Electronic Supplementary Material (ESI) for ChemComm.


Supporting Information for

# O-Functionalization of a Cobalt Carbonyl Generates a Terminal Cobalt Carbyne Complex

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## 1. Experimental Details.

### 1.1 General Considerations.

All manipulations were carried out using standard Schlenk or glovebox techniques under an $N_2$ atmosphere. Solvents were deoxygenated and dried by thoroughly sparging with $N_2$ followed by passage through an activated alumina column in a solvent purification system by SG Water, USA LLC. Ethereal solvents (THF, $Et_2O$, DME) were dried further by stirring over Na/K alloy (>2 h) and were filtered through Celite prior to use. Deuterated benzene was purchased from Cambridge Isotope Laboratories, Inc., and dried by refluxing over Ca-H then distilled and stored over Na. Deuterated THF was purchased from Cambridge Isotope Laboratories and dried over Na/K alloy and was filtered through Celite prior to use. Reagents were purchased from commercial vendors and used without further purification unless otherwise noted. $P_2^P$ was prepared according to a previously reported procedure.[1]

### 1.2 Physical Methods.

NMR spectra ($^1H$, $^{13}C$, and $^{31}P$) were collected at room temperature (25 °C unless specified) on Varian 300 or 400 MHz spectrometers. $^1H$ and $^{13}C$ chemical shifts are reported in ppm, relative to tetramethylsilane using residual proton and $^{13}C$ resonances from solvent as internal standards. $^{31}P$ chemical shifts are reported in ppm relative to 85% aqueous $H_3PO_4$. IR spectra were obtained using a Bruker Alpha Platinum ATR spectrometer with OPUS software in a glovebox under an $N_2$ atmosphere. X-band EPR spectra were obtained on a Bruker EMX spectrometer with the samples prepared in a 2-MeTHF glass.

X-Ray diffraction and combustion analysis measurements were carried out in the Beckman Institute Crystallography Facility. XRD measurements were collected using a dual source Bruker D8 Venture, four-circle diffractometer with a PHOTON II detector or a Bruker D8 KAPPA with a PHOTON 100 detector. Structures were solved using SHELXT and refined against $F^2$ on all data by full-matrix least squares with SHELXL. The crystals were mounted on a glass fiber under Paratone N oil. See below for any special refinement details for individual data sets. Combustion analysis measurements were collected using a PerkinElmer 2400 Series II CHN Elemental Analyzer by facility staff.

### 1.3 Computational Methods.

Geometry optimization and frequency calculations were carried out using the Gaussian 09 program.[2] The crystal structure coordinates of **3** and **5b** were used in the input files. Reported DFT coordinates were used in the input file for the $PhB(^tBuIm)_3CoO$ complex.[3] The crystal coordinates of **4a** were used in the input file, but the Na-coordinated DME molecules were replaced with THF molecules for optimization. For $BP_3Co(NAd)$ the crystal coordinates of the corresponding Fe

(1) Buscagan, T. M.; Oyala, P. H.; Peters, J. C. *Angew. Chem. Int. Ed.* **2017**, *56*, 6921.

(2) Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

(3) Goetz, M. K.; Hill, E. A.; Filatov, A. S.; Anderson, J. S. *J. Am. Chem. Soc.* **2018**, *140*, 13176-13180.

complex[4] were used in the input file, replacing Fe with Co. The M06-L functional[5] with def2-TZVP[6] basis set was used on Co with the def2-SVP basis set used on all other atoms.

(4) Betley, T. A.; Peters, J. C. *J. Am. Chem. Soc.* **2003**, *125*, 10782-10783.
(5) Zhao, Y.; Truhlar, D. G. *J. Chem, Phys.* **2006**, *125*, 194101.
(6) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

**2. Synthetic Details.**

**$P_2^PCoBr$ 1.** $P_2^P$ (705.5 mg, 1.43 mmol) and $CoBr_2$ (312.0 mg, 1.43 mmol) were combined in THF (40 mL) in a 100 mL Schlenk tube, rapidly turning a muddy purple-brown color. Concurrently, a solution of sodium naphthalenide was prepared by stirring naphthalene (192.0 mg, 1.50 mmol, 1.05 equiv) over an excess of Na metal in THF (12 mL) over the course of 4 h. The naphthalenide solution was pipetted away from the excess Na metal and added to the prechilled Schlenk tube at -78 °C; this mixture was warmed to room temperature and then stirred for 3 h, yielding a dark red solution. The solvent was removed *in vacuo*, and the residue was triturated and then washed with pentane (2 x 10 mL). The dark residue was extracted into benzene and filtered through celite, with iterative addition of benzene to the dark residue until no additional colored material was brought into solution (~50 mL total). Concentration of this benzene solution and then crystallization by layering with pentane overnight allowed for the isolation of the product as a dark red crystalline solid (641.9 mg, 71%); crystals suitable for XRD were grown in an analogous fashion. Additional crystalline material could be isolated from the mother liquor by removing the solvent *in vacuo*, redissolving the residue in a minimal amount of benzene and layering with pentane. $^1$H NMR (400 MHz, $C_6D_6$): δ 172.1, 94.1, 20.1, 10.1, 9.3, 8.4, 3.7, -0.8, -2.2, -8.9, -16.6. Solution magnetic moment (Evans Method): 25 °C: 2.7$\mu_B$; -80 °C: 3.0 $\mu_B$. Anal. Calcd. for $C_{30}H_{41}BrCoP_3$: C, 56.89; H, 6.52; N, 0.00. Found: C, 57.12; H, 6.52; N, < 0.1.

**$P_2^PCoBr(CO)$ 2.** $P_2^PCoBr$ **1** (244.9 mg, 0.387 mmol) was dissolved in benzene (30 mL) and transferred to a Schlenk tube. The solution was frozen and the headspace was evacuated; after thawing the solution, it was exposed to an atmosphere of CO. The tube was mixed vigorously at room temperature for 5 minutes before the solvent was removed *in vacuo*. The residue was washed with pentane (~10 mL) and the red-orange residue was extracted into benzene (~3 x 15 mL). Solvent removal by lyophilization yielded the product as an orange-red powder (244.2 mg, 95%). Consistent observation of two sets of $^{31}$P resonances (~6:1) was attributed to the presence of two isomers of this complex. Resonances for both species are noted for the $^{31}$P NMR spectrum including their approximate relative integrations. By $^1$H NMR, only the $^i$Pr methyl resonances are well resolved between the two species, so both sets are noted. Crystals suitable for XRD were grown by layering a concentrated toluene solution of **2** with pentane at -35 °C. $^1$H NMR (400 MHz, $C_6D_6$): δ 7.55 (t, *J* = 7 Hz, 2H), 7.33 (d, *J* = 7 Hz, 2H), 7.26 (dd, *J* = 11, 7 Hz, 2H), 7.08-6.85 (overlapping m, 7H), 2.68 (m, *J* = 7Hz, 2H), 2.52 (br, 2H), 1.70 (q, *J* = 7 Hz, minor isomer), 1.59 (q, *J* = 7 Hz, 6H), 1.30 (q, *J* = 7 Hz, 6H), 1.23 (q, *J* = 7 Hz, minor isomer), 1.12 (q, *J* = 7 Hz, minor isomer), 1.04 (q, *J* = 7 Hz, minor isomer), 0.94 (q, *J* = 7 Hz, 6H), 0.88 (q, *J* = 7 Hz, 6H). $^{31}$P{$^1$H} NMR (162 MHz, $C_6D_6$): δ 116.1 (t, *J* = 55 Hz, ~0.5P), 102.0 (t, *J* = 70 Hz, ~3P), 88.4 (d, *J* = 69 Hz, ~6P), 78.2 (d, *J* = 56 Hz, ~1P). $^{31}$P{$^1$H} NMR (162 MHz, $C_6D_6$, $^{13}$CO-labeled): δ 116.1 (m), 102.0 (apparent q, *J* = 70 Hz), 88.4 (dd, *J* = 70, 30 Hz), 78.2 (dd, *J* = 55, 37 Hz). $^{13}$C{$^1$H} NMR (101 MHz, $C_6D_6$, $^{13}$CO-labeled): δ 222.0 (dt, *J* = 62, 30 Hz). IR (thin film): $\nu_{CO}$ = 1928 cm$^{-1}$. IR (thin film, $^{13}$CO): $\nu_{CO}$ = 1884 cm$^{-1}$. Anal. Calcd. for $C_{31}H_{41}BrCoOP_3$: C, 56.29; H, 6.25; N, 0.00. Found: C, 57.00; H, 6.24; N, < 0.1.

**$P_2^PCo(CO)$ 3.** A solution of naphthalene (8.4 mg, 1 equiv) in THF (2 mL) was reduced by stirring over an excess of Na for 4 h. A red solution of $P_2^PCoBr(CO)$ **2** (43.5 mg, 1 equiv) in THF (3 mL) was cooled to -78 °C in the glovebox coldwell and the naphthalenide solution was decanted away from the excess Na metal and added. The mixture was allowed to stir at low temperature for an hour and then at room temperature for an additional 30 min, turning orange-red. The solvent was

removed *in vacuo*, and the residue was triturated with pentane (~1 mL) to give a red residue. The residue was then washed with pentane (3 x 1 mL) and then extracted into benzene (~5 mL). This solution was frozen and then lyophilized to yield the product as an orange-red powder (31.0 mg, 81%). Crystals suitable for XRD could be grown by evaporation of an $Et_2O$ solution of **3** into MeCy. $^1$H NMR (300 MHz, $C_6D_6$): δ 14.4 (br), 12.3 (br), 6.2 (br), 5.1 (br), 4.5 (br), -7.5 (br). IR (thin film): $\nu_{CO}$ = 1866 cm$^{-1}$. IR (thin film, $^{13}$CO): $\nu_{CO}$ = 1824 cm$^{-1}$. Solution magnetic moment (Evans Method; 25 °C): 1.8 $\mu_B$. Anal. Calcd. for $C_{31}H_{41}CoOP_3$: C, 64.03; H, 7.11; N, 0.00. Found: C, 64.07; H, 6.97; N, < 0.2.

**[$P_2^P$Co(CO)][Na(S)$_n$] 4a.** An excess of Na metal was added to a THF solution (5 mL) of $P_2^P$CoBr(CO) **2** (53.5 mg) and was stirred at room temperature turning very dark brown/black over the course of several hours. Thin film IR spectra of reaction aliquots were collected to monitor the conversion of **2** to **4** over time. Once the reaction proceeded to completion, the solvent was transferred away from remaining Na and then removed *in vacuo*. The resultant residue was triturated and then washed with pentane. Subsequent extraction into benzene and lyophilization yielded the desired product as a dark brown powder (53.2 mg; ~80% yield assuming $(S)_n$ = $(THF)_3$). Crystals suitable for XRD could be grown by dissolving the complex in a minimum of 1:1 toluene/DME and layering with pentane at -35 °C. The 12-crown-4 salt **4b** could be prepared by addition of 12-crown-4 (2 equiv) to a THF solution of the complex and then removing the solvent *in vacuo* and washing with benzene. $^{31}$P NMR spectra of the complex **4a** were consistently very broad. $^1$H NMR (400 MHz, $C_6D_6$): δ 7.81 (s, 2H), 7.59 (d, *J* = 7 Hz, 2H), 7.37 (m, 2H), 7.1-6.9 (overlapping m, 7H), 2.49 (br, 2H), 2.27 (br, 2H), 1.41 (br, 6H), 1.10 (br, 6H), 1.03 (br, 6H), 0.89 (br, 6H). $^{31}$P{$^1$H} NMR (162 Hz, $C_6D_6$/THF): δ 80-120 (br). $^{13}$C{$^1$H} NMR (101 Hz, $C_6D_6$): δ 227.2 ($^{13}$CO). IR (thin film): 1731 cm$^{-1}$. IR (thin film, $^{13}$CO): 1691 cm$^{-1}$. IR (thin film, **4b**): 1752 cm$^{-1}$. Anal. Calcd. for . $C_{47}H_{73}CoNaO_9P_3$ **4b**: C, 58.99; H, 7.69; N, 0.00. Found: C, 58.51; H, 7.74; N, < 0.25.

**$P_2^P$Co(H)(CO).** A solution of $P_2^P$CoBr(CO) **2** (39.6 mg, 1 equiv) was prepared in THF and cooled to -78 °C. A slight excess of 1 M $KHBEt_3$ in THF (66 µL, 1.1 equiv) was added and the solution was stirred at low temperature for 1 h and then warmed to room temperature and stirred for an additional 1 h. The solvent was removed and the residue was washed with pentane and then extracted into benzene, yielding the desired product upon lyophilization. The hydride product is observed as a mixture of isomers in solution, with a minor component (<5%) reproducibly observed in the $^1$H and $^{31}$P NMR spectra of this compound. Given the small fraction of the material observed as the minor isomer, NMR data is listed only for the major isomer. Crystals suitable for XRD could be grown by evaporation of an $Et_2O$ solution of the complex into MeCy. $^1$H NMR (400 MHz, $C_6D_6$): δ 7.68 (t, *J* = 7 Hz, 2H), 7.51 (m, 2H), 7.37 (d, *J* = 7 Hz, 2H), 7.09-6.93 (m, 7H), 2.26 (overlapping hept, *J* = 7 Hz, 4H), 1.30 (q, *J* = 7 Hz, 6H), 1.03 (m, 12H), 0.77 (q, *J* = 7 Hz, 6H), -11.28 (dt, *J* = 70, 50 Hz, 1H). $^{31}$P{$^1$H} NMR (162 Hz, $C_6D_6$): δ 115.3 (br, 1P), 107.4 (br, 2P). IR (thin film): $\nu_{CO}$ = 1901 cm$^{-1}$.

**$P_2^P$Co(COSi$^i$Pr$_3$) 5a.** A solution of $P_2^P$CoBr(CO) **2** (40.5 mg, 1 equiv) was stirred over an excess of Na metal in THF (5 mL) until conversion to **4** was observed with darkening of the reaction mixture. Complete conversion was confirmed by obtaining a thin film IR spectrum of a reaction aliquot. The resulting solution was decanted away from residual Na metal and cooled to -78 °C in a glovebox cold well. To the cooled solution, neat $^i$Pr$_3$SiOTf (16.5 µL, 1 equiv) was added and the

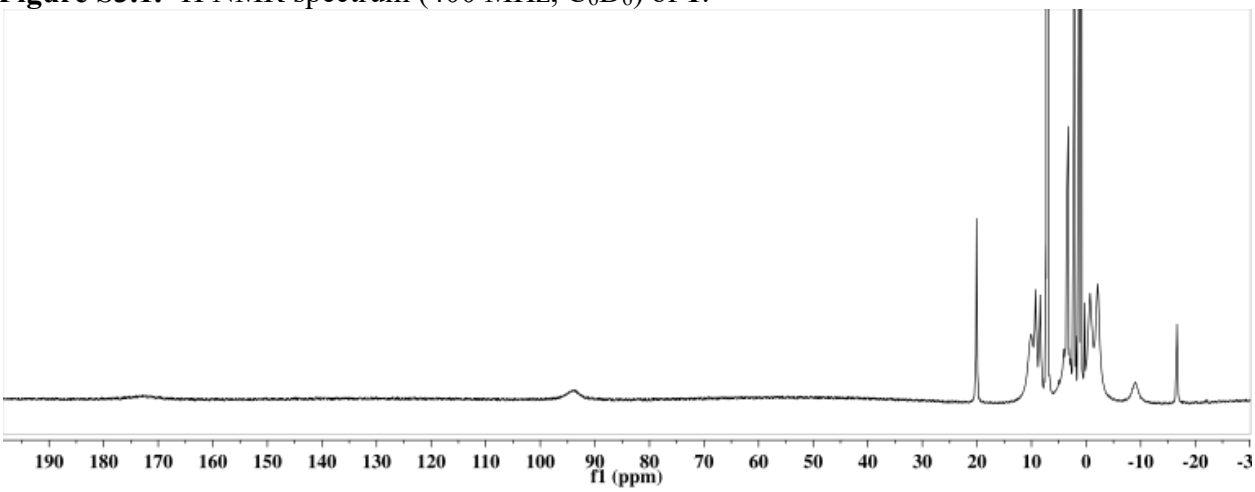
mixture was stirred at -78 °C for 15 min and then at room temperature for an additional 15 min, turning deep red. The solvent was removed *in vacuo* and then the residue was triturated with pentane (2 mL) and then extracted into pentane (5 mL). Removal of the solvent *in vacuo* yielded the product as a red foam (44.3 mg, > 95%). Minor quantities of products of unproductive reactivity (<5%) were typically observed in spectra of the isolated materials. $^{1}$H NMR (400 MHz, $C_6D_6$): δ 7.82 (t, *J* = 6 Hz, 2H), 7.75 (t, *J* = 8 Hz, 2H), 7.64 (d, *J* = 7 Hz, 2H), 7.22-7.05 (overlapping m, 7H), 2.68 (hept, *J* = 7 Hz, 2H), 2.34 (hept, *J* = 7 Hz, 2H), 1.59 (dd, *J* = 15, 7 Hz, 6H), 1.37-1.09 (overlapping m, 33H), 1.01 (dd, *J* = 12, 6 Hz, 6H). $^{31}$P{$^{1}$H} NMR (162 Hz, $C_6D_6$): δ 103.3 (br, 2P), 97.2 (br, 1P). $^{13}$C{$^{1}$H} NMR (101 Hz, $C_6D_6$): 229.8 ($^{13}$CO). IR (thin film): $\nu_{CO}$ = 1387 cm$^{-1}$. IR (thin film, $^{13}$CO): $\nu_{CO}$ = 1347 cm$^{-1}$.

**$P_2^P$Co(COSi$^t$BuPh$_2$) 5b.** As for **5a**, a solution of the reduced CO complex **4** was prepared from **2** (56.5 mg, 0.085 mmol, 1 equiv) in THF (5 mL). Neat $^t$BuPh$_2$SiOTf (33.2 mg, 1 equiv) was added to a stirring solution **4** at -78 °C and allowed to stir for 15 min and then was warmed to room temperature and stirred for an additional 15 min, turning red. The solvent was removed *in vacuo* and then the residue was triturated with pentane (2 mL) and then extracted into pentane (5 mL). Removal of the solvent *in vacuo* yielded the product as a red foam (65.8 mg, 94%). Crystals suitable for X-ray diffraction were obtained by slow evaporation of a pentane solution into MeCy. Minor quantities of products of unproductive reactivity (<5%) were typically observed in spectra of the isolated materials. $^{1}$H NMR (400 MHz, $C_6D_6$): δ 7.91 (m, 4H), 7.82-7.68 (overlapping m, 5H), 7.51 (dd, *J* = 6, 3 Hz, 2H), 7.15-7.06 (m, 8H), 7.01 (m, 4H), 2.42 (hept, *J* = 7 Hz, 2H), 2.21 (hept, *J* = 7 Hz, 2H), 1.26 (dd, *J* = 16, 7 Hz, 6H), 1.15-1.07 (dd, 6H), 1.12 (s, 9H), 1.02 (dd, *J* = 12, 7 Hz, 6H), 0.90 (dd, *J* = 12, 7 Hz, 6H). $^{31}$P{$^{1}$H} NMR (162 Hz, $C_6D_6$): δ 103.8 (br, 2P), 97.4 (br, 1P). Anal. Calcd. for $C_{47}H_{60}CoOP_3Si$: C, 68.77; H, 7.37; N, 0.00. Found: C, 68.86; H, 7.78; N, < 0.20.

**3. NMR Spectra.**

**$P_2^PCoBr$ 1.**

**Figure S3.1.** $^1H$ NMR spectrum (400 MHz, $C_6D_6$) of **1**.




**$P_2^PCoBr(CO)$ 2.**

**Figure S3.2.** $^1H$ NMR spectrum (400 MHz, $C_6D_6$) of **2**, a mixture of two isomers.

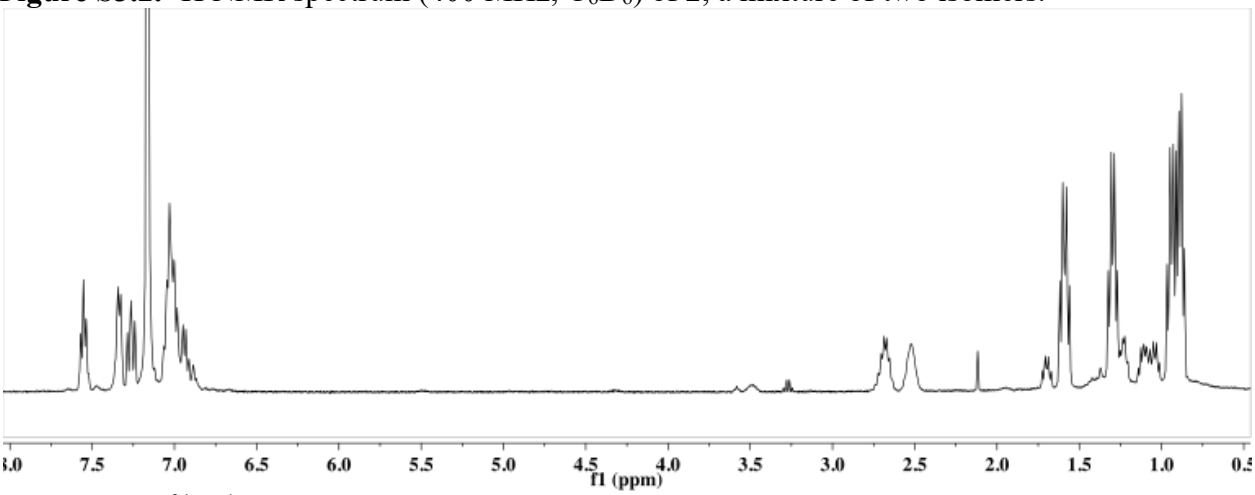



**Figure S3.3.** $^{31}P\{^1H\}$ NMR spectrum (162 MHz, $C_6D_6$) of **2**, a mixture of two isomers.

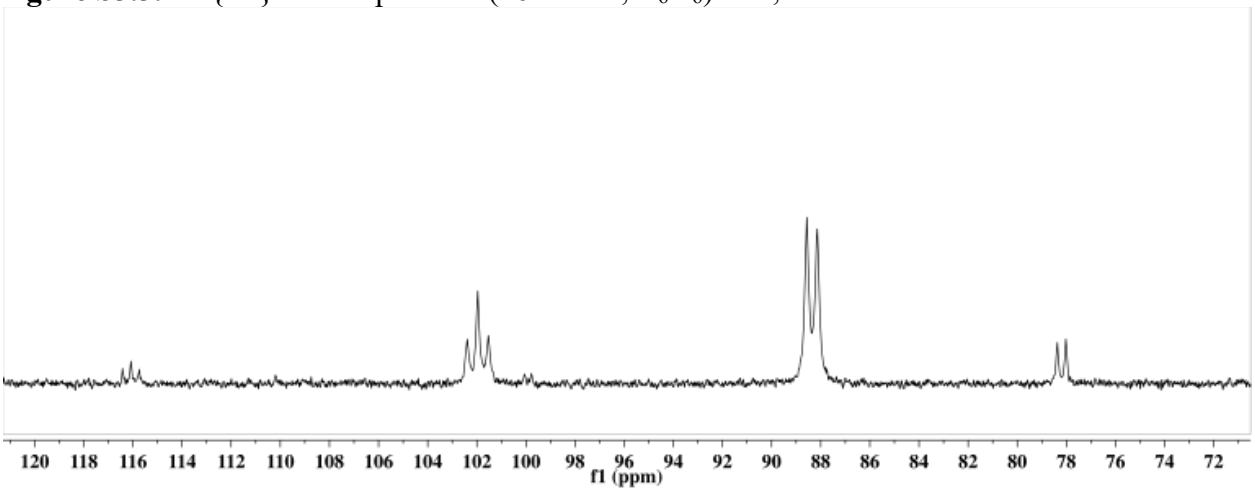


**Figure S3.4.** $^{31}P\{^{1}H\}$ NMR spectrum (162 MHz, $C_6D_6$) of **2-$^{13}$CO**, a mixture of two isomers.

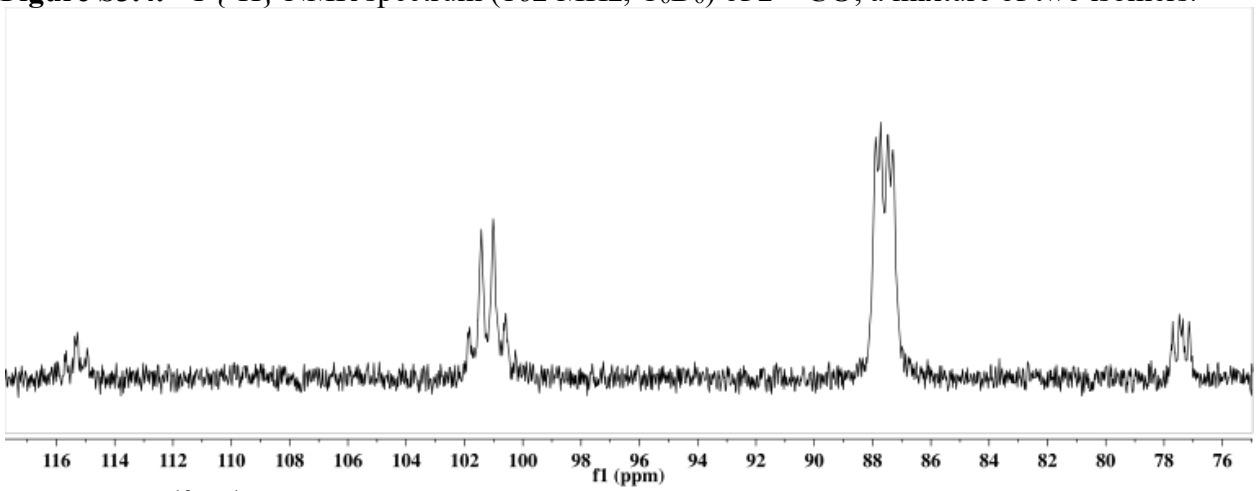
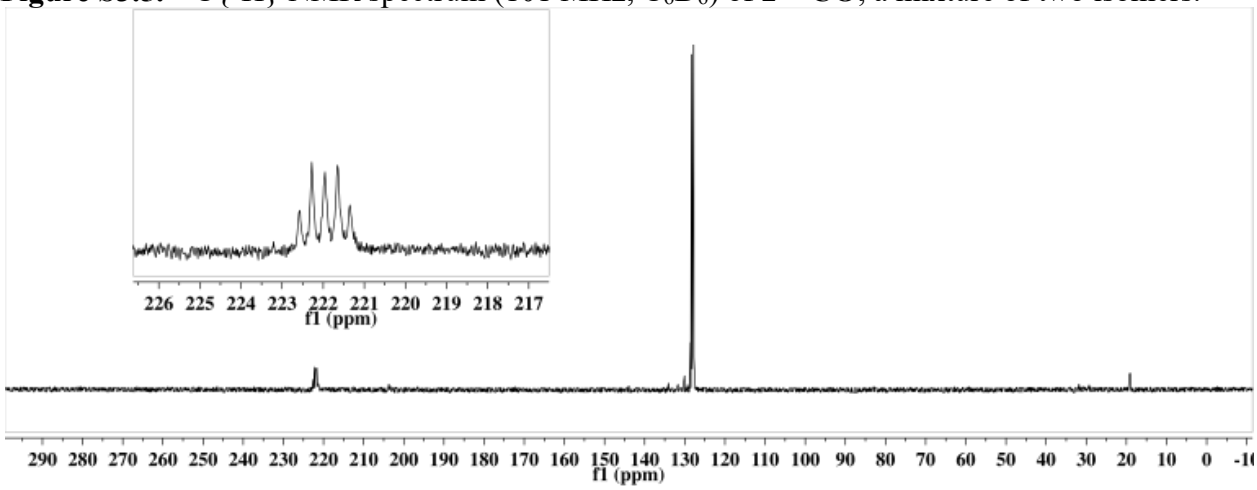
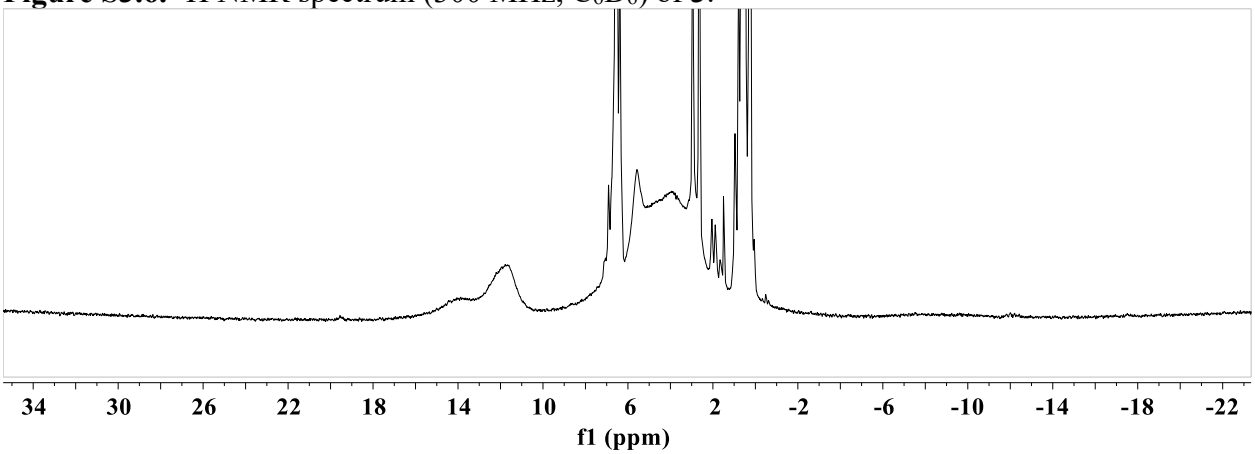



**Figure S3.5.** $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $C_6D_6$) of **2-$^{13}$CO**, a mixture of two isomers.




**$P_2^PCo(CO)$ 3.**

**Figure S3.6.** $^{1}H$ NMR spectrum (300 MHz, $C_6D_6$) of **3**.



**[$P_2^PCo(CO)$][$Na(THF)_n$] 4.**

**Figure S3.7.** $^1H$ NMR spectrum (400 MHz, $C_6D_6$) of **4a**. Spectrum obtained of crystalline material with DME, toluene, and pentane observed from the crystallization.

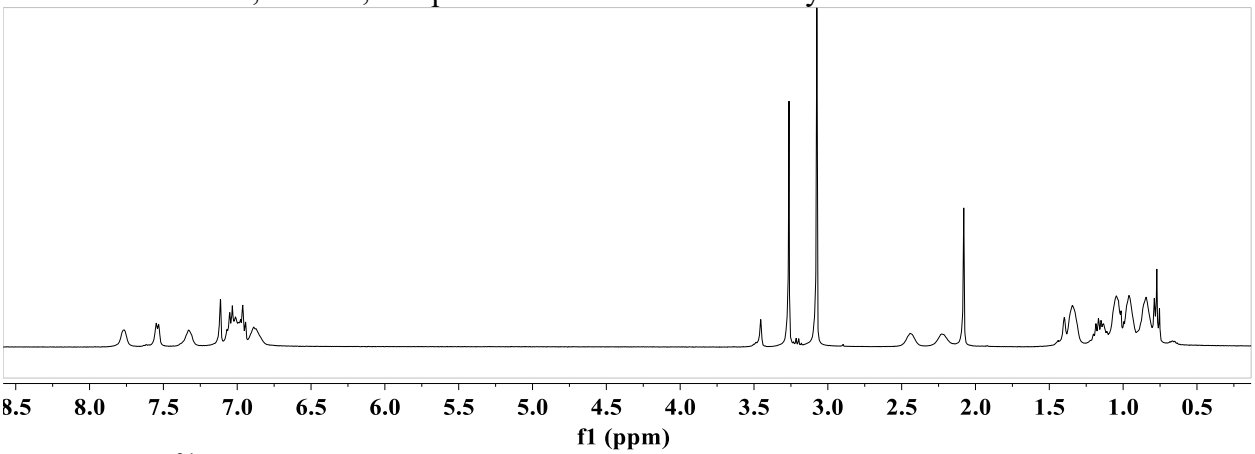



**Figure S3.8.** $^{31}P$ NMR spectrum (162 MHz, $C_6D_6$/THF) of **4a**.

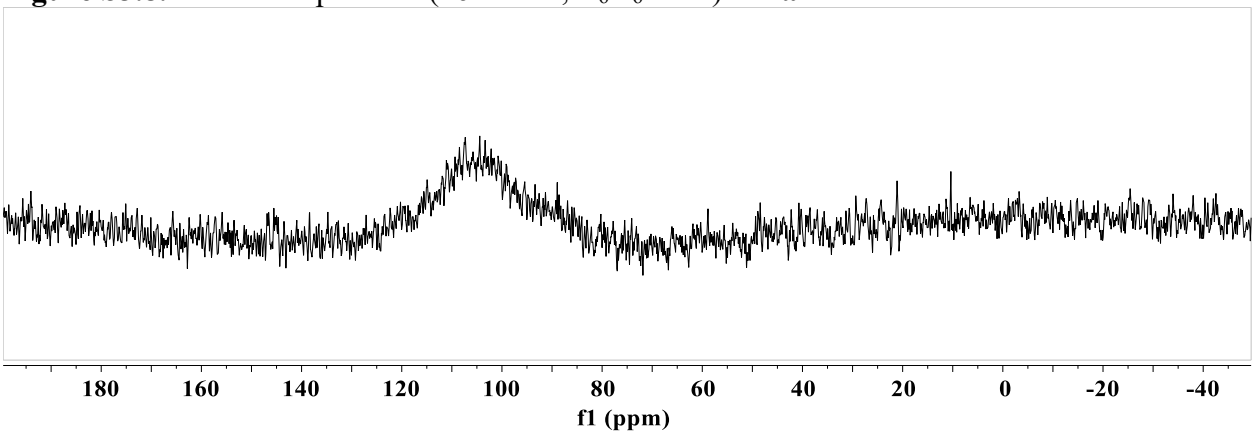
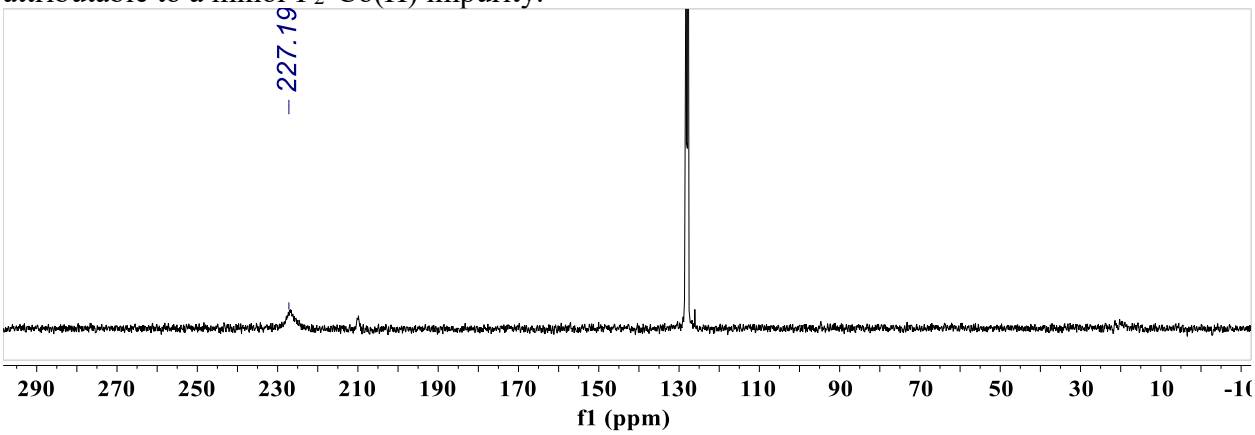



**Figure S3.9.** $^{13}C$ NMR spectrum (101 MHz, $C_6D_6$) of **4a-$^{13}$CO**. The peak at ~210 ppm is attributable to a minor $P_2^PCo(H)$ impurity.



**$P_2^PCo(H)(CO)$.**

**Figure S3.10.** $^1H$ NMR spectrum (400 MHz, $C_6D_6$) of $P_2^PCo(H)(CO)$.

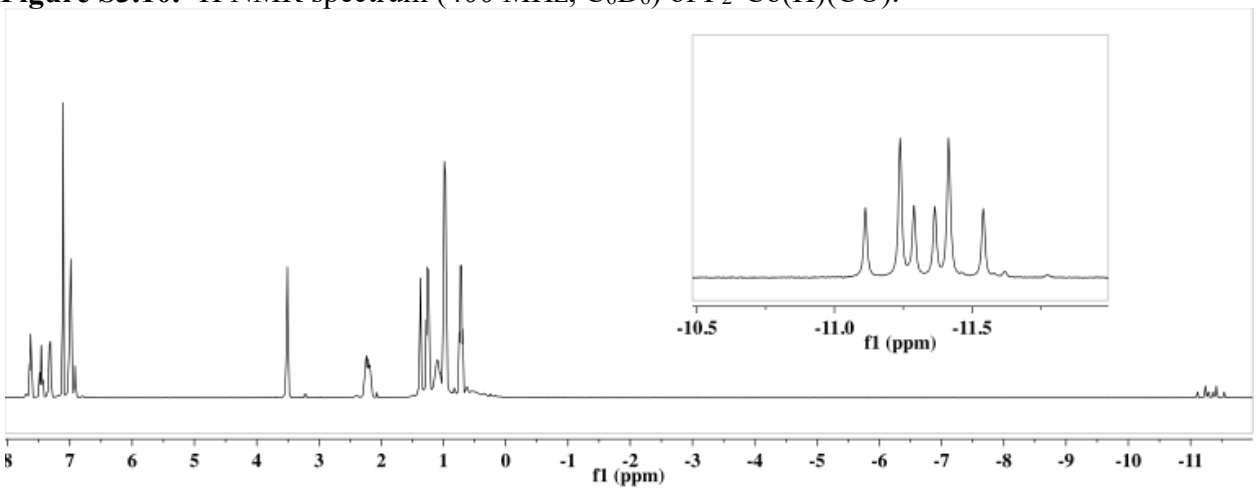
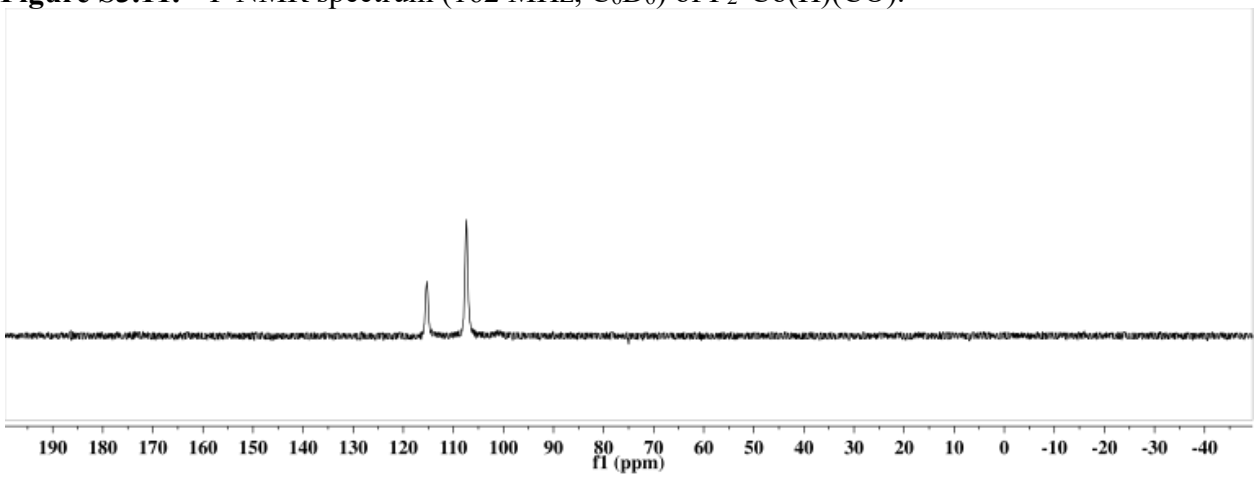



**Figure S3.11.** $^{31}P$ NMR spectrum (162 MHz, $C_6D_6$) of $P_2^PCo(H)(CO)$.




**$P_2^PCo(COSi^iPr_3)$ 5a.**

**Figure S.3.12.** $^1H$ NMR spectrum (400 MHz, $C_6D_6$) of **5a.**

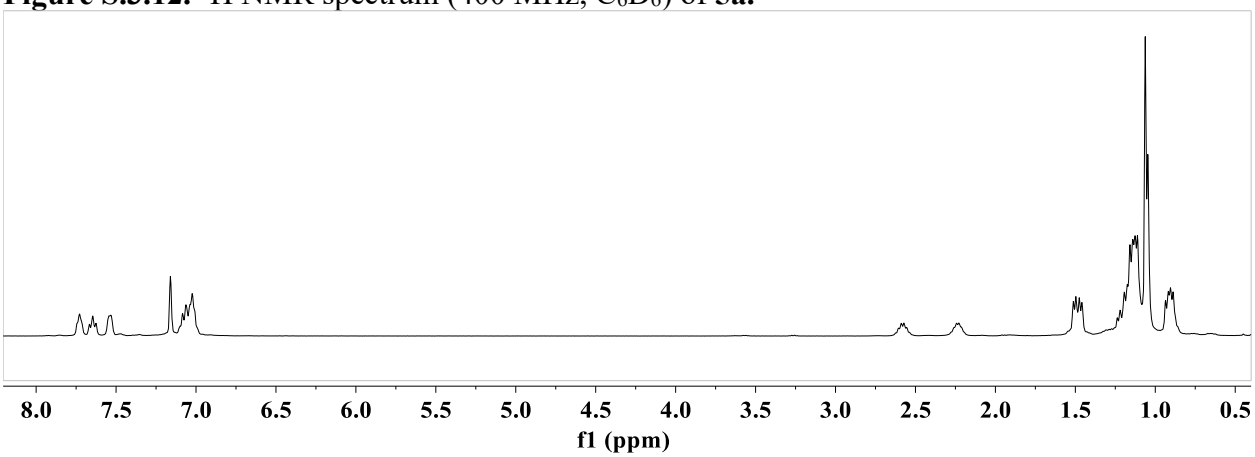


**Figure S.3.13.** $^{31}P$ NMR spectrum (162 MHz, $C_6D_6$) of **5a.**

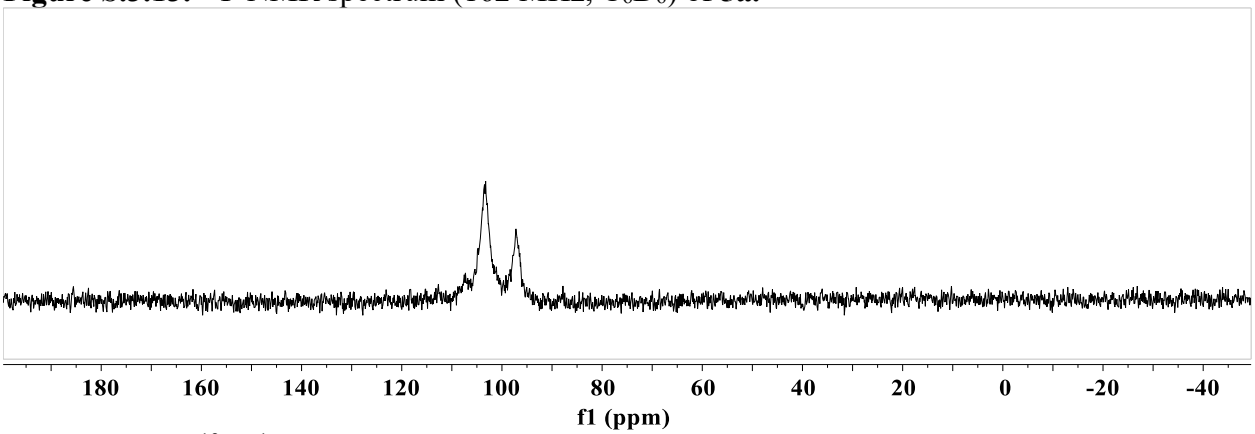



**Figure S.3.14.** $^{13}C\{^1H\}$ NMR spectrum (101 MHz, $C_6D_6$) of **5a-$^{13}$CO.** The peak at ~210 ppm is attributable to a minor $P_2^PCo(H)$ impurity.

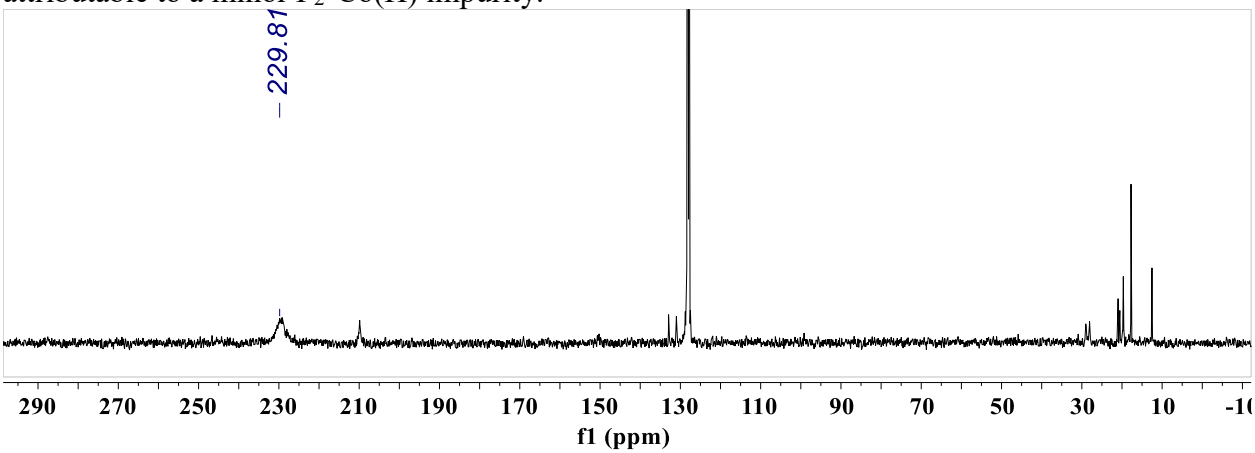
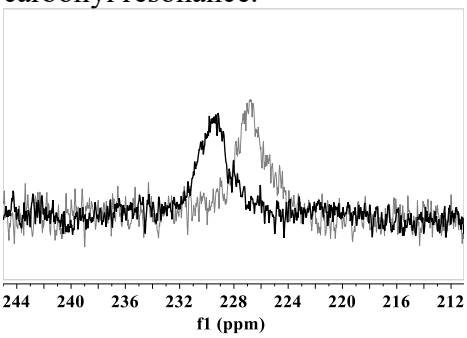



**Figure S.3.15.** $^{13}C\{^1H\}$ NMR overlay of **4** (grey) and **5a** (black) highlighting the shift in the carbonyl resonance.



**$P_2^PCo(COSi^tBuPh_2)$ 5b.**

**Figure S.3.16.** $^1H$ NMR spectrum (400 MHz, $C_6D_6$) of **5b.**

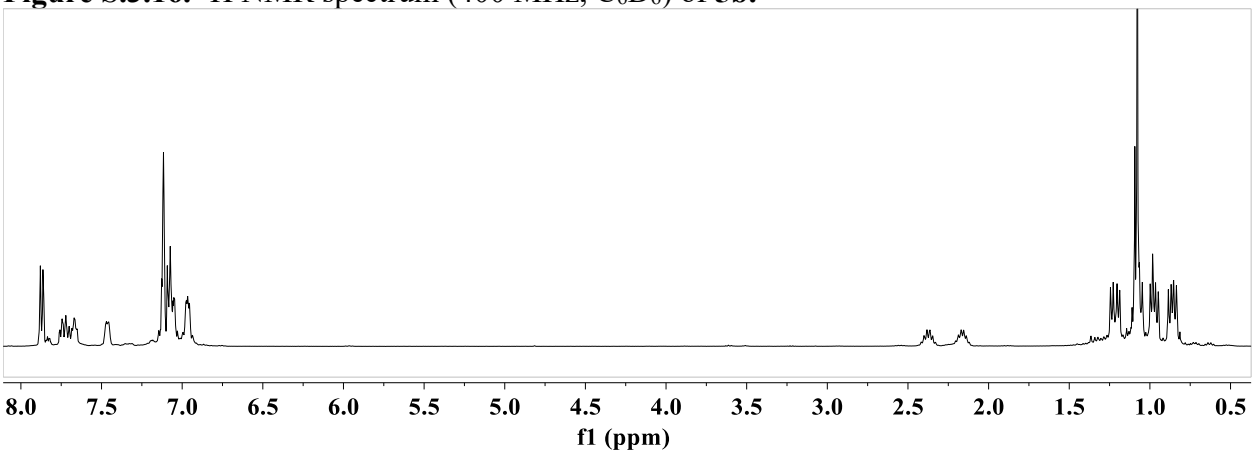
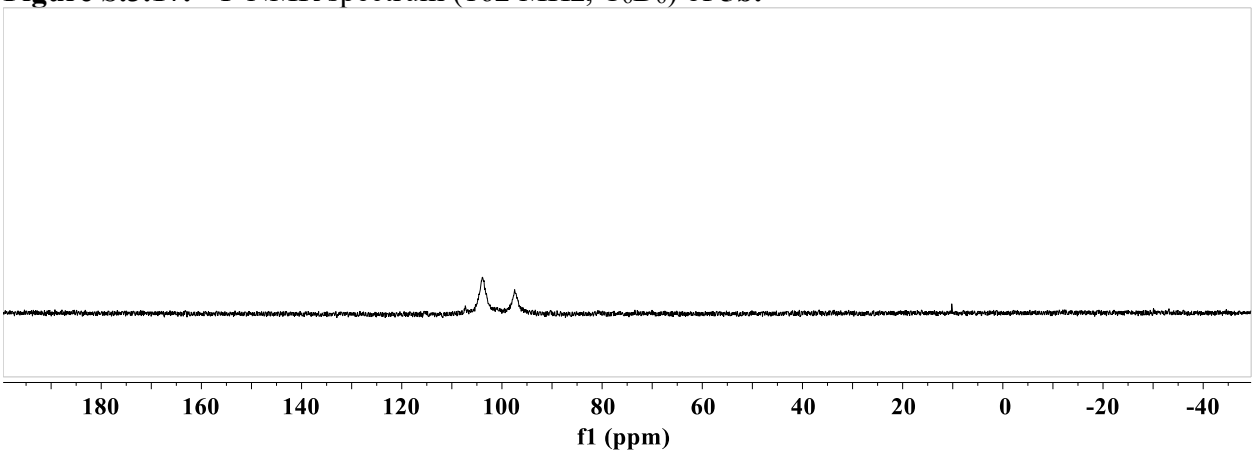



**Figure S.3.17.** $^{31}P$ NMR spectrum (162 MHz, $C_6D_6$) of **5b.**



**4. IR Spectra.**

**$P_2^PCoBr(CO)$ 2.**

**Figure S4.1.** Thin film IR spectrum of $P_2^PCoBr(CO)$ **2** ($\nu_{CO}$ = 1928 $cm^{-1}$).

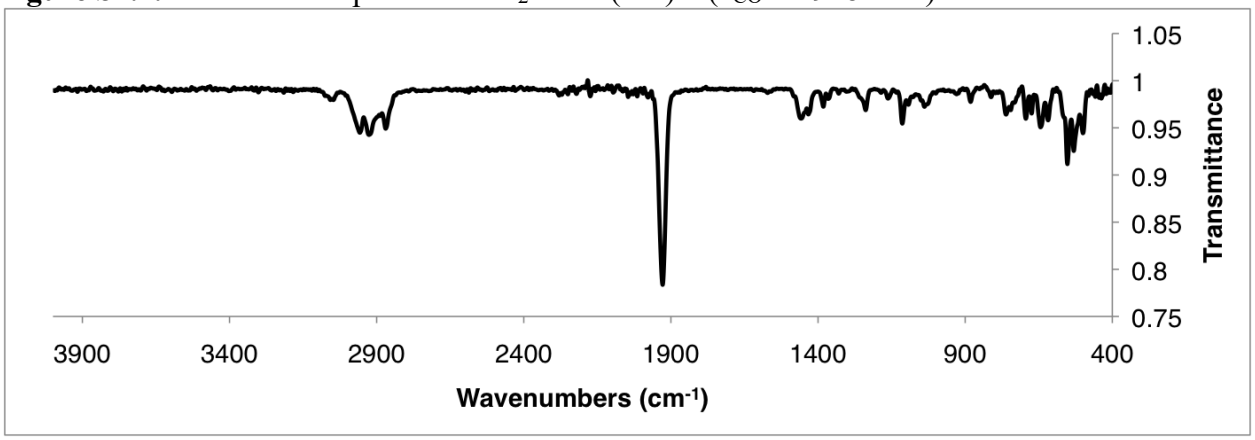
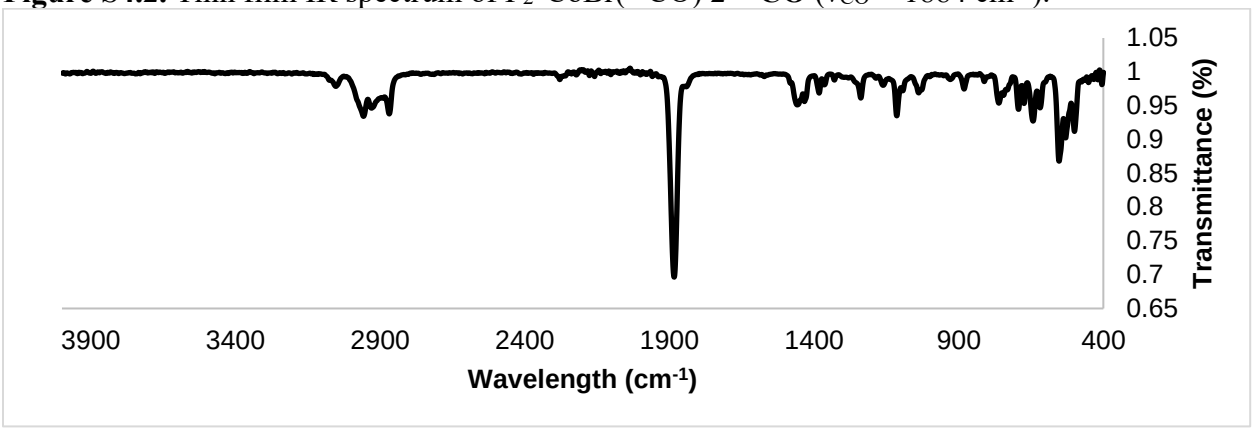



**Figure S4.2.** Thin film IR spectrum of $P_2^PCoBr(^{13}CO)$ **2-$^{13}$CO** ($\nu_{CO}$ = 1884 $cm^{-1}$).




**$P_2^PCo(CO)$ 3.**

**Figure S4.3.** Thin film IR spectrum of $P_2^PCo(CO)$ **3** ($\nu_{CO}$ = 1866 $cm^{-1}$).

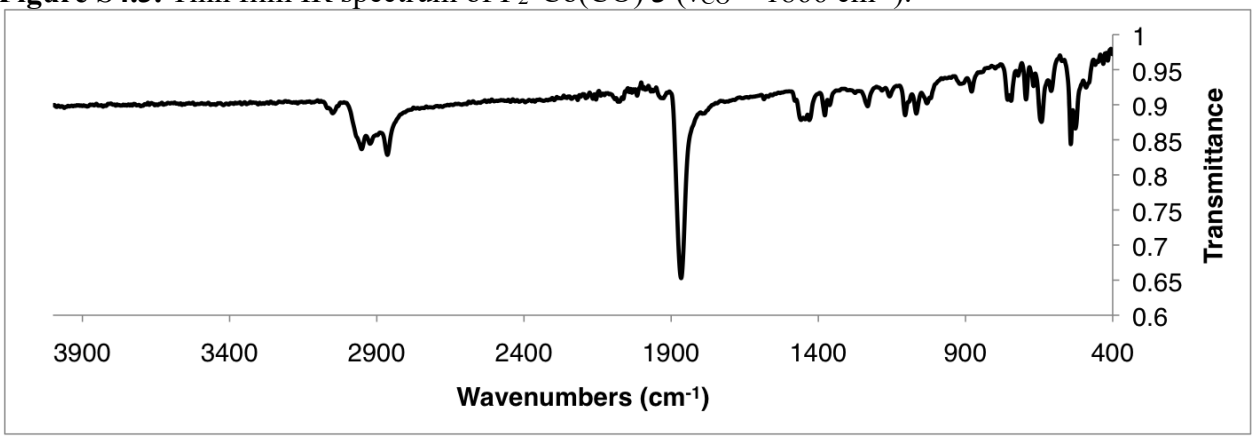
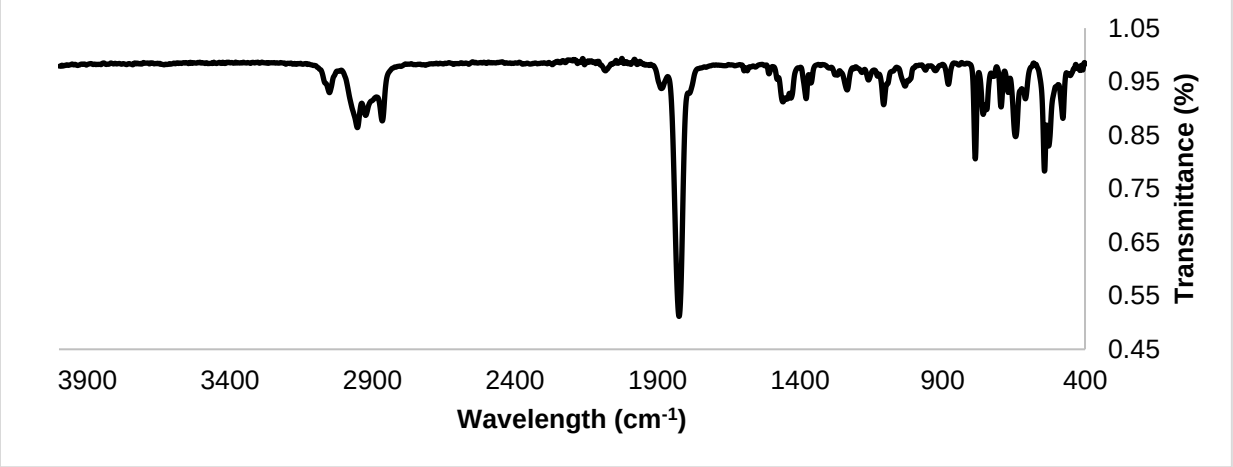


**Figure S4.4.** Thin film IR spectrum of $P_2^PCo(^{13}CO)$ **3-$^{13}$CO** ($\nu_{CO}$ = 1824 cm$^{-1}$).




**[$P_2^PCo(CO)$][$Na(THF)_n$] 4a.**

**Figure S4.5.** Thin film IR spectrum of [$P_2^PCo(CO)$][$Na(THF)_n$] **4a** ($\nu_{CO}$ = 1731 cm$^{-1}$).

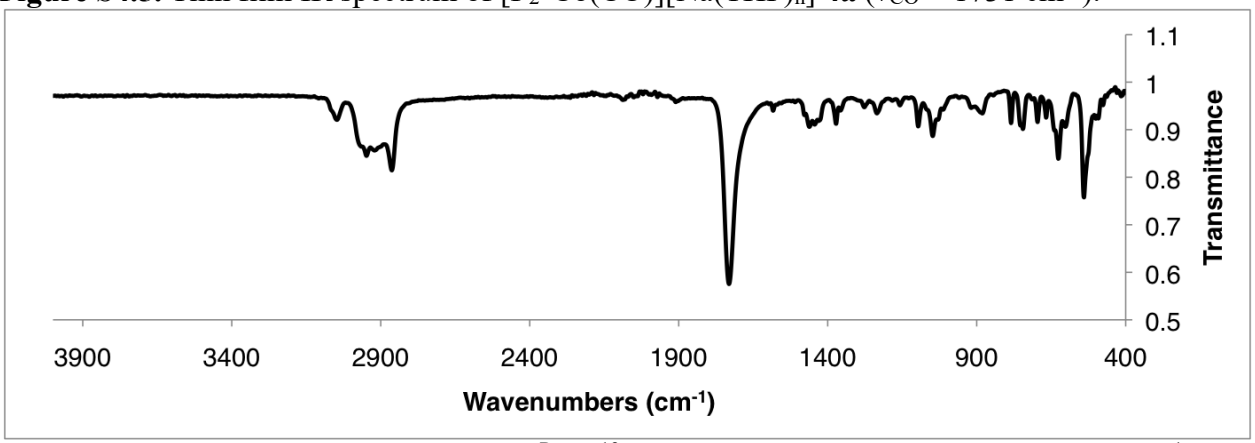
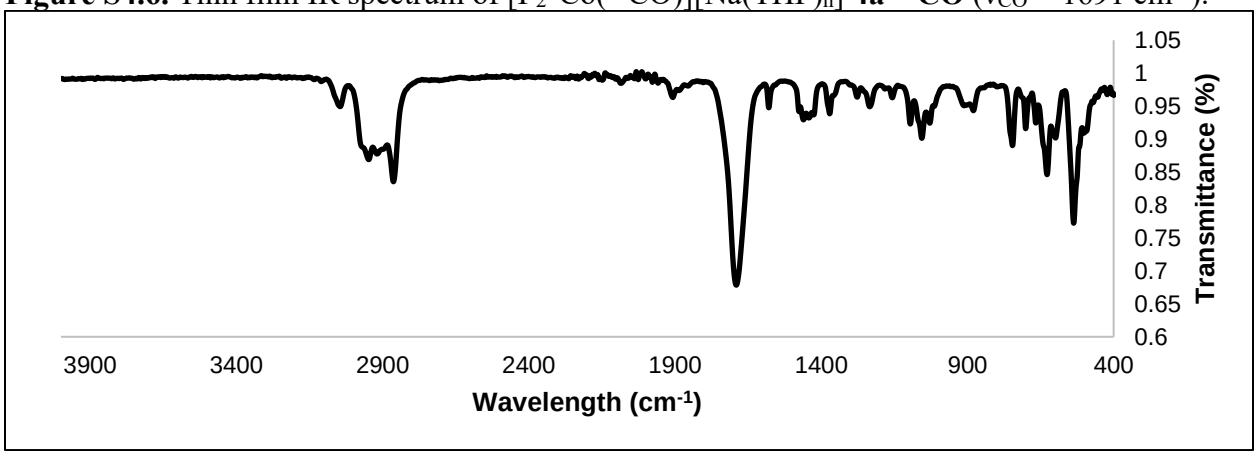
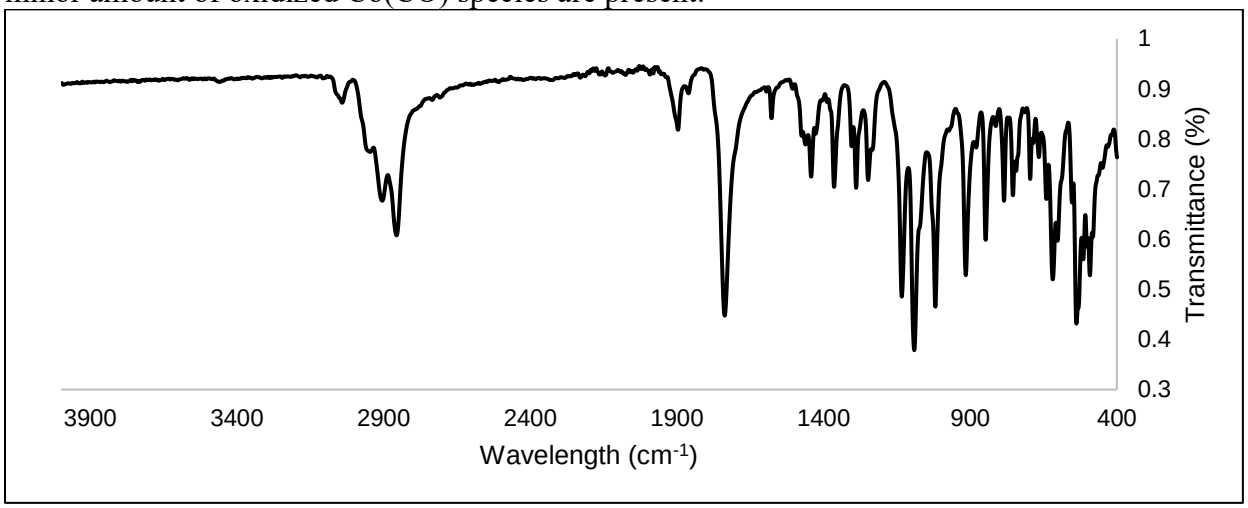



**Figure S4.6.** Thin film IR spectrum of [$P_2^PCo(^{13}CO)$][$Na(THF)_n$] **4a-$^{13}$CO** ($\nu_{CO}$ = 1691 cm$^{-1}$).



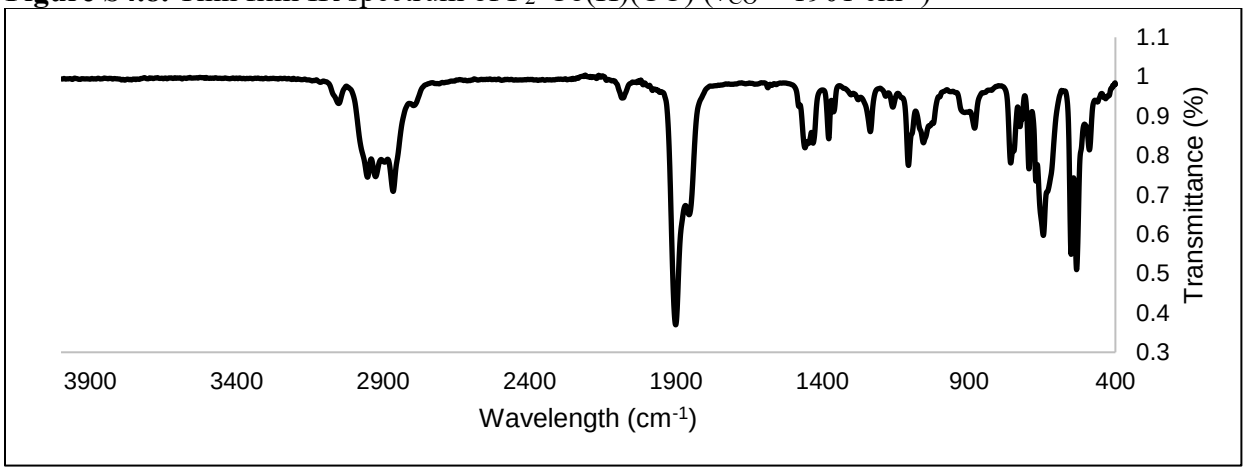
**[$P_2^PCo(CO)$][Na(12-crown-4)$_2$] 4b.**

**Figure S4.7.** Thin film IR spectrum of [$P_2^PCo(CO)$][Na(12-crown-4)$_2$] **4b** ($\nu_{CO}$ = 1752 cm$^{-1}$). A minor amount of oxidized Co(CO) species are present.




**$P_2^PCo(H)(CO)$.**

**Figure S4.8.** Thin film IR spectrum of $P_2^PCo(H)(CO)$ ($\nu_{CO}$ = 1901 cm$^{-1}$)




**$P_2^PCo(COSi^iPr_3)$ 5a.**

**Figure S4.9.** Thin film IR spectrum of $P_2^PCo(COSi^iPr_3)$ **5a** ($\nu_{CO}$ = 1387 cm$^{-1}$). A minor amount of oxidized Co(CO) species are observable.

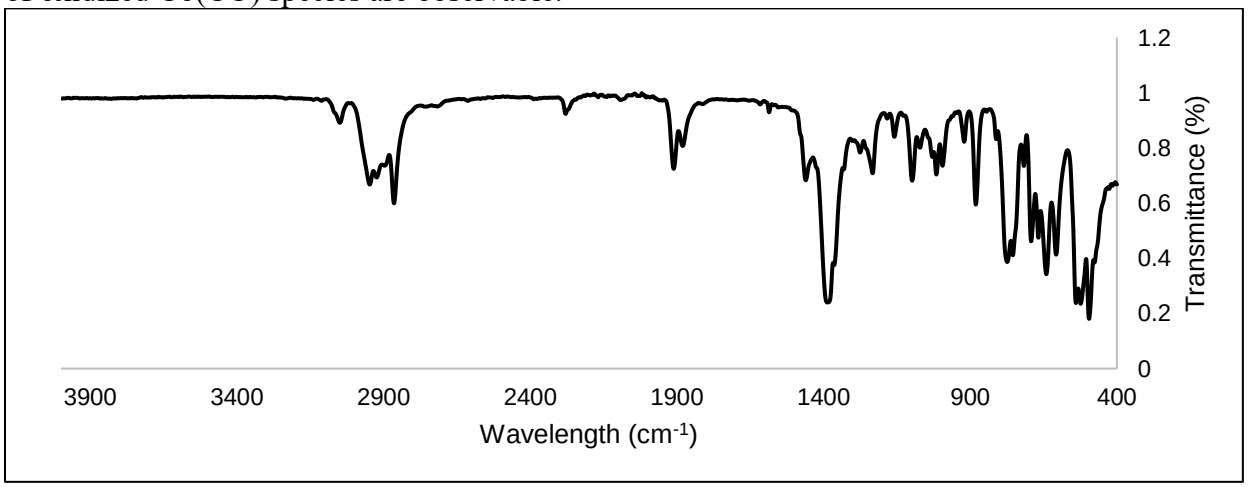


**Figure S4.10.** Thin film IR spectrum of $P_2^PCo(COSi^iPr_3)$ **5a-$^{13}$CO** ($\nu_{CO}$ = 1347 cm$^{-1}$). A minor amount of oxidized Co(CO) species are observable.

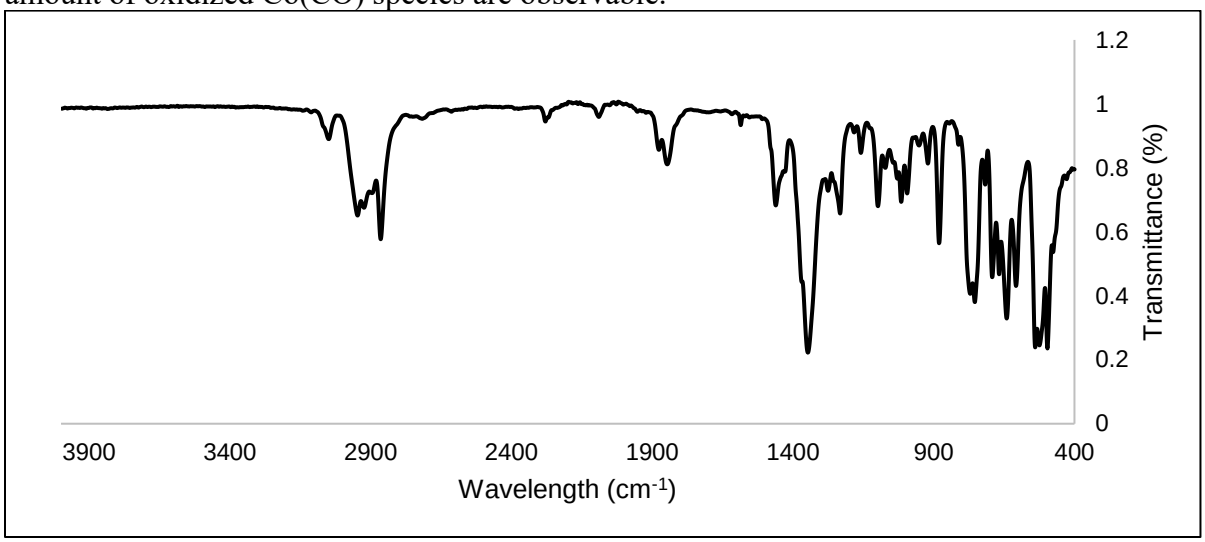
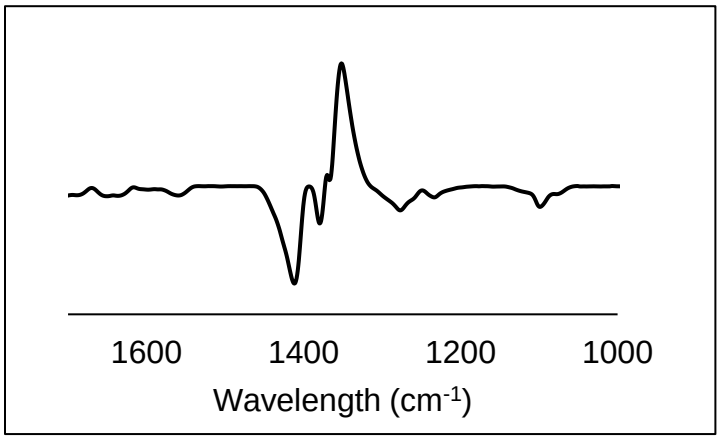
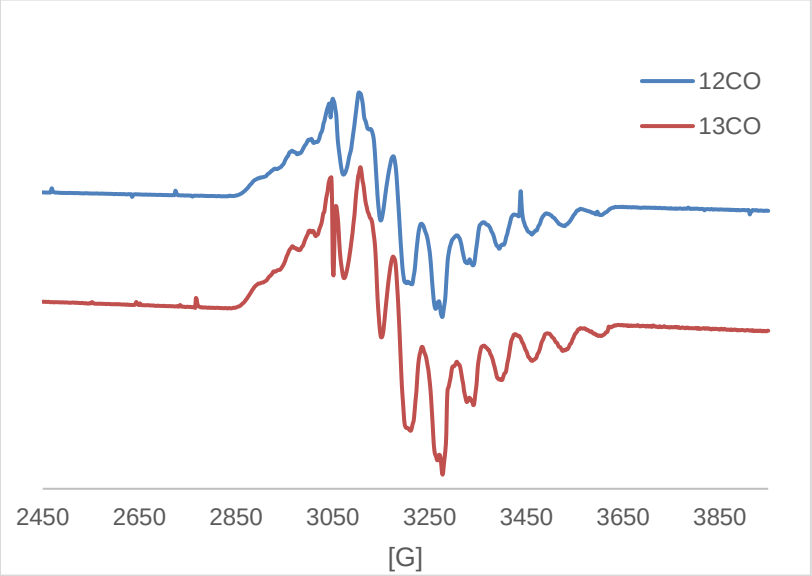



**Figure S4.11.** Solution IR difference spectrum of **5a**-**5a-$^{13}$CO** highlighting the identified CO stretch.



## 5. EPR Spectra

**Figure S4.1.** EPR spectra of $P_2^PCo(CO)$ **3** and **3-$^{13}$CO**



## 6. Crystallographic Details

| | $P_2^PCoBr$ 1 | $P_2^PCoBr(CO)$ 2 | $P_2^PCo(CO)$ 3 | $[P_2^PCo(CO)][Na(DME)_3]$ 4a | $[P_2^PCo(CO)][Na(12\text{-}c\text{-}4)_2]$ 4b |
|---|---|---|---|---|---|
| Crystal system | Triclinic | Monoclinic | Triclinic | Monoclinic | Monoclinic |
| Formula | $C_{30}H_{41}BrCoP_3$ | $C_{41.5}H_{53}BrCoOP_3$ | $C_{31}H_{41}CoOP_3$ | $C_{43}H_{71}CoNaO_7P_3$ | $C_{50}H_{76}CoNaO_9P_3$ |
| Formula weight (g/mol) | 633.37 | 799.62 | 581.51 | 874.88 | 995.99 |
| Space group | P -1 | P21/c | P -1 | P21/n | C2/c |
| a (Å) | 9.4625(5) | 10.9453(6) | 10.843(2) | 11.1659(4) | 27.599(3) |
| b (Å) | 9.5168(5) | 14.9644(8) | 16.079(3) | 16.1007(5) | 30.400(5) |
| c (Å) | 17.7628(10) | 23.9133(15) | 17.991(3) | 26.6135(8) | 18.698(2) |
| α (deg) | 100.843(2) | 90 | 109.036(7) | 90 | 90 |
| β (deg) | 96.323(2) | 101.797(3) | 92.528(7) | 97.3840(10) | 132.65 |
| γ (deg) | 102.954(2) | 90 | 90.859(8) | 90 | 90 |
| Z | 2 | 4 | 4 | 4 | 8 |
| V (Å³) | 1511.54(14) | 3834.0(4) | 2960.8(9) | 4744.9(3) | 11538(3) |
| Indep. Reflections | 6696 | 7232 | 11895 | 10157 | 16818 |
| R(int) | 3.12 | 6.77 | 6.62 | 2.09 | 5.89 |
| R1 | 1.64 | 3.13 | 2.48 | 2.68 | 5.92 |
| wR2 | 4.26 | 7.71 | 6.78 | 7.59 | 15.27 |
| GOF | 1.064 | 1.069 | 1.043 | 1.049 | 1.073 |

| | $P_2^PCo(H)(CO)$ | $P_2^PCo(COSi^tBuPh_2)$ 5b |
|---|---|---|
| Crystal system | Triclinic | Monoclinic |
| Formula | $C_{31}H_{42}CoOP_3$ | $C_{44.5}H_{56.8}CoOP_3Si$ |
| Formula weight (g/mol) | 582.51 | 787.97 |
| Space group | P-1 | P21 |
| a (Å) | 9.4357(4) | 10.4158(11) |
| b (Å) | 9.6576(6) | 16.6407(12) |
| c (Å) | 17.4658(8) | 12.8005(11) |
| α (deg) | 102.756(3) | 90 |
| β (deg) | 98.244(2) | 95.289(4) |
| γ (deg) | 103.517(3) | 90 |
| Z | 2 | 2 |
| V (Å³) | 1477.06(13) | 2209.2(3) |
| Indep. Reflections | 6375 | 9766 |
| R(int) | 4.44 | 3.89 |
| R1 | 2.07 | 3.21 |
| wR2 | 5.38 | 8.11 |
| GOF | 1.057 | 1.072 |

## Remarks on Crystal Structures:

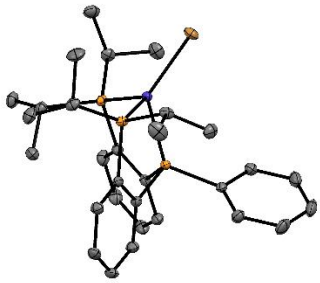


**Figure S.6.1.** Full asymmetric unit of **1**. Hydrogen atoms are omitted for clarity.

**$P_2^PCoBr$ 1.** This compound crystallizes in the absence of solvent.

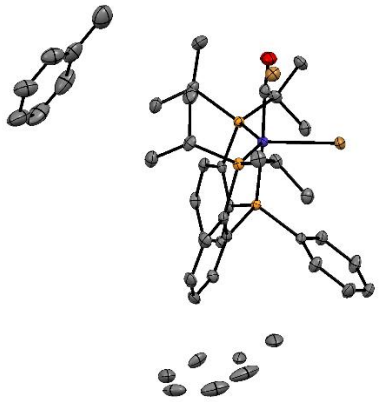


**Figure S.6.2.** Full asymmetric unit of **2** showing both toluene molecules and the Br component of the minor product isomer. Hydrogen atoms are omitted for clarity.

**$P_2^PCoBr(CO)$ 2.** This compound crystallizes with two toluene solvent molecules, one of which is modeled as disordered over two symmetry-related positions. The complex appears to co-crystallize with a component of a minor isomer with the Br occupying the axial site (~4%). Omission of this Br component resulted in elongated CO ellipsoids, with the largest residual electron density peak consistent with the presence of this atom. For the minor component, the additional CO co-ligand could not be located, but its presence is consistent with incomplete occupancy of the Br ligand located in the trigonal plane, with approximately 96% occupancy when freely refined.

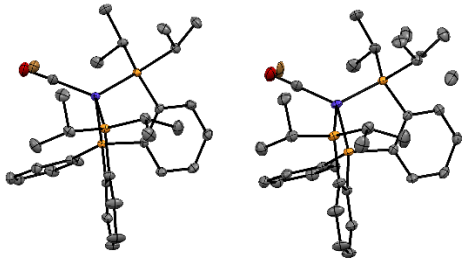


**Figure S.6.3.** Full asymmetric unit of **3** showing disordered P$^i$Pr group and minor component of **1** for both molecules. Hydrogen atoms are omitted for clarity.

**$P_2^PCo(CO)$ 3.** This compound crystallizes in the absence of solvent with two molecules of the complex in the asymmetric unit. One of the P-$^i$Pr groups on one of the molecules was modeled as disordered over two positions (73:37). For both molecules of the complex, refinement was improved by the inclusion of a very minor component of **1**, which was identified by the presence of residual electron density for the Br ligand; these refined to ~1.5% and 2.5% components for the two independent molecules.

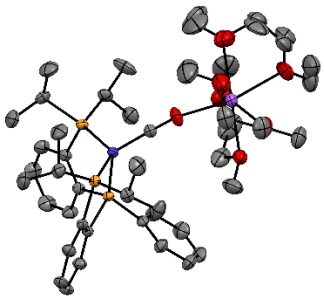


**Figure S.6.4.** Full asymmetric unit of **4a**. Hydrogen atoms are omitted for clarity.

**[$P_2^P$Co(CO)][Na(DME)$_3$] 4a.** This compound crystallizes with an O-bound Na counter cation. Three DME molecules are ligated to Na with one of these modeled as disordered over two positions (50:50).

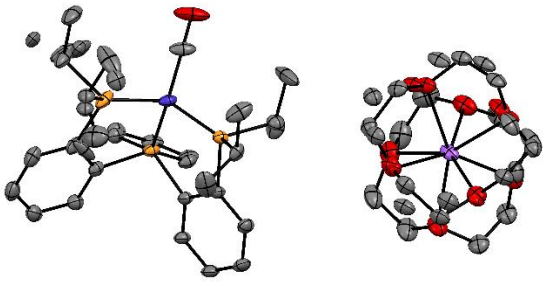


**Figure S.6.5.** Full asymmetric unit of **4b**. Hydrogen atoms are omitted for clarity.

**[$P_2^P$Co(CO)][Na(12-crown-4)$_2$] 4b.** This compound crystallizes with a fully crown-encapsulated Na counter cation and additional residual solvent electron density that could not be fully refined (likely THF and benzene/toluene molecules) that was removed by application of SQUEEZE. Two of the four ligand $^i$Pr groups were modeled in a crystallographically related disorder over two positions (62:38), with the refinement of this disorder aided by the application of an EADP constraint for one of the methine carbon positions and RIGU restraints. One of the crown ethers was modeled as fully disordered over two positions (67:33), with application of an EADP constraint on one of the oxygen atoms.

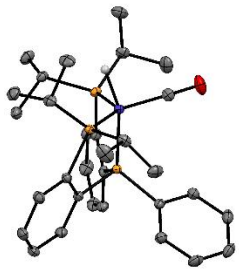


**Figure S.6.6.** Full asymmetric unit of $P_2^PCoH(CO)$. C-bound hydrogen atoms are omitted for clarity.

**$P_2^PCoH(CO)$.** This compound crystallizes in the absence of solvent.

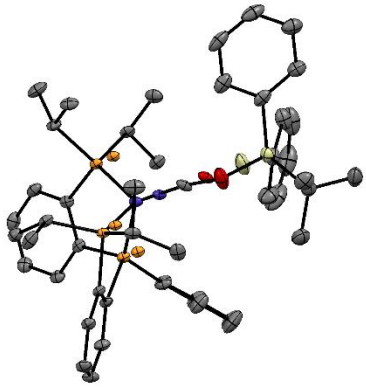


**Figure S.6.7.** Full asymmetric unit of $P_2^PCo(COSi^tBuPh_2)$ **5b**. Hydrogen atoms are omitted for clarity.

**$P_2^PCo(COSi^tBuPh_2)$ 5b.** This compound crystallizes in the absence of solvent. A minor component in the crystal lattice (~5%) was present. Within this component the core atoms were modeled best as $P_3Co(OSi)$ with their refinement aided by the application of EADP constraints. The exact identity of the minor component is ambiguous, where the most residual electron density was located at the positions of the Co and Si. Complete disorder of the remaining supporting ligand could not be reliably refined.

**7. Bond Distances and Angles.**

**$P_2^PCoBr$ 1.**

| Bond Distances (Å) | | Bond Angles (degrees) | |
|---|---|---|---|
| Co1-P1 | 2.1956(5) | P1-Co1-P2 | 86.70(1) |
| Co1-P2 | 2.2484(4) | P1-Co1-P3 | 87.19(1) |
| Co1-P3 | 2.2646(3) | P2-Co1-P3 | 118.41(2) |
| Co1-Br1 | 2.3504(3) | P1-Co1-Br1 | 130.20(2) |
| | | P2-Co1-Br1 | 118.80(1) |
| | | P3-Co1-Br1 | 111.21(1) |

**$P_2^PCoBr(CO)$ 2.**

| Bond Distances (Å) | | Bond Angles (degrees) | |
|---|---|---|---|
| Co1-P1 | 2.1673(7) | P1-Co1-P2 | 86.35(2) |
| Co1-P2 | 2.1756(6) | P1-Co1-P3 | 87.24(2) |
| Co1-P3 | 2.1835(6) | P2-Co1-P3 | 137.92(2) |
| Co1-Br1A | 2.4977(4) | P1-Co1-Br1A | 95.07(2) |
| Co1-C1 | 1.754(4) | P2-Co1-Br1A | 109.89(2) |
| | | P3-Co1-Br1 | 112.09(2) |
| | | P1-Co1-C1 | 176.0(1) |
| | | P2-Co1-C1 | 91.2(1) |
| | | P3-Co1-C1 | 92.6(1) |

**$P_2^PCo(CO)$ 3.**

| Bond Distances (Å) | | Bond Angles (degrees) | |
|---|---|---|---|
| **Molecule 1** | | | |
| Co1-P1 | 2.1344(6) | P1-Co1-P2 | 87.36(2) |
| Co1-P2 | 2.1769(5) | P1-Co1-P3 | 87.94(2) |
| Co1-P3 | 2.1922(5) | P2-Co1-P3 | 124.42(2) |
| Co1-C1 | 1.752(2) | P1-Co1-C1 | 109.40(6) |
| C1-O1 | 1.161(3) | P2-Co1-C1 | 117.85(6) |
| | | P3-Co1-C1 | 115.85(6) |
| **Molecule 2** | | | |
| Co2-P4 | 2.1301(6) | P4-Co2-P5 | 87.94(2) |
| Co2-P5 | 2.1740(5) | P4-Co2-P6 | 87.59(2) |
| Co2-P6 | 2.1753(5) | P5-Co2-P6 | 128.80(2) |
| Co2-C32 | 1.747(2) | P4-Co2-C32 | 111.08(6) |
| C32-O2 | 1.162(3) | P5-Co2-C32 | 115.86(6) |
| | | P6-Co2-C32 | 113.24(6) |

**$[P_2^PCo(CO)][Na(DME)_3]$ 4a.**

| Bond Distances (Å) | | Bond Angles (degrees) | |
|---|---|---|---|
| Co1-P1 | 2.0966(6) | P1-Co1-P2 | 89.80(2) |
| Co1-P2 | 2.1394(4) | P1-Co1-P3 | 89.23(2) |
| Co1-P3 | 2.1409(6) | P2-Co1-P3 | 126.42(2) |
| Co1-C1 | 1.716(1) | P1-Co1-C1 | 126.19(4) |
| C1-O1 | 1.187(1) | P2-Co1-C1 | 111.27(4) |
| | | P3-Co1-C1 | 112.00(4) |

**$[P_2^PCo(CO)][Na(12\text{-}c\text{-}4)_2]$ 4b.**

| Bond Distances (Å) | | Bond Angles (degrees) | |
|---|---|---|---|
| Co1-P1 | 2.0838(8) | P1-Co1-P2 | 90.20(3) |
| Co1-P2 | 2.1191(8) | P1-Co1-P3 | 89.97(3) |
| Co1-P3 | 2.1304(7) | P2-Co1-P3 | 128.03(3) |
| Co1-C1 | 1.733(3) | P1-Co1-C1 | 125.9(1) |
| C1-O1 | 1.177(4) | P2-Co1-C1 | 109.1(1) |
| | | P3-Co1-C1 | 112.3(1) |

**$P_2^PCoH(CO)$.**

| Bond Distances (Å) | | Bond Angles (degrees) | |
|---|---|---|---|
| Co1-P1 | 2.1246(5) | P1-Co1-P2 | 87.25(1) |
| Co1-P2 | 2.1387(4) | P1-Co1-P3 | 87.65(1) |
| Co1-P3 | 2.1481(3) | P2-Co1-P3 | 130.99(2) |
| Co1-C1 | 1.748(1) | P1-Co1-C1 | 111.24(4) |
| C1-O1 | 1.156(2) | P2-Co1-C1 | 117.25(4) |
| Co1-H | 1.46(2) | P3-Co1-C1 | 109.97(4) |
| | | P1-Co1-H | 158.4(8) |
| | | P2-Co1-H | 81.6(8) |
| | | P3-Co1-H | 85.8(8) |
| | | C1-Co1-H | 90.4(8) |

**$P_2^PCo(COSi^tBuPh_2)$ 5b.**

| Bond Distances (Å) | | Bond Angles (degrees) | |
|---|---|---|---|
| Co1-P1 | 2.120(1) | P1-Co1-P2 | 89.08(4) |
| Co1-P2 | 2.1617(9) | P1-Co1-P3 | 89.15(4) |
| Co1-P3 | 2.154(1) | P2-Co1-P3 | 116.58(4) |
| Co1-C1 | 1.640(4) | P1-Co1-C1 | 124.5(1) |
| C1-O1 | 1.260(5) | P2-Co1-C1 | 121.3(1) |
| | | P3-Co1-C1 | 111.1(1) |
| | | Co1-C1-O1 | 169.8(3) |
| | | C1-O1-Si1 | 137.7(3) |

## 8. DFT Calculations

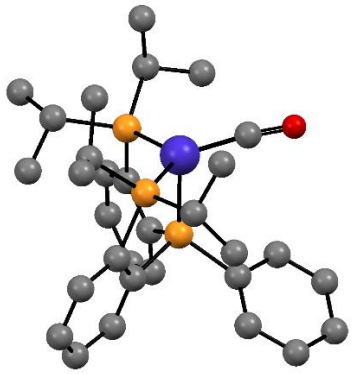


**Figure S8.1.** DFT optimized structure of $P_2^PCoCO$ **3**.

Optimized Coordinates for $P_2^PCoCO$ **3**.

| | | | |
|---|---|---|---|
| Co | -0.00373920 | -0.68403331 | -1.13110881 |
| P | -1.87398768 | -1.29740975 | -0.13861284 |
| P | -0.03676809 | 1.07695207 | 0.14191298 |
| P | 1.94878185 | -1.18329652 | -0.22032067 |
| O | -0.15144203 | 0.42470896 | -3.84313481 |
| C | -1.56014096 | 3.51219817 | 0.00676086 |
| H | -2.23053101 | 3.10296106 | 0.76821282 |
| C | -0.44140606 | 2.77932785 | -0.40975202 |
| C | 0.39440765 | 3.32667650 | -1.39751807 |
| H | 1.25777876 | 2.75204333 | -1.75059220 |
| C | -3.48008828 | -0.85564677 | -1.00175702 |
| H | -4.31027257 | -1.19426742 | -0.35454368 |
| C | 0.13160535 | 4.58048467 | -1.93718308 |
| H | 0.79480533 | 4.99161772 | -2.70197379 |
| C | -2.02331868 | 1.19571705 | 3.79240558 |
| H | -2.01389840 | 1.78644122 | 4.71156719 |
| C | -2.87196033 | 0.09683510 | 3.67355708 |
| H | -3.53163960 | -0.17772486 | 4.50042345 |
| C | 2.06214164 | -2.54589672 | 1.07911738 |
| H | 1.57955857 | -3.40188786 | 0.57094445 |
| C | -3.55616629 | -1.56406300 | -2.34495621 |
| H | -2.72944595 | -1.24626869 | -2.99958276 |
| H | -4.49804559 | -1.32423864 | -2.86187912 |
| H | -3.50112800 | -2.65856426 | -2.25840233 |
| C | -2.10968536 | -3.09358498 | 0.38119367 |
| H | -1.61671453 | -3.12741100 | 1.37038101 |
| C | -1.82869539 | 4.76626423 | -0.54480155 |
| H | -2.70603956 | 5.32633189 | -0.21149253 |
| C | -0.98375830 | 5.30541717 | -1.51247816 |
| H | -1.19596055 | 6.28770625 | -1.94119579 |
| C | -1.31891162 | -3.99208175 | -0.56315747 |

| | | | |
|---|---|---|---|
| H | -1.76215067 | -4.01445311 | -1.57066202 |
| H | -1.29238490 | -5.02994813 | -0.19656323 |
| H | -0.28085683 | -3.64445211 | -0.68239284 |
| C | -1.17214040 | 0.77497158 | 1.56241859 |
| C | 2.55128798 | 0.29792111 | 0.70166341 |
| C | 3.38568698 | -1.56701330 | -1.35292128 |
| H | 4.29072385 | -1.69254644 | -0.73152057 |
| C | -3.53798222 | -3.59442156 | 0.53798124 |
| H | -4.14485540 | -2.99230063 | 1.22730559 |
| H | -3.54178431 | -4.62549400 | 0.92454118 |
| H | -4.07249625 | -3.61731658 | -0.42301612 |
| C | -2.02620674 | -0.33932311 | 1.43786477 |
| C | -2.88133467 | -0.65755349 | 2.49923997 |
| H | -3.55957684 | -1.51115617 | 2.42255209 |
| C | -1.18326174 | 1.53847712 | 2.73375752 |
| H | -0.52040556 | 2.40392156 | 2.82717876 |
| C | 3.45106114 | -2.97755182 | 1.51842265 |
| H | 4.08911265 | -3.30666771 | 0.68632378 |
| H | 3.38210730 | -3.82353269 | 2.22030132 |
| H | 3.97881486 | -2.17346988 | 2.05327583 |
| C | -3.57274070 | 0.65081904 | -1.17921564 |
| H | -3.59876819 | 1.18695839 | -0.21893956 |
| H | -4.48457301 | 0.92397862 | -1.73166635 |
| H | -2.71286500 | 1.03315742 | -1.75478613 |
| C | 1.62459331 | 1.33732193 | 0.90017804 |
| C | 3.61514266 | -0.41533321 | -2.31816512 |
| H | 2.72523731 | -0.23564026 | -2.94079708 |
| H | 4.45674467 | -0.63438711 | -2.99255734 |
| H | 3.84642737 | 0.52501777 | -1.79552016 |
| C | 2.01304697 | 2.50299733 | 1.57101171 |
| H | 1.30361121 | 3.32895758 | 1.68417924 |
| C | 1.20229291 | -2.16700751 | 2.27542852 |
| H | 1.66500159 | -1.35519525 | 2.85944975 |
| H | 1.06774625 | -3.02194123 | 2.95550693 |
| H | 0.20520374 | -1.81561249 | 1.97056720 |
| C | 3.31053089 | 2.63342610 | 2.06199940 |
| H | 3.60779328 | 3.54599534 | 2.58447292 |
| C | 3.85902130 | 0.45131874 | 1.18066222 |
| H | 4.60490918 | -0.32787360 | 1.00009233 |
| C | 4.23468222 | 1.60809749 | 1.86271842 |
| H | 5.25953810 | 1.71645513 | 2.22633499 |
| C | 3.10131125 | -2.86755640 | -2.08862046 |
| H | 2.99836392 | -3.72770900 | -1.40961483 |
| H | 3.90783916 | -3.10703630 | -2.79797189 |
| H | 2.16678768 | -2.78972378 | -2.66864491 |
| C | -0.07928258 | -0.08910143 | -2.79735019 |

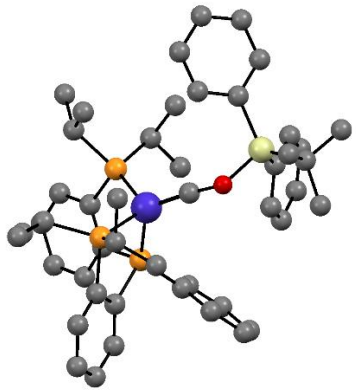


**Figure S8.2.** DFT optimized structure of $P_2^PCo(COSi^tBuPh_2)$ **5**.

Optimized coordinates for $P_2^PCo(COSi^tBuPh_2)$ **5**.

| | | | |
|---|---|---|---|
| Co | -0.45582353 | -0.55478023 | -0.22567636 |
| P | -1.98357862 | 0.92316588 | -0.02890594 |
| P | -0.70310321 | -0.99694976 | 1.89574102 |
| P | -1.83349838 | -1.71910022 | -1.42299600 |
| Si | 3.61223802 | 0.33443923 | -0.87893290 |
| O | 2.11419482 | -0.15306411 | -1.59390024 |
| C | 1.01699847 | -0.34261990 | -0.93429510 |
| C | -1.81623712 | 2.75255972 | -0.11950474 |
| C | -1.94950883 | 3.60412380 | 0.98531803 |
| H | -2.21298569 | 3.19010182 | 1.96268118 |
| C | -1.76737175 | 4.98161492 | 0.84910490 |
| H | -1.88362968 | 5.63056912 | 1.72102350 |
| C | -1.44995947 | 5.53028448 | -0.39175656 |
| H | -1.31871620 | 6.60968187 | -0.49946671 |
| C | -1.29392319 | 4.68888661 | -1.49666945 |
| H | -1.03679952 | 5.10867856 | -2.47264631 |
| C | -1.46604274 | 3.31505149 | -1.35909167 |
| H | -1.33655929 | 2.65911902 | -2.22743672 |
| C | -2.89728378 | 0.65774722 | 1.55750011 |
| C | -4.12801616 | 1.24916230 | 1.85476155 |
| H | -4.57144753 | 1.96274248 | 1.15315186 |
| C | -4.80127653 | 0.92778016 | 3.03185169 |
| H | -5.77020291 | 1.38276758 | 3.25202088 |
| C | -4.23359278 | 0.01826301 | 3.92302176 |
| H | -4.75702253 | -0.24189980 | 4.84666705 |
| C | -2.99729238 | -0.56353520 | 3.64009216 |
| H | -2.57181896 | -1.26920617 | 4.35723372 |
| C | -2.31774340 | -0.26348229 | 2.45260686 |
| C | 0.47847336 | -0.14979874 | 3.08556288 |
| H | 0.15938218 | -0.43891607 | 4.10428087 |

| | | | |
|---|---|---|---|
| C | 1.90501923 | -0.61061182 | 2.84476455 |
| H | 2.04537772 | -1.69484683 | 2.96650219 |
| H | 2.60425923 | -0.10747392 | 3.53184813 |
| H | 2.21313131 | -0.35607313 | 1.81826549 |
| C | 0.37835817 | 1.35942746 | 2.94475300 |
| H | 0.62791475 | 1.67110351 | 1.91660778 |
| H | 1.08759612 | 1.86063348 | 3.62172307 |
| H | -0.62673181 | 1.74076405 | 3.17964889 |
| C | -0.74519687 | -2.77838605 | 2.52576033 |
| H | -1.79248673 | -3.07849014 | 2.33211780 |
| C | 0.16143364 | -3.63904163 | 1.65322811 |
| H | 0.02960349 | -3.41379968 | 0.58337656 |
| H | -0.02635673 | -4.71151292 | 1.82112923 |
| H | 1.22309419 | -3.45452885 | 1.88078238 |
| C | -0.43441812 | -3.01516730 | 3.99694039 |
| H | 0.61500609 | -2.78168175 | 4.23061165 |
| H | -0.58303303 | -4.07591031 | 4.25432426 |
| H | -1.05560115 | -2.43024934 | 4.68755889 |
| C | -3.29432715 | 0.63494307 | -1.30893921 |
| C | -4.28631777 | 1.55446579 | -1.66989107 |
| H | -4.33588899 | 2.52839530 | -1.17169265 |
| C | -5.19151109 | 1.25226094 | -2.68579817 |
| H | -5.95645436 | 1.97919276 | -2.97020796 |
| C | -5.10714088 | 0.02881469 | -3.35030898 |
| H | -5.80326956 | -0.20383515 | -4.16010896 |
| C | -4.12152139 | -0.89150568 | -2.99421697 |
| H | -4.04873391 | -1.83309847 | -3.54642352 |
| C | -3.20993832 | -0.60259879 | -1.97108366 |
| C | -2.79677954 | -3.20759035 | -0.76124782 |
| H | -2.02029485 | -3.77400178 | -0.21461980 |
| C | -3.43248564 | -4.14480657 | -1.77454839 |
| H | -4.20369638 | -3.64035449 | -2.37600932 |
| H | -3.93852666 | -4.97477751 | -1.25584382 |
| H | -2.70804145 | -4.59873834 | -2.46456461 |
| C | -3.82625046 | -2.72656394 | 0.24996740 |
| H | -4.23240441 | -3.56669666 | 0.83441645 |
| H | -4.67617899 | -2.23212445 | -0.24713791 |
| H | -3.40384695 | -2.00044927 | 0.95899008 |
| C | -1.17762029 | -2.34459196 | -3.06046603 |
| H | -2.01986133 | -2.84003428 | -3.57693811 |
| C | -0.07551636 | -3.36205550 | -2.81356358 |
| H | 0.77472231 | -2.88332322 | -2.30160039 |
| H | 0.29711901 | -3.78213916 | -3.76054346 |
| H | -0.40341409 | -4.20416004 | -2.18471194 |
| C | -0.68540406 | -1.19938444 | -3.92930430 |
| H | -1.47901930 | -0.47157673 | -4.15406842 |

| | | | |
|---|---|---|---|
| H | -0.30312840 | -1.57898205 | -4.88958659 |
| H | 0.13234844 | -0.65494926 | -3.43421884 |
| C | 3.20854642 | 1.83647134 | 0.16363962 |
| C | 3.93204319 | 2.18847598 | 1.31412860 |
| H | 4.75069073 | 1.55106238 | 1.66459594 |
| C | 3.61303979 | 3.33391220 | 2.04317408 |
| H | 4.18747064 | 3.58807423 | 2.93771599 |
| C | 2.55642879 | 4.14659755 | 1.63486021 |
| H | 2.29878946 | 5.04065431 | 2.20879951 |
| C | 1.81902953 | 3.81070706 | 0.49955994 |
| H | 0.97856578 | 4.43381370 | 0.18343704 |
| C | 2.14248546 | 2.66695535 | -0.22730215 |
| H | 1.53759985 | 2.40605802 | -1.10226450 |
| C | 4.24059216 | -1.14397040 | 0.08589095 |
| C | 5.40917422 | -1.09108229 | 0.86624510 |
| H | 5.99827920 | -0.16885721 | 0.91631024 |
| C | 5.84680317 | -2.20081245 | 1.58827547 |
| H | 6.75458758 | -2.13442525 | 2.19299610 |
| C | 5.12801643 | -3.39449184 | 1.53505556 |
| H | 5.47022847 | -4.26547128 | 2.09950729 |
| C | 3.97338059 | -3.47145823 | 0.75795189 |
| H | 3.40560225 | -4.40447949 | 0.71059736 |
| C | 3.53206293 | -2.35801702 | 0.04493789 |
| H | 2.60494543 | -2.42988103 | -0.53309647 |
| C | 4.68460093 | 0.73981046 | -2.38940051 |
| C | 6.08710986 | 1.12973140 | -1.92027441 |
| H | 6.07417079 | 1.98928759 | -1.23024864 |
| H | 6.71739960 | 1.41797604 | -2.77833227 |
| H | 6.60147062 | 0.29802085 | -1.41367668 |
| C | 4.75824287 | -0.49559730 | -3.28804357 |
| H | 5.20832488 | -1.35737662 | -2.77111796 |
| H | 5.37600602 | -0.29074255 | -4.17866744 |
| H | 3.76341494 | -0.80465490 | -3.64325368 |
| C | 4.04841713 | 1.90324251 | -3.15062274 |
| H | 3.02648901 | 1.66653569 | -3.48424433 |
| H | 4.63815041 | 2.14698268 | -4.05041028 |
| H | 3.99397665 | 2.81747558 | -2.53958877 |

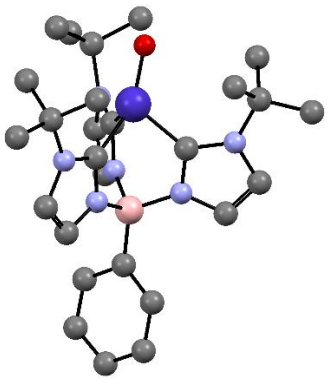


**Figure S8.3.** DFT optimized structure of Co(O).

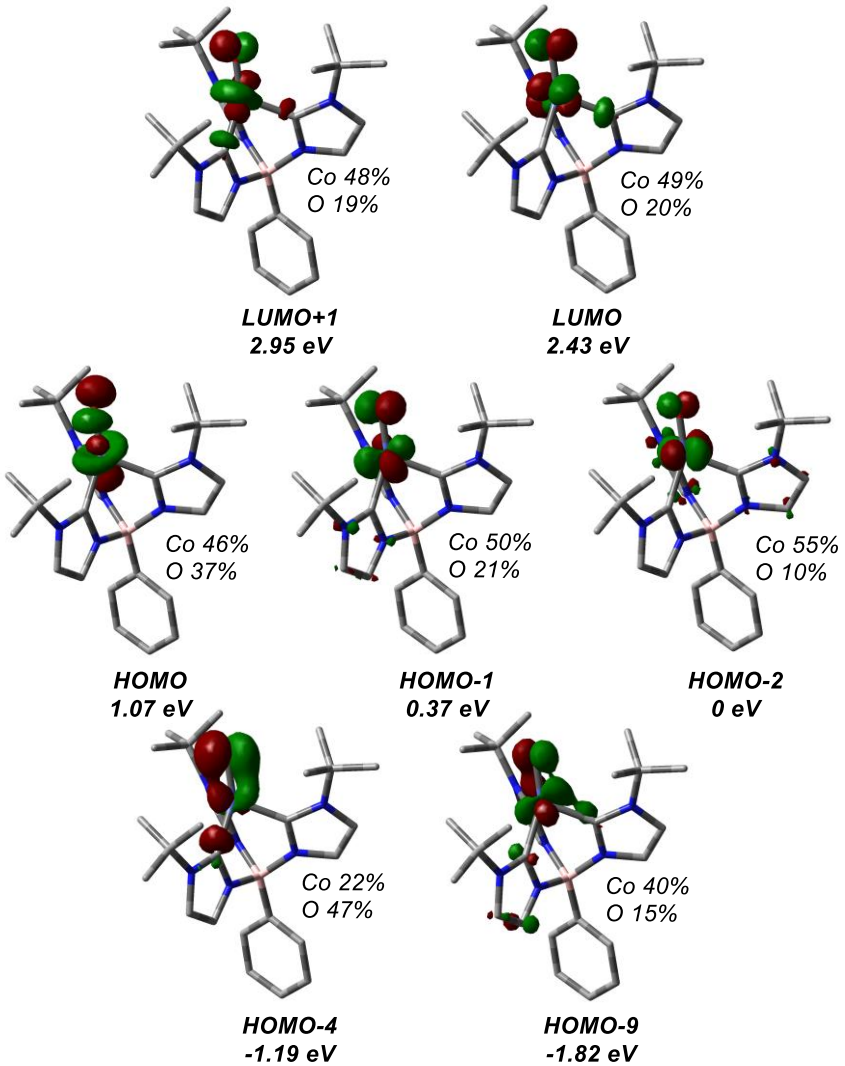



**Figure S8.4.** Depiction of MOs of the Co(O) relevant to Figure 5 of the main text. Orbital energies are listed relative to the HOMO-2 in eV. Calculated contribution of Co d-orbitals and O p-orbitals for each MO are noted. Lobal representations are shown with 0.07 isocontours.

Optimized coordinates for Co(O).

| | | | |
|---|---|---|---|
| C | -0.32852371 | 1.43037743 | -0.58181757 |
| N | -0.74902062 | 2.58448943 | -1.18762547 |
| C | 0.31451266 | 3.15626727 | -1.86704040 |
| C | 1.39802044 | 2.36276548 | -1.65777511 |
| N | 1.00106934 | 1.33043307 | -0.84293059 |
| B | 1.77225880 | 0.06266385 | -0.34265467 |
| N | 1.42395196 | -0.06696068 | 1.17054149 |
| C | 0.12697408 | -0.10216129 | 1.53852943 |
| N | 0.12252777 | -0.23164917 | 2.89780186 |
| C | 1.43027487 | -0.27873990 | 3.36204643 |
| C | 2.24012920 | -0.17430535 | 2.27283867 |
| N | 1.00466586 | -1.10748934 | -1.05346077 |
| C | -0.32672417 | -1.26883237 | -0.82944757 |
| N | -0.71710406 | -2.32466845 | -1.61168590 |
| C | 0.36775948 | -2.76879706 | -2.35062713 |
| C | 1.43266470 | -1.99835089 | -2.00663704 |
| Co | -1.29922923 | -0.00758968 | 0.23568676 |
| O | -2.95315902 | -0.08691461 | 0.02812560 |
| C | -2.13408902 | 3.15711828 | -1.17686977 |
| C | -2.08735866 | 4.57586325 | -1.73306464 |
| C | -3.03388924 | 2.29394492 | -2.05396721 |
| C | -2.63622674 | 3.20819981 | 0.26095914 |
| C | -1.10762400 | -0.33754181 | 3.73236215 |
| C | -0.71659990 | -0.41224040 | 5.20119081 |
| C | -1.97072458 | 0.89546785 | 3.48862450 |
| C | -1.85691811 | -1.60229729 | 3.32601531 |
| C | -2.08580332 | -2.93111623 | -1.71987745 |
| C | -2.59865507 | -3.25643963 | -0.32208342 |
| C | -3.00445324 | -1.95467992 | -2.44482701 |
| C | -1.99271509 | -4.22722850 | -2.51816341 |
| H | -3.09044573 | 5.01536844 | -1.65788669 |
| H | -1.40044398 | 5.22286533 | -1.16836366 |
| H | -2.63537002 | 2.23092247 | -3.07735716 |
| H | -4.03735851 | 2.73972481 | -2.10879021 |
| H | -3.13654207 | 1.28332204 | -1.63636401 |
| H | -1.95403914 | 3.79089430 | 0.89740368 |
| H | -2.74741614 | 2.19976837 | 0.67682482 |
| H | -3.62400921 | 3.68871714 | 0.28943505 |
| H | -0.16233575 | 0.47950780 | 5.52743750 |
| H | -0.11204811 | -1.30211718 | 5.42710285 |
| H | -1.62653127 | -0.47401510 | 5.81212693 |
| H | -1.41634701 | 1.81989196 | 3.70533123 |
| H | -2.86076419 | 0.86837303 | 4.13265594 |
| H | -1.22661534 | -2.49448102 | 3.45135419 |
| H | -2.75715151 | -1.72633432 | 3.94399893 |

| | | | |
|---|---|---|---|
| H | -2.17840961 | -1.54309095 | 2.27587866 |
| H | -3.56867818 | -3.76725503 | -0.39726249 |
| H | -1.90203691 | -3.92399395 | 0.20680579 |
| H | -3.98777840 | -2.42051432 | -2.60245231 |
| H | -3.15358467 | -1.04574082 | -1.84650689 |
| H | -1.29097835 | -4.94669994 | -2.07185622 |
| H | -1.70945265 | -4.06124134 | -3.56709054 |
| H | -2.98353744 | -4.69937648 | -2.52834956 |
| H | -1.80507716 | 4.60390072 | -2.79486742 |
| H | -2.59243659 | -1.69233000 | -3.43069462 |
| H | -2.31955452 | 0.92858855 | 2.44575757 |
| C | 3.36540779 | 0.06641450 | -0.50251334 |
| C | 4.12133569 | 1.24844268 | -0.41072555 |
| C | 5.51645766 | 1.23741963 | -0.39878454 |
| C | 6.20764199 | 0.02918338 | -0.46004305 |
| C | 5.48691210 | -1.16296116 | -0.50472276 |
| C | 4.09265112 | -1.13779432 | -0.51738151 |
| H | 3.61232422 | 2.21104081 | -0.30771276 |
| H | 6.06657688 | 2.17961936 | -0.32852731 |
| H | 7.30031856 | 0.01554148 | -0.45254648 |
| H | 6.01397206 | -2.12073083 | -0.51893224 |
| H | 3.55663270 | -2.09176522 | -0.50425046 |
| H | 0.22650535 | 4.07480998 | -2.43399839 |
| H | 2.40789996 | 2.45564592 | -2.04379117 |
| H | 1.68115165 | -0.37548347 | 4.41186748 |
| H | 3.32468008 | -0.16635503 | 2.20162818 |
| H | 0.30520313 | -3.58982850 | -3.05364889 |
| H | 2.45078662 | -2.01283018 | -2.38209113 |
| H | -2.74919476 | -2.34435392 | 0.26678564 |

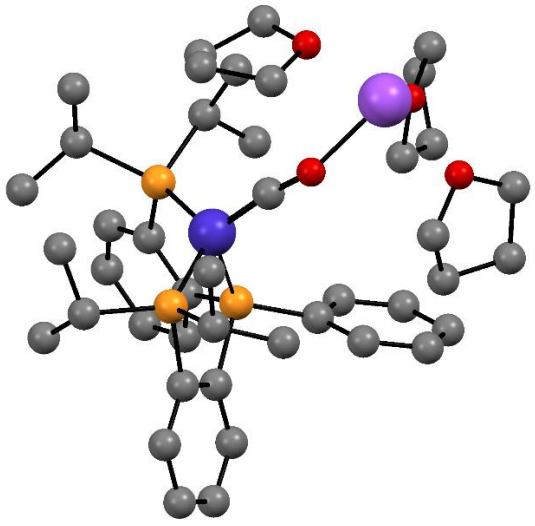


**Figure S8.5.** DFT optimized structure of the anionic Co(CO) complex **4a**.

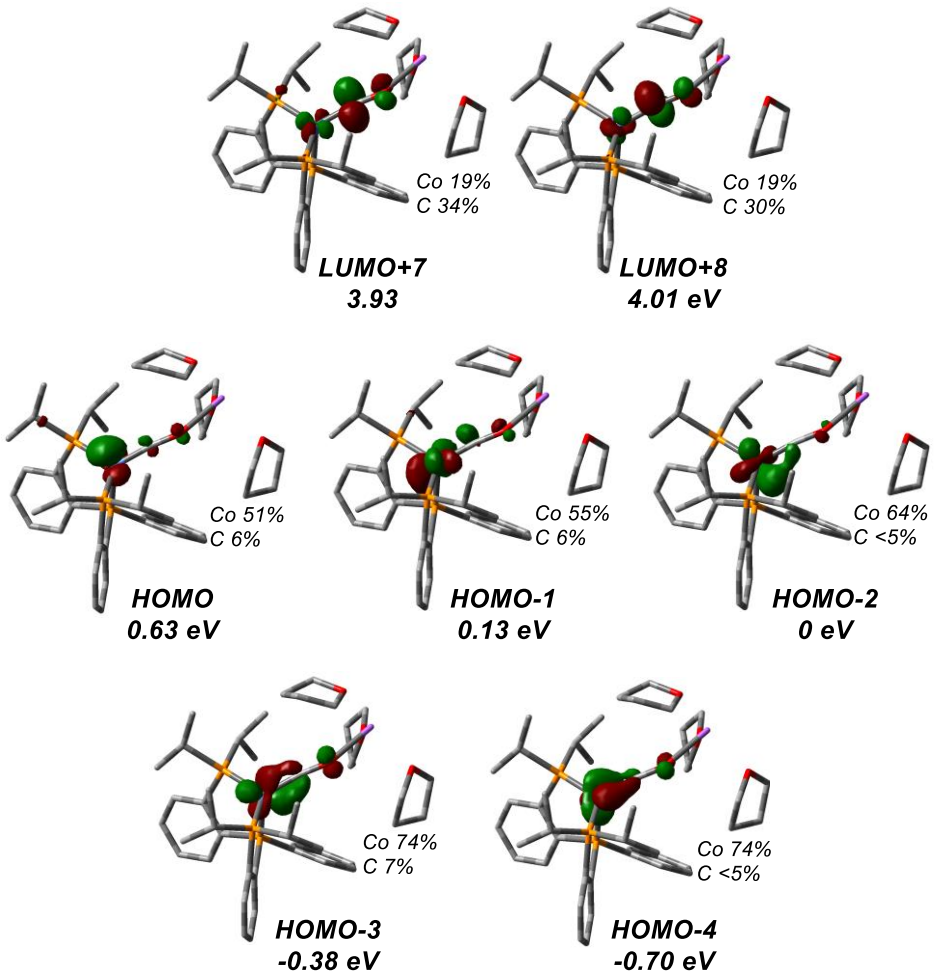



**Figure S8.6.** Depiction of MOs of the [Co(CO)][Na(THF)$_3$] relevant to Figure 5 of the main text. Orbital energies are listed relative to the HOMO in eV. Calculated contributions of Co d-orbitals and C p-orbitals for each MO are noted. Lobal representations are shown with 0.07 isocontours.

Optimized coordinates for [$P_2^PCo(CO)$][Na(THF)$_3$] **4a**.

| | | | |
|---|---|---|---|
| Co | -0.62536986 | 0.69858865 | 0.06613693 |
| P | -1.57773157 | 1.18801862 | 1.92307923 |
| P | -1.61617366 | -1.16276482 | 0.07736372 |
| P | -1.53240179 | 1.10860177 | -1.85969381 |
| Na | 4.34187214 | 0.81480924 | -0.02433994 |
| O | 2.23326925 | 0.85548486 | 0.55729858 |
| O | 4.92133365 | -0.64310596 | 1.63315916 |
| C | -0.78948460 | -2.80784669 | -0.03067047 |
| O | 3.85667330 | -0.76285179 | -1.59090831 |
| C | -2.58512749 | -1.38904434 | 1.64467275 |
| O | 4.19665841 | 3.08947297 | -0.15650994 |
| C | -2.60530306 | -0.26060130 | 2.47889327 |
| C | 1.05679951 | 0.83754237 | 0.28372391 |
| C | -2.90436338 | -1.24052673 | -1.25216313 |

| | | | |
|---|---|---|---|
| C | -3.30904332 | -0.31390549 | 3.68761532 |
| H | -3.33313610 | 0.56211094 | 4.34566283 |
| C | -2.88509075 | -0.14451688 | -2.13475467 |
| C | -0.46812403 | 1.28849696 | 3.45678471 |
| H | -1.13709031 | 1.40615624 | 4.33035884 |
| C | -3.81869482 | -0.09445182 | -3.17635715 |
| H | -3.80660305 | 0.73863283 | -3.88605387 |
| C | -3.23974194 | -2.56152682 | 2.04239156 |
| H | -3.18967452 | -3.45692206 | 1.41417082 |
| C | 0.02745883 | -3.17847967 | 1.05412072 |
| H | 0.05087194 | -2.53687621 | 1.94287261 |
| C | -0.79627027 | -3.63767873 | -1.16295046 |
| H | -1.42393003 | -3.37794997 | -2.02095872 |
| C | -0.44714070 | 0.66959147 | -3.37565157 |
| H | -0.94240741 | 1.11785944 | -4.25790327 |
| C | -2.36278611 | 2.65091742 | -2.59499594 |
| H | -2.61737783 | 2.40094495 | -3.64172344 |
| C | -3.97710342 | -1.47655752 | 4.06989515 |
| H | -4.52459043 | -1.50766461 | 5.01588830 |
| C | -3.85488614 | -2.25403956 | -1.42098276 |
| H | -3.86323048 | -3.11395940 | -0.74404709 |
| C | -4.79173703 | -2.18311046 | -2.45235335 |
| H | -5.53690771 | -2.97403765 | -2.57090208 |
| C | -2.78081450 | 2.61361475 | 2.24789540 |
| H | -2.86959938 | 2.74781337 | 3.34309736 |
| C | -3.93464548 | -2.60568089 | 3.25012831 |
| H | -4.44361817 | -3.52372725 | 3.55571661 |
| C | 0.80159720 | -4.33290153 | 1.01267388 |
| H | 1.41454506 | -4.60691244 | 1.87694075 |
| C | 0.79095796 | -5.14697802 | -0.12487409 |
| H | 1.39665027 | -6.05618675 | -0.15954589 |
| C | 0.31543203 | -0.00432383 | 3.60909761 |
| H | -0.33943909 | -0.88071983 | 3.73293290 |
| H | 0.98126694 | 0.03860171 | 4.48739540 |
| H | 0.93725951 | -0.17673108 | 2.71642868 |
| C | -3.64158155 | 3.02612462 | -1.86753951 |
| H | -4.35091602 | 2.18924865 | -1.79125792 |
| H | -4.15708430 | 3.84882646 | -2.38843159 |
| H | -3.43550978 | 3.37354738 | -0.84578146 |
| C | -4.77268248 | -1.10012376 | -3.33038907 |
| H | -5.50330570 | -1.03980090 | -4.14158366 |
| C | -0.01273639 | -4.79309440 | -1.20790154 |
| H | -0.03682710 | -5.42688885 | -2.09914227 |
| C | -0.35385230 | -0.83398229 | -3.57516100 |
| H | -0.01026073 | -1.32224425 | -2.64516107 |
| H | 0.36590689 | -1.08296757 | -4.37261047 |

| | | | |
|---|---|---|---|
| H | -1.31315857 | -1.29441612 | -3.84975071 |
| C | -1.39294177 | 3.82223879 | -2.61479794 |
| H | -0.94046956 | 3.97649897 | -1.62077287 |
| H | -1.90672670 | 4.75588096 | -2.89469874 |
| H | -0.57312997 | 3.68134466 | -3.33319553 |
| C | 0.47832918 | 2.47580880 | 3.39094417 |
| H | 1.02672317 | 2.47510298 | 2.43421514 |
| H | 1.22190322 | 2.43390771 | 4.20428252 |
| H | -0.04026661 | 3.44037741 | 3.48099529 |
| C | -2.23016226 | 3.89329808 | 1.63442549 |
| H | -1.32268917 | 4.25192615 | 2.13919124 |
| H | -2.97204257 | 4.70710914 | 1.67134033 |
| H | -1.95222041 | 3.72634652 | 0.58091800 |
| C | -4.14678983 | 2.26556197 | 1.67178444 |
| H | -4.05158427 | 1.83543656 | 0.66101702 |
| H | -4.78734928 | 3.15797956 | 1.58812467 |
| H | -4.68308541 | 1.52641216 | 2.28166490 |
| C | 0.94927823 | 1.25387285 | -3.23657165 |
| H | 0.94699890 | 2.33580391 | -3.04373963 |
| H | 1.54550697 | 1.07829462 | -4.14920183 |
| H | 1.47316651 | 0.78560527 | -2.38648652 |
| C | 4.03052077 | -0.66927608 | 2.75270661 |
| H | 4.61107133 | -0.70137460 | 3.69489056 |
| C | 5.28505806 | -1.98968658 | 1.31298652 |
| H | 5.27214733 | -2.08375967 | 0.21446944 |
| H | 6.31783643 | -2.18657618 | 1.64884009 |
| C | 2.76319796 | -1.66937474 | -1.31237276 |
| H | 2.90914978 | -2.08775942 | -0.30538961 |
| C | 4.35110027 | -0.98787096 | -2.91198074 |
| H | 4.48650409 | -0.01542762 | -3.41383104 |
| H | 5.34387941 | -1.47460370 | -2.85386320 |
| C | 3.38001122 | 3.36447365 | -1.30467216 |
| C | 3.65421416 | 3.75233630 | 0.99661992 |
| H | 4.47941599 | 4.24062714 | 1.53702995 |
| H | 1.80995847 | -1.10704209 | -1.29366351 |
| H | 3.20062276 | 2.99680920 | 1.66379731 |
| H | 3.93958340 | 4.03079001 | -1.98681366 |
| H | 3.18983940 | 2.41847333 | -1.84210547 |
| H | 3.43701845 | 0.25625716 | 2.73641194 |
| C | 4.26692603 | -2.89784848 | 2.00870901 |
| C | 3.21858796 | -1.92544178 | 2.54217091 |
| H | 3.84125360 | -3.64906761 | 1.32776134 |
| H | 4.74255379 | -3.45038872 | 2.83301794 |
| H | 2.43497661 | -1.73084330 | 1.79209056 |
| H | 2.71601684 | -2.28008622 | 3.45270218 |
| C | 2.11325554 | 4.00660520 | -0.77936905 |

| | | | |
|---|---|---|---|
| C | 2.61172076 | 4.71795826 | 0.46923083 |
| H | 3.07599968 | 5.68445413 | 0.21423131 |
| H | 1.81626850 | 4.91718339 | 1.20040338 |
| H | 1.65216502 | 4.68404479 | -1.51098555 |
| H | 1.36392670 | 3.23664380 | -0.52180556 |
| C | 2.80826659 | -2.69910378 | -2.41915678 |
| C | 3.33226216 | -1.87997481 | -3.58760420 |
| H | 3.76046851 | -2.48013465 | -4.40145010 |
| H | 2.52025857 | -1.26977152 | -4.01269915 |
| H | 3.50867959 | -3.51462159 | -2.17014481 |
| H | 1.82613350 | -3.15518033 | -2.60187365 |

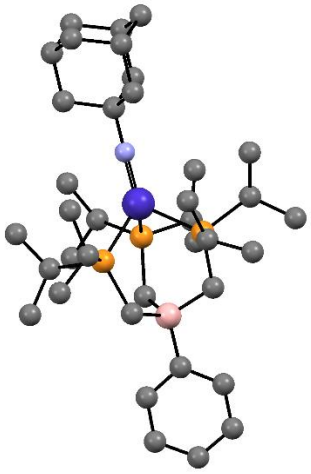


**Figure S8.7.** DFT optimized structure of [$BP_3$]Co(NAd).

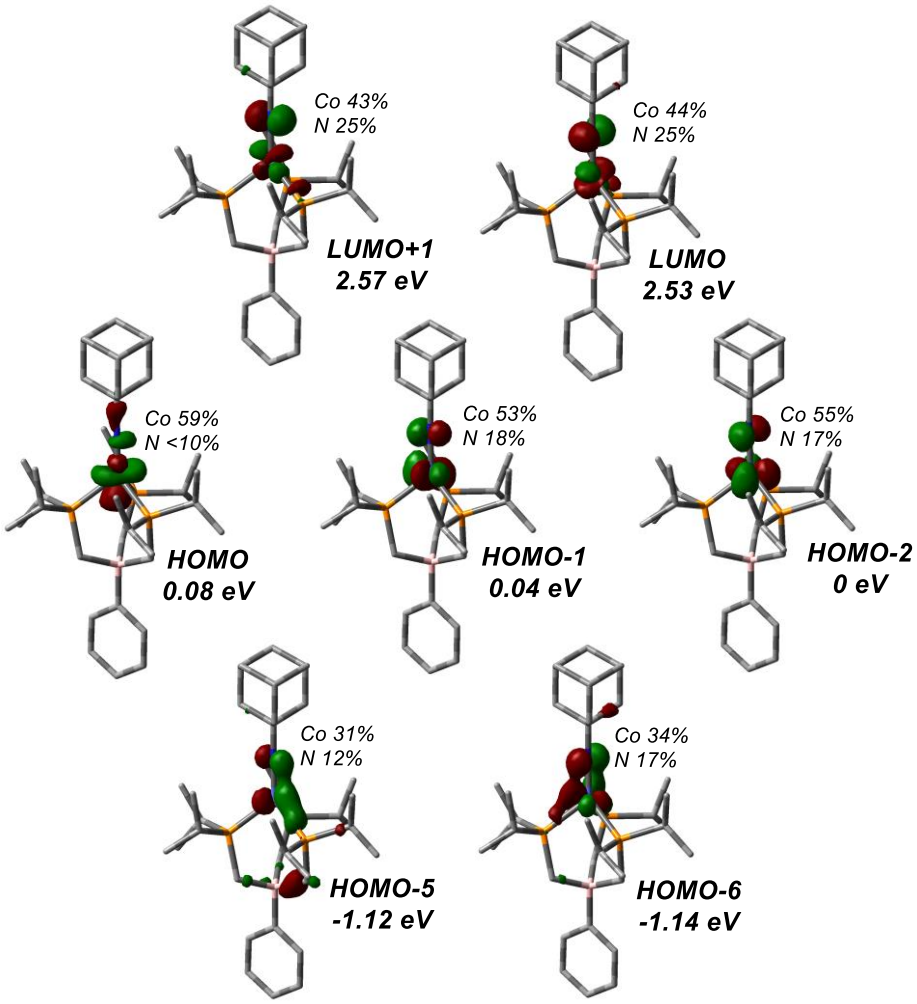



**Figure S8.8.** Depiction of MOs of [$BP_3$]Co(NAd) relevant to Figure 5 of the main text. Orbital energies are listed relative to the HOMO in eV. Calculated contributions of Co d-orbitals and N p-orbitals for each MO are noted. Lobal representations are shown with 0.07 isocontours.

Optimized coordinates for [$BP_3$]Co(NAd).

| | | | |
|---|---|---|---|
| P | -0.69223535 | 1.79102954 | -0.54345551 |
| P | -0.86732128 | -0.32694887 | 1.77760176 |
| P | -0.79233515 | -1.30378049 | -1.21333122 |
| N | 2.12089638 | -0.03340685 | 0.06087001 |
| B | -3.07584892 | 0.13246391 | -0.10795458 |
| C | -4.70351951 | 0.13410295 | -0.11899981 |
| C | -5.40877824 | -1.08475128 | -0.08980846 |
| H | -4.84465736 | -2.02667586 | -0.08286566 |
| C | -6.79978334 | -1.15096182 | -0.06435939 |
| H | -7.30213422 | -2.12284767 | -0.04247927 |
| C | -7.55429379 | 0.02343772 | -0.06648503 |
| H | -8.64652246 | -0.01848719 | -0.04897436 |
| C | -6.89253081 | 1.24878709 | -0.09013014 |

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|---|---|---|---|
| H | -7.46860047 | 2.17916698 | -0.09006516 |
| C | -5.49620980 | 1.29439074 | -0.11412046 |
| H | -5.01267905 | 2.27785978 | -0.12820555 |
| C | -2.48373729 | 1.67597262 | -0.22582951 |
| H | -2.70614671 | 2.23675865 | 0.69906109 |
| H | -3.00147682 | 2.22769957 | -1.03073701 |
| C | -2.60888917 | -0.59612209 | 1.32172520 |
| H | -2.77656870 | -1.68372082 | 1.23073437 |
| H | -3.25184321 | -0.27871241 | 2.15983018 |
| C | -2.52912419 | -0.78197414 | -1.38343664 |
| H | -2.60765227 | -0.20721509 | -2.32384728 |
| H | -3.16149407 | -1.66994380 | -1.54101894 |
| C | 0.81554514 | 1.84493666 | -2.95365439 |
| H | 0.77623771 | 1.70485291 | -4.04562272 |
| H | 1.28832265 | 0.95670863 | -2.50924251 |
| H | 1.49054029 | 2.69258992 | -2.76605415 |
| C | -0.57647729 | 2.09182885 | -2.39069506 |
| H | -1.23976664 | 1.28761619 | -2.75725399 |
| C | -1.15241120 | 3.40954869 | -2.88494734 |
| H | -0.48352132 | 4.25325391 | -2.66045180 |
| H | -2.13976797 | 3.63663539 | -2.45880440 |
| H | -1.26954226 | 3.38535859 | -3.97928347 |
| C | 1.34524372 | 3.70223108 | -0.13483175 |
| H | 1.37257496 | 4.15223148 | -1.13894731 |
| H | 1.99381433 | 2.81216141 | -0.14233817 |
| H | 1.78988997 | 4.43702981 | 0.55382630 |
| C | -0.07009856 | 3.35207654 | 0.29252534 |
| H | -0.01003784 | 3.03375859 | 1.34453695 |
| C | -1.00308413 | 4.55520523 | 0.24806241 |
| H | -0.64892928 | 5.32763108 | 0.94822562 |
| H | -2.03359502 | 4.30525811 | 0.53673735 |
| H | -1.04412117 | 5.02381963 | -0.74361529 |
| C | 0.50231792 | 1.53246251 | 3.34859583 |
| H | 0.51116358 | 2.49784570 | 3.87801910 |
| H | 1.17828543 | 1.60664398 | 2.48165410 |
| H | 0.94462583 | 0.79253762 | 4.03520302 |
| C | -0.91097496 | 1.14016308 | 2.94342655 |
| H | -1.34331099 | 1.94373173 | 2.32341425 |
| C | -1.81748584 | 0.96815429 | 4.15212239 |
| H | -1.46777647 | 0.17519910 | 4.83101121 |
| H | -2.85571158 | 0.73812134 | 3.87765794 |
| H | -1.84030222 | 1.89617620 | 4.74383199 |
| C | 1.05089769 | -2.26572382 | 2.64530592 |
| H | 1.41175719 | -2.91301443 | 3.45991615 |
| H | 1.80293324 | -1.48483545 | 2.46565011 |
| H | 1.01387399 | -2.87842837 | 1.73277477 |

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|---|---|---|---|
| C | -0.30022092 | -1.66814178 | 2.99859151 |
| H | -0.15781253 | -1.09819015 | 3.93254530 |
| C | -1.35485172 | -2.72403378 | 3.28948011 |
| H | -1.57022595 | -3.36496603 | 2.42016675 |
| H | -2.30988325 | -2.28605290 | 3.61179847 |
| H | -1.01105038 | -3.39264458 | 4.09403138 |
| C | 0.49198807 | -3.75431457 | -0.70251693 |
| H | 0.58964158 | -4.60544654 | -0.01057944 |
| H | 1.36319532 | -3.09743499 | -0.54781742 |
| H | 0.55394050 | -4.16748852 | -1.72013992 |
| C | -0.82125701 | -3.02337337 | -0.46465563 |
| H | -0.86063280 | -2.79070961 | 0.61129602 |
| C | -2.03042670 | -3.89256405 | -0.77315923 |
| H | -2.15664286 | -4.08869160 | -1.84718980 |
| H | -2.96833951 | -3.45165921 | -0.40767200 |
| H | -1.92343345 | -4.87048933 | -0.27740697 |
| C | 1.31888060 | -1.69930161 | -3.12975643 |
| H | 1.61183866 | -2.75269359 | -3.01897208 |
| H | 1.88719763 | -1.11970091 | -2.38619213 |
| H | 1.65038819 | -1.38187343 | -4.13062342 |
| C | -0.18195906 | -1.49836775 | -2.97640322 |
| H | -0.41724911 | -0.49581429 | -3.37552945 |
| C | -0.97936804 | -2.50645223 | -3.79175892 |
| H | -0.72916181 | -2.41957929 | -4.86045385 |
| H | -2.06545118 | -2.36368432 | -3.69809271 |
| H | -0.74894326 | -3.54212591 | -3.50006868 |
| C | 3.53491059 | -0.04750503 | 0.07507787 |
| C | 4.10553589 | 0.76033783 | -1.11218939 |
| H | 3.73415771 | 0.32269670 | -2.05457328 |
| H | 3.71437112 | 1.79060329 | -1.06804718 |
| C | 4.07393843 | -1.49275201 | -0.02307745 |
| H | 3.65970881 | -2.08643315 | 0.80933960 |
| H | 3.69838402 | -1.94925164 | -0.95484317 |
| C | 4.05831319 | 0.57956311 | 1.38630711 |
| H | 3.67031051 | 1.60931804 | 1.46855729 |
| H | 3.64527899 | 0.01703095 | 2.24085684 |
| C | 5.63377477 | 0.75524153 | -1.07909845 |
| H | 6.01622355 | 1.33994005 | -1.93296410 |
| C | 6.12005945 | 1.37860907 | 0.23053965 |
| H | 5.78046779 | 2.42584040 | 0.30283268 |
| H | 7.22260094 | 1.40384316 | 0.25294980 |
| C | 5.58591498 | 0.56846108 | 1.41336806 |
| H | 5.93471914 | 1.01892019 | 2.35821077 |
| C | 6.08914894 | -0.87293536 | 1.31542555 |
| H | 5.72684917 | -1.46149338 | 2.17537524 |
| H | 7.19099884 | -0.89521870 | 1.36157680 |

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|---|---|---|---|
| C | 5.60285008 | -1.49743162 | 0.00612483 |
| H | 5.96303341 | -2.53778826 | -0.06525000 |
| C | 6.13848794 | -0.68560142 | -1.17546023 |
| H | 7.24138874 | -0.70368253 | -1.18060110 |
| H | 5.81227742 | -1.13902084 | -2.12679716 |
| Co | 0.47745868 | 0.01351792 | 0.03650482 |