Electronic Supplementary Information (ESI)

A case study on the conversion of Li/Cl phosphinidenoid into phosphinidene complexes

Philip Junker,[a] Zheng-Wang Qu,[b*] Tim Kalisch,[a] Gregor Schnakenburg,[a] Arturo Espinosa Ferao,[c*] and Rainer Streubel[a*]

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Experimental Procedures

The syntheses of all compounds were performed under an argon atmosphere, using common Schlenk techniques and dry solvents. Tetrahydrofuran (THF), diethyl ether, petrol ether (40/60) and *n*-pentane were dried over sodium wire/benzophenone, CH_2Cl_2 over CaH_2, toluene over sodium and further purified by subsequent distillation. The used alcohols/amines were distilled under argon atmosphere before usage. *N,N*-Diphenylaminodichlorophosphane and *N,N*-dicyclohexylaminodichlorophosphane were synthesized according to [19] and [20]. All NMR spectra were recorded on a Bruker AVI-300 (300.1 MHz for ^{1}H, 75.5 MHz for ^{13}C, 59.6 MHz for ^{29}Si and 121.5 MHz for ^{31}P), Bruker AVI-400 (400.1 MHz for ^{1}H, 100.6 MHz for ^{13}C, 79.5 MHz for ^{29}Si and 162.0 MHz for ^{31}P) and Bruker AV III HD Prodigy 500 (500.2 MHz for ^{1}H, 125.8 MHz for ^{13}C, 99.3 MHz for ^{29}Si, and 202.5 MHz for ^{31}P) spectrometers at 25 °C. The ^{1}H and ^{13}C NMR spectra were referenced to the residual proton resonances and the ^{13}C NMR signals of the deuterated solvents; ^{31}P NMR spectra were referenced to 85% H_3PO_4 as an external standard, respectively. Melting points were determined in one-side melted off capillaries using a Büchi Type S or a Carl Roth Type MPM-2 apparatus and are uncorrected. Elemental analyses were carried out on a Vario EL gas chromatograph. Mass spectrometric data were collected on a MAT 90 Thermo Finnigan sector instrument equipped with a LIFDI ion source from Linden CMS GmbH. IR spectra of all compounds were recorded on a Thermo Nicolet 380 FT-IR spectrometer with an attenuated total reflection (ATR) attachment or a Bruker Alpha Diamond ATR FTIR spectrometer. X-ray data were collected with a Bruker D8-Venture, STOE IPDS-2T and Bruker X8-KappaApexII diffractometer. CCDC 1919557 and 1919561 contain the supplementary crystallographic data (see ESI).

*Synthesis of Complex **1a**.* $W(CO)_6$ (3,05 g, 8.69 mmol) was dissolved in THF (250 mL) before radiation was started for 1.5 h at -10 °C. The *N,N*-Diphenylaminodichlorophosphane (2.30 mg, 8.52 mmol) was added and the reaction mixture was stirred for 3 h at ambient temperature. The THF was removed in vacuo (10^{-2} mbar) and the obtained oily residue was filtered through silica (2 cm SiO_2, Ø 4 cm, r.t.) with toluene (200 mL). The toluene was removed *in vacuo* (10^{-2} mbar) and the residue washed with *n*-pentane (10 mL) at -50 °C to obtain complex **1a** as a beige/yellow solid (2.5 g, 48 %, m.p. 172 °C).

1a: ^{1}H NMR (500.1 MHz, 298.0 K, C_6D_6) δ/ppm = 6.90 (m, 1 H, *para*-H), 6.97 (t, $^{3}J_{H,H}$ = 7.8 Hz, 2 H, *meta*-H), 7.26 (d, $^{3}J_{H,H}$ = 7.8 Hz, 2 H, *ortho*-H). **^{13}C{^{1}H} NMR** (125.8 MHz, 298.0 K, C_6D_6): δ/ppm = 128.5 (d, $^{5}J_{P,C}$ = 1.4 Hz, *para*-C), 129.5 (d, $^{3}J_{P,C}$ = 6.1 Hz, *ortho*-C), 129.9 (s, *meta*-C), 144.1 ($^{2}J_{P,C}$ = 5.1 Hz, C_{quart}), 195.2 (d_{sat}, $^{1}J_{W,C}$ = 127.7 Hz, $^{1}J_{P,C}$ = 8.3 Hz, *cis*-CO), 197.9 (d_{sat}, $^{1}J_{W,C}$ = 141.2 Hz, $^{1}J_{P,C}$ = 53.2 Hz, *trans*-CO). **^{31}P NMR** (202.5 MHz, 298.0 K, C_6D_6): δ/ppm = 108.6 (s_{sat}, $^{1}J_{W,P}$ = 388.7 Hz). **MS** (EI, 70 eV, ^{184}W) m/z (%) = 592.9 (34) $[M]^{+\bullet}$, 557.9 (20) $[M\text{-}Cl]^+$, 269.0 (6) $[M\text{-}W(CO)_5]^+$, 234.0 (100) $[M\text{-}Cl\text{-}W(CO)_5]^+$, 168.0 (26) $[NPh_2]^\bullet$, 77.0 (12) $[C_6H_5]^+$. **IR** (ATR diamond) $\tilde{\nu}$/cm^{-1} = 3061 (w, *v*(CH)), 2081 (s, *v*(CO)), 1997 (m, *v*(CO)), 1980 (w, *v*(CO)), 1931 (vs, *v*(CO)). **Anal. calc.** for $C_{17}H_{10}Cl_2NO_5PW$, C 34.38 H 1.70 N 2.36; **found** C 34.73 H 1.81 N 2.46.

*Synthesis of Complex **1b**.* $W(CO)_6$ (1.50 g, 4.26 mmol) was dissolved in THF (100 mL) before radiation was started for 1 h at 10 °C. The *N,N*-dicyclohexylaminodichlorophosphane (1.20 g, 4.25 mmol) was added and the reaction mixture was stirred for 2 h at ambient temperature. The THF was removed in vacuo (10^{-2} mbar)and the obtained oily residue was filtered through alox (2 cm Al_2O_3, Ø 3 cm, r.t.) with Et_2O (200 mL). The Et_2O was removed *in vacuo* (10^{-2} mbar) and the residue washed with *n*-pentane (10 mL) at -40 °C to obtain complex **1b** as a white solid (900 mg, 35 %, m.p. 99 - 103 °C).

1b: ^{1}H NMR (400.1 MHz, 298.0 K, C_6D_6) δ/ppm = 0.83 (qt, $J_{H,H}$ = 13.0 HZ, $J_{H,H}$ = 3.5 Hz, 1H, $NCH(CH_2)(CH_2)(CH_2)$), 1.15 (qt, $J_{H,H}$ = 13.2 Hz, $J_{H,H}$ = 3.6 Hz, 2H, $NCH(CH_2)(CH_2)$), 1.41 (dt, $J_{H,H}$ = 13.6 Hz, $J_{H,H}$ = 3.2 Hz, 1H, $NCH(CH_2)(CH_2)$), 1.50 – 1.62 (m, 4H, $NCH(CH_2)$, $NCH(CH_2)(CH_2)$), 1.67 – 1.77 (m, 2H, $NCH(CH_2)(CH_2)$), 3.89 (br. d, $^{2}J_{P,H}$ = 11.0 Hz, 1H, NCH). **^{13}C{^{1}H} NMR** (100.6 MHz, 298 K, C_6D_6) δ/ppm = 25.4 (s, $NCH(CH_2(CH_2))$), 26.8 (s, $NCH(CH_2)(CH_2)$), 33.9 (d, $^{3}J_{P,C}$ = 5.6 Hz, $NCH(CH_2)$), 62.8 (d, $^{2}J_{P,C}$ = 9.8 Hz, NCH), 196.1 (d_{sat}, $^{1}J_{W,C}$ = 135.9 Hz, $^{1}J_{P,C}$ = 8.6 Hz, *cis*-CO), 198.6 (d, $^{1}J_{P,C}$ = 50.7 Hz, *trans*-CO). **^{31}P NMR** (162.1 MHz, 298.0 K, C_6D_6) δ/ppm = 118.4 (br. s). **^{31}P{^{1}H} NMR** (121.5 MHz, 193.0 K, THF) δ/ppm = 110.8 (s_{sat}, $^{1}J_{W,P}$ = 379.6 Hz) (61 %), 126.7 (s_{sat}, $^{1}J_{W,P}$ = 368.2 Hz) (39 %). **MS** (EI, 70 eV, ^{184}W) m/z (%) = 605.0 $[M]^{+\bullet}$, 570.0 $[M\text{-}Cl]^+$, 486.1 $[M\text{-}Cl\text{-}3CO]^+$, 465.0 $[M\text{-}5CO]^+$, 281.1 $[M\text{-}W(CO)_5]^+$, 246.1 (100) $[ClPN(Cy)_2]^+$, 83.1 $[C_6H_{11}]^+$. **IR** (ATR diamond) $\tilde{\nu}$/cm^{-1} = 2931 (m, *v*(CH)), 2857 (w, *v*(CH)), 2080 (m, *v*(CO)), 1949 (s, *v*(CO)), 1916 (vs, *v*(CO)). **Anal. calc.** for $C_{17}H_{22}Cl_2NO_5PW$, C 33.69 H 3.66 N 2.31; **found** C 33.80 H 3.85 N 2.48.

*Procedure for the reactions of complexes **1a,b** with MeOH.* 0.1 mmol of **1a, b** (69 mg (**a**), 61 mg (**b**)) was dissolved in 2.5 mL THF before 32 µL 12-crown-4 (2 eq.) was added. The reaction mixture was cooled down to -95/-100 °C before 0.13 mL of *tert*-butyllithium (0.22 mmol, 1.7 mol/L in *n*-hexane) was added. After 5 min 0.05 mL of MeOH (1.2 mmol, exc.) was added and reaction mixture was stirred while warming up to ambient temperature. The crude product **3a** was extracted using Et_2O (2 times with 2.5 mL) and the solvent removed in vacuo (10^{-2} mbar).

3a: ^{1}H NMR (300.1 MHz, 298 K, C_6D_6): δ / ppm = 2.99 ($^{3}J_{P,H}$ = 11.8 Hz, CH_3, 3H), 6.90-6.94 (m, Ph, 4H), 6.94-6.97 (m, Ph, 4H), 6.97-6.99 (m, Ph, 2H), 7.90 ($^{1}J_{P,H}$ = 383.3 Hz, PH, 1H). **^{13}C NMR** (75.7 MHz, 298 K, C_6D_6): δ / ppm = 59.0 (d,

$^2J_{P,C}$ = 14.3 Hz, O*C*H$_3$), 125.8 (s, Ph), 125.9 (s, Ph), 129.8 (s, Ph), 147.9 (d, $^2J_{P,C}$ = 2.7 Hz, *quart*-C), 195.8 (d, $^2J_{P,C}$ = 8.3 Hz, *cis*-CO), 198.8 (d$_{sat}$, $^1J_{W,P}$ = 82.6 Hz $^2J_{P,C}$ = 31.2 Hz, *trans*-CO). **^{31}P NMR** (121.5 MHz, 298 K, C_6D_6): δ / ppm = 112.5 (dq$_{sat}$, $^1J_{W,P}$ = 315.6 Hz, $^1J_{P,H}$ = 383.3 Hz, $^3J_{P,H}$ = 11.8 Hz). **MS** (EI, 70 eV, ^{184}W) m/z (%) = 555.0 (50) $[M]^{+\bullet}$, 527.0 (28) $[M\text{-}CO]^+$, 471 (100) $[M\text{-}3CO]^+$, 333.0 (20) $[W(CO)_5]^+$, 168.1 (50) $[NPh_2]^+$. **IR** (ATR diamond): *ν* / cm^{-1} = 1908 (vs, *ν*(CO)), 2075 (s, *ν*(CO)), 2661 (m, *ν*(PH)).

3b: ^{31}P NMR (121.5 MHz, 298.0 K, THF) δ/ppm = 87.9 (dq$_{sat}$, $^1J_{W,P}$ = 303.2 Hz, $^1J_{P,H}$ = 387.7 Hz, $^3J_{P,H}$ = 13.5 Hz).

*Procedure for the reactions of complexes **1a,b** with $MeNH_2$.* 0.1 mmol (59 mg (**a**), 61 mg (**b**) was dissolved in 2.5 mL THF before 32 µL of 12-crown-4 (2 eq.) was added. The reaction mixture was cooled down to -95/-100 °C before 0.07 mL of *tert*-butyllithium (0.12 mmol, 1.7 mol/L in *n*-hexane) was added. After 5 min 0.15 mL of $MeNH_2$ (0.3 mmol, 3 eq., 2 mol/L in THF) was added and the reaction mixture was stirred while warming up to ambient temperature. The desired product was filtered through solid phase (Ø = 1 cm, h = 3 cm SiO_2, r.t.) and the Et_2O was removed in vacuo (5 x 10^{-2} mbar). The product was obtained as an orange oil (crude product).

4a: ^{1}H NMR (300.1 MHz, 298 K, C_6D_6): δ / ppm = 2.04 ($^3J_{P,H}$ = 11.1 Hz, C*H*$_3$, 3H), 6.79-6.85 (m, Ph), 6.87-6.98 (m, Ph), 7.4 ($^1J_{P,H}$ = 407.0 Hz, $^3J_{H,H}$ = 8.5 Hz, P*H*, 1H). **^{13}C{^{1}H} NMR** (75.6 MHz, 298 K, C_6D_6): δ / ppm = 26.9 (d, $^3J_{P,C}$ = 1.7 Hz, NCH$_2$*C*H$_3$), 33.6 (d, $^2J_{P,C}$ = 10.5 Hz, N*C*H$_2$), 124.7 (s, Ph), 125.3 (d, $^3J_{P,C}$ = 4.0 Hz, Ph), 129.3 (s, Ph), 148.0 (d, $^2J_{P,C}$ = 3.0 Hz, *quart*.-C), 195.9 (d, $^2J_{P,C}$ = 7.7 Hz, *cis*-CO), 198.5 (d, $^2J_{P,C}$ = 26.1, *trans*-CO). **^{31}P NMR** (121.5 MHz, 298 K, C_6D_6): δ / ppm = 67.6 (ddq$_{sat}$, $^1J_{W,P}$ = 281.3 Hz, $^1J_{P,H}$ = 407.0 Hz, $^2J_{P,H}$ = 22.1 Hz, $^3J_{P,H}$ = 11.1 Hz). **MS** (EI, 70 eV, ^{184}W) m/z (%) = 554.0 (9) $[M]^{+\bullet}$, 526.0 (1) $[M\text{-}CO]^+$, 470.0 (3) $[M\text{-}3CO]^+$, 414.0 (2) $[M\text{-}5CO]^+$, 229.1 (6) $[M\text{-}W(CO)_5\text{-}H]^+$, 168.1 (25) $[NPh_2]^+$. **IR** (ATR diamond): *ν* / cm^{-1} = 1901.2 (vs, *ν*(CO)), 1982.3 (m, *ν*(CO)), 2071.6 (s, *ν*(CO)), 2861.2 (m, *ν*(PH)), 3320.3 (w *ν*(NH)).

*Procedure for the reactions of **1a,b** with tolane.* 0.1 mmol (59 mg (**a**), 61 mg (**b**)) was dissolved in 2 mL toluene before 90 mg (0.5 mmol) tolane was added. The reaction mixture was cooled down to -80/-85°C before 0.13 mL of *tert*-Butyllithium (0.2 mmol, 1.7 mol/L in *n*-hexane) was added and the reaction mixture was stirred while warming up to ambient temperature and was then filtered through wet silica (2 cm). After removal of the solvent under vacuum (10^{-2} mbar) the complexes were obtained as orange oils.

6a: ^{31}P NMR (121.5 MHz, 298.0 K, THF) δ/ppm = -108.3 ($^1J_{W,P}$ = 305.3 Hz). **MS** (EI, 70 eV, ^{184}W, 180°C) m/z (%) = 701.1 (10) $[M]^+$, 617-1 (8) $[M\text{-}3CO]^+$, 533.0 (7) $[M\text{-}NPh_2]^+$, 505.0 (3) $[M\text{-}NPh_2\text{-}CO]^+$, 477.0 (4) $[M\text{-}NPh_2\text{-}2CO]^+$, 449.0 (22) $[M\text{-}NPh_2\text{-}3CO]^+$, 393.0 (13) $[M\text{-}NPh_2\text{-}5CO]^+$, 209.1 (30) $[M\text{-}NPh_2\text{-}W(CO)_5]^+$, 178.1 (70) $[C_2Ph_2]^+$, 168.1 (50) $[NPh_2]^+$ (50).

6b: **^{1}H NMR** (300.1 MHz, 298.0 K, C_6D_6) δ/ppm = 0.64-0.80 (Cy, 2H), 0.89-0.98 (Cy, 2H), 1.10-1.20 (Cy, 4H), 1.51-1.61 (Cy, 4H), 1.62-1.72 (Cy, 4H), 3.12-3.29 ($^3J_{P,H}$ = 15.3 Hz, NC*H*, 2H), 6.94 – 7.05 (m, Ph), 7.47 – 7.54 (m, Ph), 7.84 – 7.89 (m, Ph) **^{13}C{^{1}H} NMR** (75.8 MHz, 298.0 K, C_6D_6) δ/ppm = 25.7 (Cy), 27.0 (Cy), 34.5 (d, $^3J_{P,C}$ = 3.2 Hz, NCH*C*H$_2$), 58.0 (d, $^2J_{P,C}$ = 6.7 Hz, N*C*H), 129.5 (Ph), 129.8 (d, $^2J_{P,C}$ = 4.4 Hz, PCC$_{Ph}$), 130.5 (Ph), 146.2 (d, $^1J_{P,C}$ = 16.8 Hz, P*C*), 197.5 (d, $^2J_{P,C}$ = 9.1 Hz, *cis*-CO), 199.3 (d, $^2J_{P,C}$ = 33.9 Hz, *trans*-CO). **^{31}P NMR** (121.5 MHz, 298.0 K, C_6D_6) δ/ppm = -115.3 (t$_{sat}$, $^1J_{W,P}$ = 306.1 Hz, $^2J_{P,H}$ = 15.6 Hz). **MS** (EI, 70 eV, ^{184}W) m/z (%) = 713.1 (0.1) $[M]^{+\bullet}$, 535.0 (28) $[M\text{-}Ph_2C_2]^+$, 507 (53) $[M\text{-}Ph_2C_2\text{-}CO]^+$, 178 (100) $[Ph_2C_2]^+$.

*Procedure for the reactions of **1b** with 1-pentene/1-hexene*. 61 mg (0.1 mmol) of **1b** was dissolved in 2 mL toluene before 0.5 mmol (70 mg 1-pentene (**7b**), 84 mg 1-hexene (**8b**)) was added. The reaction mixture was cooled down to -80/-85°C before 0.13 mL of *tert*-Butyllithium (0.2 mmol, 1.7 mol/L in *n*-hexane) was added and the reaction mixture was stirred while warming up to ambient temperature and was then filtered through wet silica (2 cm). After removal of the solvent under vacuum (10^{-2} mbar) the complexes were obtained as orange oils.

7b: ^{1}H NMR (500.1 MHz, 298.0 K, C_6D_6) δ/ppm = 0.53 (td, $^3J_{H,H}$ = 8.4 Hz, $^2J_{P,H}$ = 6.8 Hz, 1H, PC*H*), 0.93 (t, $^3J_{H,H}$ = 7.2 Hz, 3H, C*H*$_3$), 1.03-1.13 (m, 4H, NCHC*H*$_2$), 1.13-1.22 (m, 4H, NCHC*H*$_2$), 1.24-1.34 (m, 4H, NCHCH$_2$CH$_2$C*H*$_2$), 1.35-1.46 (m, 6H, NCHCH$_2$C*H*$_2$), 1.41-1.44 (m, $^3J_{P,H}$ = 3.8 Hz, 2H, CHC*H*$_2$), 1.53-1.56 (m, 2H, CHCH$_2$C*H*$_2$), 1.64-1.67 (m, 2H, PC*H*$_2$), 1.84-1.92 (m, 2H, NCHCH$_2$C*H*$_2$), 2.67-2.77 (m, 2H, NC*H*). **^{13}C{^{1}H} NMR** (125.5 MHz, 298.0 K, C_6D_6) δ/ppm = 14.0 (s, *C*H$_3$), 23.0 (d, $^3J_{P,C}$ = 6.7 Hz, CH$_2$*C*H$_2$CH$_3$), 23.4 (d, $^1J_{P,C}$ = 17.5 Hz, P*C*H), 26.8 (d, $^3J_{P,C}$ = 7.1 Hz, NCH*C*H$_2$), 31.7 (d, $^1J_{P,C}$ = 21.1 Hz, P*C*H$_2$), 33.6 (d, $^4J_{P,C}$ = 3.3 Hz, NCHCH$_2$*C*H$_2$), 34.0 ($^2J_{P,C}$ = 3.4 Hz, *C*H$_2$CH$_2$CH$_3$), 35.3 (d, $^5J_{P,C}$ = 1.5 Hz, NCHCH$_2$CH$_2$*C*H$_2$), 60.3 (d, $^2J_{P,C}$ = 3.9 Hz, N*C*H), 197.7 (d$_{sat}$, $^2J_{P,C}$ = 8.8 Hz, $^1J_{W,C}$ = 126.8 Hz, *cis*-CO), 198.9 (d, $^2J_{P,C}$ = 32.0 Hz, *trans*-CO). **^{31}P{^{1}H} NMR** (202.1 MHz, 298.0 K, C_6D_6) δ/ppm = -108.1 (s$_{sat}$, $^1J_{W,P}$ = 287.0 Hz), -111.1 (s$_{sat}$, $^1J_{W,P}$ = 281.8 Hz) [83:17]. **^{31}P NMR** (202.1 MHz, 298.0 K, C_6D_6) δ/ppm = -108.1 (br. s$_{sat}$, $^1J_{W,P}$ = 287.0, FWHM ~54 Hz), -111.1 (br. s FWHM ~49). **MS** (EI, 70 eV, ^{184}W) m/z (%) = 507.0 (1.2) $[M\text{-}CO\text{-}C_5H_{10}]^+$, 323.9 (5) $[W(CO)_5]^+$, 295.9 (1) $[W(CO)_4]^+$, 267.9 (4) $[W(CO)_3]^+$, 239.9 (3) $[W(CO)_2]^+$. **IR** (ATR Diamant): *ν* / cm^{-1} = 1904.7 (vs, *ν*(CO)), 1978.7 (m, *ν*(CO)), 2068.1 (s, *ν*(CO)), 2854.9 (m, *ν*(CH)), 2929.8 (s, *ν*(CH)). **Anal. calc.** for $C_{22}H_{32}NO_5PW$, C 43.65 H 5.33 N 2.31; **found** C 42.85 H 5.09 N 2.18.

8b: ^{1}H NMR (300.1 MHz, 298 K, C_6D_6): δ / ppm = 0.53 (m, $^3J_{H,H}$ = 7.7 Hz, $^2J_{P,H}$ = 7.6 Hz, 1H, PC*H*), 0.92 (t, $^3J_{H,H}$ = 7.2 Hz, 3H, C*H*$_3$), 1.07-1.26 (m, xH, NCHC*H*$_2$), 1.23-1.39 (m, 2H, CHCH$_2$CH$_2$C*H*$_2$), 1.34-1.53 (m, NCHCH$_2$CH$_2$C*H*$_2$), 1.40-1.52 (m, 6H, NCHCH$_2$C*H*$_2$), 1.48-1.58 (m, 2H, CHC*H*$_2$), 1.55-1.70 (m, 2H, CHCH$_2$C*H*$_2$), 1.57-1.72 (m, 2H, PC*H*$_2$), 1.60-1.73 (m, xH,

NCHC*H*$_2$), 1.84-1.95 (m, 2H, NCHCH$_2$C*H*$_2$), 2.64-2.81 (m, 2H, NC*H*). **^{13}C{^{1}H} NMR** (75.5 MHz, 298 K, C_6D_6): δ / ppm = 14.2 (s, *C*H$_3$), 22.8 (s, CH$_2$*C*H$_2$CH$_3$), 22.8 (s, P*C*H), 25.9 (s, CHCH$_2$*C*H$_2$), 25.9 (s, CH*C*H$_2$), 26.8 (d, $^3J_{P,C}$ = 4.1 Hz, NCH*C*H$_2$), 31.6 (d, $^4J_{P,C}$ = 3.3 Hz, NCHCH$_2$*C*H$_2$), 32.0 (d, $^1J_{P,C}$ = 14.0 Hz, P*C*H$_2$), 33.6 ($^4J_{P,C}$ = 3.5 Hz, NCH$_2$CH$_2$*C*H$_2$), 35.3 (d, $^5J_{P,C}$ = 1.8 Hz, NCHCH$_2$CH$_2$*C*H$_2$), 60.4 (d, $^2J_{P,C}$ = 4.1 Hz, N*C*H), 197.8 (d$_{sat}$, $^2J_{P,C}$ = 8.9 Hz), 198.9 (d, $^2J_{P,C}$ = 32.0 Hz, *trans*-CO). **^{31}P{^{1}H} NMR** (202.1 MHz, 298.0 K, C_6D_6) δ/ppm = -107.8 (s$_{sat}$, $^1J_{W,P}$ = 287.6 Hz), -110.4 (s$_{sat}$, $^1J_{W,P}$ = 281.8 Hz) [83:17]. **^{31}P NMR** (202.1 MHz, 298.0 K, C_6D_6) δ/ppm = -107.8 (br. s$_{sat}$, $^1J_{W,P}$ = 287.6, FWHM ~51 Hz), -110.4 (br. s, FWHM ~37 Hz). **MS** (EI, 70 eV, ^{184}W) m/z (%) = 536.1 (3) [M-Cy]$^+$, 508.1 (2) [M-Cy-CO]$^+$, 354.9 (1) [W(CO)$_5$-P]$^+$, 295.2 (2) [M-W(CO)$_5$]$^+$, 267.9 (4) [W(CO)$_3$]$^+$, 239.9 (2) [W(CO)$_2$]$^+$, 212.2 (4) [M-W(CO)$_5$-Cy]$^+$, 84.1 (17) [C_6H_{12}]$^+$, 56.1 (45) [C_4H_8]$^+$. **IR** (ATR diamond): *v* / cm^{-1} = 2929 (m, *v*(CH)), 2855 (m, *v*(CH)), 2068 (s, *v*(CO)), 1978 (s, *v*(CO)), 1904 (vs, *v*(CO)). **Anal. calc.** for $C_{23}H_{34}NO_5PW$, C 44.60 H 5.53 N 2.26; **found** C 44.78 H 5.65 N 2.45.

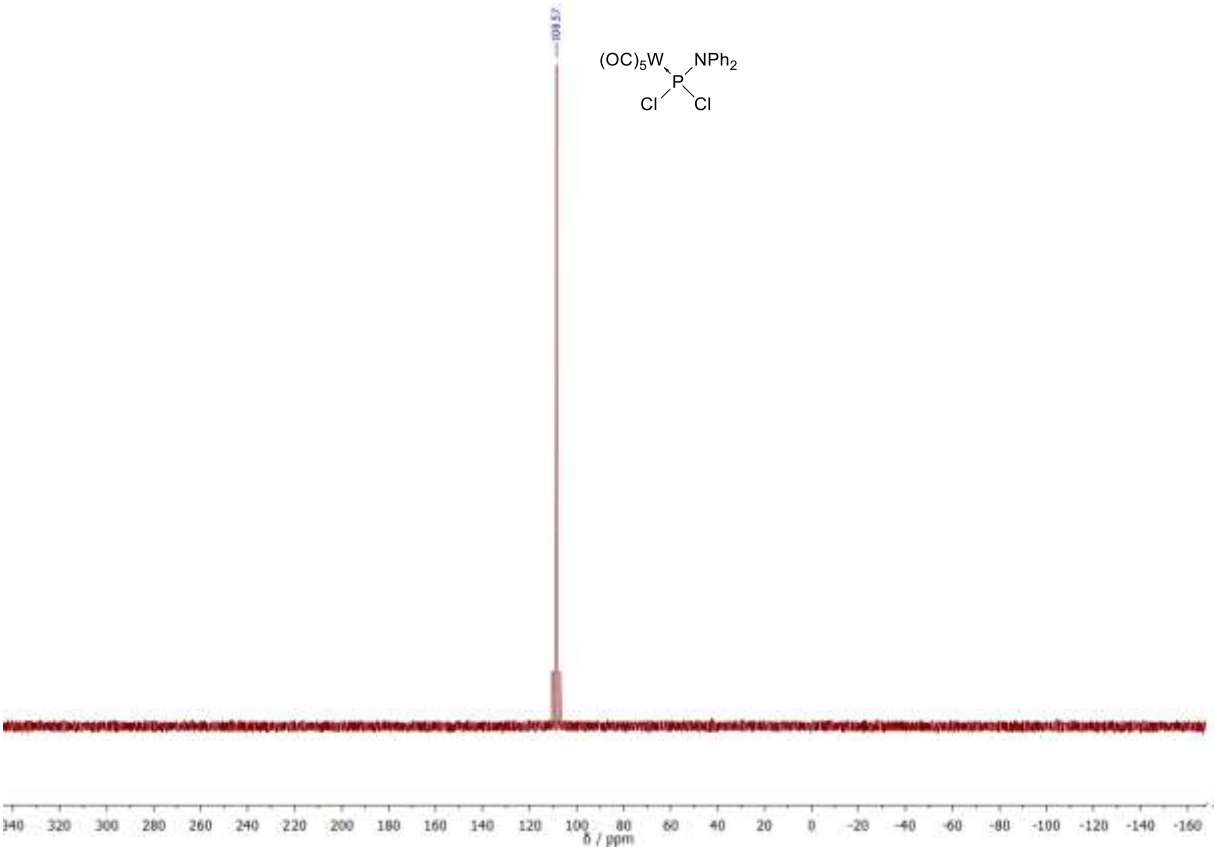


Figure S1: $^{31}P\{^{1}H\}$ NMR spectrum of **1a** in C_6D_6 at 121.5 MHz.

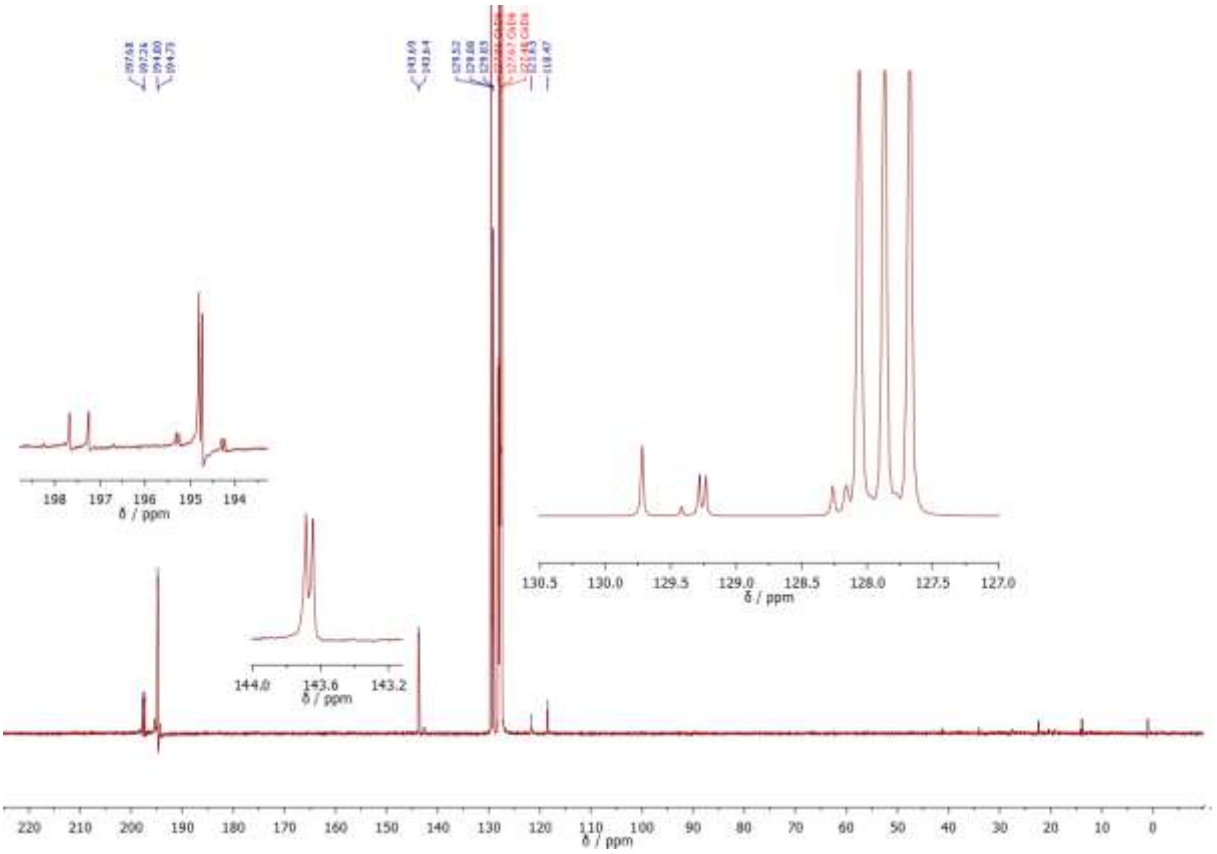


Figure S2: $^{13}C\{^{1}H\}$ NMR Spectrum of **1a** in C_6D_6 at 121.5 MHz.

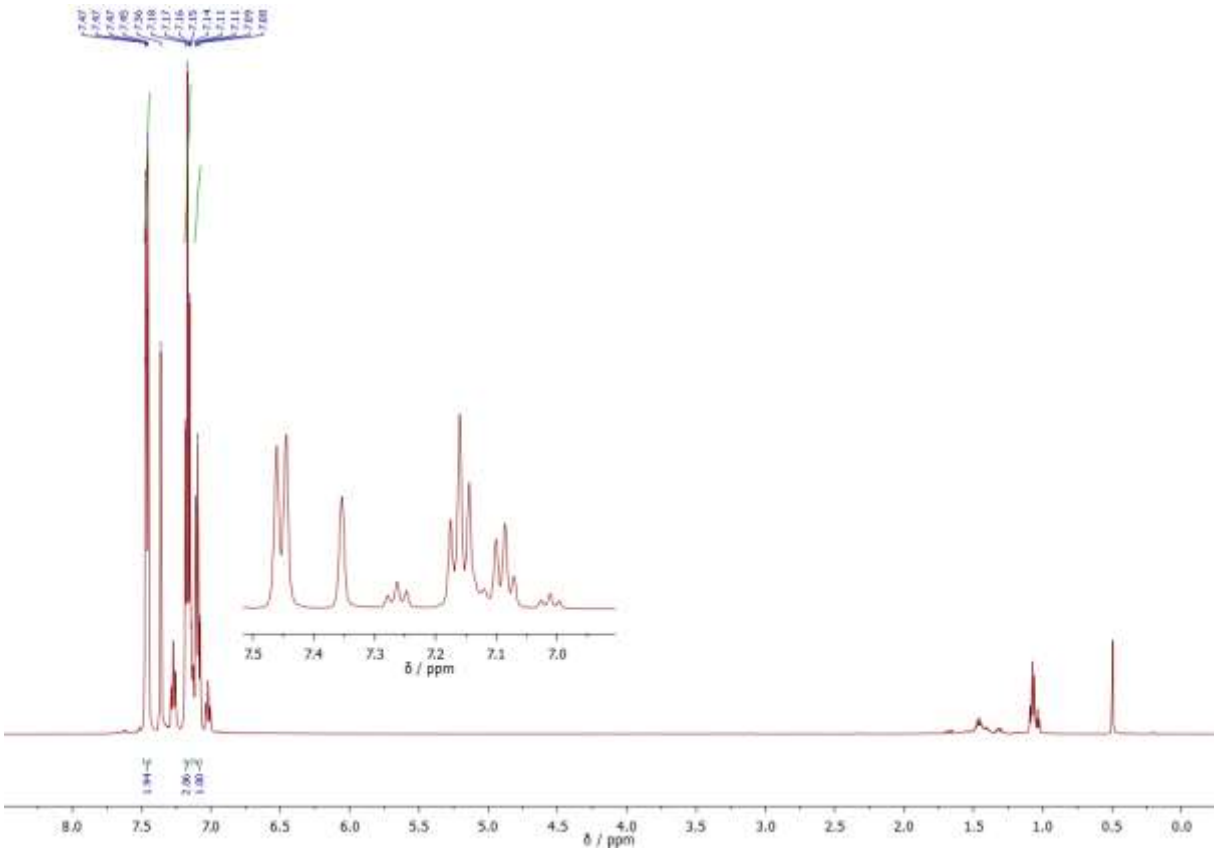


Figure S3: ^{1}H NMR Spectrum of **1a** in C_6D_6 at 500.1 MHz.

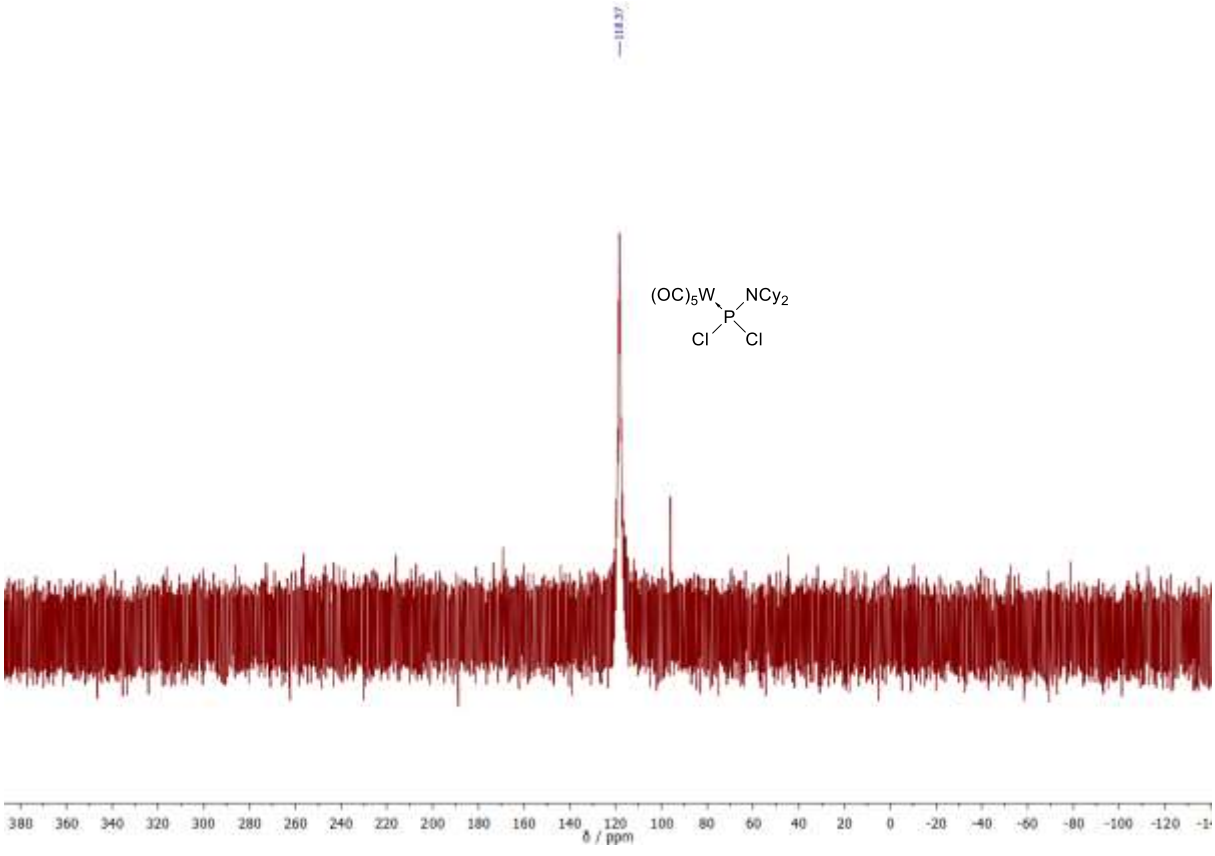


Figure S4: $^{31}P\{^{1}H\}$ NMR spectrum of **1b** in C_6D_6 at 162.0 MHz.

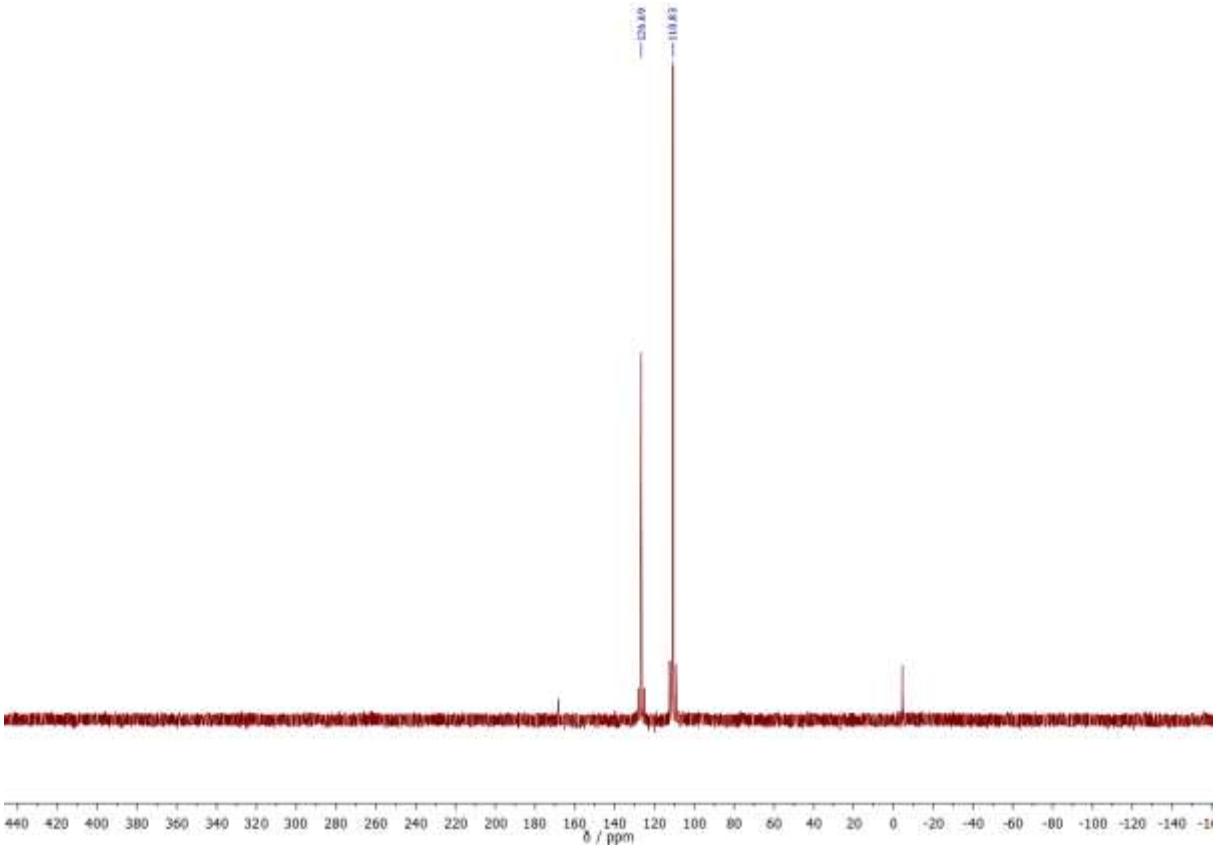


Figure S4': $^{31}P\{^{1}H\}$ NMR spectrum of **1b** at -60 °C in THF at 121.0 MHz

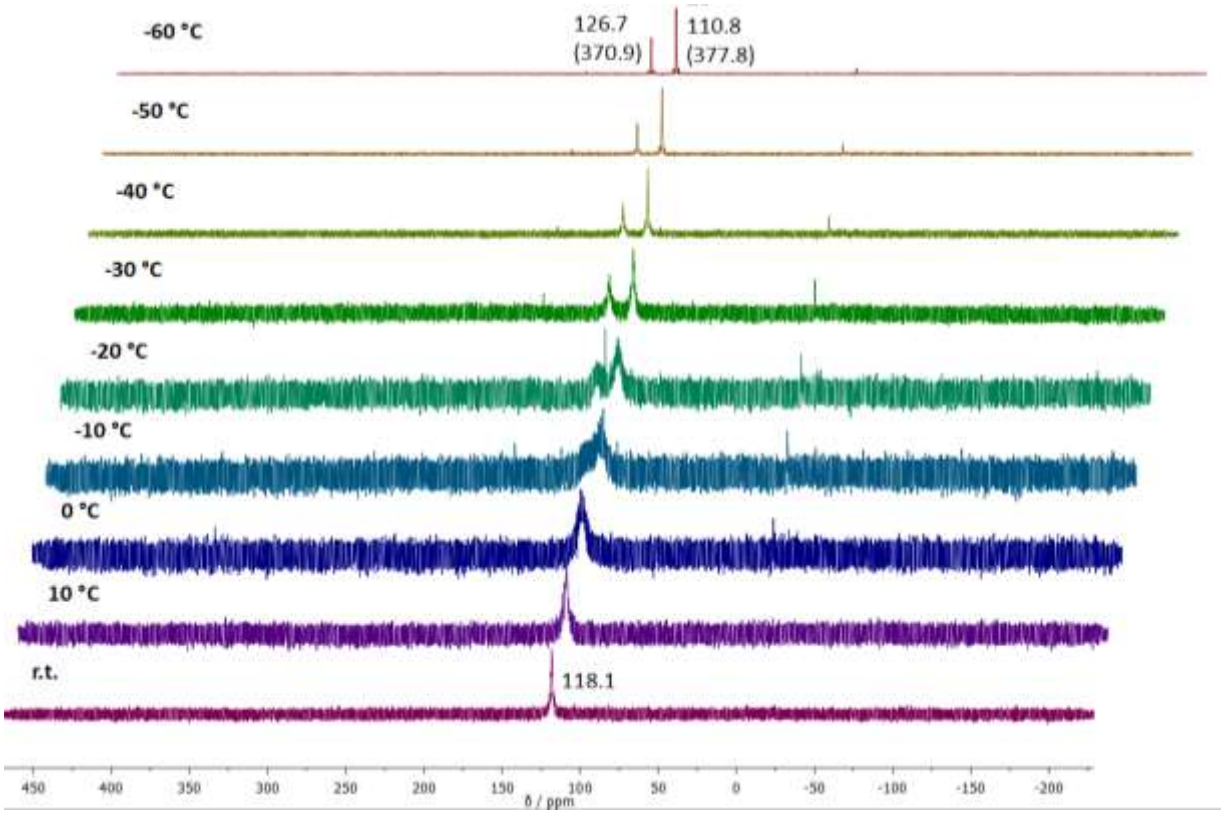


Figure S4'': $^{31}P\{^{1}H\}$ VT-NMR spectra of **1b** starting at – 60 °C in THF at 121.0 MHz. With the coalescence Temperature (Tc) taken at -10 °C, a Gibbs free energy rotation barrier of 7.3 kcal/mol could be calculated.

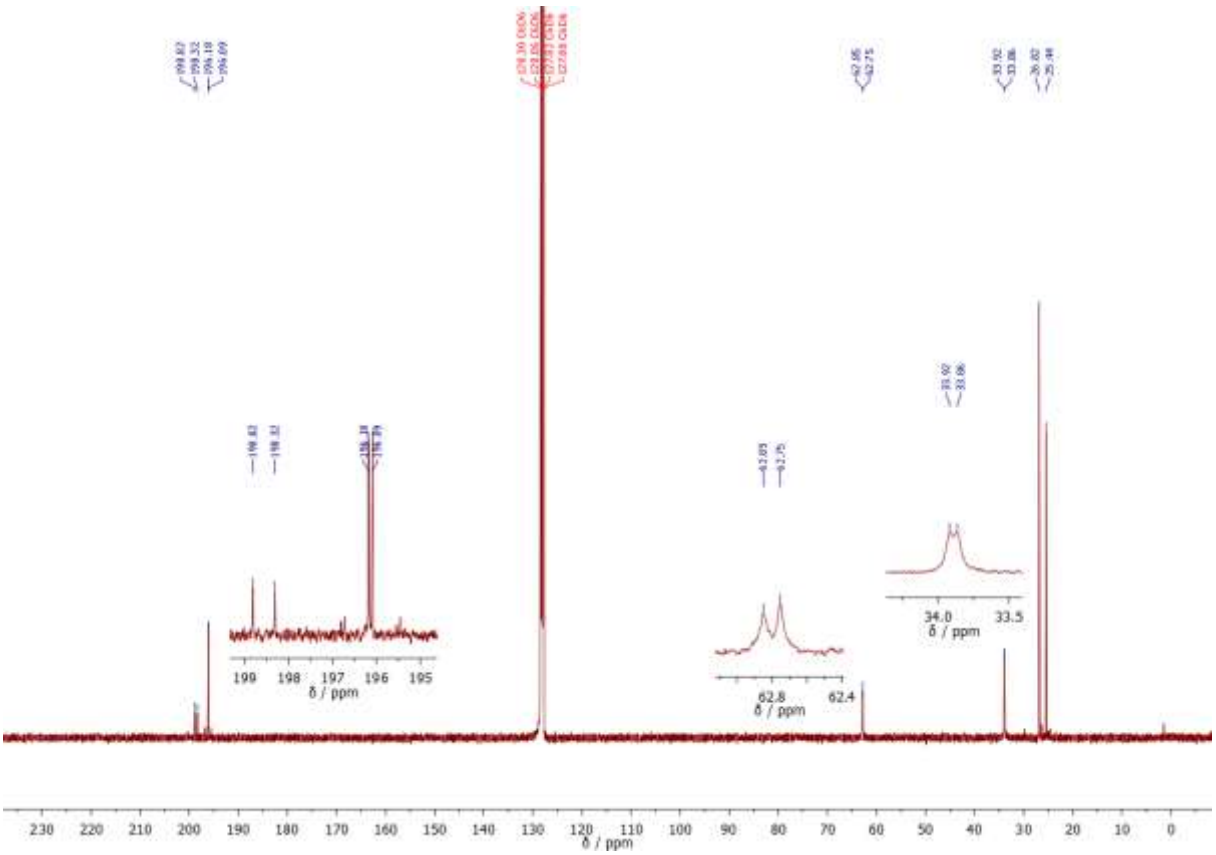


Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of **1b** in C_6D_6 at 100.6 MHz.

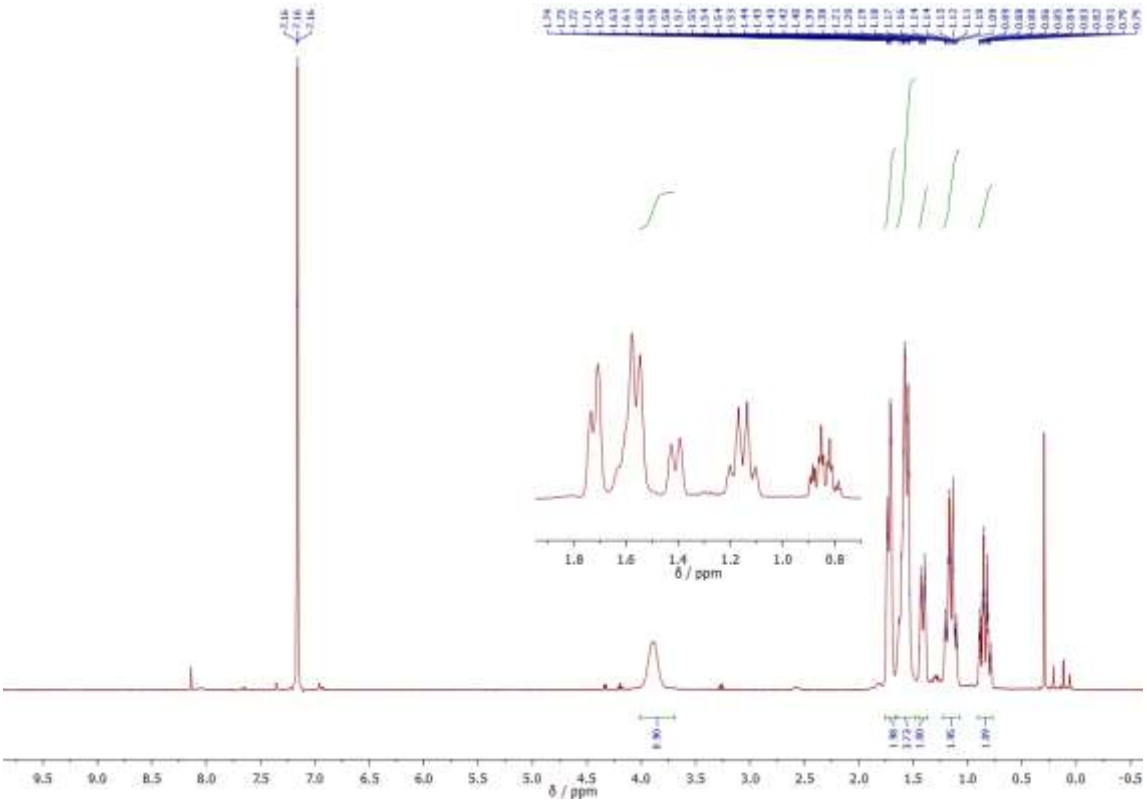


Figure S6: ^{1}H NMR spectrum of **1b** in C_6D_6 at 400.1 MHz.

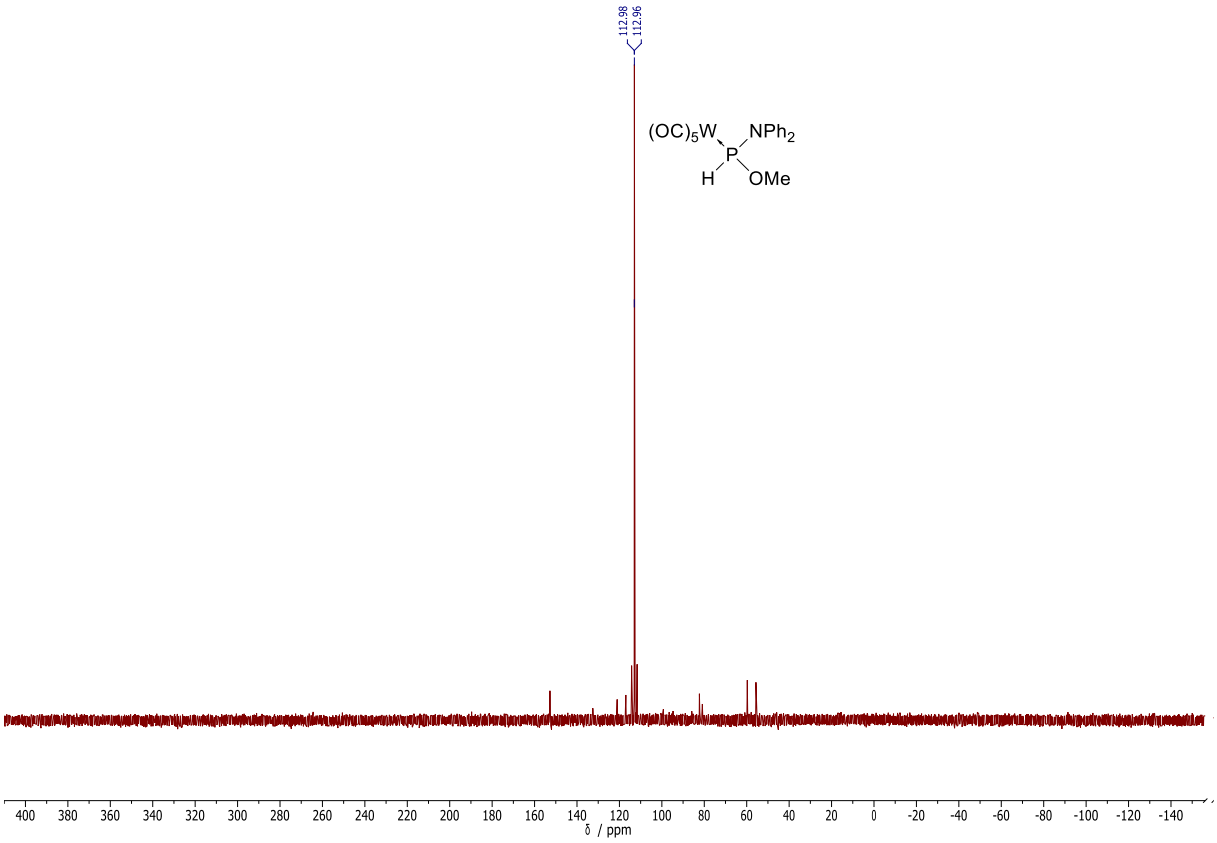
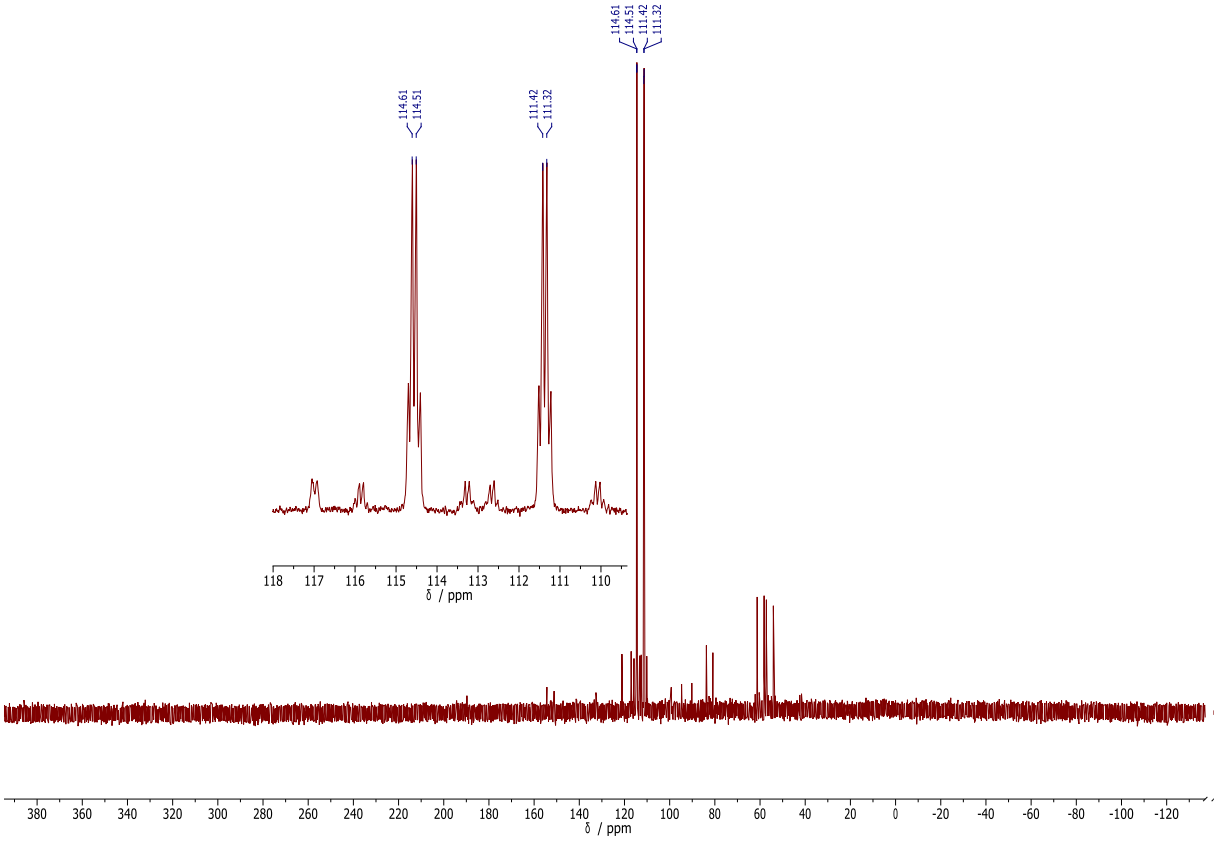


Figure S7: $^{31}P\{^{1}H\}$ NMR spectrum of **3a** in THF at 121.5 MHz.

Figure S8: ^{31}P NMR spectrum of **3a** in THF at 121.5 MHz.



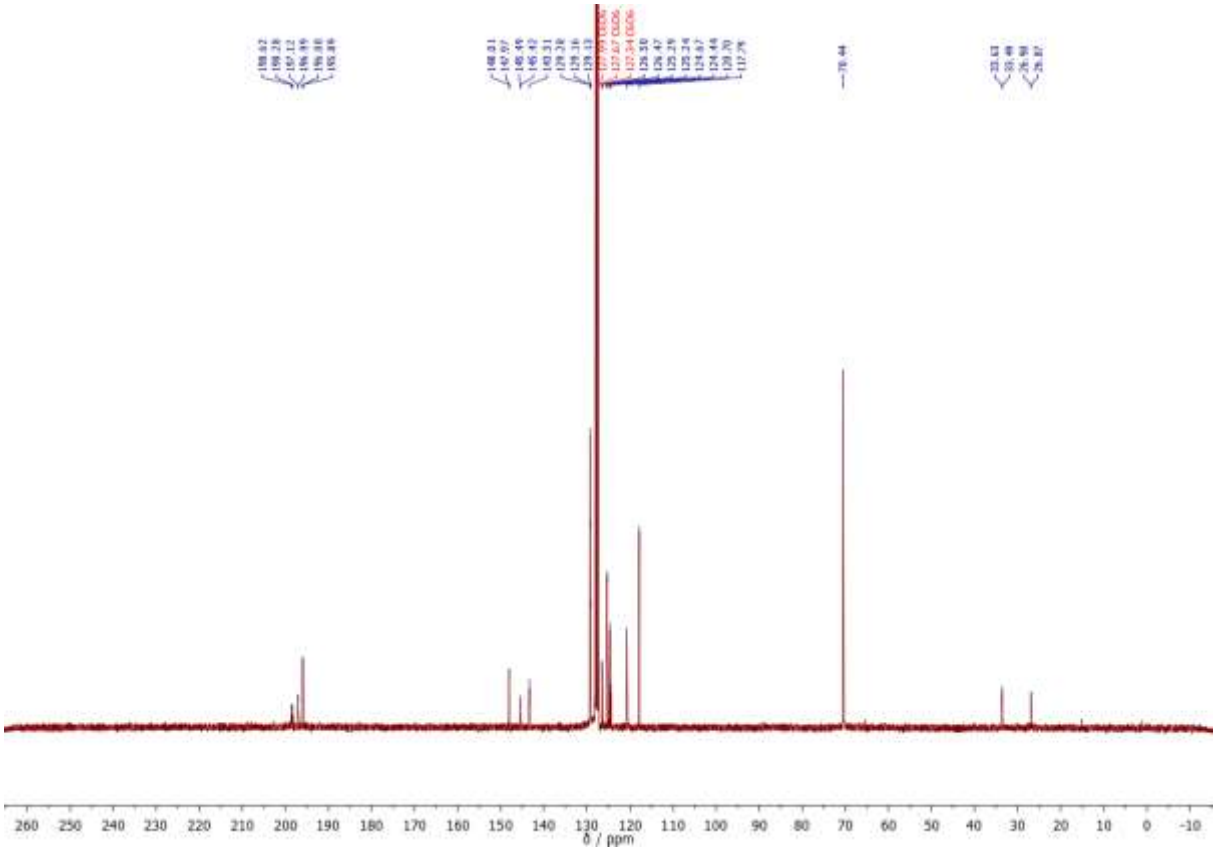


Figure S9: $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in C_6D_6 at 75.5 MHz.

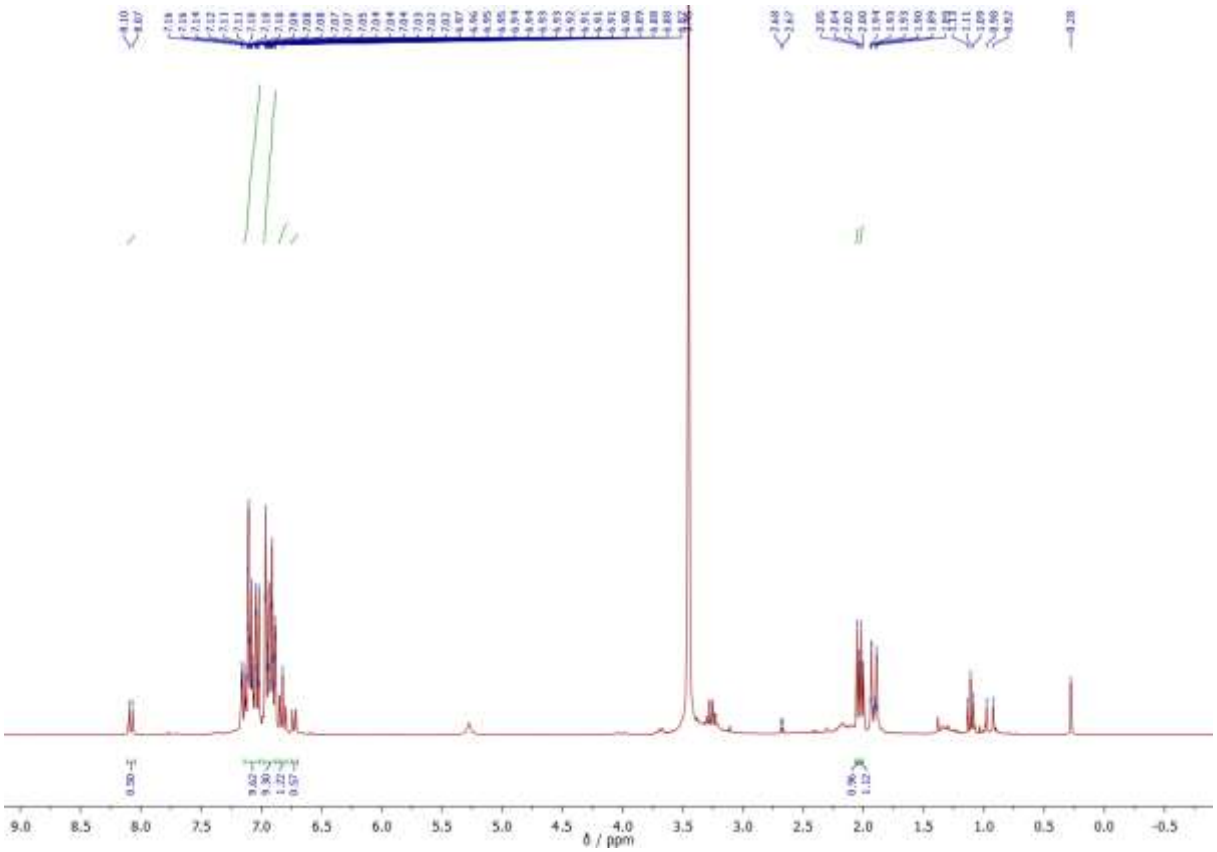


Figure S10: ^{1}H NMR spectrum of **3a** in C_6D_6 at 300.1 MHz.

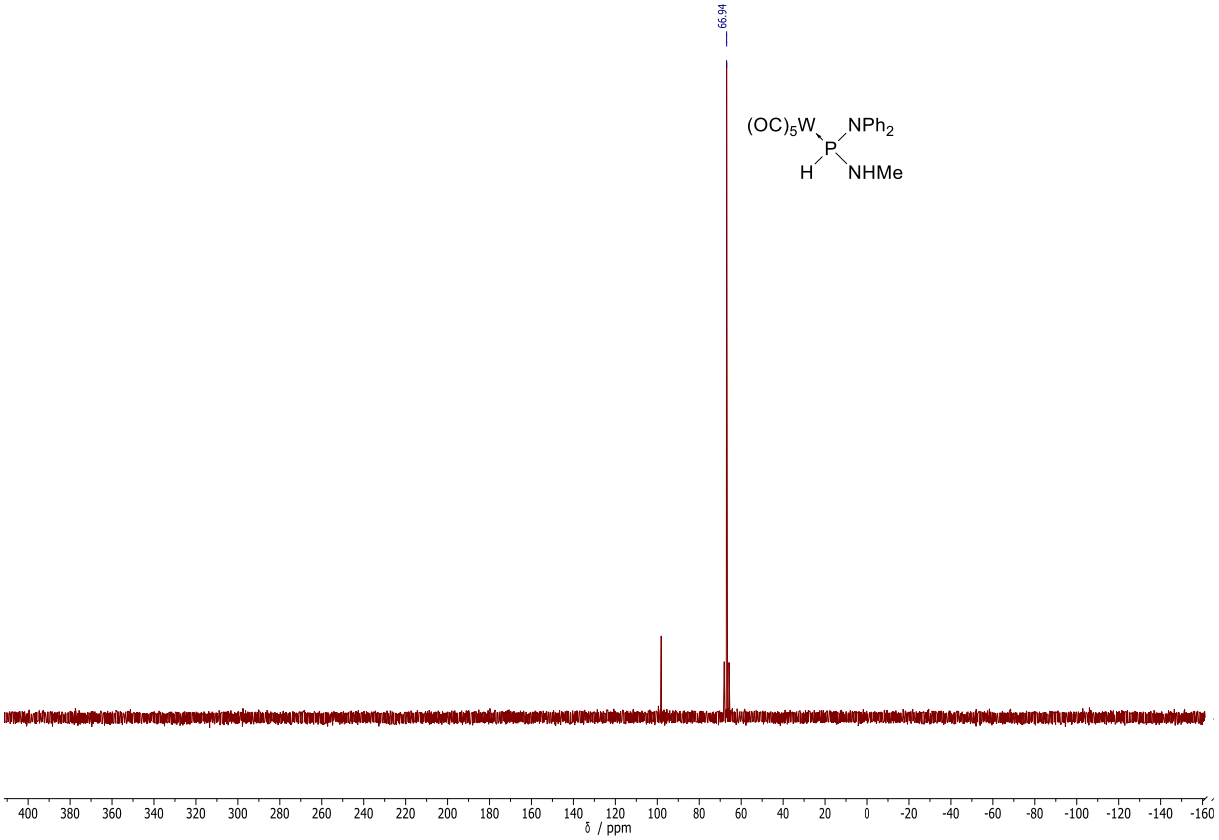


Figure S11: $^{31}P\{^{1}H\}$ NMR spectrum of **4a** in THF at 121.5 MHz.

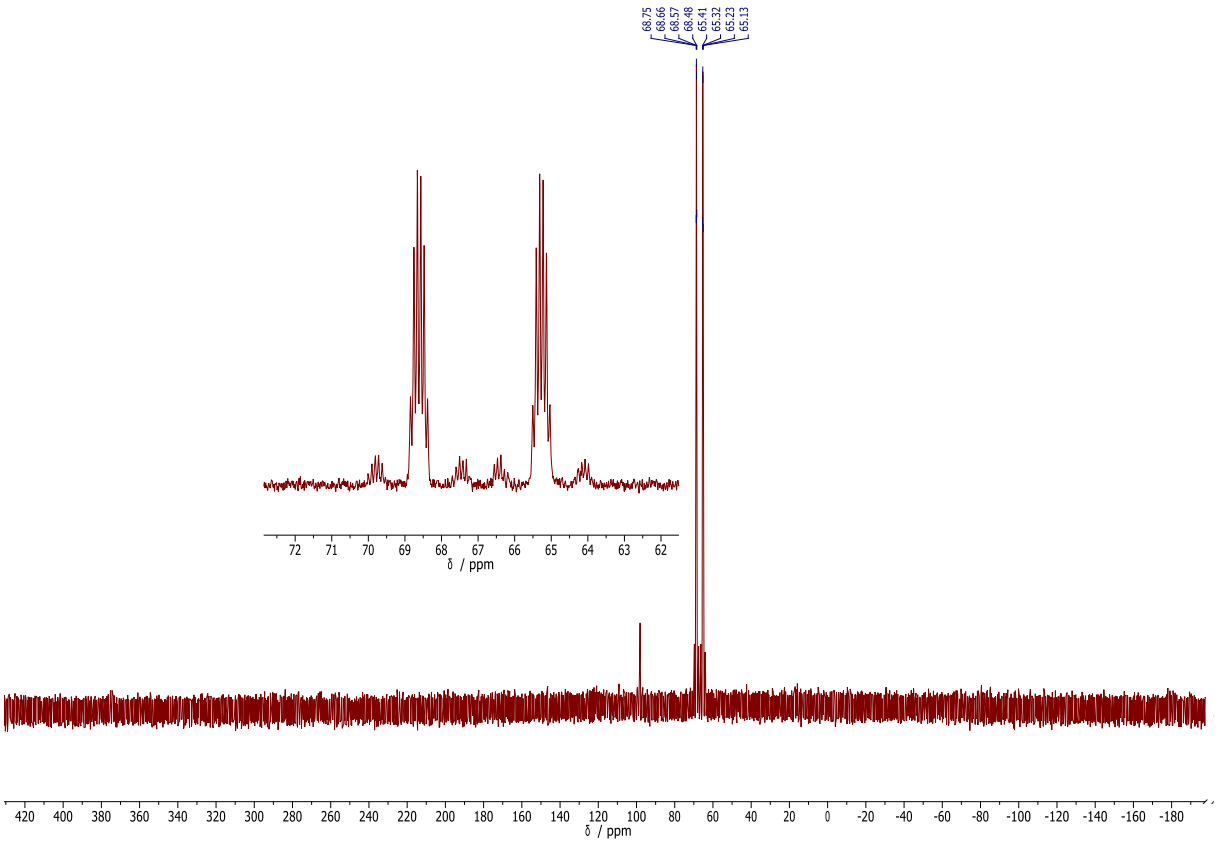


Figure S12: ^{31}P NMR spectrum of **4a** in THF at 121.5 MHz.

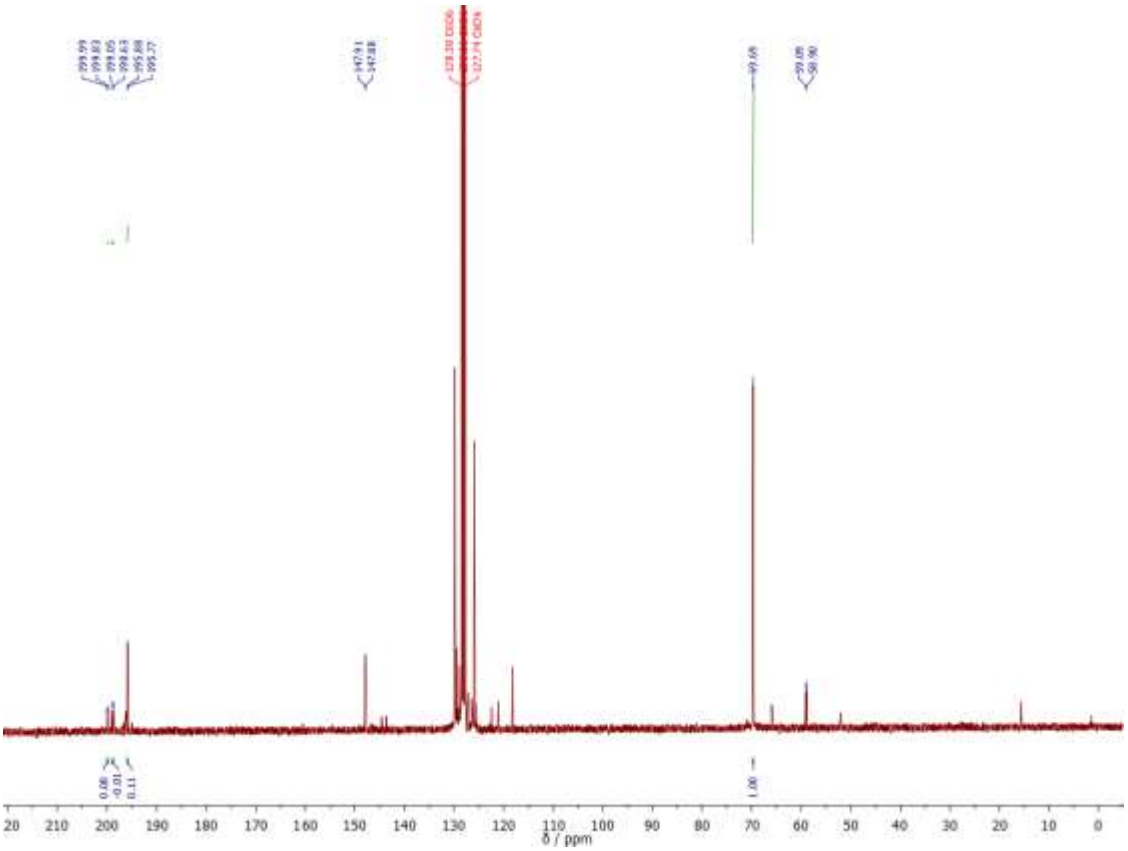


Figure S13: $^{13}C\{^{1}H\}$ NMR spectrum of **4a** in C_6D_6 at 75.5 MHz.

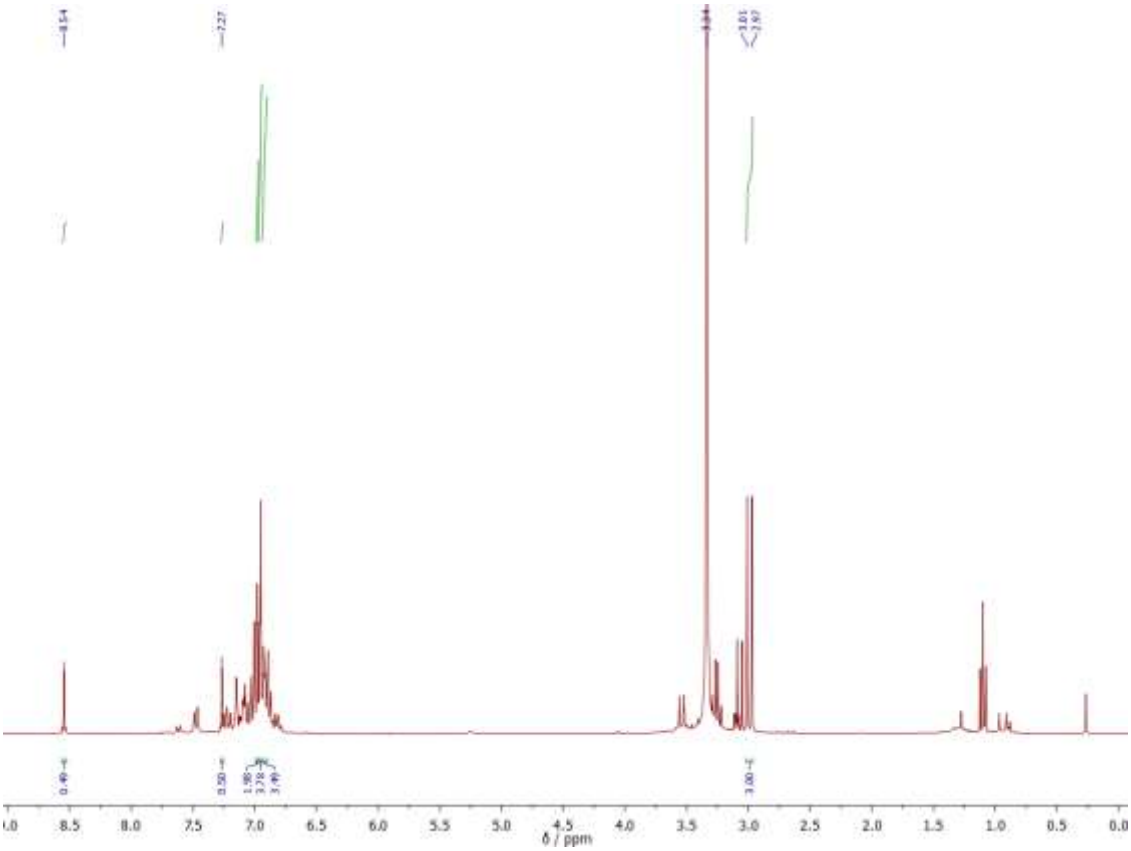


Figure S14: ^{1}H NMR spectrum of **4a** in C_6D_6 at 300.1 MHz.

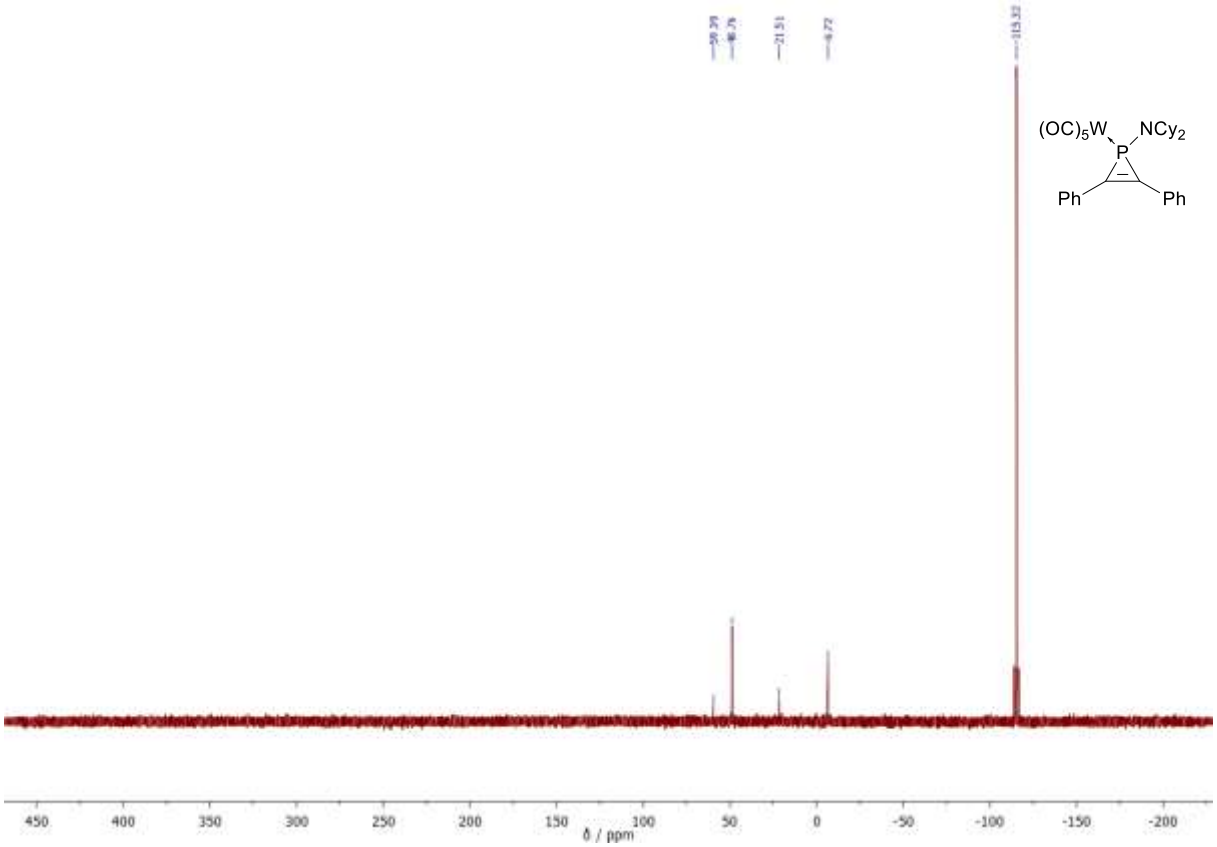


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of **6b** in C_6D_6 at 121.5 MHz.

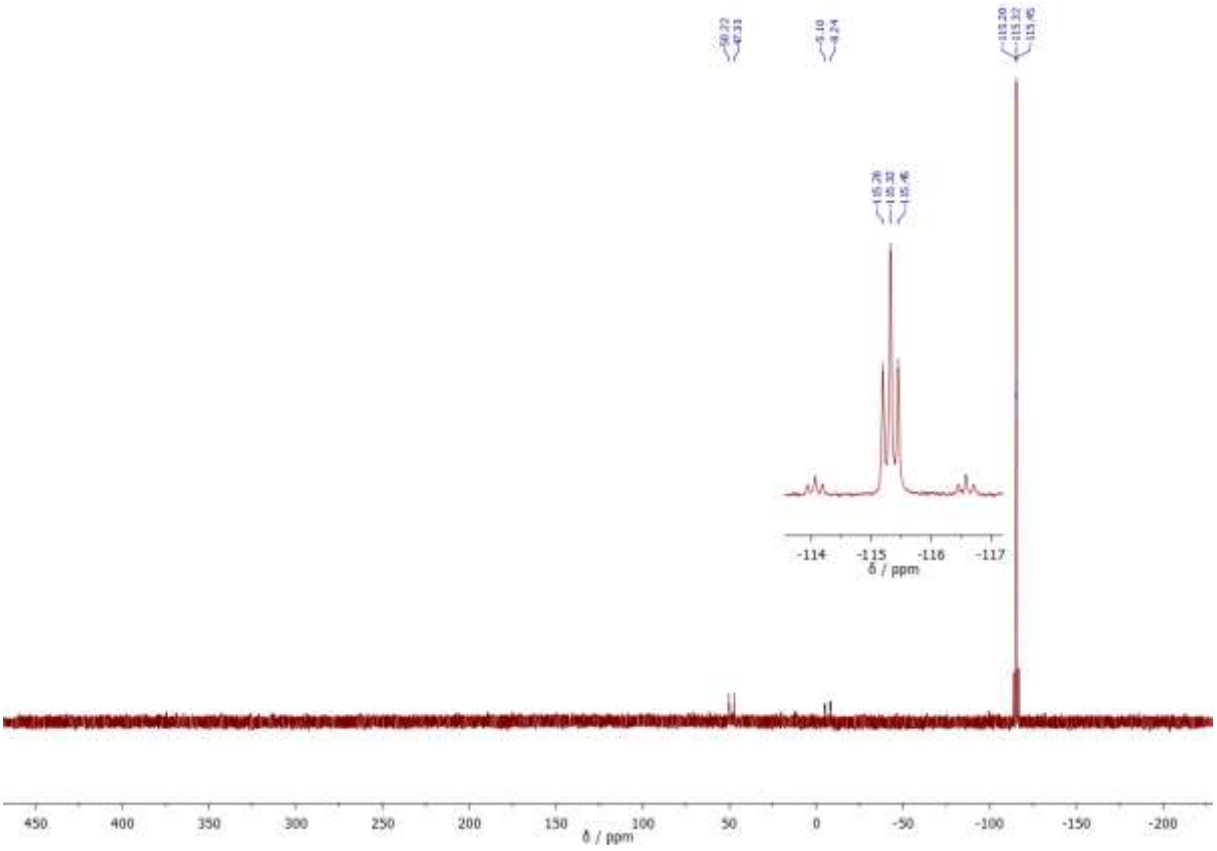


Figure S16. ^{31}P NMR spectrum of **6b** in C_6D_6 at 121.5 MHz.

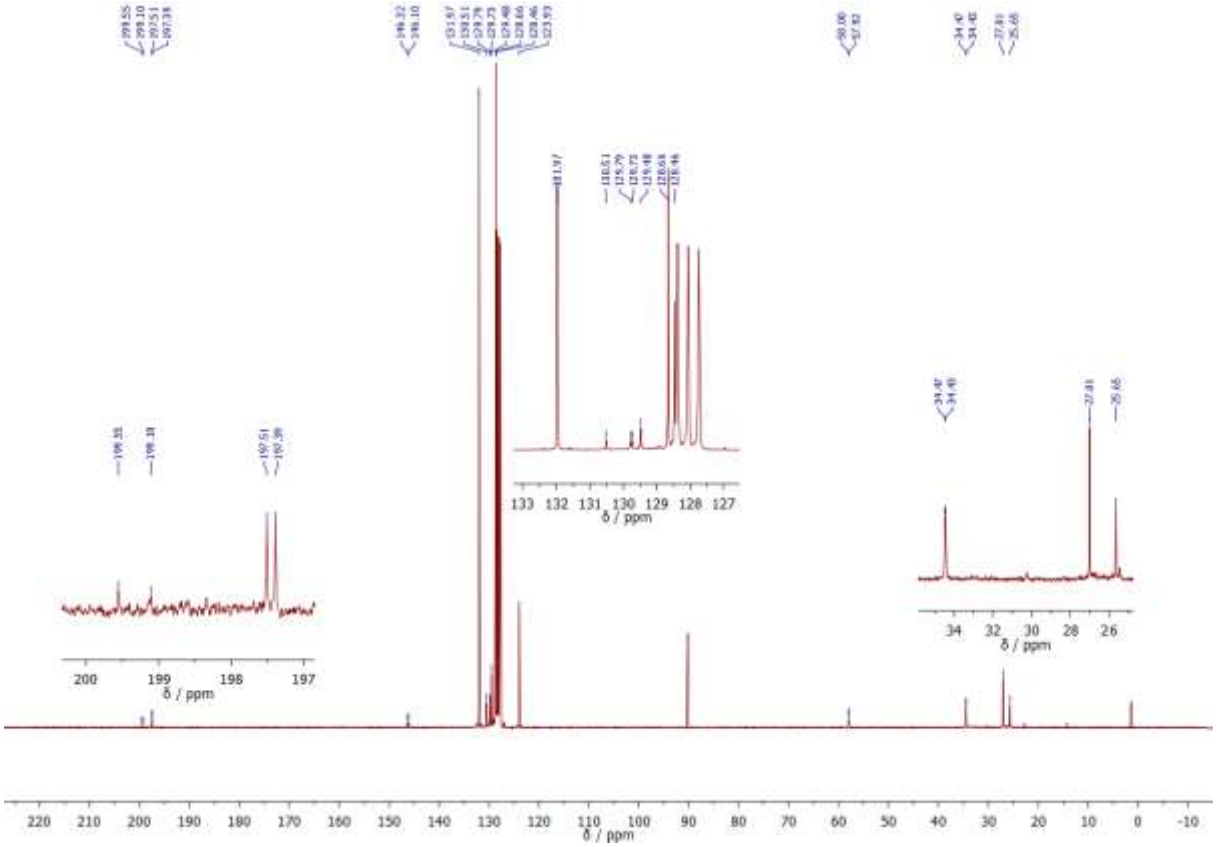


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of **6b** in C_6D_6 at 75.5 MHz.

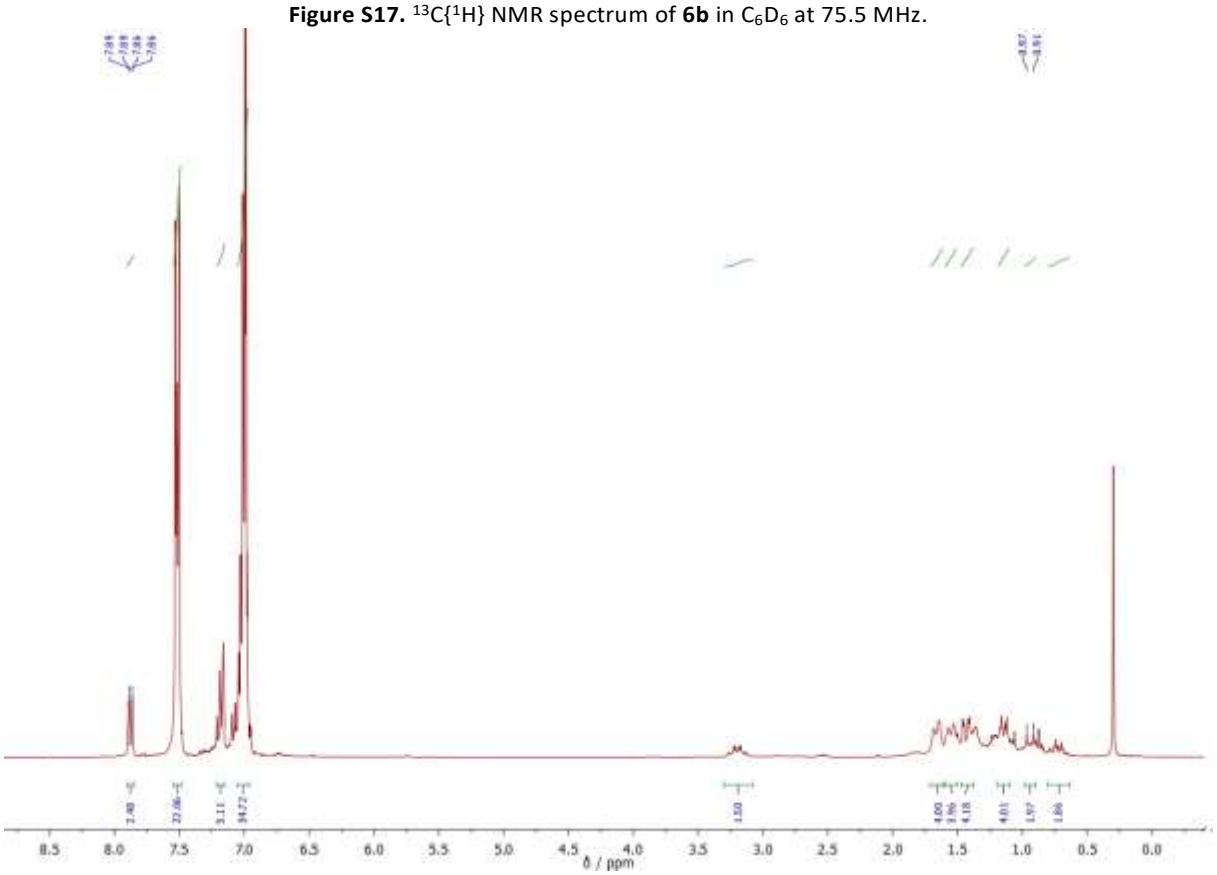


Figure S18. ^{1}H NMR spectrum of **6b** in C_6D_6 at 300.1 MHz.

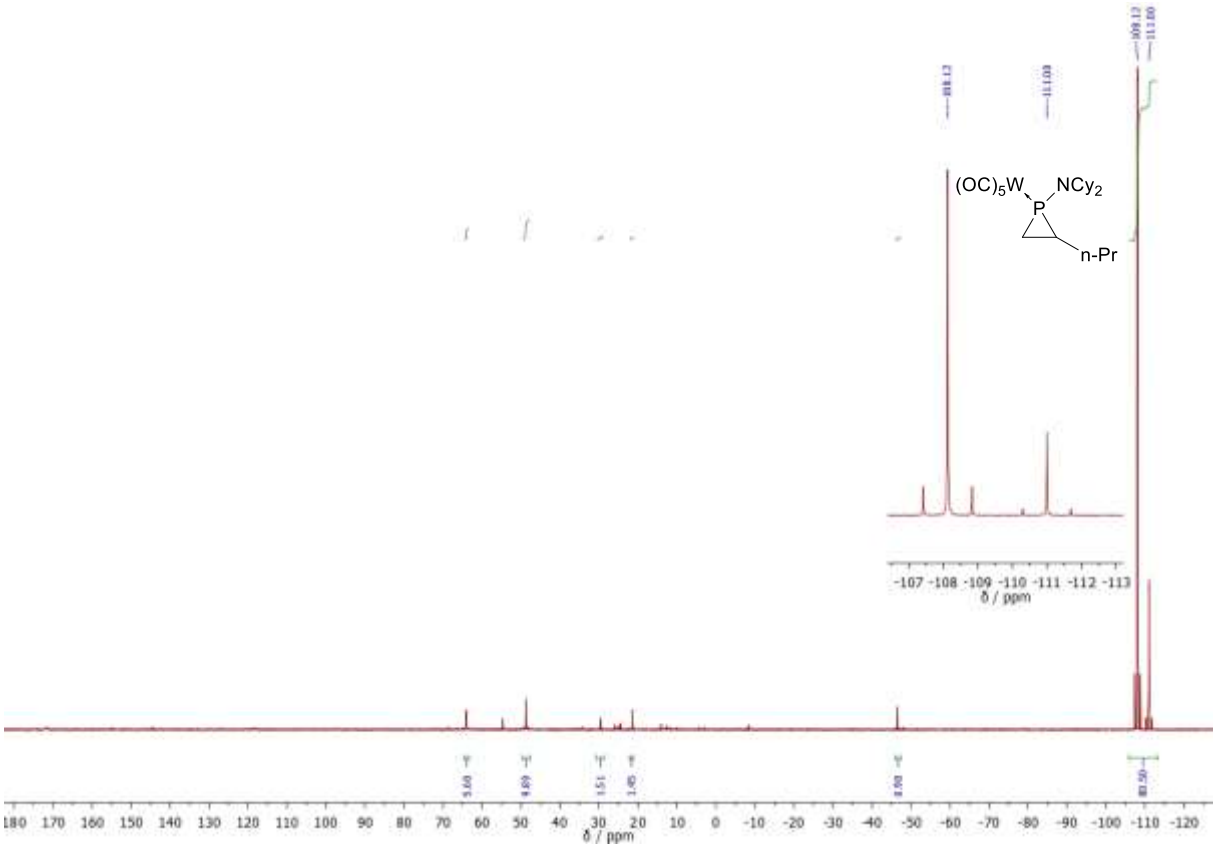


Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum of **7b** in C_6D_6 at 202.1 MHz.

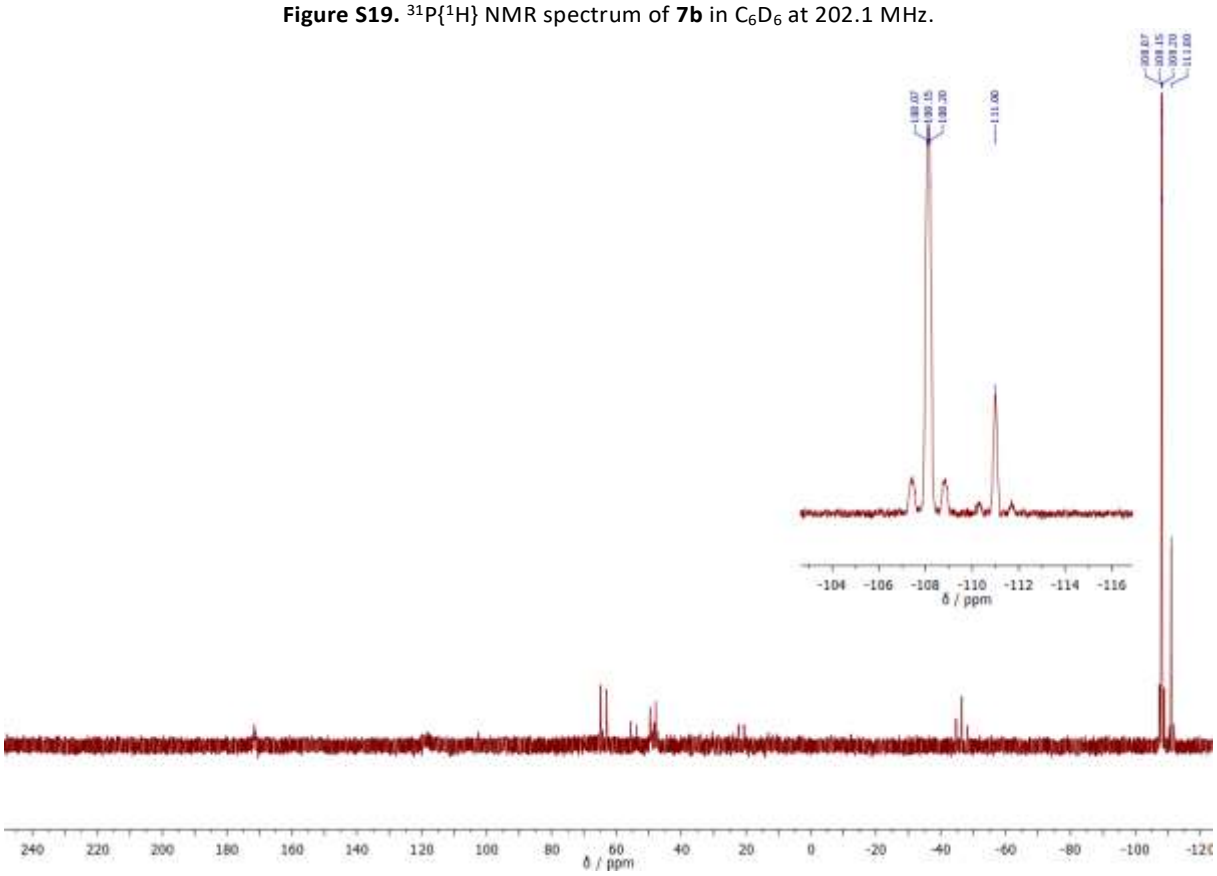


Figure S20. ^{31}P NMR spectrum of **7b** in C_6D_6 at 202.1 MHz.

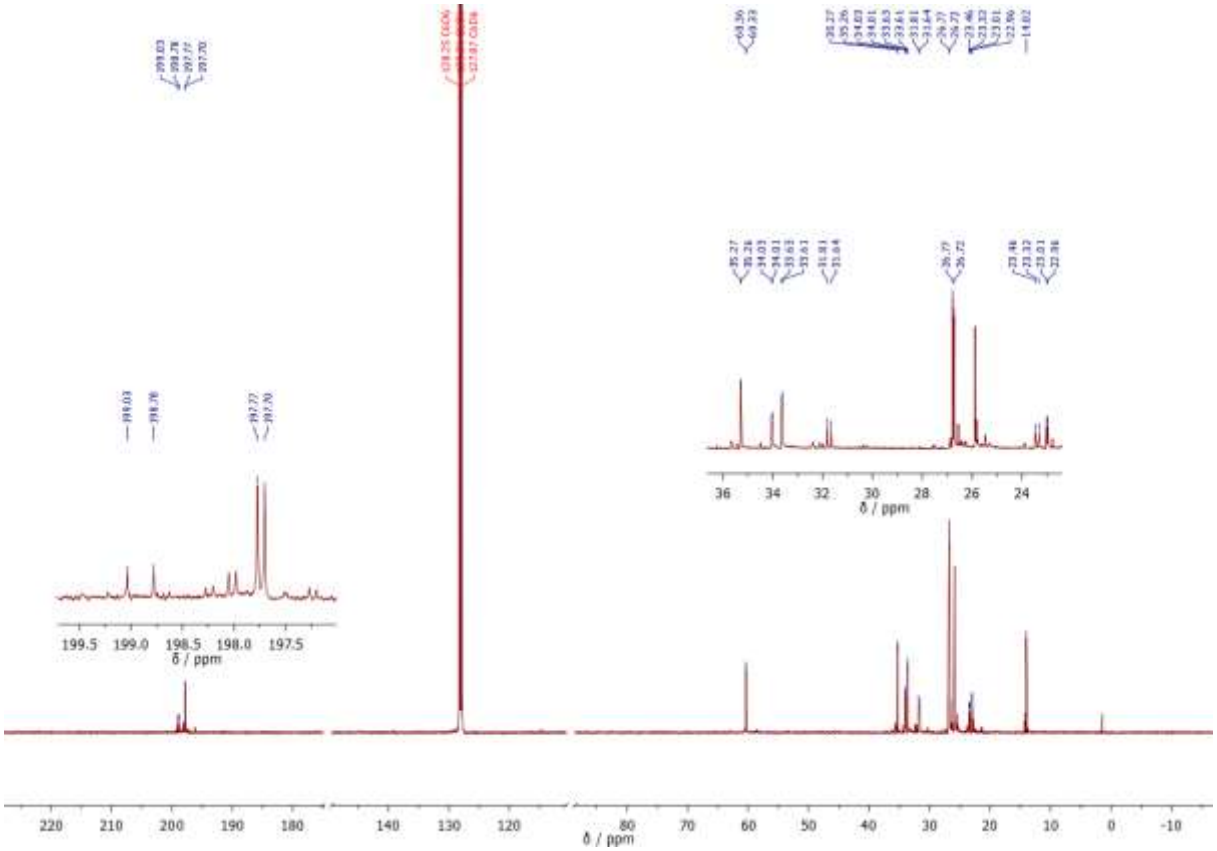


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of **7b** in C_6D_6 at 121.5 MHz.

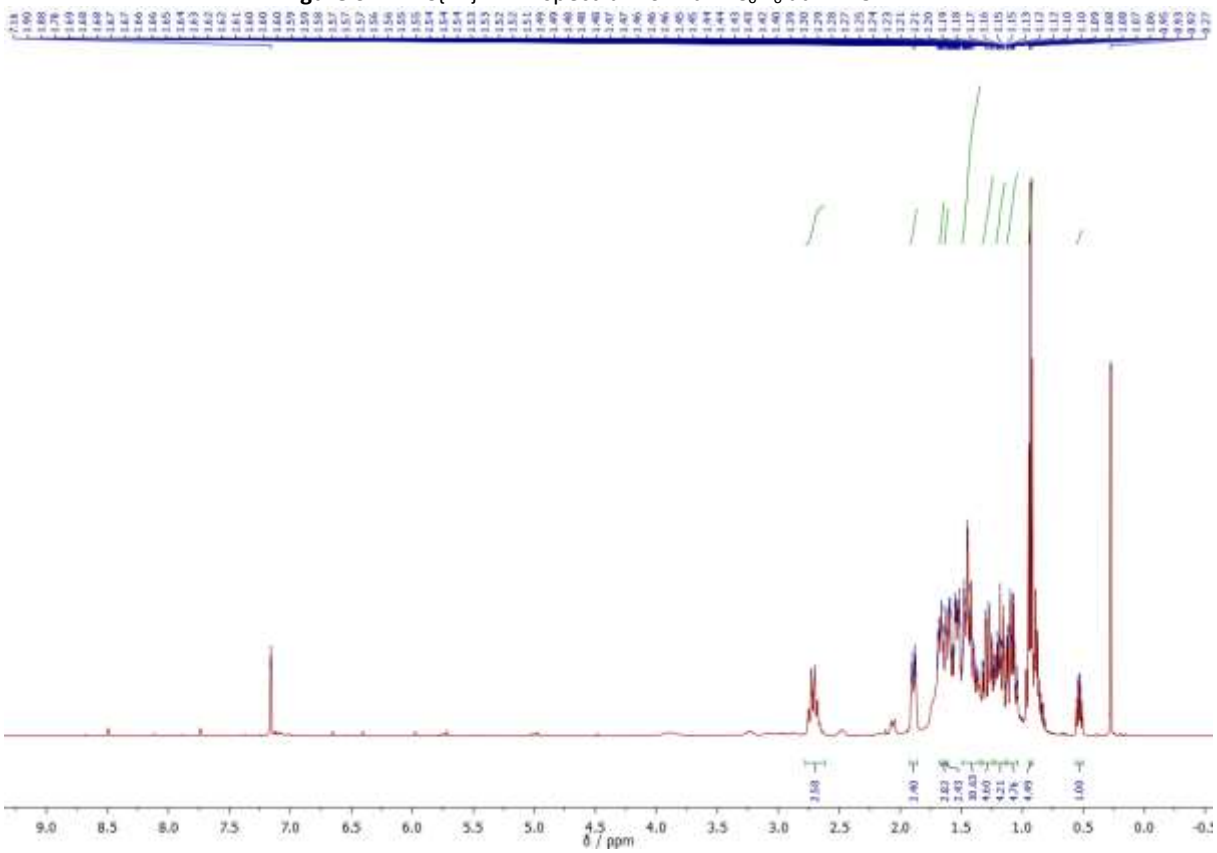


Figure S22. ^{1}H NMR spectrum of **7b** in C_6D_6 at 500.1 MHz.

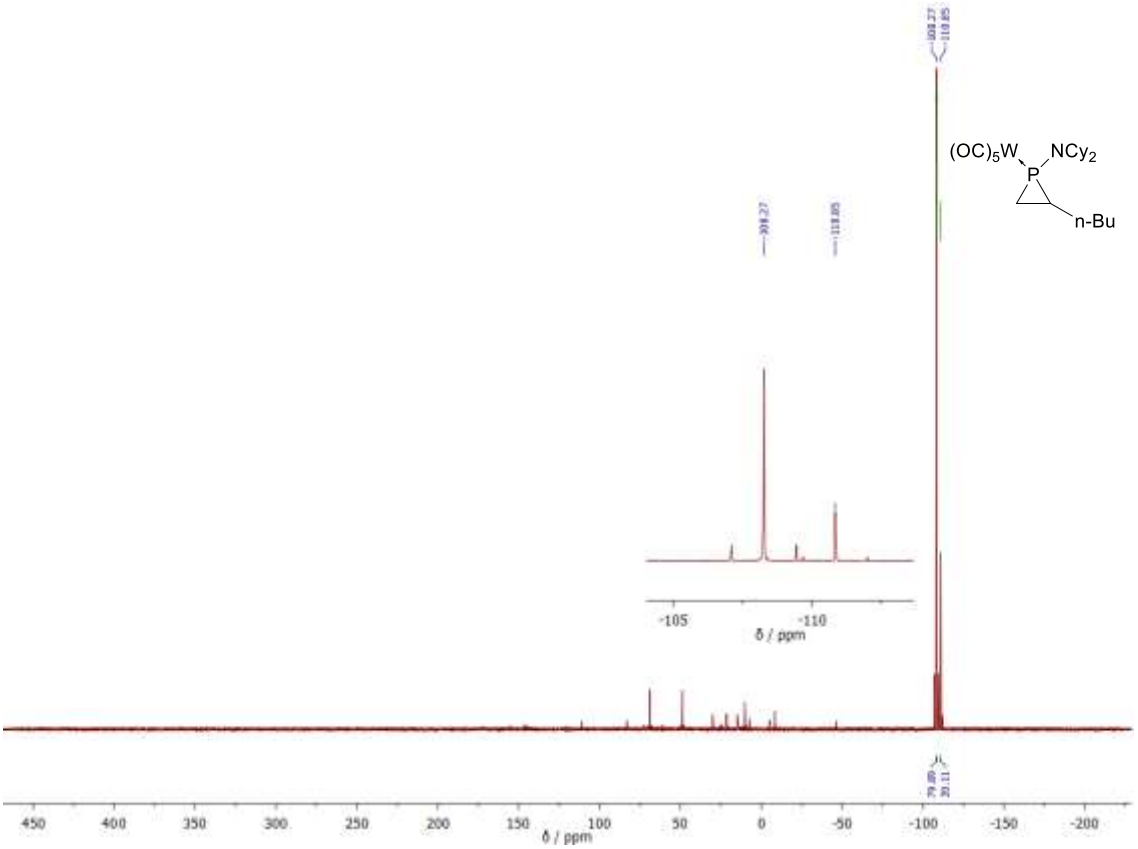


Figure S23. $^{31}P\{^{1}H\}$ NMR spectrum of **8b** in C_6D_6 at 121.5 MHz.

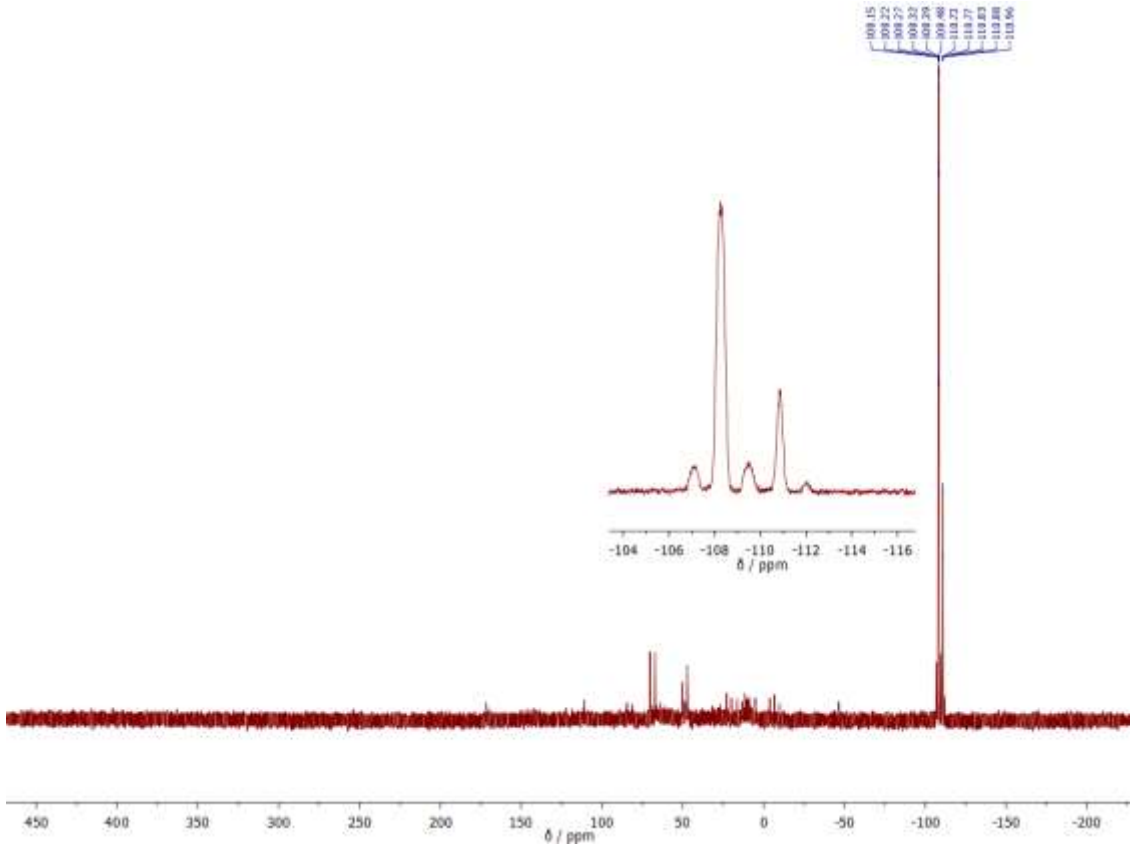


Figure S24. ^{31}P NMR spectrum of **8b** in C_6D_6 at 121.5 MHz.

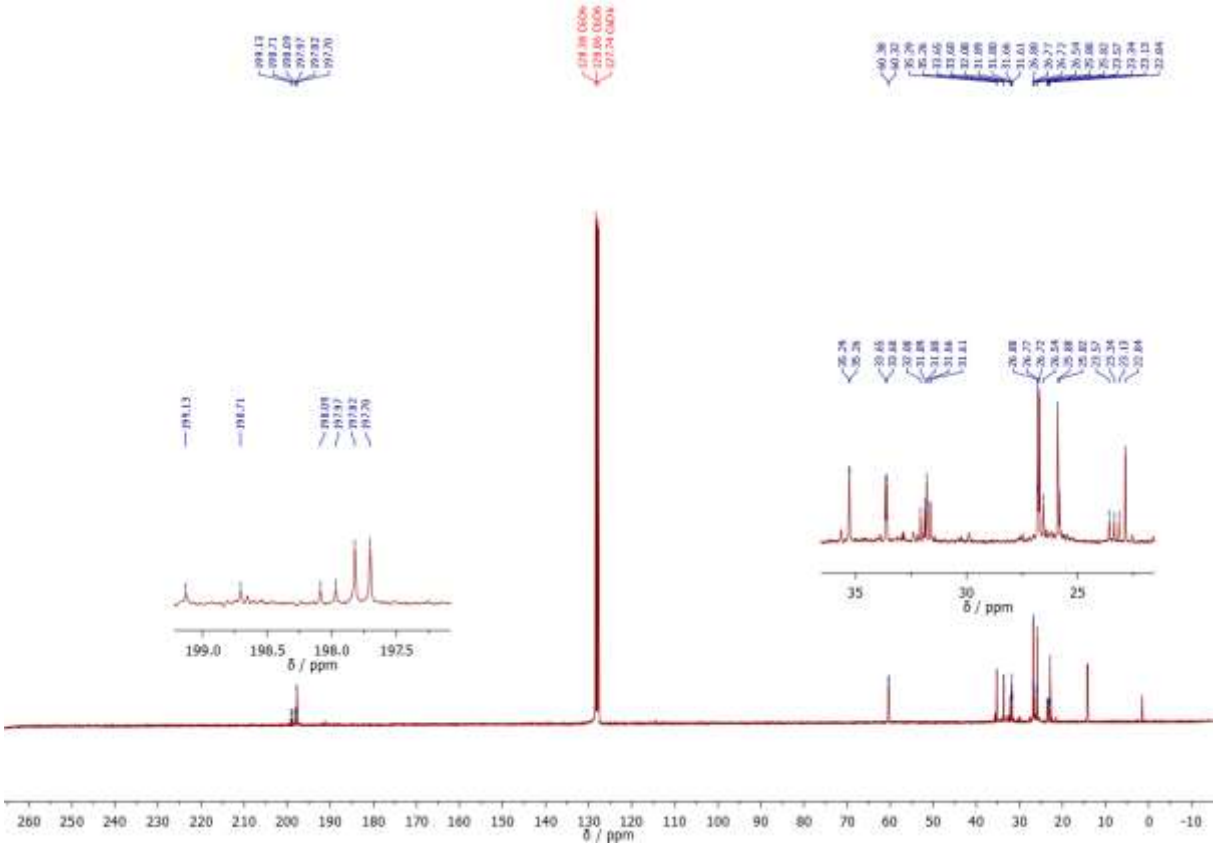


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of **8b** in C_6D_6 at 75.5 MHz.

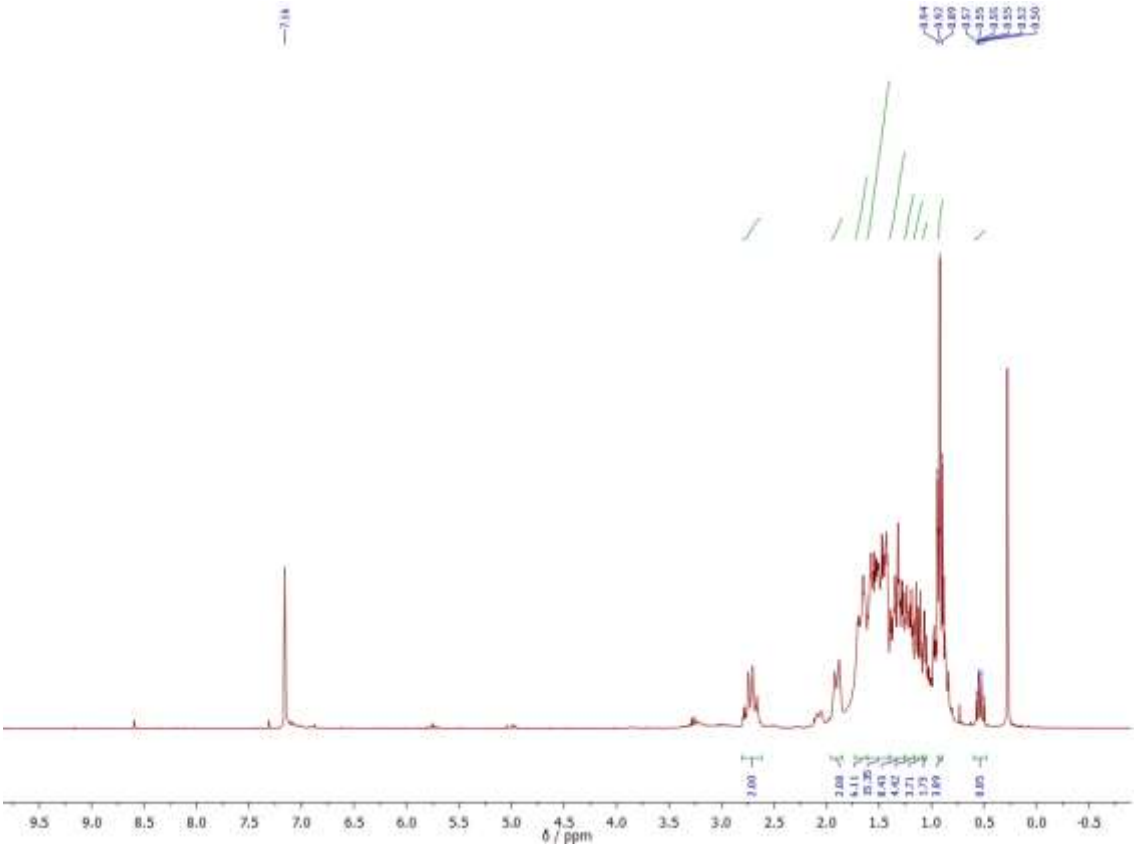


Figure S26. ^{1}H NMR spectrum of **8b** in C_6D_6 at 300.1 MHz.

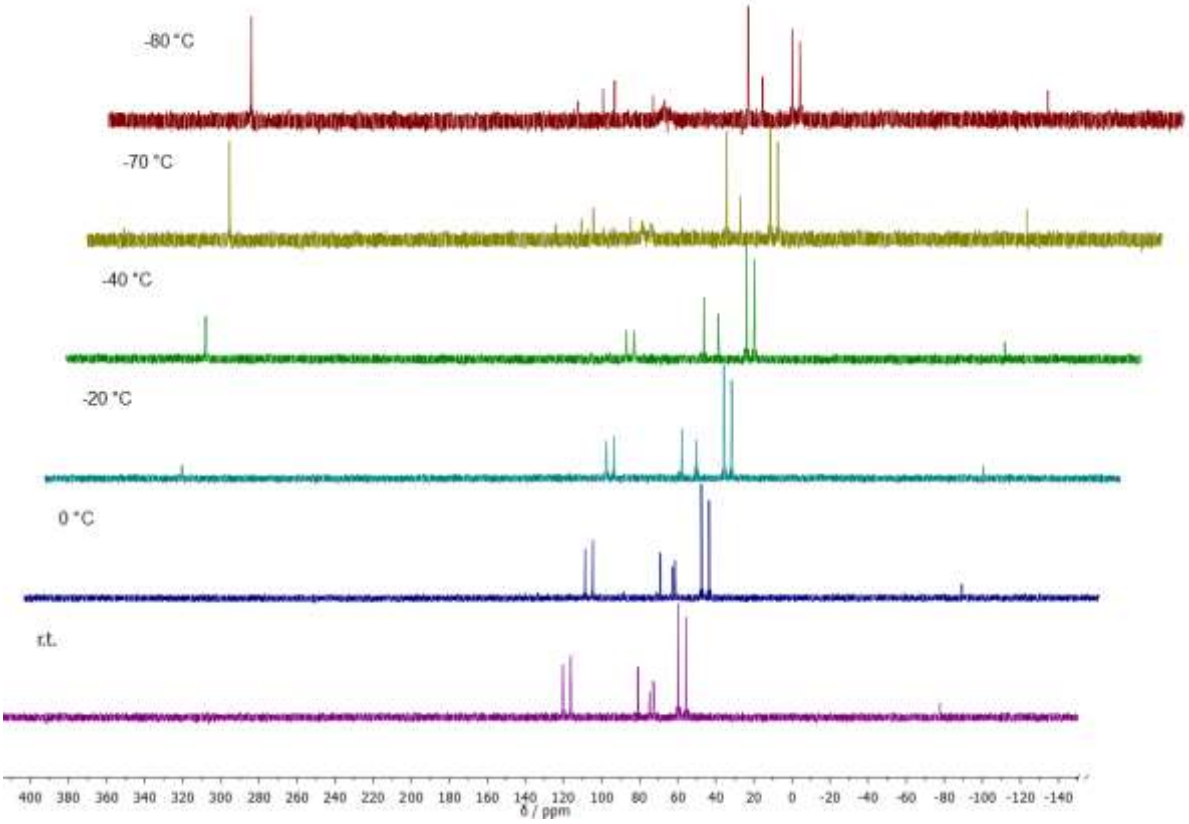


Figure S27: $^{31}P\{^{1}H\}$ NMR studies on the reaction of **1a** with ^{t}BuLi in THF at 121.1 MHz.

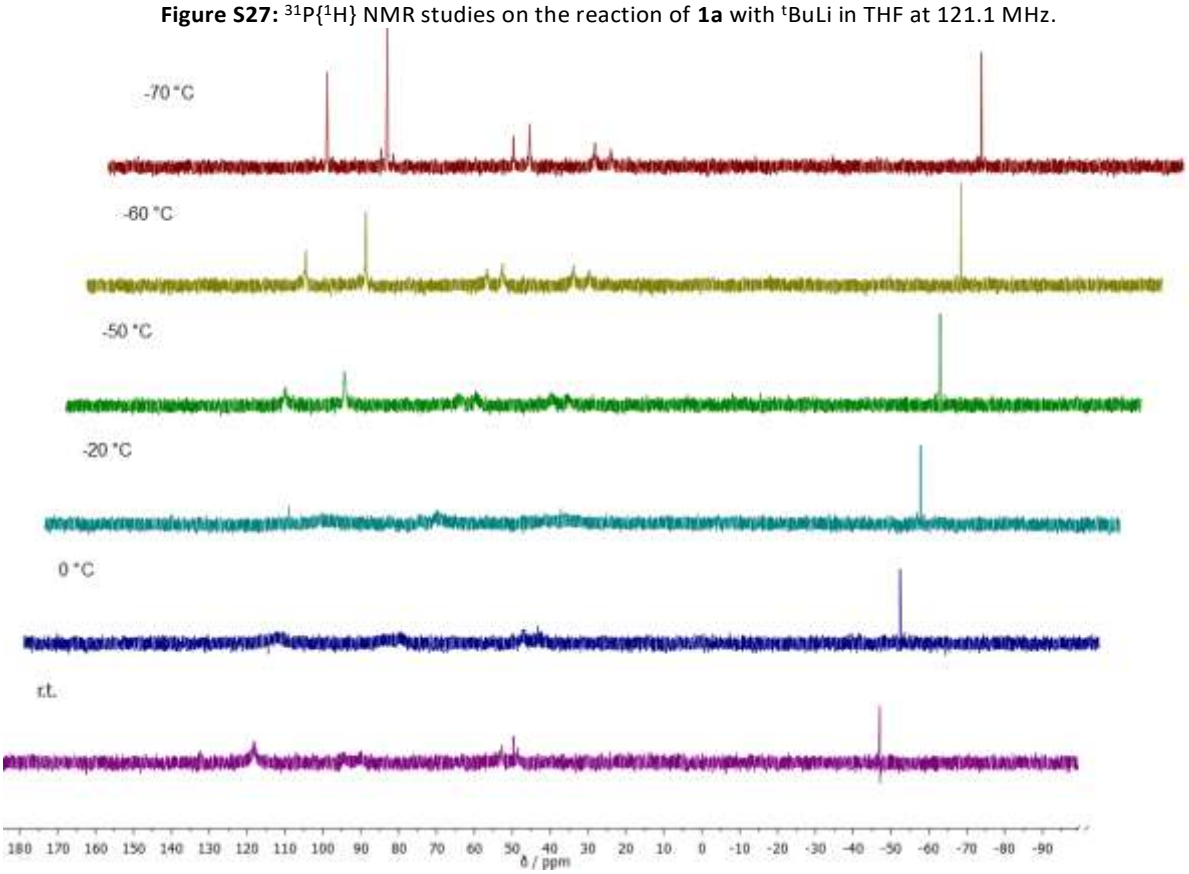


Figure S28: $^{31}P\{^{1}H\}$ NMR studies on the reaction of **1b** with ^{t}BuLi in THF at 121.1 MHz.

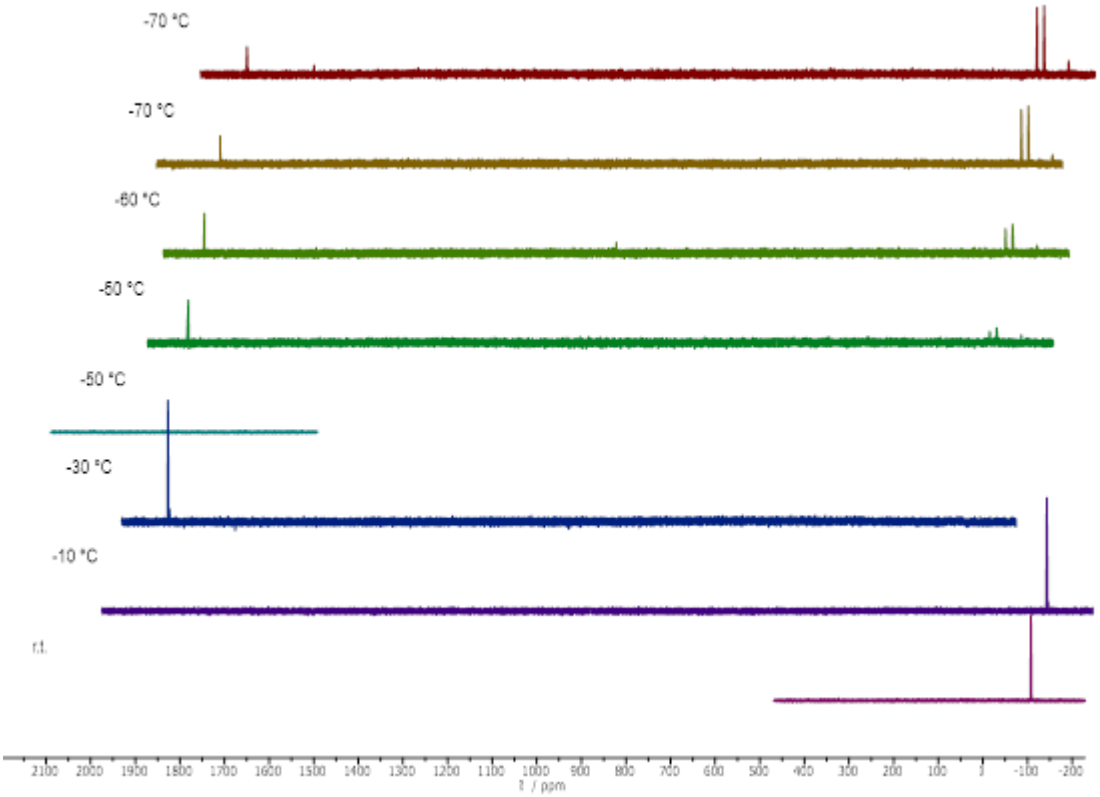
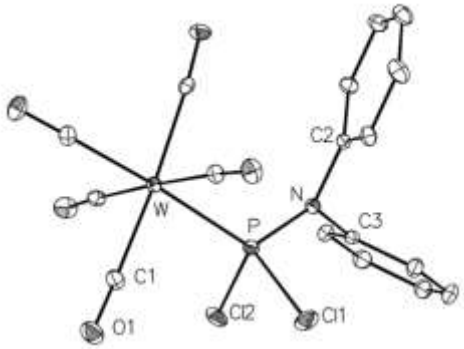


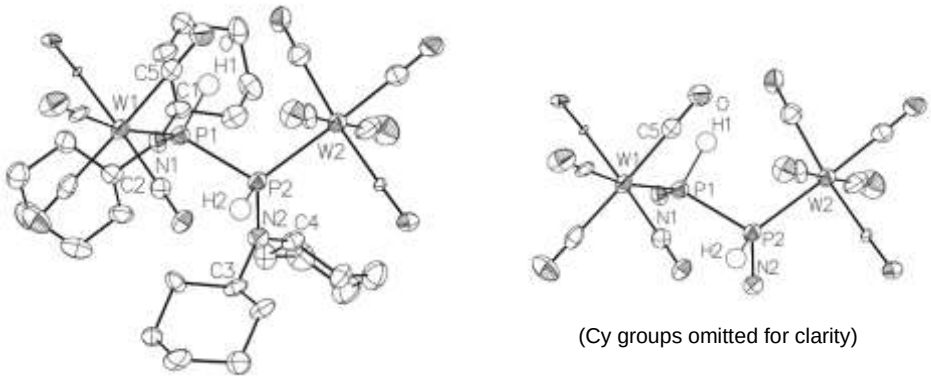
Figure S29: $^{31}P\{^{1}H\}$ NMR studies on the reaction of **1b** with ^{t}BuLi and 1-pentene in toluene at 121.1 MHz.

The signal appearing in the low-field ~1900 ppm is the expected product **8b** at -107.0 ppm "foldet" back into the spectrum due to analogues measurement of this region in the ^{31}P NMR *WIDE* spectrum. Digital measurement at -50 °C shows the lack of a real signal in that region.

Crystallographic Data



*Crystal Data for **1a**:* Suitable single crystals of **1a** were obtained from a concentrated diethylether solution at 4 °C. Data were collected with a Bruker D8-Venture diffractometer equipped with a low-temperature device at 123.0 K by using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97):$C_{17}H_{10}NO_5PCl_2W$, M_r = 593.98, crystal dimensions 0.21 × 0.14 × 0.12 mm^3, orthorhombic, space group $P2_12_12_1$, Z = 4, a = 9.085(5) Å, b = 13.306(8) Å, c = 16.740(11) Å, α = 90°, β = 90°, γ = 90°, V = 2024(2) Å^3, ρ_{calc} = 1.950 g cm^{-3}, μ = 6.078 mm^{-1}, transmission factors (min/max) 0.4745/0.7459, empirical absorption correction, 2θmax = 55.998°, no. of unique data 4866, R_{int} = 0.0499, R_1 (for I >2σ(I)) = 0.0257, wR_2 (for all data) = 0.0490, final R_1 = 0.0318, goodness of fit 1.026, ΔF (max/min) = 0.59 /−0.59 e Å^{-3}. CCDC 1919557.



(Cy groups omitted for clarity)

*Crystal Data for **cP-P**:* Suitable single crystals of **cP-P** were obtained from a concentrated diethylether solution at 4 °C. Data were collected with a Bruker Bruker APEX-II CCD diffractometer equipped with a low-temperature device at 100.0 K by using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97):$C_{34}H_{46}N_2O_8P_2W_2$, M_r = 1072.37, crystal dimensions 0.1 × 0.03 × 0.03 mm^3, triclinic, space group P-1, Z = 2, a = 11.5880(5) Å, b = 11.8529(5) Å, c = 16.5434(7) Å, α = 78.659(4)°, β = 82.857(3)°, γ = 62.420(4)°, V = 1973.28(16) Å^3, ρ_{calc} = 1.805 g cm^{-3}, μ = 5.960 mm^{-1}, transmission factors (min/max) 0.4373/0.7458, empirical absorption correction, 2θmax = 50.496°, no. of unique data 7150, R_{int} = 0.1254, R_1 (for I >2σ(I)) = 0.0843, wR_2 (for all data) = 0.2174, final R_1 = 0.1039, goodness of fit 1.078, ΔF (max/min) = 8.21 /−2.62 e Å^{-3}. CCDC 1919561. (Due to poor crystals the data/structure should only serve to confirm the connectivity.)

Supporting Information (Theory part)

1. **Computational details**
2. **Table S1.** TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in THF solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the relative electronic energies (ΔET and ΔEP) and Gibbs free-energies (ΔGT and ΔGP) at the TPSS-D3 and PW6B95-D3 levels.
3. **Table S2.** The TPSS-D3/def2-TZVP + COSMO optimized atomic Cartesian coordinates (in Å) in THF solution. Each structure is labeled by the specific name (See also **Table S1**), followed by the number of atoms, the total energy, and the detailed atomic coordinates (in double-column text list).
3. **Table S3.** The TPSS-D3/def2-TZVP + CPCM optimized atomic Cartesian coordinates (in Å) in THF solution. Each structure is labeled by the specific name (See also **Table S1**), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list). Ph: phenyl; Cy: cyclohexyl; ^{t}Bu: CMe_3; Anth: anthracenyl; Me: CH_3.
4. **Table S4.** GIAO TPSS-D3/def2-QZVP computed ^{31}P chemical shifts (in ppm) using TPSS-D3/def2-TZVP + COSMO optimized geometries (see also Table S2) , using the experimental ^{31}P NMR shift of **1a** [$W(CO)_5PCl_2NPh_2$)] at 108.6 ppm (computed shielding constant: 141.93ppm) as reference.

Computational Details: The quantum chemical DFT calculations have been performed with the TURBOMOLE 7.3 suite of programs[1] The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO(THF) level of theory, which combines the TPSS meta-GGA density functional[2] with the BJ-damped DFT-D3 dispersion correction[3, 4] and the def2-TZVP basis set,[5, 6] using the Conductor-like Screening Model (COSMO) continuum solvation model[7] for THF solvent (dielectric constant ε = 7.58 and solvent diameter R_{solv} = 3.18 Å). The density-fitting RI-J approach[5, 8, 9] is used to accelerate the geometry optimization and numerical harmonic frequency calculations[10] in solution. The optimized structures are characterized by frequency analysis to identify the nature of located stationary points (no imaginary frequency for true minima and only one imaginary frequency for transition state) and to provide thermal corrections (at 298.15 K and 1 atm) according to the modified ideal gas–rigid rotor–harmonic oscillator model.[11] This choice of dispersion-corrected meta-GGA functional makes the efficient exploration of all potential reaction paths possible.

The final solvation free energies in THF are computed with the COSMO-RS solvation model[12] (parameter file: BP_TZVP_C30_1601.ctd) using the COSMOtherm program package[13] on the above TPSS-D3 optimized structures, and corrected by +1.89 kcal·mol^{-1} to account for higher reference solute concentration of 1 mol·L^{-1} usually used in solution. To check the effects of the chosen DFT functional on the reaction energies and barriers, single-point calculations at the meta-GGA TPSS-D3[2] and hybrid-meta-GGA PW6B95-D3[14] levels are performed using a larger def2-QZVP basis set.[6, 15] The final reaction Gibbs free energies (ΔG) are determined from the electronic single-point energies plus TPSS-D3 thermal corrections and COSMO-RS solvation free energies. The computed reaction free energies from both DFT functionals are in good mutual agreement of 0.5 ± 1.7 kcal/mol (average and standard deviations, see Table S1 below). In our discussion, higher-level PW6B95-D3 Gibbs free energies (in kcal/mol, at 298.15 K and 1 mol/L standard state concentration) will be used in our discussion unless specified otherwise.

To help experimental ^{31}P NMR assignment, nuclear magnetic shielding constants for various P-containing complexes are also computed using the GIAO (Gauge Including Atomic Orbital) method at the TPSS/def2-QZVP level[16]; the final ^{31}P NMR chemical shifts are computed using the known ^{31}P NMR signal of the complex 1a [$W(CO)_5PCl_2NPh_2$)] at 108.6 ppm in C_6D_6 solution as reference.

References

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Table S1. TPSS-D3/def2-TZVP + COSMO computed imaginary frequency (ImF), zero-point energies (ZPE), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in THF solution; TPSS-D3/def2-QZVP and PW6B95-D3/def2-QZVP single-point energies (TPSS-D3 and PW6B95-D3); the relative electronic energies (ΔET and ΔEP) and Gibbs free-energies (ΔGT and ΔGP) at the TPSS-D3 and PW6B95-D3 levels.

Reactions	ImF cm^{-1}	ZPE kcal /mol	Hc kcal /mol	Gc kcal /mol	Hsol kcal /mol	Gsol kcal /mol	TPSS-D3 E_h	PW6B95-D3 E_h	ΔET kcal /mol	ΔEP kcal /mol	ΔGP kcal /mol	ΔGT kcal /mol
Solvation of LiCl in THF:												
0.5(**ClLit$_2$**)$_2$	0	148.98	158.63	131.35	-14.93	-11.42	-933.15460	-933.98397	0.0	0.0	0.0	0.0
0.5(**ClLit**)$_2$ + THF	0	147.39	156.83	116.34	-21.43	-11.55	-933.12925	-933.95752	15.9	16.6	1.5	0.8
ClLit$_3$ – THF	0	150.21	159.89	138.10	-17.84	-18.52	-933.14924	-933.97734	3.4	4.2	4.8	4.0
0.25(**ClLit**)$_4$ + THF	0	147.80	157.24	120.78	-15.96	-7.54	-933.14661	-933.97552	5.0	5.3	-1.9	-2.2
...and LiCl precipitation (computed as (LiCl)$_{28}$ nano-cluster) formation												
0.25 (**ClLit**)$_4$	0	75.75	81.50	66.17	-8.62	-6.54	-700.54275	-701.13331	0.0	0.0	0.0	0.0
LiCl + THF	0	73.88	79.66	53.84	-13.07	-5.34	-700.52549	-701.11603	10.8	10.9	-0.7	-0.7
*Solvation of Li/Cl phophinidenoid complex **2a** in THF:*												
2a$^-$ + **Lit$_4^+$**	0	435.94	470.24	368.50	-106.42	-93.13	-2892.40486	-2895.08882	0.0	0.0	0.0	0.0
2at$_3$ + THF	0	437.38	471.15	373.74	-43.56	-28.90	-2892.50589	-2895.18934	-63.4	-63.1	4.5	4.2
2at$_2$ + 2THF	0	434.91	468.87	356.84	-48.92	-28.19	-2892.48527	-2895.16635	-50.5	-48.7	2.7	0.9
5a + 0.25(**ClLit**)$_4$ + 3THF	0	433.79	467.00	338.94	-52.68	-25.03	-2892.45781	-2895.14266	-33.2	-33.8	3.3	3.9
*...with coordinating **12c4** ligand*												
2a$^-$ + **Lict$^+$** + THF	0	441.82	475.73	362.33	-118.75	-97.19	-3042.89552	-3045.72205	0.00	0.00	0.00	0.00
2at$_2$ + **12c4**	0	442.30	477.00	376.81	-52.17	-39.59	-3042.99138	-3045.81499	-60.16	-58.32	13.75	11.91
2ac + 2THF	0	441.60	475.70	364.49	-55.63	-34.03	-3042.98978	-3045.81763	-59.15	-59.98	3.44	4.27
5a.ClLic + 2THF	0	441.48	475.67	364.09	-64.67	-40.85	-3042.97456	-3045.79896	-49.60	-48.26	7.95	6.61
5a + **ClLic** + 2THF	0	440.06	474.05	347.57	-76.31	-49.53	-3042.93516	-3045.76245	-24.88	-25.35	7.54	8.02
2a-	0	142.17	159.71	108.03	-56.86	-49.17	-1954.49739	-1956.21135	0.00	0.00	0.00	0.00
5a + Cl^-	0	141.89	159.76	99.50	-88.90	-78.36	-1954.41409	-1956.12934	52.28	51.47	15.63	16.45
Lict$^+$ cation*: stable in THF*												
2**Lict$^+$** + 2THF	0	599.30	632.04	508.60	-123.77	-96.03	-2176.79624	-2179.02140	0.0	0.0	0.0	0.0
Lic$_2^+$ + **Lit$_4^+$**	0	599.72	634.22	535.12	-100.83	-89.11	-2176.83531	-2179.06618	-24.5	-28.1	5.3	8.9
Lic$^+$ + THF	0	226.26	238.58	186.33	-67.60	-52.70	-855.75738	-856.63151	0.0	0.0	0.0	0.0

Lict$^+$	0	227.60	240.28	199.69	-54.54	-47.01	-855.79427	-856.66849	-23.1	-23.2	-4.2	-4.1
*...but unstable with excess **12c4** or chloride Cl^-*												
Lict$^+$ + **12c4**	0	379.10	399.89	328.88	-72.48	-60.42	-1471.50809	-1473.00156	0.0	0.0	0.0	0.0
Lic$_2$ $^+$ + THF	0	378.00	399.43	329.26	-58.62	-46.16	-1471.53170	-1473.03093	-14.8	-18.4	-5.7	-2.1
Lict$^+$ + Cl^-	0	227.60	241.76	190.25	-121.40	-109.90	-1316.10487	-1317.31512	0.0	0.0	0.0	0.0
ClLic + THF	0	226.12	240.03	184.02	-46.93	-33.05	-1316.22782	-1317.43753	-77.2	-76.8	-8.1	-8.4
***Lic$_2$**$^+$ is more stable than **Lit$_4$**$^+$ and **Lict**$^+$, but still unstable with solvated chloride Cl^-*												
Lit$_4$ $^+$ + 2***12c4**	0	596.77	629.76	518.86	-85.42	-70.78	-2169.33511	-2171.54360	0.0	0.0	0.0	0.0
Lict$^+$ + 3THF + **12c4**	0	595.26	627.11	492.72	-94.50	-63.44	-2169.31966	-2171.52819	9.7	9.7	-11.0	-11.0
Lic$_2$ $^+$ + 4THF	0	594.16	626.65	493.09	-80.64	-49.18	-2169.34327	-2171.55756	-5.1	-8.8	-16.7	-13.1
Lic$_2$ $^+$ + Cl^-	0	305.95	325.17	265.21	-118.14	-108.05	-1699.23845	-1700.83535	0.0	0.0	0.0	0.0
ClLic + **12c4**	0	305.57	323.91	258.60	-57.53	-45.46	-1699.33779	-1700.92839	-62.3	-58.4	-2.4	-6.4
Initial Li/Cl exchange is highly exergonic												
1a + *t*Bu**Lic**	0	370.67	402.14	307.77	-54.93	-41.08	-3195.91389	-3198.76160	0.0	0.0	0.0	0.0
2ac.Cl*t*Bu	0	374.07	406.09	327.06	-47.31	-36.86	-3196.00851	-3198.85649	-59.4	-59.6	-37.9	-37.8
2ac + *t*BuCl	0	373.69	404.94	313.75	-48.46	-36.55	-3196.00105	-3198.85025	-54.7	-55.6	-45.1	-44.2
*Solvation of tBuLi: tetrameric (tBuLi)$_4$ in THF but neutral monomeric tBu**Lic** with excess **12c4***												
***t*BuLic** + **12c4**	0	378.18	399.24	328.80	-50.02	-38.40	-1396.92766	-1398.34536	0.0	0.0	0.0	0.0
0.25*(*t*BuLi)$_4$ + 2***12c4**	0	378.04	398.96	325.81	-39.61	-29.25	-1396.92914	-1398.34807	-0.9	-1.7	4.9	5.7
*t*Bu$^-$ + **Lic$_2$**$^+$	0	376.86	398.55	329.20	-109.40	-99.27	-1396.81878	-1398.24221	68.3	64.7	4.3	7.9
*Facile lithilation of **1a** with **tBuLic***												
1a + ***t*BuLic**	0	370.67	402.14	307.77	-54.93	-41.08	-3195.91389	-3198.76160	0.0	0.0	0.0	0.0
1a.*t*BuLic	0	372.65	405.26	323.99	-49.64	-38.86	-3195.99773	-3198.84309	-52.6	-51.2	-34.6	-36.1
2ac. Cl*t*Bu	0	374.07	406.09	327.06	-47.31	-36.86	-3196.00851	-3198.85649	-59.4	-59.6	-37.9	-37.8
2ac + *t*BuCl	0	373.69	404.94	313.75	-48.46	-36.55	-3196.00105	-3198.85025	-54.7	-55.6	-45.1	-44.2
***tBuLic** as potential hydride H^- source*												
5a + ***t*BuLic** + THF	0	440.63	473.64	363.16	-61.47	-41.47	-2507.92118	-2510.33722	0.0	0.0	0.0	0.0
TSh + THF	18i	441.23	474.30	379.07	-59.72	-41.75	-2507.96527	-2510.36821	-27.7	-19.5	-5.7	-13.9
2ah$^-$ + CH_2CMe_2 + **Lict**$^+$	0	441.49	474.39	364.29	-114.68	-97.57	-2507.93275	-2510.35093	-7.3	-8.6	-61.7	-60.3
…and tBuCl as potential H^+ source aided by Li^+												
2a$^-$ + *t*BuCl + **Lict**$^+$ - THF	0	373.92	404.97	311.59	-111.57	-99.71	-3195.90679	-3198.75467	0.0	0.0	0.0	0.0

2a^{-} + *t*BuClLic^{+}	0	374.25	405.16	311.93	-113.45	-97.00	-3195.89452	-3198.74147	7.7	8.3	9.4	8.9
TSp	181i	368.77	401.70	319.30	-52.77	-40.33	-3195.97750	-3198.81532	-44.4	-38.1	25.2	18.9
2aH + **ClLic** + *t*Bue	0	370.49	401.93	295.31	-68.40	-50.89	-3195.97773	-3198.82864	-44.5	-46.4	-13.9	-12.0
*Li^{+} aided H^{+} transfer from MeOH (or **oH**) to **2a**$^{-}$*												
Lict^{+} + MeOH	0	259.16	274.54	216.95	-66.45	-51.81	-971.59213	-972.58014	0.0	0.0	0.0	0.0
HoLic^{+} + THF	0	260.39	275.15	217.10	-71.88	-51.10	-971.58660	-972.57504	3.5	3.2	2.2	2.4
2a^{-} + **HoLic**$^{+}$	0	330.51	359.11	270.51	-121.40	-99.27	-2693.48013	-2695.94418	0.0	0.0	0.0	0.0
TS1	71i	326.33	355.67	280.65	-42.02	-32.30	-2693.58070	-2696.03851	-63.1	-59.2	16.0	12.1
2aH + MeOLic	0	326.79	355.95	265.75	-57.94	-43.71	-2693.53576	-2695.99766	-34.9	-33.6	17.2	15.9
TS2	0	328.71	358.02	283.38	-43.79	-34.02	-2693.58324	-2696.03882	-64.7	-59.4	16.8	11.5
3a + **ClLic**	0	328.57	357.39	268.78	-63.06	-48.71	-2693.59766	-2696.06126	-73.8	-73.5	-24.6	-24.9
*…Alternative mechanism via MeOH trapping of **5a** is kinetically 4.7kcal/mol less favorable (**TS3**).*												
2a^{-} + **Lict**$^{+}$ + THF	0	441.82	475.73	362.33	-118.75	-97.19	-3042.89552	-3045.72205	0.00	0.00	0.00	0.00
5a + **ClLic** + 2THF	0	440.06	474.05	347.57	-76.31	-49.53	-3042.93516	-3045.76245	-24.88	-25.35	7.54	8.02
5a + 3MeOH	0	236.57	261.06	160.72	-57.76	-29.88	-1841.49707	-1843.21767	0.0	0.0	0.0	0.0
TS3a + MeOH	731i	236.03	259.87	183.99	-39.17	-24.18	-1841.51342	-1843.22281	-10.3	-3.2	22.0	14.9
TS31	307i	238.68	262.11	198.54	-28.66	-21.00	-1841.54865	-1843.25704	-32.4	-24.7	16.3	8.7
TS32	198i	238.52	261.83	198.40	-29.51	-21.50	-1841.54791	-1843.25574	-31.9	-23.9	16.5	8.5
TS3	273i	238.39	261.72	198.39	-29.63	-21.57	-1841.54776	-1843.25545	-31.8	-23.7	16.6	8.5
3a + 2MeOH	0	237.62	261.61	173.89	-47.28	-26.26	-1841.56941	-1843.28924	-45.4	-44.9	-30.0	-30.5
…but trapping of electrophilic **5a** with PhCCPh is *kinetically 1.3 kcal/mol more facile (**TS4**) than trapping of **2a**$^{-}$ with MeOH.*												
5a + PhCCPh	0	262.19	285.49	207.72	-38.60	-26.90	-2033.92024	-2035.89713	0.0	0.0	0.0	0.0
TS4	-136	260.38	284.61	219.57	-32.92	-24.12	-2033.93014	-2035.90049	-6.2	-2.1	10.6	6.5
5a	0	262.21	286.05	222.27	-33.07	-24.42	-2033.99088	-2035.96810	-44.3	-44.5	-29.4	-29.2
…trapping of **5a** with more nucleophilic C_2H_4 (**TS5**) is more facile												
5a + C_2H_4	0	173.71	192.59	127.66	-25.02	-16.63	-1572.74510	-1574.20656	0.0	0.0	0.0	0.0
TS5	91i	174.40	192.92	139.36	-23.30	-16.55	-1572.75588	-1574.21317	-6.8	-4.1	5.7	3.1
7a	0	176.01	194.00	141.75	-23.26	-16.70	-1572.79760	-1574.26179	-32.9	-34.7	-22.5	-20.8
*… and even more facile with $MeNH_2$ (or **nH**)*												
5a + $MeNH_2$	0	181.46	200.58	134.13	-27.41	-18.08	-1590.02521	-1591.50134	0.00	0.00	0.00	0.00
5a.nH	0	184.53	203.09	149.66	-37.99	-24.37	-1590.05333	-1591.52886	-17.65	-17.27	-9.92	-10.30

5a.nH + **nH**	0	224.10	245.39	174.85	-43.36	-26.97	-1685.97506	-1687.54749	-17.65	-17.27	-9.92	-10.30
TSn2	869i	222.35	243.57	184.64	-43.85	-29.20	-1685.98678	-1687.55373	-25.00	-21.18	-8.16	-11.98
4a + $MeNH_2$	0	221.60	243.10	171.98	-31.01	-20.19	-1686.01140	-1687.58455	-40.46	-40.52	-29.26	-29.20

Table S2. The TPSS-D3/def2-TZVP + COSMO optimized atomic Cartesian coordinates (in Å) in THF solution. Each structure is labeled by the specific name (See also **Table S1**), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list). Ph: phenyl; Cy: cyclohexyl. **9** as possible diphosphane (complex) side products.

12c4 12-crown-4 ligand *c*-$(C_2H_4O)_4$
28
Energy = -615.6885361593

O	-0.2904976	-2.3428677	-0.6138394
O	0.5660503	1.0894427	1.4833774
O	-1.6362858	-0.8171597	1.4764910
O	1.9126711	-0.4335819	-0.6082963
C	0.2034286	0.3424507	2.6451410
C	1.0516711	-2.7294689	-0.3171562
C	-1.2629300	-2.1846869	1.6515247
C	-1.2636436	-2.8704844	0.2940288
C	-1.2826404	0.0265202	2.5780238
C	1.9735901	1.1138102	1.2223787
C	2.0014511	-1.7932060	-1.0488531
C	2.5112027	-0.1963172	0.6667682
H	0.4057632	0.9294603	3.5561346
H	0.7907935	-0.5828911	2.7119333
H	-0.2736007	-2.2609029	2.1218873
H	1.2347811	-3.7637199	-0.6520059
H	1.2361152	-2.6963274	0.7647699
H	-1.1149966	-3.9520384	0.4389816
H	-1.8471167	0.9514803	2.4279688
H	-2.2305406	-2.7138632	-0.1934584
H	2.2994796	-1.0242140	1.3563200
H	-1.9833273	-2.6951898	2.3115399
H	-1.5968216	-0.4249572	3.5319892
H	1.7463066	-1.7710465	-2.1126510
H	2.5339905	1.3751311	2.1335568
H	2.1181659	1.9085982	0.4846068
H	3.0304624	-2.1705987	-0.9424640
H	3.6065127	-0.1225194	0.5663079

1a $[W(CO)_5]PCl_2NPh_2$
37
Energy = -2414.610287300

P	1.8419615	0.6414101	-0.3873341
Cl	3.7230221	1.6042948	-0.3557328
N	0.7111282	1.8388381	-0.0742397
C	0.3480043	2.8773545	-1.0183503
C	-0.6892612	2.6499591	-1.9229262
C	1.0162947	4.1020516	-0.9854731
C	-1.0596015	3.6615681	-2.8086143
H	-1.1931225	1.6890933	-1.9292704
C	0.6426265	5.1078542	-1.8765069
H	1.8153120	4.2610040	-0.2685109
C	-0.3931511	4.8886114	-2.7876879
H	-1.8686027	3.4901394	-3.5122811
H	1.1610677	6.0618857	-1.8584995
H	-0.6824079	5.6746927	-3.4789710
C	0.3241250	2.0588126	1.2986873
C	-1.0235785	2.2903640	1.5898648
C	1.2758458	2.0413746	2.3218442
C	-1.4153049	2.4851184	2.9113750
H	-1.7523828	2.3103809	0.7860706
C	0.8701011	2.2124267	3.6466821
H	2.3271536	1.9185653	2.0834038
C	-0.4736983	2.4342184	3.9442308
H	-2.4629629	2.6609032	3.1368678
H	1.6113204	2.1877524	4.4397898
H	-0.7881754	2.5749756	4.9738114
W	1.8135999	-1.5392660	0.7962428
C	3.3897190	-2.0731573	-0.4211887
O	4.2698067	-2.3873058	-1.0979311
C	3.1271138	-0.8423081	2.2288182
O	3.8511181	-0.4465302	3.0350281
C	1.8491137	-3.3980185	1.6162962
O	1.8744065	-4.4628099	2.0678038
C	0.2243200	-1.0941017	2.0446316
O	-0.6668868	-0.9256982	2.7553257
C	0.4543047	-2.1769793	-0.6178014
O	-0.3181369	-2.5248931	-1.4009680
Cl	1.6758839	0.4650518	-2.4302917

1b $[W(CO)_5]PCl_2NCy_2$
49
Energy = -2421.864473646

P	1.7816711	0.7083713	0.5979806
Cl	1.8074204	1.8186222	2.3405499
N	0.8646772	1.5971796	-0.4447616
W	1.3571047	-1.7287261	1.0375797
C	3.2622925	-1.8337666	1.8314916
O	4.3145450	-1.9193381	2.2945488
C	0.6234393	-1.2432850	2.9053230
O	0.2101097	-0.9888732	3.9512674
C	1.0945106	-3.6921625	1.4633836
O	0.9437306	-4.8133026	1.7098316
C	-0.5777034	-1.6855555	0.3338237
O	-1.6755987	-1.7012435	-0.0253026
C	2.0929812	-2.2130539	-0.8281279
O	2.5020999	-2.4929714	-1.8709766
Cl	3.8287450	0.9960233	0.0605103
C	0.4346364	0.8546736	-1.6764975

C	-1.0457214	1.0868392	-1.9944298
C	1.3300349	1.1614112	-2.8839996
H	0.5562191	-0.2079213	-1.4337162
C	-1.4603461	0.2228851	-3.1953788
H	-1.2130488	2.1432875	-2.2408506
H	-1.6547742	0.8532361	-1.1159575
C	0.9019641	0.3127372	-4.0909512
H	1.2504129	2.2261277	-3.1410469
H	2.3758208	0.9651748	-2.6253403
C	-0.5824573	0.5149525	-4.4191815
H	-2.5163107	0.4014960	-3.4262791
H	-1.3678245	-0.8381516	-2.9254793
H	1.5264716	0.5647930	-4.9553029
H	1.0819222	-0.7473881	-3.8656405
H	-0.8744380	-0.1306414	-5.2554248
H	-0.7449136	1.5532745	-4.7414804
C	0.7168006	3.0884915	-0.5226860
C	-0.3823151	3.5936949	0.4226583
C	2.0234370	3.8787705	-0.3860920
H	0.3614779	3.2596492	-1.5448360
C	-0.6283213	5.0918307	0.1958813
H	-0.0845133	3.4245166	1.4613746
H	-1.2977252	3.0187515	0.2474549
C	1.7484379	5.3753072	-0.6015654
H	2.4584123	3.7309466	0.6068922
H	2.7501454	3.5138811	-1.1183362
C	0.6695801	5.8923233	0.3582083
H	-1.3930633	5.4478069	0.8954895
H	-1.0241243	5.2476689	-0.8181804
H	2.6805878	5.9368440	-0.4730042
H	1.4178668	5.5378278	-1.6375707
H	0.4838704	6.9580196	0.1806271
H	1.0279906	5.7963212	1.3928762

2ac $[W(CO)_5]PClNPh_2Li$(**12c4**)

65

Energy = -2577.681892130

P	0.2727039	0.2706366	-0.1909634
Cl	0.5068613	0.7371932	-2.3649055
N	0.5075360	1.8042256	0.5585547
C	1.7424523	2.4888708	0.7084818
C	2.7774248	2.3021832	-0.2173834
C	1.9528865	3.3378613	1.8070152
C	4.0117034	2.9206707	-0.0257435
H	2.5999459	1.6858249	-1.0895871
C	3.1863822	3.9592284	1.9845655
H	1.1574200	3.4903920	2.5293965
C	4.2277052	3.7493370	1.0762402
H	4.8049537	2.7560208	-0.7500228
H	3.3381141	4.5999877	2.8491107
H	5.1904242	4.2301381	1.2237240
C	-0.6643542	2.4437292	1.0870178
C	-1.4077473	1.8036922	2.0835841
C	-1.0576344	3.7049418	0.6261222
C	-2.5419848	2.4193851	2.6133609
H	-1.0782856	0.8354472	2.4495718
C	-2.1917748	4.3154045	1.1574220
H	-0.4701509	4.1964357	-0.1435911
C	-2.9367989	3.6766202	2.1530455
H	-3.1078404	1.9197937	3.3947869
H	-2.4975192	5.2915730	0.7918618
H	-3.8165704	4.1586860	2.5698054
W	2.0854966	-1.4543971	0.4391658
C	3.3789397	-0.8442881	-1.0462403
O	4.0983412	-0.5007807	-1.8849156
C	3.0409806	-0.2285507	1.7995681
O	3.6067072	0.3852875	2.5999304
C	3.3042621	-2.9495721	1.0173296
O	4.0053342	-3.8179084	1.3565212
C	0.7125722	-1.9415881	1.8795540
O	-0.0791580	-2.1913029	2.6914042
C	1.1958934	-2.7369526	-0.8906201
O	0.7344941	-3.4953419	-1.6378721
Li	-2.2419195	-0.1964258	-0.3636792
O	-3.3971774	1.4676092	-0.9900590
O	-2.2019486	-2.3620321	-0.3719729
O	-3.8337925	-0.4784374	0.8713493
C	-3.0177680	1.7082719	-2.3556980
C	-4.7519055	1.0241339	-0.8023997
C	-3.1002212	-2.7288748	0.6942000
C	-2.5932396	-2.8904013	-1.6585550
C	-4.8289132	0.5457308	0.6352901
C	-4.3198422	-1.8250191	0.7012251
H	-3.6900748	2.4387753	-2.8225046
H	-2.0128762	2.1267400	-2.2835463
H	-5.4521761	1.8530605	-0.9734628
H	-4.9865818	0.2091808	-1.4990612
H	-2.5286351	-2.5982816	1.6161089
H	-3.4004006	-3.7793749	0.6059425
H	-2.1004755	-3.8550797	-1.8244245
H	-3.6799585	-3.0317000	-1.6817304
H	-4.5779259	1.3632667	1.3137251
H	-5.8284021	0.1661031	0.8721159
H	-4.9879001	-2.0866493	1.5320319
H	-4.8786079	-1.9045443	-0.2409976
O	-2.6585902	-0.6201317	-2.2271841
C	-2.1936368	-1.8821242	-2.7212293
H	-2.6760147	-2.1341596	-3.6729763
H	-1.1087606	-1.8319227	-2.8632169
C	-2.9832582	0.4049860	-3.1698849
H	-3.9477034	0.1701543	-3.6393455
H	-2.2151282	0.4806919	-3.9477147

2ahH $[W(CO)_5]PH_2NPh_2$

37

Energy = -1495.272228598

P	2.0449860	0.7943701	-0.2425410
H	3.2895875	1.4290696	0.0069550
H	2.0635675	0.9156764	-1.6420015
N	0.8671098	2.0003975	0.0763206
C	0.3653502	2.8381568	-0.9725328
C	-0.1976312	2.2706787	-2.1204531
C	0.4361504	4.2302747	-0.8448097
C	-0.6674298	3.0930823	-3.1447334
H	-0.2805925	1.1906490	-2.2040585
C	-0.0538129	5.0459271	-1.8631038
H	0.8708529	4.6632929	0.0509038
C	-0.6005198	4.4818746	-3.0189461
H	-1.1024526	2.6452604	-4.0334215
H	0.0042548	6.1255060	-1.7578622
H	-0.9751806	5.1203280	-3.8133200
C	0.4881332	2.2506192	1.4211085
C	-0.8103937	2.6901481	1.7189974
C	1.3912656	2.0115409	2.4652939
C	-1.1944694	2.8677335	3.0441075
H	-1.5122051	2.8764444	0.9123846
C	0.9894596	2.1704122	3.7921427
H	2.4144365	1.7198717	2.2465336
C	-0.3035314	2.5982877	4.0886985
H	-2.2046809	3.2014466	3.2636526
H	1.6983316	1.9703832	4.5903328
H	-0.6153479	2.7262927	5.1207470
W	1.7347579	-1.5206418	0.6713705
C	3.3408409	-2.0926722	-0.4791203
O	4.2408901	-2.4303415	-1.1220929
C	2.9904475	-1.0818273	2.2443518
O	3.6901838	-0.8180218	3.1257004
C	1.5287244	-3.4394389	1.2983166
O	1.4185540	-4.5399054	1.6452337
C	0.1076474	-1.0055422	1.8437138
O	-0.8110405	-0.7793580	2.5028446
C	0.4639315	-1.8385463	-0.9152411
O	-0.2513593	-1.9884227	-1.8115312

2ah⁻ $[W(CO)_5]PHNPh_2^-$

36

Energy = -1494.785485374

P	1.3435755	-0.7865603	-0.5645346
H	2.0130784	-0.8472208	-1.8119247
N	2.7605891	-0.0676524	0.2687701
C	2.5957188	0.4018009	1.5755251
C	1.3858874	0.1987740	2.2710825
C	3.6146669	1.1362007	2.2213075
C	1.2067073	0.7110436	3.5548009
H	0.5917982	-0.3764897	1.8054817
C	3.4255835	1.6352798	3.5054159
H	4.5517506	1.3158698	1.7043528
C	2.2213347	1.4296854	4.1890911
H	0.2642274	0.5314898	4.0664151
H	4.2279663	2.1996429	3.9748181
H	2.0806194	1.8202721	5.1927931
C	4.0699057	-0.3603198	-0.2087429
C	4.4556486	0.0613914	-1.4879997
C	4.9737402	-1.1022367	0.5654124
C	5.7131865	-0.2688931	-1.9902736
H	3.7610702	0.6465411	-2.0833829
C	6.2332325	-1.4220832	0.0627662
H	4.6790622	-1.4289930	1.5566321
C	6.6088194	-1.0132455	-1.2189068
H	5.9962118	0.0634797	-2.9856640
H	6.9180005	-2.0083598	0.6702055
H	7.5882747	-1.2710655	-1.6119406
W	1.2255483	-3.3689970	0.0341281
C	2.9515387	-3.5327726	-1.0750715
O	3.9047837	-3.6189623	-1.7306905
C	2.3031921	-3.1328999	1.7677621
O	2.9043452	-3.0280106	2.7558216
C	1.0946703	-5.3385646	0.3648773
O	1.0251436	-6.4953122	0.5401536
C	-0.4815462	-2.9410841	1.0797635
O	-1.4472479	-2.6649418	1.6677521
C	0.1339336	-3.5128242	-1.6949857
O	-0.4876103	-3.5795557	-2.6758391

2aH $[W(CO)_5]PClHNPh_2$

37

Energy = -1954.945218471

P	2.0290385	1.1162317	0.9539504
Cl	1.6107200	2.1876359	2.7403260
N	1.2854392	1.9561126	-0.2969038
C	1.7152395	3.2446942	-0.7624328
C	2.6201131	4.0276324	-0.0321268
C	1.2255805	3.7228667	-1.9866174
C	3.0449479	5.2565402	-0.5374442
H	2.9745109	3.7082417	0.9407303
C	1.6526926	4.9549583	-2.4768332
H	0.5165205	3.1309840	-2.5542000
C	2.5678348	5.7285722	-1.7601000
H	3.7434180	5.8512724	0.0444667
H	1.2667197	5.3061337	-3.4292745
H	2.8961963	6.6891629	-2.1447802
C	-0.0219925	1.4968375	-0.7285829
C	-0.1310183	0.6639198	-1.8422302
C	-1.1584552	1.9201384	-0.0381084

C	-1.3925703	0.2479660	-2.2677550
H	0.7639304	0.3600570	-2.3730863
C	-2.4168804	1.4977446	-0.4667534
H	-1.0524634	2.5695292	0.8249544
C	-2.5344584	0.6645074	-1.5811814
H	-1.4800972	-0.4036603	-3.1317866
H	-3.3031104	1.8162722	0.0733779
H	-3.5152742	0.3367875	-1.9119057
W	1.7888737	-1.3511454	1.1797399
C	1.3677951	-1.1771871	3.1953007
O	1.1362393	-1.0996233	4.3218781
C	-0.2498555	-1.3982294	0.8209420
O	-1.3887282	-1.5010242	0.6774619
C	1.7608216	-3.3721625	1.3529328
O	1.7549909	-4.5257179	1.4494581
C	2.2257932	-1.5517997	-0.8232976
O	2.4879163	-1.6916451	-1.9398845
C	3.7969557	-1.3772874	1.6252089
O	4.9208477	-1.4085197	1.8909030
H	3.3274594	1.6263422	0.7956589

2at$_2$ [W(CO)$_5$]PClNPh$_2$Li(THF)$_2$

63

Energy = -2427.176632048

P	0.4895927	0.6677786	0.2865176
Cl	1.1749677	0.3032414	-1.9580474
N	0.0717975	-0.9009352	0.8094211
C	-1.1915371	-1.5394272	0.5858135
C	-1.8200275	-1.4501100	-0.6569369
C	-1.7994031	-2.2457944	1.6300844
C	-3.0738458	-2.0324331	-0.8448682
H	-1.3142420	-0.9371949	-1.4671401
C	-3.0453418	-2.8351203	1.4328458
H	-1.3008754	-2.3142764	2.5923046
C	-3.6917866	-2.7236884	0.1980859
H	-3.5615644	-1.9508371	-1.8120133
H	-3.5208250	-3.3690556	2.2507706
H	-4.6683048	-3.1757904	0.0511006
C	1.1181566	-1.7266844	1.3424496
C	1.9953480	-1.2120101	2.3052873
C	1.2755747	-3.0450150	0.8971226
C	3.0328097	-2.0010165	2.7993563
H	1.8447429	-0.2010209	2.6705672
C	2.3102190	-3.8312744	1.4023856
H	0.5907131	-3.4445089	0.1558424
C	3.1964557	-3.3131159	2.3495284
H	3.7018276	-1.5944414	3.5526256
H	2.4284650	-4.8504526	1.0454457
H	4.0006225	-3.9292674	2.7406995
W	-1.4208392	2.3513674	0.1588882
C	-2.2513466	1.5817409	-1.5668663
O	-2.7166695	1.1863627	-2.5482321
C	-2.7039313	1.2172640	1.3133483
O	-3.4572295	0.6357342	1.9687245
C	-2.7716615	3.8539922	0.1799453
O	-3.5490641	4.7200956	0.1949846
C	-0.5532212	3.1197255	1.8539856
O	-0.0567979	3.5624691	2.8038992
C	-0.1816659	3.4756833	-1.0285044
O	0.4926794	4.1224219	-1.7143098
Li	2.9333177	0.6203377	-0.3783717
O	4.2193950	-0.7441921	-0.5521802
O	3.6888965	2.2245925	0.3351589
C	4.0765111	-1.9379305	-1.3863393
C	5.4860557	-0.7895395	0.1679143
C	3.5688406	2.4519207	1.7757199
C	3.7366097	3.5082146	-0.3610437
C	5.2294066	-2.8526777	-0.9858508
H	3.0888592	-2.3603632	-1.1923196
H	4.1415512	-1.6224040	-2.4330692
C	6.3108971	-1.8517883	-0.5482476
H	5.2791636	-1.0681777	1.2079688
H	5.9168533	0.2137753	0.1349618
C	3.7375357	3.9557437	1.9737092
H	2.5753199	2.1046332	2.0806721
H	4.3352010	1.8512078	2.2731230
C	3.2137215	4.5240096	0.6456769
H	3.1275006	3.4177704	-1.2631080
H	4.7778869	3.7084106	-0.6397374
H	4.9345985	-3.4853935	-0.1430427
H	5.5479078	-3.4941781	-1.8110210
H	7.0666431	-2.2958090	0.1044815
H	6.8123062	-1.4212556	-1.4216191
H	3.1799343	4.3155681	2.8415806
H	4.7938471	4.2106348	2.1074945
H	2.1197901	4.5374763	0.6403783
H	3.5756837	5.5340748	0.4397217

2at$_3$ [W(CO)$_5$]PClNPh$_2$Li(THF)$_3$

76

Energy = -2659.786264299

P	0.2039937	0.1376733	-0.8482015
Cl	0.5905125	0.9753382	-2.8982338
N	-0.0084192	-1.5428209	-1.1500824
C	-1.1976799	-2.1014445	-1.7301812
C	-1.6607835	-1.6733565	-2.9773882
C	-1.8750853	-3.1169724	-1.0444670
C	-2.7946573	-2.2654751	-3.5356916
H	-1.1309046	-0.8844247	-3.4981945
C	-3.0043831	-3.7045806	-1.6085609
H	-1.5090369	-3.4365389	-0.0734603
C	-3.4657154	-3.2844607	-2.8594705

H	-3.1513477	-1.9277245	-4.5045642
H	-3.5306757	-4.4852500	-1.0661216
H	-4.3471790	-3.7432925	-3.2979616
C	1.0530556	-2.4693126	-0.9209215
C	1.8684272	-2.3442042	0.2112268
C	1.2618238	-3.5462429	-1.7959168
C	2.8823520	-3.2678739	0.4563555
H	1.6797532	-1.5349396	0.9073252
C	2.2711861	-4.4728055	-1.5387464
H	0.6306230	-3.6548395	-2.6718588
C	3.0900744	-4.3398167	-0.4144673
H	3.4941654	-3.1640975	1.3486723
H	2.4221972	-5.2989089	-2.2280913
H	3.8729692	-5.0656141	-0.2156704
W	-1.9658210	1.1226387	0.1265830
C	-3.4094841	-0.0020794	-0.8407045
O	-4.3386619	-0.5258879	-1.2857882
C	-1.6856670	-0.4090574	1.4644690
O	-1.4867261	-1.2967129	2.1837647
C	-3.5218300	1.9141529	1.1314042
O	-4.4171145	2.3751208	1.7180484
C	-0.8370648	2.3976549	1.2561636
O	-0.2924837	3.1557136	1.9498487
C	-2.0657770	2.4890856	-1.4105101
O	-2.1137425	3.2304420	-2.2970775
Li	2.6670659	0.8913247	-0.4957645
O	4.0137187	-0.1028878	-1.4648507
O	2.9817953	2.7905001	-0.8943622
O	3.0611085	0.8968722	1.4163608
C	4.0180474	-0.4470605	-2.8757504
C	5.1206652	-0.7901988	-0.8103581
C	2.3876079	3.8560711	-0.1147037
C	3.1481368	3.3297776	-2.2337815
C	2.2449868	0.5399876	2.5578875
C	4.2913065	1.4294509	1.9666811
C	4.5776196	-1.8600541	-2.9123634
H	2.9902179	-0.3509526	-3.2287906
H	4.6623605	0.2607118	-3.4161595
C	5.6688602	-1.8037123	-1.8286821
H	4.7114183	-1.2674834	0.0826363
H	5.8691529	-0.0472340	-0.5166264
C	1.3303059	4.4403932	-1.0435057
H	1.9988688	3.4098819	0.7996643
H	3.1643980	4.5928246	0.1346509
C	1.9955539	4.3373363	-2.4374896
H	3.1181636	2.4856858	-2.9224325
H	4.1289997	3.8175748	-2.2879469
C	2.4991761	1.6393333	3.6012585
H	1.2134697	0.4810687	2.2055830
H	2.5635944	-0.4443742	2.9261885
C	3.8540986	2.2695776	3.1721988
H	4.7773470	1.9960393	1.1712153
H	4.9336640	0.5917927	2.2694975
H	3.7967042	-2.5734442	-2.6369003
H	4.9742057	-2.1278350	-3.8952774
H	5.8489093	-2.7783691	-1.3686202
H	6.6112190	-1.4453512	-2.2540369
H	0.4318371	3.8202593	-1.0065507
H	1.0583941	5.4650121	-0.7774445
H	1.2843247	3.9793803	-3.1841795
H	2.3854173	5.3044007	-2.7662684
H	1.7026389	2.3851871	3.5779111
H	2.5413219	1.2185754	4.6083774
H	3.7167503	3.3138815	2.8816009
H	4.5994576	2.2358342	3.9702513

2a⁻ $[W(CO)_5]PClNPh_2^-$

36

Energy = -1954.464329645

P	1.1684966	-1.1760060	0.3020863
Cl	1.3269457	-0.1010716	-1.6689328
N	2.5711890	-0.5955405	1.1314912
C	2.4088620	0.5741811	1.9394927
C	1.3413778	0.6654857	2.8427426
C	3.3052615	1.6464849	1.8281545
C	1.1662718	1.8167149	3.6093920
H	0.6568534	-0.1720107	2.9341626
C	3.1310149	2.7908620	2.6051444
H	4.1330839	1.5776643	1.1293210
C	2.0596612	2.8856092	3.4971470
H	0.3355246	1.8712487	4.3080014
H	3.8302365	3.6167324	2.5030159
H	1.9251226	3.7790114	4.1003886
C	3.9091868	-1.0429061	0.9230423
C	4.3690175	-1.3684298	-0.3569722
C	4.7719456	-1.1804375	2.0200832
C	5.6639307	-1.8557081	-0.5330920
H	3.7079606	-1.2220225	-1.2027876
C	6.0669158	-1.6573263	1.8364138
H	4.4155596	-0.9236571	3.0133017
C	6.5190095	-2.0051248	0.5597960
H	6.0046903	-2.1122890	-1.5327161
H	6.7208161	-1.7741581	2.6967097
H	7.5266905	-2.3865458	0.4207162
W	1.3148297	-3.7144760	-0.2679804
C	2.3848095	-3.3852220	-1.9958423
O	2.9873632	-3.2058290	-2.9688276
C	3.0567075	-4.1174457	0.7573830
O	4.0079987	-4.4288317	1.3399540
C	1.1385689	-5.6768918	-0.6595836
O	1.0344245	-6.8183254	-0.8912039
C	0.2888022	-3.9154786	1.4967839

O	-0.2844038	-4.0170987	2.5015768
C	-0.4327511	-3.3441003	-1.2805611
O	-1.4252863	-3.1536122	-1.8505455

2bhH $[W(CO)_5]PH_2NCy_2$

49

Energy = -1502.525255606

P	1.4937712	1.0332556	0.7799174
N	0.6473233	1.7341045	-0.4849219
W	1.3459567	-1.4564869	1.2202395
C	3.2033519	-1.2960980	2.0937231
O	4.2451642	-1.2080700	2.5871932
C	0.4594427	-0.9949663	3.0207350
O	-0.0361423	-0.7262468	4.0297118
C	1.2992829	-3.4303072	1.6700934
O	1.2774018	-4.5603886	1.9323338
C	-0.5290009	-1.6023397	0.3761645
O	-1.5873371	-1.7021479	-0.0781330
C	2.2514178	-1.8661578	-0.5836399
O	2.7697524	-2.1052291	-1.5898144
C	0.4246478	0.9593611	-1.7267031
C	-1.0124545	1.1147495	-2.2405552
C	1.4510790	1.2751957	-2.8248527
H	0.5570301	-0.0908588	-1.4397717
C	-1.2408123	0.2342619	-3.4778179
H	-1.2005573	2.1628970	-2.5095424
H	-1.7121550	0.8526685	-1.4400617
C	1.2100089	0.4068306	-4.0685220
H	1.3736260	2.3360771	-3.1004547
H	2.4632933	1.1150751	-2.4343177
C	-0.2272441	0.5577423	-4.5830858
H	-2.2651200	0.3691176	-3.8439264
H	-1.1407403	-0.8222606	-3.1917804
H	1.9291739	0.6720586	-4.8521436
H	1.3922430	-0.6457901	-3.8115682
H	-0.3890504	-0.0954169	-5.4486255
H	-0.3836948	1.5905988	-4.9259341
C	0.4913269	3.2125508	-0.5674465
C	-0.6099506	3.7095536	0.3784619
C	1.7990298	3.9848738	-0.3499466
H	0.1631029	3.4109418	-1.5944148
C	-0.8298673	5.2208476	0.2172636
H	-0.3215823	3.4924210	1.4161643
H	-1.5335875	3.1565610	0.1765727
C	1.5717982	5.4938632	-0.5222455
H	2.1724317	3.7966715	0.6662748
H	2.5627520	3.6237126	-1.0482451
C	0.4756387	5.9997145	0.4245061
H	-1.5970780	5.5621669	0.9217679
H	-1.2129135	5.4216074	-0.7936408
H	2.5103552	6.0318505	-0.3458737
H	1.2765231	5.6979670	-1.5613581
H	0.3061208	7.0716963	0.2690311
H	0.8109743	5.8748947	1.4640405
H	1.0897335	1.8432274	1.8603811
H	2.8389358	1.4923878	0.7344569

2bh$^-$ $[W(CO)_5]PHNCy_2^-$

48

Energy = -1502.021875903

P	1.5083985	0.3555475	-0.9540995
H	0.1451584	0.3193906	-1.4123019
N	1.5353975	1.8953116	-0.1530406
W	1.4332849	-1.6235188	0.8245653
C	1.9556997	-0.3737637	2.3658187
O	2.2780234	0.3191061	3.2411681
C	-0.5480708	-1.1322414	1.0016603
O	-1.6699139	-0.8261908	1.0487661
C	1.3607578	-3.1840080	2.0749141
O	1.2980263	-4.0977451	2.8094050
C	0.9767281	-2.8042534	-0.7874108
O	0.7276569	-3.4623300	-1.7141630
C	3.4251806	-1.8080426	0.3820788
O	4.5512314	-1.8647293	0.0961876
C	0.4529100	2.2680464	0.7673038
C	0.9003382	3.2095981	1.8972940
C	-0.8001518	2.8397902	0.0778539
H	0.1591686	1.3237588	1.2427177
C	-0.2321540	3.3850557	2.9204707
H	1.1600176	4.1968589	1.4909058
H	1.7977575	2.8028016	2.3741688
C	-1.9415933	3.0354278	1.0860418
H	-0.5467858	3.8059497	-0.3818959
H	-1.1090044	2.1624575	-0.7272820
C	-1.5031639	3.9298363	2.2537678
H	0.0894976	4.0541158	3.7286586
H	-0.4531049	2.4114538	3.3808137
H	-2.8220017	3.4626573	0.5888109
H	-2.2406548	2.0528694	1.4768093
H	-2.3118934	4.0177944	2.9904217
H	-1.3024339	4.9432500	1.8758175
C	2.2775888	2.9846003	-0.8186483
C	3.7874827	2.7031278	-0.7833496
C	1.8237976	3.2769549	-2.2615356
H	2.0970712	3.8909666	-0.2262830
C	4.5994796	3.8395415	-1.4191493
H	3.9692142	1.7628596	-1.3226319
H	4.0899715	2.5392479	0.2574294
C	2.6312271	4.4218909	-2.8893330
H	1.9599515	2.3586508	-2.8496015
H	0.7529943	3.5101269	-2.2713358
C	4.1355473	4.1225644	-2.8541070

H	5.6688915	3.5933230	-1.4046441
H	4.4762947	4.7532999	-0.8181601
H	2.3001903	4.5959706	-3.9213100
H	2.4380261	5.3519792	-2.3333827
H	4.7023130	4.9601611	-3.2806066
H	4.3414496	3.2422623	-3.4798479

2bH $[W(CO)_5]PHClNCy_2$

49

Energy = -1962.203083537

P	1.6863411	0.9878642	0.6275696
N	0.8089978	1.7268331	-0.5574225
W	1.2871489	-1.4031038	1.2640497
C	3.0892259	-1.3724305	2.2715272
O	4.0865026	-1.3839483	2.8512205
C	0.3423603	-0.6777168	2.9438371
O	-0.1880327	-0.2507228	3.8771323
C	1.0103716	-3.3139043	1.8882104
O	0.8548671	-4.4031707	2.2506473
C	-0.5417218	-1.5084675	0.3249166
O	-1.5814827	-1.6089662	-0.1695730
C	2.2411510	-2.0277061	-0.4572602
O	2.7728545	-2.3605902	-1.4267709
C	0.5375395	0.9721520	-1.8081717
C	-0.9285812	1.0861897	-2.2416405
C	1.4900301	1.3646895	-2.9461365
H	0.7295490	-0.0788420	-1.5551849
C	-1.1821400	0.2060861	-3.4745809
H	-1.1613579	2.1286721	-2.4948336
H	-1.5828736	0.7962122	-1.4139943
C	1.2276672	0.4963482	-4.1853789
H	1.3357018	2.4223820	-3.1998267
H	2.5262920	1.2570004	-2.6089259
C	-0.2394266	0.5799724	-4.6258793
H	-2.2279410	0.3037803	-3.7865953
H	-1.0269420	-0.8474977	-3.2035744
H	1.8924073	0.8050169	-4.9999836
H	1.4762540	-0.5479415	-3.9492111
H	-0.4136637	-0.0773527	-5.4855407
H	-0.4606326	1.6052813	-4.9546363
C	0.5462992	3.1977613	-0.5711508
C	-0.5275420	3.5639366	0.4613543
C	1.8027581	4.0597758	-0.4017079
H	0.1409264	3.4008758	-1.5683653
C	-0.8782295	5.0559963	0.3779665
H	-0.1508496	3.3333150	1.4677569
H	-1.4149197	2.9433115	0.2975937
C	1.4398270	5.5489658	-0.4983519
H	2.2565010	3.8627618	0.5782047
H	2.5445019	3.7887767	-1.1596400
C	0.3721649	5.9305994	0.5347694
H	-1.6214851	5.3036703	1.1442099
H	-1.3436633	5.2605019	-0.5965966
H	2.3422646	6.1550981	-0.3607614
H	1.0616657	5.7633894	-1.5081077
H	0.1080493	6.9896006	0.4330966
H	0.7833413	5.7972842	1.5454220
H	1.5858258	1.9660224	1.6298230
Cl	3.7846100	1.3113186	0.2793930

2b⁻ $[W(CO)_5]PClNCy_2^-$

48

Energy = -1961.713259038

P	1.8361840	0.2956373	-0.9362532
Cl	0.0117825	0.0755644	-2.3734222
N	1.6199223	1.8159915	-0.2516447
W	1.3435393	-1.6557619	0.7509015
C	1.7113984	-0.5721230	2.4507156
O	1.9448838	-0.0126050	3.4426073
C	-0.6412121	-1.1038950	0.7453146
O	-1.7527347	-0.7762911	0.7337961
C	1.0365267	-3.2715124	1.9002366
O	0.8443048	-4.2105990	2.5721339
C	1.0485228	-2.8027849	-0.9343533
O	0.9033547	-3.4864953	-1.8588719
C	3.3576188	-2.0036813	0.6155147
O	4.5034345	-2.1739140	0.5240586
C	0.6234787	2.1486872	0.7862593
C	1.2161913	2.9801374	1.9337175
C	-0.6295262	2.8255803	0.2071855
H	0.3190686	1.1831250	1.2009813
C	0.1657433	3.2008572	3.0319952
H	1.5475711	3.9580153	1.5584505
H	2.0968944	2.4689002	2.3352298
C	-1.6759437	3.0621419	1.3056828
H	-0.3493922	3.7896087	-0.2413428
H	-1.0332150	2.1950773	-0.5912141
C	-1.0922980	3.8755092	2.4686225
H	0.5935047	3.8033507	3.8426829
H	-0.1081648	2.2295793	3.4669306
H	-2.5525164	3.5703342	0.8852003
H	-2.0219455	2.0900882	1.6837943
H	-1.8423785	4.0006835	3.2595334
H	-0.8316638	4.8824384	2.1109546
C	2.2376053	2.9844107	-0.9420542
C	3.7635533	2.9627480	-0.7815561
C	1.8433597	3.1017365	-2.4203116
H	1.8577991	3.8764293	-0.4285926
C	4.4168745	4.1864664	-1.4372900
H	4.1365151	2.0394050	-1.2456487
H	4.0114229	2.9118297	0.2851791
C	2.4905739	4.3357397	-3.0639270

H	2.1706913	2.1920633	-2.9398618
H	0.7527587	3.1391067	-2.5077777
C	4.0172954	4.3057529	-2.9140178
H	5.5078582	4.1269543	-1.3382474
H	4.0988612	5.0956095	-0.9053717
H	2.2113220	4.3925380	-4.1232780
H	2.1002225	5.2455128	-2.5833832
H	4.4626534	5.2052808	-3.3572747
H	4.4158636	3.4428634	-3.4664568

9acCl {[W(CO)$_5$]PClNPh$_2$}$_2$ (one P-P)

72

Energy = -3908.707022113

P	1.0586954	0.5977892	-0.4574890
Cl	0.3965657	1.9730286	-1.9109906
N	0.9842184	1.4843388	0.9789615
C	-0.1856370	2.1995098	1.4554973
C	-1.2437861	1.5178700	2.0530560
C	-0.1894921	3.5964568	1.3993052
C	-2.3111012	2.2352920	2.5973886
C	-1.2529727	4.3061783	1.9499286
C	-2.3163779	3.6279121	2.5515187
C	2.2123715	1.9400388	1.6023642
C	2.4524886	1.5959401	2.9343703
C	3.0971200	2.7728708	0.9168805
C	3.6057792	2.0567324	3.5661049
C	4.2570846	3.2200125	1.5489521
C	4.5157118	2.8575630	2.8714810
W	3.2440585	-0.3670393	-1.3171113
C	3.8897479	1.5124148	-1.8326318
O	4.3107323	2.5238212	-2.2035638
C	4.2183756	-0.2871589	0.5015005
O	4.8470292	-0.2818094	1.4691995
C	4.9804926	-1.0189655	-2.1200995
O	5.9769614	-1.3840635	-2.5811005
C	2.8087804	-2.3721945	-1.0458257
O	2.6939260	-3.5186004	-1.0099028
H	-1.2142817	0.4385483	2.1188973
H	0.6417038	4.1189126	0.9381152
H	-3.1282212	1.6993644	3.0690550
H	-1.2541605	5.3908315	1.9022428
H	-3.1429587	4.1842781	2.9827284
H	1.7355344	0.9847507	3.4735284
H	2.8597244	3.0873375	-0.0923126
H	3.7961725	1.7845567	4.5997776
H	4.9485658	3.8608929	1.0104816
H	5.4178735	3.2069305	3.3642760
P	-0.9418027	-0.6308914	-0.5044527
Cl	-0.2667552	-1.9130708	-2.0347459
N	-0.8805657	-1.6056290	0.8744780
C	0.2849377	-2.3495466	1.3162504
C	1.3380804	-1.7064143	1.9632674
C	0.2892971	-3.7404461	1.1745271
C	2.4007803	-2.4564081	2.4715538
C	1.3481648	-4.4831262	1.6894722
C	2.4064832	-3.8435923	2.3404102
C	-2.1150138	-2.1005556	1.4541907
C	-2.3713155	-1.8405235	2.8021276
C	-2.9903514	-2.8896208	0.7075307
C	-3.5313005	-2.3408949	3.3900582
C	-4.1570797	-3.3762566	1.2965076
C	-4.4317747	-3.0974226	2.6359848
W	-3.1199954	0.3863919	-1.3221638
C	-2.6868795	2.3706548	-0.9237583
O	-2.5728786	3.5125891	-0.8157292
C	-3.7636724	-1.4566934	-1.9574564
O	-4.1841695	-2.4420955	-2.3932269
C	-4.8475664	1.0893024	-2.1002601
O	-5.8387508	1.4841371	-2.5480426
C	-4.1118374	0.1946754	0.4786497
O	-4.7508167	0.1287755	1.4373237
H	1.3080131	-0.6331366	2.0948890
H	-0.5379849	-4.2333074	0.6753485
H	3.2138207	-1.9507609	2.9820716
H	1.3497083	-5.5628255	1.5754531
H	3.2293705	-4.4258080	2.7436553
H	-1.6617957	-1.2635170	3.3869263
H	-2.7404628	-3.1401964	-0.3164268
H	-3.7343427	-2.1340299	4.4363812
H	-4.8411980	-3.9826848	0.7107922
H	-5.3391240	-3.4776616	3.0952448
C	2.3875266	-0.4713378	-3.1906017
O	1.9683565	-0.5229845	-4.2640580
C	-2.2467520	0.6044156	-3.1781090
O	-1.8186684	0.7210351	-4.2428884

9ac$^-$ {[W(CO)$_5$]PNPh$_2$}$_2$Cl$^-$ (P-P-Cl)

71

Energy = -3448.572295063

P	0.6511862	0.7449523	0.2501776
Cl	-0.6308993	2.3876327	0.9825181
N	1.5020080	0.3038067	1.6819613
C	2.5162099	1.1357517	2.2408535
C	3.5722431	0.5509840	2.9619796
C	2.5050174	2.5290943	2.0731582
C	4.5910417	1.3421692	3.4838751
H	3.5992320	-0.5237804	3.1012814
C	3.5346441	3.3103771	2.5958856
H	1.6831847	3.0039582	1.5551290
C	4.5854008	2.7276513	3.3022962
H	5.4027707	0.8660099	4.0273070
H	3.5040413	4.3865257	2.4484563

H	5.3851970	3.3400461	3.7082345
C	1.3138726	-0.9688702	2.3399017
C	1.7428528	-2.1495735	1.7254345
C	0.7988888	-0.9995936	3.6356494
C	1.6353945	-3.3606052	2.4060460
H	2.1568348	-2.1099778	0.7244890
C	0.6948870	-2.2143682	4.3141705
H	0.4952180	-0.0721970	4.1073180
C	1.1103568	-3.3960592	3.7001478
H	1.9655401	-4.2771543	1.9255815
H	0.2841596	-2.2345759	5.3194885
H	1.0221152	-4.3426292	4.2252886
W	2.2367705	1.5025894	-1.6208909
C	2.6948861	-0.4987506	-1.8484060
O	3.0739265	-1.5889624	-1.9027574
C	0.7957104	1.5866461	-3.0868037
O	0.1186687	1.7332205	-4.0139518
C	3.4807775	1.9929215	-3.1196494
O	4.1980133	2.2743305	-3.9926489
C	1.8669545	3.4728379	-1.1673730
O	1.6818634	4.5805901	-0.8905109
C	3.9411871	1.5734915	-0.4623032
O	4.9881950	1.6230353	0.0267360
P	-0.6552131	-0.9808787	-0.0367057
N	-0.8726565	-0.9938799	-1.7770624
C	-0.1512822	-1.9872498	-2.5067817
C	0.1669631	-3.2194652	-1.9182724
C	0.2747746	-1.7369392	-3.8206770
C	0.9182313	-4.1635213	-2.6156759
H	-0.1646778	-3.4228252	-0.9046242
C	1.0149230	-2.6896324	-4.5160453
H	0.0236772	-0.7943593	-4.2920714
C	1.3503290	-3.9065720	-3.9180664
H	1.1578969	-5.1099572	-2.1380306
H	1.3446190	-2.4698532	-5.5281605
H	1.9371216	-4.6430351	-4.4595038
C	-1.8989974	-0.2683045	-2.4391653
C	-2.2338612	1.0207661	-2.0121853
C	-2.6150314	-0.8352118	-3.5066934
C	-3.2463022	1.7364752	-2.6465619
H	-1.6911021	1.4646954	-1.1842475
C	-3.6222855	-0.1131013	-4.1390308
H	-2.3867528	-1.8447294	-3.8305877
C	-3.9454058	1.1802530	-3.7173685
H	-3.4873311	2.7356236	-2.2948248
H	-4.1688233	-0.5719632	-4.9591194
H	-4.7338183	1.7400442	-4.2125445
W	-2.8877173	-1.0365508	1.2844745
C	-2.2304848	0.0109875	2.9280631
O	-1.9753498	0.6200173	3.8799076
C	-3.7112207	0.7526301	0.6670835
O	-4.2682283	1.7443798	0.4511697
C	-4.6030909	-1.3691750	2.2569932
O	-5.6098202	-1.5732052	2.8150411
C	-3.6552691	-2.0459985	-0.3354680
O	-4.1236754	-2.6460369	-1.2075463
C	-2.2126306	-2.8252474	2.0435468
O	-1.9214204	-3.8558484	2.4844119

9aH {[W(CO)$_5$]PHNPh$_2$}$_2$ (PH-PH)

72

Energy = -2989.376919887

P	1.0704644	0.9325299	-0.3964068
H	1.7125002	0.9470402	-1.6495397
N	0.7859376	2.6233052	-0.3038053
C	0.0811933	3.1283936	0.8209097
C	-0.7571315	2.2878087	1.5643713
C	0.2636314	4.4564423	1.2345084
C	-1.3816466	2.7536590	2.7209405
C	-0.3780453	4.9189345	2.3784985
C	-1.1963729	4.0718979	3.1332264
C	1.0915729	3.4962562	-1.3996141
C	0.0993131	4.3337738	-1.9199059
C	2.3839919	3.5259574	-1.9313637
C	0.4113434	5.2157347	-2.9506559
C	2.6820756	4.3955605	-2.9803091
C	1.7013172	5.2501839	-3.4845177
W	2.4096644	-0.0909689	1.4699925
C	4.0148621	0.7277763	0.4810722
O	4.9095717	1.2019211	-0.0767233
C	2.2787106	1.6269120	2.6183599
O	2.2769698	2.5511259	3.3065930
C	3.6559086	-0.8344827	2.8835672
O	4.3825710	-1.2557655	3.6807543
C	0.7891672	-0.8356529	2.5118893
O	-0.0830971	-1.2297727	3.1570901
H	-0.9247362	1.2612005	1.2459939
H	0.9166184	5.1114629	0.6679043
H	-2.0206564	2.0836796	3.2867732
H	-0.2234014	5.9471078	2.6925802
H	-1.6858708	4.4386613	4.0299681
H	-0.9040567	4.2968873	-1.5080897
H	3.1572802	2.8911200	-1.5096171
H	-0.3621784	5.8633855	-3.3510844
H	3.6886684	4.4170112	-3.3872404
H	1.9380548	5.9339829	-4.2939173
P	-0.9154164	0.1311343	-1.3186893
H	-1.5150292	1.4044704	-1.2753207
N	-0.5710714	0.1336412	-3.0007869
C	-0.7898615	1.2969378	-3.8103206
C	-2.0535090	1.8930974	-3.8531372
C	0.2588502	1.8202581	-4.5741198

C	-2.2663906	3.0087966	-4.6625535
C	0.0317026	2.9195509	-5.3972731
C	-1.2293869	3.5174274	-5.4450705
C	0.1134699	-0.9835727	-3.5493658
C	0.8974419	-1.8044676	-2.7286844
C	-0.0359889	-1.3099614	-4.9054539
C	1.5003646	-2.9515981	-3.2438051
C	0.5839458	-2.4455209	-5.4158603
C	1.3478741	-3.2771078	-4.5901873
W	-2.3603174	-1.7438701	-0.4677759
C	-3.8819467	-0.6737954	-1.3420751
O	-4.7305723	-0.0730776	-1.8473117
C	-0.8312307	-2.8747721	0.3382392
O	-0.0177610	-3.5720901	0.7676688
C	-3.6949743	-3.1438200	0.1338253
O	-4.4726910	-3.9319784	0.4730592
C	-2.7292849	-0.7754485	1.3089011
O	-3.0169940	-0.2698121	2.3077309
H	-2.8710411	1.4711402	-3.2766057
H	1.2393261	1.3574486	-4.5275894
H	-3.2510662	3.4655914	-4.6946766
H	0.8489404	3.3220596	-5.9874194
H	-1.4000727	4.3795184	-6.0825907
H	1.0385763	-1.5547789	-1.6793444
H	-0.6462988	-0.6819812	-5.5455747
H	2.0967603	-3.5786261	-2.5891095
H	0.4550267	-2.6919334	-6.4657883
H	1.8204708	-4.1665636	-4.9948748
C	2.7047958	-1.8456252	0.4379788
O	2.9535820	-2.8378548	-0.1003250
C	-2.1556247	-2.8258665	-2.2215940
O	-2.1192816	-3.4787156	-3.1704569

9a⁻ $\{[W(CO)_5]PNPh_2\}_2H^-$ (P-P-H)

71

Energy = -2988.903040015

P	0.9760502	0.0396269	0.3108978
H	1.0046540	0.3165555	1.6927728
N	2.1844402	-1.2236909	0.3170514
C	2.3208829	-2.0318711	1.4913900
C	2.7415976	-1.4504238	2.6916062
C	2.0108958	-3.3957594	1.4486903
C	2.8384682	-2.2271787	3.8459411
H	2.9952809	-0.3943540	2.7152509
C	2.1214006	-4.1686386	2.6014668
H	1.6715381	-3.8359661	0.5170923
C	2.5305792	-3.5889107	3.8053456
H	3.1648018	-1.7683166	4.7751669
H	1.8642123	-5.2235547	2.5621747
H	2.6062703	-4.1925892	4.7053724
C	2.6830857	-1.7221905	-0.9088897
C	2.0227471	-1.4703945	-2.1180201
C	3.8887703	-2.4435357	-0.9324468
C	2.5725992	-1.8928916	-3.3274709
H	1.0589555	-0.9707947	-2.1144340
C	4.4159772	-2.8868338	-2.1404551
H	4.4090555	-2.6428720	-0.0012497
C	3.7695141	-2.6066578	-3.3493918
H	2.0435565	-1.6771828	-4.2515402
H	5.3503435	-3.4421475	-2.1388728
H	4.1914260	-2.9467238	-4.2906563
W	1.8750029	2.1793593	-0.8705731
C	1.5559671	1.5995638	-2.8213748
O	1.4142568	1.3421728	-3.9408410
C	0.0655454	3.1603916	-0.8659914
O	-0.9025426	3.7935832	-0.8977471
C	2.7114257	3.8726190	-1.5411807
O	3.2135737	4.8577035	-1.9103741
C	2.2372990	2.7701283	1.0640818
O	2.4672527	3.0945041	2.1513249
C	3.7338160	1.2912203	-0.9187821
O	4.8007152	0.8477471	-0.9478649
P	-0.9318993	-1.0698748	0.6056898
N	-1.1963211	-1.9658088	-0.8821087
C	-0.8711130	-3.3538686	-0.8251903
C	-0.1605596	-3.9677666	-1.8674814
C	-1.2098696	-4.1120360	0.3046297
C	0.2275151	-5.3015988	-1.7639556
H	0.1057166	-3.3885601	-2.7437486
C	-0.8151137	-5.4452375	0.4044248
H	-1.7614590	-3.6393235	1.1107500
C	-0.0895528	-6.0482340	-0.6254054
H	0.7987519	-5.7528036	-2.5709477
H	-1.0777520	-6.0134593	1.2926703
H	0.2240804	-7.0850635	-0.5437174
C	-1.6918188	-1.4215695	-2.0865991
C	-2.4764999	-2.1963033	-2.9600481
C	-1.4310322	-0.0858016	-2.4196267
C	-2.9671689	-1.6440511	-4.1387321
H	-2.7011909	-3.2266404	-2.7045053
C	-1.9292224	0.4605868	-3.6003613
H	-0.8364059	0.5202148	-1.7424574
C	-2.6974213	-0.3115311	-4.4703709
H	-3.5765511	-2.2566451	-4.7985645
H	-1.7137125	1.4984884	-3.8361559
H	-3.0848618	0.1157608	-5.3908007
W	-2.8652976	0.5305821	1.2439186
C	-3.2338656	1.5763517	-0.4978004
O	-3.5790827	2.2203495	-1.3966904
C	-4.0011179	-1.0157808	0.5040745
O	-4.6113697	-1.9043610	0.0797757
C	-4.4576140	1.4989933	1.9843580

O	-5.3913055	2.0532277	2.4176509
C	-2.6964616	-0.4139053	3.0609176
O	-2.6433426	-0.9235636	4.1008249
C	-1.5769191	1.9825305	1.9164128
O	-0.8663974	2.8011585	2.3309127

9b0W^{-} $[W(CO)_5]PNCy_2PHNCy_2^{-}$
84
Energy = -2369.057247372

P	-1.2223756	-0.0590101	-0.2624043
N	-1.8846224	0.9150594	0.9865264
C	-3.2602847	1.3961497	0.7522739
C	-4.3251085	0.4220057	1.2900643
C	-3.5091068	2.8121696	1.2944976
H	-3.3682484	1.4352161	-0.3395795
C	-5.7464625	0.8996971	0.9599854
H	-4.2113319	0.3317682	2.3803660
H	-4.1410976	-0.5704154	0.8602979
C	-4.9253188	3.2892302	0.9401688
H	-3.4004513	2.8175284	2.3879123
H	-2.7581015	3.4941161	0.8868595
C	-5.9891287	2.3232153	1.4784692
H	-6.4879304	0.2073981	1.3788243
H	-5.8815904	0.8890166	-0.1314225
H	-5.0907306	4.2983894	1.3378561
H	-5.0191868	3.3577441	-0.1531290
H	-6.9931741	2.6650712	1.1969959
H	-5.9478619	2.3194451	2.5776741
C	-1.3979105	0.9639881	2.3819859
C	-0.9129587	-0.3895408	2.9123174
C	-0.3024383	2.0280236	2.5439005
H	-2.2560908	1.2607531	3.0015098
C	-0.4431961	-0.2799294	4.3690368
H	-0.0753065	-0.7244441	2.2888701
H	-1.7139054	-1.1324619	2.8147352
C	0.1845886	2.1352624	3.9936975
H	0.5345884	1.7398424	1.8965412
H	-0.6774298	2.9913211	2.1818526
C	0.6640245	0.7728760	4.5115271
H	-0.0877241	-1.2574453	4.7196396
H	-1.2916892	-0.0002338	5.0118929
H	0.9900185	2.8770651	4.0625780
H	-0.6363545	2.4940909	4.6336815
H	0.9864683	0.8500128	5.5578257
H	1.5362547	0.4538823	3.9233545
H	-1.0865216	-1.3383324	0.3730837
P	1.0066007	0.2885731	-0.2122812
N	1.4543693	-1.1203249	-1.1126807
W	1.4281581	2.5186095	-1.6100832
C	-0.5180333	3.1319263	-1.3815435
O	-1.6184645	3.5052943	-1.3548657
C	1.9910688	3.3428872	0.1878623
O	2.3350223	3.8509949	1.1752770
C	1.9098687	4.2310801	-2.5110356
O	2.1949223	5.2362527	-3.0486735
C	3.3013341	1.7304848	-1.8731080
O	4.3619277	1.2797662	-2.0294873
C	0.8236442	1.7995176	-3.4309608
O	0.4590874	1.4996590	-4.4961868
C	0.9713111	-1.4198994	-2.4647288
C	2.1200256	-1.5499905	-3.4812510
C	0.0552243	-2.6573329	-2.5156649
H	0.3618373	-0.5561067	-2.7512761
C	1.6044757	-1.8362161	-4.8994230
H	2.7873492	-2.3660429	-3.1693366
H	2.7105935	-0.6278072	-3.4624601
C	-0.4622444	-2.9163843	-3.9370957
H	0.6131832	-3.5396543	-2.1697465
H	-0.7782929	-2.5053066	-1.8205666
C	0.6985655	-3.0737500	-4.9275143
H	2.4501181	-1.9650672	-5.5872194
H	1.0332819	-0.9685477	-5.2546217
H	-1.1015929	-3.8084921	-3.9500173
H	-1.0898791	-2.0692502	-4.2492387
H	0.3155851	-3.2416615	-5.9422565
H	1.2865600	-3.9627529	-4.6548250
C	2.2585571	-2.1531360	-0.4362443
C	3.6211216	-1.6062303	0.0176357
C	1.5153078	-2.7958683	0.7464083
H	2.4474593	-2.9392675	-1.1807920
C	4.4631341	-2.6697836	0.7350342
H	3.4307666	-0.7598699	0.6926381
H	4.1533199	-1.2080870	-0.8527009
C	2.3608562	-3.8593667	1.4584883
H	1.2636234	-1.9906727	1.4494911
H	0.5691290	-3.2193017	0.3912439
C	3.7027637	-3.2776960	1.9207260
H	5.4120027	-2.2329337	1.0720103
H	4.7181882	-3.4729116	0.0267541
H	1.8071954	-4.2714143	2.3121652
H	2.5520101	-4.6970090	0.7705569
H	4.3089921	-4.0515595	2.4088974
H	3.5156301	-2.4937702	2.6690359

9bHww $\{[W(CO)_5]PHNCy_2\}_2$ (PH-PH)
96
Energy = -3003.883790195

P	-0.9871575	-0.2446888	0.3632371
N	-1.5948634	0.7391513	1.5687590
W	-2.4390612	-1.4630482	-1.2957107
C	-3.6161207	0.1735311	-1.7117250
O	-4.2814015	1.0570585	-1.9881005

C	-1.2243295	-1.0466496	-2.9106893
O	-0.6084578	-0.9209923	-3.8600153
C	-3.5762570	-2.5937547	-2.5778333
O	-4.1968350	-3.2351902	-3.2802214
C	-1.2519636	-3.0948472	-0.8474288
O	-0.6013039	-3.9727312	-0.5404021
C	-3.6562642	-2.0531246	0.2623885
O	-4.3006408	-2.4719479	1.1003629
C	-2.6129839	1.7169561	1.2108030
C	-4.0133329	1.2832521	1.6579400
C	-2.3033467	3.1154599	1.7523170
H	-2.6147817	1.7743629	0.1176126
C	-5.0642704	2.2891280	1.1961689
H	-4.0503733	1.1991224	2.7454905
H	-4.2339295	0.3013075	1.2335530
C	-3.3549265	4.1149320	1.2756745
H	-2.2960239	3.1106992	2.8433896
H	-1.3127807	3.4275139	1.4171379
C	-4.7465508	3.6834653	1.7270566
H	-6.0487749	1.9727373	1.5451302
H	-5.0903396	2.3129274	0.1050839
H	-3.1241372	5.1053555	1.6731754
H	-3.3377818	4.1797030	0.1855343
H	-5.4896915	4.3954503	1.3644584
H	-4.7928285	3.6800340	2.8184265
C	-1.3741495	0.4955344	2.9891763
C	-1.8283172	-0.8944997	3.4453963
C	0.0821588	0.7468741	3.3829346
H	-1.9860770	1.2212859	3.5308800
C	-1.6412554	-1.0428190	4.9527560
H	-1.2489427	-1.6715317	2.9451533
H	-2.8772003	-1.0414425	3.1804195
C	0.2814429	0.5612088	4.8848373
H	0.7389131	0.0634926	2.8399224
H	0.3562460	1.7647275	3.1044096
C	-0.1797273	-0.8226263	5.3304565
H	-1.9598366	-2.0394674	5.2623099
H	-2.2678057	-0.3158734	5.4752413
H	1.3360409	0.6989374	5.1301994
H	-0.2878944	1.3227978	5.4236972
H	-0.0569528	-0.9220835	6.4103164
H	0.4375470	-1.5855337	4.8522510
H	-0.3975041	-1.1890428	1.2000744
P	1.0613430	0.4390275	-0.3293869
N	0.9072572	2.0458007	-0.7826682
W	3.0201627	-0.9720492	0.4996597
C	1.9279822	-1.9720658	1.9355634
O	1.4461670	-2.6682714	2.6979748
C	2.3317625	-2.3289181	-0.8982277
O	1.9577383	-3.0506736	-1.6906216
C	4.5437579	-2.2476286	0.9934967
O	5.3828985	-2.9698138	1.2478993
C	4.2314869	-0.2278549	-1.0004484
O	4.9241673	0.0382166	-1.8611251
C	3.7253676	0.3431906	1.9225692
O	4.1630741	0.9832647	2.7566231
C	1.3982608	3.0509594	0.1558965
C	2.1301349	4.2163352	-0.5120874
C	0.2902369	3.6001821	1.0584311
H	2.1342899	2.5469397	0.7928846
C	2.7613960	5.0980009	0.5630489
H	1.4413952	4.8298806	-1.0952622
H	2.8963921	3.8343175	-1.1847405
C	0.8915156	4.5052221	2.1311893
H	-0.4243512	4.1698526	0.4610019
H	-0.2443472	2.7715241	1.5290531
C	1.6866000	5.6439597	1.4986161
H	3.2961665	5.9255738	0.0923674
H	3.4843434	4.5165688	1.1391177
H	0.0945649	4.9120630	2.7560568
H	1.5491032	3.9165397	2.7741920
H	2.1503342	6.2470585	2.2807968
H	1.0103650	6.2916537	0.9356913
C	0.3188767	2.4770595	-2.0424579
C	1.1059085	1.9358817	-3.2344602
C	-1.1567335	2.0997894	-2.1922961
H	0.3849614	3.5670237	-2.0682353
C	0.5446332	2.4745694	-4.5472660
H	1.0531835	0.8464321	-3.2279539
H	2.1529061	2.2276492	-3.1384850
C	-1.7207430	2.6655791	-3.4921526
H	-1.2445681	1.0117146	-2.2105347
H	-1.7287112	2.4719049	-1.3409859
C	-0.9356818	2.1335788	-4.6869323
H	1.1021950	2.0512665	-5.3848044
H	0.6716589	3.5596469	-4.5775495
H	-2.7720023	2.3880610	-3.5853852
H	-1.6649365	3.7568858	-3.4738102
H	-1.3272915	2.5641439	-5.6102116
H	-1.0556813	1.0503405	-4.7459267
H	0.4833857	-0.1151817	-1.4861070

9bH $(PHNCy_2)_2$ (PH-PH)

74

Energy = -1735.245108125

P	2.0862013	-0.7625191	-1.2690567
H	2.6357481	0.5394844	-1.5252675
N	2.1010020	-0.8597343	0.4250148
P	0.0472757	0.0099425	-1.7344468
H	0.5189998	0.4814293	-3.0058284
N	-0.8291258	-1.3821030	-2.1472363
C	2.7816544	-2.0095995	1.0596215

C	2.0792334	-3.3317340	0.7228461
C	4.2769640	-2.0928346	0.7127572
H	2.6959711	-1.8499328	2.1419199
C	2.7497900	-4.5220161	1.4213544
H	2.1208200	-3.4719058	-0.3665548
H	1.0209539	-3.2565067	0.9981349
C	4.9495818	-3.2808623	1.4149240
H	4.3698848	-2.2050883	-0.3770535
H	4.7685520	-1.1515047	0.9837482
C	4.2421502	-4.5987061	1.0727408
H	2.2426275	-5.4540526	1.1435639
H	2.6390648	-4.4120586	2.5101017
H	6.0090574	-3.3307644	1.1359677
H	4.9141068	-3.1249957	2.5032166
H	4.7146871	-5.4337868	1.6040284
H	4.3518004	-4.7979810	-0.0029465
C	1.7018237	0.2686552	1.2862384
C	0.6585909	-0.1387027	2.3382561
C	2.8988421	0.9723448	1.9461433
H	1.2156191	0.9889805	0.6159266
C	0.1986945	1.0787235	3.1528934
H	1.0908816	-0.8836200	3.0203201
H	-0.1883109	-0.6142349	1.8332484
C	2.4405597	2.1857330	2.7689668
H	3.4174275	0.2617625	2.6049816
H	3.6125516	1.2777558	1.1716834
C	1.3888491	1.7875047	3.8132273
H	-0.5304416	0.7682060	3.9109642
H	-0.3165136	1.7840722	2.4849772
H	3.3033719	2.6566372	3.2553414
H	2.0080426	2.9355914	2.0910935
H	1.0467680	2.6727487	4.3630355
H	1.8481583	1.1110129	4.5484864
C	-2.2202710	-1.5118614	-1.6629050
C	-2.2770322	-1.5851992	-0.1310035
C	-3.1432268	-0.3982020	-2.1831042
H	-2.5886495	-2.4665883	-2.0589373
C	-3.7141797	-1.7652047	0.3750729
H	-1.8592093	-0.6510799	0.2700833
H	-1.6311417	-2.4010064	0.2136367
C	-4.5821817	-0.5800814	-1.6802729
H	-2.7471826	0.5656928	-1.8326989
H	-3.1128947	-0.3811835	-3.2785942
C	-4.6293632	-0.6503203	-0.1482810
H	-3.7253178	-1.7870561	1.4716624
H	-4.0990362	-2.7373243	0.0338212
H	-5.2135192	0.2387652	-2.0460014
H	-4.9957622	-1.5105627	-2.0962214
H	-5.6588857	-0.8110729	0.1939983
H	-4.2988323	0.3126018	0.2669553
C	-0.3455126	-2.3612875	-3.1376039
C	-0.3203488	-3.7933755	-2.5810709
C	-1.1184201	-2.2999994	-4.4650939
H	0.6952969	-2.0795082	-3.3413947
C	0.2665616	-4.7725757	-3.6076025
H	-1.3413466	-4.1096750	-2.3268358
H	0.2621348	-3.8034490	-1.6541047
C	-0.5372053	-3.2848169	-5.4906935
H	-2.1729937	-2.5487648	-4.2810679
H	-1.0895967	-1.2751406	-4.8540413
C	-0.4998131	-4.7151324	-4.9358373
H	0.2535737	-5.7916558	-3.2025532
H	1.3201449	-4.5146128	-3.7873968
H	-1.1226734	-3.2494262	-6.4174273
H	0.4851437	-2.9724622	-5.7474813
H	-0.0432018	-5.3928906	-5.6673025
H	-1.5291712	-5.0659486	-4.7729173

9bw0⁻ $[W(CO)_5]PHNCy_2PNCy_2^-$

84

Energy = -2369.052935256

P	1.1805275	-0.0192028	-0.7854496
H	0.1574417	0.2634279	0.1437947
N	1.9312944	-1.2609777	0.1639122
W	2.3545812	2.2240711	-1.4406629
C	3.8851568	2.2172653	-0.0940347
O	4.7734175	2.3268442	0.6542646
C	3.4728912	1.1131631	-2.7609900
O	4.1199700	0.4666830	-3.4776067
C	3.0661921	3.9977140	-2.0349684
O	3.4802896	5.0411351	-2.3722481
C	0.8246359	2.4948954	-2.8263304
O	0.0195060	2.8444887	-3.5846958
C	1.1288024	2.9650810	0.0178196
O	0.4156638	3.3186057	0.8669546
P	0.3559673	-0.6472603	-2.6817118
N	-1.1485484	-1.4807431	-2.4414297
C	3.0656415	-1.9349835	-0.4900318
C	4.4422679	-1.3585404	-0.1227270
C	3.0316959	-3.4502772	-0.2511270
H	2.9031101	-1.7740365	-1.5669545
C	5.5630124	-2.0658184	-0.8970465
H	4.6131116	-1.4816107	0.9565066
H	4.4488386	-0.2852833	-0.3330198
C	4.1516983	-4.1591599	-1.0245446
H	3.1456644	-3.6584257	0.8226816
H	2.0508717	-3.8302579	-0.5513343
C	5.5277007	-3.5822504	-0.6653570
H	6.5387642	-1.6570405	-0.6058395
H	5.4388138	-1.8610351	-1.9696283
H	4.1239976	-5.2375795	-0.8236351
H	3.9770261	-4.0304239	-2.1025429

H	6.3128553	-4.0761985	-1.2517060
H	5.7394427	-3.7902698	0.3938182
C	1.9196446	-1.2277059	1.6421722
C	2.3171929	0.1305963	2.2427193
C	0.5674823	-1.6978751	2.2007196
H	2.6734913	-1.9593964	1.9646519
C	2.3060693	0.0998508	3.7765090
H	1.6122222	0.8947307	1.8913948
H	3.3049922	0.4167503	1.8719238
C	0.5605809	-1.7162349	3.7350576
H	-0.2226503	-1.0265454	1.8381499
H	0.3449489	-2.6927195	1.8031202
C	0.9412474	-0.3479612	4.3128075
H	2.5691666	1.0892192	4.1704000
H	3.0787007	-0.5980935	4.1321074
H	-0.4255547	-2.0288271	4.0997940
H	1.2817011	-2.4670469	4.0905475
H	0.9523788	-0.3844497	5.4091365
H	0.1801546	0.3908744	4.0231865
C	-2.3866867	-0.6894012	-2.2572193
C	-2.3575491	0.2621466	-1.0492861
C	-2.7085867	0.1043944	-3.5352483
H	-3.1954712	-1.4183539	-2.0939697
C	-3.6576618	1.0659359	-0.9149388
H	-1.5165990	0.9529177	-1.1940304
H	-2.1569832	-0.3070426	-0.1341890
C	-3.9995344	0.9244007	-3.4081558
H	-1.8574089	0.7714509	-3.7281763
H	-2.7719661	-0.5955428	-4.3779680
C	-3.9451770	1.8610692	-2.1945343
H	-3.5904841	1.7415642	-0.0524120
H	-4.4977494	0.3822534	-0.7190768
H	-4.1706407	1.4990541	-4.3276946
H	-4.8569891	0.2434433	-3.2948502
H	-4.8856127	2.4185004	-2.0979078
H	-3.1449205	2.5992027	-2.3460084
C	-1.2769812	-2.9175963	-2.1523737
C	-0.3030891	-3.7684356	-2.9719130
C	-1.1157533	-3.2358955	-0.6571737
H	-2.2971803	-3.2044615	-2.4580453
C	-0.5176072	-5.2653535	-2.7029667
H	0.7223010	-3.4777441	-2.7075479
H	-0.4339544	-3.5395201	-4.0364162
C	-1.3102202	-4.7288396	-0.3600056
H	-0.1097066	-2.9109731	-0.3629156
H	-1.8270619	-2.6373300	-0.0750323
C	-0.3716502	-5.5946423	-1.2109260
H	0.1932659	-5.8582540	-3.2922948
H	-1.5252939	-5.5545539	-3.0369246
H	-1.1464231	-4.9272269	0.7076636
H	-2.3519721	-5.0089504	-0.5774430
H	-0.5693095	-6.6596986	-1.0336500
H	0.6665257	-5.4083326	-0.9037834

9bwW^{-} {[W(CO)$_5$]PNCy$_2$}$_2$H^{-} (P-P-H)

95

Energy = -3003.384415783

P	-1.0838080	-0.2944239	0.4125416
N	-1.8246712	0.7352604	1.5465282
W	-2.4843530	-1.6717633	-1.2600682
C	-3.7118778	-0.1407650	-1.8608909
O	-4.4213398	0.6970038	-2.2427926
C	-1.2096732	-1.2253688	-2.8408483
O	-0.6132405	-1.0792893	-3.8219507
C	-3.4278099	-2.9327076	-2.5192694
O	-3.9768496	-3.6741053	-3.2269040
C	-1.2377290	-3.1875806	-0.6457367
O	-0.5601583	-4.0544003	-0.2825816
C	-3.7900472	-2.2473764	0.2016827
O	-4.5430010	-2.6415453	0.9955444
C	-3.0697182	1.4395324	1.1865882
C	-4.3066348	0.8937291	1.9191541
C	-2.9796479	2.9601875	1.3795634
H	-3.2049158	1.2510914	0.1160471
C	-5.5888749	1.5784300	1.4249011
H	-4.1950803	1.0749859	2.9973464
H	-4.3696160	-0.1872319	1.7753679
C	-4.2589452	3.6540478	0.8891472
H	-2.8250181	3.1876153	2.4437531
H	-2.1118418	3.3450366	0.8387067
C	-5.5040186	3.1002806	1.5923767
H	-6.4557769	1.1802880	1.9660753
H	-5.7374186	1.3389821	0.3629673
H	-4.1785745	4.7366368	1.0458429
H	-4.3559808	3.4944545	-0.1943793
H	-6.4086897	3.5792285	1.1981676
H	-5.4517939	3.3433243	2.6636178
C	-1.4316116	0.6943514	2.9736184
C	-1.8229177	-0.6222119	3.6710746
C	0.0639880	0.9752292	3.1574264
H	-1.9867451	1.5097037	3.4572470
C	-1.4317804	-0.6030004	5.1553329
H	-1.3062278	-1.4540334	3.1755865
H	-2.8968438	-0.7968221	3.5552575
C	0.4656237	0.9751643	4.6372027
H	0.6396798	0.2141731	2.6147328
H	0.3087197	1.9347664	2.6966166
C	0.0685539	-0.3352135	5.3272377
H	-1.7088302	-1.5548033	5.6247404
H	-2.0010236	0.1844535	5.6713493
H	1.5450252	1.1448471	4.7233552
H	-0.0315361	1.8147156	5.1454762

H	0.3305933	-0.2993742	6.3918575
H	0.6352228	-1.1642483	4.8819210
H	-0.5307490	-1.2264298	1.3118731
P	0.8404788	0.3005365	-0.7172532
N	1.0088828	1.9973177	-0.7714566
W	2.8887539	-0.9626908	0.3467119
C	1.8358731	-2.0766372	1.7108923
O	1.2937728	-2.7371032	2.4988910
C	2.3862293	-2.3132529	-1.1277613
O	2.1224348	-3.0717628	-1.9619555
C	4.5294825	-2.0158154	0.7928414
O	5.5002359	-2.6190987	1.0501436
C	3.9423570	0.1164601	-1.0494099
O	4.5500600	0.6828786	-1.8594876
C	3.3697684	0.3465177	1.8518681
O	3.6932800	1.0221040	2.7420404
C	1.6451502	2.8318610	0.2570722
C	2.9003011	3.5529562	-0.2632327
C	0.6827125	3.8436906	0.8966757
H	1.9558893	2.1310821	1.0370979
C	3.5889333	4.3524200	0.8528578
H	2.6143133	4.2369239	-1.0752057
H	3.5877531	2.8175952	-0.6894260
C	1.3690328	4.6331585	2.0195853
H	0.3219432	4.5455225	0.1313313
H	-0.1894606	3.3066365	1.2773756
C	2.6234216	5.3501509	1.5048661
H	4.4664194	4.8753192	0.4523386
H	3.9545278	3.6550061	1.6189041
H	0.6662176	5.3531951	2.4573135
H	1.6561804	3.9390073	2.8226847
H	3.1218606	5.8831510	2.3241465
H	2.3269961	6.1059132	0.7627501
C	0.4340070	2.6927524	-1.9443939
C	1.1134796	2.2637558	-3.2532461
C	-1.0847665	2.4936381	-2.0288000
H	0.6278560	3.7637547	-1.7979254
C	0.5019897	2.9727066	-4.4692784
H	0.9934605	1.1769615	-3.3510206
H	2.1887381	2.4654592	-3.1814818
C	-1.6967988	3.1938179	-3.2474292
H	-1.2760877	1.4123230	-2.0847653
H	-1.5466970	2.8514364	-1.1029425
C	-1.0134541	2.7419373	-4.5443511
H	0.9874300	2.6230690	-5.3890945
H	0.6961474	4.0539269	-4.3993295
H	-2.7740999	2.9930173	-3.2896917
H	-1.5789512	4.2825191	-3.1387965
H	-1.4385746	3.2748763	-5.4042259
H	-1.2068008	1.6716746	-4.6987119

9b$^-$ $PHNCy_2PNCy_2^-$

73

Energy = -1734.712172121

P	0.6474595	-2.8495822	0.3110697
H	1.1439743	-4.1566708	0.6159398
N	1.7901243	-2.1042405	1.4205629
P	1.2125208	-2.6621711	-1.8104597
N	-0.2497298	-2.0458624	-2.5591885
C	3.2186730	-2.4360435	1.2965531
C	4.0279590	-1.4791941	0.4023300
C	3.8955424	-2.5884447	2.6700857
H	3.2415790	-3.4243757	0.8162897
C	5.4788928	-1.9561034	0.2513957
H	4.0240191	-0.4760362	0.8536345
H	3.5210632	-1.4119483	-0.5677981
C	5.3506258	-3.0591132	2.5230710
H	3.8816151	-1.6244759	3.1983846
H	3.3159169	-3.2964251	3.2744598
C	6.1565616	-2.1158823	1.6190614
H	6.0473820	-1.2573345	-0.3760041
H	5.4849201	-2.9256305	-0.2684544
H	5.8246627	-3.1398752	3.5098729
H	5.3577178	-4.0672229	2.0832076
H	7.1817319	-2.4896785	1.4989732
H	6.2293639	-1.1299219	2.1015216
C	1.4768063	-0.7650626	1.9442359
C	1.1319400	0.2754668	0.8629477
C	0.3413950	-0.8391589	2.9769782
H	2.3767686	-0.4119049	2.4688315
C	0.8392873	1.6519565	1.4732781
H	0.2467694	-0.0820057	0.3236792
H	1.9387149	0.3287749	0.1257482
C	0.0221960	0.5341313	3.5836713
H	-0.5456292	-1.2441465	2.4703116
H	0.6214468	-1.5550071	3.7590979
C	-0.3012263	1.5665771	2.4953508
H	0.5898280	2.3713843	0.6822833
H	1.7438772	2.0317891	1.9725599
H	-0.8128726	0.4506099	4.2913531
H	0.8917247	0.8852205	4.1601322
H	-0.4910619	2.5495633	2.9456802
H	-1.2227058	1.2662813	1.9762244
C	-0.6196758	-0.6336267	-2.4275962
C	-0.8820511	0.0390502	-3.7892307
C	-1.8091230	-0.3853716	-1.4775282
H	0.2629824	-0.1516962	-1.9875410
C	-1.1854597	1.5365885	-3.6324244
H	-1.7333661	-0.4505670	-4.2843918
H	-0.0047484	-0.1156293	-4.4288160
C	-2.1096657	1.1118366	-1.3218428
H	-2.7010294	-0.8889322	-1.8784386

H	-1.5865875	-0.8496936	-0.5094648
C	-2.3691074	1.7684760	-2.6838399
H	-1.3858166	1.9910622	-4.6117631
H	-0.2975422	2.0410676	-3.2232481
H	-2.9684520	1.2628315	-0.6543801
H	-1.2495166	1.6039560	-0.8464524
H	-2.5568575	2.8433557	-2.5626131
H	-3.2766704	1.3324268	-3.1275414
C	-1.3083063	-2.9500102	-3.0371233
C	-0.8060210	-3.8203360	-4.2005688
C	-1.9133866	-3.8398458	-1.9370746
H	-2.1178451	-2.3157359	-3.4297521
C	-1.8892080	-4.7644252	-4.7399537
H	0.0525590	-4.3968673	-3.8276969
H	-0.4329290	-3.1631177	-4.9960144
C	-3.0089034	-4.7672159	-2.4802798
H	-1.0938069	-4.4338893	-1.5094524
H	-2.2946328	-3.2085696	-1.1272615
C	-2.4738398	-5.6392123	-3.6233824
H	-1.4794515	-5.3924391	-5.5423646
H	-2.7014930	-4.1706333	-5.1866727
H	-3.4062463	-5.3975671	-1.6736414
H	-3.8510624	-4.1647420	-2.8550693
H	-3.2671742	-6.2869491	-4.0193289
H	-1.6849130	-6.2976327	-3.2315048

3a $[W(CO)_5]PHOMeNPh_2$

41

Energy = -1609.903934296

P	0.5720613	0.2725614	-0.4405475
N	0.5866596	1.7706749	0.3787283
C	1.7802049	2.5494709	0.3989339
C	2.6414307	2.5451866	-0.7070556
C	2.1212862	3.2863765	1.5408760
C	3.8497936	3.2399261	-0.6518021
H	2.3614725	2.0118720	-1.6097861
C	3.3186537	3.9948441	1.5761734
H	1.4548785	3.2878128	2.3971742
C	4.1944555	3.9677055	0.4866394
H	4.5145190	3.2186615	-1.5105787
H	3.5777833	4.5567058	2.4688409
H	5.1324590	4.5130082	0.5241607
C	-0.5563547	2.2331563	1.1149486
C	-1.1617010	1.4144421	2.0730758
C	-1.0615283	3.5151011	0.8717927
C	-2.2892164	1.8652745	2.7613164
H	-0.7434505	0.4356244	2.2887840
C	-2.1741061	3.9675082	1.5776859
H	-0.5781758	4.1492721	0.1344636
C	-2.7973055	3.1417649	2.5181586
H	-2.7576167	1.2221703	3.5007091
H	-2.5622150	4.9629438	1.3825441
H	-3.6682397	3.4945118	3.0623225
W	2.3926529	-1.3760456	-0.0153558
C	3.3216250	-0.7661074	-1.7534970
O	3.8330276	-0.3971856	-2.7207740
C	3.5947793	-0.0786152	1.0581037
O	4.3133802	0.5734843	1.6821723
C	3.7762591	-2.8267215	0.3128638
O	4.5555415	-3.6656859	0.4938118
C	1.4052389	-1.8460431	1.7242717
O	0.8388344	-2.0826108	2.7054658
C	1.2562284	-2.7322881	-1.0619269
O	0.6294456	-3.5093590	-1.6454741
H	-0.7361756	-0.0778760	-0.0431417
O	0.3553775	0.5524187	-2.0303790
C	-0.7422180	1.4094871	-2.4447057
H	-0.7955468	1.3313816	-3.5304719
H	-1.6805526	1.0689677	-1.9932519
H	-0.5369304	2.4416196	-2.1485500

3b $[W(CO)_5]PHOMeNCy_2$

53

Energy = -1617.155996358

P	1.6667184	1.0441143	0.7337534
N	0.8773862	1.7545698	-0.5449004
W	1.3149936	-1.4308459	1.1930342
C	3.1597912	-1.4447071	2.1087670
O	4.1840221	-1.4702321	2.6436920
C	0.4663880	-0.8010254	2.9602910
O	-0.0100812	-0.4374412	3.9484947
C	1.0686346	-3.3682420	1.7284837
O	0.9298781	-4.4764459	2.0430372
C	-0.5660597	-1.4695045	0.3559309
O	-1.6352999	-1.5369150	-0.0788799
C	2.1573411	-2.0083073	-0.5959942
O	2.6236772	-2.3435586	-1.6009529
C	0.5725364	0.9783124	-1.7693729
C	-0.9010011	1.0999824	-2.1805959
C	1.5009136	1.3258963	-2.9413272
H	0.7534341	-0.0686083	-1.4974746
C	-1.1956287	0.1956758	-3.3860695
H	-1.1267112	2.1398611	-2.4520119
H	-1.5406693	0.8383933	-1.3324750
C	1.1988439	0.4373396	-4.1570679
H	1.3654255	2.3814584	-3.2147697
H	2.5442484	1.2034395	-2.6302237
C	-0.2762802	0.5322745	-4.5668621
H	-2.2474914	0.2974914	-3.6763501
H	-1.0452488	-0.8534323	-3.0951611
H	1.8494554	0.7190551	-4.9929471
H	1.4372758	-0.6054073	-3.9049964

H	-0.4780888	-0.1403500	-5.4086464
H	-0.4916219	1.5535712	-4.9120939
C	0.5990893	3.2195809	-0.5876775
C	-0.5485182	3.6022238	0.3575447
C	1.8377847	4.0884242	-0.3329807
H	0.2688311	3.4185449	-1.6139130
C	-0.8894032	5.0942849	0.2326731
H	-0.2502160	3.3835499	1.3917081
H	-1.4238815	2.9830940	0.1345980
C	1.4868754	5.5759352	-0.4776582
H	2.2156858	3.9005602	0.6795310
H	2.6342230	3.8060087	-1.0305551
C	0.3471192	5.9707020	0.4702042
H	-1.6857281	5.3520141	0.9405282
H	-1.2825103	5.2897763	-0.7753557
H	2.3769716	6.1853876	-0.2830616
H	1.1822370	5.7767698	-1.5149218
H	0.0924043	7.0288234	0.3381774
H	0.6839170	5.8484478	1.5095479
H	1.2754586	1.9021098	1.7745237
O	3.2437529	1.5234684	0.8275661
C	4.2190638	0.9460016	-0.0625878
H	5.1975299	1.1425798	0.3769185
H	4.0688661	-0.1352913	-0.1586535
H	4.1531320	1.4170622	-1.0482352

3ohH $[W(CO)_5]PH_2OMe$
19
Energy = -1092.102438425

P	1.3195398	1.0868747	0.9714481
O	0.7402730	1.5638667	-0.4726191
W	1.3240921	-1.3808868	1.2879301
C	3.2336379	-1.2626949	2.0513941
O	4.3059377	-1.1832587	2.4749237
C	0.5411588	-1.1289051	3.1765981
O	0.0992464	-0.9759625	4.2334033
C	1.3214992	-3.4016054	1.5268771
O	1.3192080	-4.5523111	1.6602474
C	-0.5851874	-1.4298298	0.5073428
O	-1.6534688	-1.4533004	0.0692126
C	2.1012704	-1.5674573	-0.6139921
O	2.5360087	-1.6684910	-1.6791291
C	0.6992574	2.9899605	-0.7484502
H	0.2879970	3.0931790	-1.7525429
H	0.5930400	1.8843395	1.8890804
H	2.5493005	1.7824192	1.0703191
H	0.0541550	3.4931418	-0.0207785
H	1.7104205	3.4080083	-0.7079713

4a $[W(CO)_5]PH(NHMe)NPh_2$
42
Energy = -1590.021118953

P	2.6089781	1.0030405	0.1588273
N	1.2558158	1.9941564	-0.2445122
C	1.3747736	3.0492315	-1.2084786
C	1.0052778	4.3526226	-0.8548417
C	1.8605712	2.7898914	-2.4947565
C	1.1290488	5.3868441	-1.7795802
H	0.6223348	4.5443183	0.1430687
C	2.0022475	3.8343690	-3.4102582
H	2.1115686	1.7732647	-2.7821292
C	1.6354997	5.1338307	-3.0579351
H	0.8409358	6.3953642	-1.4974613
H	2.3829667	3.6254774	-4.4056177
H	1.7381518	5.9433501	-3.7746369
C	-0.0002602	1.7760757	0.3806789
C	-0.0681993	1.3102172	1.7013917
C	-1.1891526	1.9767159	-0.3370607
C	-1.3016512	1.0060401	2.2776034
H	0.8400800	1.2003349	2.2837667
C	-2.4164037	1.6914685	0.2535187
H	-1.1421760	2.3402982	-1.3586819
C	-2.4813693	1.1925042	1.5582373
H	-1.3342613	0.6361589	3.2986333
H	-3.3291922	1.8426979	-0.3159701
H	-3.4419970	0.9597083	2.0078590
W	2.2767650	-1.4908270	0.1709426
C	0.2251937	-1.4361691	-0.0932063
O	-0.9159032	-1.4968997	-0.2541928
C	2.5129897	-1.3925990	-1.8715382
O	2.6356920	-1.3069831	-3.0185798
C	2.1664266	-3.5135688	0.1254864
O	2.1226643	-4.6728525	0.1019565
C	4.3112485	-1.6290511	0.4338597
O	5.4539834	-1.7284776	0.5822543
C	1.9803776	-1.4611058	2.2051642
O	1.8003650	-1.4209774	3.3481208
H	3.4344257	1.5372131	-0.8456356
C	3.7563119	3.0003278	1.6678318
H	2.8821316	3.5989761	1.9533110
H	4.5264059	3.1024726	2.4358971
H	4.1494718	3.3861865	0.7231913
N	3.4296654	1.5782790	1.4995477
H	3.2538209	1.0782362	2.3649141

4b $[W(CO)_5]PH(NHMe)NCy_2$
54
Energy = -1597.270022588

P	1.7586380	1.1476892	0.6696083
N	0.8315714	1.8317282	-0.5532860
W	1.3800755	-1.3227092	1.2034239
C	3.2779466	-1.3738198	2.0049359

O	4.3322475	-1.4217493	2.4758800
C	0.6621968	-0.6337668	3.0050746
O	0.2577140	-0.2346877	4.0122035
C	1.1040285	-3.2373727	1.7876259
O	0.9493869	-4.3361469	2.1315782
C	-0.5449563	-1.2962277	0.4787032
O	-1.6405894	-1.3202588	0.1079698
C	2.0915304	-1.9665622	-0.6179968
O	2.4861252	-2.3445234	-1.6389720
C	0.5682577	1.0668858	-1.7905179
C	-0.9005635	1.1493081	-2.2292014
C	1.5038666	1.4554397	-2.9458215
H	0.7746500	0.0211007	-1.5297978
C	-1.1469867	0.2505488	-3.4495643
H	-1.1509723	2.1849588	-2.4954984
H	-1.5490535	0.8607423	-1.3967850
C	1.2509991	0.5758138	-4.1789071
H	1.3385928	2.5103628	-3.2064990
H	2.5452865	1.3635141	-2.6175295
C	-0.2197351	0.6291415	-4.6115267
H	-2.1966120	0.3230146	-3.7569118
H	-0.9686044	-0.7968747	-3.1679364
H	1.9049700	0.8895546	-5.0008933
H	1.5183174	-0.4624087	-3.9371170
H	-0.3873359	-0.0390137	-5.4644521
H	-0.4615929	1.6473976	-4.9482482
C	0.4931797	3.2789368	-0.5704094
C	-0.6717415	3.5933328	0.3796352
C	1.6840671	4.2094857	-0.2954006
H	0.1578184	3.4898116	-1.5929421
C	-1.0909582	5.0662966	0.2703422
H	-0.3607307	3.3747673	1.4107029
H	-1.5126863	2.9308515	0.1498859
C	1.2600492	5.6794725	-0.4279868
H	2.0488285	4.0451808	0.7285352
H	2.5036255	3.9761003	-0.9847403
C	0.0968730	6.0051841	0.5179201
H	-1.9008995	5.2767681	0.9782879
H	-1.4919024	5.2501012	-0.7367950
H	2.1163769	6.3321336	-0.2228919
H	0.9515186	5.8723874	-1.4652742
H	-0.2123177	7.0494731	0.3924059
H	0.4364293	5.8935674	1.5575774
H	1.3973218	2.0169518	1.7131014
C	4.3624568	0.8954070	-0.2242178
H	5.3678459	0.9554403	0.2012873
H	4.0938132	-0.1593710	-0.3226418
H	4.3740102	1.3438733	-1.2263355
N	3.4086692	1.5453784	0.6802823
H	3.6066039	2.5343847	0.8087745

4nCl $[W(CO)_5]PCl_2NHMe$

20

Energy = -1991.563233259

P	1.7047664	0.7277347	0.7740577
Cl	1.5426856	1.9608176	2.4308249
N	0.7205966	1.4937152	-0.3022528
W	1.3709109	-1.6965499	1.1035187
C	3.2650849	-1.8298660	1.9223034
O	4.3198226	-1.8999568	2.3812349
C	0.5861258	-1.3680880	2.9870683
O	0.1459335	-1.1810355	4.0354641
C	1.1008040	-3.7048421	1.3214207
O	0.9461201	-4.8442440	1.4382065
C	-0.5240923	-1.5318821	0.3148683
O	-1.5887448	-1.4352550	-0.1220307
C	2.1580029	-1.9909484	-0.7802682
O	2.5987958	-2.1505499	-1.8346999
Cl	3.6609320	1.2647506	0.2287542
C	0.8223311	2.9007947	-0.7202043
H	-0.1328976	3.2000898	-1.1545806
H	0.3242590	0.8641037	-0.9948468
H	1.0216080	3.5173078	0.1576014
H	1.6229462	3.0431525	-1.4533091

4nhH $[W(CO)_5]PH_2NHMe$

20

Energy = -1072.221748023

P	1.3622839	1.0807990	0.9682085
N	0.5288492	1.6475027	-0.3806939
W	1.3383278	-1.4114989	1.2874200
C	3.2119308	-1.2887670	2.1347029
O	4.2633070	-1.2127393	2.6089113
C	0.4795413	-1.1454548	3.1425309
O	-0.0033288	-0.9836027	4.1796496
C	1.3260084	-3.4257623	1.5319129
O	1.3196198	-4.5771772	1.6694308
C	-0.5405807	-1.4743802	0.4414322
O	-1.5946797	-1.5133182	-0.0307463
C	2.1968629	-1.6101181	-0.5727213
O	2.6790214	-1.7183640	-1.6187801
C	0.6141246	3.0635356	-0.7703625
H	-0.0958778	3.2500366	-1.5795512
H	0.8103719	1.8908603	1.9818295
H	2.6462104	1.6891155	0.9444338
H	0.5497442	1.0020423	-1.1640137
H	0.3346514	3.6829242	0.0867383
H	1.6207426	3.3534955	-1.1010517

4n $[W(CO)_5]PH(NHMe)_2$

25

Energy = -1166.966703847

P	1.6952235	1.1802893	0.8201246
N	0.7348127	1.6934506	-0.4616806
W	1.3561546	-1.2712158	1.3305550
C	3.2252299	-1.3259094	2.1925429
O	4.2730834	-1.3575562	2.6805151
C	0.5525679	-0.7369763	3.1516830
O	0.1056919	-0.4218390	4.1701637
C	1.0845118	-3.2398426	1.7307574
O	0.9298574	-4.3683382	1.9551778
C	-0.5189701	-1.1598876	0.4862851
O	-1.5738067	-1.0999394	0.0164526
C	2.1748489	-1.7147050	-0.5030905
O	2.6382154	-1.9546436	-1.5367966
C	0.6269281	3.0908526	-0.8993448
H	-0.3239006	3.2355851	-1.4199726
H	1.2923554	2.1615066	1.7473011
C	3.8145777	2.9773721	0.6517170
H	3.8454782	3.3368098	-0.3842550
H	3.1565710	3.6334210	1.2293171
H	4.8200454	3.0387657	1.0776749
N	3.3209351	1.5998986	0.7635157
H	3.9327613	0.8995939	0.3573148
H	0.6366662	3.7366362	-0.0161938
H	1.4451971	3.3942218	-1.5640122
H	0.6189973	1.0133027	-1.2063107

5a2 $\{[W(CO)_5]PNPh_2\}_2$ (one P=P)

70

Energy = -2988.165322093

P	-0.3801503	-0.8832381	0.1625470
N	-2.0485619	-0.5546467	-0.0663670
C	-2.9440648	-1.0810681	0.9126025
C	-4.1356632	-1.7180916	0.5407840
C	-2.5908062	-1.0006256	2.2650965
C	-4.9580157	-2.2645132	1.5214842
H	-4.4036302	-1.7951444	-0.5072268
C	-3.4102866	-1.5686564	3.2383364
H	-1.6794964	-0.4786612	2.5451816
C	-4.5996584	-2.1983935	2.8718603
H	-5.8779544	-2.7608991	1.2265827
H	-3.1233819	-1.5042899	4.2835115
H	-5.2443567	-2.6330585	3.6295736
C	-2.5308850	-0.0522001	-1.3132878
C	-1.8390630	-0.3344003	-2.4982643
C	-3.6973178	0.7227936	-1.3594444
C	-2.3015793	0.1656717	-3.7134276
H	-0.9447538	-0.9504112	-2.4662605
C	-4.1633640	1.1994559	-2.5821992
H	-4.2342235	0.9428757	-0.4435474
C	-3.4683071	0.9298419	-3.7632907
H	-1.7549308	-0.0591539	-4.6246260
H	-5.0679783	1.7999612	-2.6071397
H	-3.8314884	1.3130142	-4.7117631
W	0.5105438	-3.1781227	0.2301911
C	1.1083515	-3.0801250	-1.7513477
O	1.3951293	-3.1124839	-2.8664747
C	2.3487215	-2.5336471	0.9117906
O	3.3825800	-2.2252480	1.3211571
C	1.1791267	-5.0943277	0.2665666
O	1.5569160	-6.1885249	0.2828944
C	-0.1143642	-3.4060261	2.1882368
O	-0.4432450	-3.5708273	3.2807738
C	-1.3222501	-3.8458772	-0.4382484
O	-2.3348629	-4.2336232	-0.8308366
P	0.4543059	0.9800469	0.1841970
N	2.0972879	0.6743742	-0.2031672
C	2.4733555	0.2321257	-1.5083596
C	1.6895741	0.5735892	-2.6180156
C	3.6287286	-0.5400746	-1.6865602
C	2.0509934	0.1350766	-3.8899164
H	0.8035806	1.1875475	-2.4832125
C	3.9932207	-0.9548257	-2.9651591
H	4.2363923	-0.8057851	-0.8287803
C	3.2068852	-0.6256603	-4.0715096
H	1.4342837	0.4058735	-4.7419600
H	4.8903794	-1.5534417	-3.0928419
H	3.4911965	-0.9606356	-5.0641239
C	3.0731169	1.1596547	0.7184128
C	2.8362639	1.0192865	2.0913081
C	4.2291467	1.8162583	0.2748062
C	3.7354221	1.5480458	3.0152150
H	1.9523804	0.4818039	2.4249902
C	5.1318095	2.3228127	1.2048758
H	4.4070299	1.9398417	-0.7878329
C	4.8892994	2.1974185	2.5767111
H	3.5383783	1.4374821	4.0771811
H	6.0232193	2.8351141	0.8547604
H	5.5960402	2.6013976	3.2950540
W	-0.4333631	3.2621392	0.4516988
C	-2.2163163	2.5766086	1.2327288
O	-3.2188861	2.2496147	1.7011616
C	0.3354947	3.3834890	2.3675688
O	0.7446399	3.4873583	3.4403397
C	-1.1029666	5.1683824	0.6421244
O	-1.4819716	6.2573837	0.7453639
C	1.3403144	3.9845947	-0.3124748
O	2.3166097	4.4083572	-0.7563776
C	-1.1776424	3.2648972	-1.4821940
O	-1.5478180	3.3513259	-2.5695087

5aBe $[W(CO)_5]PNPh_2CH_2CMe_2$ (PC_2 ring)

47

Energy = -1651.413337049

P	-0.3626546	-0.1376185	1.1778756
N	-1.9491195	-0.0337358	0.5165139
C	-2.9551841	-1.0051849	0.7994239
C	-2.6426001	-2.3677999	0.8557603
C	-4.2680954	-0.5854899	1.0532935
C	-3.6322261	-3.2996989	1.1686097
H	-1.6272608	-2.6959182	0.6570492
C	-5.2553821	-1.5234285	1.3463076
H	-4.5078056	0.4727530	1.0137993
C	-4.9427402	-2.8842739	1.4095964
H	-3.3769145	-4.3545950	1.2111045
H	-6.2698775	-1.1868342	1.5401191
H	-5.7129978	-3.6122507	1.6457535
C	-2.1762844	0.9722874	-0.4612123
C	-1.4650675	2.1802207	-0.3995212
C	-3.0578303	0.7503747	-1.5305117
C	-1.6206420	3.1402232	-1.3984586
H	-0.7940406	2.3699628	0.4326832
C	-3.2205729	1.7238129	-2.5113717
H	-3.6015883	-0.1861560	-1.5942256
C	-2.4998736	2.9207979	-2.4582862
H	-1.0555345	4.0657787	-1.3379555
H	-3.9032587	1.5359012	-3.3353049
H	-2.6232504	3.6704366	-3.2338819
W	1.6167775	-0.4998093	-0.3446386
C	0.9353661	-2.4092076	-0.6978425
O	0.5490579	-3.4800964	-0.9014883
C	0.6029489	0.1383785	-2.0337428
O	0.1128343	0.4573395	-3.0279307
C	3.2270694	-0.8144011	-1.5224359
O	4.1569470	-0.9982332	-2.1923562
C	2.2088963	1.4433113	0.0086220
O	2.5236713	2.5399528	0.1929482
C	2.6952937	-1.1991212	1.2570444
O	3.3150040	-1.6144682	2.1420123
C	-0.6005882	-0.7786899	2.8640066
H	0.2080010	-1.3948428	3.2494890
H	-1.5942224	-1.1407154	3.1155632
C	-0.3895985	0.7318557	2.8256498
C	-1.5910899	1.5931037	3.1627677
H	-1.7382810	1.6010209	4.2503115
H	-1.4370082	2.6252677	2.8327294
H	-2.5041794	1.2115537	2.6992594
C	0.9372794	1.2599561	3.3365147
H	0.9375800	1.2576534	4.4339907
H	1.7785435	0.6473170	3.0012586
H	1.1028918	2.2864207	2.9949240

5a.ClLic adduct of **6a** and **ClLic**

65

Energy = -2577.674629487

P	0.2311415	0.1319137	0.1081486
Cl	-0.3666142	0.3976488	-2.1596877
N	0.2998095	1.7629464	0.6207679
C	1.4058862	2.6578864	0.4208378
C	1.9285084	2.8780891	-0.8545756
C	1.9281954	3.3483960	1.5201780
C	2.9796638	3.7790631	-1.0258289
H	1.4999928	2.3545084	-1.7010068
C	2.9825379	4.2411372	1.3435541
H	1.5084357	3.1735794	2.5057701
C	3.5123934	4.4610526	0.0685619
H	3.3781371	3.9526855	-2.0209732
H	3.3936220	4.7639363	2.2027903
H	4.3328438	5.1598100	-0.0685593
C	-0.9170615	2.3817727	1.0601214
C	-1.7924844	1.6879205	1.9059490
C	-1.2445292	3.6802203	0.6471263
C	-2.9875535	2.2778991	2.3129658
H	-1.5245886	0.6901406	2.2387105
C	-2.4376797	4.2677337	1.0664394
H	-0.5658623	4.2217277	-0.0038246
C	-3.3180086	3.5705774	1.8966354
H	-3.6548427	1.7298958	2.9726535
H	-2.6817661	5.2735086	0.7349232
H	-4.2460566	4.0312958	2.2226368
W	2.5228481	-1.0407076	0.2145818
C	3.7337770	0.2343950	-0.8533525
O	4.5171088	0.8624032	-1.4330830
C	2.8621892	0.0287111	1.9389545
O	3.0328492	0.6085400	2.9268046
C	4.1611347	-2.1813815	0.4899958
O	5.1103844	-2.8398827	0.6504441
C	1.4839412	-2.4403365	1.3050664
O	0.9372609	-3.2564001	1.9197738
C	1.9940064	-2.0349621	-1.5017429
O	1.6729336	-2.6141666	-2.4531268
Li	0.9003517	0.6351862	-4.1368043
O	2.0189398	2.4029966	-4.2772384
O	0.2492137	-0.7364597	-5.5870921
O	-0.4907352	1.8451942	-5.1678208
C	3.4149951	2.0816951	-4.4600200
C	1.4724082	3.2619495	-5.2965837
C	-0.8804166	-0.1824782	-6.2945301
C	1.3545227	-1.1021482	-6.4368343
C	-0.0334922	3.2103536	-5.1250838
C	-0.6882430	1.3097556	-6.4889692
H	3.9514640	2.9285751	-4.9011495
H	3.8064470	1.8860595	-3.4611625
H	1.8438299	4.2858793	-5.1627213
H	1.7734556	2.9074578	-6.2913292

H	-1.7463131	-0.3687728	-5.6547809
H	-1.0222290	-0.6911177	-7.2543665
H	1.1120939	-2.0138664	-6.9973592
H	1.5648022	-0.2969982	-7.1536124
H	-0.3119756	3.5753101	-4.1331851
H	-0.5364854	3.8145954	-5.8884005
H	-1.5758037	1.7605506	-6.9510620
H	0.1829096	1.5199023	-7.1242321
O	2.7533940	-0.1746581	-4.6863532
C	2.5314783	-1.3397821	-5.5106799
H	3.4352037	-1.5857718	-6.0790484
H	2.3081930	-2.1499918	-4.8150286
C	3.5471010	0.8445269	-5.3248150
H	3.1794224	1.0303792	-6.3429050
H	4.5941458	0.5214409	-5.3843930

5a.nH $[W(CO)_5]PNPh_2.NH_2Me$ (P..N adduct)
42
Energy = -1589.992184618

P	-0.0281470	1.2492114	-1.2004682
N	-1.3483722	1.3566462	-0.1016103
W	1.4214104	-0.8660742	-0.9219436
C	-1.4389251	0.7165634	1.1748520
C	-2.4450872	2.2172197	-0.4536591
C	2.5655582	-0.1313366	-2.4560590
C	2.5505429	0.0882368	0.4911867
C	2.6029391	-2.5038476	-0.9712496
C	0.3450761	-1.8494843	0.5475714
C	0.0901475	-1.6374379	-2.2912334
C	-2.5991163	-0.0015508	1.4944163
C	-0.4038355	0.7932088	2.1113846
C	-3.0103657	3.0575316	0.5156749
C	-2.9493573	2.2369730	-1.7598445
O	3.2293418	0.2236142	-3.3389131
O	3.1401492	0.6901810	1.2923831
O	3.2975056	-3.4369526	-0.9997697
O	-0.1911156	-2.5189550	1.3212882
O	-0.6827151	-2.0441056	-3.0507322
C	-2.7138852	-0.6349207	2.7283582
H	-3.4029728	-0.0600903	0.7667302
C	-0.5185256	0.1513266	3.3443840
H	0.4935943	1.3576667	1.8878423
C	-4.0615653	3.9089953	0.1773417
H	-2.6266704	3.0365742	1.5312163
C	-3.9935322	3.0986229	-2.0932025
H	-2.5188650	1.5754559	-2.5047973
C	-1.6731544	-0.5643600	3.6590863
H	-3.6140536	-1.1975787	2.9591794
H	0.2970806	0.2171972	4.0587148
C	-4.5559680	3.9385518	-1.1285564
H	-4.4889434	4.5565739	0.9380168
H	-4.3786625	3.1002734	-3.1091398
H	-1.7619556	-1.0653014	4.6183700
H	-5.3739763	4.6032424	-1.3901863
H	1.3643369	2.5663396	0.4848244
N	1.0247595	2.7550338	-0.4608924
C	2.1652508	3.1380225	-1.3411805
H	2.6027101	4.0756254	-0.9960673
H	2.9088790	2.3431334	-1.3065156
H	1.7867990	3.2452948	-2.3586481
H	0.3655896	3.5338982	-0.3872465

5a $[W(CO)_5]PNPh_2$ (partial P=N double-bond)
35
Energy = -1494.041307738

P	1.1322091	-1.4111780	0.5842248
N	2.5284380	-0.6592902	1.1704567
C	2.4099066	0.5655913	1.9189073
C	1.3764927	0.7211868	2.8486403
C	3.3330985	1.5970599	1.7090698
C	1.2531128	1.9198960	3.5491697
H	0.6933362	-0.1027666	3.0294228
C	3.2042258	2.7891900	2.4171572
H	4.1339755	1.4655244	0.9889556
C	2.1642076	2.9566222	3.3357520
H	0.4553204	2.0335284	4.2769511
H	3.9164847	3.5906789	2.2450568
H	2.0714154	3.8856929	3.8902242
C	3.8787312	-1.1258211	0.9789651
C	4.3650692	-1.3234123	-0.3140175
C	4.6940380	-1.3546035	2.0903220
C	5.6653007	-1.7904472	-0.4970783
H	3.7301334	-1.0892184	-1.1610964
C	5.9919178	-1.8225670	1.8995691
H	4.3049478	-1.1854018	3.0893984
C	6.4776958	-2.0476954	0.6089084
H	6.0434086	-1.9448073	-1.5032469
H	6.6216483	-2.0214563	2.7614801
H	7.4889365	-2.4166824	0.4666097
W	1.3395847	-3.7443370	-0.1966545
C	2.3953765	-3.3385511	-1.9322736
O	2.9903105	-3.1365110	-2.8997281
C	3.1271281	-4.1795695	0.7496399
O	4.1037256	-4.5103595	1.2666610
C	1.1663679	-5.7070330	-0.7570797
O	1.0667797	-6.8182560	-1.0641206
C	0.3270411	-4.2187299	1.5450080
O	-0.2391382	-4.5018542	2.5103143
C	-0.4453771	-3.3736396	-1.1516083
O	-1.4511937	-3.1918142	-1.6914094

5b $[W(CO)_5]PNCy_2$ (partial P=N double-bond)

47

Energy = -1501.301826426

P	2.2676779	0.3009610	-0.5539300
N	1.7091981	1.8133860	-0.1749758
W	1.3385233	-1.6239470	0.7370827
C	1.5144568	-0.6952859	2.5718199
O	1.6227165	-0.1874460	3.6044567
C	-0.6147367	-0.9805894	0.5659029
O	-1.7111335	-0.6295494	0.4629626
C	0.7222588	-3.3530799	1.6388913
O	0.3665914	-4.3276715	2.1542006
C	1.1997173	-2.5526309	-1.1003512
O	1.1307579	-3.0829616	-2.1245975
C	3.2967436	-2.2590358	0.8755809
O	4.3905293	-2.6244888	0.9488765
C	0.7108417	2.1489246	0.8703575
C	1.3168765	3.0257399	1.9766003
C	-0.5554607	2.7799986	0.2724151
H	0.4341971	1.1888270	1.3122623
C	0.2733998	3.2837356	3.0734051
H	1.6455821	3.9853051	1.5576173
H	2.2000955	2.5270519	2.3899704
C	-1.5863461	3.0377558	1.3811184
H	-0.3073325	3.7303461	-0.2171849
H	-0.9664594	2.1127619	-0.4926314
C	-0.9993479	3.9142601	2.4945777
H	0.7081499	3.9301053	3.8440064
H	0.0188238	2.3325681	3.5600763
H	-2.4758683	3.5087841	0.9481759
H	-1.9076314	2.0769892	1.8056387
H	-1.7407959	4.0626561	3.2879811
H	-0.7604305	4.9068872	2.0873879
C	2.2425870	2.9895303	-0.9411715
C	3.7551808	3.1507017	-0.7446427
C	1.8806918	2.8998192	-2.4290696
H	1.7459255	3.8687594	-0.5185864
C	4.2665978	4.3837354	-1.5008956
H	4.2483221	2.2452137	-1.1217026
H	3.9794739	3.2269223	0.3251978
C	2.3958158	4.1326500	-3.1830435
H	2.3375425	1.9887386	-2.8373585
H	0.7947990	2.8008818	-2.5372264
C	3.9074840	4.3112340	-2.9907949
H	5.3513402	4.4693046	-1.3701715
H	3.8206414	5.2884254	-1.0634226
H	2.1515565	4.0393534	-4.2473233
H	1.8743649	5.0273979	-2.8138945
H	4.2495785	5.2161111	-3.5063466
H	4.4328853	3.4613908	-3.4482920

6a $[W(CO)_5]PNPh_2C_2Ph_2$: **6a** + PhCCPh

59

Energy = -2033.902245424

P	-0.2666964	0.6391877	0.2419101
N	-1.3623636	-0.1463474	1.3355185
C	-0.8643294	-0.9099932	2.4099009
C	-1.6068328	-1.9597580	2.9746396
C	0.4028887	-0.6133265	2.9408624
C	-1.0738724	-2.7044262	4.0248254
H	-2.5928879	-2.1931876	2.5878764
C	0.9320302	-1.3753576	3.9786125
H	0.9664585	0.2283308	2.5498277
C	0.2006745	-2.4308428	4.5266389
H	-1.6623444	-3.5142140	4.4475707
H	1.9177922	-1.1328172	4.3655113
H	0.6122960	-3.0228112	5.3382657
C	-2.6761405	-0.3943178	0.8024984
C	-2.9045778	-1.4930028	-0.0335024
C	-3.7016424	0.5156416	1.0661066
C	-4.1600775	-1.6729390	-0.6131139
H	-2.0988886	-2.1947773	-0.2265857
C	-4.9549984	0.3337337	0.4806330
H	-3.5027897	1.3645146	1.7125390
C	-5.1842314	-0.7568040	-0.3602958
H	-4.3355187	-2.5221205	-1.2667640
H	-5.7492808	1.0480875	0.6756866
H	-6.1589701	-0.8932294	-0.8191706
W	1.4900202	-0.7191681	-0.9478635
C	2.8794916	-0.2356929	0.4909038
O	3.6583669	0.0342621	1.3026990
C	1.0279913	-2.4384792	0.0981174
O	0.7819782	-3.4216882	0.6510354
C	2.8955316	-1.7281146	-1.9922097
O	3.7044845	-2.2997480	-2.5975507
C	0.0681180	-1.2059277	-2.3579919
O	-0.7255958	-1.4854069	-3.1508178
C	1.9194551	1.0123861	-1.9752862
O	2.1496944	1.9913734	-2.5447178
C	-0.2480566	2.3989344	0.5493128
C	-1.1156541	2.0545450	-0.4145844
C	-2.0291895	2.4891425	-1.4429868
C	-2.7491884	1.5292216	-2.1759451
C	-2.1999056	3.8534580	-1.7466081
C	-3.6253111	1.9222843	-3.1814272
H	-2.6223724	0.4786452	-1.9365462
C	-3.0736390	4.2410018	-2.7571692
H	-1.6354020	4.6021928	-1.2010687
C	-3.7912823	3.2783590	-3.4743461
H	-4.1814697	1.1726628	-3.7364466
H	-3.1962278	5.2950404	-2.9884134

H	-4.4758723	3.5857064	-4.2595018
C	0.3488774	3.4558965	1.3276582
C	1.5393994	3.2067764	2.0343225
C	-0.2377631	4.7334880	1.4071063
C	2.1395993	4.2121712	2.7851892
H	1.9938405	2.2226407	1.9750140
C	0.3588718	5.7324348	2.1698160
H	-1.1695859	4.9298772	0.8871957
C	1.5502721	5.4772921	2.8557574
H	3.0637624	4.0111496	3.3186266
H	-0.1048675	6.7125209	2.2313440
H	2.0149429	6.2609629	3.4466950

7a electrophilic adduct of **5a** and C_2H_4
41
Energy = -1572.729649920

P	0.5324823	1.1093108	0.7060124
N	-0.1951063	0.4437463	2.1143278
C	0.6164331	-0.1764120	3.1152479
C	0.3943715	0.1175794	4.4659827
C	1.6486724	-1.0478254	2.7534906
C	1.1976136	-0.4659258	5.4439696
H	-0.4056181	0.7987717	4.7395618
C	2.4630537	-1.6114179	3.7357311
H	1.8087231	-1.2840583	1.7055621
C	2.2377346	-1.3274283	5.0837190
H	1.0193050	-0.2341735	6.4901308
H	3.2645983	-2.2844650	3.4454593
H	2.8670426	-1.7731403	5.8481674
C	-1.6084099	0.3076518	2.1464311
C	-2.2155661	-0.7452404	2.8486576
C	-2.4127830	1.2035126	1.4264075
C	-3.6000454	-0.8875418	2.8295366
H	-1.6017959	-1.4536809	3.3943244
C	-3.7969640	1.0384922	1.3972951
H	-1.9578042	2.0351718	0.8972001
C	-4.4010662	-0.0032451	2.1010523
H	-4.0541694	-1.7095974	3.3758553
H	-4.4014449	1.7379888	0.8271448
H	-5.4796178	-0.1266636	2.0826137
W	0.2911481	0.0063449	-1.5331792
C	2.0974929	-0.9217300	-1.1978641
O	3.1133431	-1.4399489	-1.0064785
C	-0.6940858	-1.5688696	-0.6310293
O	-1.2343862	-2.4528435	-0.1233382
C	0.1479335	-0.9013880	-3.3363150
O	0.0728073	-1.4213513	-4.3705974
C	-1.5134802	0.9512379	-1.8666926
O	-2.5181675	1.4779957	-2.0837784
C	1.2724479	1.6107563	-2.3658021
O	1.8234872	2.5210795	-2.8190290
C	0.7642026	2.8969264	1.0410775
C	1.9717863	2.0185372	1.3410651
H	2.8215703	2.0828871	0.6680607
H	2.2351597	1.8582152	2.3821511
H	0.8141434	3.5544892	0.1773551
H	0.2215976	3.2997743	1.8906231

C_2H_4 : ethylene
6
Energy = -78.63740833140

C	-1.8253213	0.1356016	0.0000007
C	-0.4928300	0.1355848	0.0000086
H	-2.3971511	1.0606878	-0.0000141
H	-2.3971716	-0.7894743	-0.0000104
H	0.0789993	-0.7895021	-0.0000353
H	0.0790194	1.0606615	0.0000354

ClLic ClLi(12-crown-4)
30
Energy = -1083.609609229

Cl	0.0045386	-0.0004779	3.1100263
Li	0.0045994	-0.0010435	0.8821557
O	-1.3023837	-1.4258092	-0.0541579
O	1.3121384	1.4251092	-0.0545691
O	1.4272779	-1.3058340	-0.0572052
C	-2.4899163	-0.7488024	-0.5109293
C	-0.6046555	-2.1511402	-1.0816997
C	2.4988611	0.7475567	-0.5128825
C	0.6127760	2.1498088	-1.0815871
C	0.7532133	-2.4995471	-0.5016717
C	2.1368962	-0.6060912	-1.0941707
H	-3.0254700	-1.3603324	-1.2464935
H	-3.1141644	-0.6221664	0.3770851
H	-1.1593950	-3.0620160	-1.3434228
H	-0.5027225	-1.5336372	-1.9844064
H	3.1245158	0.6210775	0.3742173
H	3.0342280	1.3584337	-1.2492162
H	1.1660542	3.0615641	-1.3435930
H	0.5105862	1.5324726	-1.9843885
H	0.6341727	-3.1169184	0.3921661
H	1.3637958	-3.0391045	-1.2351874
H	3.0413208	-1.1624324	-1.3745268
H	1.5042990	-0.4975565	-1.9856871
O	-1.4185213	1.3042754	-0.0555536
C	-0.7443695	2.4979236	-0.4998818
H	-1.3558509	3.0386209	-1.2319227
H	-0.6226780	3.1138447	0.3945862
C	-2.1294963	0.6052728	-1.0921841
H	-1.4979752	0.4973679	-1.9844724
H	-3.0344508	1.1615555	-1.3707293

ClLit$_3$ ClLi(THF)$_3$
41
Energy = -1165.708873408

Cl	0.8615771	0.1133934	-0.6681205
Li	2.9325778	0.9661965	-0.3029879
O	4.2833469	0.1942249	-1.5031032
O	2.9749768	2.9219029	-0.5903930
O	3.5431290	0.7104578	1.5498454
C	3.7995009	-0.4132910	-2.7375651
C	5.4066808	-0.5831437	-0.9850177
C	1.7027399	3.6094490	-0.4781088
C	3.6754626	3.5045935	-1.7246865
C	2.8121309	-0.2310380	2.3925325
C	3.9167521	1.8370078	2.3782166
C	4.2854604	-1.8542297	-2.6764421
H	2.7126125	-0.3037973	-2.7375381
H	4.2366989	0.1262073	-3.5884326
C	5.6608065	-1.6914770	-2.0092166
H	5.1118204	-0.9782454	-0.0077365
H	6.2573943	0.0925545	-0.8559975
C	1.2616955	3.7910578	-1.9243523
H	1.0453942	2.9652874	0.1083501
H	1.8558713	4.5699290	0.0342456
C	2.5908291	4.1022460	-2.6494540
H	4.2529882	2.6982560	-2.1800486
H	4.3613985	4.2747653	-1.3529400
C	2.3075607	0.5740622	3.6098180
H	2.0091929	-0.6340647	1.7715688
H	3.4964410	-1.0344461	2.6884155
C	2.7137023	2.0290427	3.2927961
H	4.1185374	2.6733402	1.7071370
H	4.8232166	1.5855964	2.9470401
H	3.6156576	-2.4472788	-2.0445534
H	4.3419666	-2.3191666	-3.6641512
H	6.0221116	-2.6084080	-1.5367221
H	6.4019548	-1.3689129	-2.7481137
H	0.8338396	2.8493779	-2.2801828
H	0.5216168	4.5869217	-2.0436287
H	2.6214934	3.6596240	-3.6479016
H	2.7345893	5.1813007	-2.7543241
H	1.2285486	0.4687237	3.7443978
H	2.7991309	0.2308707	4.5247754
H	1.9163601	2.5432340	2.7468997
H	2.9508450	2.6062503	4.1904898

(ClLit)$_4$ [ClLi(THF)]$_4$
60
Energy = -2802.065823960

Cl	1.8228550	-0.0029614	1.2819008
Li	0.0024251	-1.5066636	1.0527409
O	-0.0215481	-2.9001799	2.3787330
C	1.0214676	-2.9002468	3.3906994
C	-1.2565527	-3.0999999	3.1208337
C	0.4407953	-2.0665549	4.5359229
C	-1.0945989	-2.2727188	4.4068455
Cl	-1.8337894	-0.0076777	1.2805055
Li	-0.0133828	1.4953283	1.0517085
O	0.0139092	2.8913410	2.3734063
C	1.2542101	3.0988665	3.1045956
C	-1.0205565	2.8879578	3.3940825
C	1.1070140	2.2747176	4.3944825
C	-0.4260085	2.0590737	4.5355455
H	1.2094815	-3.9384047	3.6934686
H	1.9160599	-2.4764851	2.9328567
H	-1.3574610	-4.1711699	3.3347727
H	-2.0747612	-2.7707919	2.4791569
H	0.8278116	-2.3870337	5.5062623
H	0.6992149	-1.0145106	4.3925655
H	-1.5138810	-2.7999256	5.2672353
H	-1.6072244	-1.3131162	4.3085956
H	2.0684420	2.7713268	2.4570182
H	1.3520980	4.1711151	3.3143848
H	-1.9168681	2.4591365	2.9443563
H	-1.2112204	3.9256404	3.6968473
H	1.6251252	1.3181371	4.2957617
H	1.5289440	2.8076951	5.2500142
H	-0.6788091	1.0052924	4.3949832
H	-0.8076567	2.3778389	5.5085692
Cl	0.0002967	1.8222385	-1.2812136
Li	-1.5054459	0.0034629	-1.0525128
O	-2.8985591	-0.0181713	-2.3790415
C	-2.8980370	1.0257578	-3.3900438
C	-3.0996460	-1.2523145	-3.1221971
C	-2.0653139	0.4454054	-4.5361614
C	-2.2723268	-1.0899644	-4.4081117
Cl	-0.0088510	-1.8345398	-1.2803206
Li	1.4961012	-0.0159088	-1.0512764
O	2.8920059	0.0101679	-2.3732073
C	3.1015944	1.2507565	-3.1033101
C	2.8868444	-1.0233573	-3.3948269
C	2.2768895	1.1061680	-4.3931172
C	2.0588520	-0.4263790	-4.5356928
H	-3.9361397	1.2150046	-3.6922356
H	-2.4732721	1.9195384	-2.9315533
H	-4.1709329	-1.3520019	-3.3361542
H	-2.7711755	-2.0714093	-2.4812762
H	-2.3861577	0.8333172	-5.5060230
H	-1.0130302	0.7031003	-4.3932761
H	-2.7997354	-1.5084106	-5.2687816
H	-1.3129973	-1.6031760	-4.3101850
H	2.7756263	2.0649873	-2.4549366
H	4.1739725	1.3469305	-3.3132239

H	2.4566081	-1.9193753	-2.9458722
H	3.9241839	-1.2154320	-3.6978776
H	1.3211378	1.6256433	-4.2935797
H	2.8102878	1.5281556	-5.2483605
H	1.0046720	-0.6776529	-4.3953881
H	2.3770132	-0.8075672	-5.5090947

Cl^- chloride anion
1
Energy = -460.3887073905

Cl	-0.0000765	0.0000001	0.0674709

HnLic$^+$ $MeNH_2Li$(12-crown-4)
36
Energy = -719.1216738832

Li	-0.1657800	-0.0291633	-0.0253254
O	0.6504972	0.9750059	1.6224217
C	0.2582765	0.2807448	2.8243876
C	2.0795489	1.0862696	1.4424665
C	-1.2227162	-0.0091993	2.6754707
H	0.4436654	0.9132514	3.7014251
H	0.8362199	-0.6463497	2.9328717
C	2.6211549	-0.1672373	0.7829814
H	2.5765122	1.2716100	2.4008806
H	2.2255936	1.9502734	0.7895527
O	-1.4654799	-0.7384038	1.4518737
H	-1.7828771	0.9238404	2.5760841
H	-1.6020312	-0.5664517	3.5388145
O	1.8706567	-0.3295219	-0.4377774
H	2.4902299	-1.0452785	1.4292348
H	3.6888379	-0.0563516	0.5560703
C	-1.2971936	-2.1661825	1.5718011
C	2.0357542	-1.6187200	-1.0671043
C	-1.2725043	-2.7055445	0.1547515
H	-0.3628305	-2.3952632	2.1009894
H	-2.1334512	-2.5966003	2.1367078
C	1.0688582	-2.6198480	-0.4651667
H	1.8069613	-1.4608401	-2.1238660
H	3.0701480	-1.9661915	-0.9715668
O	-0.2442646	-2.0418868	-0.6118743
H	-1.1186204	-3.7900847	0.1510332
H	-2.2116234	-2.4747359	-0.3541414
H	1.1199077	-3.5777712	-0.9975988
H	1.2896651	-2.7969146	0.5957371
N	-1.0320922	1.1762798	-1.4091575
C	-0.5646525	0.8695270	-2.7854082
H	-2.0490964	1.0904827	-1.3790547
H	0.5185207	1.0090697	-2.8274621
H	-0.7861782	-0.1775244	-3.0066456
H	-1.0323074	1.5005543	-3.5502542
H	-0.8460421	2.1599870	-1.2088087

Hn $MeNH_2$
7
Energy = -95.91823399162

C	-0.0967579	0.8009561	3.4598507
H	0.6668728	1.5460297	3.2153894
H	-1.0838673	1.2829835	3.3839090
H	0.0543210	0.4940076	4.4996816
N	0.0781007	-0.3733228	2.5809540
H	-0.6497410	-1.0579618	2.7875704
H	-0.0815486	-0.0934519	1.6128332

HoLic$^+$ MeOHLi(12-crown-4)
35
Energy = -738.9924998212

Li	-0.2504482	-0.2081157	-0.1038057
O	0.5774657	0.9648669	1.4157262
C	0.2343437	0.3819869	2.6893186
C	1.9962034	1.1034178	1.1840668
C	-1.2425370	0.0478424	2.6057621
H	0.4249791	1.1005688	3.4960733
H	0.8374261	-0.5172523	2.8711767
C	2.5595830	-0.1866129	0.6200723
H	2.5136176	1.3872275	2.1067604
H	2.0953926	1.9110867	0.4546313
O	-1.4947448	-0.7990332	1.4614597
H	-1.8263794	0.9550708	2.4329664
H	-1.5895905	-0.4344787	3.5256922
O	1.7726563	-0.4846881	-0.5518553
H	2.4825105	-1.0059720	1.3466986
H	3.6136298	-0.0622717	0.3427819
C	-1.2881162	-2.2051776	1.7146473
C	1.9581371	-1.8218876	-1.0659750
C	-1.2797611	-2.8791168	0.3565804
H	-0.3367939	-2.3587328	2.2406239
H	-2.1007684	-2.5969094	2.3386734
C	1.0420908	-2.7883275	-0.3403820
H	1.6901950	-1.7692666	-2.1240895
H	3.0054698	-2.1288907	-0.9748567
O	-0.2912428	-2.2606472	-0.4958954
H	-1.0901359	-3.9535431	0.4530741
H	-2.2370460	-2.7275208	-0.1480340
H	1.1043899	-3.7900490	-0.7832315
H	1.3012664	-2.8589803	0.7243019
O	-1.0163436	0.8609934	-1.4957620
C	-0.2779714	1.4635843	-2.5851741
H	-1.9573812	1.0640324	-1.6051135
H	0.7694117	1.2085389	-2.4214555
H	-0.6120138	1.0575932	-3.5447208
H	-0.4000233	2.5508420	-2.5743409

Ho MeOH
6
Energy = -115.7944957160

H	-0.0167505	-0.0798849	1.6886658
O	0.0868426	-0.3691789	2.6089528
C	-0.0856265	0.7846988	3.4505439
H	0.6412692	1.5710323	3.2097064
H	-1.1009396	1.1942718	3.3697081
H	0.0818657	0.4480587	4.4760684

Lic$_2^+$ Li(12-crown-4)$_2^+$
57
Energy = -1238.900467273

Li	-0.0003150	0.0005907	0.0007573
O	-0.5697131	1.8735502	1.3425857
O	0.5695662	-1.8724804	1.3423322
O	1.8724055	0.5699129	1.3424621
O	-1.8725964	-0.5688720	1.3425340
C	1.5176303	-1.5980735	2.3821053
C	-1.5176602	1.5990639	2.3824294
C	1.5984390	1.5181563	2.3821503
C	0.6252513	2.5258760	1.8022174
C	2.5251947	-0.6248489	1.8020158
C	-0.6253037	-2.5248432	1.8021053
C	-2.5252827	0.6258886	1.8023344
C	-1.5984604	-1.5171493	2.3821198
H	2.0175145	-2.5263016	2.6943400
H	1.0140583	-1.1688799	3.2589412
H	1.1696363	1.0148290	3.2593055
H	-2.0175809	2.5272449	2.6947518
H	-1.0139867	1.1698902	3.2592322
H	0.3852022	3.3002305	2.5421342
H	2.9898507	-1.0587564	0.9141080
H	1.0592397	2.9905210	0.9143845
H	-1.1696344	-1.0137519	3.2592222
H	2.5267894	2.0180670	2.6939315
H	3.2996635	-0.3846090	2.5417295
H	-2.9899772	1.0599083	0.9145401
H	-0.3851430	-3.2991723	2.5420243
H	-1.0594127	-2.9894984	0.9143448
H	-3.2996536	0.3855218	2.5421177
H	-2.5267255	-2.0171543	2.6939976
O	0.5693279	1.8729761	-1.3411695
O	-0.5704726	-1.8728327	-1.3412944
O	-1.8731823	0.5697605	-1.3412224
O	1.8719174	-0.5694992	-1.3410959
C	-1.5186956	-1.5984890	-2.3809630
C	1.5175857	1.5987643	-2.3808073
C	-1.5985218	1.5176830	-2.3810222
C	-0.6255038	2.5254456	-1.8009188
C	-2.5259753	-0.6249614	-1.8008138
C	0.6243497	-2.5252254	-1.8010273
C	2.5248380	0.6251805	-1.8007161
C	1.5974570	-1.5173986	-2.3809084
H	-2.0190595	-2.5266351	-2.6926694
H	-1.0152823	-1.1699009	-3.2582245
H	-1.1690058	1.0139844	-3.2576047
H	2.0179348	2.5269391	-2.6924518
H	1.0141615	1.1702595	-3.2580996
H	-0.3853379	3.2998328	-2.5407398
H	-2.9905790	-1.0588654	-0.9128650
H	-1.0595622	2.9901513	-0.9131201
H	1.1680876	-1.0136455	-3.2575350
H	-2.5266275	2.0175324	-2.6936561
H	-3.3004833	-0.3846998	-2.5404744
H	2.9894665	1.0590210	-0.9127509
H	0.3842465	-3.2994562	-2.5410431
H	1.0583541	-2.9901045	-0.9133063
H	3.2992393	0.3847422	-2.5404052
H	2.5256242	-2.0172346	-2.6934332

LiClm $(LiCl)_{28}$ nano-cluster
56
Energy = -13101.51894196

Li	4.7101014	2.0818359	-0.0645311
Li	4.6112011	-1.1347229	-1.9934664
Li	4.6879550	-1.1994903	1.7448033
Li	-3.8971741	-0.9263781	1.5803666
Li	-3.9450773	-0.7250583	-1.5386545
Li	-3.8712608	1.8767837	0.2053839
Li	-3.5951888	1.7681553	-3.2228729
Li	-3.6416862	-3.6291342	0.2488602
Li	-3.4738989	2.0599865	3.2103889
Li	2.2150416	-0.0425504	-0.0497925
Li	2.5068039	-0.0245313	3.4920674
Li	1.8384768	-2.9359043	2.5512524
Li	2.4433334	3.0126094	-1.8402075
Li	1.9294860	3.6531644	1.1792460
Li	1.7495501	-0.8330248	-3.8440888
Li	2.3375832	-3.1358719	-1.8125928
Li	-0.8602253	-4.3188913	2.6670511
Li	-0.7597551	0.7993001	-1.9217346
Li	-0.9249313	-0.1080939	-5.0653621
Li	-0.2813359	3.3888894	-3.8707770
Li	-0.4003751	-5.0321200	-0.9882679
Li	-0.7740529	-2.0518699	0.3051955
Li	-0.4884116	-2.8991836	-3.1375972
Li	-0.1375022	1.6586416	4.8799052
Li	-0.6845689	1.2978259	1.6694217
Li	-0.6945426	4.4643949	2.4600478
Li	-0.3026539	4.1931887	-0.9476068
Li	-0.2966607	-1.2600914	4.1017578

Cl	-5.1459703	1.3398049	-1.6490218
Cl	-5.1929089	-2.0357154	-0.0976833
Cl	-5.0918742	0.9923465	2.0653562
Cl	3.7266098	0.9898190	-1.8880296
Cl	3.7286372	-2.0810810	3.5785408
Cl	3.7990455	0.9684237	1.7332176
Cl	3.7116869	-2.1704093	-0.0981380
Cl	3.7510601	4.1162158	-0.1702924
Cl	3.5754160	-2.2420055	-3.6562742
Cl	-2.5402479	-0.3134082	-3.4366672
Cl	-1.9608010	3.0760507	-2.2689949
Cl	-2.1778779	0.0454944	0.0489458
Cl	-2.0792371	-3.4610513	-1.4352511
Cl	-2.4914600	-2.7925459	2.1106551
Cl	-2.3971124	3.2466045	1.5060112
Cl	-1.8878170	0.5088787	3.8308093
Cl	1.1678282	4.7080765	-2.7616757
Cl	1.2547119	-0.0210730	5.4376887
Cl	0.3581960	-3.4626619	4.3555811
Cl	0.7534468	-0.7849958	1.8835600
Cl	0.8226165	2.8117070	3.1341626
Cl	0.4418785	5.4934495	0.8142438
Cl	0.7494638	2.0215809	-0.2961327
Cl	0.1917186	-2.0594182	-5.1829002
Cl	0.6334675	-4.1515291	0.8710372
Cl	0.6752996	-1.2782117	-1.6337930
Cl	0.9721106	-4.7527439	-2.7505286
Cl	0.6518823	1.2905387	-4.0426222

Lict^{+} Li(12-crown-4)(THF)$^{+}$

42

Energy = -855.7938526787

Li	-0.2318508	-0.2069760	-0.1113055
O	-0.2616409	-2.2367719	-0.5271365
O	-1.0024250	0.9911602	-1.3806540
O	0.5597888	0.9642999	1.4204598
O	-1.4974623	-0.8041933	1.4333421
O	1.8002879	-0.4678175	-0.5401848
C	0.2124553	0.3753953	2.6890620
C	-0.3605848	1.2854040	-2.6616058
C	1.0672017	-2.7707969	-0.3516758
C	-1.3038745	-2.2150187	1.6666653
C	-1.2682771	-2.8659363	0.2968976
C	-1.7496577	2.1631867	-0.9240823
C	-0.4709342	2.7965217	-2.8301086
C	-1.2608068	0.0258637	2.5922363
C	-1.8016527	3.1014747	-2.1248108
C	1.9778491	1.1191194	1.2004026
C	2.0013152	-1.8030596	-1.0520139
C	2.5624459	-0.1657151	0.6460453
H	0.6676268	0.9194609	-2.6083808
H	0.3892339	1.0936594	3.4995419
H	0.8231496	-0.5183189	2.8738046
H	-0.3667395	-2.3836065	2.2130552
H	0.3568688	3.2992334	-2.3181897
H	-1.2061847	2.6049758	-0.0807961
H	1.1326724	-3.7695810	-0.8004350
H	1.3057453	-2.8494683	0.7171528
H	-1.0812995	-3.9420266	0.3797685
H	-0.9040106	0.7445912	-3.4442496
H	-1.8543482	0.9291800	2.4317308
H	-0.4633152	3.0954188	-3.8810230
H	-2.7299591	1.8175569	-0.5867928
H	-2.2145113	-2.7048533	-0.2248035
H	2.4787528	-0.9864161	1.3707953
H	-2.1332723	-2.6136105	2.2639181
H	-1.6063543	-0.4750969	3.5027203
H	1.7627822	-1.7493103	-2.1172464
H	-1.8979037	4.1474755	-1.8244530
H	2.4839559	1.4128575	2.1264524
H	2.0740100	1.9237729	0.4671710
H	-2.6450341	2.8448283	-2.7743955
H	3.0458632	-2.1101622	-0.9333754
H	3.6205671	-0.0320850	0.3891793

Lic^{+} Li(12-crown-4)$^{+}$

29

Energy = -623.1790335421

Li	-0.1833361	-0.2571869	-0.0373083
O	-0.2619833	-2.2370187	-0.5119998
O	0.5647317	0.9571896	1.4199508
O	-1.4834096	-0.8124067	1.4379530
O	1.7890415	-0.4730366	-0.5267693
C	0.2124909	0.3797563	2.6974386
C	1.0683550	-2.7813447	-0.3581337
C	-1.3079225	-2.2270040	1.6780078
C	-1.2674569	-2.8783735	0.3086754
C	-1.2584304	0.0229774	2.5989075
C	1.9887461	1.1145422	1.2112604
C	1.9985831	-1.8056193	-1.0524730
C	2.5699863	-0.1687548	0.6509376
H	0.3849800	1.1093019	3.4975336
H	0.8280747	-0.5081665	2.8916226
H	-0.3774221	-2.4022759	2.2333322
H	1.1235039	-3.7723936	-0.8237486
H	1.3140859	-2.8777914	0.7074051
H	-1.0704140	-3.9520928	0.3891903
H	-1.8584705	0.9209592	2.4344710
H	-2.2133146	-2.7234504	-0.2157167
H	2.4972218	-0.9914580	1.3742859
H	-2.1472043	-2.6134443	2.2685485
H	-1.6024040	-0.4812108	3.5074480

H	1.7616009	-1.7420119	-2.1170838
H	2.4853203	1.3965971	2.1451769
H	2.0904128	1.9262871	0.4874138
H	3.0443604	-2.1061306	-0.9328468
H	3.6230840	-0.0333129	0.3775632

Lit$_4$ $^+$ Li(THF)$_4$$^+$

53

Energy = -937.8922194929

Li	-0.3885753	-0.0906300	-0.0801932
O	0.6371916	1.0782378	1.0761203
O	0.8174045	-0.9427398	-1.3197664
O	-1.7078200	0.9809485	-0.9935922
O	-1.2119905	-1.4337095	1.0241193
C	1.2614383	2.2953318	0.5681594
C	0.4843092	1.1728582	2.5269635
C	0.3764858	-2.0407324	-2.1803507
C	2.2435708	-1.0815827	-1.0474011
C	-2.4962302	2.0073471	-0.3266091
C	-1.7111369	1.2230784	-2.4370745
C	-2.5782035	-1.3899340	1.5400218
C	-0.4730482	-2.5088017	1.6754661
C	1.0863320	3.3231061	1.6778979
H	0.7632806	2.5536408	-0.3695035
H	2.3198189	2.0874362	0.3697045
C	1.2157288	2.4493824	2.9352209
H	-0.5870439	1.2229587	2.7518814
H	0.9038390	0.2660550	2.9701910
C	1.6348150	-2.8429854	-2.5149104
H	-0.3556777	-2.6298831	-1.6171979
H	-0.1091094	-1.6087139	-3.0593131
C	2.5535743	-2.5469035	-1.3186175
H	2.7953130	-0.4182591	-1.7250566
H	2.4092591	-0.7643245	-0.0154127
C	-2.5388989	3.1682806	-1.3099628
H	-2.0028116	2.2367726	0.6209828
H	-3.4987130	1.6094126	-0.1259291
C	-2.6246773	2.4296705	-2.6548876
H	-0.6778868	1.4227633	-2.7404636
H	-2.0652298	0.3147537	-2.9318941
C	-2.7337570	-2.6497272	2.3871866
H	-2.6855045	-0.4792047	2.1415128
H	-3.2554137	-1.3425774	0.6840796
C	-1.3026772	-2.8783908	2.8981131
H	0.5266676	-2.1332709	1.9091532
H	-0.3901385	-3.3474614	0.9734389
H	0.0915059	3.7789368	1.6255806
H	1.8360842	4.1164310	1.6293141
H	0.7756986	2.9073993	3.8240040
H	2.2700541	2.2366509	3.1388255
H	1.4182426	-3.9066230	-2.6390138
H	2.0898750	-2.4731969	-3.4393623
H	2.2780526	-3.1623608	-0.4553209
H	3.6103785	-2.7120440	-1.5417049
H	-1.6158624	3.7551444	-1.2489829
H	-3.3878380	3.8328733	-1.1323398
H	-2.2990543	3.0393436	-3.5005967
H	-3.6533022	2.1035159	-2.8378601
H	-3.4605501	-2.5155440	3.1917390
H	-3.0531733	-3.4927247	1.7655832
H	-1.0793371	-2.2031844	3.7310570
H	-1.1233349	-3.9055977	3.2239112

MeOLic or MeOLi(**12c4**)

34

Energy = -738.5003735239

Li	0.0376864	-0.2788982	0.9976040
O	-1.2939046	-1.6081356	-0.1295689
O	1.3435564	1.2467146	0.0919861
O	1.4522237	-1.5004536	-0.1467281
C	-2.4764512	-0.8783706	-0.5060210
C	-0.6023989	-2.2171615	-1.2318820
C	2.5156687	0.5959650	-0.4277911
C	0.6319327	2.0368760	-0.8726968
C	0.7566589	-2.6334012	-0.7004632
C	2.1440108	-0.7014974	-1.1211807
H	-3.0364941	-1.4179316	-1.2794648
H	-3.0821639	-0.8199344	0.4016237
H	-1.1598686	-3.0932714	-1.5908923
H	-0.5017343	-1.5061455	-2.0631793
H	3.1455812	0.3892867	0.4412298
H	3.0568259	1.2579658	-1.1149494
H	1.1798977	2.9664198	-1.0799065
H	0.5176350	1.4862745	-1.8166736
H	0.6346311	-3.3343842	0.1292183
H	1.3527327	-3.1087189	-1.4889580
H	3.0465182	-1.2237148	-1.4667686
H	1.4995072	-0.5131022	-1.9905860
O	-1.4042235	1.1348488	0.1043222
C	-0.7178094	2.3470598	-0.2532078
H	-1.3253960	2.9520521	-0.9374584
H	-0.5810776	2.8901980	0.6850740
C	-2.1149132	0.5171824	-0.9790536
H	-1.4878837	0.4791296	-1.8805083
H	-3.0225293	1.0906115	-1.2141243
O	0.0492696	-0.3525992	2.7733528
C	-0.0869199	0.7729180	3.5637471
H	0.6246658	1.5922812	3.2983168
H	-1.1013346	1.2363086	3.5062258
H	0.0835399	0.5753097	4.6485767

PhCCPh tolane

24
Energy = -539.7930404158

C	-2.0291365	0.0000010	0.0014459
C	-2.7461547	-1.2150390	0.0106082
C	-2.7461276	1.2150589	-0.0077172
C	-4.1378372	-1.2091383	0.0092352
H	-2.1998051	-2.1530625	0.0192023
C	-4.1378080	1.2091674	-0.0094492
H	-2.1997540	2.1530923	-0.0131230
C	-4.8389834	0.0000115	-0.0014681
H	-4.6780932	-2.1514737	0.0168550
H	-4.6780442	2.1515139	-0.0171410
H	-5.9250402	0.0000163	-0.0041362
C	-0.6091815	-0.0000111	0.0007776
C	0.6091409	0.0000193	0.0000673
C	2.0291274	0.0000169	-0.0005938
C	2.7461344	-1.2150483	-0.0099586
C	2.7461551	1.2150721	0.0083832
C	4.1378212	-1.2091602	-0.0096929
H	2.1997579	-2.1530726	-0.0177008
C	4.1378414	1.2091519	0.0089838
H	2.1997972	2.1531180	0.0146768
C	4.8389864	-0.0000156	0.0003106
H	4.6780602	-2.1515009	-0.0176425
H	4.6780974	2.1514881	0.0162950
H	5.9250432	-0.0000264	0.0018103

Be CH_2=CMe_2
12
Energy = -157.3223473943

C	-0.0001678	1.4626299	0.0000016
C	-0.0000130	0.1238090	-0.0000014
H	-0.0002377	2.0305389	0.9277415
H	-0.0002876	2.0305406	-0.9277395
C	0.0000040	-0.6768534	-1.2764859
C	0.0001414	-0.6768528	1.2764849
H	0.8800913	-1.3320785	-1.3219179
H	-0.8804670	-1.3315529	-1.3221953
H	0.0003365	-0.0305136	-2.1586817
H	-0.8798030	-1.3322704	1.3219091
H	0.8807544	-1.3313608	1.3222055
H	-0.0003394	-0.0305110	2.1586792

***t*BuLi** (*t*BuLi)$_4$ tretramer
56
Energy = -661.9537502791

C	-0.1967287	-0.3314666	2.2067120
C	-1.1735672	-1.4781766	2.5366672
C	1.1515151	-0.6989938	2.8590346
C	-0.7169539	0.9189563	2.9445000
H	-2.1957814	-1.3001685	2.1591196
H	-0.8350065	-2.4429456	2.1311132
H	-1.2890656	-1.6228580	3.6293925
H	1.8936978	0.1067695	2.7624604
H	1.0458762	-0.8973870	3.9443118
H	1.6010249	-1.6166611	2.4404607
H	-0.7745156	0.7590418	4.0397069
H	-0.0661084	1.8017670	2.8159000
H	-1.7278722	1.2037442	2.6195706
C	0.2061221	-1.9751608	-1.0402204
C	0.7100818	-1.8191678	-2.4893803
C	1.1968097	-2.9176279	-0.3271370
C	-1.1382915	-2.7267269	-1.1200493
H	0.0469621	-1.1966423	-3.1154216
H	1.7169817	-1.3792679	-2.5352744
H	0.7719717	-2.7939089	-3.0132068
H	0.8720861	-3.1691457	0.6931799
H	1.3113494	-3.8806369	-0.8636357
H	2.2171371	-2.5021096	-0.2575006
H	-1.0324542	-3.7132769	-1.6137422
H	-1.5726497	-2.9449744	-0.1287581
H	-1.8927708	-2.1718757	-1.6969401
C	1.8155269	1.2514496	-0.4058027
C	1.9250755	2.4569779	0.5499352
C	3.1188083	0.4422706	-0.2480095
C	1.8213428	1.8225066	-1.8383399
H	1.0616532	3.1417373	0.4841305
H	2.0233319	2.1488918	1.6009629
H	2.8108171	3.0839898	0.3249197
H	3.1794961	-0.3939552	-0.9600841
H	4.0178550	1.0659178	-0.4234562
H	3.2496815	0.0250426	0.7657135
H	2.7384361	2.4086530	-2.0470778
H	1.7952714	1.0402715	-2.6171138
H	0.9738684	2.4995134	-2.0203846
C	-1.8240649	1.0578534	-0.7601682
C	-1.9407459	0.9973278	-2.2967776
C	-3.1251557	0.4524772	-0.1947024
C	-1.8293217	2.5512424	-0.3751518
H	-1.0781046	1.4501926	-2.8161978
H	-2.0442870	-0.0333980	-2.6660812
H	-2.8261224	1.5515630	-2.6671704
H	-3.1809405	0.5333890	0.9008265
H	-4.0256145	0.9627604	-0.5908314
H	-3.2578611	-0.6119346	-0.4557735
H	-2.7461102	3.0658226	-0.7256804
H	-1.8037193	2.7178751	0.7158734
H	-0.9814979	3.0981470	-0.8131676
Li	0.1287073	0.2210598	-1.4459330
Li	-1.1894351	-0.8195512	0.2656366
Li	-0.1331173	1.2952218	0.6805301
Li	1.1963768	-0.6944147	0.4985121

*t*BuCl Me_3CCl
14
Energy = -618.1970674978

C	-1.2655558	-0.7306721	0.7955134
C	-0.0000013	-0.0000380	0.3626850
H	-2.1591297	-0.2186151	0.4286643
H	-1.2686632	-1.7607349	0.4292182
H	-1.3015817	-0.7510603	1.8916698
C	1.2655516	-0.7306786	0.7955078
C	0.0000080	1.4612935	0.7956051
H	2.1591392	-0.2185032	0.4288557
H	1.3014365	-0.7512728	1.8916663
H	1.2687464	-1.7606762	0.4290355
H	0.0001321	1.5026254	1.8917865
H	0.8903376	1.9791399	0.4289763
H	-0.8904108	1.9791228	0.4291692
Cl	-0.0000089	0.0000694	-1.5133819

***t*BuLic** $Me_3CLi(12\text{-crown-4})$
42
Energy = -781.1842671954

Li	-0.2005240	-0.1282800	-0.1844102
O	-0.2381696	-2.3052233	-0.4563365
O	0.7262388	0.9320348	1.4913748
O	-1.4280066	-0.7814147	1.4985785
O	1.9159433	-0.5940972	-0.4641613
C	0.3319421	0.3447705	2.7410665
C	1.0703057	-2.8619072	-0.2519347
C	-1.2406422	-2.1819492	1.7541315
C	-1.2550829	-2.8605633	0.3968920
C	-1.1561258	0.0704271	2.6259311
C	2.1483543	0.9803747	1.2806592
C	2.0383117	-1.9368233	-0.9656560
C	2.6527468	-0.3460812	0.7436949
H	0.5324265	1.0401729	3.5678784
H	0.8920900	-0.5822516	2.9259143
H	-0.2878635	-2.3558513	2.2728623
H	1.1222350	-3.8750191	-0.6739098
H	1.3004609	-2.9220060	0.8206958
H	-1.1258578	-3.9448049	0.5018889
H	-1.6907560	1.0011202	2.4203692
H	-2.2018323	-2.6578789	-0.1101543
H	2.4872960	-1.1542605	1.4694047
H	-2.0534324	-2.5656444	2.3861238
H	-1.5428443	-0.3735444	3.5514723
H	1.7816799	-1.8754135	-2.0263468
H	2.6711593	1.2487824	2.2069693
H	2.3055618	1.7664276	0.5377274
H	3.0689862	-2.2983756	-0.8637118
H	3.7285993	-0.2906175	0.5274797
C	-1.1399169	1.1259346	-1.5725515
C	-2.1219564	2.0322246	-0.8375694
C	-0.1217585	2.0123991	-2.2814057
C	-1.9130721	0.3519077	-2.6341553
H	-2.9079163	1.4579805	-0.3231121
H	-1.6209902	2.6484231	-0.0750433
H	-2.6517156	2.7482104	-1.5241599
H	0.6065756	1.4235895	-2.8596975
H	-0.5980133	2.7279900	-3.0066729
H	0.4528922	2.6296042	-1.5729672
H	-2.4368663	1.0243445	-3.3679663
H	-1.2560056	-0.3017801	-3.2278682
H	-2.6923121	-0.2891712	-2.1933604

***t*BuLit$_2$** $Me_3CLi(THF)_2$
40
Energy = -630.6769465552

Li	0.6356448	0.4252955	-3.4722488
O	-0.5184374	1.7902001	-4.2320487
O	0.5801451	-1.0566756	-4.7441684
C	-1.4566686	2.4257841	-3.3261353
C	-1.2209761	1.6741779	-5.4978328
C	-0.5753298	-1.9224157	-4.5339896
C	1.7754061	-1.8799771	-4.9355912
C	-2.7859644	1.7316662	-3.6211657
H	-1.0754831	2.2729060	-2.3156173
H	-1.4962856	3.4995960	-3.5531565
C	-2.6954052	1.3991125	-5.1354221
H	-0.7359799	0.8725554	-6.0562950
H	-1.1113247	2.6199486	-6.0424776
C	0.0038755	-3.2701887	-4.1268295
H	-1.1999443	-1.4584133	-3.7656972
H	-1.1385058	-1.9864959	-5.4735051
C	1.2863205	-3.3281828	-4.9718057
H	2.4455966	-1.6940390	-4.0897289
H	2.2577934	-1.5578314	-5.8622051
H	-2.8636816	0.8147301	-3.0300228
H	-3.6425016	2.3663896	-3.3813579
H	-2.9643690	0.3571207	-5.3242146
H	-3.3611259	2.0304563	-5.7290092
H	0.2451181	-3.2690520	-3.0591006
H	-0.6817619	-4.0960731	-4.3321806
H	2.0314590	-4.0199251	-4.5715120
H	1.0504583	-3.6283232	-5.9980429
C	0.9305897	0.1304763	-1.4146544
C	1.3209027	1.3854932	-0.6325663
C	-0.3600333	-0.4116507	-0.7941974
C	2.0213545	-0.9147994	-1.1692457
H	1.4448431	1.1800474	0.4621269
H	2.2746839	1.8105756	-0.9784490
H	0.5655258	2.1825099	-0.7109504

H	-1.1988910	0.2960547	-0.8816463
H	-0.6839169	-1.3552928	-1.2600526
H	-0.2466538	-0.6272200	0.2997069
H	3.0029703	-0.5912119	-1.5471900
H	2.1598468	-1.1344234	-0.0789979
H	1.7911638	-1.8784176	-1.6484228

***t*BuLit$_3$** $Me_3CLi(THF)_3$
53
Energy = -863.2859060538

Li	-0.3642253	0.1130433	-2.8471011
O	-0.1530842	-1.8659717	-2.6269425
O	-2.2575096	0.3238308	-3.5497646
O	0.5984019	0.3167082	-4.6015314
C	0.1908855	-2.3850990	-1.3230953
C	0.3019553	-2.8582414	-3.5729146
C	-2.8630313	-0.8338489	-4.1757245
C	-3.1679197	0.6939454	-2.4860659
C	0.1704069	1.2495436	-5.6212626
C	2.0416433	0.3077262	-4.6730370
C	1.5909143	-2.9798747	-1.5035415
H	0.1379998	-1.5455303	-0.6294721
H	-0.5423732	-3.1542231	-1.0399107
C	1.6237139	-3.4038214	-2.9982833
H	0.4023744	-2.3576237	-4.5368669
H	-0.4563943	-3.6499872	-3.6476299
C	-3.5282736	-1.6331251	-3.0350831
H	-3.6049926	-0.4875784	-4.9072882
H	-2.0679838	-1.3708545	-4.6947869
C	-3.5486660	-0.6394247	-1.8425952
H	-4.0408621	1.2001603	-2.9227164
H	-2.6262273	1.3745814	-1.8293857
C	1.1868484	2.4015879	-5.5722176
H	0.1907130	0.7390246	-6.5942551
H	-0.8535280	1.5352823	-5.3788750
C	2.4416353	1.7712519	-4.9058961
H	2.3512495	-0.3328840	-5.5109069
H	2.4095610	-0.1140975	-3.7362313
H	2.3482553	-2.2168295	-1.3058365
H	1.7664594	-3.8195500	-0.8263049
H	2.4844507	-2.9635414	-3.5077205
H	1.6816477	-4.4888459	-3.1166178
H	-4.5359538	-1.9473899	-3.3196251
H	-2.9477280	-2.5246589	-2.7888970
H	-4.5212856	-0.5966748	-1.3453333
H	-2.7918405	-0.9136406	-1.1022273
H	1.3981209	2.7845283	-6.5738518
H	0.8048431	3.2263519	-4.9661190
H	3.3312152	1.8459890	-5.5363891
H	2.6554901	2.2620838	-3.9534214
C	0.1884355	1.3099395	-1.1505431
C	1.6752402	1.0925636	-0.8662737
C	0.0257941	2.7631865	-1.5994015
C	-0.5444165	1.1637136	0.1815823
H	2.2997928	1.2401731	-1.7599216
H	2.0680099	1.8031409	-0.0916406
H	1.8869166	0.0807626	-0.4885662
H	0.4057748	3.4911709	-0.8347873
H	0.5761720	2.9758375	-2.5278119
H	-1.0264671	3.0316052	-1.7817262
H	-1.6241037	1.3588673	0.0960376
H	-0.4362955	0.1570481	0.6144386
H	-0.1595883	1.8778218	0.9563691

***t*Bu$^-$** Me_3C^- anion
13
Energy = -157.9511652535

C	-1.2247968	-0.7071638	0.7685848
C	-0.0002595	-0.0001147	0.2144241
H	-2.1672042	-0.2277139	0.4620789
H	-1.2804866	-1.7631383	0.4624136
H	-1.2308616	-0.7104927	1.9013167
C	1.2248519	-0.7072510	0.7686581
C	-0.0000366	1.4144307	0.7687163
H	2.1670870	-0.2275253	0.4621554
H	1.2309691	-0.7106519	1.9014659
H	1.2806398	-1.7631695	0.4623754
H	0.0000386	1.4213619	1.9015117
H	0.8865728	1.9905135	0.4622554
H	-0.8865051	1.9908454	0.4623968

THF *c*-C_4H_8O solvent
13
Energy = -232.5925767060

O	-0.0232633	0.0049832	-1.2561122
C	0.1576323	1.1732537	-0.4153786
C	-0.1579139	-1.1731542	-0.4183970
C	0.2209204	-0.7343577	0.9965100
C	-0.2236577	0.7364535	0.9980885
H	1.2097707	1.4880729	-0.4643996
H	-0.4714906	1.9757797	-0.8128748
H	-1.1996301	-1.5196441	-0.4643926
H	0.4936350	-1.9547486	-0.8222421
H	-0.2712193	-1.3359849	1.7655039
H	1.3048491	-0.8031003	1.1415513
H	-1.3078392	0.8069993	1.1408101
H	0.2688629	1.3359052	1.7686234

6a
59
Energy = -2033.901696528

P	-0.2759893	0.1143798	-0.6357018

N	-1.3931645	-0.9875986	0.0851264
C	-1.5730768	-2.2845413	-0.4526258
C	-1.3653741	-2.5261027	-1.8177729
C	-1.9273305	-3.3533223	0.3856139
C	-1.4670058	-3.8188395	-2.3300071
H	-1.1336131	-1.6982044	-2.4794203
C	-2.0517992	-4.6362370	-0.1382846
H	-2.0930741	-3.1705859	1.4427663
C	-1.8107072	-4.8809966	-1.4944616
H	-1.2911967	-3.9884609	-3.3884416
H	-2.3228223	-5.4555289	0.5217915
H	-1.8970818	-5.8870593	-1.8934858
C	-2.2427689	-0.5321453	1.1437186
C	-3.6322458	-0.5329290	0.9764085
C	-1.6827800	-0.0514132	2.3303256
C	-4.4519439	-0.0483098	1.9935549
H	-4.0577744	-0.9082270	0.0505170
C	-2.5059315	0.4521428	3.3365050
H	-0.6045334	-0.0694733	2.4557057
C	-3.8915911	0.4539226	3.1719979
H	-5.5298947	-0.0466750	1.8588940
H	-2.0622986	0.8384729	4.2492497
H	-4.5333973	0.8430742	3.9568872
W	2.0635036	-0.6644958	-1.1567896
C	2.5306968	-0.3401476	0.8191297
O	2.7792268	-0.1627890	1.9354199
C	1.7050307	-2.6471771	-0.6886331
O	1.5743528	-3.7599725	-0.4133432
C	3.9841828	-1.1352586	-1.5748995
O	5.0903077	-1.3927556	-1.8150399
C	1.5090667	-1.0155280	-3.1103036
O	1.1832239	-1.2176664	-4.2011938
C	2.4468966	1.3093862	-1.5914244
O	2.6604713	2.4207953	-1.8269257
C	-0.7591709	1.7525005	-0.1480156
C	-1.1428310	1.4736164	-1.4044273
C	-1.7654097	1.9814108	-2.6026677
C	-1.9351055	1.1337403	-3.7116368
C	-2.1812514	3.3238232	-2.7002284
C	-2.5158951	1.6079410	-4.8837772
H	-1.6033177	0.1025186	-3.6442173
C	-2.7535247	3.7964724	-3.8763523
H	-2.0398063	3.9923249	-1.8574318
C	-2.9271068	2.9403390	-4.9687156
H	-2.6447216	0.9426460	-5.7321942
H	-3.0663222	4.8342604	-3.9443831
H	-3.3781523	3.3126431	-5.8837521
C	-0.7529283	2.7359515	0.9139013
C	0.2691292	2.7195882	1.8778251
C	-1.7782964	3.6915514	1.0184515
C	0.2760781	3.6484029	2.9130642
H	1.0559679	1.9757836	1.8042918
C	-1.7766213	4.6089087	2.0653803
H	-2.5903908	3.6878444	0.2986096
C	-0.7488116	4.5936175	3.0118384
H	1.0750370	3.6322008	3.6484757
H	-2.5802491	5.3349776	2.1464200
H	-0.7495041	5.3117134	3.8266004

6a1

59

Energy = -2033.902245424

P	-0.2666964	0.6391877	0.2419101
N	-1.3623636	-0.1463474	1.3355185
C	-0.8643294	-0.9099932	2.4099009
C	-1.6068328	-1.9597580	2.9746396
C	0.4028887	-0.6133265	2.9408624
C	-1.0738724	-2.7044262	4.0248254
H	-2.5928879	-2.1931876	2.5878764
C	0.9320302	-1.3753576	3.9786125
H	0.9664585	0.2283308	2.5498277
C	0.2006745	-2.4308428	4.5266389
H	-1.6623444	-3.5142140	4.4475707
H	1.9177922	-1.1328172	4.3655113
H	0.6122960	-3.0228112	5.3382657
C	-2.6761405	-0.3943178	0.8024984
C	-2.9045778	-1.4930028	-0.0335024
C	-3.7016424	0.5156416	1.0661066
C	-4.1600775	-1.6729390	-0.6131139
H	-2.0988886	-2.1947773	-0.2265857
C	-4.9549984	0.3337337	0.4806330
H	-3.5027897	1.3645146	1.7125390
C	-5.1842314	-0.7568040	-0.3602958
H	-4.3355187	-2.5221205	-1.2667640
H	-5.7492808	1.0480875	0.6756866
H	-6.1589701	-0.8932294	-0.8191706
W	1.4900202	-0.7191681	-0.9478635
C	2.8794916	-0.2356929	0.4909038
O	3.6583669	0.0342621	1.3026990
C	1.0279913	-2.4384792	0.0981174
O	0.7819782	-3.4216882	0.6510354
C	2.8955316	-1.7281146	-1.9922097
O	3.7044845	-2.2997480	-2.5975507
C	0.0681180	-1.2059277	-2.3579919
O	-0.7255958	-1.4854069	-3.1508178
C	1.9194551	1.0123861	-1.9752862
O	2.1496944	1.9913734	-2.5447178
C	-0.2480566	2.3989344	0.5493128
C	-1.1156541	2.0545450	-0.4145844
C	-2.0291895	2.4891425	-1.4429868
C	-2.7491884	1.5292216	-2.1759451
C	-2.1999056	3.8534580	-1.7466081

C	-3.6253111	1.9222843	-3.1814272
H	-2.6223724	0.4786452	-1.9365462
C	-3.0736390	4.2410018	-2.7571692
H	-1.6354020	4.6021928	-1.2010687
C	-3.7912823	3.2783590	-3.4743461
H	-4.1814697	1.1726628	-3.7364466
H	-3.1962278	5.2950404	-2.9884134
H	-4.4758723	3.5857064	-4.2595018
C	0.3488774	3.4558965	1.3276582
C	1.5393994	3.2067764	2.0343225
C	-0.2377631	4.7334880	1.4071063
C	2.1395993	4.2121712	2.7851892
H	1.9938405	2.2226407	1.9750140
C	0.3588718	5.7324348	2.1698160
H	-1.1695859	4.9298772	0.8871957
C	1.5502721	5.4772921	2.8557574
H	3.0637624	4.0111496	3.3186266
H	-0.1048675	6.7125209	2.2313440
H	2.0149429	6.2609629	3.4466950

6b

71

Energy = -2041.149061379

P	-0.3650176	0.4312401	-0.0824710
N	-1.4104090	-0.4967025	0.8592287
W	1.6952815	-0.6657562	-1.0839279
C	2.4770029	-0.9952060	0.7915630
O	2.9492182	-1.1837695	1.8321287
C	0.7441029	-2.4893108	-1.0644448
O	0.2002570	-3.5099427	-1.0744720
C	3.3583114	-1.4856171	-1.8829560
O	4.3172196	-1.9541196	-2.3431545
C	0.9522040	-0.3507743	-2.9768071
O	0.5493361	-0.1896425	-4.0494158
C	2.5413618	1.2132398	-1.1053579
O	2.9983067	2.2746225	-1.1187674
C	-0.3470693	2.1639497	0.3953140
C	-1.1057482	1.9501110	-0.6838762
C	-1.9660753	2.5314077	-1.6890085
C	-2.2101323	1.8465403	-2.8921810
C	-2.6024554	3.7673834	-1.4677972
C	-3.0551301	2.3884172	-3.8554934
H	-1.7229918	0.8931717	-3.0669235
C	-3.4572701	4.2998346	-2.4280345
H	-2.4444076	4.2906784	-0.5305251
C	-3.6837654	3.6148810	-3.6254255
H	-3.2290935	1.8527457	-4.7839198
H	-3.9512497	5.2490463	-2.2421040
H	-4.3507334	4.0333756	-4.3733244
C	0.2501477	3.0989982	1.3130599
C	1.0863671	2.6044868	2.3315043
C	0.0477554	4.4891581	1.2130199
C	1.6974339	3.4711199	3.2313980
H	1.2517730	1.5330269	2.3982289
C	0.6639539	5.3533877	2.1122131
H	-0.5817694	4.8857259	0.4234947
C	1.4862340	4.8482870	3.1246822
H	2.3400429	3.0773772	4.0132614
H	0.5048619	6.4242730	2.0256743
H	1.9626272	5.5271730	3.8258231
C	-0.8467892	-0.9494017	2.1498335
C	-1.4066555	-0.1817007	3.3573501
C	-0.9689559	-2.4644335	2.3597347
H	0.2278986	-0.7218692	2.0883368
C	-0.6919620	-0.6045940	4.6484352
H	-2.4801118	-0.3949944	3.4493659
H	-1.3009802	0.8957069	3.1881527
C	-0.2582007	-2.8890419	3.6539883
H	-2.0292477	-2.7428851	2.4226780
H	-0.5467582	-2.9869480	1.4962973
C	-0.7964534	-2.1195649	4.8673291
H	-1.1127069	-0.0625776	5.5034010
H	0.3684236	-0.3208753	4.5815630
H	-0.3737180	-3.9688394	3.8031515
H	0.8187550	-2.6946160	3.5517713
H	-0.2505327	-2.4106426	5.7725104
H	-1.8504392	-2.3880905	5.0274456
C	-2.8531261	-0.6671003	0.5944657
C	-3.7009930	0.5885534	0.8694339
C	-3.0758111	-1.1803642	-0.8343107
H	-3.1857462	-1.4522470	1.2857043
C	-5.1858602	0.3236178	0.5866031
H	-3.3586553	1.4025951	0.2224841
H	-3.5525010	0.9156250	1.9032999
C	-4.5624209	-1.4071580	-1.1383108
H	-2.6756858	-0.4378680	-1.5376928
H	-2.5027320	-2.1029742	-0.9758068
C	-5.3898551	-0.1462161	-0.8591102
H	-5.7680494	1.2320577	0.7814898
H	-5.5591227	-0.4486771	1.2748985
H	-4.6819497	-1.7237003	-2.1812701
H	-4.9364184	-2.2291872	-0.5114339
H	-6.4516307	-0.3394431	-1.0528564
H	-5.0755974	0.6534363	-1.5450117

7b

62

Energy = -1697.993538034

P	-0.3494869	0.2683852	-0.1463386
N	-1.4508855	-0.1956356	1.0428575
W	1.2773771	-1.2598679	-1.3920104
C	2.2695035	-1.4532224	0.4029897

O	2.8271205	-1.5560557	1.4110876
C	0.2120251	-2.9790740	-1.0105796
O	-0.3418310	-3.9801159	-0.8366556
C	2.6501468	-2.4100936	-2.3181108
O	3.4493645	-3.0635903	-2.8515965
C	0.2155246	-1.0444397	-3.1442629
O	-0.3800049	-0.9497543	-4.1310395
C	2.4392861	0.3775813	-1.8399270
O	3.1280962	1.2708861	-2.0986028
C	-0.8765902	-0.6407988	2.3362335
C	-1.6780681	-0.0922615	3.5251367
C	-0.7127547	-2.1650646	2.4397841
H	0.1263961	-0.1935210	2.3801972
C	-1.0284754	-0.4948814	4.8572248
H	-2.7004798	-0.4919416	3.4876653
H	-1.7512114	0.9978815	3.4407665
C	-0.0696389	-2.5646216	3.7748838
H	-1.6962771	-2.6455891	2.3518614
H	-0.1057124	-2.5198265	1.6012471
C	-0.8710781	-2.0171534	4.9624465
H	-1.6278315	-0.1116832	5.6913523
H	-0.0383926	-0.0233343	4.9318487
H	0.0120923	-3.6560581	3.8357792
H	0.9536032	-2.1656522	3.8141231
H	-0.3804717	-2.2829592	5.9062528
H	-1.8662013	-2.4841992	4.9745866
C	-2.8332453	-0.6193025	0.7110029
C	-3.8374491	0.5369635	0.8523239
C	-2.9464355	-1.2589669	-0.6781735
H	-3.1013031	-1.3885191	1.4471357
C	-5.2710537	0.0586155	0.5862184
H	-3.5807509	1.3191062	0.1270186
H	-3.7499401	0.9790551	1.8498430
C	-4.3820412	-1.7201463	-0.9672595
H	-2.6411887	-0.5241030	-1.4369637
H	-2.2560941	-2.1037182	-0.7509843
C	-5.3856701	-0.5716848	-0.8073520
H	-5.9696645	0.8972433	0.6881077
H	-5.5528397	-0.6853313	1.3454573
H	-4.4366625	-2.1417483	-1.9775740
H	-4.6438012	-2.5286713	-0.2701489
H	-6.4055238	-0.9339649	-0.9816820
H	-5.1827397	0.1960987	-1.5677777
C	0.2465091	1.9214142	0.3816223
H	1.2576684	2.1764242	0.0761355
H	-0.0188810	2.2455924	1.3832028
C	-0.8338993	1.9681493	-0.6823520
H	-1.8114318	2.2536412	-0.3033502
C	-0.5418151	2.4443938	-2.0884800
C	-1.7019849	2.1656148	-3.0503949
H	0.3715636	1.9655320	-2.4620893
H	-0.3341532	3.5237917	-2.0602150
C	-1.3956672	2.6059027	-4.4839254
H	-1.9297443	1.0929809	-3.0335795
H	-2.6002674	2.6806378	-2.6852026
H	-1.1830820	3.6804955	-4.5268489
H	-0.5211465	2.0742403	-4.8759711
H	-2.2401522	2.4010917	-5.1501851

7b1

62

Energy = -1697.991747922

P	-0.6289955	0.3239379	-0.1676410
N	-1.6696497	-0.1602545	1.0731120
W	1.1193392	-1.0784717	-1.4064819
C	2.1489538	-1.1598696	0.3739377
O	2.7179871	-1.1957147	1.3805791
C	0.2846819	-2.9169519	-1.0075563
O	-0.1084310	-3.9904182	-0.8287278
C	2.5739314	-2.0782562	-2.3787526
O	3.4189009	-2.6424984	-2.9429734
C	-0.0426200	-0.9406429	-3.1031413
O	-0.7157629	-0.8672375	-4.0403026
C	2.1197061	0.6531529	-1.8836174
O	2.7285627	1.5978106	-2.1611417
C	-1.0113151	-0.4999813	2.3611496
C	-1.7836683	0.0938215	3.5475794
C	-0.7674533	-2.0039597	2.5545586
H	-0.0306403	-0.0048608	2.3280128
C	-1.0567448	-0.1878814	4.8709319
H	-2.7887839	-0.3477615	3.5865457
H	-1.9093593	1.1710910	3.3913652
C	-0.0410756	-2.2783674	3.8787894
H	-1.7304378	-2.5321767	2.5539859
H	-0.1868807	-2.3896659	1.7096387
C	-0.8137545	-1.6900657	5.0661361
H	-1.6377183	0.2193010	5.7066344
H	-0.0904055	0.3361854	4.8684903
H	0.1000651	-3.3576603	4.0083828
H	0.9605522	-1.8280180	3.8391687
H	-0.2660856	-1.8663790	5.9994085
H	-1.7810382	-2.2043470	5.1591521
C	-2.9790398	-0.7980300	0.7860242
C	-4.0384319	0.2299224	0.3658212
C	-2.9036167	-1.9362562	-0.2398321
H	-3.3019457	-1.2314704	1.7406694
C	-5.4107703	-0.4360582	0.1960990
H	-3.7426688	0.6748006	-0.5928918
H	-4.0779415	1.0363956	1.1065381
C	-4.2742321	-2.5965643	-0.4459344
H	-2.5428493	-1.5292859	-1.1965026
H	-2.1729922	-2.6781344	0.0911531

C	-5.3431900	-1.5688890	-0.8360714
H	-6.1532869	0.3128216	-0.1031347
H	-5.7396300	-0.8437832	1.1628643
H	-4.1964965	-3.3803510	-1.2083911
H	-4.5739241	-3.0915772	0.4889652
H	-6.3203031	-2.0565914	-0.9325767
H	-5.0971119	-1.1451067	-1.8202583
C	-0.1746717	2.0460833	0.2695769
H	0.8093277	2.3711344	-0.0570473
H	-0.4608295	2.3928523	1.2575906
C	-1.2630728	1.9455015	-0.7836175
H	-2.2559885	2.1721932	-0.4067858
C	-1.0011766	2.3895549	-2.2069979
C	-0.9346018	3.9185259	-2.3396803
H	-1.7901726	1.9942543	-2.8587058
H	-0.0581566	1.9583593	-2.5625490
C	-0.6421323	4.3597737	-3.7768638
H	-1.8846594	4.3519247	-2.0012028
H	-0.1571346	4.3025017	-1.6670683
H	0.3177723	3.9563458	-4.1201330
H	-1.4196953	4.0031093	-4.4624063
H	-0.5971216	5.4512012	-3.8547454

8b

65

Energy = -1737.331115916

P	-0.3097475	0.3573861	-0.0618823
N	-1.4597598	-0.1348724	1.0681572
W	1.2886193	-1.1571130	-1.3661429
C	2.2259303	-1.4941195	0.4367731
O	2.7525425	-1.6801302	1.4496270
C	0.1529914	-2.8545911	-1.1127656
O	-0.4401852	-3.8431744	-1.0127269
C	2.6439033	-2.3008278	-2.3240312
O	3.4344256	-2.9507199	-2.8747756
C	0.2842394	-0.8108360	-3.1312224
O	-0.2777386	-0.6496658	-4.1290648
C	2.5191890	0.4588417	-1.6908084
O	3.2468087	1.3384501	-1.8815973
C	-0.9407328	-0.6787023	2.3470149
C	-1.7520485	-0.1670482	3.5455012
C	-0.8414669	-2.2118725	2.3639948
H	0.0780712	-0.2776764	2.4431522
C	-1.1561441	-0.6729539	4.8674485
H	-2.7884814	-0.5206937	3.4585979
H	-1.7790407	0.9282343	3.5237867
C	-0.2482583	-2.7131368	3.6879761
H	-1.8412127	-2.6452766	2.2263414
H	-0.2286565	-2.5428642	1.5199912
C	-1.0588720	-2.2037804	4.8862237
H	-1.7634840	-0.3159508	5.7073710
H	-0.1513149	-0.2458252	4.9954244
H	-0.2093214	-3.8086110	3.6867955
H	0.7880729	-2.3573731	3.7744569
H	-0.6034410	-2.5427917	5.8241817
H	-2.0709597	-2.6312910	4.8472554
C	-2.8470925	-0.4830152	0.6741902
C	-3.8079430	0.7055090	0.8459994
C	-2.9426507	-1.0459585	-0.7490852
H	-3.1684211	-1.2765827	1.3614391
C	-5.2508346	0.3012466	0.5148461
H	-3.4982466	1.5111491	0.1686577
H	-3.7329712	1.0932392	1.8670025
C	-4.3857773	-1.4308246	-1.1043442
H	-2.5838652	-0.2868680	-1.4591579
H	-2.2851427	-1.9141587	-0.8450692
C	-5.3480919	-0.2524277	-0.9122637
H	-5.9177945	1.1621952	0.6401384
H	-5.5855137	-0.4677781	1.2261184
H	-4.4250950	-1.7959917	-2.1371285
H	-4.7014333	-2.2636958	-0.4601458
H	-6.3756836	-0.5639321	-1.1332431
H	-5.0930081	0.5442861	-1.6258004
C	0.3450466	1.9433723	0.5893032
H	1.3739802	2.1705417	0.3238783
H	0.0687869	2.2136531	1.6038604
C	-0.7051556	2.1091414	-0.4922281
H	-1.6789103	2.4116114	-0.1167504
C	-0.3644746	2.6523958	-1.8623649
C	-1.4991365	2.4265152	-2.8663934
H	0.5538642	2.1801133	-2.2315054
H	-0.1469946	3.7265166	-1.7758927
C	-1.1516814	2.8870432	-4.2848385
H	-1.7505278	1.3581681	-2.8841389
H	-2.4002019	2.9508264	-2.5187873
C	-2.2807411	2.6143602	-5.2832541
H	-0.9184807	3.9601763	-4.2712309
H	-0.2388919	2.3732177	-4.6144876
H	-2.0128446	2.9510289	-6.2905404
H	-2.5030428	1.5419821	-5.3334603
H	-3.1998785	3.1337092	-4.9866937

8b1

65

Energy = -1737.329552805

P	-0.6657376	0.2693916	-0.1990752
N	-1.6586311	-0.3084724	1.0353469
W	1.1642366	-1.0231617	-1.4239548
C	2.2287279	-1.0094929	0.3380739
O	2.8218622	-0.9916337	1.3312577
C	0.3937749	-2.8756450	-0.9641629
O	0.0071047	-3.9435996	-0.7423659

C	2.6584828	-1.9701213	-2.3922820
O	3.5237150	-2.5055071	-2.9538700
C	-0.0124683	-0.9935712	-3.1159752
O	-0.6906889	-0.9865318	-4.0522768
C	2.0403535	0.7655375	-1.9363982
O	2.5668442	1.7543367	-2.2275699
C	-0.9842711	-0.5946653	2.3262714
C	-1.8398525	-0.1522369	3.5212440
C	-0.5487027	-2.0604301	2.4775431
H	-0.0758971	0.0251334	2.3241109
C	-1.0911884	-0.3760085	4.8434330
H	-2.7718972	-0.7333885	3.5326596
H	-2.1136544	0.9020389	3.4015343
C	0.1967377	-2.2820512	3.8009008
H	-1.4335714	-2.7098451	2.4453359
H	0.0848886	-2.3375950	1.6296228
C	-0.6544810	-1.8385352	4.9972082
H	-1.7273622	-0.0745468	5.6837612
H	-0.2025391	0.2707086	4.8673120
H	0.4769097	-3.3374215	3.8975045
H	1.1314370	-1.7040874	3.7877083
H	-0.0949233	-1.9704547	5.9307938
H	-1.5466441	-2.4774393	5.0639846
C	-2.9497991	-0.9848136	0.7575751
C	-4.1462000	-0.0364890	0.9459936
C	-3.0015984	-1.6323705	-0.6317427
H	-3.0405955	-1.7918463	1.4966647
C	-5.4735681	-0.7807181	0.7461579
H	-4.0734815	0.7756867	0.2112921
H	-4.1009071	0.4221217	1.9385502
C	-4.3313131	-2.3679322	-0.8515705
H	-2.8864755	-0.8527346	-1.3986466
H	-2.1631920	-2.3251195	-0.7469813
C	-5.5311880	-1.4369192	-0.6390661
H	-6.3133675	-0.0887732	0.8793021
H	-5.5733784	-1.5562840	1.5192947
H	-4.3514775	-2.7977754	-1.8596907
H	-4.3948043	-3.2077104	-0.1452560
H	-6.4676151	-1.9941588	-0.7597757
H	-5.5221043	-0.6530585	-1.4099002
C	-0.4167789	2.0439820	0.1870580
H	0.5203162	2.4763320	-0.1541659
H	-0.7434218	2.3846522	1.1645419
C	-1.4810245	1.7794661	-0.8661529
H	-2.4991026	1.8976983	-0.5048999
C	-1.2610888	2.2155083	-2.2993844
C	-1.4140011	3.7329932	-2.4764031
H	-1.9730785	1.6923211	-2.9495037
H	-0.2593604	1.9150827	-2.6281639
C	-1.1657931	4.1842602	-3.9198397
H	-2.4231709	4.0355354	-2.1644472
H	-0.7120569	4.2470051	-1.8058188
C	-1.3186452	5.6976454	-4.1013855
H	-0.1557977	3.8764715	-4.2226640
H	-1.8635401	3.6602152	-4.5868259
H	-1.1348923	5.9943649	-5.1397231
H	-2.3300601	6.0235594	-3.8309679
H	-0.6105967	6.2413167	-3.4646724

2m^{-} [W(CO)$_5$]PMeCl^{-}
17
Energy = -1476.015784454

P	1.1662412	-1.2294617	0.5800005
Cl	0.7498292	-0.1124896	-1.2390375
W	1.1967910	-3.7519119	-0.1270338
C	2.4420833	-3.1014789	-1.6261321
O	3.1504230	-2.6795607	-2.4417855
C	2.8133296	-4.0068700	1.1050906
O	3.7263521	-4.1410666	1.8122294
C	1.2494453	-5.6805743	-0.6871545
O	1.3034334	-6.7983874	-1.0296002
C	-0.0492694	-4.1290291	1.4557584
O	-0.7546139	-4.3100891	2.3616450
C	-0.4506028	-3.3721096	-1.3007233
O	-1.3860666	-3.1540259	-1.9505234
C	2.9461476	-0.6995420	0.7333718
H	3.0013308	0.3842922	0.8792888
H	3.3466560	-1.1922386	1.6280108
H	3.5597692	-0.9819666	-0.1272208

5m [W(CO)$_5$]PMe
16
Energy = -1015.568645854

P	1.1577103	-1.4269238	0.7571402
W	1.1927385	-3.6983282	-0.0696547
C	2.4125514	-3.0705538	-1.6181338
O	3.1091053	-2.6924481	-2.4547696
C	2.9151615	-4.0162032	1.0304887
O	3.8816529	-4.1514056	1.6437845
C	1.1983590	-5.6549126	-0.7864773
O	1.2350531	-6.7344947	-1.1880114
C	-0.0318353	-4.2602466	1.5064760
O	-0.7257629	-4.5613969	2.3755180
C	-0.5425195	-3.2950744	-1.1284977
O	-1.5170985	-3.0652400	-1.6988717
C	2.8496310	-0.6917783	0.7864497
H	2.7987981	0.3497678	0.4478248
H	3.1284043	-0.6501512	1.8518640
H	3.6223840	-1.2360486	0.2399871

TS1 transition structure: H^{+} transfer to **2a**$^{-}$
71

Energy = -2693.470412842

P	0.4582151	-0.3979597	0.2661513
Cl	-0.2709012	-0.5693896	2.2844283
N	0.7220031	-2.0023758	-0.2182909
C	-0.3927102	-2.8819403	-0.4639449
C	-1.3805419	-2.5339977	-1.3892195
C	-0.4872442	-4.0904194	0.2384637
C	-2.4575459	-3.3927830	-1.6073317
H	-1.3206240	-1.5893878	-1.9141857
C	-1.5634422	-4.9459246	0.0086487
H	0.2808823	-4.3536440	0.9588774
C	-2.5539617	-4.6013224	-0.9151719
H	-3.2269384	-3.1051614	-2.3169493
H	-1.6304042	-5.8799871	0.5599255
H	-3.3927833	-5.2686592	-1.0913187
C	1.9916683	-2.6353088	0.0128152
C	2.6617815	-2.4934219	1.2300211
C	2.5560474	-3.3990167	-1.0140815
C	3.9135037	-3.0852115	1.4066279
H	2.1952480	-1.9344477	2.0338422
C	3.7971208	-4.0015636	-0.8254442
H	2.0229548	-3.5045567	-1.9541104
C	4.4843647	-3.8393849	0.3814869
H	4.4346187	-2.9624349	2.3516822
H	4.2375641	-4.5848632	-1.6290000
H	5.4577288	-4.3006147	0.5202093
W	2.3379602	1.2885253	0.2389833
C	2.9527944	0.7142450	2.1197431
O	3.3217572	0.4117022	3.1728701
C	3.7445042	0.0399831	-0.6146012
O	4.5643158	-0.6001569	-1.1161365
C	3.6987516	2.7822237	0.2676753
O	4.4759205	3.6462388	0.2945716
C	1.8018985	1.8914566	-1.6556188
O	1.5612355	2.2675364	-2.7221832
C	0.9202999	2.5403837	1.0509942
O	0.1260399	3.2474822	1.5070323
Li	-3.5357534	0.6182220	-0.4316563
O	-3.4213075	-0.3536032	1.3927026
C	-3.8946059	0.4134758	2.5049402
C	-3.9004578	-1.7060731	1.3296678
C	-3.4325283	1.8378159	2.2472313
H	-3.4578150	0.0365975	3.4400605
H	-4.9897093	0.3488585	2.5808423
C	-5.1781495	-1.7527609	0.5113058
H	-4.0649977	-2.1098068	2.3355150
H	-3.1123962	-2.2776767	0.8351098
O	-3.8604718	2.2820790	0.9466182
H	-2.3414872	1.8707284	2.2145366
H	-3.7960926	2.5141121	3.0307085
O	-4.8625396	-1.1533652	-0.7565414
H	-5.9822085	-1.1932264	1.0095954
H	-5.5121553	-2.7896930	0.3660128
C	-5.2255583	2.7181740	0.8838547
C	-6.0086451	-0.7493469	-1.5215278
C	-5.5714556	2.7936974	-0.5918635
H	-5.8843658	2.0120337	1.4078940
H	-5.3330593	3.7051096	1.3551371
C	-6.4923801	0.6175907	-1.0745971
H	-5.6678543	-0.7032278	-2.5595174
H	-6.8152704	-1.4887860	-1.4419413
O	-5.3770914	1.5126012	-1.2235514
H	-6.6012604	3.1430406	-0.7358761
H	-4.8850673	3.4764290	-1.0995705
H	-7.3318020	0.9540622	-1.6986272
H	-6.8258216	0.5934162	-0.0282859
O	-1.9691199	0.6755662	-1.2790847
C	-1.5098558	0.7363616	-2.5854312
H	-0.8198476	-0.0237201	-0.3995628
H	-2.1756553	0.2105914	-3.3028913
H	-1.4006124	1.7744229	-2.9539507
H	-0.5055972	0.2708235	-2.7023933

TS2 transition structure of Cl/O exchange 71

Energy = -2693.475741956

P	-0.5210313	0.7596768	-0.6464527
Cl	0.4654506	2.6452795	0.0795843
N	-2.1230952	1.4359653	-0.0245903
C	-2.8206552	2.3098788	-0.9042253
C	-3.3942454	1.7978078	-2.0766841
C	-2.9049559	3.6874551	-0.6479355
C	-4.0300938	2.6486233	-2.9819992
H	-3.3527311	0.7285829	-2.2603632
C	-3.5508624	4.5314149	-1.5477569
H	-2.4557680	4.0817927	0.2579867
C	-4.1127850	4.0175779	-2.7213943
H	-4.4731920	2.2373584	-3.8850536
H	-3.6073651	5.5967374	-1.3393415
H	-4.6141478	4.6788848	-3.4224932
C	-2.4189449	1.5282006	1.3447340
C	-1.4586187	1.2403924	2.3328711
C	-3.7294974	1.8340383	1.7668560
C	-1.8100260	1.2171346	3.6818367
H	-0.4328297	1.0470469	2.0474089
C	-4.0652243	1.8274611	3.1157458
H	-4.4876861	2.0538307	1.0220330
C	-3.1116121	1.5103626	4.0891751
H	-1.0480445	0.9778289	4.4194322
H	-5.0863999	2.0587994	3.4085688
H	-3.3787999	1.4983976	5.1419785
W	-0.7682244	-1.7474105	0.0767010

C 0.0937774 -1.5912721 1.9419504
O 0.5137819 -1.5311177 3.0201007
C -2.6046922 -1.4722188 0.9643364
O -3.6625822 -1.4634482 1.4332363
C -1.0729846 -3.7127834 0.3480933
O -1.2532952 -4.8528446 0.4910630
C -1.7420462 -1.8130955 -1.7250374
O -2.3075971 -1.8434933 -2.7370776
C 0.9329590 -2.3117494 -0.9422922
O 1.7891825 -2.7683509 -1.5742562
Li 2.6976144 0.7785627 -0.2785349
O 3.6823454 2.6122481 0.2133078
C 4.1463458 2.6212788 1.5734052
C 4.6657793 3.0057276 -0.7600384
C 3.0673795 1.9380205 2.3954448
H 4.2895510 3.6547030 1.9160840
H 5.1066633 2.0931534 1.6519424
C 5.4179610 1.7852786 -1.2498738
H 5.3525732 3.7499290 -0.3413522
H 4.1058720 3.4588176 -1.5828717
O 2.7906365 0.6252349 1.8688624
H 2.1274909 2.4860735 2.3111394
H 3.3647970 1.8755701 3.4489205
O 4.4200117 0.8892361 -1.7692906
H 5.9682282 1.3127896 -0.4255436
H 6.1330675 2.0532294 -2.0393775
C 3.7481359 -0.3667954 2.2837101
C 4.8866659 -0.4565417 -1.9705421
C 3.6062487 -1.5306924 1.3239521
H 4.7642651 0.0458998 2.2368737
H 3.5402258 -0.6781607 3.3155978
C 4.9764381 -1.1995540 -0.6495752
H 4.1360310 -0.9277448 -2.6096674
H 5.8551866 -0.4610952 -2.4856178
O 3.6982474 -1.0367499 -0.0230659
H 4.3697740 -2.2916232 1.5161235
H 2.6191905 -1.9885605 1.4118069
H 5.1812219 -2.2633716 -0.8277580
H 5.7699410 -0.7949954 -0.0062203
O 1.0938365 0.4664180 -1.4585530
C 1.3138631 1.1502303 -2.6943123
H -1.0054348 1.1071302 -1.9174946
H 1.5717275 2.2046577 -2.5253903
H 2.1362039 0.6551717 -3.2175422
H 0.4132343 1.1035705 -3.3232350

TS3a.xyz
47
Energy = -1725.640424683

TS3 : TS of **5a** trapping with 3MeOH

53
Energy = -1841.466770942
P -0.6229708 0.7125796 -0.1970088
N 0.6301608 1.8913598 -0.0682393
W 0.1106791 -1.6768091 0.3596249
C 1.9621351 1.6821898 -0.5232738
C 0.2947451 3.1735730 0.4770280
C 0.3209284 -2.0542009 -1.6531602
C 2.1460897 -1.3365656 0.5456993
C 0.5039316 -3.5850976 0.8963629
C -0.0969891 -1.0236606 2.2939801
C -1.8656842 -2.1944609 0.3331079
C 2.2100184 0.8945462 -1.6561166
C 3.0432029 2.2399327 0.1753714
C -0.4432282 3.2636161 1.6631016
C 0.6808244 4.3464429 -0.1846528
O 0.4416893 -2.2225118 -2.7918998
O 3.2846118 -1.2606275 0.7277142
O 0.7229548 -4.6884576 1.1971811
O -0.2190912 -0.6048351 3.3681812
O -2.9773631 -2.5340217 0.3652049
C 3.5197063 0.6582344 -2.0724943
H 1.3764860 0.4670616 -2.2022387
C 4.3466815 2.0064031 -0.2532165
H 2.8556549 2.8458670 1.0563014
C -0.8205892 4.5107864 2.1617373
H -0.7104614 2.3534276 2.1918717
C 0.3123820 5.5900169 0.3251267
H 1.2643679 4.2775700 -1.0977432
C 4.5941599 1.2117973 -1.3767551
H 3.6957698 0.0397354 -2.9482126
H 5.1751555 2.4361474 0.3031931
C -0.4472064 5.6791180 1.4951111
H -1.3935796 4.5673116 3.0830823
H 0.6107648 6.4924570 -0.2012577
H 5.6133449 1.0274118 -1.7032390
H -0.7363410 6.6497301 1.8872252
H -3.6806628 0.9389195 -0.8803682
O -3.5282950 0.5538153 -1.9581659
C -4.2476628 -0.6648823 -2.3228907
H -5.3079519 -0.4528116 -2.1929422
H -4.0292839 -0.8719146 -3.3702523
H -3.9391354 -1.4947060 -1.6864277
H -2.4903267 0.4628886 -2.0206286
O -0.9969665 0.7549255 -1.9439314
C -0.9346480 2.0708999 -2.5520032
H 0.1050908 2.4011087 -2.6074158
H -1.3470262 1.9733843 -3.5581763
H -1.5152856 2.8001707 -1.9739032
O -3.5644182 1.4086241 0.3218082
C -3.9535542 2.8056587 0.4504177

H	-2.5274906	1.3306952	0.4020550
H	-3.4129138	3.4250222	-0.2712849
H	-5.0261894	2.8568398	0.2645473
H	-3.7314167	3.1358298	1.4661240

TS4 : TS of **5a** trapping with tolane PhCCPh

59

Energy = -2033.841305067

P	0.3382083	-0.1228510	0.4429653
N	-0.9392830	-0.0288362	1.5560737
C	-0.6970509	-0.0909767	2.9764612
C	-1.7303831	-0.4922021	3.8361431
C	0.5580253	0.2174363	3.5124487
C	-1.5002464	-0.5880211	5.2080209
H	-2.7079727	-0.7350434	3.4354218
C	0.7780671	0.1173345	4.8843654
H	1.3605888	0.5306448	2.8588304
C	-0.2472179	-0.2849098	5.7426794
H	-2.3101774	-0.9057383	5.8584513
H	1.7583671	0.3666383	5.2809300
H	-0.0734574	-0.3570951	6.8121069
C	-2.3219158	0.1996514	1.1974658
C	-3.1034368	-0.8348568	0.6853412
C	-2.8830384	1.4566916	1.4373131
C	-4.4429272	-0.5998011	0.3726866
H	-2.6723040	-1.8205814	0.5626110
C	-4.2195184	1.6882604	1.1176045
H	-2.2688778	2.2432863	1.8649895
C	-5.0002124	0.6621203	0.5787730
H	-5.0487003	-1.4061129	-0.0296737
H	-4.6501363	2.6703129	1.2892667
H	-6.0412675	0.8446495	0.3299278
W	-0.1744307	-0.7779740	-1.9521898
C	1.7282575	-1.5407578	-1.8124871
O	2.8038271	-1.9644454	-1.7611532
C	-0.9299769	-2.5312820	-1.1923017
O	-1.3237354	-3.5483437	-0.8032438
C	-0.3090818	-1.6065985	-3.7930413
O	-0.3870394	-2.0916175	-4.8454476
C	-2.0653210	0.0189192	-2.2238865
O	-3.1050924	0.4509681	-2.4808800
C	0.6750680	0.8971599	-2.8185840
O	1.1918628	1.7724133	-3.3653901
C	1.6673972	1.9506751	0.6400671
C	0.7800412	2.5135878	-0.0101250
C	-0.0425050	3.3350894	-0.8278184
C	-1.3888604	3.0357156	-1.0905941
C	0.5333463	4.4867783	-1.4072248
C	-2.1450799	3.8644830	-1.9123783
H	-1.8254569	2.1497329	-0.6502493
C	-0.2322077	5.3105161	-2.2248296
H	1.5762029	4.7162866	-1.2140678
C	-1.5717426	5.0028868	-2.4820861
H	-3.1831844	3.6159893	-2.1116345
H	0.2199386	6.1924752	-2.6687881
H	-2.1632660	5.6467518	-3.1261769
C	2.8364782	1.7444468	1.4434359
C	3.5825320	0.5544746	1.3858714
C	3.2562875	2.7826762	2.2989430
C	4.7223115	0.4066921	2.1703597
H	3.2474153	-0.2490941	0.7395765
C	4.3948190	2.6226467	3.0829768
H	2.6775288	3.6996411	2.3459738
C	5.1299980	1.4359607	3.0227281
H	5.2926096	-0.5160123	2.1192800
H	4.7057764	3.4245677	3.7460044
H	6.0157683	1.3132141	3.6389016

TS5 : TS of **5a** trapping with C_2H_4

41

Energy = -1572.688589670

P	1.1289683	0.0884598	0.7132354
N	0.1007969	-0.1008727	2.0394683
C	0.6995213	-0.2219002	3.3448341
C	0.1708753	0.5043460	4.4187367
C	1.8214704	-1.0356547	3.5323095
C	0.7761359	0.4238100	5.6717418
H	-0.7032281	1.1296999	4.2675176
C	2.4234548	-1.1056336	4.7876340
H	2.2073710	-1.6122537	2.6974651
C	1.9051713	-0.3766690	5.8606016
H	0.3659122	0.9941475	6.4999981
H	3.2905016	-1.7441694	4.9289301
H	2.3727375	-0.4384736	6.8386912
C	-1.3382475	-0.0549445	2.0183708
C	-2.0557929	-1.1051869	2.5986915
C	-2.0090958	1.0198880	1.4376039
C	-3.4479629	-1.0839785	2.5717859
H	-1.5214987	-1.9326281	3.0553452
C	-3.4033158	1.0358304	1.4127088
H	-1.4378509	1.8369404	1.0148624
C	-4.1258127	-0.0174270	1.9747039
H	-4.0045753	-1.9076082	3.0090383
H	-3.9214598	1.8738347	0.9561322
H	-5.2113102	-0.0080691	1.9495990
W	0.1200900	-0.1234578	-1.5941692
C	1.1709101	-1.8970226	-1.6193270
O	1.7548260	-2.8945671	-1.6493673
C	-1.5651588	-1.1552848	-0.9840353
O	-2.5104574	-1.7587795	-0.7118610
C	-0.4123819	-0.4558058	-3.5226726
O	-0.7125850	-0.6450707	-4.6277924

C	-0.9440292	1.6416288	-1.5808897
O	-1.5372731	2.6341391	-1.5905687
C	1.7923811	0.8922323	-2.2220373
O	2.7328190	1.4660799	-2.5780464
C	1.2280420	2.9024345	0.7115782
C	2.2266780	2.2289620	1.3352745
H	3.1703305	2.0307651	0.8370749
H	2.1899185	2.0145276	2.3999362
H	1.3057039	3.1969513	-0.3293744
H	0.3173828	3.1759867	1.2347032

TSh : TS of hydride transfer from ***t*BuLic** to **5a**
77
Energy = -2275.270449600

Li	-0.0867280	-0.3925070	-4.4128260
O	1.9563720	-0.0607220	-4.7811820
O	-1.4403750	-1.8098880	-5.1427270
O	-0.2141140	0.2890890	-6.3891900
C	2.7482000	-1.0226610	-4.0533210
C	2.1796300	-0.0621630	-6.2034670
C	-1.8853330	-1.3782280	-6.4453760
C	-0.8380810	-3.1201510	-5.1272150
C	1.0759560	0.7916050	-6.7975140
C	-0.7303070	-0.7700820	-7.2185080
H	3.7624490	-1.0790310	-4.4640020
H	2.7924020	-0.6478230	-3.0283640
H	3.1648410	0.3640410	-6.4316170
H	2.1438140	-1.0874080	-6.5953370
H	-2.6510140	-0.6217370	-6.2555310
H	-2.3306820	-2.2123350	-6.9984650
H	-1.6096680	-3.8883160	-5.2611590
H	-0.1061390	-3.2118850	-5.9410980
H	1.1312610	1.8082620	-6.4010230
H	1.1506800	0.8251810	-7.8901050
H	-1.0765860	-0.3625850	-8.1767170
H	0.0521250	-1.5146020	-7.4173560
O	0.7448830	-2.1611560	-3.5705610
C	-0.1677540	-3.2565010	-3.7737310
H	0.3516160	-4.2173190	-3.6897670
H	-0.9058770	-3.1775860	-2.9718650
C	2.0726200	-2.3804860	-4.0775320
H	2.0324460	-2.7902260	-5.0959070
H	2.6097610	-3.0904190	-3.4357710
C	-0.9244430	-0.0362920	-1.9259050
C	-1.0091560	0.9997910	-2.9414020
H	-1.5583150	-0.9059140	-2.1301840
H	0.0897610	-0.3640730	-1.6874010
H	-1.3498500	0.3350170	-0.8888580
C	-0.0157730	2.1290770	-2.9117370
C	-2.3909450	1.3705230	-3.4078080
H	-0.0160580	2.6842890	-3.8590940
H	-0.2541960	2.8698390	-2.1208240
H	1.0064520	1.7788690	-2.7266140
H	-2.8998460	2.0140580	-2.6613610
H	-2.3679710	1.9361370	-4.3482030
H	-3.0235810	0.4858270	-3.5510260
P	-1.3170840	0.5127640	1.2166470
N	-0.5681640	2.0823890	1.1063780
C	-1.2693450	3.1837590	0.5567900
C	-2.6745780	3.1743650	0.4564170
C	-0.5699070	4.2917490	0.0390240
C	-3.3483040	4.2428370	-0.1245910
H	-3.2224190	2.3216480	0.8429870
C	-1.2601170	5.3586480	-0.5376880
H	0.5119630	4.3219340	0.0959110
C	-2.6511890	5.3477740	-0.6252790
H	-4.4334560	4.2132980	-0.1812630
H	-0.6943880	6.2013470	-0.9266310
H	-3.1842600	6.1787210	-1.0775320
C	0.8193900	2.3090330	1.4019190
C	1.8129610	1.8745220	0.5228500
C	1.1683540	3.0066300	2.5610050
C	3.1550820	2.1122340	0.8153500
H	1.5202570	1.3575560	-0.3832550
C	2.5110990	3.2509150	2.8469540
H	0.3846200	3.3457650	3.2320510
C	3.5081390	2.8015060	1.9781300
H	3.9250610	1.7617070	0.1333700
H	2.7789850	3.7822120	3.7560290
H	4.5541250	2.9849890	2.2068200
W	0.2278300	-1.4469770	1.8741690
C	1.6737390	-1.2442240	0.4247800
O	2.5155700	-1.2327130	-0.3756880
C	1.3671770	-0.3721390	3.2188340
O	2.0158050	0.1702010	4.0090320
C	1.1587260	-3.1456820	2.4234760
O	1.6977130	-4.1342180	2.7370040
C	-1.1820310	-1.7724000	3.3413470
O	-1.9613180	-1.9897730	4.1705500
C	-0.9227240	-2.4826980	0.5265020
O	-1.5671240	-3.0771060	-0.2354230

TSn2 : TS of **5a** trapping with 2 $MeNH_2$
49
Energy = -1685.923504682

P	-1.1411998	0.4579983	0.0388674
N	-0.3787198	2.0249761	-0.1595579
W	0.5759327	-1.5107018	-0.0198291
C	0.7521542	2.3013483	-0.9687936
C	-0.8764557	3.0930640	0.6530981
C	0.2902743	-1.6626329	-2.0361898
C	2.3121840	-0.4107756	-0.3116673

C	1.7697753	-3.1298423	0.0921094
C	0.7151699	-1.0658497	1.9847879
C	-0.9957794	-2.7436568	0.3707256
C	0.9158819	1.6941368	-2.2222687
C	1.7533113	3.1771565	-0.5137164
C	-1.1586460	2.8955605	2.0103314
C	-1.1034983	4.3550670	0.0847745
O	0.0816363	-1.6900579	-3.1807869
O	3.3474037	0.0888732	-0.4244730
O	2.4482564	-4.0766462	0.1430986
O	0.7628257	-0.7716957	3.1040929
O	-1.8702341	-3.4761475	0.6147819
C	2.0527520	1.9394581	-2.9909439
H	0.1505076	1.0327392	-2.6076692
C	2.8818241	3.4253668	-1.2886809
H	1.6441116	3.6504638	0.4568682
C	-1.6787550	3.9372833	2.7794098
H	-0.9694334	1.9237125	2.4552810
C	-1.6098141	5.3959021	0.8602050
H	-0.8777681	4.5129936	-0.9658351
C	3.0440846	2.8059722	-2.5316551
H	2.1562260	1.4511504	-3.9561093
H	3.6492151	4.0954273	-0.9102011
C	-1.9063163	5.1922998	2.2110543
H	-1.8915632	3.7688112	3.8316818
H	-1.7838584	6.3667080	0.4037045
H	3.9297645	2.9966160	-3.1303415
H	-2.3047907	6.0035462	2.8134177
H	-2.9634698	-0.7543090	-1.3429248
N	-3.7572718	-1.7332790	-1.2662582
C	-3.5185394	-2.6851720	-2.3856255
H	-2.4856548	-3.0304702	-2.3323617
H	-4.1942596	-3.5396758	-2.3237126
H	-3.6748606	-2.1595723	-3.3286209
H	-4.7217295	-1.3988238	-1.2775217
N	-2.1420973	0.3263734	-1.4896219
C	-3.0152876	1.5039025	-1.7201689
H	-2.4244750	2.3949361	-1.9478312
H	-3.6974137	1.3004609	-2.5516972
H	-3.5887878	1.6882353	-0.8083067
H	-3.6202330	-2.1995661	-0.3673662
H	-1.5801299	0.1579996	-2.3269074

TSn3 : TS of **5a** trapping with 3 $MeNH_2$

56

Energy = -1781.855768329

P	-0.6535864	0.9067880	-0.1080057
N	0.6678636	2.0434954	-0.0467496
W	0.0673945	-1.4917906	0.5727017
C	2.0096296	1.7561178	-0.4159957
C	0.3805853	3.3666022	0.4164350
C	0.1380625	-1.9407785	-1.4175361
C	2.1261798	-1.2812495	0.6268538
C	0.4164509	-3.3675800	1.2236975
C	0.0164081	-0.6339677	2.4395714
C	-1.9164014	-1.9652424	0.7405318
C	2.3034191	0.9806459	-1.5456069
C	3.0716582	2.2349387	0.3681895
C	-0.4928902	3.5765860	1.4917309
C	0.9550936	4.4766060	-0.2208032
O	0.1796653	-2.0854823	-2.5717963
O	3.2758283	-1.3040049	0.7465567
O	0.6103111	-4.4585567	1.5851530
O	-0.0132974	-0.0845575	3.4594321
O	-3.0168973	-2.3026665	0.9015315
C	3.6243851	0.6901478	-1.8844775
H	1.4989176	0.6006415	-2.1634374
C	4.3883467	1.9474088	0.0230112
H	2.8533920	2.8291606	1.2501073
C	-0.8026460	4.8720116	1.9044993
H	-0.9260614	2.7196306	1.9968602
C	0.6530443	5.7682529	0.2060396
H	1.6380589	4.3212407	-1.0505654
C	4.6749031	1.1730250	-1.1055049
H	3.8279187	0.0841833	-2.7629168
H	5.1960921	2.3184545	0.6480533
C	-0.2323765	5.9759028	1.2669718
H	-1.4813199	5.0161613	2.7408867
H	1.1043202	6.6163084	-0.3021579
H	5.7036343	0.9460322	-1.3687557
H	-0.4696317	6.9836397	1.5952892
H	-3.9286146	0.2650409	-1.1131184
N	-3.5637644	0.0949808	-2.0810214
C	-3.7084226	-1.3197513	-2.4947986
H	-4.7479289	-1.6560584	-2.4389043
H	-3.3491250	-1.4354933	-3.5198659
H	-3.0996960	-1.9431668	-1.8383200
H	-2.2636164	0.4818114	-2.0127677
N	-1.0776473	0.9181220	-1.9140220
C	-1.0928698	2.2818413	-2.5016280
H	-0.0885367	2.7097892	-2.5235284
H	-1.4937690	2.2353410	-3.5179893
H	-1.7307742	2.9148038	-1.8799461
N	-4.0714765	0.9245479	0.6745065
C	-4.7266101	2.2374906	0.8265807
H	-3.0595212	1.0320260	0.8138378
H	-4.3050329	2.9280669	0.0896429
H	-5.7969475	2.1354325	0.6246669
H	-4.6013590	2.6840238	1.8231047
H	-0.4765399	0.3111675	-2.4758210
H	-4.0882271	0.7000782	-2.7129320
H	-4.4039957	0.2777438	1.3885874

TSp : TS of H^+ transfer from *t*BuCl

79

Energy = -3195.860208485

Cl	4.3149087	3.0359829	0.7843620
Li	5.0410615	1.0633210	-0.0229304
O	3.6045588	-0.3687515	-0.8019500
O	7.1634391	0.8846044	0.0677256
O	5.2454876	-0.5842215	1.3555935
C	3.5785987	-0.2482209	-2.2386559
C	3.8980683	-1.6942026	-0.3257791
C	7.5179365	0.0417476	1.1811189
C	7.6759762	0.4412675	-1.2016208
C	4.1953835	-1.5491283	1.1542772
C	6.5712449	-1.1393691	1.2702594
H	3.0952194	-1.1202492	-2.6913968
H	2.9794029	0.6422684	-2.4438287
H	3.0353336	-2.3536357	-0.4895540
H	4.7596105	-2.1113597	-0.8632155
H	7.4142845	0.6736510	2.0666307
H	8.5573463	-0.2963516	1.0973564
H	8.7578931	0.6200530	-1.2555313
H	7.4929164	-0.6334294	-1.3355514
H	3.3234058	-1.1531633	1.6783037
H	4.4648213	-2.5152684	1.5958372
H	6.7857969	-1.7403385	2.1635137
H	6.6568606	-1.7861408	0.3866604
O	5.5191526	1.0899788	-2.1017198
C	6.9436970	1.2563693	-2.2504833
H	7.2637110	0.9751282	-3.2602391
H	7.1310461	2.3218205	-2.0957834
C	4.9852705	-0.0643613	-2.7737808
H	5.6056434	-0.9477114	-2.5703452
H	4.9662816	0.1046737	-3.8583677
C	1.2362127	1.7509589	0.2794421
C	1.5482171	2.4774362	1.4423028
H	1.1799182	2.3395245	-0.6360451
H	1.7533913	0.8006264	0.1528605
H	0.0496750	1.3817077	0.3949576
C	1.9791314	1.7758903	2.6861525
C	1.1464187	3.9089277	1.5534951
H	2.5943897	2.4281388	3.3084949
H	1.0815263	1.5064035	3.2628537
H	2.5279767	0.8602806	2.4634609
H	0.1298582	3.9473875	1.9757881
H	1.8056091	4.4527492	2.2336525
H	1.1242651	4.4010914	0.5793104
P	-1.6308583	0.4680646	0.5389917
Cl	-1.7572888	1.1892988	2.6022848
N	-2.8921933	1.2932163	-0.2510551
C	-2.6306089	2.6395752	-0.6799512
C	-1.5604975	2.8967848	-1.5419806
C	-3.4233117	3.6947692	-0.2157691
C	-1.2646412	4.2074558	-1.9143141
H	-0.9759164	2.0640557	-1.9213109
C	-3.1303018	5.0018751	-0.6018666
H	-4.2556610	3.4859470	0.4491336
C	-2.0465819	5.2646597	-1.4440764
H	-0.4315960	4.4008565	-2.5842966
H	-3.7437193	5.8188752	-0.2325018
H	-1.8180520	6.2849818	-1.7373547
C	-4.2497554	0.8443382	-0.2726333
C	-4.8148985	0.2158444	0.8404868
C	-5.0082658	1.0167587	-1.4373051
C	-6.1200589	-0.2723150	0.7756157
H	-4.2352945	0.1289482	1.7525952
C	-6.3154537	0.5403983	-1.4892383
H	-4.5644148	1.5111136	-2.2962108
C	-6.8744057	-0.1149336	-0.3876445
H	-6.5489440	-0.7657611	1.6432218
H	-6.8950143	0.6675086	-2.3993262
H	-7.8909901	-0.4939367	-0.4360507
W	-1.6104893	-2.0687323	0.4803563
C	-2.8764047	-2.2127958	2.1050289
O	-3.5788825	-2.2956875	3.0182398
C	-3.2235586	-2.2083659	-0.8066742
O	-4.1044701	-2.3383287	-1.5414160
C	-1.3882400	-4.0750591	0.4069054
O	-1.2586572	-5.2307012	0.3688839
C	-0.3602439	-1.8584156	-1.1339742
O	0.3513532	-1.7401356	-2.0417481
C	-0.0122414	-1.9285137	1.7583457
O	0.8934459	-1.8613244	2.4789171

Table S3. The TPSS-D3/def2-TZVP + CPCM optimized atomic Cartesian coordinates (in Å) in THF solution. Each structure is labeled by the specific name (See also **Table S1**), followed by the number of atoms, the total energy (in hartrees), and the detailed atomic coordinates (in double-column text list). Ph: phenyl; Cy: cyclohexyl; ^{t}Bu: CMe_3; Anth: anthracenyl; Me: CH_3.

2-Me$^-$ $[W(CO)_5]PClMe$
17
Energy = -1476.018777763869
P -1,7966572 2,1661176 0,7609881
Cl -1,1785783 1,2023492 1,0935170
C 1,1063694 0,5949706 4,0062284
O 1,8710301 0,2148964 4,8066333
C 1,2995126 1,7394644 1,2500184
O 2,0857417 2,0369626 0,4510014
C -0,0809099 3,1735484 3,3596577
O -0,0443282 4,2562378 3,7808500
C -1,8122654 0,9057504 3,7788614
O -2,7614504 0,7145307 4,4216648
C -0,3779159 -0,6003781 1,7730633
O -0,5117776 -1,6515844 1,3013546
W -0,1693465 1,2688758 2,6076583
C -1,1961340 3,8699118 0,3069750
H -1,7405477 4,2375041 -0,5688945
H -1,4274730 4,5208904 1,1591677
H -0,1204699 3,9147523 0,1129891

2-^{t}Bu$^-$ $[W(CO)_5]PCl^{t}Bu$
26
Energy = -1594.031168028574
P -1,2739131 0,3418998 0,9356328
Cl -1,3294055 1,5123540 -0,8986185
C 1,1934870 -3,3924298 -0,2408407
O 1,7515119 -4,3591357 -0,5934380
C 1,3485966 -0,4758425 -0,8588807
O 1,9713662 0,2519775 -1,5114786
C 1,6588868 -1,5141549 1,8060042
O 2,4965732 -1,4490082 2,6105282
C -0,9549754 -2,7212352 1,6770923
O -1,6392713 -3,2466138 2,4551790
C -1,1365220 -1,9976348 -1,1649969
O -1,9005492 -2,1736427 -2,0193979
W 0,2406934 -1,7256822 0,3412901
C -0,3818768 1,5926859 2,0478756
C -0,3301753 0,8952807 3,4201213
H 0,2729345 -0,0163816 3,3867167
H 0,1159080 1,5735231 4,1591095
H -1,3365171 0,6298652 3,7657418
C -1,2557568 2,8542806 2,1637620
H -0,8103288 3,5471426 2,8909474
H -1,3317686 3,3697384 1,2014192
H -2,2670879 2,6015025 2,5012212

C 1,0241179 1,9779915 1,5813165
H 1,6838995 1,1068182 1,5573441
H 0,9932866 2,4122661 0,5768213
H 1,4582860 2,7220351 2,2642280

2-Ph$^-$ $[W(CO)_5]PClPh$
24
Energy = -1667.877312903094
P -1,4538875 0,4138344 0,9622697
Cl -1,6043492 1,4661054 -0,9181685
C 1,2313182 -3,2433676 0,0401754
O 1,9162988 -4,1545926 -0,2237582
C 1,3118740 -0,3032953 -0,4608639
O 1,9856962 0,4947184 -0,9625034
C 1,1091321 -1,3653909 2,2216190
O 1,6996738 -1,2136615 3,2085337
C -1,2899797 -2,8042206 1,4838643
O -2,0818153 -3,4283717 2,0608747
C -1,0013919 -1,9213301 -1,2611381
O -1,6126743 -2,0772163 -2,2341405
W 0,0775070 -1,6602453 0,4711734
C -0,3888201 1,5871450 1,8890682
C -0,3638510 1,4057055 3,2864775
C 0,3714147 2,6325752 1,3422984
C 0,4131921 2,2236983 4,1024788
H -0,9568387 0,6099259 3,7345679
C 1,1403587 3,4593731 2,1640998
H 0,3630921 2,7961430 0,2693859
C 1,1706595 3,2594693 3,5456503
H 0,4205558 2,0585390 5,1769988
H 1,7223855 4,2624754 1,7181346
H 1,7703494 3,9044839 4,1819023

2-Anth$^-$ $[W(CO)_5]PClAnth$
36
Energy = -1975.344916160436
P -1,3162184 -0,0505676 1,4667530
Cl -2,1592992 1,1431701 -0,1661834
C 1,4229254 -3,1222239 -0,6361713
O 2,1124122 -3,8849445 -1,1933311
C 1,1539077 -0,1499134 -0,5940764
O 1,6083996 0,7902615 -1,0969247

C 1,5837405 -1,8005848 1,8807574
O 2,3250785 -1,8778107 2,7717507
C -0,8085381 -3,2247312 1,2777343
O -1,4373009 -4,0253646 1,8358722
C -1,1009794 -1,8731281 -1,2299724
O -1,8682010 -1,9701189 -2,0929861
W 0,2670840 -1,7759411 0,3046629
C -0,4213418 1,3329419 2,2949339
C -1,1837265 2,3417351 3,0081053
C 0,9565139 1,3965462 2,3530024
C -2,5826815 2,3552967 3,0291889
C -0,4792539 3,3823316 3,7292355
C 1,6449511 2,4004741 3,0861770
H 1,5411376 0,6630919 1,8113570
C -3,3101870 3,3443422 3,7057043
H -3,1232039 1,5706422 2,5072287
C -1,2040468 4,3734405 4,4045330
C 0,9475920 3,3754869 3,7495580
H 2,7315776 2,3944602 3,0976918
C -4,7374787 3,3531145 3,7207512
C -2,6038601 4,3883330 4,4099392
H -0,6609429 5,1494474 4,9407051
H 1,4641943 4,1588399 4,2989642
C -5,4283141 4,3344064 4,3875769
H -5,2660793 2,5652523 3,1896720
C -3,3580885 5,3910282 5,0908557
C -4,7305244 5,3654272 5,0801718
H -6,5147834 4,3310753 4,3907956
H -2,8223161 6,1765871 5,6185827
H -5,2948484 6,1336968 5,6015846

2-NH_2^- $[W(CO)_5]PClNH_2$
16
Energy = -1492.086131680954
P -1,8000511 2,1777467 0,7404140
Cl -1,1615585 1,0206992 -1,1247805
C 1,1008475 0,6187603 3,9852518
O 1,8630890 0,2515824 4,7929344
C 1,3009450 1,7296423 1,2195252
O 2,0954417 2,0139738 0,4235746
C -0,0986146 3,1878464 3,3189852
O -0,0689128 4,2707657 3,7374638
C -1,8179744 0,9155567 3,7488237
O -2,7667257 0,7250297 4,3918481
C -0,3748655 -0,6034047 1,7658007
O -0,4996399 -1,6649693 1,3164358
N -1,2623829 3,7489809 0,4182722
H -0,2756132 3,9888090 0,4516948
H -1,7511994 4,2704802 -0,3041549
W -0,1747852 1,2774008 2,5763110

2-NMe_2^- $[W(CO)_5]PClNMe_2$
22
Energy = -1570.745391823646
P -0,2293171 -0,0079409 -0,0845211
N 0,0134297 1,0799635 1,1857596
C -0,5942734 2,4077608 1,2938173
H 0,0441155 3,0538395 1,9082965
H -0,7008491 2,8459632 0,3034797
H -1,5865083 2,3470007 1,7647283
C 0,2665052 0,4961007 2,5113629
H -0,6687940 0,3763961 3,0784595
H 0,7367757 -0,4819626 2,3913508
H 0,9348807 1,1551778 3,0790621
W -0,3116525 1,2073241 -2,3938113
C 0,9223429 2,6721901 -1,6577527
O 1,6484153 3,4785534 -1,2431227
C -2,0181561 2,1940026 -1,7974254
O -2,9891498 2,7283180 -1,4583390
C -0,3379643 2,0631533 -4,2131524
O -0,3645636 2,5769035 -5,2634667
C 1,3578989 0,1142857 -2,8659837
O 2,2992893 -0,5153918 -3,1235116
C -1,4721479 -0,3641332 -3,0390035
O -2,1082577 -1,2590641 -3,4112431
Cl -2,4321195 -0,6305405 0,2487164

2-NCy_2^- $[W(CO)_5]PClNCy_2$
48
Energy = -1961.711687519924
P -1,2720060 0,5465614 1,1062147
Cl -1,8474214 1,5714956 -0,9334909
C 1,1870803 -3,0993888 -0,3148482
O 1,7763254 -4,0381738 -0,6892316
C 1,1597988 -0,2231724 -1,0145116
O 1,6754064 0,4792469 -1,7784034
C 1,5963863 -1,1981439 1,7890585
O 2,3764801 -1,0976013 2,6445215
C -0,9032636 -2,5503355 1,6621983
O -1,5413116 -3,1432207 2,4309508
C -1,2765866 -1,7903912 -1,0877512
O -2,1073276 -2,0102373 -1,8658028
N -0,4114265 1,7510535 1,9093655
W 0,1964249 -1,4679930 0,3132749
C -1,2706108 2,6402448 2,7479577
C -1,1184883 2,3624634 4,2541866
C -1,1758775 4,1422338 2,4472121
H -2,2924327 2,3358241 2,4852548
C -2,1830338 3,1326992 5,0488125
H -0,1235118 2,6613672 4,5998892
H -1,2142482 1,2833168 4,4220565
C -2,2390021 4,9064270 3,2526911

H	-0,1836441	4,5252892	2,7146742
H	-1,3191007	4,3111595	1,3750852
C	-2,1067289	4,6370015	4,7569952
H	-2,0587946	2,9428846	6,1219725
H	-3,1798452	2,7622480	4,7697123
H	-2,1554542	5,9805484	3,0471734
H	-3,2371764	4,5916619	2,9166680
H	-2,8891136	5,1728361	5,3085607
H	-1,1402922	5,0251471	5,1100675
C	1,0099566	2,0741767	1,6372096
C	1,2208500	3,1363135	0,5400893
C	1,8339978	2,4053883	2,8888427
H	1,4133338	1,1409213	1,2315490
C	2,7119600	3,2454983	0,1889944
H	0,8640846	4,1133118	0,8807871
H	0,6302197	2,8566476	-0,3372584
C	3,3225110	2,5265383	2,5275628
H	1,4967499	3,3528209	3,3268247
H	1,6895111	1,6233833	3,6414977
C	3,5498935	3,5742784	1,4308011
H	2,8562475	4,0088722	-0,5854420
H	3,0568002	2,2925039	-0,2340746
H	3,9002900	2,7780634	3,4254097
H	3,6861779	1,5515339	2,1749148
H	4,6146116	3,6259125	1,1711373
H	3,2623008	4,5652836	1,8112411

2-NPh$_2^-$ [W(CO)$_5$]PClNPh$_2$
36
Energy = -1954.468902360317

P	-1,2535309	-0,7212214	2,1265412
Cl	-3,4833193	-0,6446822	1,7394394
C	0,7743216	-1,6992701	-1,8838316
O	1,2999059	-2,0456352	-2,8689078
C	0,8993378	0,6666804	-0,3237247
O	1,5413642	1,6209507	-0,4625830
C	1,3903281	-1,8516599	0,9651347
O	2,2469705	-2,2574778	1,6354760
C	-1,1268245	-2,9078129	-0,1045926
O	-1,6744168	-3,9301947	-0,0743734
C	-1,7186954	-0,2833771	-1,2125304
O	-2,6095196	0,1872432	-1,7843480
W	-0,1348561	-1,1111225	-0,1906328
N	-0,9518655	0,8605525	2,7503271
C	-0,8326786	2,0558777	1,9797348
C	-1,6425565	2,2767637	0,8612530
C	0,1229067	3,0168583	2,3402266
C	-1,4809481	3,4327112	0,0974202
H	-2,4017457	1,5453785	0,6112032
C	0,2731419	4,1731259	1,5788892
H	0,7497580	2,8455717	3,2104854
C	-0,5237039	4,3856323	0,4495570
H	-2,1135550	3,5891763	-0,7722315
H	1,0260668	4,9045416	1,8603953
H	-0,3993622	5,2851536	-0,1465900
C	-1,0531580	1,0280242	4,1697849
C	-1,8207212	2,0698961	4,7093984
C	-0,3974749	0,1400210	5,0328404
C	-1,9330110	2,2144485	6,0918471
H	-2,3290050	2,7591559	4,0422371
C	-0,5220044	0,2842685	6,4143223
H	0,2075523	-0,6562418	4,6105546
C	-1,2887416	1,3215680	6,9521732
H	-2,5367906	3,0223533	6,4965801
H	-0,0049946	-0,4092984	7,0719743
H	-1,3790745	1,4353405	8,0286506

2-N(SiH$_3$)$_2^-$ [W(CO)$_5$]PClN(SiH$_3$)$_2$
22
Energy = -2073.597721301266

P	-1,3738883	-0,1668918	1,8177684
Cl	-2,7634116	0,9492228	0,5215758
C	1,3541035	-2,6507587	-0,9473036
O	2,0458471	-3,3018218	-1,6271618
C	0,6049216	0,1341354	-0,9534431
O	0,8396435	1,0212859	-1,6616737
C	1,7149143	-1,1370348	1,5269640
O	2,5630062	-0,9638672	2,2993205
C	-0,3181818	-3,1506360	1,3427040
O	-0,5997503	-4,0860146	1,9686732
C	-1,4820264	-1,8562045	-0,9479324
O	-2,4247455	-2,0627309	-1,5896551
N	-0,5389648	1,1627369	2,5810876
W	0,1766277	-1,5062767	0,2162620
Si	-1,1867613	1,3353072	4,1939580
H	-0,4858252	2,4673143	4,8587358
H	-2,6448286	1,6164598	4,1747775
H	-0,9539558	0,1082768	4,9957279
Si	0,5184928	2,2806509	1,7609302
H	1,7966624	1,6479313	1,3595812
H	-0,1327984	2,8257531	0,5470974
H	0,8118188	3,3979626	2,6940062

5-Me [W(CO)$_5$]PMe
16
Energy = -1015.569266519900

P	-1,7606135	2,2180007	0,9469284
C	1,1329130	0,5158253	3,9446603
O	1,8943267	0,0907978	4,6985967
C	1,3374373	1,7955765	1,2745850
O	2,1757176	2,0917388	0,5411033
C	0,0022988	3,2291441	3,3521495

O 0,1037702 4,3051535 3,7533084
C -1,8017326 0,8908558 3,8224415
O -2,6965164 0,6412340 4,5043333
C -0,4951199 -0,5469233 1,7335152
O -0,6773545 -1,5875804 1,2719261
W -0,2068160 1,3256072 2,5697351
C -1,2189582 3,8688551 0,3281763
H -1,4257343 3,9447303 -0,7455127
H -1,8910731 4,5896894 0,8222058
H -0,1854452 4,1471952 0,5435476

5-^{t}Bu [W(CO)$_5$]P^{t}Bu
25
Energy = -1133.580826442887
P -1,1758845 0,1072127 1,2628923
C 1,1858040 -3,3126573 -0,4406866
O 1,7395398 -4,2135573 -0,9010300
C 1,3884850 -0,4125330 -0,7487086
O 2,0620611 0,2695400 -1,3879873
C 1,6286680 -1,5452760 1,8837709
O 2,4329882 -1,4903824 2,7093738
C -0,9479929 -2,9716880 1,5301856
O -1,5949224 -3,6916596 2,1549263
C -1,2237284 -1,8306430 -1,1006205
O -2,0260757 -1,9291616 -1,9223953
W 0,2053764 -1,6785039 0,3899407
C -0,3164979 1,5554885 2,0858357
C -0,3006456 1,0932787 3,5700013
H 0,3937876 0,2638182 3,7279721
H 0,0241181 1,9427486 4,1852749
H -1,2963116 0,7910619 3,9165538
C -1,2272064 2,7935087 1,9532024
H -0,8087232 3,6188731 2,5438539
H -1,2968116 3,1204459 0,9103917
H -2,2375182 2,5823768 2,3178131
C 1,0995881 1,8957312 1,6158557
H 1,7779092 1,0458019 1,7197069
H 1,0983708 2,2128044 0,5686852
H 1,4972223 2,7225715 2,2187917

5-Ph [W(CO)$_5$]PPh
23
Energy = -1207.432754107932
P -1,0924067 -0,1857344 1,7953479
C 1,1728831 -3,0402875 -0,8623977
O 1,7332675 -3,7846072 -1,5441833
C 0,9828198 -0,0918664 -0,7028880
O 1,4071364 0,8040164 -1,2927261
C 1,8310605 -1,6024099 1,6359768
O 2,7320198 -1,5527459 2,3545313
C -0,6290352 -3,2458312 1,4369101
O -1,1071488 -4,1154535 2,0241414
C -1,4605210 -1,7627382 -0,8673280
O -2,3936546 -1,8205606 -1,5422558
W 0,2028862 -1,6825444 0,3635814
C -0,2408085 1,2718400 2,4192457
C -1,0201898 2,1272058 3,2407640
C 1,1041821 1,6341288 2,1703037
C -0,4796729 3,2877066 3,7845513
H -2,0544476 1,8596837 3,4404019
C 1,6425192 2,7915377 2,7144119
H 1,7228694 0,9993660 1,5469748
C 0,8518762 3,6205656 3,5218783
H -1,0898230 3,9316615 4,4107672
H 2,6767773 3,0553834 2,5145453
H 1,2775105 4,5257838 3,9453458

5-anth [W(CO)$_5$]PAnth
35
Energy = -1514.905123317359
P -1,1079222 0,3862284 0,9040766
C 1,0383991 -3,4587960 -0,0992054
O 1,5515384 -4,4651383 -0,3466157
C 1,7646280 -0,6632883 -0,4961830
O 2,6617756 -0,1165016 -0,9704995
C 1,0817427 -1,5511959 2,1979831
O 1,5793541 -1,4669283 3,2367234
C -1,4199544 -2,7182654 1,1893069
O -2,2935060 -3,3232439 1,6360438
C -0,8674017 -1,6301974 -1,4301011
O -1,4571003 -1,6106865 -2,4228569
W 0,1564591 -1,6548298 0,3612295
C -0,3177183 1,5038894 2,0605489
C -1,1187478 2,4210226 2,8626240
C 1,0716812 1,6738762 2,0576503
C -2,4982087 2,2863093 3,0050507
C -0,4563756 3,4966116 3,5684918
C 1,7034733 2,7357977 2,7319562
H 1,6808465 0,9879541 1,4803517
C -3,2583742 3,1797027 3,7797970
H -3,0056071 1,4641900 2,5051225
C -1,2066690 4,3857988 4,3491609
C 0,9562714 3,6275648 3,4713024
H 2,7816395 2,8439152 2,6655474
C -4,6706758 3,0494258 3,9083294
C -2,5960514 4,2593199 4,4715451
H -0,6937739 5,1866301 4,8769997
H 1,4389065 4,4437970 4,0026726
C -5,3895670 3,9356963 4,6743871
H -5,1686265 2,2361172 3,3870043
C -3,3756805 5,1558772 5,2604917
C -4,7363218 4,9988817 5,3575037

H -6,4666464 3,8279521 4,7642446
H -2,8705362 5,9640061 5,7831644
H -5,3237510 5,6862070 5,9592520

5-NH_2 [$W(CO)_5$]PNH_2
15
Energy = -1031.662193219029
P -1,7805257 2,1786190 0,8942282
C 1,0888139 0,5433816 3,9819431
O 1,8209356 0,1185047 4,7698863
C 1,3626006 1,7772339 1,2884626
O 2,2042876 2,0573825 0,5485092
C -0,0279578 3,2339496 3,3467096
O 0,0439848 4,3176803 3,7404841
C -1,8131479 0,9313874 3,7851337
O -2,7282617 0,7077506 4,4535474
C -0,4244649 -0,5342087 1,7125921
O -0,5697147 -1,5730404 1,2287091
N -1,2784568 3,6100177 0,2491059
H -0,4242025 4,1047870 0,4941257
H -1,8342936 4,0812139 -0,4598453
W -0,1892968 1,3293406 2,5718082

5-NMe_2 [$W(CO)_5$]$PNMe_2$
21
Energy = -1110.326669544871
P -1,4037257 1,6815726 -0,1962570
N -0,5181664 1,4656754 1,1857809
C 0,8906937 1,0741543 1,3197366
H 0,9533452 0,1470811 1,8995621
H 1,3262584 0,9260574 0,3353454
H 1,4335189 1,8612536 1,8540358
C -1,1618282 1,6783377 2,4977304
H -1,1059868 0,7531337 3,0809908
H -0,6300620 2,4701890 3,0359249
H -2,2028372 1,9631683 2,3458057
C 1,4301365 2,3717173 -1,7954979
O 2,3620988 2,9783176 -1,4809187
C -1,1591007 3,0522629 -2,9683077
O -1,6801061 4,0244767 -3,3128484
C 0,5048689 1,0480113 -4,2514882
O 0,9369555 0,9004754 -5,3156169
C 0,6267400 -0,4567411 -1,7275075
O 1,1022506 -1,4488810 -1,3739136
C -1,9446976 0,2695400 -2,9054271
O -2,8997279 -0,3018654 -3,2165389
W -0,2449280 1,3047632 -2,3613906

5-NCy_2 [$W(CO)_5$]$PNCy_2$
47
Energy = -1501.295167090530
P -1,1594509 0,3509613 1,4131379
C 1,0810888 -3,0729910 -0,5244812
O 1,5846306 -3,9982008 -1,0070278
C 1,1828849 -0,2039587 -1,0071232
O 1,7297818 0,4548993 -1,7829128
C 1,7453803 -1,2730691 1,6897451
O 2,6014862 -1,2001988 2,4637132
C -0,7918351 -2,6935548 1,6288802
O -1,3493264 -3,4094868 2,3445394
C -1,3793727 -1,5951594 -0,9862561
O -2,2693095 -1,6953557 -1,7167967
N -0,4035676 1,7328140 1,9437629
W 0,2013610 -1,4350435 0,3300678
C -1,2864174 2,6515303 2,7491210
C -1,1436765 2,4030365 4,2607326
C -1,1750202 4,1400985 2,4042919
H -2,2988222 2,3311073 2,4760738
C -2,2169712 3,1960935 5,0200031
H -0,1531636 2,7080916 4,6102916
H -1,2480257 1,3284545 4,4506843
C -2,2483996 4,9225198 3,1795177
H -0,1865982 4,5275842 2,6747718
H -1,3099903 4,2844600 1,3277394
C -2,1335071 4,6917786 4,6910390
H -2,0993185 3,0308678 6,0971281
H -3,2104759 2,8180322 4,7416294
H -2,1559775 5,9890902 2,9451421
H -3,2422983 4,6021050 2,8378248
H -2,9229902 5,2407426 5,2174443
H -1,1719853 5,0882691 5,0466552
C 1,0322376 2,0486139 1,6977809
C 1,2266048 3,0635315 0,5553016
C 1,8262203 2,4433737 2,9496212
H 1,4433041 1,1012659 1,3385912
C 2,7205523 3,1862623 0,2216893
H 0,8432654 4,0452010 0,8445269
H 0,6573986 2,7295423 -0,3188396
C 3,3153998 2,5783262 2,5946405
H 1,4661196 3,3985057 3,3471358
H 1,6896784 1,6846196 3,7269177
C 3,5321339 3,5859852 1,4597336
H 2,8534745 3,9198320 -0,5815234
H 3,0914132 2,2250341 -0,1569053
H 3,8728078 2,8784258 3,4891981
H 3,7041093 1,5978600 2,2878247
H 4,5975575 3,6494063 1,2096278
H 3,2185095 4,5847968 1,7948402

5-NPh_2 [$W(CO)_5$]$PNPh_2$
35
Energy = -1494.042914613830

P	-0,7613058	0,5218718	0,4024372
C	1,2720936	-3,4811424	0,6973467
O	1,8147780	-4,5023295	0,6453188
C	2,0009069	-0,7685070	-0,0220020
O	2,9466480	-0,2664994	-0,4534169
C	1,0953311	-1,3330081	2,6548944
O	1,5961701	-1,2206476	3,6885218
C	-1,3464118	-2,5529765	1,6345521
O	-2,2639498	-3,0485856	2,1285387
C	-0,3931840	-2,0629490	-1,1237684
O	-0,7705772	-2,3022384	-2,1901477
W	0,3144019	-1,6689497	0,7679970
N	-0,9777885	1,5251329	1,7436269
C	-1,3415176	2,9049273	1,5405672
C	-2,3012686	3,4986479	2,3698126
C	-0,7433420	3,6412497	0,5126096
C	-2,6753766	4,8221590	2,1489362
H	-2,7568445	2,9221630	3,1683090
C	-1,1280959	4,9638093	0,2973137
H	0,0298688	3,1795741	-0,0936354
C	-2,0948664	5,5575570	1,1116716
H	-3,4272970	5,2776057	2,7865312
H	-0,6563883	5,5348780	-0,4967520
H	-2,3861235	6,5906034	0,9472482
C	-0,8526509	1,1279567	3,1234773
C	0,0531724	1,7970566	3,9506920
C	-1,6559361	0,1031190	3,6256614
C	0,1719176	1,4122771	5,2842764
H	0,6625236	2,5986045	3,5449577
C	-1,5341655	-0,2727122	4,9624871
H	-2,3819149	-0,3703222	2,9741155
C	-0,6175749	0,3766464	5,7917145
H	0,8862986	1,9184247	5,9265860
H	-2,1613665	-1,0672322	5,3553377
H	-0,5222640	0,0814356	6,8322838

5-N(SiH$_3$)$_2$ [W(CO)$_5$]PN(SiH$_3$)$_2$

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Energy = -1613.162081395819

P	-0,9419350	-0,5146647	2,1467372
C	1,1253404	-2,6560383	-1,2281093
O	1,6092760	-3,2748352	-2,0745056
C	0,5621029	0,1916254	-0,7943981
O	0,7215901	1,1406817	-1,4323023
C	2,1199050	-1,2971146	1,1917723
O	3,1467534	-1,1706455	1,7008016
C	-0,0376274	-3,2960963	1,3348681
O	-0,2171895	-4,2821674	1,9076170
C	-1,5801437	-1,7837679	-0,6045212
O	-2,6123075	-1,9232012	-1,1004519
N	-0,5597674	1,0459887	2,6452849
W	0,2715141	-1,5440623	0,2880315
Si	-1,6000580	1,6038233	3,9937773
H	-1,4467680	3,0765828	4,0551729
H	-3,0006456	1,2369150	3,7064072
H	-1,1398165	0,9892772	5,2580439
Si	0,6976653	2,1525909	2,0364281
H	1,8175878	1,3656197	1,4929585
H	0,1086501	3,0229034	0,9952890
H	1,1411462	2,9687078	3,1887772

Table S4. GIAO TPSS-D3/def2-QZVP computed ^{31}P chemical shifts (in ppm) using TPSS-D3/def2-TZVP + COSMO optimized geometries (see Table S2) , using the experimental ^{31}P NMR shift of **1a** [$W(CO)_5PCl_2NPh_2$)] at 108.6 ppm (computed shielding constant: 141.93ppm) as reference. **9** as possible diphosphane (complex) side products.

Compound	Shift	Atom	Compound	Shift	Atom
1a	108.6	1	**5a.nH**	339.8	1
1b	112.2	1	**5b**	1053.8	1
2a$^-$	346.5	1	**6a,a'**	-133.2, -139.1	1
2ac	281.3	1	**6b**	-158.1	1
2ah$^-$	46.0	1	**7b,b'**	-133.1, -140.0	1
2aH	38.5	1	**7a**	-140.4	1
2ahH	-33.4	1	**8b,b'**	-134.7, -135.6	1
2at$_2$	406.1	1	**9a$^-$**	39.0	1
2at$_3$	280.2	1	**9a$^-$**	136.4	37
2b$^-$	313.7	1	**9ac-**	216.5	1
2bh$^-$	-60.0	1	**9ac$^-$**	120.1	37
2bH	40.2	1	**9acCl**	121.8	1
2bhH	-78.3	1	**9acCl**	121.7	35
3a	83.0	1	**9aH**	47.6	1
3b	58.4	1	**9aH**	47.3	35
3ohH	22.0	1	**9b$^-$**	33.3	1
4a	38.4	1	**9b$^-$**	44.1	4
4anH	79.1	1	**9b0W$^-$**	-38.2	1
4b	6.8	1	**9b0W$^-$**	13.3	38
4n	20.2	1	**9bH**	-51.8	1
4nCl	118.9	1	**9bH**	-51.1	4
4nhH	-51.2	1	**9bHww**	8.4	1
5a	1183.9	1	**9bHww**	8.4	49
5a$_2$	287.7	1	**9bwW$^-$**	5.0	1
5a$_2$	287.9	36	**9bwW$^-$**	171.4	49
5aBe	-100.2	1			