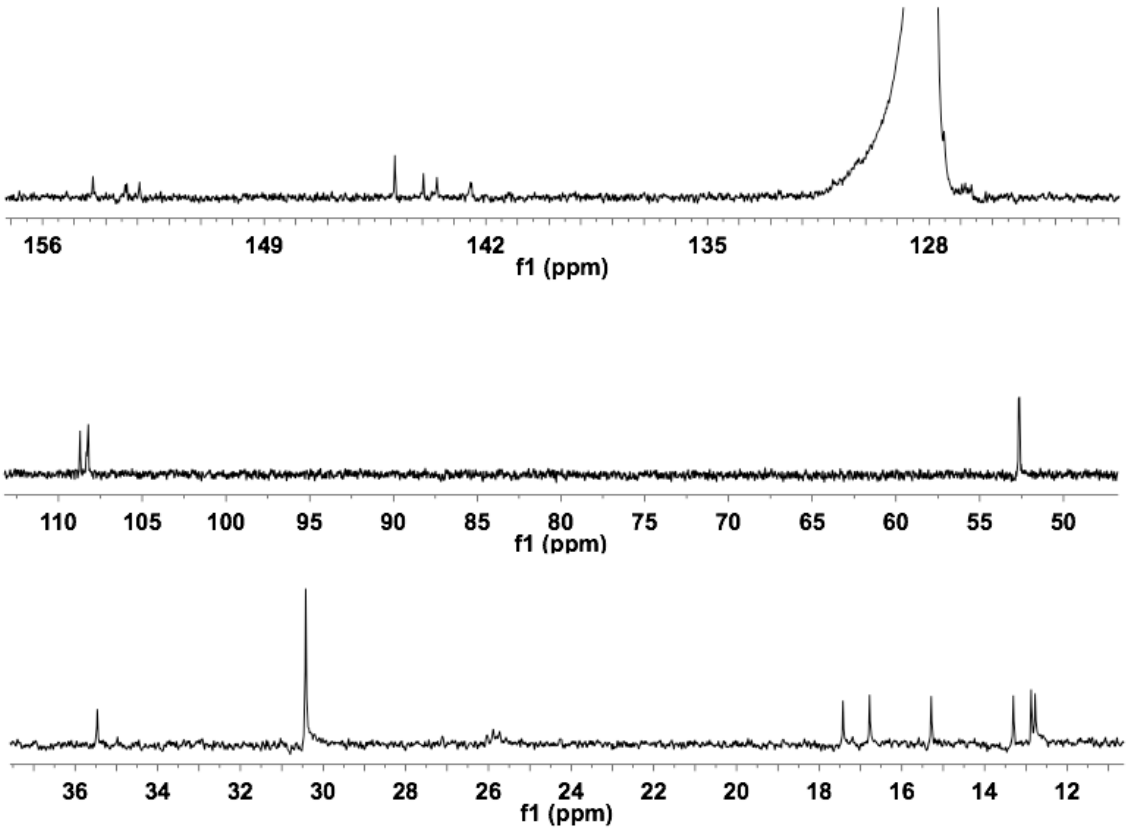


Figure S-56. $^{13}C\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)Br **(7c)** in C$_6$D$_6$.

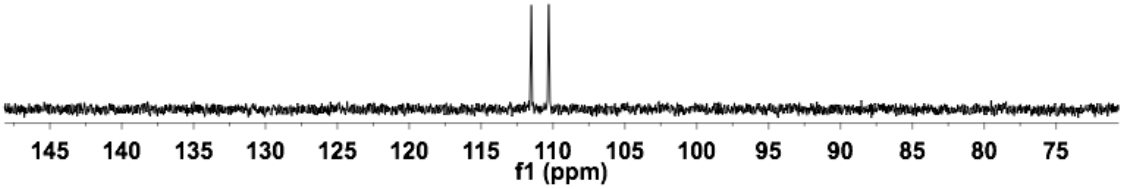


Figure S-57. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)Br **(7c)** in C_6D_6.

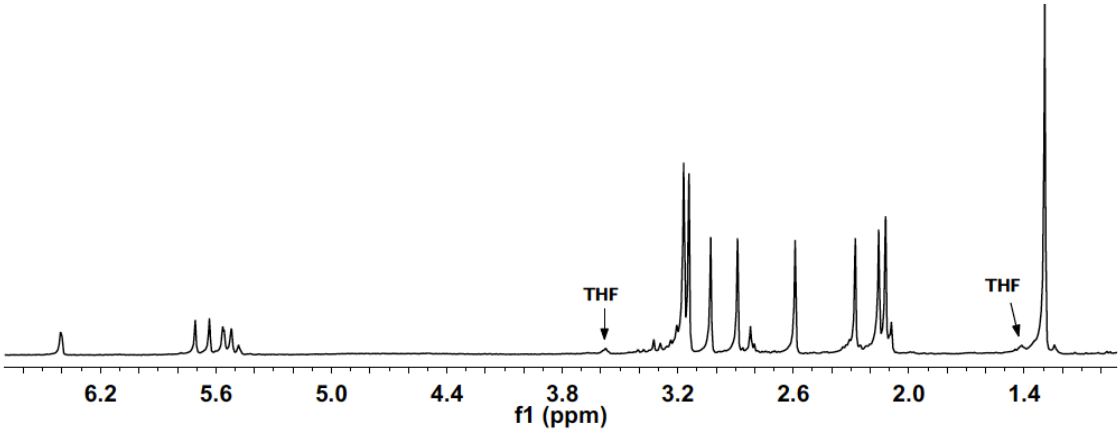


Figure S-58. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)Br **(7d)** in C_6D_6.

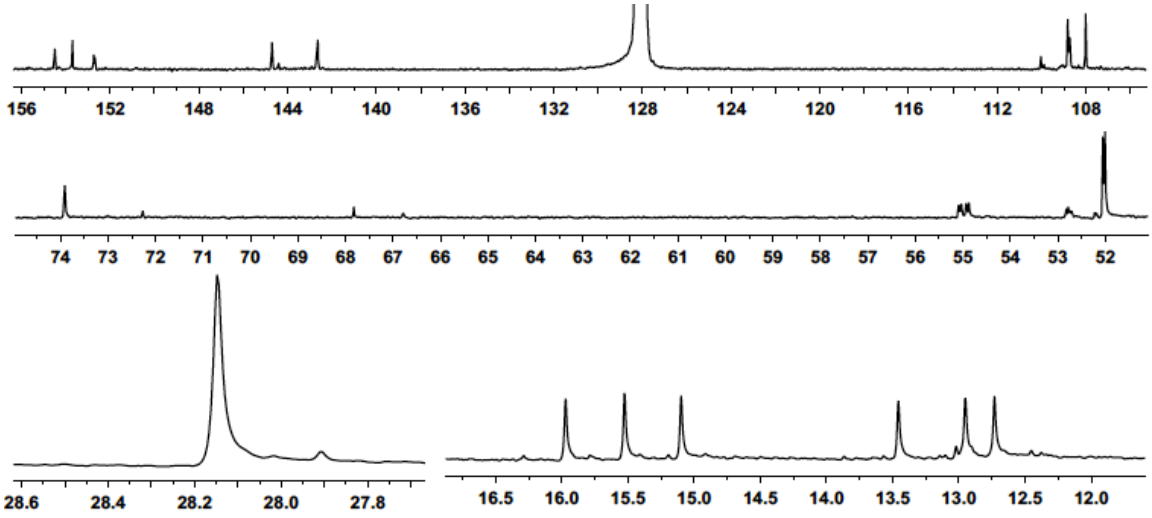


Figure S-59. $^{13}C\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)Br **(7d)** in C_6D_6.

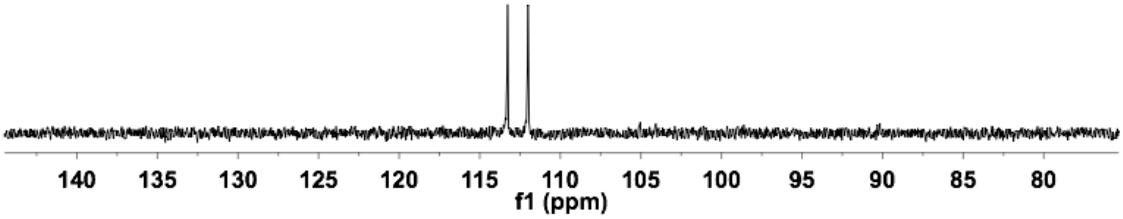


Figure S-60. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)Br **(7d)** in C$_6$D$_6$.

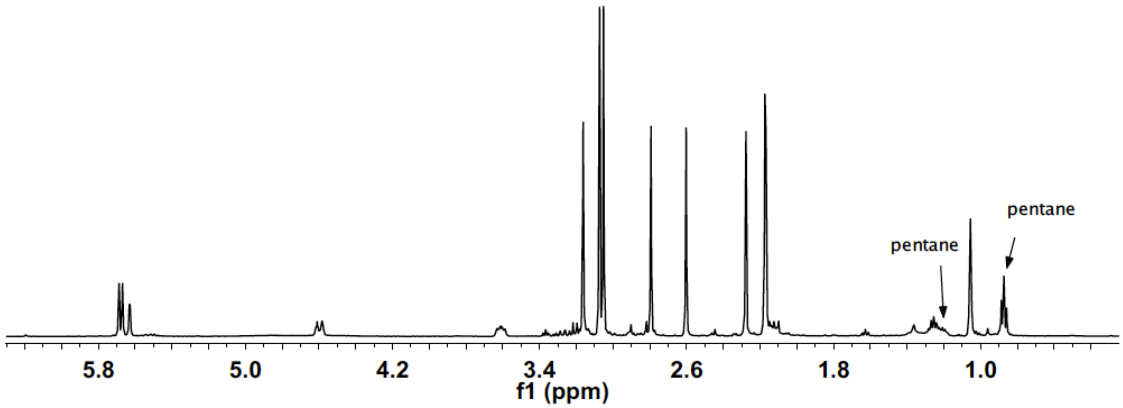


Figure S-61. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)Br **(7e)** in C$_6$D$_6$.

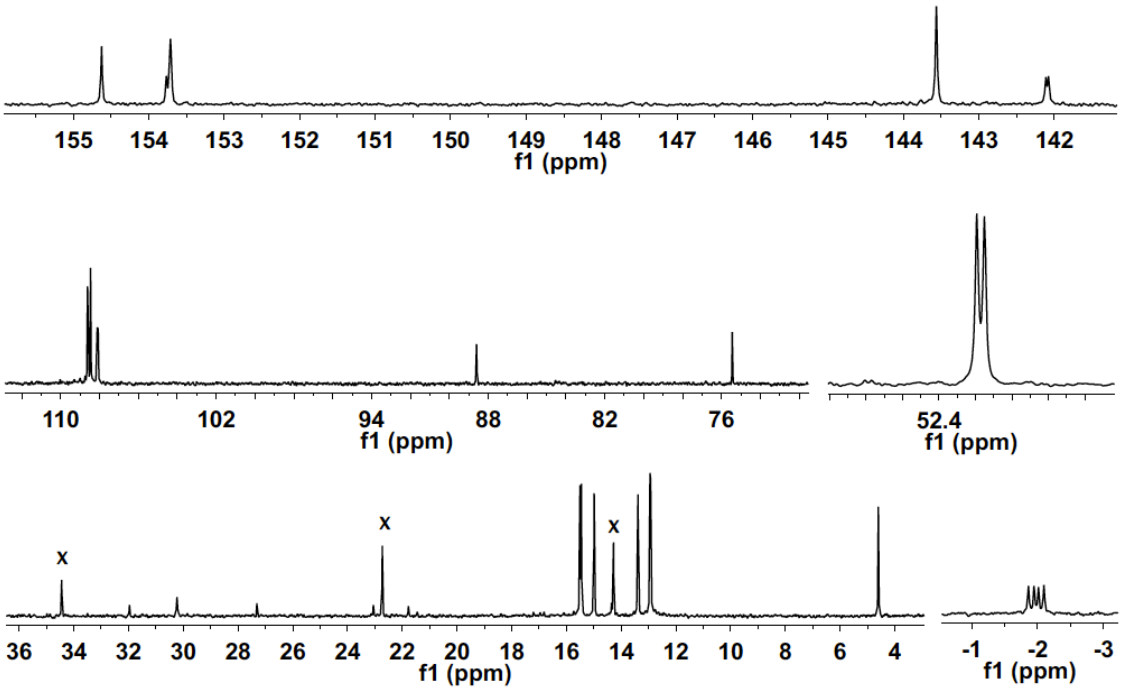


Figure S-62. $^{13}C\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)Br **(7e)** in C$_6$D$_6$. **X** denotes pentane.

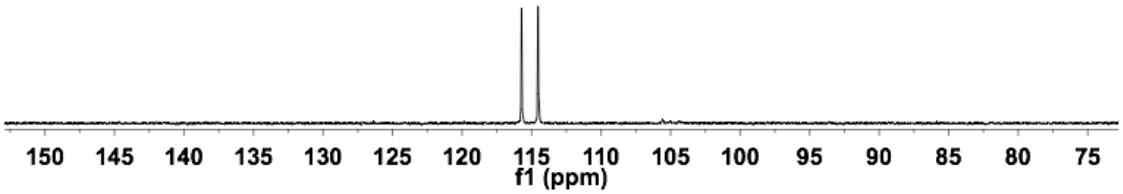


Figure S-63. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)Br **(7e)** in C$_6$D$_6$.

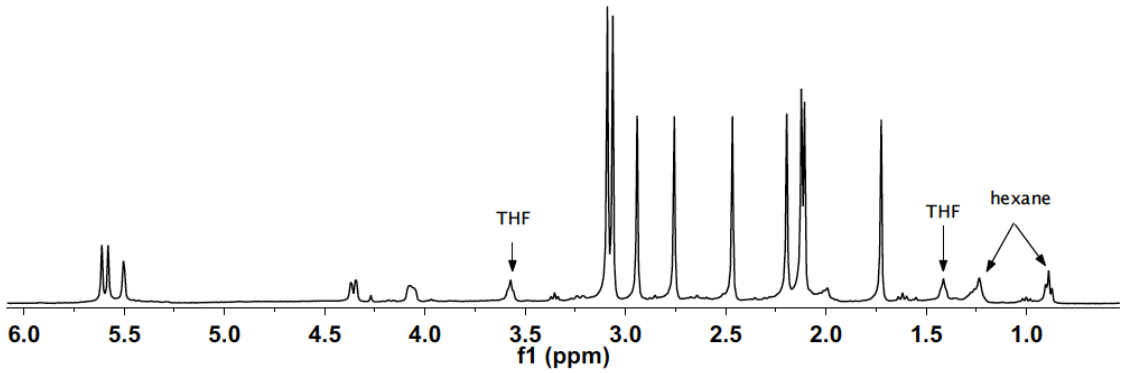


Figure S-64. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)Br **(7f)** in C_6D_6.

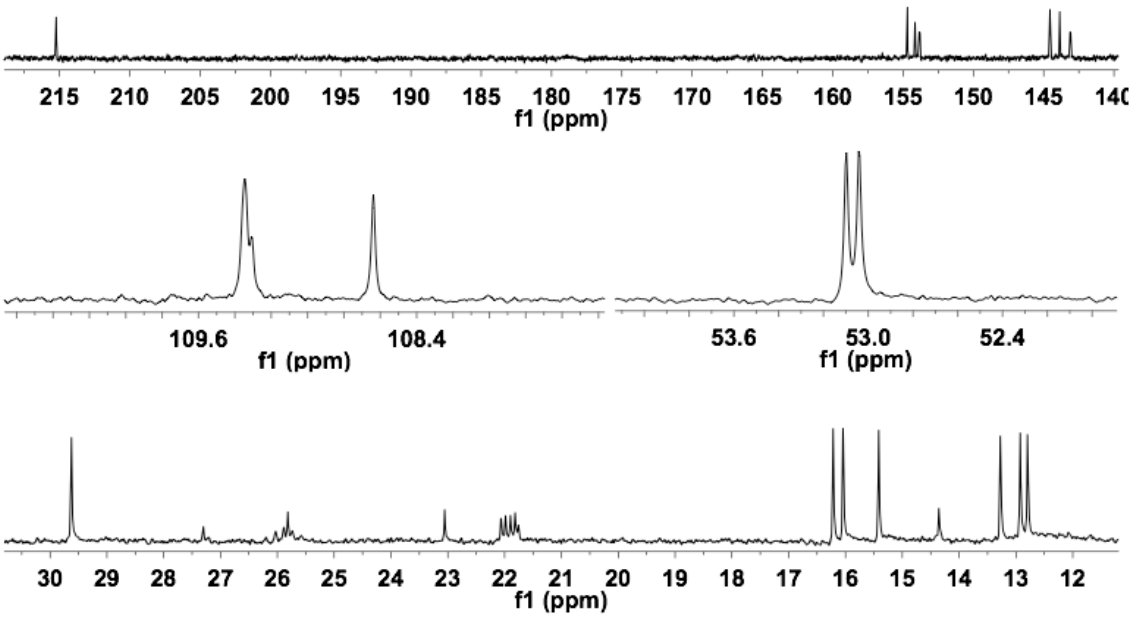


Figure S-65. $^{13}C\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)Br **(7f)** in C_6D_6.

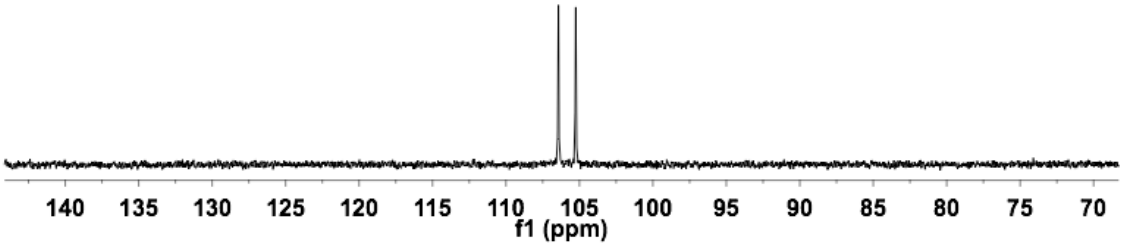


Figure S-66. $^{31}P\{^{1}H\}$ NMR for Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)Br **(7f)** in C_6D_6.

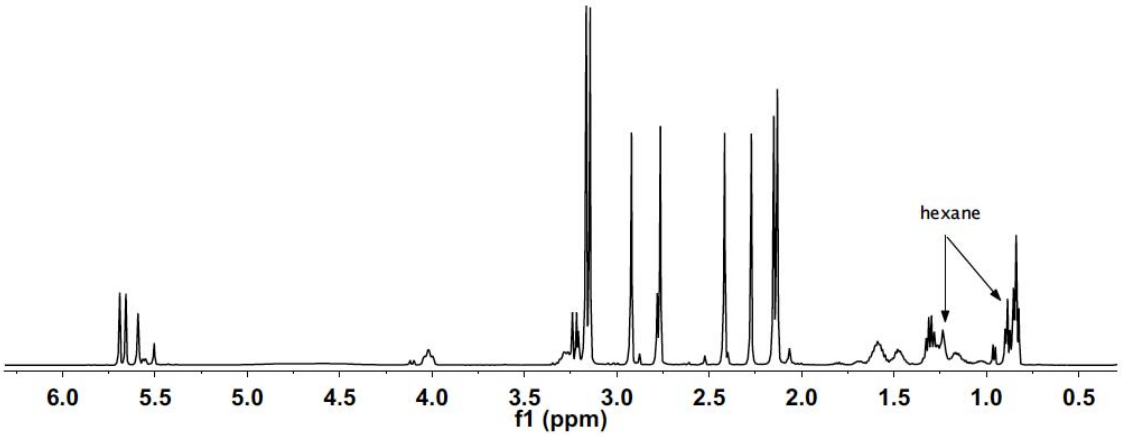


Figure S-67. ^{1}H NMR for Tp'Rh[P(OMe)$_3$](*n*-pentyl)Cl **(7p)** in C_6D_6.

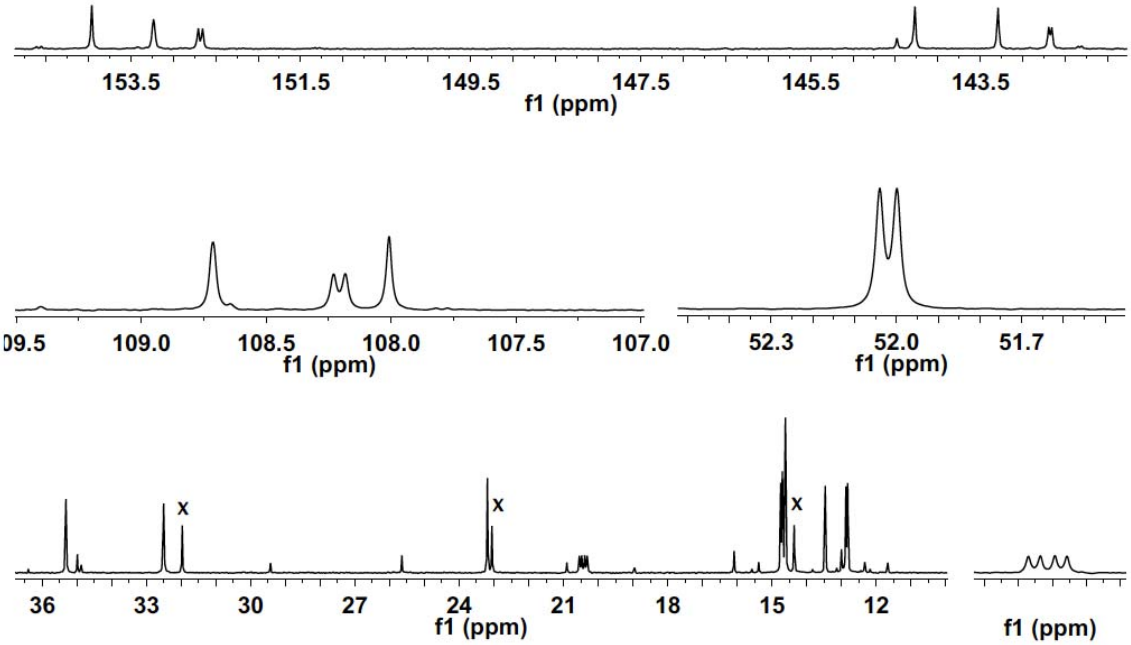


Figure S-68. ^{13}C{^{1}H} NMR for Tp'Rh[P(OMe)$_3$](*n*-pentyl)Cl **(7p)**. X denotes hexane.

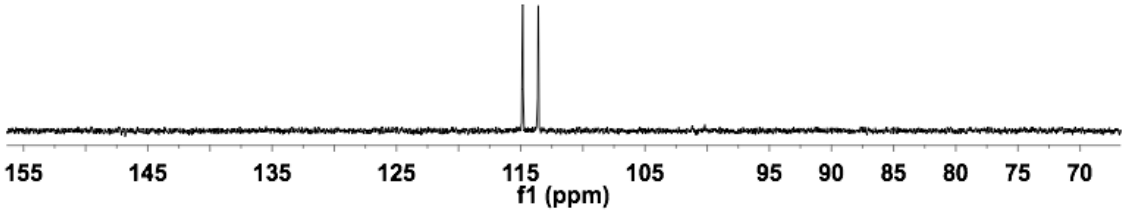


Figure S-69. ^{31}P{^{1}H} NMR for Tp'Rh[P(OMe)$_3$](*n*-pentyl)Cl **(7p)**.

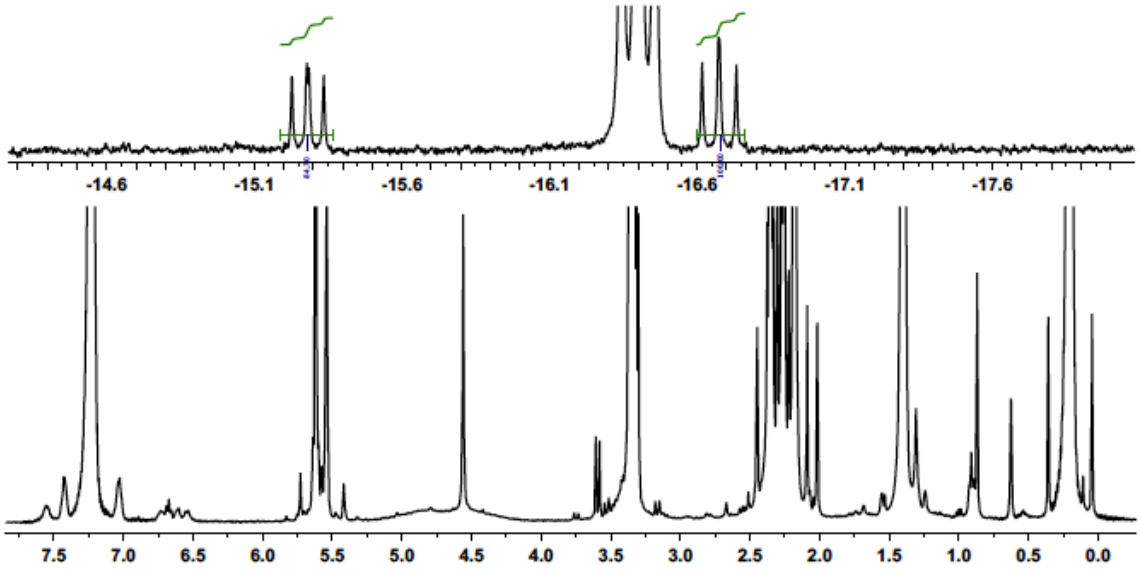


Figure S-70. ^{1}H NMR for competition between methane and benzene in C_6D_{12}.

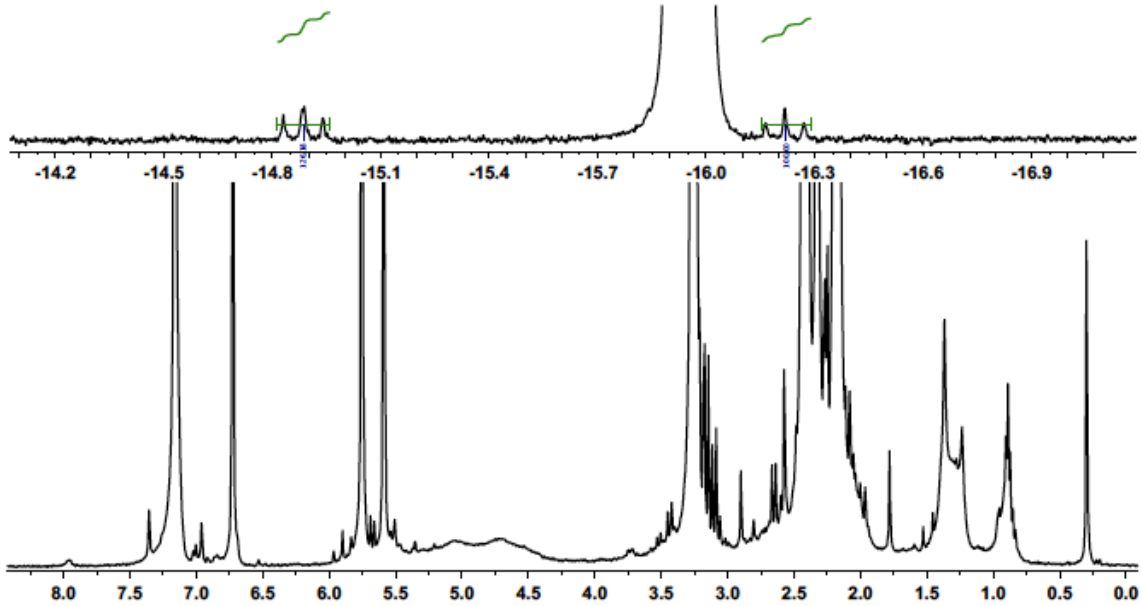


Figure S-71. ^{1}H NMR for competition between mesitylene and benzene.

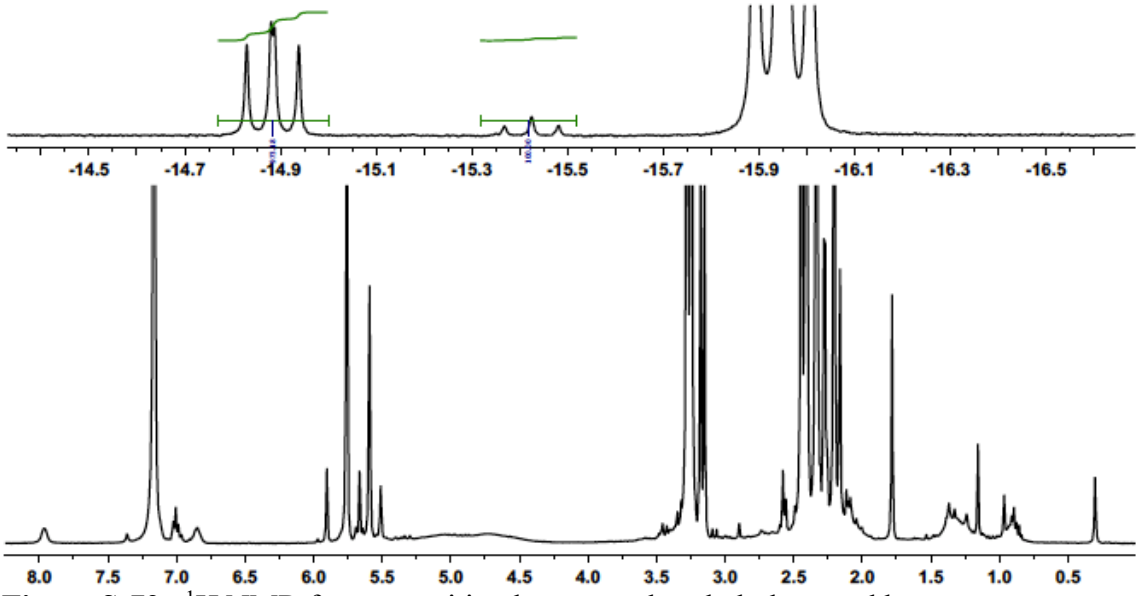


Figure S-72. ^{1}H NMR for competition between *t*-butylethylene and benzene.

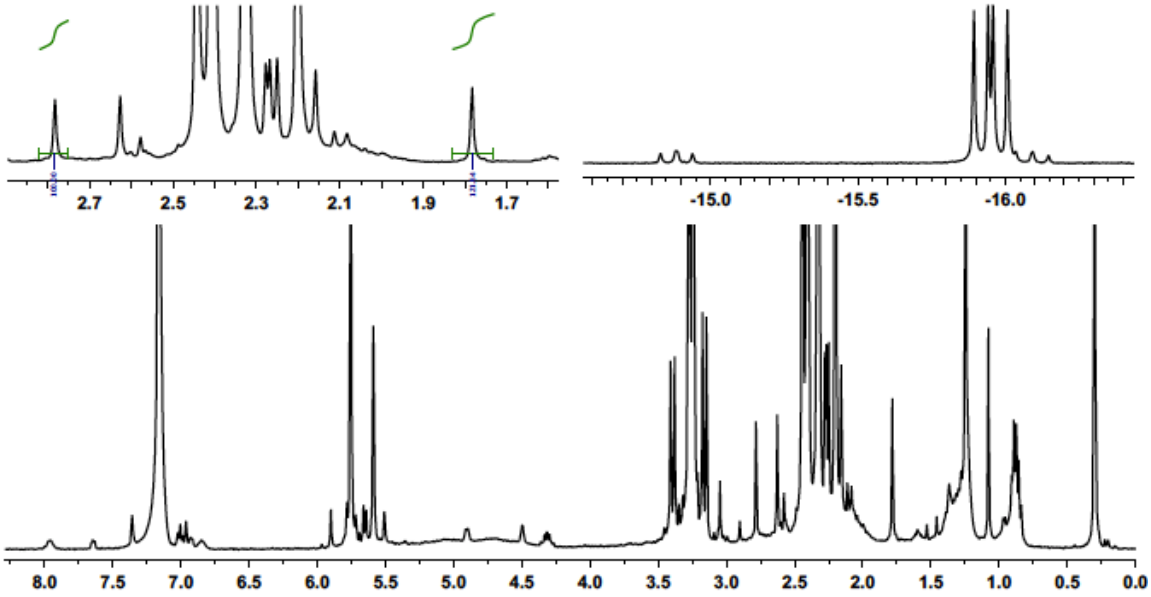


Figure S-73. ^{1}H NMR for competition between *t*-butylmethylether and benzene. Due to overlap of **6d** with **2** in hydride area, the ratio was calculated based on the integration of pzCH_3 area for **6d** and **6a** (integration from 2.750 to 2.820 for **6d**; 1.733 to 1.830 for **6a**). The ratio of **6a** and **6d** is 1.2164.

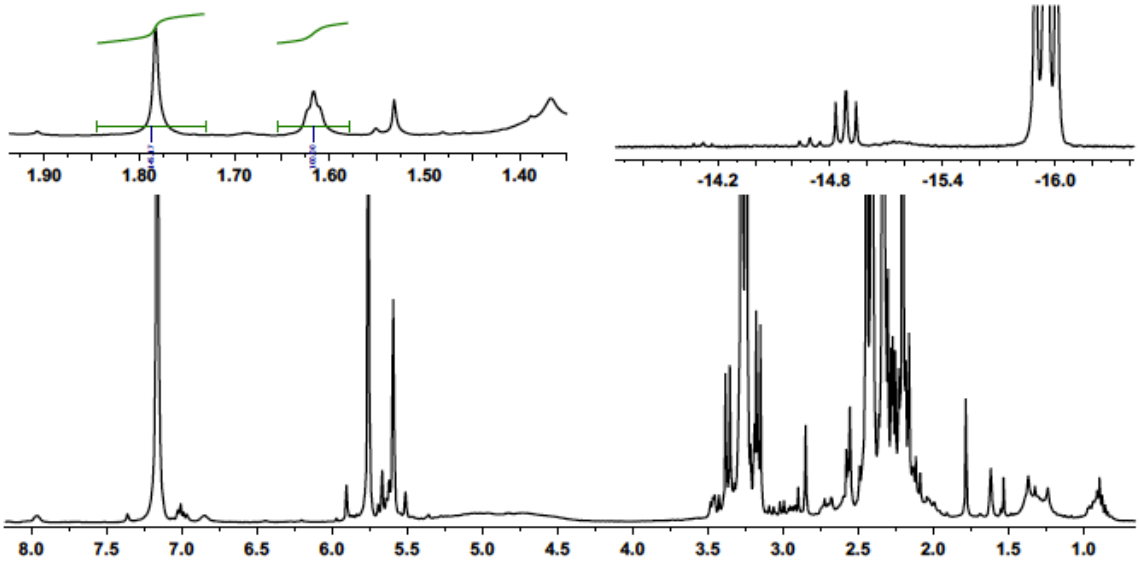


Figure S-74. ^{1}H NMR for competition between 2-butyne and benzene. Due to overlap of **6e** with **2** in hydride area, the ratio was calculated based on the integration of CH_3 area for **6e** and pzCH_3 area for **6a** (integration from 1.730 to 1.844 for **6a**; 1.579 to 1.655 for **6e**). The ratio of **6a** and **6e** is 1.4517.

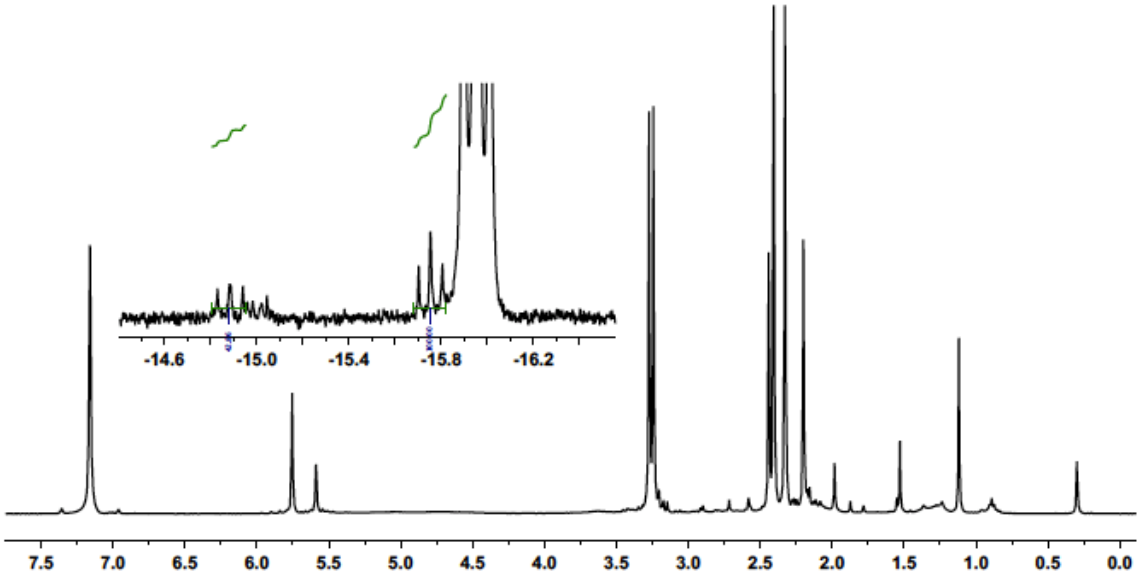


Figure S-75. ^{1}H NMR for competition between acetone and benzene.

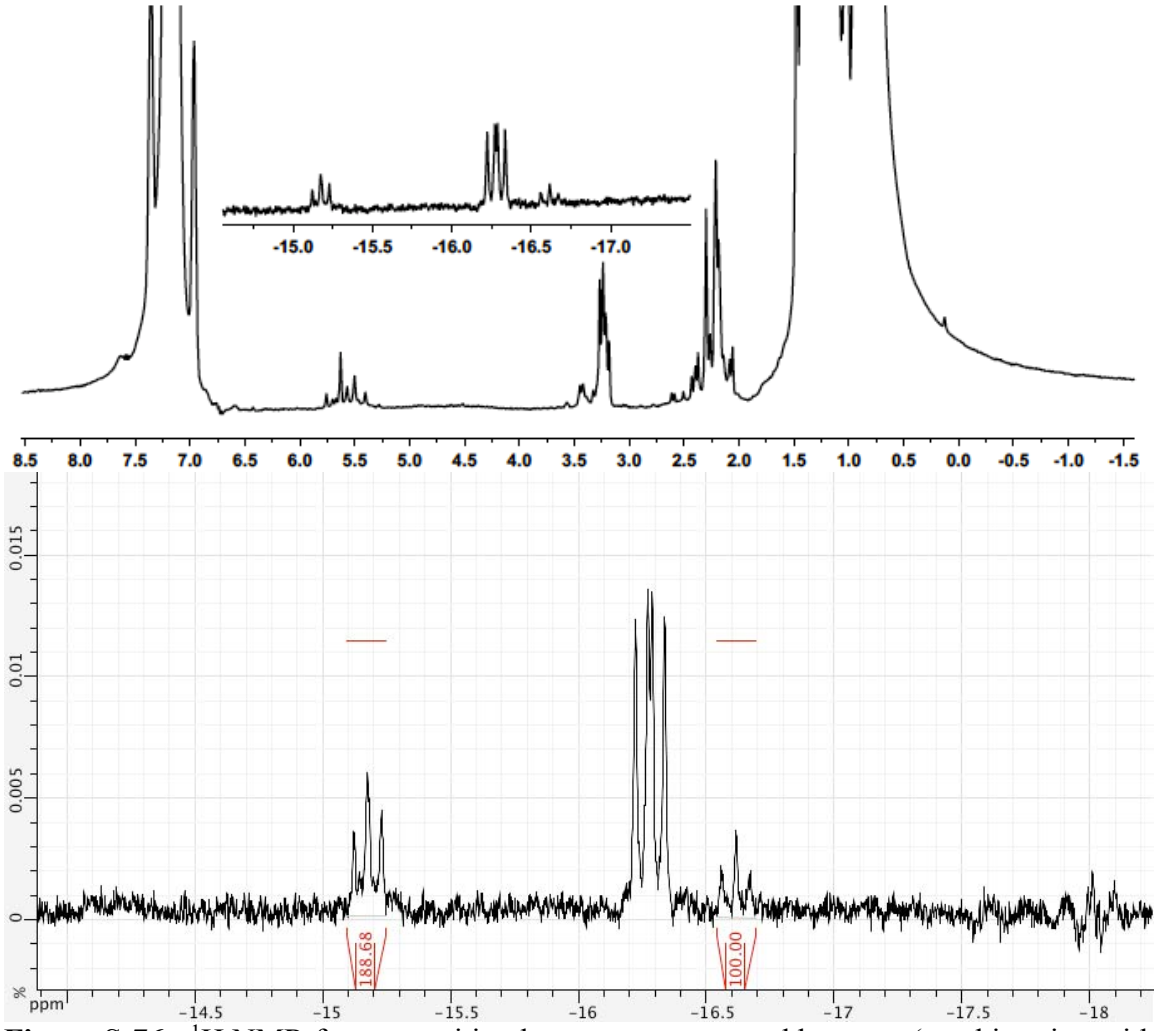


Figure S-76. ^{1}H NMR for competition between pentane and benzene (preshimming with C_6D_6).

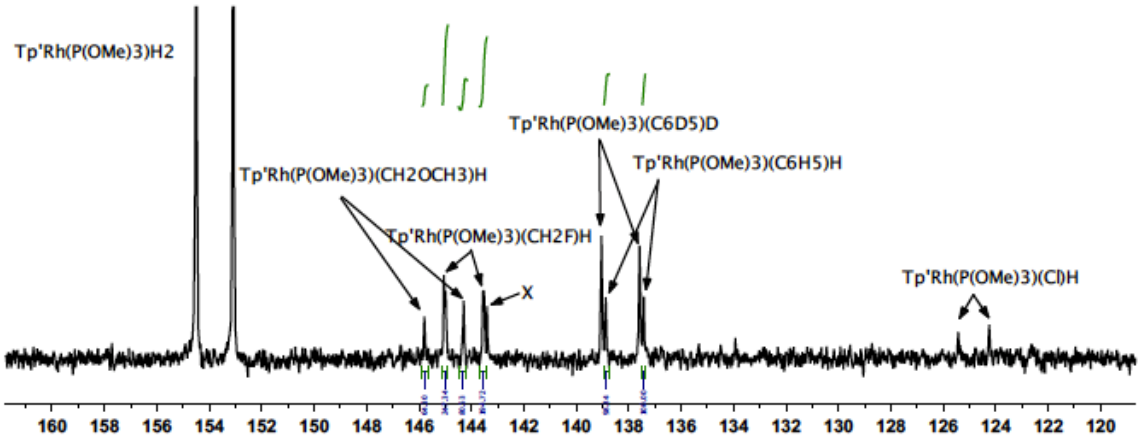


Figure S-77. $^{31}P\{^{1}H\}$ NMR for competition between fluoromethane, dimethylether and benzene (due to the ambiguity of assignment in ^{1}H NMR, integration of $^{31}P\{^{1}H\}$ NMR resonances is used instead to calculate the ratio of Tp'Rh(P(OMe)$_3$)(CH$_2$F)H **(6g)** and Tp'Rh(P(OMe)$_3$)(CH$_2$OMe)H **(6h)** relative to Tp'Rh(P(OMe)$_3$)(C$_6$H$_5$)H **(6a)**). **X** denotes

an unknow compound, which probably has a set of doublet signals (the other singlet peak is presumably overlapping with that of Tp'Rh(P(OMe)$_3$)(CH$_2$F)H **(6g)** at 145.05 ppm.

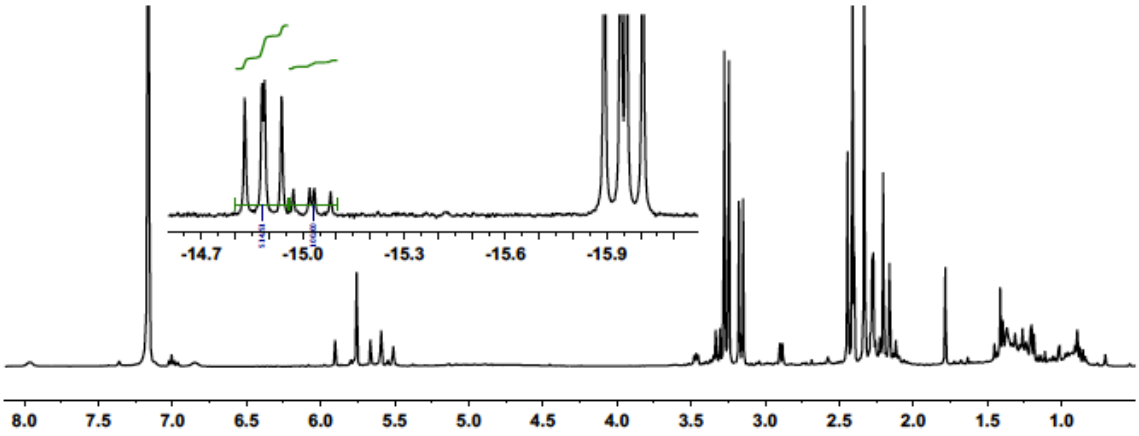


Figure S-78. ^{1}H NMR for competition between *t*-butylacetylene and benzene.

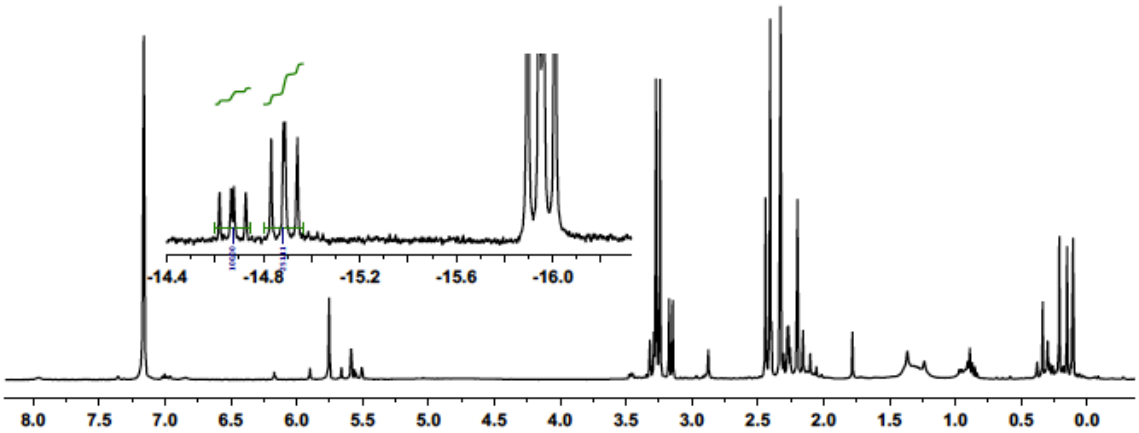
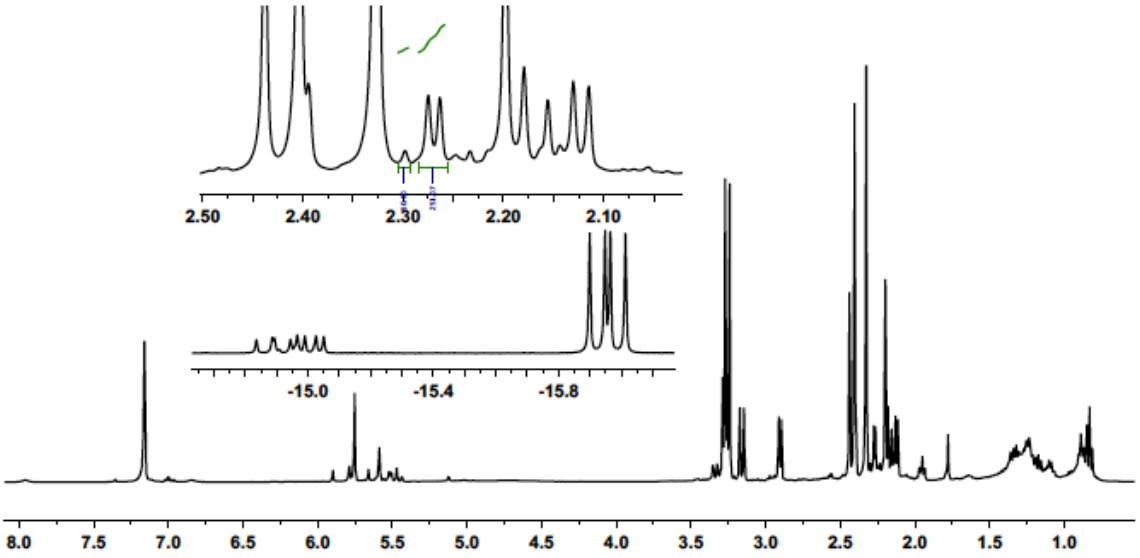


Figure S-79. ^{1}H NMR for competition between ethynyltrimethylsilane and benzene.



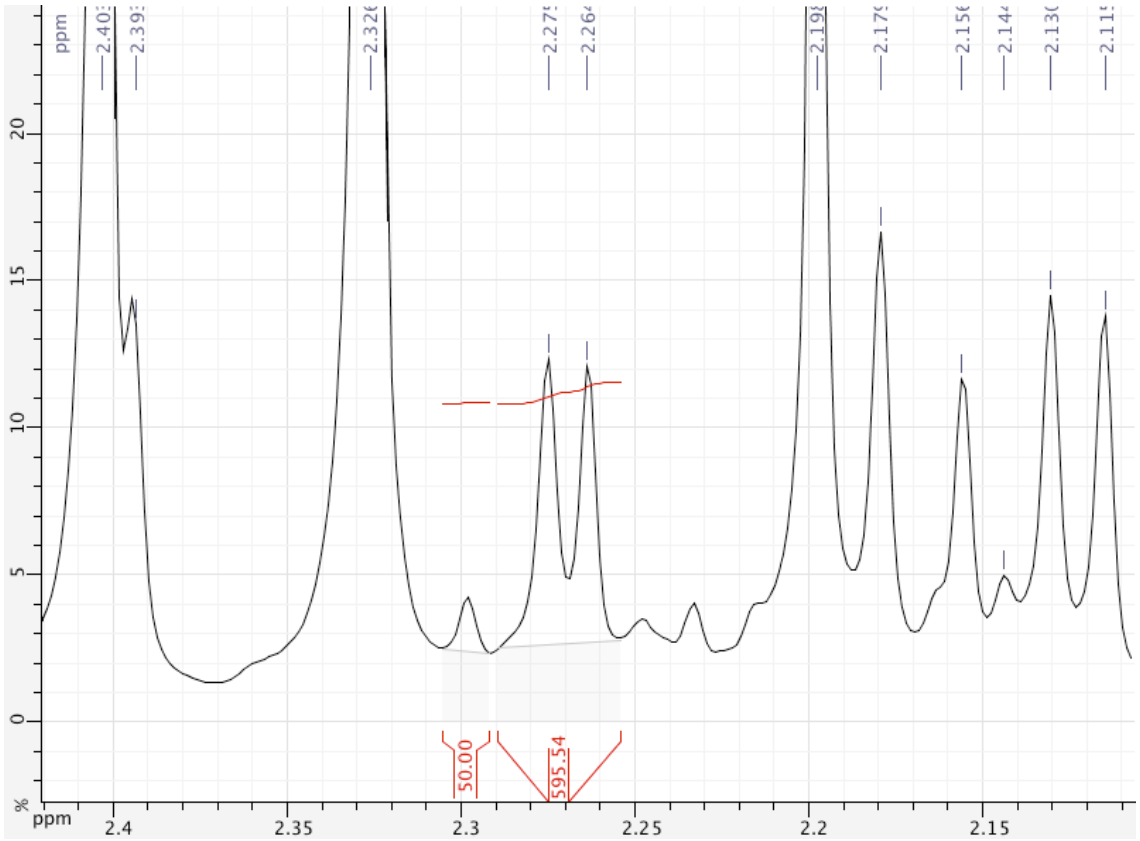


Figure S-80. ^{1}H NMR for competition between 1-octyne and benzene. Due to overlap of **6a** and **6k** in hydride area, the ratio was calculated based on the integration of pzCH_3 area for **6a** and **6k** (integration from 2.256 to 2.285 for **6a**; 2.292 to 2.305 for **6k**). The ratio of **6a** and **6k** is 5.9554.

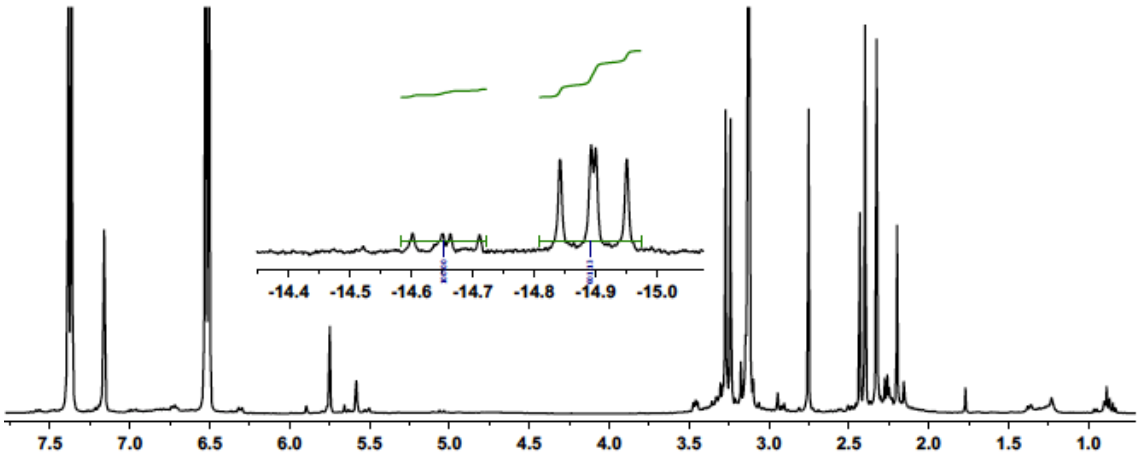


Figure S-81. ^{1}H NMR for competition between 4-ethynylanisole and benzene.

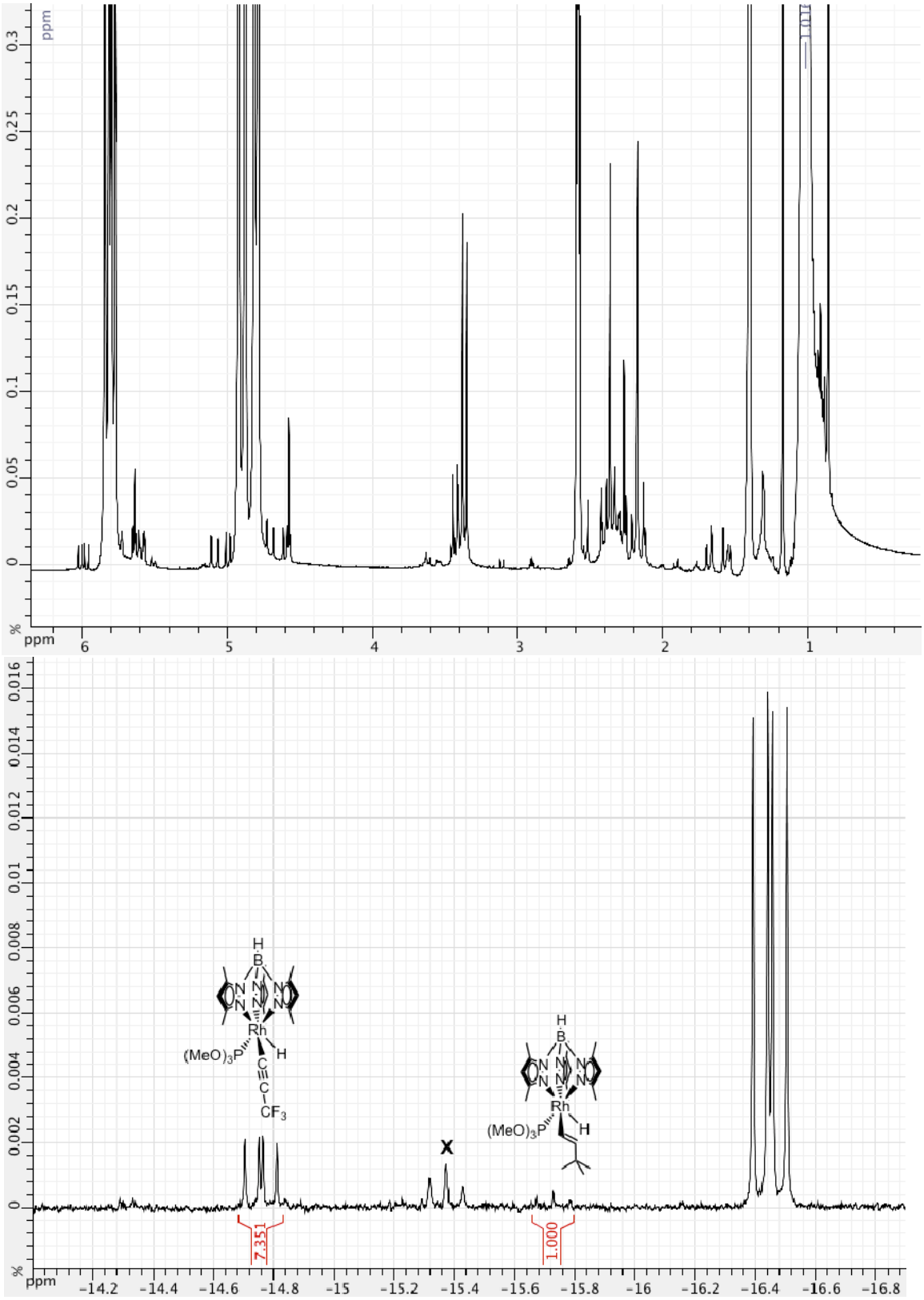


Figure S-82. ^{1}H NMR of 3,3,3-trifluoro-1-propyne vs *t*-butylethylene in C_6D_{12}. **X** denotes an unknown hydride.

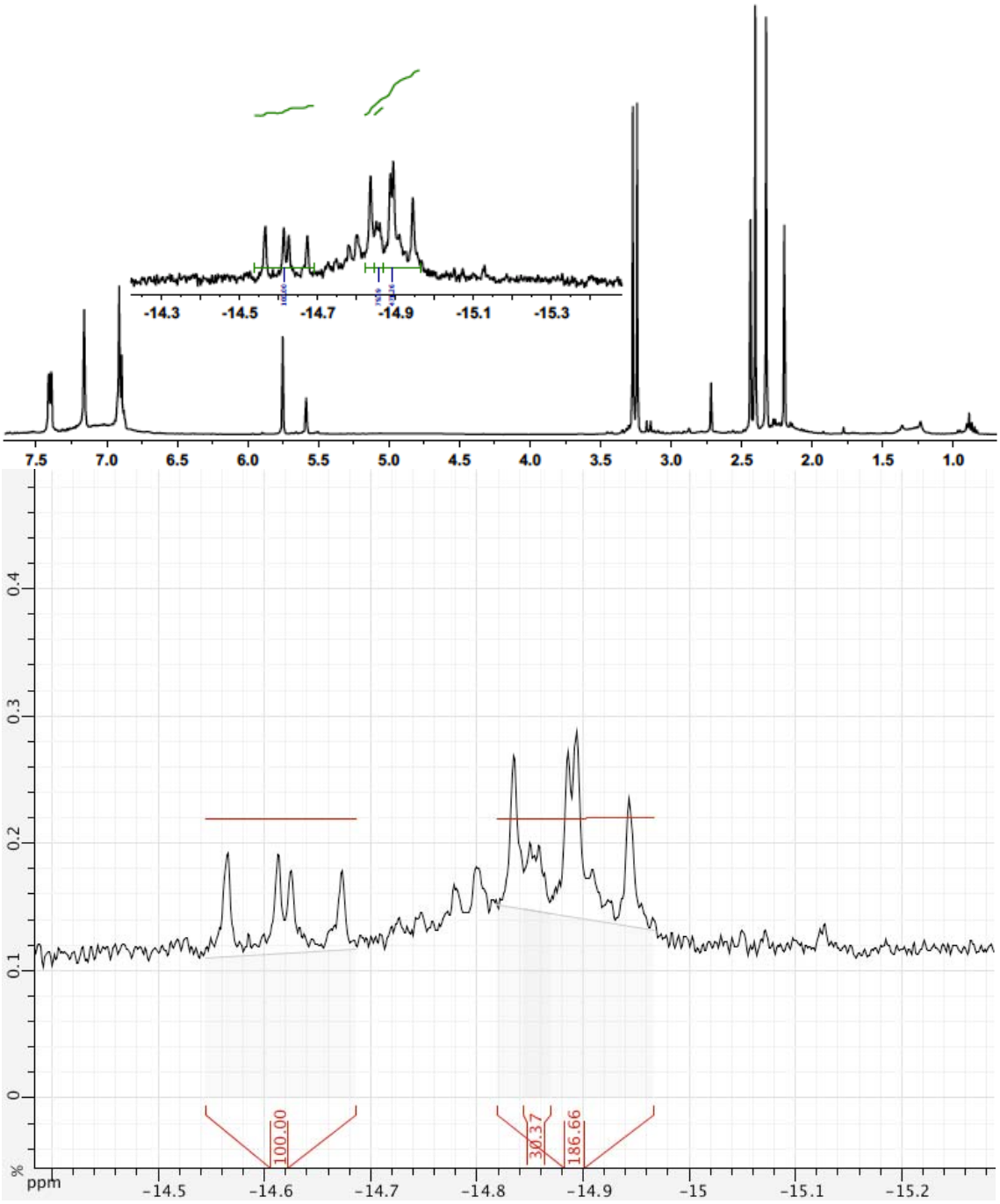


Figure S-83. ^{1}H NMR of phenylacetylene vs benzene. The ratio of **6a** and **6m** is approximately (1.8666-0.3037): 1 due to overlapping with an unknown hydride.

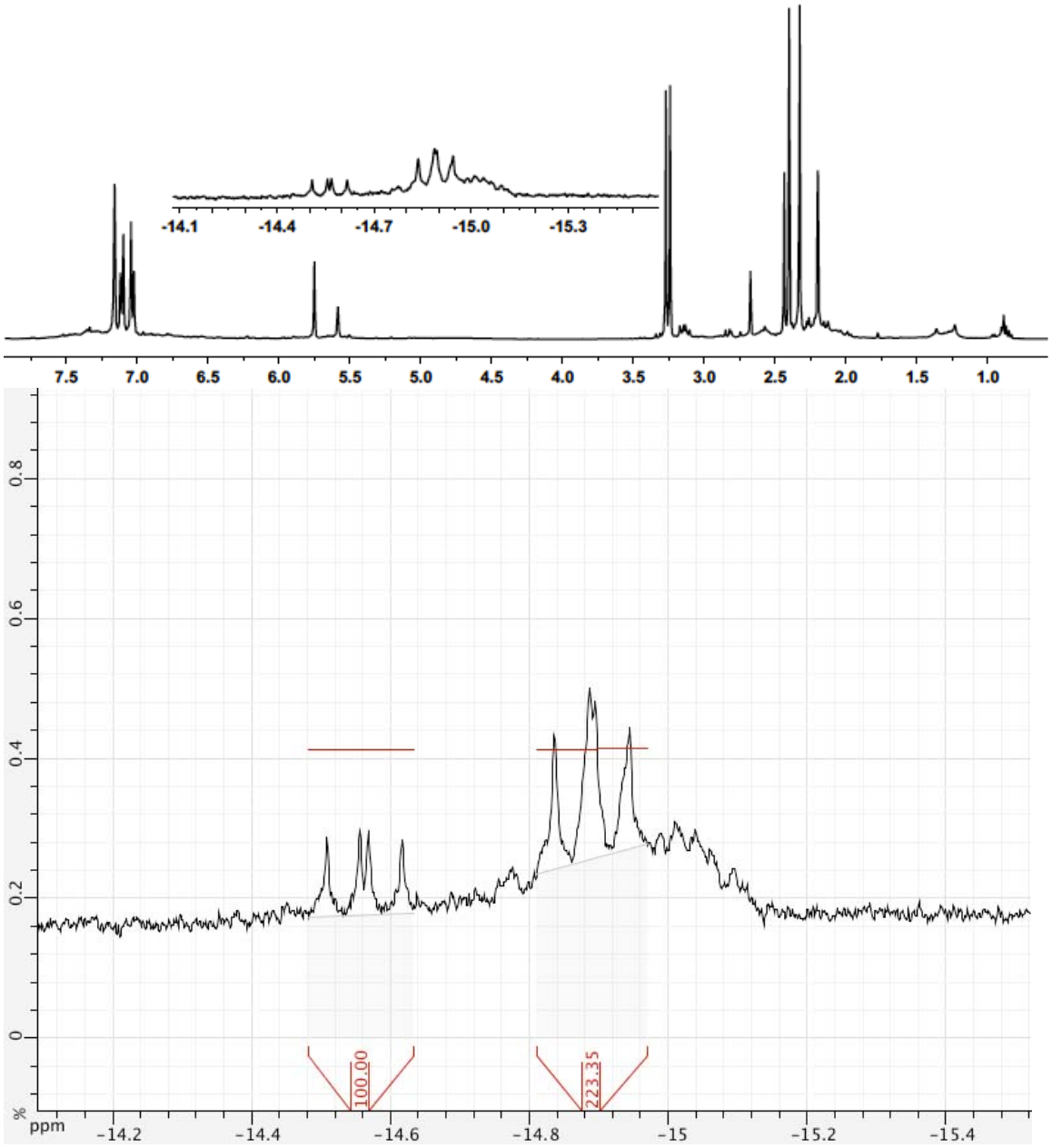


Figure S-84. ^{1}H NMR of 4-ethynyl-α,α,α-trifluorotoluene vs benzene.

Table S-3. Summary of kinetic selectivity data

substrate2: substrate 1	n_2: n_1	I_2: I_1	k_2: k_1	$\Delta\Delta G_{oa}^{\ddagger}$
benzene:methane	0.5781	0.8475	1.4660	0.2152
benzene: mesitylene	0.6852	1.2618	1.8416	0.3193
benzene: *t*-butylethylene	1.3891	9.7329	7.0066	1.0955
benzene: *t*-butyl methyl ether	0.4642	1.2164	2.6205	0.5038
benzene: 2-butyne	1.1489	1.4517	1.2636	0.1316
benzene: acetone	0.1548	0.4286	2.7689	0.5427
benzene: pentane	0.5556	1.8868	3.3961	0.6710
benzene: fluoromethane	0.6659	0.5051	0.7585	-0.1556
benzene: dimethylether	2.2642	1.4493	0.6401	-0.2510
benzene: *t*-butylacetylene	1.0536	5.1445	4.8826	0.8922
benzene: ethynyltrimethylsilane	0.7510	2.5111	3.3439	0.6792
benzene: 1-octyne	1.4271	5.9554	4.1731	0.8039
benzene: 4-ethynylanisole	2.2068	6.0107	2.7237	0.5638
t-butylethylene: 3,3,3-trifluoro-1-propyne	5.1870	0.1360	0.02623	-1.9040
benzene: phenylacetylene	1.1186	1.5629	1.3972	0.1882
benzene: 4-ethynyl-α,α,α-trifluorotoluene	1.8765	2.2335	1.1903	0.09801

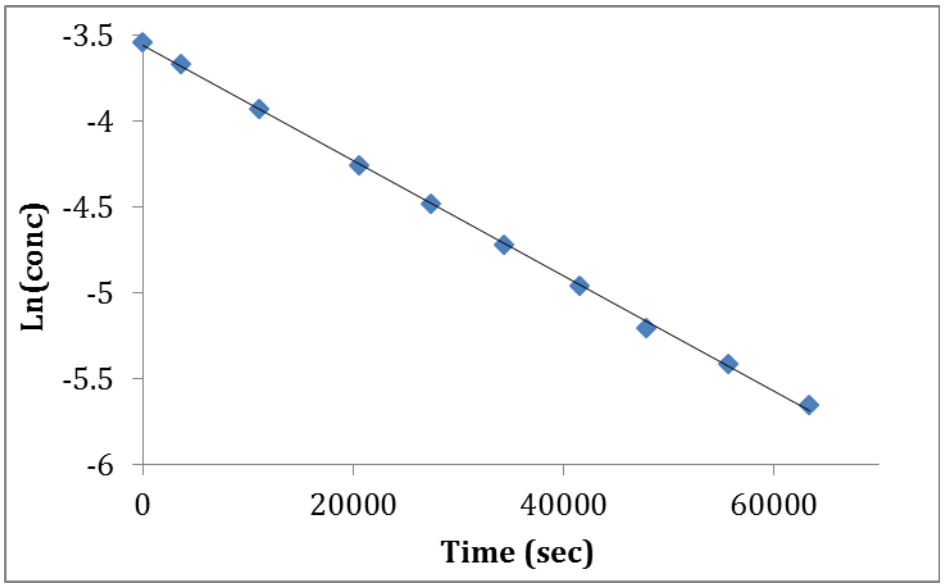


Figure S-85: Reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 70.0 °C.

Table S-4: Kinetic data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 70.0 °C. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	21.4127	-3.540350443
3600	18.873	-3.666602318
11010	14.5922	-3.923847508
20615	10.4599	-4.256785749
27335	8.3437	-4.482827884
34355	6.5949	-4.718038024
41555	5.1753	-4.960437339
47869	4.057	-5.203890863
55605	3.2802	-5.416430251
63355	2.5932	-5.651442013

Table S-5. Regression data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 70.0 °C.

Regression Statistics	
Multiple R	0.999656466
R Square	0.999313051
Adjusted R Square	0.999227182
Standard Error	0.02042887
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.856861555	4.856861555	11637.6964	6.09082E-14
Residual	8	0.00333871	0.000417339		
Total	9	4.860200265			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.55480812	0.011506939	-308.927336	1.3497E-17
Slope	-3.36476E-05	3.11904E-07	-107.8781553	6.09082E-14

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.581343169	-3.52827307	-3.581343169	-3.52827307
-3.43668E-05	-3.29283E-05	-3.43668E-05	-3.29283E-05

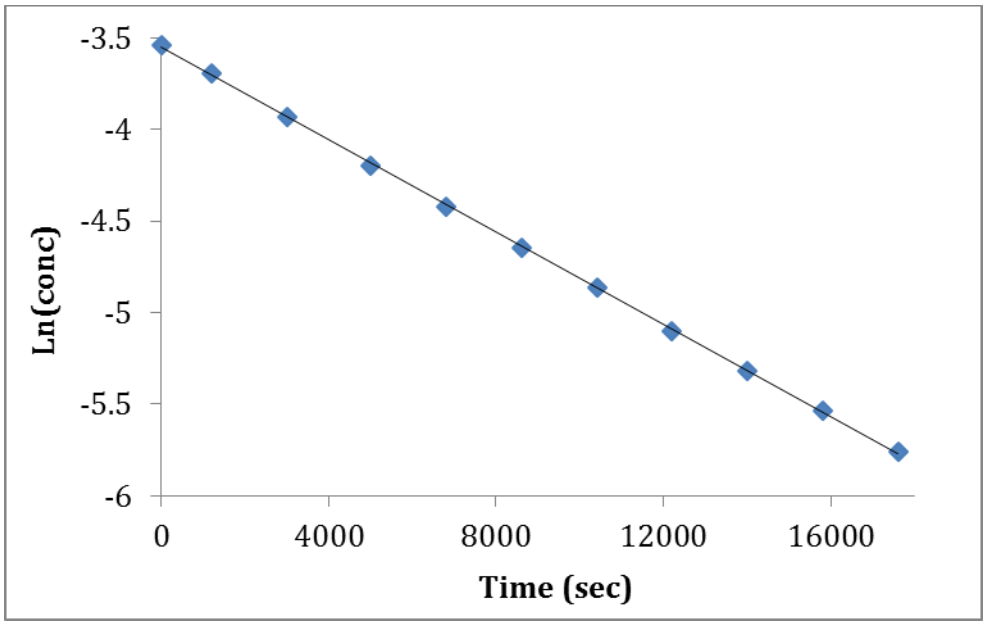


Figure S-86: Reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 80.0 °C.

Table S-6: Kinetic data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 80.0 °C. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	24.9791	-3.540350443
1200	21.4785	-3.691337483
3000	16.8973	-3.931236072
5010	12.9893	-4.194263977
6810	10.3475	-4.421644974
8610	8.2878	-4.643605364
10410	6.6451	-4.864510177
12210	5.2575	-5.09873429
14010	4.2174	-5.319171094
15810	3.3905	-5.537412515
17610	2.7125	-5.760519199

Table S-7. Regression data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 80.0 °C.

Regression Statistics	
Multiple R	0.99992897
R Square	0.999857945
Adjusted R Square	0.999842162
Standard Error	0.009435767
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.640009179	5.640009179	63346.90078	1.25561E-18
Residual	9	0.000801303	8.90337E-05		
Total	10	5.640810482			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.551578757	0.005165178	-687.6004959	1.48187E-22
Slope	-1.26061E-04	5.0086E-07	-251.6881022	1.25561E-18

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.563263201	-3.539894313	-3.563263201	-3.539894313
-1.27194E-04	-1.24928E-04	-1.27194E-04	-1.24928E-04

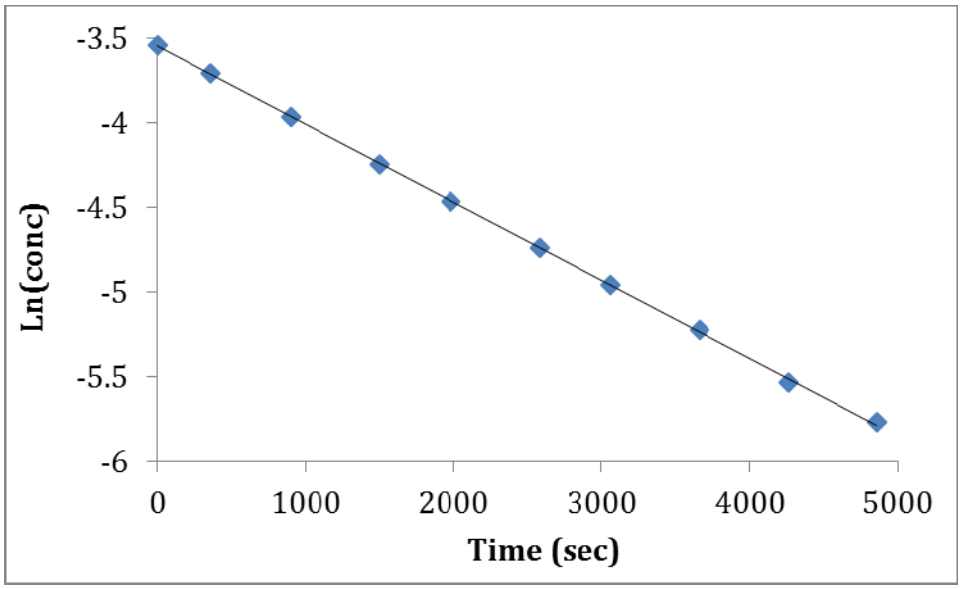


Figure S-87. Reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 90.0 °C.

Table S-8. Kinetic data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 90.0 °C. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	28.6911	-3.540350443
360	24.2074	-3.710279042
900	18.8072	-3.962697638
1500	14.1422	-4.247774178
1980	11.401	-4.463236342
2580	8.6787	-4.736065665
3060	6.9611	-4.956599905
3660	5.3255	-5.224430809
4260	3.9228	-5.530131729
4860	3.1067	-5.763376344

Table S-9. Regression data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 90.0 °C.

Regression Statistics	
Multiple R	0.999889224
R Square	0.99977846
Adjusted R Square	0.999750767
Standard Error	0.012018205
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.214586504	5.214586504	36102.7806	6.58732E-16
Residual	8	0.001155498	0.000144437		
Total	9	5.215742002			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.548364046	0.006772589	-523.9302275	1.97235E-19
Slope	-4.59901E-04	2.42044E-06	-190.0073172	6.58732E-16

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.563981664	-3.532746428	-3.563981664	-3.532746428
-4.65482E-04	-4.54319E-04	-4.65482E-04	-4.54319E-04

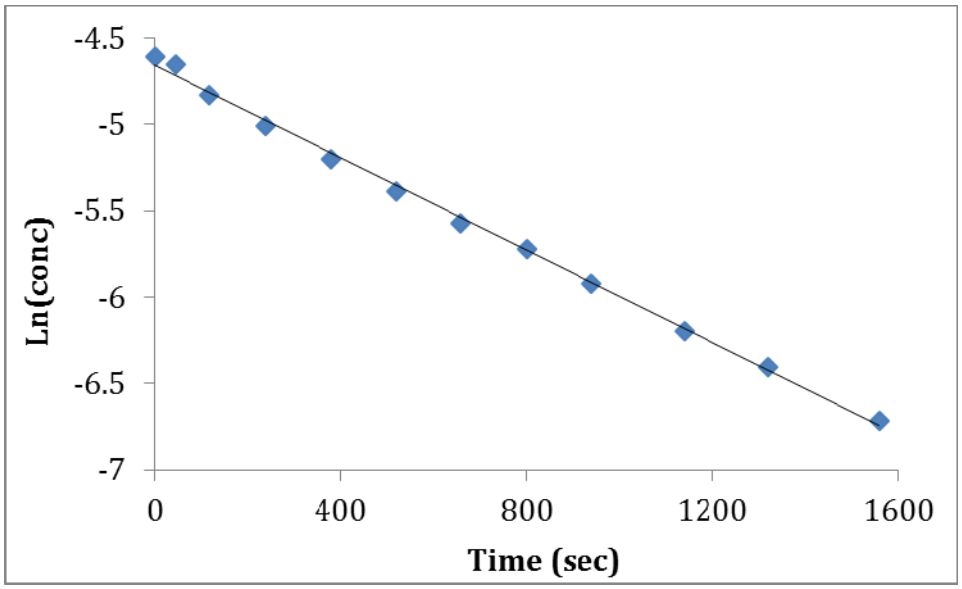


Figure S-88: Reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 100.0 °C.

Table S-10: Kinetic data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 100.0 °C. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	8.9777	-4.608285052
46	8.5655	-4.655286269
120	7.1925	-4.82998996
240	6.0184	-5.008207333
380	4.9624	-5.201139282
520	4.1073	-5.390262898
660	3.4168	-5.574324336
800	2.9387	-5.72506147
940	2.4172	-5.920418931
1140	1.8328	-6.197183924
1320	1.4904	-6.403984236
1560	1.0942	-6.713005274

Table S-11. Regression data for reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)** at 100.0 °C.

Regression Statistics	
Multiple R	0.998784654
R Square	0.997570786
Adjusted R Square	0.997327864
Standard Error	0.035895379
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.291209341	5.291209341	4106.557059	2.08387E-14
Residual	10	0.012884782	0.001288478		
Total	11	5.304094124			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-4.656586762	0.016984045	-274.1741849	1.02464E-20
Slope	-1.33939E-03	2.0901E-05	-64.08242395	2.08387E-14

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-4.694429573	-4.618743951	-4.694429573	-4.618743951
-1.38596E-03	-1.29282E-03	-1.38596E-03	-1.29282E-03

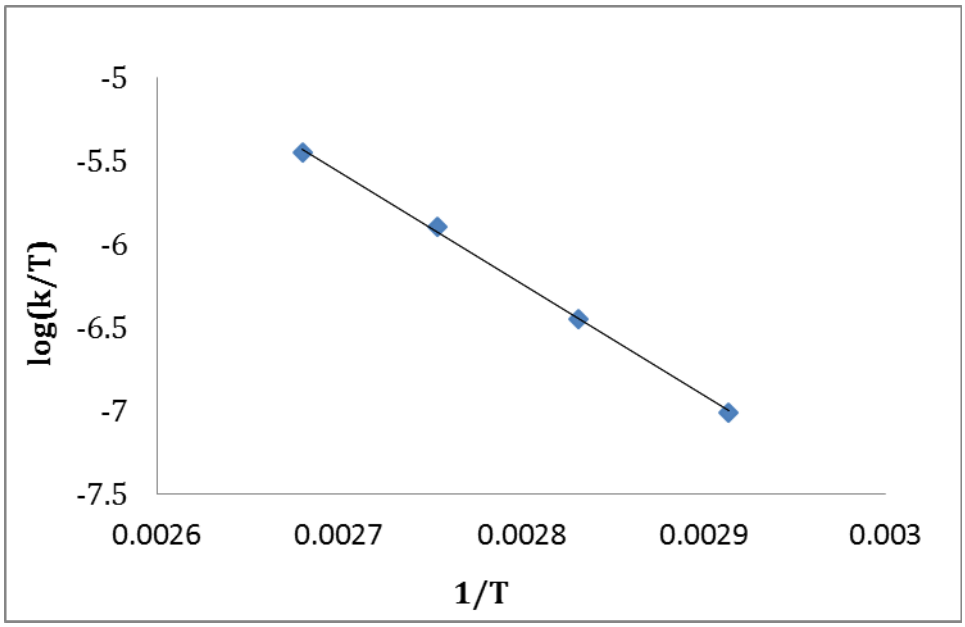


Figure S-89. Eyring Plot for Reductive Elimination of benzene in Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)**.

Table S-12: Kinetic data for Eyring Plot of reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)**.

T	*k*, s^{-1}	1/T	log(*k*/T)
373.15	1.33939E-03	0.002679887	-5.444977204
363.15	4.59901E-04	0.002753683	-5.89742192
353.15	1.26061E-04	0.002831658	-6.447379772
343.15	3.36476E-05	0.002914177	-7.00853022
Calculated:			
303.15	7.92057E-08		

Table S-13. Regression data for Eyring Plot of reductive elimination of benzene from Tp'Rh[P(OMe)$_3$](C$_6$H$_5$)H **(6a)**.

Regression Statistics	
Multiple R	0.999628512
R Square	0.999257162
Adjusted R Square	0.998885743
Standard Error	0.022611266
Observations	4

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.375507532	1.375507532	2690.377367	3.71488E-04
Residual	2	0.001022539	0.000511269		
Total	3	1.37653007			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	12.56785555	0.362001335	34.71770499	0.000828625
Slope	-6715.00185	129.4611726	-51.86884775	3.71488E-04

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
11.01028952	14.12542159	11.01028952	14.12542159
-7272.028317	-6157.975382	-7272.028317	-6157.975382

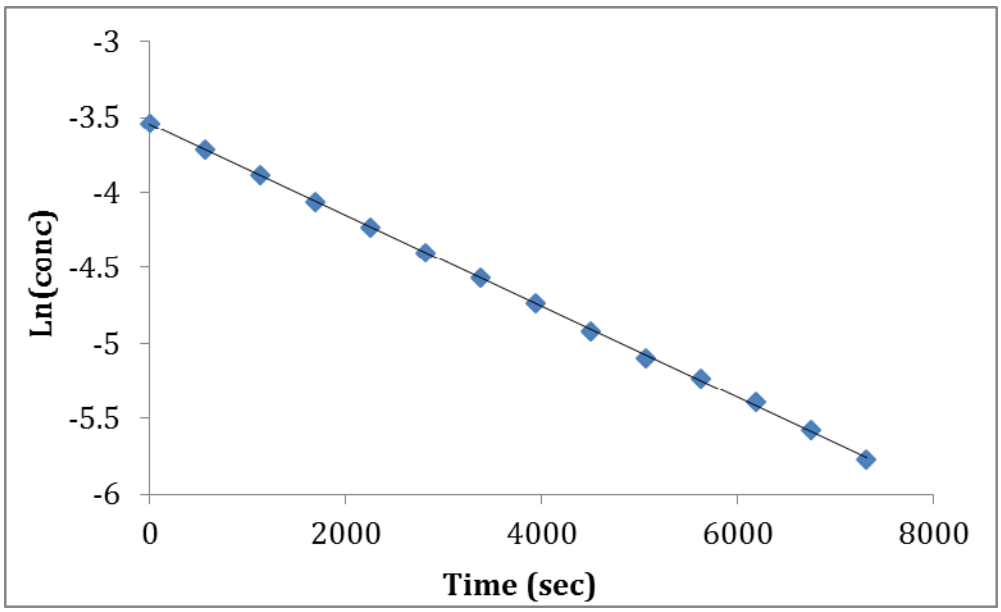


Figure S-90: Reductive elimination of methane from Tp'Rh[P(OMe)$_3$](CH$_3$)H **(4)** at 30.0 °C.

Table S-14: Kinetic data for reductive elimination of methane from Tp'Rh[P(OMe)$_3$](CH$_3$)H **(4)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	11.2194	-3.540350443
563	9.3612	-3.721421378
1125	7.9671	-3.882674304
1689	6.6719	-4.060090189
2252	5.6266	-4.230489514
2814	4.759	-4.397957304
3376	4.0198	-4.566762716
3938	3.3905	-4.737017463
4500	2.8177	-4.922073916
5063	2.3645	-5.097428283
5625	2.0635	-5.233591296
6187	1.7556	-5.395184187
6750	1.4648	-5.576276151
7312	1.2066	-5.770188379

Table S-15. Regression data for reductive elimination of methane from Tp'Rh[P(OMe)$_3$](CH$_3$)H **(4)**.

Regression Statistics	
Multiple R	0.999872438
R Square	0.999744892
Adjusted R Square	0.999723633
Standard Error	0.011815775
Observations	14

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	6.565535578	6.565535578	47026.83122	6.21882E-23
Residual	12	0.001675351	0.000139613		
Total	13	6.567210928			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.547714346	0.005992909	-591.9853476	3.63568E-28
Slope	-0.000302057	1.39289E-06	-216.8567067	6.21882E-23

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.560771773	-3.534656919	-3.560771773	-3.534656919
-3.05092E-04	-2.99022E-04	-3.05092E-04	-2.99022E-04

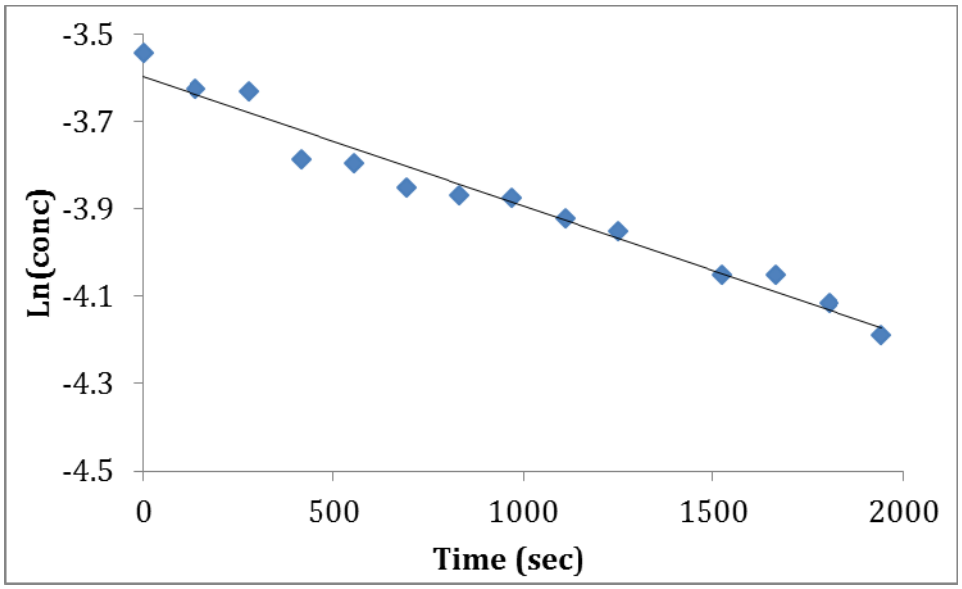


Figure S-91: Reductive elimination of mesitylene from Tp'Rh[P(OMe)$_3$](CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$)H **(6b)** at 19.7 °C.

Table S-16: Kinetic data for reductive elimination of mesitylene from Tp'Rh[P(OMe)$_3$](CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$)H **(6b)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	425.95	-3.540350443
138	391.69	-3.624201701
277	389.05	-3.630964541
416	333.12	-3.786169626
555	330.24	-3.794852749
693	312.53	-3.849971947
832	307.42	-3.866457521
971	305.27	-3.873475781
1110	291.47	-3.919735327
1249	282.55	-3.950816885
1526	255.62	-4.050980445
1665	255.63	-4.050941325
1804	239.91	-4.114408559
1943	222.6	-4.189295973

Table S-17. Regression data for reductive elimination of mesitylene from Tp'Rh[P(OMe)$_3$](CH$_2$C$_6$H$_3$-3,5-(CH$_3$)$_2$)H **(6b)**.

Regression Statistics	
Multiple R	0.98249958
R Square	0.965305425
Adjusted R Square	0.96241421
Standard Error	0.037067318
Observations	14

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.458740148	0.458740148	333.8753962	3.99430E-10
Residual	12	0.016487833	0.001373986		
Total	13	0.475227981			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.595107042	0.018218064	-197.3374943	1.92814E-22
Slope	-2.96769E-04	1.62415E-05	-18.27225756	3.99430E-10

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.634800793	-3.555413292	-3.634800793	-3.555413292
-3.32157E-04	-2.61382E-04	-3.32157E-04	-2.61382E-04

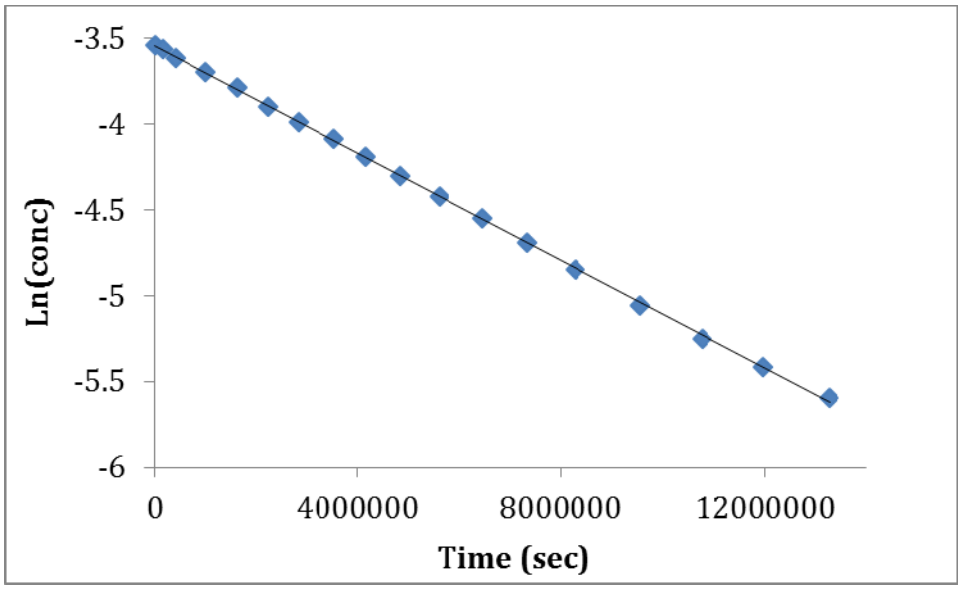


Figure S-92: Reductive elimination of 3,3-dimethyl-1-butene from Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)H **(6c)** at 30.0 °C.

Table S-18: Kinetic data for reductive elimination of 3,3-dimethyl-1-butene from Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)H **(6c)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	8.1881	-3.540350443
173190	7.9959	-3.564103413
416060	7.5726	-3.618495854
1020100	6.9929	-3.698136975
1624920	6.3931	-3.78781304
2231520	5.7194	-3.899168419
2840230	5.2406	-3.986596328
3524890	4.7236	-4.090461103
4148010	4.2714	-4.191090681
4838290	3.825	-4.301473856
5607990	3.3833	-4.424180759
6452550	2.9801	-4.551075467
7315890	2.5979	-4.688328897
8276570	2.2203	-4.845390002
9557290	1.7972	-5.056802426
10777470	1.4792	-5.251530923
11973250	1.2499	-5.419968776
13277020	1.0505	-5.593766082

Table S-19. Regression data for reductive elimination of 3,3-dimethyl-1-butene from Tp'Rh[P(OMe)$_3$](CH=CHC(CH$_3$)$_3$)H **(6c)**.

Regression Statistics	
Multiple R	0.999870033
R Square	0.999740082
Adjusted R Square	0.999723837
Standard Error	0.010954511
Observations	18

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.385108676	7.385108676	61541.89645	4.09108E-30
Residual	16	0.001920021	0.000120001		
Total	17	7.387028698			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.542776563	0.004190609	-845.4086023	1.23856E-38
Slope	-1.56703E-07	6.31673E-10	-248.0763924	4.09108E-30

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.551660256	-3.53389287	-3.551660256	-3.53389287
-1.58042E-07	-1.55364E-07	-1.58042E-07	-1.55364E-07

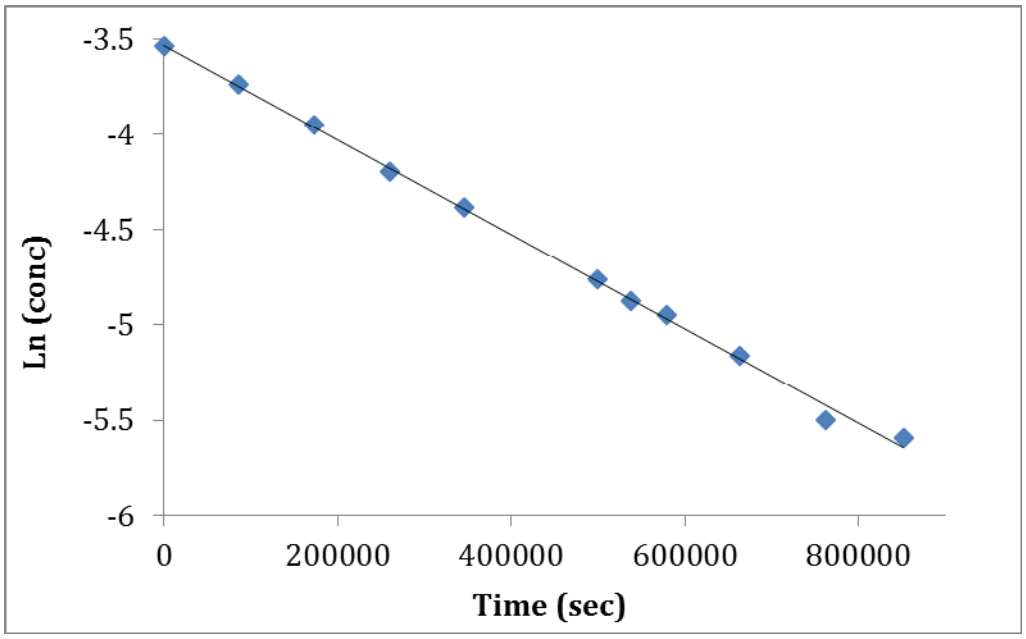


Figure S-93: Reductive elimination of 2-methoxy-2-methylpropane from Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)H **(6d)** at 30.0 °C.

Table S-20: Kinetic data for reductive elimination of 2-methoxy-2-methylpropane from Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)H **(6d)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	7.989	-3.540350443
86400	6.5438	-3.739898002
172800	5.3103	-3.948767708
259560	4.1533	-4.19451284
345940	3.4364	-4.383991627
498730	2.3513	-4.763447672
538330	2.111	-4.87125427
579730	1.9628	-4.944044013
662650	1.5798	-5.161117782
762610	1.1268	-5.499034282
851700	1.0229	-5.595774308

Table S-21. Regression data for reductive elimination of 2-methoxy-2-methylpropane from Tp'Rh[P(OMe)$_3$](CH$_2$OC(CH$_3$)$_3$)H **(6d)**.

Regression Statistics	
Multiple R	0.999004967
R Square	0.998010925
Adjusted R Square	0.997789916
Standard Error	0.032675535
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.821387108	4.821387108	4515.715662	1.80744E-13
Residual	9	0.009609215	0.001067691		
Total	10	4.830996323			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.53286791	0.018736553	-188.5548498	1.68842E-17
Slope	-2.47573E-06	3.68418E-08	-67.19907486	1.80744E-13

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.575252937	-3.490482883	-3.575252937	-3.490482883
-2.55907E-06	-2.39239E-06	-2.55907E-06	-2.39239E-06

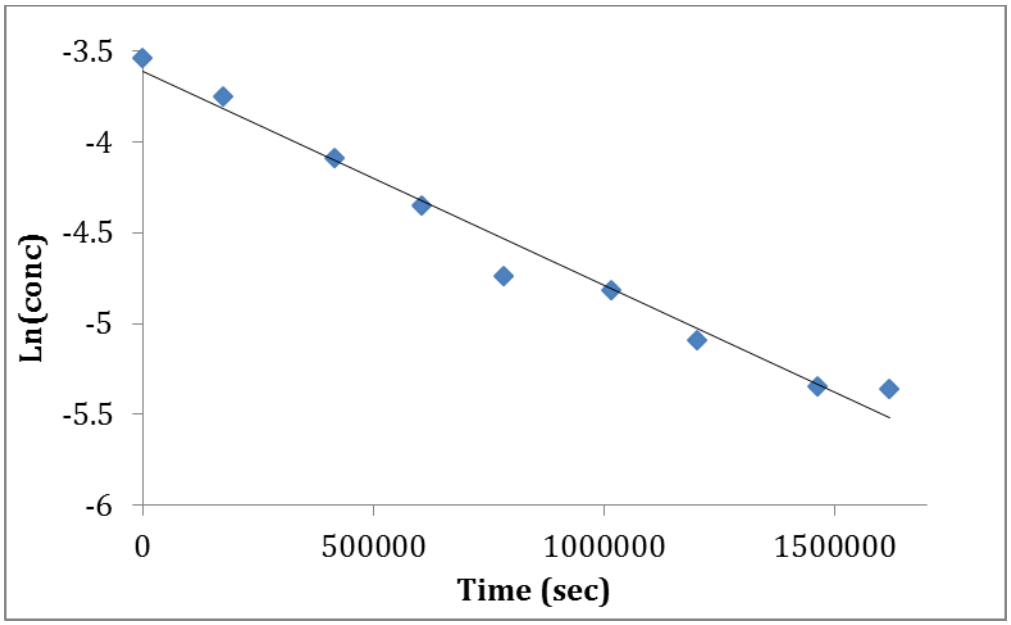


Figure S-94: Reductive elimination of 2-butyne from Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)H **(6e)** at 30.0 °C.

Table S-22: Kinetic data for reductive elimination of 2-butyne from Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)H **(6e)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	2.4829	-3.540350443
173190	2.0171	-3.748116839
416060	1.4347	-4.088821907
603690	1.1048	-4.350113352
781155	0.7503	-4.737059827
1016125	0.6921	-4.8178025
1200325	0.5278	-5.08881553
1462525	0.4092	-5.34332892
1618925	0.4023	-5.360334875

Table S-23. Regression data for reductive elimination of 2-butyne from Tp'Rh[P(OMe)$_3$](CH$_2$C≡CCH$_3$)H **(6e)**.

Regression Statistics	
Multiple R	0.988545639
R Square	0.97722248
Adjusted R Square	0.973968548
Standard Error	0.108177284
Observations	9

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.514448571	3.514448571	300.3205488	5.23707E-07
Residual	7	0.081916273	0.011702325		
Total	8	3.596364843			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.612518779	0.065680095	-55.00172848	1.72194E-10
Slope	-1.17740E-06	6.79412E-08	-17.32975905	5.23707E-07

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.767827526	-3.457210032	-3.767827526	-3.457210032
-1.33806E-06	-1.01675E-06	-1.33806E-06	-1.01675E-06

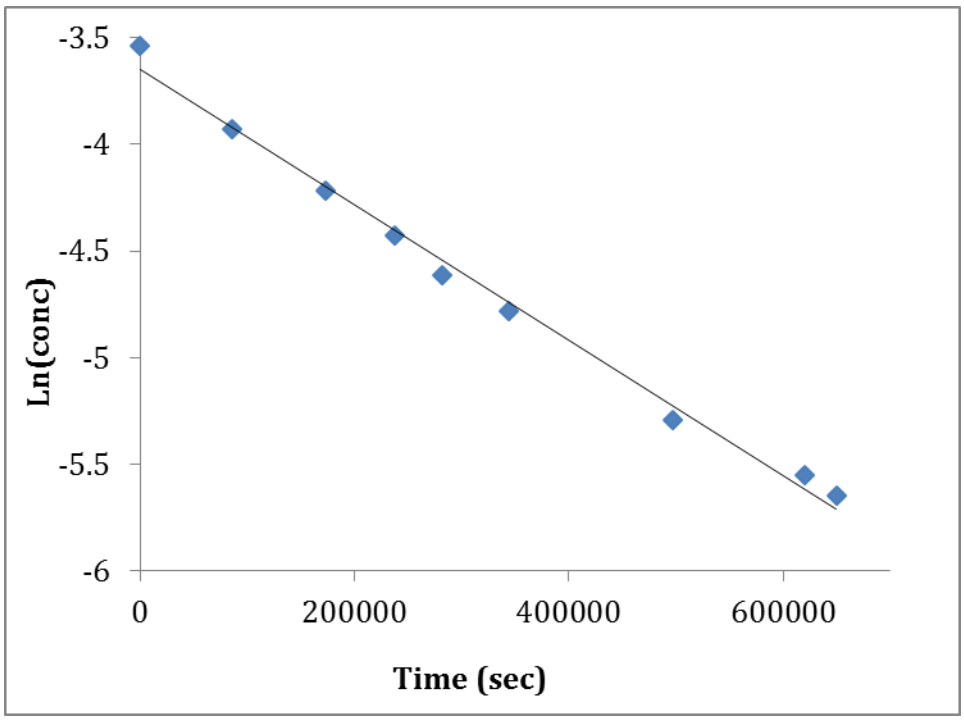


Figure S-95: Reductive elimination of acetone from Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)H **(6f)** at 30.0 °C.

Table S-24: Kinetic data for reductive elimination of acetone from Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)H **(6f)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	9.0563	-3.540350443
86460	6.1564	-3.9263189
172860	4.6086	-4.215886968
237600	3.7391	-4.42496615
281370	3.0918	-4.615057646
343620	2.6147	-4.782661723
496410	1.5728	-5.290953621
620430	1.2101	-5.55310809
649410	1.1012	-5.647410597

Table S-25. Regression data for reductive elimination of acetone from Tp'Rh[P(OMe)$_3$](CH$_2$C(O)CH$_3$)H **(6f)**.

Regression Statistics	
Multiple R	0.996167527
R Square	0.992349742
Adjusted R Square	0.991256848
Standard Error	0.068006788
Observations	9

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.199438465	4.199438465	908.0017736	1.14313E-08
Residual	7	0.032374462	0.004624923		
Total	8	4.231812927			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.648312184	0.040683907	-89.67457699	5.64825E-12
Slope	-3.17223E-06	1.05274E-07	-30.13306778	1.14313E-08

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.744514338	-3.55211003	-3.744514338	-3.55211003
-3.42116E-06	-2.92330E-06	-3.42116E-06	-2.92330E-06

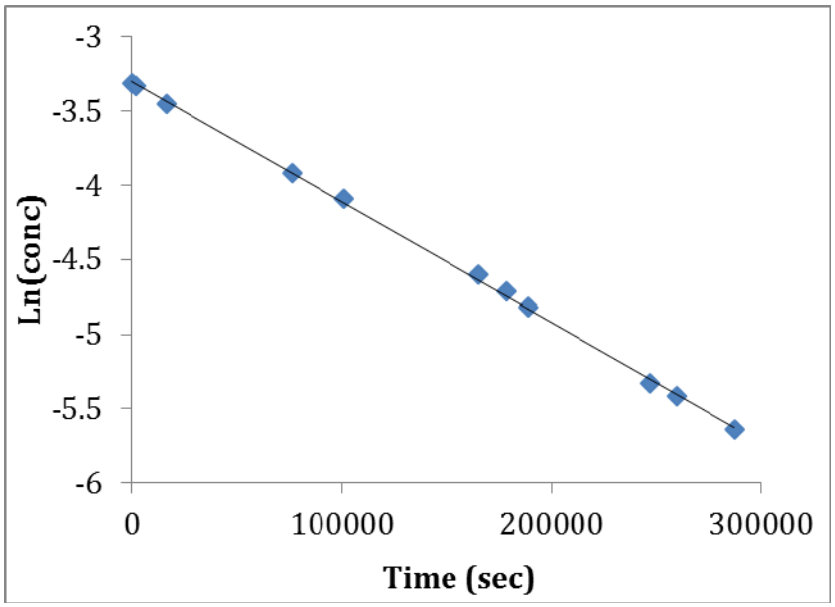


Figure S-96: Reductive elimination of fluoromethane from Tp'Rh[P(OMe)$_3$](CH$_2$F)H **(6g)** at 66.9 °C.

Table S-26: Kinetic data for reductive elimination of fluoromethane from Tp'Rh[P(OMe)$_3$](CH$_2$F)H **(6g)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	7.3789	-3.310620862
1740	7.2058	-3.334359181
16640	6.422	-3.449515842
76480	4.0307	-3.91530538
100900	3.388	-4.089005661
165110	2.0361	-4.598209225
178430	1.8116	-4.715035005
188630	1.6399	-4.814610174
246690	0.9795	-5.32995848
259800	0.902	-5.412386197
287080	0.7189	-5.639278451

Table S-27. Regression data for reductive elimination of dimethylether from Tp'Rh[P(OMe)$_3$](CH$_2$F)H **(6g)**.

Regression Statistics	
Multiple R	0.999628338
R Square	0.999256815
Adjusted R Square	0.999174238
Standard Error	0.024534368
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.284037689	7.284037689	12101.03307	2.15203E-15
Residual	9	0.005417417	0.000601935		
Total	10	7.289455106			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.299994706	0.012577197	-262.3791926	8.63523E-19
Slope	-8.08961E-06	7.35388E-08	-110.0046957	2.15203E-15

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.328446301	-3.27154311	-3.328446301	-3.27154311
-8.25597E-06	-7.92325E-06	-8.25597E-06	-7.92325E-06

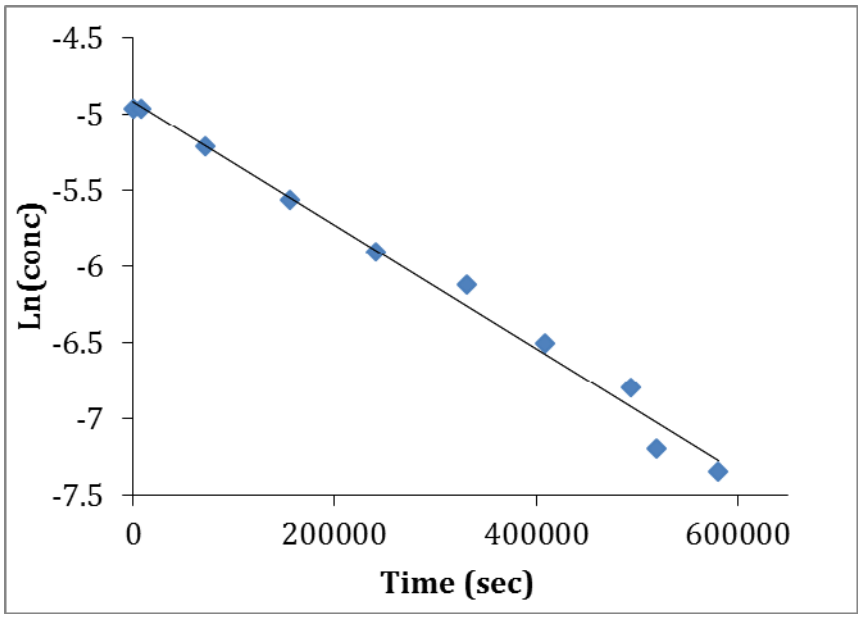


Figure S-97: Reductive elimination of dimethylether from Tp'Rh[P(OMe)$_3$](CH$_2$OMe)H **(6h)** at 30.0 °C.

Table S-28: Kinetic data for reductive elimination of dimethylether from Tp'Rh[P(OMe)$_3$](CH$_2$OMe)H **(6h)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	1.4702	-4.96024174
8790	1.4647	-4.963989743
72230	1.1374	-5.21689523
156090	0.8024	-5.565788228
241130	0.5719	-5.904431314
330720	0.4598	-6.122603853
408940	0.3127	-6.508151201
493170	0.234	-6.79807435
519250	0.1575	-7.193970007
580200	0.135	-7.348120687

Table S-29. Regression data for reductive elimination of dimethylether from Tp'Rh[P(OMe)$_3$](CH$_2$OMe)H **(6h)**.

Regression Statistics

Multiple R	0.994707297
R Square	0.989442606
Adjusted R Square	0.988122932
Standard Error	0.096692132
Observations	10

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.009808229	7.009808229	749.7627515	3.41136E-09
Residual	8	0.074794948	0.009349368		
Total	9	7.084603176			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-4.915430698	0.05173778	-95.00660169	1.68191E-13
Slope	-4.06614E-06	1.48498E-07	-27.38179599	3.41136E-09

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-5.034738234	-4.796123163	-5.034738234	-4.796123163
-4.40857E-06	-3.72370E-06	-4.40857E-06	-3.72370E-06

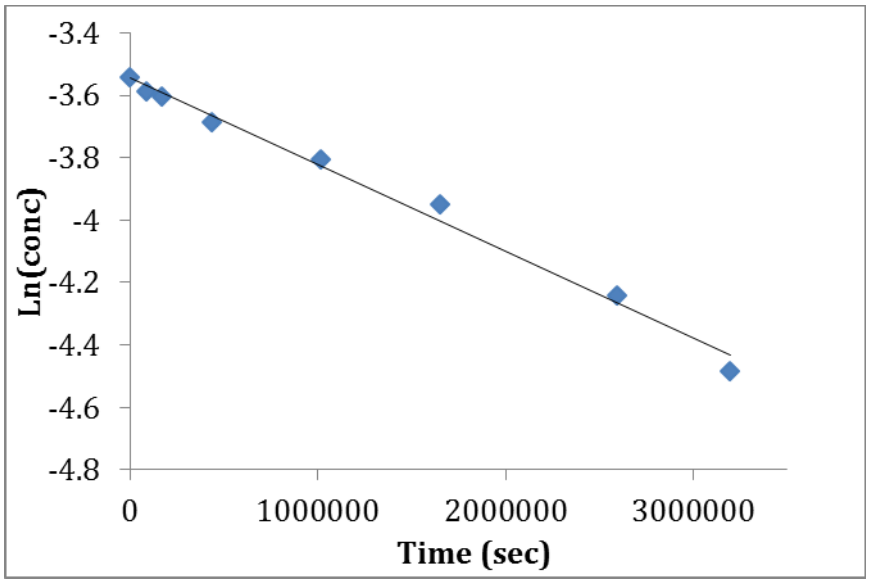


Figure S-98: Reductive elimination of *t*-butylacetylene from Tp'Rh[P(OMe)$_3$](C≡CC(CH$_3$)$_3$)H **(6i)** at 140.0 °C.

Table S-30: Kinetic data for reductive elimination of *t*-butylacetylene from Tp'Rh[P(OMe)$_3$](C≡CC(CH$_3$)$_3$)H **(6i)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	12.2928	-3.540350443
87950	11.7238	-3.587743205
172070	11.5189	-3.605375004
434780	10.624	-3.686248575
1019620	9.4318	-3.80527721
1652740	8.183	-3.947305337
2591875	6.1097	-4.239486496
3195625	4.7876	-4.483334926

Table S-31. Regression data for reductive elimination of *t*-butylacetylene from Tp'Rh[P(OMe)$_3$](C≡CC(CH$_3$)$_3$)H **(6i)**.

Regression Statistics	
Multiple R	0.995141947
R Square	0.990307494
Adjusted R Square	0.988692077
Standard Error	0.036272654
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.806573471	0.806573471	613.034982	2.85590E-07
Residual	6	0.007894233	0.001315705		
Total	7	0.814467703			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.543992934	0.01814698	-195.2938109	1.21617E-12
Slope	-2.77801E-07	1.122E-08	-24.75954325	2.85590E-07

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.588396995	-3.499588873	-3.588396995	-3.499588873
-3.05256E-07	-2.50347E-07	-3.05256E-07	-2.50347E-07

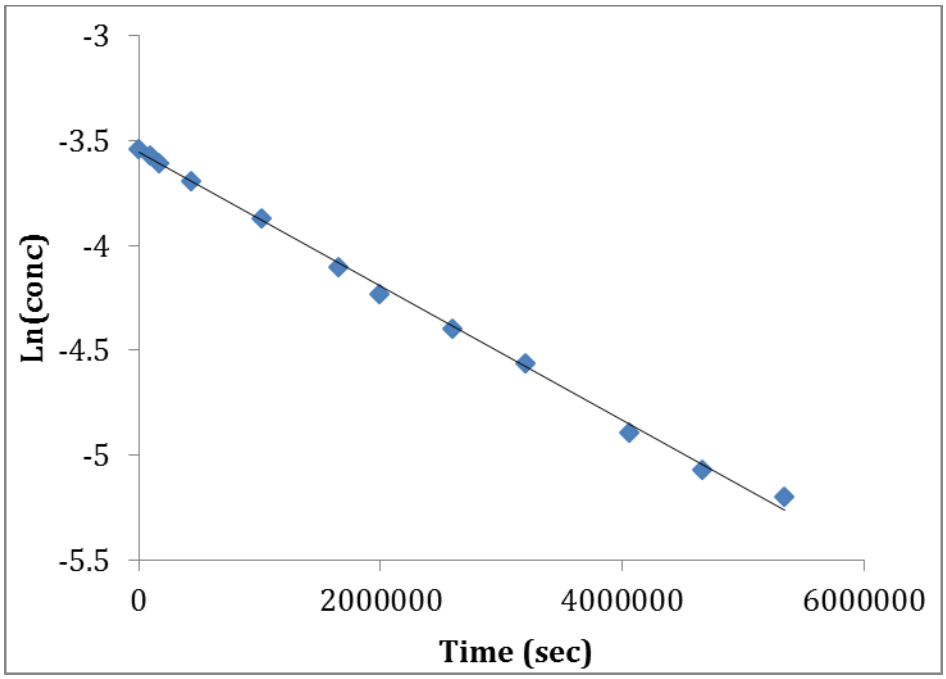


Figure S-99: Reductive elimination of ethynyltrimethylsilane from Tp'Rh[P(OMe)$_3$](C≡CSi(CH$_3$)$_3$)H **(6j)** at 140.0 °C.

Table S-32: Kinetic data for reductive elimination of ethynyltrimethylsilane from Tp'Rh[P(OMe)$_3$](C≡CSi(CH$_3$)$_3$)H **(6j)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	6.5571	-3.540350443
87950	6.3694	-3.569393601
172070	6.1323	-3.607328992
434780	5.6375	-3.69145817
1019620	4.7227	-3.868518205
1652740	3.7333	-4.103606314
1994155	3.2874	-4.230801896
2592025	2.7912	-4.394427264
3195775	2.368	-4.558853158
4056795	1.6969	-4.892095818
4659855	1.4254	-5.066446399
5340395	1.2468	-5.200318606

Table S-33. Regression data for reductive elimination of ethynyltrimethylsilane from Tp'Rh[P(OMe)$_3$](C≡CSi(CH$_3$)$_3$)H **(6j)**.

Regression Statistics	
Multiple R	0.998885874
R Square	0.997772989
Adjusted R Square	0.997550288
Standard Error	0.029663012
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.942211917	3.942211917	4480.324392	1.34932E-14
Residual	10	0.008798943	0.000879894		
Total	11	3.95101086			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.556137399	0.013182045	-269.7712986	1.20467E-20
Slope	-3.19364E-07	4.77125E-09	-66.93522535	1.34932E-14

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.585508826	-3.526765973	-3.585508826	-3.526765973
-3.29995E-07	-3.08733E-07	-3.29995E-07	-3.08733E-07

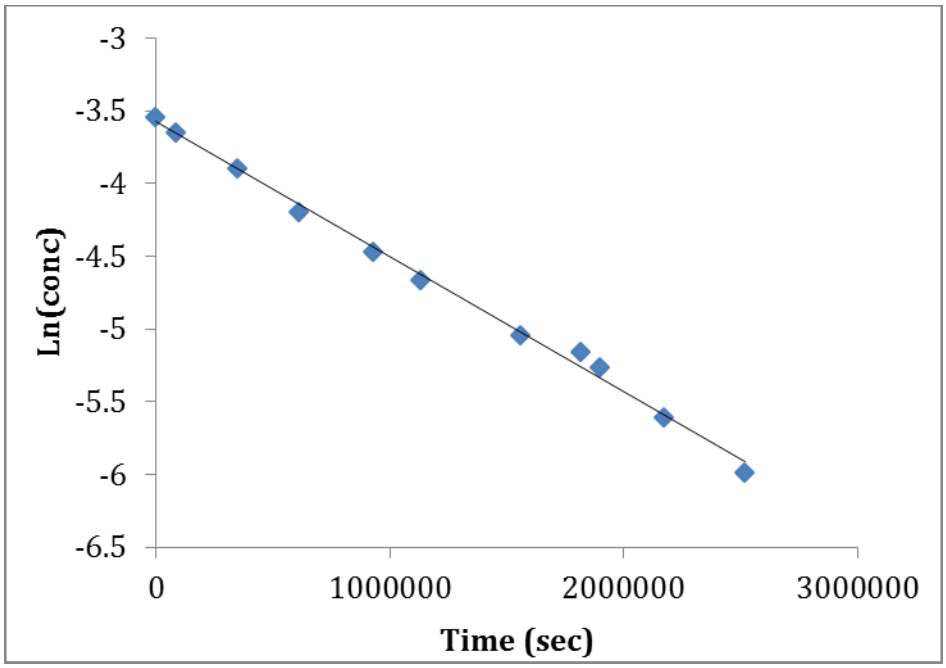


Figure S-100: Reductive elimination of 1-octyne from Tp'Rh[P(OMe)$_3$](C≡C*n*-hexyl)H **(6k)** at 140.0 °C.

Table S-34: Kinetic data for reductive elimination of 1-octyne from Tp'Rh[P(OMe)$_3$](C≡C*n*-hexyl)H **(6k)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	104.7394	-3.540350443
84120	93.9668	-3.648884275
346830	73.6877	-3.891989911
608610	54.4849	-4.193902204
930340	41.437	-4.467651602
1131340	33.9516	-4.666889822
1561420	23.373	-5.040244293
1815890	20.8082	-5.156478664
1897390	18.6346	-5.266805736
2172730	13.2655	-5.606659123
2518930	9.0796	-5.985795665

Table S-35. Regression data for reductive elimination of 1-octyne from Tp'Rh[P(OMe)$_3$](C≡C*n*-hexyl)H **(6k)**.

Regression Statistics	
Multiple R	0.997844483
R Square	0.995693612
Adjusted R Square	0.995215124
Standard Error	0.055895064
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	6.501326686	6.501326686	2080.918522	5.84864E-12
Residual	9	0.028118323	0.003124258		
Total	10	6.52944501			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.574175232	0.029500616	-121.1559526	9.02982E-16
Slope	-9.29759E-07	2.03818E-08	-45.61708586	5.84864E-12

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.640910261	-3.507440202	-3.640910261	-3.507440202
-9.75866E-07	-8.83653E-07	-9.75866E-07	-8.83653E-07

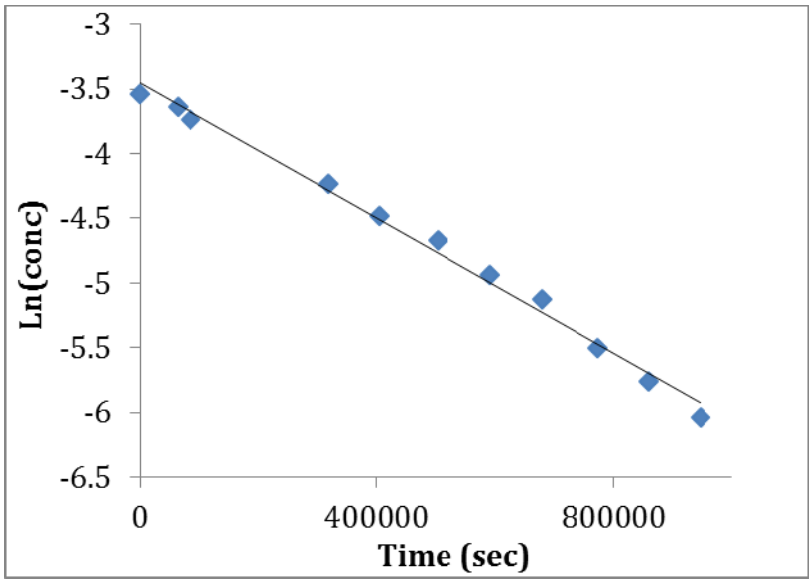


Figure S-101: Reductive elimination of 1-octyne from 3,3,3-trifluoro-1-propyne from Tp'Rh[P(OMe)$_3$](C≡CCF$_3$)H **(6l)** at 140.0 °C.

Table S-36: Kinetic data for reductive elimination of 3,3,3-trifluoro-1-propyne from Tp'Rh[P(OMe)$_3$](C≡CCF$_3$)H **(6l)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	2.7102	-3.540350443
63210	2.4647	-3.63530278
85710	2.2205	-3.73964048
319180	1.3497	-4.23749053
405580	1.0583	-4.480709029
504280	0.8716	-4.674797552
591220	0.6705	-4.937104452
679180	0.5558	-5.124719638
774640	0.3811	-5.502066347
858760	0.2931	-5.764614307
947500	0.2229	-6.038404915

Table S-37. Regression data for reductive elimination of 3,3,3-trifluoro-1-propyne from Tp'Rh[P(OMe)$_3$](C≡CCF$_3$)H **(6l)**.

Regression Statistics	
Multiple R	0.996250732
R Square	0.992515521
Adjusted R Square	0.991683912
Standard Error	0.078805843
Observations	11

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.411994273	7.411994273	1193.488497	7.04435E-11
Residual	9	0.055893248	0.006210361		
Total	10	7.467887521			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.459340214	0.043006869	-80.43692332	3.59172E-14
Slope	-2.60505E-06	7.5406E-08	-34.54690286	7.04435E-11

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.55662851	-3.362051917	-3.55662851	-3.362051917
-2.77563E-06	-2.43446E-06	-2.77563E-06	-2.43446E-06

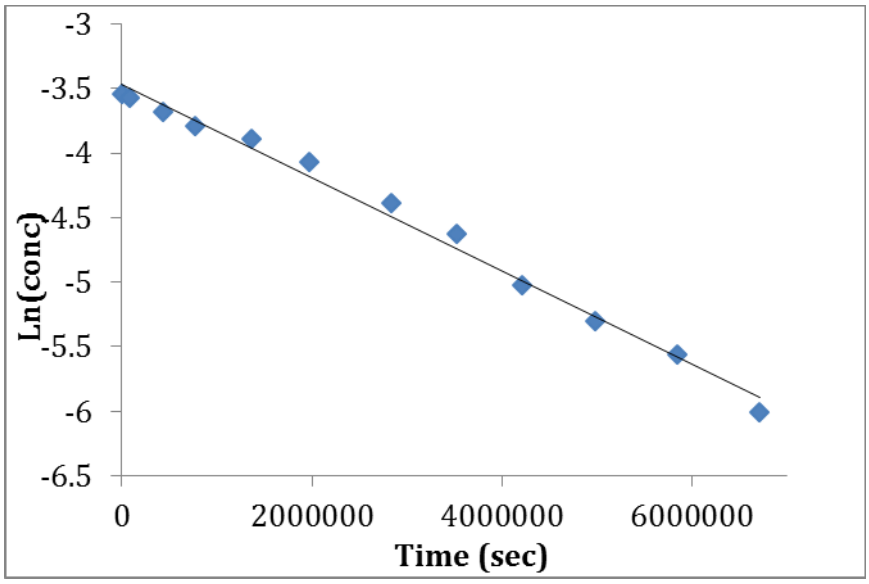


Figure S-102: Reductive elimination of phenylacetylene from Tp'Rh[P(OMe)$_3$](C≡CPh)H **(6m)** at 140.0 °C.

Table S-38: Kinetic data for reductive elimination of phenylacetylene from Tp'Rh[P(OMe)$_3$](C≡CPh)H **(6m)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	19.9765	-3.540350443
87680	19.3025	-3.574672405
428540	17.4249	-3.677006808
769160	15.6267	-3.785926036
1362260	14.108	-3.888165013
1970210	11.7469	-4.07131765
2831230	8.6044	-4.382633325
3525920	6.7434	-4.626342777
4206730	4.5219	-5.025974766
4981750	3.4248	-5.30386395
5842390	2.6415	-5.563560088
6708350	1.6864	-6.012310946

Table S-39. Regression data for reductive elimination of phenylacetylene from Tp'Rh[P(OMe)$_3$](C≡CPh)H **(6m)**.

Regression Statistics

Multiple R	0.995229128
R Square	0.990481018
Adjusted R Square	0.989529119
Standard Error	0.086543769
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.793404828	7.793404828	1040.532452	1.93100E-11
Residual	10	0.074898239	0.007489824		
Total	11	7.868303067			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.467146009	0.039506312	-87.76182443	9.02530E-16
Slope	-3.62117E-07	1.12259E-08	-32.25728526	1.93100E-11

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.555171557	-3.379120461	-3.555171557	-3.379120461
-3.87130E-07	-3.37104E-07	-3.87130E-07	-3.37104E-07

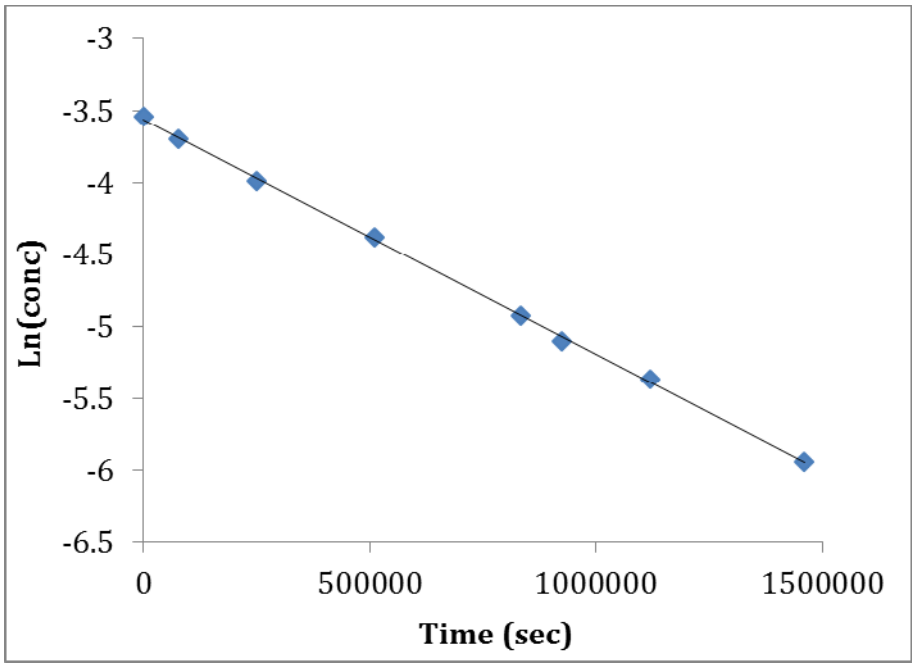


Figure S-103: Reductive elimination of 4-ethynylanisole from Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OMe)H **(6n)** at 140.0 °C.

Table S-40: Kinetic data for reductive elimination of 4-ethynylanisole from Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-OMe)H **(6n)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	119.13	-3.540350443
76410	102.21	-3.693536257
248760	76.15	-3.987860698
510540	51.79	-4.373368696
832270	29.9	-4.922707296
922710	24.94	-5.104092837
1120070	19.28	-5.361497488
1460930	10.82	-5.939169503

Table S-41. Regression data for reductive elimination of 4-ethynylanisole from Tp'Rh[P(OMe)$_3$](C≡CC$_6$H$_4$-*p*-OMe)H **(6n)**.

Regression Statistics	
Multiple R	0.999653306
R Square	0.999306732
Adjusted R Square	0.999191187
Standard Error	0.024275607
Observations	8

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.096698784	5.096698784	8648.659182	1.04152E-10
Residual	6	0.00353583	0.000589305		
Total	7	5.100234614			

	Coefficients	*Standror*	*t Stat*	*P-value*
Intercept	-3.561515947	0.014214978	-250.5467123	2.72811E-13
Slope	-1.63012E-06	1.75285E-08	-92.99816763	1.04152E-10

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.596298744	-3.526733149	-3.596298744	-3.526733149
-1.67301E-06	-1.58723E-06	-1.67301E-06	-1.58723E-06

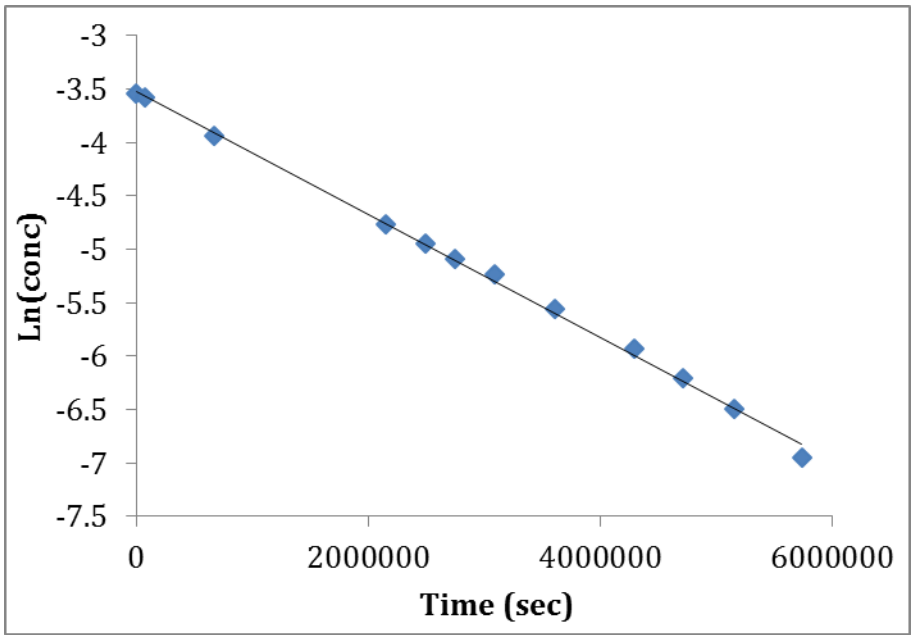


Figure S-104: Reductive elimination of 4-ethynyl-α,α,α-trifluorotoluene from Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-CF_3)H **(6o)** at 30.0 °C.

Table S-42: Kinetic data for reductive elimination of 4-ethynyl-α,α,α-trifluorotoluene from Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-CF_3)H **(6o)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	14.2337	-3.540350443
74450	13.6825	-3.579845191
676730	9.5521	-3.93920181
2148520	4.1828	-4.764981957
2489320	3.482	-4.948355994
2749810	3.0358	-5.085487854
3089700	2.6092	-5.236919174
3607815	1.8883	-5.560285882
4297025	1.3005	-5.93321403
4719755	0.9956	-6.200372544
5155745	0.7456	-6.489528851
5741400	0.4728	-6.945045648

Table S-43. Regression data for reductive elimination of 4-ethynyl-α,α,α-trifluorotoluene from Tp'Rh[P(OMe)$_3$](C≡CC_6H_4-*p*-CF_3)H **(6o)**.

Regression Statistics	
Multiple R	0.999027598
R Square	0.998056142
Adjusted R Square	0.997861756
Standard Error	0.051434589
Observations	12

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	13.58316616	13.58316616	5134.408971	6.83558E-15
Residual	10	0.02645517	0.002645517		
Total	11	13.60962133			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.519598229	0.027583421	-127.5983222	2.14501E-17
Slope	-5.75202E-07	8.0274E-09	-71.65479029	6.83558E-15

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.58105792	-3.458138537	-3.58105792	-3.458138537
-5.93088E-07	-5.57315E-07	-5.93088E-07	-5.57315E-07

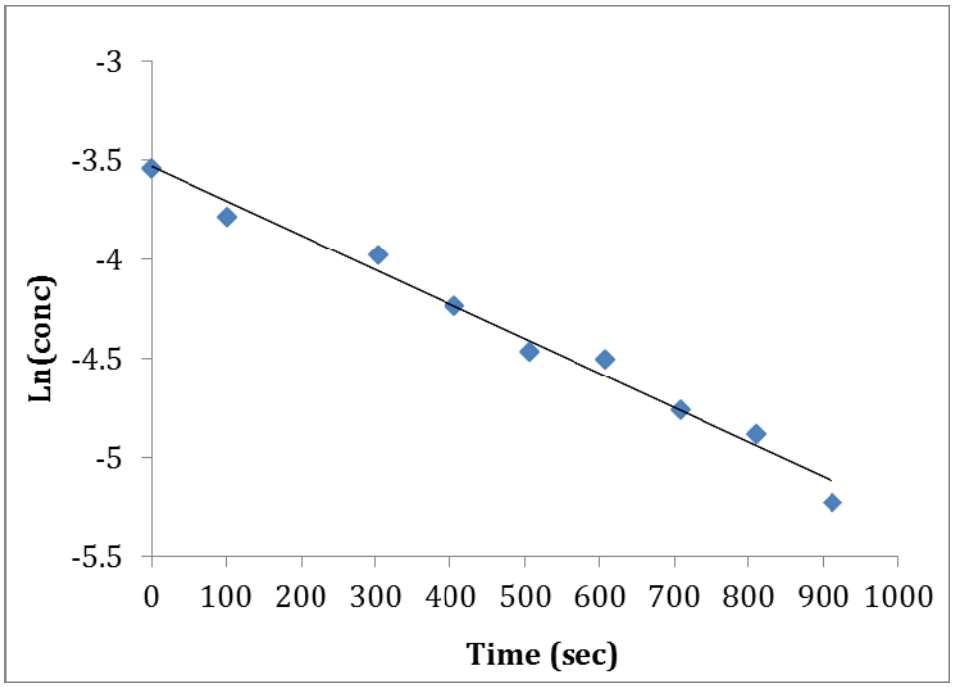


Figure S-105: Reductive elimination of *n*-pentane from Tp'Rh[P(OMe)$_3$](*n*-pentyl)H **(6p)** at 25.3 °C.

Table S-44: Kinetic data for reductive elimination of *n*-pentane from Tp'Rh[P(OMe)$_3$](*n*-pentyl)H **(6p)**. Hydride integration was measured relative to an internal standard (hexamethyldisiloxane).

Time (sec)	Hydride Area	Ln(conc)
0	20.48	-3.540350443
101	16.03	-3.785337277
304	13.2	-3.979582414
405	10.24	-4.233497624
506	8.13	-4.46423832
608	7.82	-4.503114689
709	6.07	-4.756440638
810	5.36	-4.880835268
912	3.78	-5.230075234

Table S-45. Regression data for reductive elimination of *n*-pentane from Tp'Rh[P(OMe)$_3$](*n*-pentyl)H **(6p)**.

Regression Statistics	
Multiple R	0.991755451
R Square	0.983578875
Adjusted R Square	0.981233
Standard Error	0.074683273
Observations	9

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.338573387	2.338573387	419.2801641	1.66202E-07
Residual	7	0.039043139	0.005577591		
Total	8	2.377616526			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	-3.534554904	0.047997083	-73.64103612	2.23972E-11
Slope	-1.73650E-03	8.48055E-05	-20.4763318	1.66202E-07

Lower 95%	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
-3.64804997	-3.421059838	-3.64804997	-3.421059838
-1.93704E-03	-1.53597E-03	-1.93704E-03	-1.53597E-03

Table S46. Summary of thermodynamic data. All values are in kcal mol^{-1}.

Data for plot of M-R vs C-H bond strengths-P(OMe)3

$D_{rel}(Rh\text{-}C) = [\Delta H(Rh\text{-}R2) - \Delta H(Rh\text{-}R1)] = \Delta G° + RT\ \ln(H1/H2) + [\Delta H(R2\text{-}H) - \Delta H(R1\text{-}H)]$							$\Delta\Delta G° \approx \Delta\Delta H° - RT\ \ln(H1/H2)$			
			T= -10 to +10		T = 20 to 140				corr. for ΔS	
R	D(C-H)[a]	k_{PhH}/k_{RH}	T_{comp}	$\Delta\Delta G_{oa}^{\ddagger}$ vs PhH	$\Delta G_{re}^{\ddagger}$	T_{re}(R-H)	ΔG^0 vs PhH	#H	D_{rel}(M-C)	line calc
c-pentyl	95.6									
Ph [b]	112.9	1	283	0	27.61	303	0.01	6	0.0	0.42
t-butylvinyl [c]	111.1	7.01	283	1.10	27.20	303	1.51	1	-2.3	-2.38
methyl	105.0	1.47	283	0.22	22.64	303	5.20	4	-12.9	-11.83
n-pentyl	100.2	3.40	276	0.67	21.24	298	7.10	6	-19.8	-19.28
CF_3-acetylene [d,e]	*135.4*	**0.18**	263	**-0.81**	35.01	413	-9.33	1	32.9	35.30
1-octyne [e]	*131.0*	4.17	283	0.80	35.86	413	-8.57	1	27.7	28.48
trimethylsilylacetylene [e]	*131.6*	3.34	283	0.68	36.74	413	-9.58	1	29.3	29.35
t-butylacetylene [e]	*131.4*	4.88	283	0.89	36.85	413	-9.47	1	29.0	29.10
phenylacetylene [e]	*133.2*	1.40	283	0.19	36.63	413	-9.95	1	31.3	31.89
p-CF_3phenylacetylene [e]	*127.8*	1.19	283	0.10	36.25	413	-9.67	1	25.6	23.52
p-MeOphenylacetylene [e]	*122.7*	2.72	283	0.56	35.40	413	-8.35	1	19.2	15.61
mesityl	89.4	1.84	263	0.32	21.86	293	6.18	9	-29.9	-28.11
CH2C(O)CH3	96.0	2.77	268	0.54	25.39	303	2.77	6	-19.7	-18.52
CH2CCCH3	90.7	1.26	283	0.13	25.98	303	1.77	6	-24.0	-26.22
CH2O^{t}Bu [f]	93.0	2.62	263	0.50	25.53	303	2.59	3	-22.1	-22.88
CH2OCH3	96.1	0.64	283	-0.25	25.24	303	2.13	6	-18.9	-18.37
CH2F	101.3	0.76	283	-0.16	27.92	340	-0.84	3	-10.4	-10.82
CHF2	103.2									
CH2CF3	106.7									

Notes:

ΔG^0 calculated using: $\Delta G_{re}^{\ddagger}$ for benzene at same T as $\Delta G_{re}^{\ddagger}$ for substrate R-H

$\Delta\Delta G^{\ddagger}$ calculated at temperature at which competition was carried out.

A positive $\Delta\Delta G^{\ddagger}$ or ΔG^0 means benzene is kinetically or thermodynamically favored.

Competion ratios in **bold** are calculated using two separate competition ratios.

	expt
slope of Phenyl to pentyl+ acetylenes =	1.55
slope of Mesitylene to CF2H2 =	1.45

[a] D(C-H) from Luo, Y.-R. Comprehensive Handbook of Chemical Bond Energies, 2007

[b] $\Delta G_{re}^{\ddagger}$=30.74-0.303*10.30=27.6; Calcd using ΔH=30.74 kcal/mol and ΔS=10.30 e.u. from Eyring Plot. k(303) = 7.92x10^{-8} s^{-1}

[c] D(C-H) for propene

[d] Data for CF_3-acetylene competition $k_{PhH}/k_{RH} = (k_{PhH}/k_{t\text{-butylethylene}})(k_{t\text{-butylethylene}}/k_{CF3\text{-acetylene}})$

[e] Terminal C-H bond strengths *in italics* for alkynes and nitriles were calculated using DFT; B3LYP/6-31g**

[f] D(C-H) for MeOEt

Table S47. Summary of DFT calculated thermodynamic data (and notes for experimental calculations).

Data for plot of M-R vs C-H bond strengths	Tp*Rh(CNAr)(H)(R) model	
	M062x DFT:	
R	Drogbh Cycle	Experimental Notes
c-pentyl	-26.67	
Ph[a]	0.00	
1-butynyl[a]	-4.18	
methyl[a]	-18.76	
n-pentyl	-28.04	
CF_3-acetylene[a]	36.63	$k_{rel}/k_{Ph} = (k_{rel}/k_{Ph})^{\Delta H_{rel}/\Delta H_{Ph}}$; ΔH_{rel}=7.0069*0.036229=0.16376
1-octyne[a]	26.88	
3-methylphenylacetylene[a]	31.38	
1-butylacetylene[a]	26.64	
phenylacetylene[a]	27.71	
p-CF$_3$phenylacetylene[a]	31.16	
p-MeOphenylacetylene[a]	23.71	
neopentyl	-29.57	
CH$_2$OCH$_3$	-18.95	
CH$_2$CCCH$_3$	-25.55	
CH$_2$OPh[a]	-19.63	
CH$_2$OCH$_3$	-19.23	
CH$_2$F	-12.72	
CHF$_2$	-5.03	
CH$_2$CF$_3$	-7.37	

Computational Details.

Calculations were done using the Gaussian 09 set of programs (Revision A.02).[1] Homolytic Rh-C bond energies were calculated from the reaction:

$$Tp'Rh[P(OMe)_3](R)(H) \rightarrow Tp'Rh[P(OMe)_3](H)\cdot + R\cdot$$

C-H bond energies in terminal alkynes and the corresponding Rh-C bond energies in $Tp'Rh(PMe_3)(C{\equiv}CR)(H)$ were calculated previously with the functionals B3LYP and M06-2X, respectively.[2-3] Here Rh-C bond energies in $Tp'Rh[P(OMe)_3](R)(H)$ complexes were calculated with the functional M06-2X using the same basis set (6-31g**), Stuttgart core potentials, and augmentation functions as the B3LYP calculations.[4-5] X-ray crystallographic structures were used as the starting points for the calculations if a corresponding or similar structure was available. Heavy atoms of rhodium, phosphorous and silicon were treated with the core potentials described by the Stuttgart group, with additional *d*, and *f* polarization functions (alpha for Rh=1.350, P= 0.387, Si=0.284). The remaining atoms (C, H, N, B, O, and F) were represented by 6-31g(d,p) basis set.[6-7] The geometry optimizations were performed without any symmetry constraints, and the local minima were checked by frequency calculations.

Calculation of C-H Bond Strengths:

As reported previously the choice of calculation method has little influence in calculating C-H bond strengths for terminal alkynes. Alkynyl C-H bond strengths were calculated by comparing the enthalpies of the organic molecule with the corresponding radicals. Enthalpy values were taken at 298 K and 1 atm using the harmonic oscillator approximation as implemented by Gaussian 09. Two methods of M06-2X and B3LYP were used in the calculation. Using methods of M06-2X vs B3LYP led to a difference in bond energy with less than 5 kcal/mol in energy for the same alkyne. However, calculation with M06-2X method gave more congregated bond energies spanning a narrower range of 5.8 kcal/mol in comparison with B3LYP, which gave a differentiation of 12.7 kcal/mol for calculated bond energies.

For the other substrates, literature recorded C-H bond strengths were used in plotting against experimental and calculated Rh-C bond strengths, which ensures the direct

comparison between experimental and calculated Rh-C bond energies by sharing the same set of C-H bond energy values. When comparing the performance of method choice (choosing M06-2X or B3LYP in alkynyl C-H bond energy calculation) in $R_{M\text{-}C/C\text{-}H}$ among the three systems of [Tp′Rh(L)] (L = $P(OMe)_3$, PMe_3 and CNMe), using one unified method (M06-2X) to calculate both C-H and Rh-C bond energies does not necessarily produce a better match with the experimental results. Therefore, it is reasonable to keep in our final plots the existing calculated C-H bond strengths for terminal alkynes using M06-2X, especially considering that systematic errors due to the chosen functional itself in calculating alkynyl C-H bonds is mostly cancelled out between experimental and calculated correlations.

Calculation of Rh-C Bond Strengths: Effect of Method and Model:

The model of Tp'Rh[$P(OMe)_3$](R)(H) was chosen as previously it was found that replacing Tp' with Tp have little influence in Tp'Rh(PMe_3)(R)(H) system but make big difference in Tp'Rh(CNMe)(R)(H) case. In the previous computation for the Tp'Rh(PMe_3)(R)(H) model, the available X-ray crystal structures for Tp'Rh(PMe_3)(C≡CR)(H) species enabled us to directly compare the reliability of DFT methods. Comparison between calculated (M06-2X or B3LYP) and crystal structures led to RMSD values of 4.4-5.1 for all atoms in all five complexes. DFT calculated bond distances were slightly off by less than 0.1 Å in the coordination atmosphere around rhodium. The model choice here is out of concern at least in terminal alkyne activation as both methods produced almost identical molecular structures with small RMSD values of less than 0.6 for all atoms.

Computational References:

1. Gaussian 09, Revision A.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji,H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.;

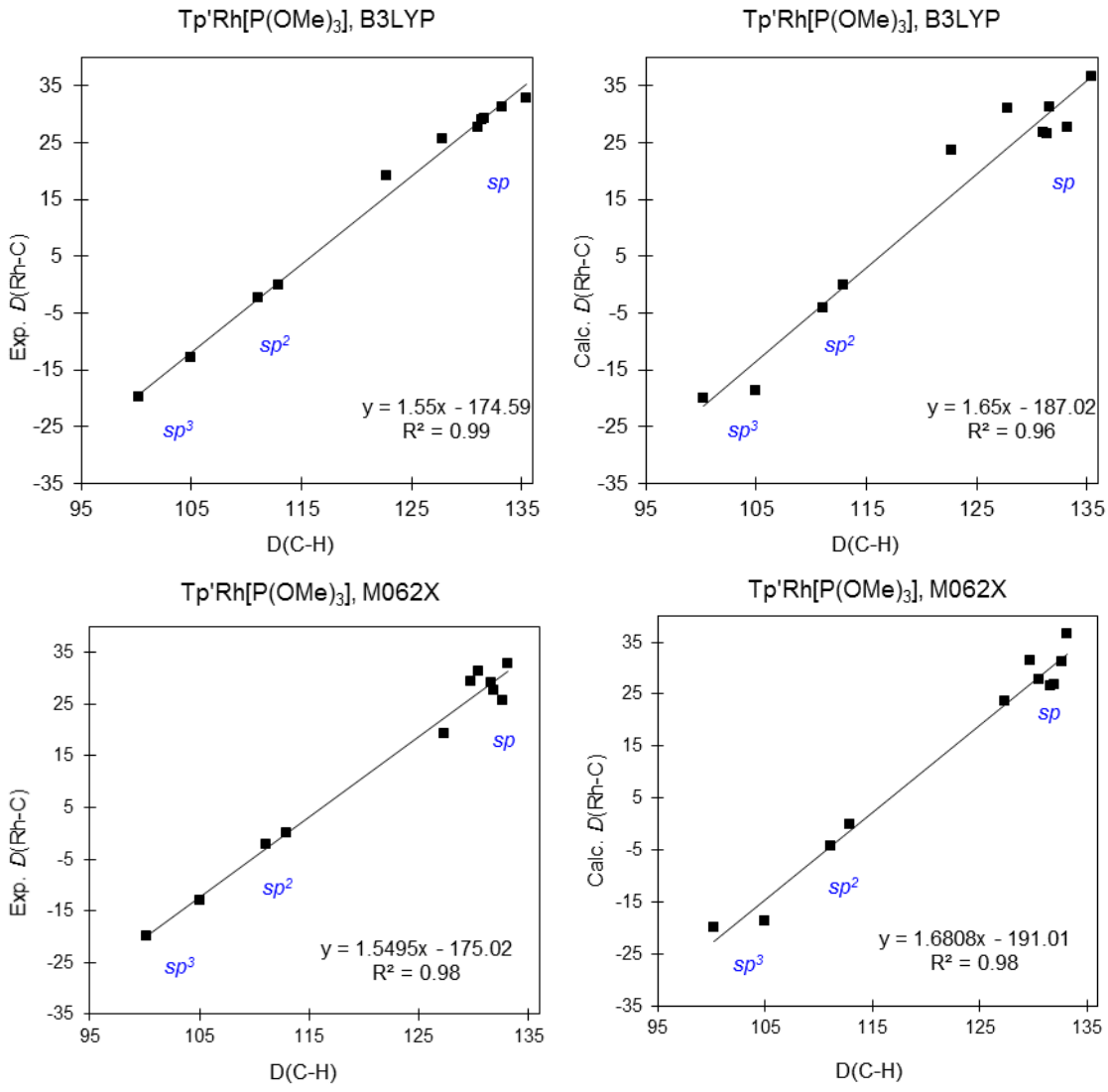
Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

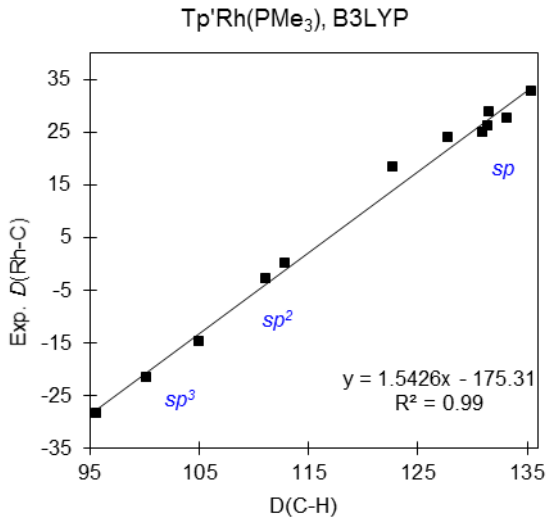
2. Choi, G.; Morris, J.; Brennessel, W. W.; Jones, W. D. *J. Am. Chem. Soc.*, **2012**, *134*, 9276-9284.
3. Jiao, Y; Morris, J; Brennessel, W. W.; Jones, W. D. *J. Am. Chem. Soc.* **2013**, *135*, Article ASAP, DOI: 10.1021/ja4080985.
4. Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215–241.
5. Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, 56, 2257-2261.
6. Andrae, D., Häussermann, U., Dolg, M., Stoll, H. and Preuss, H. *Theor. Chim. Acta* **1990**, *77*, 123-141.
7. Ehlers, A. W.; Böhme, M.; Dapprich, S.; Gobbi, A.; Höllwarth, A.; Jonas, V.; Köhler, K. F.; Stegmann, R.; Veldkamp, A.; Frenking, G. *Chem. Phys. Lett.* **1993**, *208*, 111-114.

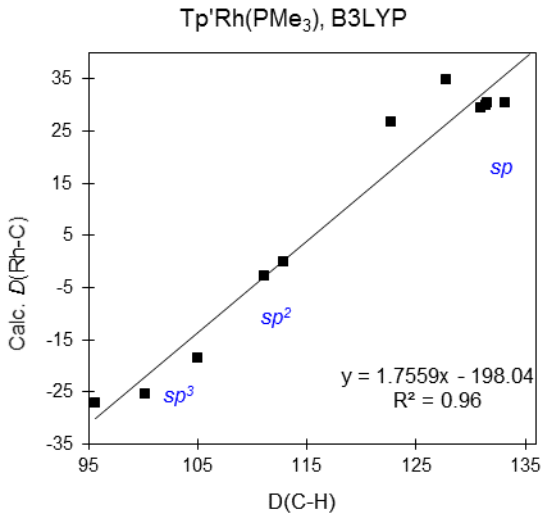
Table S48. Summary of alkynyl C-H bond energies in terminal alkynes calculated with different methods.

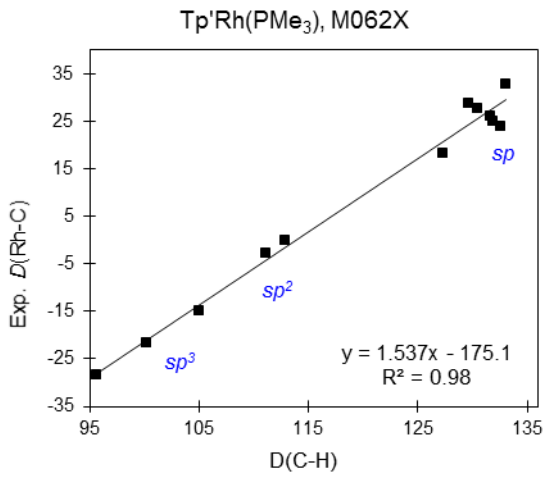
R	M06-2X calc. D(C-H)	B3LYP calc. D(C-H)
CF_3-acetylene	133.1	135.4
1-octyne	131.9	131.0
trimethylsilylacetylene	129.7	131.6
t-butylacetylene	131.6	131.4
phenylacetylene	130.5	133.2
p-CF_3phenylacetylene	132.6	127.8
p-MeOphenylacetylene	127.3	122.7

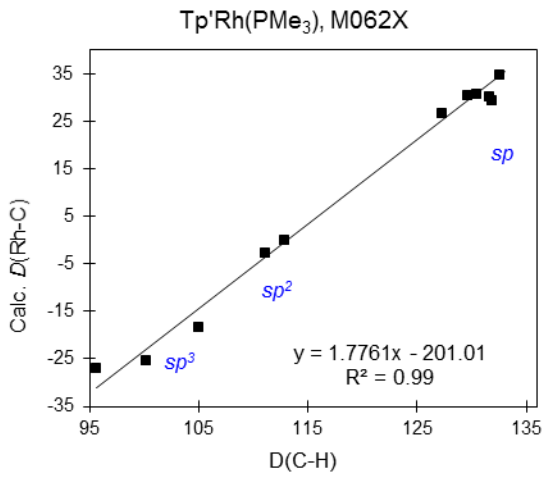
Figure S-106. Plots of *D*(Rh-C) vs. *D*(C-H) in activation of nonsubstituted hydrocarbons at [Tp′Rh(L)] (L = $P(OMe)_3$, PMe_3 and CNR), in which C-H bond strengths of terminal alkynes were calculated using M06-2X vs B3LYP methods.

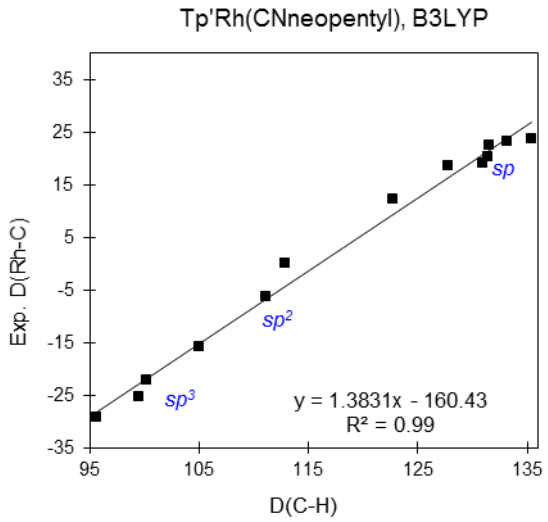


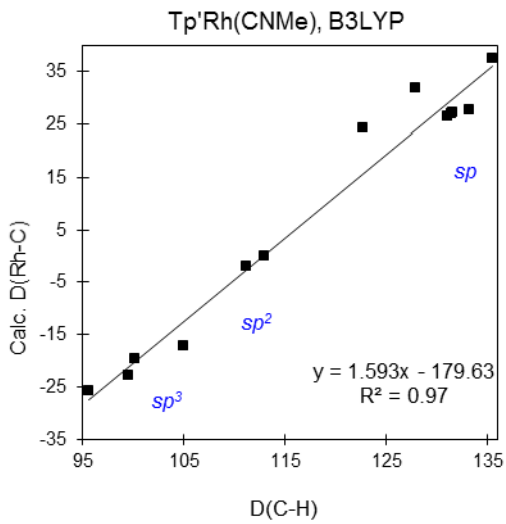


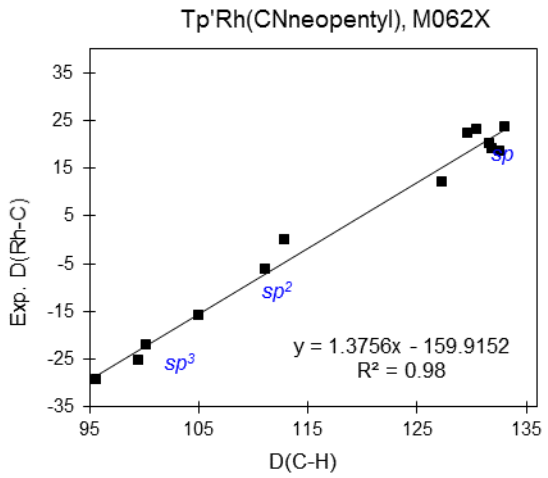







Tp'Rh(CNneopentyl), B3LYP
Exp. D(Rh-C)
D(C-H)
sp
sp²
sp³
y = 1.3831x - 160.43
R² = 0.99


Tp'Rh(CNMe), B3LYP
Calc. D(Rh-C)
D(C-H)
sp
sp²
sp³
y = 1.593x - 179.63
R² = 0.97


Tp'Rh(CNneopentyl), M062X
Exp. D(Rh-C)
D(C-H)
sp
sp²
sp³
y = 1.3756x - 159.9152
R² = 0.98

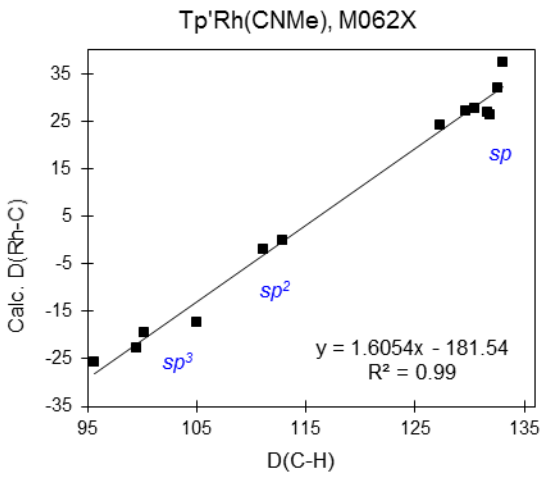

Tp'Rh(CNMe), M062X
Calc. D(Rh-C)
D(C-H)
sp
sp²
sp³
y = 1.6054x - 181.54
R² = 0.99

Table S49. Calculated energies for Tp'Rh[P(OMe)$_3$](R)H complexes and fragments.

R	Lit D(C-H) kcal/mol	calc D(Rh-C) kcal/mol
c-pentyl	95.60	42.84
Ph	112.90	69.51
t-butylvinyl	111.09	65.33
methyl	105.00	50.75
n-pentyl	100.19	49.47
CF_3-acetylene	135.40	106.14
1-octyne	131.00	96.39
trimethylsilylacetylene	131.56	100.89
t-butylacetylene	131.40	96.15
phenylacetylene	133.20	97.21
p-CF_3phenylacetylene	127.80	100.67
p-MeOphenylacetylene	122.70	93.22
mesityl	89.40	39.94
$CH_2C(O)CH_3$	96.00	50.56
CH_2CCCH_3	90.70	43.96
CH2O*t*Bu	93.00	49.88
CH_2OCH_3	96.10	50.28
CH_2F	101.30	56.79
CHF_2	103.20	64.48
CH_2CF_3	106.70	62.14

Table S50. Calculated coordinates for Tp'Rh[P(OMe)$_3$](R)H complexes and fragments. The following is a list of xyz coordinates of species used for the calculation of C-H and Rh-C bond strengths. Molecules R-H are followed by the corresponding radicals.

Tp'Rh[P(OMe)$_3$]H

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.407095	0.470795	-0.354906
2	7	0	0.522588	-1.411339	-0.911423
3	7	0	1.804222	-1.647663	-0.550757
4	7	0	1.636664	1.335488	-1.037916
5	7	0	2.736356	0.701615	-0.568489
6	7	0	0.621017	0.108520	1.627569
7	7	0	1.901400	-0.324156	1.599786
8	6	0	0.092519	-2.461704	-1.605757
9	6	0	1.123943	-3.408751	-1.697611
10	1	0	1.093761	-4.367850	-2.192378
11	6	0	2.195920	-2.853528	-1.016849
12	6	0	2.051640	2.330844	-1.816858
13	6	0	3.458157	2.351219	-1.844721
14	1	0	4.096671	3.031564	-2.388514
15	6	0	3.855843	1.296275	-1.043508
16	6	0	0.260956	0.209165	2.905952
17	6	0	1.337817	-0.164106	3.727565
18	1	0	1.363652	-0.196324	4.806496
19	6	0	2.362110	-0.499218	2.858305
20	5	0	2.615958	-0.601365	0.254855
21	1	0	3.710484	-1.034568	0.474677
22	6	0	3.743117	-0.983381	3.165778
23	1	0	3.877637	-1.030598	4.247643
24	1	0	3.919114	-1.980163	2.752224
25	1	0	4.504121	-0.315799	2.752534
26	6	0	-1.101784	0.675518	3.308784
27	1	0	-1.821269	0.509693	2.501397
28	1	0	-1.442785	0.134748	4.194808
29	1	0	-1.093577	1.745087	3.542318
30	6	0	3.564125	-3.412278	-0.789889
31	1	0	3.775147	-3.536787	0.275901
32	1	0	3.641152	-4.388363	-1.271569
33	1	0	4.336988	-2.760404	-1.206327
34	6	0	5.237068	0.819676	-0.724295
35	1	0	5.413986	0.788039	0.354160
36	1	0	5.415612	-0.185456	-1.116975
37	1	0	5.965705	1.497197	-1.172621

38	6	0	1.089570	3.224979	-2.531073
39	1	0	1.463138	3.454814	-3.532218
40	1	0	0.113316	2.744798	-2.613069
41	1	0	0.949853	4.175566	-2.004564
42	6	0	-1.294161	-2.506610	-2.163131
43	1	0	-1.497743	-3.487868	-2.595988
44	1	0	-2.033866	-2.307736	-1.382584
45	1	0	-1.422935	-1.747141	-2.939354
46	15	0	-1.530440	2.264261	0.146910
47	1	0	-1.104513	0.605395	-1.707305
48	8	0	-1.733604	3.330114	-1.083593
49	6	0	-2.474218	4.527347	-0.879344
50	1	0	-3.539183	4.301646	-0.765237
51	1	0	-2.112131	5.068608	0.001378
52	1	0	-2.330261	5.143496	-1.767814
53	8	0	-0.949252	3.235426	1.351502
54	6	0	0.447912	3.543457	1.311134
55	1	0	0.661495	4.130237	2.205314
56	1	0	1.049530	2.629270	1.308962
57	1	0	0.686553	4.135855	0.420917
58	8	0	-3.046387	2.062274	0.741313
59	6	0	-3.592961	2.849071	1.797934
60	1	0	-3.063948	2.655946	2.733813
61	1	0	-3.541867	3.918478	1.578472
62	1	0	-4.636118	2.545365	1.892966

Tp'Rh[P(OMe)$_3$](R)H R = methyl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.466099	0.428488	-0.376871
2	7	0	0.511682	-1.432657	-0.931610
3	7	0	1.784765	-1.645532	-0.526518
4	7	0	1.514487	1.318608	-1.000179
5	7	0	2.638127	0.727042	-0.532101
6	7	0	0.542268	0.050247	1.672783
7	7	0	1.840480	-0.332060	1.631077
8	6	0	0.135155	-2.483147	-1.659341
9	6	0	1.193452	-3.404262	-1.722044
10	1	0	1.206886	-4.353317	-2.236602
11	6	0	2.223001	-2.836118	-0.992410
12	6	0	1.891802	2.330675	-1.780753
13	6	0	3.295139	2.401712	-1.808630
14	1	0	3.906171	3.105973	-2.353288

15	6	0	3.732976	1.361674	-1.007727
16	6	0	0.197148	0.117600	2.958813
17	6	0	1.298659	-0.217518	3.764678
18	1	0	1.337186	-0.256260	4.843179
19	6	0	2.324132	-0.502883	2.881837
20	5	0	2.559365	-0.581504	0.287581
21	1	0	3.667832	-0.979166	0.503007
22	6	0	3.727696	-0.931082	3.170826
23	1	0	3.877252	-0.971504	4.251042
24	1	0	3.938031	-1.921099	2.756969
25	1	0	4.457318	-0.235411	2.747527
26	6	0	-1.184232	0.472363	3.407990
27	1	0	-1.714718	1.036295	2.640021
28	1	0	-1.768199	-0.429674	3.616785
29	1	0	-1.144504	1.062245	4.328407
30	6	0	3.595937	-3.364244	-0.724445
31	1	0	3.781314	-3.474185	0.347583
32	1	0	3.704598	-4.343193	-1.194104
33	1	0	4.366581	-2.701114	-1.127169
34	6	0	5.130716	0.935164	-0.690197
35	1	0	5.312957	0.920415	0.387712
36	1	0	5.340645	-0.067243	-1.073862
37	1	0	5.834323	1.632317	-1.148186
38	6	0	0.906594	3.201150	-2.493451
39	1	0	1.350464	3.588663	-3.413378
40	1	0	0.007662	2.634903	-2.747080
41	1	0	0.602938	4.050239	-1.873494
42	6	0	-1.221175	-2.580906	-2.280342
43	1	0	-1.175981	-3.192663	-3.183888
44	1	0	-1.940668	-3.037968	-1.594650
45	1	0	-1.592473	-1.587331	-2.540183
46	15	0	-1.455221	2.317476	-0.051148
47	1	0	-1.067473	0.554044	-1.751799
48	8	0	-2.165343	2.975892	-1.361272
49	6	0	-2.786246	4.255684	-1.284391
50	1	0	-3.684296	4.210964	-0.660120
51	1	0	-2.092078	5.004084	-0.891843
52	1	0	-3.072886	4.522012	-2.301747
53	8	0	-0.509316	3.595562	0.386894
54	6	0	0.427251	3.379269	1.448530
55	1	0	-0.082801	3.036137	2.357298
56	1	0	1.175702	2.637612	1.155031
57	1	0	0.902628	4.341812	1.639798
58	8	0	-2.631085	2.365683	1.100851
59	6	0	-2.938739	3.497809	1.908070
60	1	0	-2.742790	3.236199	2.952729

61	1	0	-2.337130	4.368424	1.636947
62	1	0	-3.999876	3.729766	1.789688
63	6	0	-2.158974	-0.580796	0.153886
64	1	0	-2.899288	-0.640548	-0.649024
65	1	0	-1.824849	-1.594270	0.400955
66	1	0	-2.647289	-0.152654	1.032464

Tp'Rh[P(OMe)$_3$](R)H R = phenyl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.489563	0.547205	-0.352564
2	7	0	0.443108	-1.331901	-0.919308
3	7	0	1.689954	-1.589104	-0.454580
4	7	0	1.497689	1.365104	-1.082998
5	7	0	2.617399	0.744267	-0.634055
6	7	0	0.567524	0.187040	1.691495
7	7	0	1.875785	-0.148860	1.618483
8	6	0	0.013259	-2.420055	-1.558285
9	6	0	1.007995	-3.409402	-1.500295
10	1	0	0.968378	-4.401350	-1.924726
11	6	0	2.054933	-2.845413	-0.793211
12	6	0	1.881895	2.242331	-2.013031
13	6	0	3.279542	2.201577	-2.149412
14	1	0	3.889356	2.791389	-2.817447
15	6	0	3.709379	1.231936	-1.263360
16	6	0	0.278595	0.348424	2.984780
17	6	0	1.428752	0.122649	3.758958
18	1	0	1.515948	0.167268	4.834432
19	6	0	2.424270	-0.195100	2.852367
20	5	0	2.527816	-0.505922	0.267392
21	1	0	3.630078	-0.927425	0.466615
22	6	0	3.854654	-0.551867	3.103928
23	1	0	4.060612	-0.485687	4.173500
24	1	0	4.079049	-1.569139	2.771667
25	1	0	4.535965	0.123462	2.579164
26	6	0	-1.086350	0.714689	3.469629
27	1	0	-1.834586	0.435029	2.727014
28	1	0	-1.308736	0.184383	4.399038
29	1	0	-1.168324	1.789772	3.658022
30	6	0	3.379586	-3.439090	-0.434490
31	1	0	3.546414	-3.424365	0.645923
32	1	0	3.412667	-4.475851	-0.773290
33	1	0	4.204909	-2.897236	-0.904861

34	6	0	5.097481	0.739689	-1.003975
35	1	0	5.359198	0.810349	0.055073
36	1	0	5.215150	-0.305514	-1.303649
37	1	0	5.805735	1.341932	-1.575367
38	6	0	0.928800	3.087813	-2.794593
39	1	0	1.331118	3.250445	-3.797397
40	1	0	-0.045843	2.604950	-2.872289
41	1	0	0.776149	4.062897	-2.324470
42	6	0	-1.328707	-2.500339	-2.212647
43	1	0	-1.301440	-3.239299	-3.016693
44	1	0	-2.104246	-2.790447	-1.496074
45	1	0	-1.611919	-1.531165	-2.628586
46	15	0	-1.459949	2.426417	0.187923
47	1	0	-1.109276	0.746665	-1.710302
48	6	0	-2.164977	-0.459324	0.084360
49	6	0	-3.392146	-0.279648	-0.573879
50	6	0	-2.083589	-1.512467	1.008201
51	6	0	-4.484568	-1.107881	-0.318982
52	6	0	-3.175468	-2.340604	1.270526
53	6	0	-4.383599	-2.143725	0.606664
54	1	0	-3.502662	0.521266	-1.299605
55	1	0	-1.143048	-1.696676	1.521591
56	1	0	-5.417780	-0.943060	-0.850731
57	1	0	-3.074930	-3.147301	1.991489
58	1	0	-5.233085	-2.789670	0.805893
59	8	0	-1.296942	3.595158	-0.933759
60	6	0	-1.866045	4.882272	-0.685589
61	1	0	-2.951066	4.840933	-0.796651
62	1	0	-1.614794	5.230692	0.320509
63	1	0	-1.438347	5.557182	-1.427987
64	8	0	-0.926439	3.137732	1.571675
65	6	0	0.479705	3.368503	1.718232
66	1	0	0.739462	3.166224	2.759390
67	1	0	1.069826	2.709895	1.073889
68	1	0	0.694767	4.413200	1.474952
69	8	0	-3.060537	2.575910	0.447448
70	6	0	-3.701214	2.121666	1.639393
71	1	0	-3.704590	1.029742	1.685477
72	1	0	-3.210476	2.544777	2.519367
73	1	0	-4.728825	2.482453	1.582969

Tp'Rh[P(OMe)$_3$](R)H R = *n*-pentyl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	45	0	-0.616106	0.591058	-0.738279
2	7	0	0.704014	-0.972099	-1.475882
3	7	0	1.959410	-1.045110	-0.975637
4	7	0	1.221722	1.866485	-1.136105
5	7	0	2.406535	1.413708	-0.663653
6	7	0	0.360314	0.166965	1.322616
7	7	0	1.702672	0.004152	1.320490
8	6	0	0.571397	-1.938049	-2.383545
9	6	0	1.770137	-2.664381	-2.465074
10	1	0	1.983809	-3.508617	-3.103319
11	6	0	2.627921	-2.065181	-1.559100
12	6	0	1.461210	3.005241	-1.785782
13	6	0	2.833561	3.302198	-1.720037
14	1	0	3.342918	4.150725	-2.152030
15	6	0	3.401602	2.263406	-1.004290
16	6	0	-0.043692	0.071193	2.589683
17	6	0	1.064689	-0.148670	3.425546
18	1	0	1.066646	-0.275903	4.497906
19	6	0	2.157729	-0.189042	2.579183
20	5	0	2.507726	0.022498	0.004119
21	1	0	3.656009	-0.217023	0.243413
22	6	0	3.600065	-0.409024	2.907914
23	1	0	3.710055	-0.529312	3.987009
24	1	0	3.990273	-1.306415	2.420114
25	1	0	4.219435	0.434390	2.590541
26	6	0	-1.484007	0.164558	2.981909
27	1	0	-2.110139	0.383327	2.115536
28	1	0	-1.824428	-0.778650	3.421638
29	1	0	-1.631918	0.946109	3.735707
30	6	0	4.045937	-2.410002	-1.233575
31	1	0	4.174192	-2.615605	-0.167534
32	1	0	4.337540	-3.299760	-1.793941
33	1	0	4.728439	-1.597490	-1.498415
34	6	0	4.835339	2.033247	-0.646770
35	1	0	4.969778	1.925764	0.433025
36	1	0	5.226302	1.127521	-1.118930
37	1	0	5.432856	2.881637	-0.984470
38	6	0	0.380309	3.781071	-2.468653
39	1	0	0.797008	4.328990	-3.316984
40	1	0	-0.402546	3.111292	-2.831383
41	1	0	-0.083543	4.500599	-1.787648
42	6	0	-0.699459	-2.151916	-3.140523
43	1	0	-0.494558	-2.680558	-4.073650
44	1	0	-1.411735	-2.747972	-2.559614
45	1	0	-1.172853	-1.194482	-3.369565

46	15	0	-1.874164	2.275900	-0.236981
47	1	0	-1.179612	0.800532	-2.119673
48	8	0	-2.638589	2.979230	-1.492735
49	6	0	-3.445656	4.135295	-1.290272
50	1	0	-4.334458	3.885595	-0.702345
51	1	0	-2.877249	4.927403	-0.794739
52	1	0	-3.756900	4.473138	-2.278695
53	8	0	-1.125338	3.611296	0.373220
54	6	0	-0.209788	3.420539	1.456958
55	1	0	-0.693610	2.899069	2.291810
56	1	0	0.659758	2.844513	1.128544
57	1	0	0.096070	4.416303	1.779665
58	8	0	-3.071520	2.033115	0.866679
59	6	0	-3.547019	3.005606	1.790695
60	1	0	-3.349770	2.639031	2.802716
61	1	0	-3.056865	3.972496	1.654264
62	1	0	-4.625527	3.116867	1.653985
63	6	0	-2.187067	-0.714449	-0.472534
64	1	0	-2.612468	-0.956129	-1.454215
65	1	0	-3.001895	-0.255024	0.100162
66	6	0	-1.781476	-2.009456	0.231857
67	1	0	-0.991178	-2.526580	-0.325801
68	1	0	-1.346491	-1.787987	1.212934
69	6	0	-2.963189	-2.963789	0.421269
70	1	0	-3.766615	-2.446061	0.965044
71	1	0	-3.382993	-3.229659	-0.560103
72	6	0	-2.587301	-4.238563	1.173558
73	1	0	-2.180113	-3.965511	2.155854
74	1	0	-1.775156	-4.746079	0.637795
75	6	0	-3.764342	-5.193831	1.351315
76	1	0	-4.161740	-5.507902	0.380872
77	1	0	-4.579176	-4.709741	1.899309
78	1	0	-3.477271	-6.093307	1.902813

Tp'Rh[P(OMe)$_3$](R)H R = *c*-pentyl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.929762	1.210133	-0.073018
2	7	0	1.010003	0.281235	0.367461
3	7	0	1.907387	0.971873	1.107885
4	7	0	0.475090	2.946474	-0.560301
5	7	0	1.335893	3.317888	0.416246
6	7	0	-0.855009	2.001076	2.100688

7	7	0	0.365387	2.362938	2.560208
8	6	0	1.615555	-0.821371	-0.072759
9	6	0	2.932953	-0.853322	0.410249
10	1	0	3.676965	-1.616320	0.236927
11	6	0	3.082927	0.306228	1.150586
12	6	0	0.589826	3.830430	-1.550505
13	6	0	1.539025	4.806789	-1.199873
14	1	0	1.861436	5.652280	-1.789301
15	6	0	1.995712	4.442074	0.054224
16	6	0	-1.697900	2.079970	3.132120
17	6	0	-1.005729	2.499926	4.279848
18	1	0	-1.409527	2.657681	5.268954
19	6	0	0.306582	2.665758	3.876008
20	5	0	1.595543	2.393625	1.631187
21	1	0	2.537810	2.804530	2.245192
22	6	0	1.493914	3.095526	4.677465
23	1	0	1.188172	3.266529	5.711034
24	1	0	2.277557	2.333064	4.671784
25	1	0	1.930545	4.019980	4.289679
26	6	0	-3.152329	1.749347	3.024418
27	1	0	-3.519537	1.915078	2.010680
28	1	0	-3.339591	0.698724	3.270773
29	1	0	-3.728049	2.363925	3.721552
30	6	0	4.286561	0.811030	1.880107
31	1	0	4.072850	0.986584	2.937793
32	1	0	5.086672	0.072492	1.807972
33	1	0	4.648184	1.751770	1.455226
34	6	0	3.032008	5.094039	0.913024
35	1	0	2.637019	5.338903	1.902874
36	1	0	3.900564	4.444991	1.056483
37	1	0	3.367990	6.017445	0.438358
38	6	0	-0.197834	3.712465	-2.816206
39	1	0	0.409682	4.033496	-3.665849
40	1	0	-0.507002	2.677073	-2.975338
41	1	0	-1.099678	4.331250	-2.784287
42	6	0	0.925338	-1.814417	-0.949719
43	1	0	1.655169	-2.502803	-1.380360
44	1	0	0.189868	-2.400810	-0.390115
45	1	0	0.396133	-1.305989	-1.759877
46	15	0	-2.684773	2.190188	-0.863419
47	1	0	-0.882769	0.607147	-1.452550
48	8	0	-2.948810	1.953753	-2.453936
49	6	0	-4.029013	2.601969	-3.118834
50	1	0	-4.988679	2.215177	-2.762148
51	1	0	-3.983186	3.685339	-2.975597
52	1	0	-3.923632	2.369639	-4.178622

53	8	0	-2.699072	3.838079	-0.852281
54	6	0	-2.340462	4.493066	0.369188
55	1	0	-3.022340	4.207536	1.179757
56	1	0	-1.314701	4.244244	0.654197
57	1	0	-2.429987	5.563452	0.181221
58	8	0	-4.137195	1.844053	-0.166066
59	6	0	-5.241832	2.739753	-0.088347
60	1	0	-5.471650	2.905855	0.968692
61	1	0	-5.023167	3.699130	-0.563433
62	1	0	-6.103610	2.274499	-0.572743
63	6	0	-2.671347	-1.314831	-0.562692
64	6	0	-2.115271	-0.363950	0.504275
65	6	0	-3.248399	-2.460250	0.275227
66	6	0	-1.498301	-1.297794	1.573815
67	6	0	-2.183976	-2.678693	1.367914
68	1	0	-1.875443	-1.690792	-1.216281
69	1	0	-4.191441	-2.132575	0.729802
70	1	0	-2.997406	0.087684	0.972182
71	1	0	-1.672466	-0.896854	2.578547
72	1	0	-0.415490	-1.388827	1.473327
73	1	0	-2.613008	-3.077995	2.291107
74	1	0	-1.450206	-3.415004	1.019853
75	1	0	-3.457742	-3.367884	-0.298955
76	1	0	-3.416221	-0.828620	-1.203336

Tp'Rh[P(OMe)$_3$](R)H R = *t*BuCHCH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.531673	0.587276	-0.333226
2	7	0	0.312578	-1.306148	-0.940845
3	7	0	1.563863	-1.625656	-0.536544
4	7	0	1.483557	1.365779	-0.972729
5	7	0	2.578229	0.682643	-0.566368
6	7	0	0.507585	0.150992	1.695155
7	7	0	1.775722	-0.316675	1.617050
8	6	0	-0.155580	-2.320781	-1.665754
9	6	0	0.818316	-3.331141	-1.723138
10	1	0	0.748057	-4.279418	-2.234528
11	6	0	1.894728	-2.852546	-0.996938
12	6	0	1.901096	2.363738	-1.751506
13	6	0	3.302795	2.331178	-1.840490
14	1	0	3.940985	2.999488	-2.399139
15	6	0	3.695693	1.244799	-1.077769

16	6	0	0.206335	0.251122	2.990604
17	6	0	1.307008	-0.155921	3.765092
18	1	0	1.375246	-0.193773	4.842235
19	6	0	2.284274	-0.512632	2.854722
20	5	0	2.434740	-0.620359	0.254087
21	1	0	3.519110	-1.093397	0.437226
22	6	0	3.663687	-1.033727	3.104649
23	1	0	3.840736	-1.084673	4.180235
24	1	0	3.797089	-2.034903	2.685901
25	1	0	4.425489	-0.387164	2.660351
26	6	0	-1.123761	0.727699	3.481131
27	1	0	-1.811257	0.893416	2.651083
28	1	0	-1.569224	-0.015294	4.149377
29	1	0	-1.013775	1.654614	4.057173
30	6	0	3.215963	-3.499358	-0.729214
31	1	0	3.396945	-3.614750	0.342979
32	1	0	3.232035	-4.489281	-1.188155
33	1	0	4.041895	-2.914558	-1.143621
34	6	0	5.069877	0.710540	-0.828102
35	1	0	5.287932	0.643987	0.241085
36	1	0	5.194446	-0.289522	-1.253050
37	1	0	5.804485	1.372913	-1.289051
38	6	0	0.952284	3.320363	-2.400616
39	1	0	1.397117	3.723759	-3.313024
40	1	0	0.016478	2.818233	-2.657198
41	1	0	0.710514	4.155606	-1.736351
42	6	0	-1.507756	-2.299570	-2.302172
43	1	0	-1.506494	-2.919783	-3.201489
44	1	0	-2.271474	-2.675533	-1.616370
45	1	0	-1.784187	-1.277644	-2.569836
46	15	0	-1.414712	2.524479	0.076772
47	1	0	-1.136451	0.778207	-1.699251
48	8	0	-2.137262	3.231761	-1.200745
49	6	0	-2.729401	4.522017	-1.076433
50	1	0	-3.612016	4.479547	-0.430578
51	1	0	-2.009913	5.245905	-0.683551
52	1	0	-3.035670	4.819762	-2.079148
53	8	0	-0.411230	3.756579	0.508848
54	6	0	0.566574	3.485915	1.520098
55	1	0	0.086226	3.153020	2.447748
56	1	0	1.267198	2.718620	1.179701
57	1	0	1.090621	4.425246	1.698797
58	8	0	-2.551631	2.574699	1.259688
59	6	0	-2.805601	3.693438	2.102930
60	1	0	-2.604186	3.393230	3.135407
61	1	0	-2.176908	4.549350	1.845977

62	1	0	-3.859148	3.967561	2.008432
63	6	0	-2.263434	-0.275008	0.147027
64	1	0	-3.178921	0.067893	-0.339282
65	6	0	-2.344782	-1.295904	1.004707
66	1	0	-1.432621	-1.649333	1.496247
67	6	0	-3.594983	-2.053303	1.420765
68	6	0	-3.832394	-1.811243	2.919948
69	6	0	-3.356383	-3.554891	1.199603
70	1	0	-3.211046	-3.777373	0.137781
71	1	0	-2.463442	-3.889970	1.737757
72	1	0	-4.210534	-4.141255	1.557331
73	1	0	-2.959219	-2.120102	3.505430
74	1	0	-4.697945	-2.382665	3.275328
75	1	0	-4.014021	-0.749173	3.114671
76	6	0	-4.833816	-1.617766	0.638212
77	1	0	-4.691917	-1.767102	-0.437477
78	1	0	-5.704625	-2.202998	0.952179
79	1	0	-5.057155	-0.559746	0.808117

Tp'Rh[P(OMe)$_3$](R)H R = α-mesityl

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-4.088516	-0.379956	2.461538
2	7	0	-1.933445	-0.342980	2.160970
3	7	0	-1.140316	-0.888187	3.114608
4	7	0	-3.510836	0.266610	4.545838
5	7	0	-2.532940	-0.435533	5.164543
6	7	0	-3.705823	-2.550784	3.213289
7	7	0	-2.641003	-2.703744	4.035388
8	6	0	-1.141799	0.177952	1.224187
9	6	0	0.199347	-0.042562	1.578093
10	1	0	1.079018	0.256921	1.028366
11	6	0	0.159113	-0.719117	2.783893
12	6	0	-3.917923	1.213778	5.390696
13	6	0	-3.192934	1.113216	6.590030
14	1	0	-3.282302	1.738292	7.466028
15	6	0	-2.318262	0.056968	6.405132
16	6	0	-4.256955	-3.756728	3.063621
17	6	0	-3.538296	-4.704051	3.810916
18	1	0	-3.735115	-5.762605	3.893583
19	6	0	-2.513580	-3.995473	4.411525
20	5	0	-1.728772	-1.512671	4.399638
21	1	0	-0.836004	-1.904047	5.094224

22	6	0	-1.427749	-4.488735	5.314020
23	1	0	-1.559726	-5.558424	5.485008
24	1	0	-0.438936	-4.329687	4.875284
25	1	0	-1.444440	-3.980036	6.281707
26	6	0	-5.449964	-4.007582	2.197232
27	1	0	-6.063451	-3.110878	2.100105
28	1	0	-5.146137	-4.308207	1.189495
29	1	0	-6.056150	-4.814933	2.617570
30	6	0	1.291454	-1.203622	3.631845
31	1	0	1.247687	-2.286034	3.780439
32	1	0	2.236400	-0.961887	3.142578
33	1	0	1.284613	-0.733350	4.619142
34	6	0	-1.284296	-0.489065	7.337318
35	1	0	-1.428679	-1.557615	7.517930
36	1	0	-0.274685	-0.354964	6.939018
37	1	0	-1.348325	0.032930	8.293497
38	6	0	-4.981165	2.201705	5.032289
39	1	0	-4.840324	3.121821	5.603916
40	1	0	-4.941682	2.437962	3.966742
41	1	0	-5.979385	1.809422	5.249089
42	6	0	-1.675452	0.870599	0.013449
43	1	0	-0.975521	1.643572	-0.312097
44	1	0	-1.818223	0.171653	-0.816227
45	1	0	-2.644883	1.329245	0.219656
46	15	0	-6.218976	-0.202448	2.809600
47	1	0	-4.209546	1.028990	1.953890
48	8	0	-6.850619	1.286258	2.592877
49	6	0	-8.247117	1.514576	2.753754
50	1	0	-8.807972	1.023566	1.952276
51	1	0	-8.592777	1.159982	3.729181
52	1	0	-8.394863	2.592593	2.685819
53	8	0	-6.764594	-0.461278	4.342521
54	6	0	-6.282527	-1.614031	5.041163
55	1	0	-6.539474	-2.534202	4.502600
56	1	0	-5.197843	-1.561550	5.168853
57	1	0	-6.777539	-1.611716	6.012775
58	8	0	-7.195988	-1.188839	1.927793
59	6	0	-8.462593	-1.684071	2.354205
60	1	0	-8.418388	-2.777204	2.343709
61	1	0	-8.713387	-1.343250	3.361496
62	1	0	-9.225302	-1.349255	1.647479
63	6	0	-4.381861	-1.082436	0.554449
64	1	0	-3.434444	-1.593716	0.338909
65	1	0	-5.147005	-1.864399	0.614723
66	6	0	-4.735442	-0.205186	-0.623636
67	6	0	-4.263105	-0.562990	-1.892617

68	6	0	-5.564686	0.917016	-0.537489
69	6	0	-4.593855	0.158314	-3.039750
70	6	0	-5.917420	1.657134	-1.667609
71	6	0	-5.428878	1.268261	-2.914244
72	1	0	-3.617954	-1.436352	-1.985239
73	1	0	-5.934509	1.240541	0.430371
74	1	0	-5.699145	1.839913	-3.800061
75	6	0	-4.041414	-0.250620	-4.382261
76	1	0	-2.978347	0.000147	-4.462398
77	1	0	-4.133211	-1.329712	-4.535424
78	1	0	-4.564461	0.254648	-5.197690
79	6	0	-6.788469	2.880873	-1.529893
80	1	0	-7.323339	3.095855	-2.458629
81	1	0	-7.524878	2.752719	-0.731481
82	1	0	-6.188701	3.763022	-1.281638

Tp'Rh[P(OMe)$_3$](R)H R = CH_3OCH_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-3.966562	-0.349735	2.296967
2	7	0	-1.805060	-0.460321	2.124308
3	7	0	-1.086115	-0.884203	3.188896
4	7	0	-3.481829	0.552604	4.312216
5	7	0	-2.561300	-0.084619	5.072413
6	7	0	-3.747811	-2.396374	3.371442
7	7	0	-2.729730	-2.480898	4.260797
8	6	0	-0.949565	-0.124755	1.159530
9	6	0	0.362514	-0.345875	1.612754
10	1	0	1.281167	-0.172560	1.072620
11	6	0	0.234034	-0.825046	2.904038
12	6	0	-3.892689	1.621194	4.994529
13	6	0	-3.229657	1.668283	6.232914
14	1	0	-3.339286	2.411752	7.008356
15	6	0	-2.387336	0.570500	6.242307
16	6	0	-4.362371	-3.580091	3.370186
17	6	0	-3.732719	-4.444030	4.281497
18	1	0	-3.993609	-5.467590	4.506434
19	6	0	-2.695662	-3.708600	4.825271
20	5	0	-1.774465	-1.292208	4.512356
21	1	0	-0.940734	-1.621550	5.306042
22	6	0	-1.679956	-4.120123	5.842907
23	1	0	-1.878300	-5.146781	6.155325
24	1	0	-0.665579	-4.073658	5.437187

25	1	0	-1.709950	-3.477901	6.727170
26	6	0	-5.533369	-3.885811	2.491514
27	1	0	-6.003451	-2.969500	2.132132
28	1	0	-5.224862	-4.467223	1.616756
29	1	0	-6.272521	-4.479716	3.037713
30	6	0	1.299028	-1.225225	3.874195
31	1	0	1.185955	-2.266993	4.186730
32	1	0	2.277010	-1.110656	3.403995
33	1	0	1.275862	-0.605659	4.775046
34	6	0	-1.422215	0.125368	7.294396
35	1	0	-1.629734	-0.896136	7.624881
36	1	0	-0.391578	0.150374	6.929566
37	1	0	-1.496809	0.788229	8.158017
38	6	0	-4.897084	2.583226	4.444482
39	1	0	-4.709204	3.583134	4.842554
40	1	0	-4.834905	2.620525	3.354711
41	1	0	-5.918229	2.294339	4.710784
42	6	0	-1.394704	0.401872	-0.168467
43	1	0	-0.819872	1.294335	-0.429468
44	1	0	-1.226559	-0.340801	-0.955579
45	1	0	-2.457306	0.654095	-0.158707
46	15	0	-6.099277	0.002905	2.373908
47	1	0	-3.966078	0.979949	1.596732
48	8	0	-6.597696	1.456959	1.845429
49	6	0	-7.979746	1.797892	1.847839
50	1	0	-8.523969	1.197040	1.112558
51	1	0	-8.416006	1.664622	2.842254
52	1	0	-8.039409	2.848223	1.562584
53	8	0	-6.805158	0.030757	3.865987
54	6	0	-6.468515	-1.020382	4.776226
55	1	0	-6.743236	-1.999257	4.363532
56	1	0	-5.397958	-1.010282	5.000412
57	1	0	-7.044056	-0.836845	5.684206
58	8	0	-7.047498	-1.079376	1.575137
59	6	0	-8.375173	-1.430780	1.951402
60	1	0	-8.394325	-2.502609	2.172452
61	1	0	-8.709497	-0.877384	2.832110
62	1	0	-9.041917	-1.226157	1.110355
63	6	0	-4.194335	-1.193317	0.483056
64	1	0	-3.195753	-1.546152	0.173250
65	1	0	-4.857493	-2.071364	0.537386
66	8	0	-4.704016	-0.295859	-0.490156
67	6	0	-4.775961	-0.894163	-1.756953
68	1	0	-3.780260	-1.210013	-2.106492
69	1	0	-5.432292	-1.777773	-1.747804
70	1	0	-5.179959	-0.156870	-2.454088

Tp'Rh[P(OMe)$_3$](R)H R = *t*BuOCH$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.174291	-2.344178	-2.006655
2	7	0	1.104263	-0.597276	-1.897529
3	7	0	2.152351	-0.497841	-2.746703
4	7	0	1.803132	-3.437481	-2.154774
5	7	0	2.723161	-2.939810	-3.013015
6	7	0	0.031703	-2.069000	-4.306318
7	7	0	1.279550	-1.780784	-4.746780
8	6	0	1.131871	0.459666	-1.086821
9	6	0	2.227363	1.271490	-1.428639
10	1	0	2.527355	2.198454	-0.963239
11	6	0	2.851125	0.628912	-2.483223
12	6	0	2.343418	-4.501436	-1.562230
13	6	0	3.643421	-4.702872	-2.057991
14	1	0	4.341782	-5.476261	-1.774731
15	6	0	3.850046	-3.686643	-2.974076
16	6	0	-0.758460	-2.116360	-5.380139
17	6	0	-0.004290	-1.860601	-6.537378
18	1	0	-0.355791	-1.828705	-7.557984
19	6	0	1.287591	-1.648130	-6.092061
20	5	0	2.464816	-1.616144	-3.769082
21	1	0	3.444532	-1.320090	-4.390206
22	6	0	2.515802	-1.327285	-6.883039
23	1	0	2.260892	-1.289192	-7.943479
24	1	0	2.937768	-0.360599	-6.595174
25	1	0	3.294607	-2.081781	-6.742845
26	6	0	-2.227912	-2.385074	-5.297821
27	1	0	-2.487466	-2.864319	-4.353011
28	1	0	-2.800260	-1.453843	-5.366197
29	1	0	-2.542774	-3.026417	-6.126515
30	6	0	4.075399	1.028728	-3.242632
31	1	0	3.865669	1.149255	-4.308979
32	1	0	4.446020	1.979219	-2.855429
33	1	0	4.869490	0.283530	-3.143284
34	6	0	5.062048	-3.385773	-3.796846
35	1	0	4.828286	-3.364259	-4.864713
36	1	0	5.494942	-2.416249	-3.534562
37	1	0	5.816004	-4.155843	-3.625474
38	6	0	1.612747	-5.296490	-0.526985
39	1	0	2.323238	-5.714092	0.190323

40	1	0	0.902176	-4.664861	0.011107
41	1	0	1.052847	-6.122631	-0.976428
42	6	0	0.125453	0.673022	0.000289
43	1	0	0.632470	0.936047	0.932482
44	1	0	-0.552364	1.495401	-0.251499
45	1	0	-0.474133	-0.225358	0.164170
46	15	0	-1.440772	-4.094460	-1.841481
47	1	0	-0.218238	-2.420922	-0.505294
48	8	0	-1.683840	-4.657069	-0.336039
49	6	0	-2.530197	-5.779579	-0.115329
50	1	0	-3.569632	-5.528021	-0.348409
51	1	0	-2.206985	-6.638584	-0.711034
52	1	0	-2.452442	-6.022477	0.944422
53	8	0	-0.898322	-5.489668	-2.538223
54	6	0	-0.412621	-5.402062	-3.880910
55	1	0	-1.198088	-5.045236	-4.559111
56	1	0	0.446854	-4.727960	-3.938545
57	1	0	-0.118843	-6.411874	-4.169321
58	8	0	-2.952962	-3.975528	-2.488917
59	6	0	-3.686665	-5.055551	-3.055029
60	1	0	-3.899051	-4.811660	-4.100853
61	1	0	-3.130797	-5.995188	-3.011332
62	1	0	-4.630910	-5.159601	-2.513939
63	6	0	-1.831442	-1.202549	-1.913280
64	1	0	-1.500608	-0.153838	-1.890841
65	1	0	-2.411002	-1.357826	-2.831810
66	8	0	-2.622025	-1.511977	-0.777770
67	6	0	-3.886543	-0.858252	-0.652034
68	6	0	-4.542417	-1.568849	0.527711
69	6	0	-4.745311	-1.038420	-1.907984
70	1	0	-4.391487	-0.423007	-2.739921
71	1	0	-4.724262	-2.087961	-2.217507
72	1	0	-5.778937	-0.749157	-1.695783
73	1	0	-4.682088	-2.627008	0.286721
74	1	0	-5.514020	-1.124910	0.763374
75	1	0	-3.895995	-1.500427	1.406538
76	6	0	-3.688254	0.625644	-0.336055
77	1	0	-3.079236	0.735959	0.566299
78	1	0	-3.186184	1.141351	-1.160002
79	1	0	-4.652512	1.115919	-0.170160

Tp'Rh[P(OMe)$_3$](R)H R = MeCCCH$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	45	0	-0.481348	0.400913	-0.385773
2	7	0	0.522196	-1.437305	-0.967080
3	7	0	1.795954	-1.631956	-0.555159
4	7	0	1.467087	1.309056	-1.034027
5	7	0	2.598233	0.758072	-0.534738
6	7	0	0.549396	0.075105	1.656032
7	7	0	1.832580	-0.350768	1.615877
8	6	0	0.147814	-2.513399	-1.654805
9	6	0	1.208068	-3.433594	-1.686115
10	1	0	1.224236	-4.398843	-2.169660
11	6	0	2.236618	-2.837499	-0.977740
12	6	0	1.827991	2.334037	-1.806183
13	6	0	3.227629	2.456874	-1.793915
14	1	0	3.826862	3.182917	-2.322767
15	6	0	3.681161	1.433464	-0.980411
16	6	0	0.164284	0.041316	2.930640
17	6	0	1.227407	-0.406830	3.734633
18	1	0	1.232695	-0.536114	4.806826
19	6	0	2.269763	-0.651941	2.859162
20	5	0	2.552418	-0.563177	0.268624
21	1	0	3.670405	-0.939630	0.473105
22	6	0	3.649143	-1.153244	3.146870
23	1	0	3.773681	-1.269759	4.224869
24	1	0	3.831751	-2.122454	2.674192
25	1	0	4.413582	-0.461052	2.783832
26	6	0	-1.220892	0.395145	3.364464
27	1	0	-1.740155	0.961045	2.589985
28	1	0	-1.800964	-0.514440	3.548942
29	1	0	-1.198716	0.981928	4.287932
30	6	0	3.612933	-3.350707	-0.697812
31	1	0	3.799103	-3.439849	0.376091
32	1	0	3.728802	-4.337533	-1.149061
33	1	0	4.379535	-2.690020	-1.112074
34	6	0	5.084309	1.058430	-0.624501
35	1	0	5.234517	1.043141	0.458294
36	1	0	5.342948	0.067185	-1.007294
37	1	0	5.773799	1.784930	-1.057586
38	6	0	0.835420	3.166929	-2.552477
39	1	0	1.284109	3.537344	-3.477147
40	1	0	-0.050336	2.578788	-2.801433
41	1	0	0.511089	4.027449	-1.959256
42	6	0	-1.216052	-2.650903	-2.247696
43	1	0	-1.194139	-3.357251	-3.080256
44	1	0	-1.921930	-3.019196	-1.496374
45	1	0	-1.574882	-1.685674	-2.612823

46	15	0	-1.441906	2.315211	-0.055076
47	1	0	-1.101452	0.509816	-1.754375
48	8	0	-2.155465	2.975513	-1.361480
49	6	0	-2.763893	4.261696	-1.279732
50	1	0	-3.653140	4.225971	-0.642528
51	1	0	-2.057270	5.004259	-0.898509
52	1	0	-3.061827	4.527745	-2.293810
53	8	0	-0.471174	3.574936	0.368001
54	6	0	0.471422	3.354632	1.425184
55	1	0	-0.030490	2.985493	2.327979
56	1	0	1.229201	2.629774	1.116290
57	1	0	0.930880	4.321776	1.631364
58	8	0	-2.611404	2.386930	1.101758
59	6	0	-2.873869	3.512547	1.934213
60	1	0	-2.648000	3.234614	2.968371
61	1	0	-2.269180	4.377534	1.652532
62	1	0	-3.934691	3.760432	1.852270
63	6	0	-2.203794	-0.602276	0.177418
64	1	0	-2.774902	-0.875683	-0.714229
65	1	0	-2.853233	0.025121	0.794419
66	6	0	-1.828193	-1.792083	0.924723
67	6	0	-1.448890	-2.758017	1.548813
68	6	0	-0.916685	-3.891633	2.304159
69	1	0	-0.222267	-3.539763	3.073921
70	1	0	-1.709253	-4.462753	2.796757
71	1	0	-0.368856	-4.571621	1.644879

Tp'Rh[P(OMe)$_3$](R)H R = MeC(O)CH$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.404112	0.064191	-0.327776
2	7	0	0.517130	-1.828145	-0.901479
3	7	0	1.768539	-2.094713	-0.462129
4	7	0	1.596366	0.877363	-0.875423
5	7	0	2.686678	0.248814	-0.375308
6	7	0	0.523951	-0.415409	1.762194
7	7	0	1.806120	-0.850526	1.736836
8	6	0	0.142466	-2.835111	-1.689275
9	6	0	1.175832	-3.783730	-1.753205
10	1	0	1.183071	-4.709705	-2.308265
11	6	0	2.192063	-3.276131	-0.963333
12	6	0	2.025602	1.896424	-1.619613
13	6	0	3.430145	1.934059	-1.589597

14	1	0	4.077667	2.635980	-2.093480
15	6	0	3.812846	0.868829	-0.794194
16	6	0	0.157730	-0.365590	3.044210
17	6	0	1.227052	-0.768956	3.861108
18	1	0	1.242198	-0.834470	4.938915
19	6	0	2.257722	-1.073461	2.991090
20	5	0	2.550495	-1.078042	0.404387
21	1	0	3.641739	-1.513075	0.634174
22	6	0	3.637103	-1.564201	3.296338
23	1	0	3.761207	-1.641212	4.377824
24	1	0	3.818783	-2.549396	2.858128
25	1	0	4.401541	-0.885240	2.909060
26	6	0	-1.209107	0.047351	3.491468
27	1	0	-1.673113	0.728838	2.776746
28	1	0	-1.864879	-0.822882	3.600199
29	1	0	-1.149866	0.539221	4.466262
30	6	0	3.539440	-3.854027	-0.670039
31	1	0	3.687020	-4.003106	0.403044
32	1	0	3.634146	-4.820573	-1.167510
33	1	0	4.341698	-3.202293	-1.027009
34	6	0	5.187387	0.403653	-0.432603
35	1	0	5.323713	0.351310	0.650925
36	1	0	5.393418	-0.590561	-0.839200
37	1	0	5.922659	1.099975	-0.838984
38	6	0	1.091222	2.804396	-2.351716
39	1	0	1.577914	3.190849	-3.250167
40	1	0	0.185154	2.269589	-2.644843
41	1	0	0.787058	3.650707	-1.729680
42	6	0	-1.188289	-2.872690	-2.369002
43	1	0	-1.084792	-3.279094	-3.377823
44	1	0	-1.889548	-3.512600	-1.823053
45	1	0	-1.611517	-1.868003	-2.437068
46	15	0	-1.310756	2.017694	0.029291
47	1	0	-0.954016	0.256417	-1.712137
48	8	0	-1.895029	2.850255	-1.235078
49	6	0	-3.165444	3.494111	-1.204734
50	1	0	-3.923191	2.823716	-0.795804
51	1	0	-3.110339	4.425894	-0.631685
52	1	0	-3.411996	3.725830	-2.240919
53	8	0	-0.262138	3.180949	0.554057
54	6	0	0.604365	2.862581	1.643930
55	1	0	0.032937	2.525388	2.517856
56	1	0	1.317316	2.083863	1.359283
57	1	0	1.134877	3.782254	1.893491
58	8	0	-2.470990	2.063458	1.191057
59	6	0	-2.813039	3.248637	1.906747

60	1	0	-2.765030	3.016146	2.974356
61	1	0	-2.124239	4.067468	1.685028
62	1	0	-3.833315	3.539376	1.645048
63	6	0	-2.151305	-0.874956	0.168452
64	1	0	-1.966112	-1.956036	0.161074
65	1	0	-2.389898	-0.610633	1.208585
66	6	0	-3.398620	-0.559849	-0.606064
67	8	0	-3.663679	0.556291	-1.016548
68	6	0	-4.380978	-1.695966	-0.825838
69	1	0	-4.588675	-2.205301	0.119931
70	1	0	-5.304005	-1.313415	-1.261692
71	1	0	-3.937242	-2.436508	-1.498507

Tp'Rh[P(OMe)$_3$](R)H R = CH_2F

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.447071	0.428594	-0.348292
2	7	0	0.509048	-1.435964	-0.913587
3	7	0	1.782645	-1.663011	-0.517954
4	7	0	1.545778	1.307747	-0.971799
5	7	0	2.662568	0.700038	-0.508255
6	7	0	0.569195	0.071306	1.700900
7	7	0	1.852926	-0.358035	1.648950
8	6	0	0.128547	-2.460673	-1.676391
9	6	0	1.185782	-3.381747	-1.768061
10	1	0	1.196817	-4.314512	-2.311586
11	6	0	2.217592	-2.838830	-1.023606
12	6	0	1.933722	2.318595	-1.748162
13	6	0	3.337849	2.373357	-1.777452
14	1	0	3.956758	3.073085	-2.319024
15	6	0	3.764323	1.324358	-0.981977
16	6	0	0.245651	0.174360	2.991254
17	6	0	1.344274	-0.188952	3.787389
18	1	0	1.396371	-0.210571	4.865737
19	6	0	2.346675	-0.524728	2.895992
20	5	0	2.567417	-0.612743	0.303113
21	1	0	3.670540	-1.024699	0.518015
22	6	0	3.739088	-0.993352	3.175875
23	1	0	3.893853	-1.038505	4.255129
24	1	0	3.918376	-1.988451	2.759953
25	1	0	4.485330	-0.318138	2.748429
26	6	0	-1.111045	0.596681	3.458681
27	1	0	-1.650561	1.128654	2.674179

28	1	0	-1.712219	-0.271462	3.747612
29	1	0	-1.024694	1.243475	4.336761
30	6	0	3.589975	-3.377520	-0.774804
31	1	0	3.780125	-3.512313	0.293490
32	1	0	3.693165	-4.345741	-1.267237
33	1	0	4.360628	-2.707691	-1.166292
34	6	0	5.157260	0.880761	-0.666850
35	1	0	5.338791	0.857467	0.411046
36	1	0	5.356738	-0.121387	-1.056751
37	1	0	5.868567	1.573117	-1.120127
38	6	0	0.954685	3.201438	-2.454374
39	1	0	1.398166	3.587516	-3.375016
40	1	0	0.049727	2.644046	-2.707015
41	1	0	0.660159	4.051078	-1.831158
42	6	0	-1.224012	-2.538149	-2.311542
43	1	0	-1.127039	-2.810737	-3.365577
44	1	0	-1.841712	-3.301083	-1.827468
45	1	0	-1.745244	-1.581957	-2.242511
46	15	0	-1.470724	2.314776	-0.060855
47	1	0	-1.031605	0.554549	-1.730598
48	8	0	-2.180562	2.933529	-1.385127
49	6	0	-2.881076	4.172534	-1.325144
50	1	0	-3.800074	4.063686	-0.741217
51	1	0	-2.251691	4.958934	-0.898460
52	1	0	-3.140136	4.430663	-2.351797
53	8	0	-0.558478	3.620828	0.365721
54	6	0	0.381454	3.440622	1.430590
55	1	0	-0.129075	3.146463	2.356050
56	1	0	1.121346	2.678523	1.167894
57	1	0	0.868866	4.404851	1.577130
58	8	0	-2.641283	2.329295	1.093301
59	6	0	-3.031544	3.472750	1.847825
60	1	0	-2.899210	3.237641	2.908317
61	1	0	-2.430120	4.349825	1.596797
62	1	0	-4.086981	3.678275	1.654965
63	6	0	-2.113475	-0.540806	0.192805
64	1	0	-1.924165	-1.615922	0.089341
65	1	0	-2.385602	-0.322585	1.231311
66	9	0	-3.232108	-0.237536	-0.586962

Tp'Rh[P(OMe)$_3$](R)H R = CHF_2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	45	0	-0.492409	0.397555	-0.254196
2	7	0	0.484616	-1.423082	-0.883180
3	7	0	1.776420	-1.618396	-0.526941
4	7	0	1.447616	1.329630	-0.970425
5	7	0	2.596968	0.762568	-0.536983
6	7	0	0.586692	0.009613	1.725449
7	7	0	1.893801	-0.330579	1.640598
8	6	0	0.096224	-2.470145	-1.607273
9	6	0	1.166976	-3.371698	-1.721276
10	1	0	1.173969	-4.315578	-2.245180
11	6	0	2.214216	-2.796917	-1.023898
12	6	0	1.781329	2.348885	-1.761842
13	6	0	3.180564	2.450225	-1.831299
14	1	0	3.760285	3.166969	-2.393478
15	6	0	3.663417	1.419373	-1.044237
16	6	0	0.261179	-0.001744	3.018517
17	6	0	1.387554	-0.338769	3.786016
18	1	0	1.445384	-0.433305	4.860145
19	6	0	2.405248	-0.548498	2.872140
20	5	0	2.567457	-0.556884	0.270170
21	1	0	3.688911	-0.938954	0.440368
22	6	0	3.824077	-0.954642	3.113775
23	1	0	4.003443	-1.016195	4.188405
24	1	0	4.040693	-1.931720	2.673067
25	1	0	4.528997	-0.236391	2.686723
26	6	0	-1.130531	0.248561	3.504640
27	1	0	-1.598983	1.091092	2.990726
28	1	0	-1.753472	-0.635463	3.334597
29	1	0	-1.119516	0.454433	4.577079
30	6	0	3.603099	-3.308772	-0.812383
31	1	0	3.827483	-3.431254	0.250842
32	1	0	3.707265	-4.279975	-1.298766
33	1	0	4.350827	-2.630653	-1.233064
34	6	0	5.078157	1.020930	-0.769023
35	1	0	5.290878	1.005056	0.303196
36	1	0	5.296813	0.024747	-1.163602
37	1	0	5.754003	1.734362	-1.243347
38	6	0	0.761203	3.200491	-2.447418
39	1	0	1.161743	3.570554	-3.393956
40	1	0	-0.144791	2.624197	-2.651628
41	1	0	0.489045	4.063727	-1.831603
42	6	0	-1.285106	-2.590265	-2.161055
43	1	0	-1.287903	-3.279782	-3.007782
44	1	0	-1.976610	-2.961338	-1.401088
45	1	0	-1.654078	-1.616600	-2.489603
46	15	0	-1.436818	2.329519	0.096976

47	1	0	-1.140192	0.531682	-1.610376
48	8	0	-2.198081	3.017555	-1.165435
49	6	0	-2.319075	4.418297	-1.412859
50	1	0	-3.362338	4.714093	-1.276210
51	1	0	-1.674683	5.004287	-0.755815
52	1	0	-2.028611	4.589646	-2.451569
53	8	0	-0.455659	3.576581	0.523125
54	6	0	0.500902	3.331014	1.563438
55	1	0	0.000218	2.986485	2.474763
56	1	0	1.230378	2.582451	1.242785
57	1	0	0.994169	4.284202	1.753799
58	8	0	-2.559693	2.339360	1.294587
59	6	0	-3.336168	3.510897	1.529568
60	1	0	-3.824970	3.378980	2.495072
61	1	0	-2.700554	4.401826	1.563072
62	1	0	-4.095237	3.621281	0.750300
63	6	0	-2.124625	-0.539609	0.386064
64	1	0	-2.615820	-0.056530	1.237021
65	9	0	-3.097045	-0.713625	-0.570125
66	9	0	-1.788146	-1.806389	0.805562

Tp'Rh[P(OMe)$_3$](R)H R = CH_2CF_3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.485328	0.450637	-0.459555
2	7	0	0.496996	-1.423342	-1.001098
3	7	0	1.750544	-1.632215	-0.529802
4	7	0	1.469319	1.309812	-1.070819
5	7	0	2.590974	0.741095	-0.570440
6	7	0	0.472268	0.052649	1.636150
7	7	0	1.784011	-0.283487	1.607261
8	6	0	0.165444	-2.478530	-1.746071
9	6	0	1.226278	-3.397742	-1.745257
10	1	0	1.268097	-4.348476	-2.255153
11	6	0	2.214521	-2.824182	-0.966256
12	6	0	1.846569	2.304227	-1.875209
13	6	0	3.249036	2.387124	-1.883079
14	1	0	3.860769	3.081508	-2.439333
15	6	0	3.685672	1.373662	-1.048184
16	6	0	0.119960	0.123396	2.921997
17	6	0	1.229561	-0.159524	3.735443
18	1	0	1.262788	-0.183492	4.814506
19	6	0	2.268729	-0.419661	2.861247

20	5	0	2.510980	-0.551784	0.273672
21	1	0	3.619802	-0.937939	0.504247
22	6	0	3.684175	-0.797208	3.162474
23	1	0	3.831202	-0.810145	4.243643
24	1	0	3.926636	-1.788656	2.770336
25	1	0	4.393411	-0.088273	2.726874
26	6	0	-1.272072	0.422128	3.381051
27	1	0	-1.810046	1.033278	2.656456
28	1	0	-1.838549	-0.503438	3.527377
29	1	0	-1.244264	0.945650	4.340713
30	6	0	3.572461	-3.350297	-0.627394
31	1	0	3.711424	-3.435484	0.453802
32	1	0	3.695272	-4.340470	-1.069109
33	1	0	4.363067	-2.700652	-1.012961
34	6	0	5.082767	0.968587	-0.701657
35	1	0	5.249966	0.979837	0.378647
36	1	0	5.307524	-0.039837	-1.060120
37	1	0	5.785691	1.662476	-1.165416
38	6	0	0.869042	3.148012	-2.628551
39	1	0	1.325491	3.503714	-3.555011
40	1	0	-0.027620	2.575466	-2.875209
41	1	0	0.558283	4.015996	-2.040081
42	6	0	-1.139325	-2.582864	-2.466138
43	1	0	-1.022531	-3.219196	-3.346020
44	1	0	-1.918541	-3.024411	-1.836904
45	1	0	-1.485413	-1.598673	-2.781889
46	15	0	-1.361367	2.400217	-0.074048
47	1	0	-1.061086	0.606777	-1.836943
48	8	0	-2.089770	3.112514	-1.335622
49	6	0	-2.871567	4.287537	-1.145672
50	1	0	-3.779991	4.047514	-0.585591
51	1	0	-2.297760	5.063954	-0.629616
52	1	0	-3.145033	4.641213	-2.139448
53	8	0	-0.303937	3.601605	0.314047
54	6	0	0.621188	3.348829	1.377434
55	1	0	0.101943	3.001752	2.279319
56	1	0	1.354540	2.596260	1.075021
57	1	0	1.117659	4.297318	1.584804
58	8	0	-2.429848	2.491850	1.168250
59	6	0	-2.655140	3.643550	1.976156
60	1	0	-2.515449	3.349791	3.020591
61	1	0	-1.962675	4.452740	1.732924
62	1	0	-3.684083	3.981245	1.831305
63	6	0	-2.207306	-0.520851	0.056898
64	1	0	-1.991841	-1.591418	-0.017583
65	1	0	-2.464195	-0.313240	1.099692

66	6	0	-3.461254	-0.271852	-0.723125
67	9	0	-3.911191	0.996813	-0.601254
68	9	0	-3.342417	-0.496826	-2.047576
69	9	0	-4.474462	-1.063856	-0.304715

Tp'Rh[P(OMe)$_3$](R)H R = *t*BuCC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.938264	0.501930	-0.340513
2	7	0	0.129440	-1.263197	-0.984241
3	7	0	1.478708	-1.273190	-0.871070
4	7	0	0.656341	1.493088	-1.525948
5	7	0	1.935704	1.178470	-1.199148
6	7	0	0.530785	0.447878	1.434374
7	7	0	1.828123	0.205922	1.140677
8	6	0	-0.246521	-2.421688	-1.521367
9	6	0	0.893266	-3.207288	-1.759773
10	1	0	0.927773	-4.197503	-2.188546
11	6	0	1.967064	-2.445055	-1.334471
12	6	0	0.706892	2.358792	-2.540943
13	6	0	2.049019	2.635459	-2.851655
14	1	0	2.418497	3.295431	-3.622191
15	6	0	2.797282	1.860119	-1.986945
16	6	0	0.438767	0.530865	2.762027
17	6	0	1.707455	0.343913	3.335260
18	1	0	1.959320	0.348642	4.385324
19	6	0	2.565304	0.133394	2.270238
20	5	0	2.252432	-0.053393	-0.313257
21	1	0	3.427895	-0.275173	-0.352536
22	6	0	4.034405	-0.146363	2.274145
23	1	0	4.403198	-0.128901	3.300942
24	1	0	4.255257	-1.128352	1.846392
25	1	0	4.588917	0.597757	1.695894
26	6	0	-0.857211	0.792710	3.455641
27	1	0	-1.650031	0.208973	2.981922
28	1	0	-0.785172	0.507270	4.507559
29	1	0	-1.121236	1.853454	3.403278
30	6	0	3.425882	-2.771844	-1.353542
31	1	0	3.856485	-2.744734	-0.348735
32	1	0	3.565703	-3.774473	-1.760740
33	1	0	3.987350	-2.067196	-1.973419
34	6	0	4.282801	1.719891	-1.890736
35	1	0	4.636447	1.887418	-0.870144

36	1	0	4.611707	0.722252	-2.194828
37	1	0	4.757066	2.452507	-2.545834
38	6	0	-0.499497	2.867759	-3.261918
39	1	0	-0.294930	2.876352	-4.335544
40	1	0	-1.364323	2.234466	-3.066262
41	1	0	-0.755665	3.885719	-2.956290
42	6	0	-1.677915	-2.755825	-1.787766
43	1	0	-1.745298	-3.504296	-2.580436
44	1	0	-2.156104	-3.149096	-0.887249
45	1	0	-2.233536	-1.863752	-2.083918
46	15	0	-2.057021	2.305492	0.201857
47	1	0	-1.868933	0.447858	-1.520822
48	8	0	-2.326053	3.285877	-1.067449
49	6	0	-3.030033	4.513395	-0.864809
50	1	0	-4.083945	4.313817	-0.664039
51	1	0	-2.596642	5.074958	-0.032072
52	1	0	-2.925306	5.082537	-1.789380
53	8	0	-1.342518	3.294302	1.305015
54	6	0	0.003410	3.706749	1.031383
55	1	0	0.680702	2.848724	1.027321
56	1	0	0.056723	4.219791	0.064361
57	1	0	0.279925	4.397061	1.828628
58	8	0	-3.558397	2.288012	0.814352
59	6	0	-3.843631	2.004861	2.183568
60	1	0	-3.636771	0.955176	2.398952
61	1	0	-3.260675	2.658359	2.837719
62	1	0	-4.907237	2.208007	2.316104
63	6	0	-2.287282	-0.558364	0.592102
64	6	0	-3.096706	-1.256924	1.177633
65	6	0	-4.050888	-2.109534	1.915657
66	6	0	-3.980229	-3.548061	1.379569
67	1	0	-2.967731	-3.948637	1.484272
68	1	0	-4.670199	-4.193958	1.934229
69	1	0	-4.255919	-3.576878	0.321263
70	6	0	-5.480542	-1.574049	1.736625
71	1	0	-5.755015	-1.555855	0.678580
72	1	0	-6.192891	-2.210789	2.273218
73	1	0	-5.567459	-0.555921	2.127679
74	6	0	-3.686539	-2.107004	3.409489
75	1	0	-4.374011	-2.749760	3.970741
76	1	0	-2.665887	-2.471452	3.556818
77	1	0	-3.749843	-1.095252	3.824260

Tp'Rh[P(OMe)$_3$](R)H R = SiMe$_3$CC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.906172	0.555300	-0.420238
2	7	0	0.165421	-1.214059	-1.037313
3	7	0	1.509920	-1.220393	-0.864823
4	7	0	0.676082	1.536954	-1.611155
5	7	0	1.959541	1.211362	-1.313102
6	7	0	0.516508	0.481694	1.373821
7	7	0	1.830485	0.359091	1.078686
8	6	0	-0.194766	-2.402923	-1.515537
9	6	0	0.950177	-3.204215	-1.657714
10	1	0	0.997234	-4.218615	-2.024066
11	6	0	2.009245	-2.420693	-1.234566
12	6	0	0.704520	2.335526	-2.680955
13	6	0	2.039202	2.553206	-3.061809
14	1	0	2.391806	3.153832	-3.886920
15	6	0	2.804022	1.815569	-2.178461
16	6	0	0.417233	0.587707	2.699327
17	6	0	1.701950	0.550068	3.269538
18	1	0	1.954823	0.605469	4.317958
19	6	0	2.573987	0.396279	2.206572
20	5	0	2.272321	0.032307	-0.359803
21	1	0	3.449327	-0.183665	-0.373458
22	6	0	4.063710	0.265953	2.211588
23	1	0	4.434973	0.393193	3.229687
24	1	0	4.382231	-0.715656	1.849738
25	1	0	4.535416	1.020110	1.575792
26	6	0	-0.890767	0.729841	3.408654
27	1	0	-1.675961	0.209499	2.856240
28	1	0	-0.818361	0.292318	4.407342
29	1	0	-1.169086	1.782985	3.515989
30	6	0	3.464942	-2.755626	-1.169464
31	1	0	3.851452	-2.667391	-0.150430
32	1	0	3.613345	-3.783257	-1.505017
33	1	0	4.059329	-2.096034	-1.807807
34	6	0	4.288245	1.639666	-2.133548
35	1	0	4.689227	1.857293	-1.140401
36	1	0	4.577175	0.616351	-2.389449
37	1	0	4.753482	2.317508	-2.850985
38	6	0	-0.516751	2.841277	-3.378993
39	1	0	-0.364753	2.771888	-4.459170
40	1	0	-1.394379	2.256918	-3.103827
41	1	0	-0.718910	3.885442	-3.128471
42	6	0	-1.616220	-2.749360	-1.818321

43	1	0	-1.656537	-3.500220	-2.610699
44	1	0	-2.116941	-3.143999	-0.930091
45	1	0	-2.170042	-1.862303	-2.132124
46	15	0	-1.943486	2.389031	0.191550
47	1	0	-1.829498	0.534846	-1.609620
48	8	0	-2.013819	3.503570	-0.988690
49	6	0	-2.648544	4.756960	-0.721406
50	1	0	-3.729100	4.622352	-0.647025
51	1	0	-2.268325	5.192818	0.207030
52	1	0	-2.407447	5.408723	-1.561657
53	8	0	-1.252832	3.187183	1.448332
54	6	0	0.129863	3.554458	1.349559
55	1	0	0.639873	3.018156	0.543163
56	1	0	0.190463	4.631579	1.171272
57	1	0	0.611097	3.299919	2.296288
58	8	0	-3.486835	2.426415	0.681848
59	6	0	-3.892495	2.048816	2.000964
60	1	0	-3.736913	0.978536	2.147222
61	1	0	-3.342329	2.629119	2.745899
62	1	0	-4.955843	2.282417	2.063067
63	6	0	-2.268758	-0.502050	0.470913
64	6	0	-3.089713	-1.217577	1.036636
65	14	0	-4.242581	-2.292372	1.963385
66	6	0	-4.164093	-4.048752	1.290011
67	1	0	-3.149405	-4.449540	1.371142
68	1	0	-4.836874	-4.713135	1.841913
69	1	0	-4.453558	-4.073924	0.235165
70	6	0	-6.000779	-1.634101	1.802273
71	1	0	-6.311488	-1.608665	0.754040
72	1	0	-6.708204	-2.262194	2.353439
73	1	0	-6.075640	-0.616364	2.197469
74	6	0	-3.740508	-2.280483	3.780442
75	1	0	-4.393279	-2.920748	4.382327
76	1	0	-2.711709	-2.633351	3.897614
77	1	0	-3.792881	-1.266190	4.189759

Tp'Rh[P(OMe)$_3$](R)H R = *n*-hexylCC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.634772	-0.055438	-0.706592
2	7	0	0.415184	-1.887699	-1.159491
3	7	0	1.766933	-1.875515	-1.068391
4	7	0	0.872577	0.762261	-2.103043

5	7	0	2.173562	0.481024	-1.837179
6	7	0	0.901836	0.106941	0.994209
7	7	0	2.195814	-0.067933	0.643627
8	6	0	0.035686	-3.119332	-1.490939
9	6	0	1.175522	-3.931197	-1.617170
10	1	0	1.207389	-4.978259	-1.878640
11	6	0	2.252184	-3.107213	-1.342003
12	6	0	0.836504	1.431228	-3.257568
13	6	0	2.147156	1.611863	-3.730765
14	1	0	2.450305	2.115086	-4.636722
15	6	0	2.965114	0.986646	-2.809296
16	6	0	0.880311	0.393550	2.295978
17	6	0	2.195665	0.418895	2.792124
18	1	0	2.509936	0.614188	3.806672
19	6	0	3.003884	0.113579	1.711462
20	5	0	2.551013	-0.572923	-0.767073
21	1	0	3.726306	-0.791557	-0.826280
22	6	0	4.491002	-0.030872	1.648909
23	1	0	4.920636	0.229718	2.617610
24	1	0	4.785118	-1.056232	1.407601
25	1	0	4.927562	0.624641	0.890549
26	6	0	-0.386785	0.645406	3.047835
27	1	0	-1.203347	0.075245	2.599605
28	1	0	-0.268392	0.333355	4.088239
29	1	0	-0.650372	1.707879	3.037017
30	6	0	3.711783	-3.431643	-1.332486
31	1	0	4.162158	-3.225571	-0.357639
32	1	0	3.846771	-4.491124	-1.555960
33	1	0	4.258545	-2.850189	-2.080148
34	6	0	4.452222	0.830711	-2.820029
35	1	0	4.898633	1.174329	-1.883353
36	1	0	4.745166	-0.213277	-2.962723
37	1	0	4.870533	1.418934	-3.638444
38	6	0	-0.426415	1.840672	-3.944369
39	1	0	-0.335798	1.631979	-5.013485
40	1	0	-1.281015	1.296023	-3.543831
41	1	0	-0.623283	2.908227	-3.819314
42	6	0	-1.398475	-3.494712	-1.674100
43	1	0	-1.486841	-4.277536	-2.431201
44	1	0	-1.824182	-3.863433	-0.737111
45	1	0	-1.986940	-2.627023	-1.977262
46	15	0	-1.668358	1.828190	-0.281875
47	1	0	-1.631989	-0.229745	-1.820790
48	8	0	-1.829918	2.775631	-1.593044
49	6	0	-2.485234	4.039194	-1.462022
50	1	0	-3.564741	3.895740	-1.388674

51	1	0	-2.126540	4.573389	-0.577261
52	1	0	-2.242016	4.607868	-2.360270
53	8	0	-0.929772	2.802310	0.814943
54	6	0	0.438071	3.167668	0.592730
55	1	0	0.941236	2.472253	-0.086175
56	1	0	0.469469	4.178792	0.176968
57	1	0	0.946812	3.140786	1.558577
58	8	0	-3.183407	1.917542	0.288553
59	6	0	-3.504385	1.700811	1.665241
60	1	0	-3.340203	0.653822	1.924621
61	1	0	-2.905667	2.356785	2.302028
62	1	0	-4.560497	1.951770	1.768321
63	6	0	-1.941953	-0.995134	0.400991
64	6	0	-2.726662	-1.628231	1.085116
65	6	0	-3.667983	-2.389229	1.916166
66	1	0	-3.369146	-2.324255	2.971492
67	1	0	-4.667629	-1.937767	1.852426
68	6	0	-3.766427	-3.867696	1.519469
69	1	0	-2.771700	-4.323324	1.601272
70	1	0	-4.056865	-3.933063	0.463551
71	6	0	-4.762955	-4.639256	2.379648
72	1	0	-4.475496	-4.553783	3.436881
73	1	0	-5.754740	-4.173964	2.292972
74	6	0	-4.863630	-6.114899	2.002315
75	1	0	-5.143003	-6.201159	0.943203
76	1	0	-3.873847	-6.582448	2.096099
77	6	0	-5.868936	-6.887192	2.853557
78	1	0	-6.856902	-6.419781	2.755958
79	1	0	-5.590020	-6.796765	3.911019
80	6	0	-5.955982	-8.361202	2.468064
81	1	0	-4.984525	-8.851893	2.584640
82	1	0	-6.259124	-8.473120	1.422259
83	1	0	-6.679585	-8.898727	3.086404

Tp'Rh[P(OMe)$_3$](R)H R = *p*-MeOC$_6$H$_4$CC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.934582	0.301348	-0.558099
2	7	0	0.136806	-1.502285	-1.072032
3	7	0	1.482720	-1.500078	-0.912472
4	7	0	0.648367	1.216302	-1.799719
5	7	0	1.931996	0.904135	-1.488608
6	7	0	0.500990	0.333885	1.232630

7	7	0	1.812864	0.181049	0.943317
8	6	0	-0.227415	-2.714080	-1.485842
9	6	0	0.917071	-3.521298	-1.598684
10	1	0	0.961064	-4.552600	-1.915093
11	6	0	1.979608	-2.717041	-1.226637
12	6	0	0.676233	1.964193	-2.905649
13	6	0	2.010353	2.163364	-3.297770
14	1	0	2.362116	2.724944	-4.150340
15	6	0	2.775859	1.467530	-2.381658
16	6	0	0.406677	0.532760	2.547335
17	6	0	1.692386	0.523617	3.116124
18	1	0	1.948902	0.649768	4.157435
19	6	0	2.560015	0.290218	2.064092
20	5	0	2.248240	-0.224291	-0.476519
21	1	0	3.424957	-0.442314	-0.484628
22	6	0	4.048777	0.148955	2.074372
23	1	0	4.424570	0.351719	3.078574
24	1	0	4.358472	-0.860557	1.789568
25	1	0	4.523907	0.847762	1.380677
26	6	0	-0.901315	0.730410	3.242649
27	1	0	-1.686065	0.175442	2.723933
28	1	0	-0.834269	0.365069	4.269954
29	1	0	-1.177665	1.789091	3.272343
30	6	0	3.436521	-3.046837	-1.161401
31	1	0	3.835180	-2.906330	-0.152993
32	1	0	3.582978	-4.089950	-1.446207
33	1	0	4.022126	-2.419545	-1.839254
34	6	0	4.260209	1.294866	-2.329187
35	1	0	4.660276	1.552994	-1.345413
36	1	0	4.550604	0.262407	-2.543557
37	1	0	4.725153	1.943715	-3.073181
38	6	0	-0.545976	2.438686	-3.623246
39	1	0	-0.389843	2.336925	-4.700196
40	1	0	-1.419528	1.855978	-3.331970
41	1	0	-0.757887	3.488174	-3.405231
42	6	0	-1.650723	-3.078448	-1.759155
43	1	0	-1.696347	-3.841413	-2.539745
44	1	0	-2.134720	-3.468264	-0.859237
45	1	0	-2.218529	-2.201865	-2.075862
46	15	0	-2.003166	2.148487	-0.056520
47	1	0	-1.860592	0.210927	-1.741544
48	8	0	-2.114785	3.185442	-1.302961
49	6	0	-2.786491	4.432984	-1.109577
50	1	0	-3.864917	4.273862	-1.056628
51	1	0	-2.442506	4.920350	-0.192545
52	1	0	-2.539436	5.052310	-1.972381

53	8	0	-1.324223	3.044435	1.140027
54	6	0	0.051485	3.425115	1.007313
55	1	0	0.591838	2.770320	0.316246
56	1	0	0.098522	4.458186	0.651455
57	1	0	0.510618	3.345699	1.994669
58	8	0	-3.543531	2.179062	0.445596
59	6	0	-3.932162	1.863482	1.786126
60	1	0	-3.771812	0.802588	1.985016
61	1	0	-3.375877	2.480376	2.496225
62	1	0	-4.995169	2.097933	1.850528
63	6	0	-2.300518	-0.713415	0.388052
64	6	0	-3.126404	-1.415055	0.949080
65	6	0	-4.093264	-2.236749	1.615985
66	6	0	-5.458519	-1.895562	1.612627
67	6	0	-3.710381	-3.401836	2.289091
68	6	0	-6.392495	-2.685499	2.257897
69	6	0	-4.642898	-4.206482	2.939591
70	6	0	-5.991295	-3.847695	2.925783
71	1	0	-5.773472	-1.000081	1.085461
72	1	0	-2.660584	-3.677781	2.299838
73	1	0	-7.447137	-2.431701	2.258391
74	1	0	-4.306877	-5.101933	3.448743
75	8	0	-6.984842	-4.557493	3.526540
76	6	0	-6.623236	-5.750020	4.183248
77	1	0	-6.167857	-6.467478	3.489525
78	1	0	-5.925269	-5.559135	5.007851
79	1	0	-7.545698	-6.170705	4.583078

Tp'Rh[P(OMe)$_3$](R)H R = CF_3CC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.943279	0.434355	-0.513226
2	7	0	0.085858	-1.365941	-1.084448
3	7	0	1.436721	-1.385383	-0.998387
4	7	0	0.648819	1.370223	-1.722004
5	7	0	1.922825	1.055747	-1.371828
6	7	0	0.508420	0.425767	1.262416
7	7	0	1.796636	0.121192	0.984452
8	6	0	-0.315724	-2.546290	-1.555045
9	6	0	0.811406	-3.352860	-1.780176
10	1	0	0.825856	-4.362811	-2.161085
11	6	0	1.902384	-2.583230	-1.415019
12	6	0	0.715892	2.211574	-2.756866

13	6	0	2.062806	2.473914	-3.056301
14	1	0	2.444770	3.113964	-3.837382
15	6	0	2.796614	1.714984	-2.164682
16	6	0	0.399714	0.496390	2.590799
17	6	0	1.648532	0.240354	3.178226
18	1	0	1.885096	0.226221	4.231621
19	6	0	2.511155	-0.001320	2.123426
20	5	0	2.225070	-0.164099	-0.463892
21	1	0	3.397245	-0.401062	-0.495670
22	6	0	3.965745	-0.347123	2.145954
23	1	0	4.322898	-0.340983	3.176878
24	1	0	4.146763	-1.340818	1.726662
25	1	0	4.559622	0.367683	1.569977
26	6	0	-0.889228	0.801417	3.281767
27	1	0	-1.610035	-0.008210	3.137540
28	1	0	-0.714876	0.927987	4.352175
29	1	0	-1.322731	1.726155	2.893357
30	6	0	3.356901	-2.926757	-1.449084
31	1	0	3.805463	-2.874075	-0.453273
32	1	0	3.478844	-3.942834	-1.827319
33	1	0	3.914334	-2.247634	-2.100182
34	6	0	4.279958	1.569256	-2.047300
35	1	0	4.620018	1.745513	-1.023643
36	1	0	4.607660	0.567008	-2.337158
37	1	0	4.766301	2.292868	-2.703400
38	6	0	-0.478346	2.708177	-3.505970
39	1	0	-0.255358	2.698374	-4.575769
40	1	0	-1.346506	2.077909	-3.315099
41	1	0	-0.739731	3.731218	-3.222556
42	6	0	-1.755489	-2.882987	-1.774721
43	1	0	-1.843056	-3.651297	-2.545804
44	1	0	-2.218122	-3.255078	-0.856477
45	1	0	-2.316439	-1.999357	-2.085997
46	15	0	-2.085813	2.260464	-0.053115
47	1	0	-1.872236	0.341520	-1.695001
48	8	0	-2.363349	3.167383	-1.370185
49	6	0	-3.100590	4.386566	-1.237063
50	1	0	-4.149298	4.169186	-1.028326
51	1	0	-2.684655	5.003850	-0.435814
52	1	0	-3.006631	4.905143	-2.191662
53	8	0	-1.402688	3.309940	1.008088
54	6	0	-0.046796	3.704299	0.749896
55	1	0	0.622532	2.840395	0.784421
56	1	0	0.028382	4.188860	-0.230020
57	1	0	0.218529	4.414994	1.532428
58	8	0	-3.588927	2.217026	0.545338

59	6	0	-3.894877	1.994895	1.924617
60	1	0	-3.644374	0.972401	2.209210
61	1	0	-3.364053	2.716934	2.550318
62	1	0	-4.970189	2.146114	2.018447
63	6	0	-2.256145	-0.585150	0.472888
64	6	0	-3.028871	-1.275249	1.108303
65	6	0	-3.913171	-2.089858	1.920187
66	9	0	-5.072773	-1.458835	2.188564
67	9	0	-4.228389	-3.252181	1.325852
68	9	0	-3.361423	-2.395256	3.109165

Tp'Rh[P(OMe)$_3$](R)H R = phenylCC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.936177	0.302908	-0.538980
2	7	0	0.127310	-1.509712	-1.031660
3	7	0	1.474603	-1.507076	-0.884856
4	7	0	0.636560	1.194903	-1.808549
5	7	0	1.922301	0.887133	-1.501735
6	7	0	0.515056	0.366898	1.238709
7	7	0	1.823796	0.201913	0.941663
8	6	0	-0.242534	-2.727262	-1.423292
9	6	0	0.899668	-3.537757	-1.534570
10	1	0	0.939050	-4.574054	-1.834883
11	6	0	1.966788	-2.729495	-1.185004
12	6	0	0.656813	1.926846	-2.925285
13	6	0	1.988161	2.120560	-3.329103
14	1	0	2.334140	2.669861	-4.191976
15	6	0	2.759999	1.437995	-2.408258
16	6	0	0.432397	0.586918	2.550990
17	6	0	1.722401	0.578997	3.109670
18	1	0	1.987803	0.719899	4.146847
19	6	0	2.580335	0.324029	2.054731
20	5	0	2.245956	-0.226342	-0.475432
21	1	0	3.422123	-0.446445	-0.490618
22	6	0	4.068267	0.173998	2.055795
23	1	0	4.452617	0.387184	3.054574
24	1	0	4.369712	-0.840946	1.781727
25	1	0	4.542388	0.861081	1.349815
26	6	0	-0.868010	0.804211	3.254725
27	1	0	-1.662703	0.251550	2.749224
28	1	0	-0.795943	0.448463	4.285057
29	1	0	-1.134446	1.865632	3.276403

30	6	0	3.423743	-3.060591	-1.128286
31	1	0	3.831963	-2.905046	-0.125925
32	1	0	3.565932	-4.108267	-1.398011
33	1	0	4.003823	-2.444961	-1.821409
34	6	0	4.244735	1.266672	-2.362919
35	1	0	4.650887	1.539495	-1.385613
36	1	0	4.534372	0.231340	-2.564006
37	1	0	4.704597	1.904715	-3.119310
38	6	0	-0.570463	2.390109	-3.641487
39	1	0	-0.421395	2.272912	-4.717853
40	1	0	-1.441437	1.810767	-3.336018
41	1	0	-0.781929	3.442400	-3.437152
42	6	0	-1.668924	-3.094170	-1.676106
43	1	0	-1.723852	-3.866784	-2.446477
44	1	0	-2.142268	-3.473117	-0.765925
45	1	0	-2.239944	-2.221425	-1.997696
46	15	0	-2.000361	2.159994	-0.059339
47	1	0	-1.872757	0.193154	-1.712611
48	8	0	-2.123356	3.174081	-1.323032
49	6	0	-2.793837	4.424895	-1.146876
50	1	0	-3.872406	4.267388	-1.092303
51	1	0	-2.449902	4.924411	-0.236404
52	1	0	-2.545900	5.032310	-2.017847
53	8	0	-1.311520	3.076451	1.115255
54	6	0	0.063269	3.454437	0.965257
55	1	0	0.597848	2.787850	0.281102
56	1	0	0.107565	4.481301	0.591657
57	1	0	0.530048	3.391267	1.950213
58	8	0	-3.536304	2.198352	0.455571
59	6	0	-3.914664	1.909017	1.805022
60	1	0	-3.765474	0.849475	2.018965
61	1	0	-3.343314	2.529637	2.499639
62	1	0	-4.973956	2.157581	1.876557
63	6	0	-2.291658	-0.693212	0.439054
64	6	0	-3.108965	-1.380930	1.029183
65	6	0	-4.059188	-2.186670	1.738300
66	6	0	-5.428417	-1.878018	1.704650
67	6	0	-3.637629	-3.298850	2.484382
68	6	0	-6.345796	-2.657923	2.398751
69	6	0	-4.559793	-4.075475	3.175271
70	6	0	-5.916228	-3.758774	3.136717
71	1	0	-5.756834	-1.023200	1.121195
72	1	0	-2.579411	-3.538919	2.510349
73	1	0	-7.401560	-2.407296	2.361923
74	1	0	-4.219451	-4.933116	3.747450
75	1	0	-6.634142	-4.367033	3.677484

Tp'Rh[P(OMe)$_3$](R)H R = *p*-CF$_3$C$_6$H$_4$CC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.931431	0.279841	-0.541410
2	7	0	0.144885	-1.520746	-1.041140
3	7	0	1.492087	-1.507691	-0.893408
4	7	0	0.630866	1.188314	-1.805889
5	7	0	1.919441	0.893051	-1.497834
6	7	0	0.515354	0.348855	1.238479
7	7	0	1.825607	0.195165	0.941872
8	6	0	-0.214151	-2.738158	-1.443575
9	6	0	0.934772	-3.537733	-1.560680
10	1	0	0.983311	-4.570959	-1.869917
11	6	0	1.994772	-2.723233	-1.203601
12	6	0	0.644935	1.922915	-2.921222
13	6	0	1.974788	2.131544	-3.322159
14	1	0	2.316099	2.686452	-4.183276
15	6	0	2.752471	1.454902	-2.401889
16	6	0	0.430475	0.565057	2.551463
17	6	0	1.719986	0.565949	3.110751
18	1	0	1.983684	0.706360	4.148407
19	6	0	2.580544	0.320771	2.055548
20	5	0	2.252574	-0.222427	-0.476787
21	1	0	3.430418	-0.432329	-0.492320
22	6	0	4.069649	0.183435	2.057112
23	1	0	4.451461	0.396246	3.056896
24	1	0	4.379874	-0.827868	1.779567
25	1	0	4.538225	0.877204	1.354029
26	6	0	-0.871331	0.771324	3.255840
27	1	0	-1.663042	0.216406	2.748314
28	1	0	-0.797473	0.411629	4.284633
29	1	0	-1.144136	1.830974	3.282192
30	6	0	3.454498	-3.042208	-1.149088
31	1	0	3.860987	-2.891348	-0.145346
32	1	0	3.605847	-4.086318	-1.427332
33	1	0	4.029280	-2.415899	-1.837003
34	6	0	4.238790	1.298977	-2.354700
35	1	0	4.640388	1.573025	-1.375878
36	1	0	4.539377	0.267332	-2.558530
37	1	0	4.693162	1.944179	-3.108261
38	6	0	-0.585124	2.374166	-3.640357
39	1	0	-0.433334	2.254686	-4.716057

40	1	0	-1.452307	1.789210	-3.334961
41	1	0	-0.804637	3.425526	-3.439917
42	6	0	-1.637303	-3.114307	-1.700977
43	1	0	-1.685262	-3.884996	-2.473568
44	1	0	-2.109984	-3.499982	-0.793324
45	1	0	-2.213648	-2.244907	-2.022411
46	15	0	-2.002946	2.134493	-0.056553
47	1	0	-1.864682	0.169641	-1.717642
48	8	0	-2.130243	3.149742	-1.317486
49	6	0	-2.806086	4.397997	-1.139191
50	1	0	-3.883894	4.235580	-1.085060
51	1	0	-2.463955	4.897293	-0.227995
52	1	0	-2.560497	5.007502	-2.009242
53	8	0	-1.318093	3.048104	1.121176
54	6	0	0.055265	3.433901	0.973035
55	1	0	0.593406	2.772286	0.286916
56	1	0	0.093979	4.462174	0.603075
57	1	0	0.521329	3.369659	1.958172
58	8	0	-3.539271	2.160885	0.458837
59	6	0	-3.914601	1.880313	1.810645
60	1	0	-3.758458	0.823497	2.033428
61	1	0	-3.346705	2.509222	2.500434
62	1	0	-4.975402	2.122409	1.881606
63	6	0	-2.283230	-0.725560	0.430263
64	6	0	-3.103726	-1.409436	1.021278
65	6	0	-4.061502	-2.195739	1.736512
66	6	0	-5.428232	-1.871245	1.692115
67	6	0	-3.653234	-3.295258	2.509416
68	6	0	-6.355231	-2.618897	2.402876
69	6	0	-4.581624	-4.043753	3.219309
70	6	0	-5.931150	-3.703290	3.168327
71	1	0	-5.745698	-1.024639	1.092008
72	1	0	-2.598246	-3.545308	2.546703
73	1	0	-7.408722	-2.360200	2.375269
74	1	0	-4.262932	-4.886861	3.822951
75	6	0	-6.945251	-4.529629	3.899299
76	9	0	-7.965536	-3.779461	4.346097
77	9	0	-7.481537	-5.479659	3.115041
78	9	0	-6.410844	-5.156616	4.958478
