Supplementary Information

Cp*Co(IPr): Synthesis and Reactivity of an Unsaturated Co(I) Complex

*John Andjaba,[a] Jesse W. Tye,[b] Pony Yu,[c] Iraklis Pappas,[c] and Christopher A. Bradley[a]**

chris.bradley@ttu.edu

[a] *Department of Science, Mount St. Mary's University, Emmitsburg, MD 21727*
[b] *Department of Chemistry, Ball State University, Muncie, IN 47306*
[c] *Department of Chemistry, Princeton University, Princeton, NJ 08544*

-Supplementary Information-

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Additional Experimental Details

General Considerations. All air- and moisture-sensitive manipulations were carried out using standard vacuum line, Schlenk or cannula techniques or in a Vacuum Atmospheres OMNI inert atmosphere drybox containing an atmosphere of purified nitrogen. Solvents for air- and moisture-sensitive manipulations were initially dried and deoxygenated using literature procedures.[1] Benzene-d_6 and toluene-d_8 for NMR spectroscopy were purchased from Cambridge Isotope Labs and were distilled from sodium metal under an atmosphere of nitrogen and stored over 4 Å molecular sieves or sodium metal. Methanol-d_1 was purchased from Cambridge Isotope labs, stored in a refrigerator, and used as received. Trimethylphosphine was purchased from Strem and used as received. Sodium hydride was purchased from Strem and rinsed with hexanes in a glovebox and dried to any remove oil coating. Lithium aluminum hydride was purchased from Aldrich and used as received. Potassium tert-butoxide was purchased from Aldrich and dried overnight under vacuum on a Schlenk line prior to use. DMAP was purchased from Aldrich, recrystallized from ether, and dried overnight on a Schlenk line before use. Carbon monoxide, ethylene, and hydrogen were purchased from Aldrich and dried on a Schlenk line using a liquid nitrogen trap prior to use (In the case of ethylene, the cooled trap was slowly warmed to admit dry ethylene to the line). Deuterium gas was purchased from Cambridge Isotope Labs and dried on a Schlenk line using a liquid nitrogen cooled trap prior to use. **1**[2] and IPr•HCl[3] were prepared according to literature procedures.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker 400 MHz Spectrometer. Initial ^{1}H NMR experiments were conducted on site on an Anasazi 90 MHz NMR spectrometer. All chemical shifts are reported relative to $SiMe_4$ using ^{1}H (residual) or ^{13}C NMR chemical shifts of the solvent as a secondary standard. Fourier-Transform Infrared (FT-IR) Spectroscopy was performed on a Shimadzu IRAffinity-1 spectrometer using a liquid cell purchased from Pike Technologies. UV-visible data were collected on a Shimadzu UV-1800 spectrometer using a sealable quartz cell. LIFDI[4] and LIFDI/Exact Mass Spectrometry were performed by the High Resolution Mass Spectrometry Facility at the University of California, Riverside.

Single crystals suitable for X-ray diffraction were coated with polyisobutylene oil in a drybox and were quickly transferred to the goniometer head of a Bruker Apex II detector system equipped with a molybdenum X-ray tube (λ = 0.71073 Å). Data was collected at 100 K. Preliminary data revealed the crystal system. A hemisphere routine was used for data collection and determination of lattice constants. The space group was identified and the data were processed using the Bruker AXS SHELXTL software and corrected for absorption using SADABS. The structures were solved using direct methods (SHELXS) completed by subsequent Fourier transformation and refinement by full-matrix least-squares procedures. Initial crystallographic determinations were collected on site at 170 K on a Rigaku XtaLAB mini.

Modified preparation of IPr. A 100 mL round-bottomed flask was charged with 1.20 g (2.82 mmol) of IPr•HCl and approximately 40 mL of THF. While stirring, 0.204 g (8.50 mmol) of NaH was added, along with a small spatula head (~20 mg) of potassium tert-butoxide. The resulting reaction mixture was stirred for 16 hours. Solvent was then removed *in vacuo* from the light brown mixture. The resulting solid was extracted with ether (3 x 25 mL) and filtered through Celite. Removal of the solvent *in vacuo* afforded 0.740 g (68%) of IPr as a light brown solid. Spectral data match previous reports of the complex (Figures S22 and S23).[3]

Preparation of Cp*Co(IPr) (2). A 100 mL round-bottomed flask was charged with 0.234 g (0.487 mmol) of **1** and approximately 35 mL of toluene. While stirring, 0.379 g (0.975 mmol) of IPr was added and the reaction mixture was stirred for 24 hours. Solvent removal *in vacuo* affords 0.528 g (93%) of **2** as a red solid. Recrystallization of **2** in toluene at -25 °C affords (0.346 g, 61%) of analytically pure **2**. LIFDI exact mass spectrum for $C_{37}H_{51}N_2Co$: calcd. 582.34 *m/z*; found 582.3388 *m/z*. ^{1}H NMR (benzene-d_6): δ = -9.84 (br, 4H, C*H*Me$_2$), 2.35 (br, 15H, Cp*), 5.20 (br, 24H, CH*Me$_2$*), 6.67 (br, 2H, NHC/Ar), 8.76 (br, 2H, Ar/NHC), and 10.57 (br, 4H, Ar). Magnetic susceptibility (benzene-d_6, 25 °C): μ_{eff} = 2.6(1). UV-visible (toluene, nm, [ε, cm^{-1}M^{-1}]): 440 (3000), 800 (250).[5]

Preparation of Cp*Co(IPr)(CO) (3). A sealable thick walled vessel was charged with 0.200 g (0.343 mmol) of **2** and approximately 10 mL of toluene in a glovebox. The vessel was sealed, removed from the glovebox, and attached to a Schlenk line. The reaction mixture was then frozen in liquid nitrogen, evacuated, and predried carbon monoxide was admitted to the vessel. The vessel was then allowed to warm to ambient temperature and stirred for 3 hours. Solvent and excess carbon monoxide were removed from the green solution *in vacuo* on a Schlenk line. Inside a glovebox, the solid was extracted with ether and filtered through Celite. Solvent was removed *in vacuo* and the material was recrystallized in pentane at -25 ºC to give 0.136 g (65%) of **3** as a green solid. LIFDI exact mass spectrum for $C_{38}H_{51}N_2OCo$: calcd. 610.33 *m/z*; found 610.335 *m/z*. ^{1}H NMR (benzene-d_6): δ = 1.03 (d, 12H, 8 Hz, CH*Me$_2$*), 1.51 (d, 12H, 8 Hz, CH*Me$_2$*), 1.53 (s, 15H, Cp* *Me*), 3.06 (sept, 4H, 8 Hz, C*H*Me$_2$), 6.60 (s, 2H, IPr *H*), 7.18-7.25 (6H, Ar). ^{13}C NMR (benzene-d_6): δ = 10.86 (Cp* *Me*), 22.95, 26.73, 28.79 (CHMe$_2$), 91.24 (Cp*), 123.94, 124.49, 129.40, 138.36, and 146.95 (Ar/NHC), 220.48 (*C*O). The Co-C_{NHC} resonance was not observed. IR (ether, cm^{-1}): 1884 (CO).

Reaction of 2 with DMAP. A J. Young NMR tube was charged with 0.020 g (0.0343 mmol) of **2** and then dissolved in 0.5 mL of benzene-d_6. The tube was then charged with 0.008 g (0.0655 mmol) of DMAP and the reaction mixture was monitored by ^{1}H NMR spectroscopy. No reaction was observed at ambient temperature for three days or heating at 65 ºC for one week.

Reaction of Cp*Co(IPr) (2) with PMe$_3$. A sealable thick walled vessel was charged with 0.200 g (0.343 mmol) of **2** and approximately 10 mL of toluene in a glovebox. Trimethylphosphine (0.060 g, 0.789 mmol) was then added to the stirring solution, the vessel was sealed, removed from the glovebox, and heated at 65 ºC for 16 hours in an oil bath. The solvent was then removed *in vacuo* on a Schlenk line. Inside a glovebox, the red solid was extracted with ether and filtered through Celite. Solvent was removed *in vacuo* and the resulting solid was recrystallized in pentane at -25 ºC to give 0.083 g (70%) of **4** as a red solid. Crude reaction mixtures analyzed by ^{1}H and ^{13}C NMR spectroscopy revealed a mixture of **4** and IPr.

Mass spectra of the product mixture and comparison to independently prepared **4** (Figures S10 and S11) and IPr (Figures S23 and S24) establish their formation. LIFDI mass spectrum for $C_{16}H_{33}P_2Co$: calcd. 346 *m/z*; found 346 *m/z*.

Independent Preparation of Cp*Co(PMe$_3$)$_2$ (4). A 50 mL round-bottomed flask was charged with 0.100 g (0.208 mmol) of **1** and approximately 15 mL of pentane. While stirring, 0.80 g (1.05 mmol) of trimethylphosphine was added. The resulting reaction mixture was stirred for 16 hours. Filtration through Celite followed by solvent removal of the pentane *in vacuo* and subsequent recrystallization from pentane at -25 °C afforded 0.044 g (63%) of **4** as a dark red solid. Spectral data match previous reports of the complex (Figures S10 and S11).

Reaction of 2 with ethylene. A sealable thick walled vessel was charged with 0.200 g (0.343 mmol) of **2** and approximately 10 mL of toluene in a glovebox. The vessel was sealed, removed from the glovebox, and frozen in liquid nitrogen. The vessel was then charged with excess ethylene (previously dried in a liquid N_2 cooled trap) and the reaction mixture was allowed to warm to ambient temperature and stirred for three hours. The solvent and excess ethylene was then removed *in vacuo* on a Schlenk line. Inside a glovebox, the resulting solid was dissolved in pentane and filtered through Celite. Solvent removal followed by recrystallization from pentane at -25 ºC yields 0.047 g (55%) of **5** as a dark red solid. Crude reaction mixtures monitored by ^{1}H and ^{13}C NMR spectroscopy revealed a mixture of **5** and IPr. Mass spectra of the product mixture and comparison to independently prepared **5** (Figures S15 and S16) and IPr (Figures S23 and S24) establish their formation. LIFDI mass spectrum for $C_{14}H_{23}Co$: calcd. 250 *m/z*; found 250 *m/z*.

Independent Preparation of Cp*Co(η^2-CH$_2$=CH$_2$)$_2$ (5). A sealable thick walled vessel was charged with 0.100 g (0.208 mmol) of **1** and approximately 15 mL of pentane in a glovebox. The vessel was sealed, removed from the glovebox, and frozen in liquid nitrogen. The vessel was then charged with excess ethylene (previously dried in a liquid N_2 cooled trap) and the reaction mixture was allowed to warm to ambient temperature and stirred for three hours. The solvent was then removed *in vacuo* on a Schlenk line. Inside a glovebox, the resulting solid was dissolved in pentane and filtered through Celite. Solvent removal *in vacuo* followed by recrystallization from pentane at -25 ºC yields 0.073 g (70%) of **5** as a dark red solid. Spectral data match previous reports of the complex (Figures S15 and S16).

Characterization of Cp*CoH$_2$ (2-^{c}H$_2$). A J. Young tube was charged with 0.020 g (0.034 mmol) of **2** and then dissolved in 0.5 mL of benzene-d_6. The tube was then charged with excess dihydrogen (previously dried in a liquid N_2 cooled trap) and the reaction mixture was monitored by ^{1}H NMR spectroscopy, resulting in complete conversion to **2-^{c}H$_2$** in less than 5 minutes. A similar method, using 0.018 g (0.031 mmol) of **2** and **D**$_2$ resulted in formation of **2-^{c}D$_2$**, based on spectral comparison and a ^{2}H NMR spectrum of the sample. ^{1}H NMR (benzene-d_6): δ = -17.78 (br s, 2H, Co-*H*), 1.05 (d, 12H, 8 Hz, CH*Me*$_2$), 1.50 (d, 12H, 8 Hz, CH*Me*$_2$), 1.68 (s, 15H, Cp* *Me*), 3.02 (sept, 4H, 8 Hz, C*H*Me$_2$), 6.46 (s, 2H, IPr *H*), 7.20 (d, 2H, 8 Hz, Ar), and 7.27 (d, 4H, 8 Hz, Ar). ^{13}C NMR (benzene-d_6): δ = 11.88 (Cp* *Me*), 22.73, 25.84, 28.85 (CHMe$_2$), 89.70 (Cp*), 123.42, 123.86, 129.10, 139.50, and 146.62. The Co-C$_{NHC}$ resonance was not observed. ^{2}H NMR (benzene): δ = -17.58 (Zr-*D*).

Generation of HD gas and addition to 2. A sealable thick walled vessel was charged with 0.200 g (5.27 mmol) of lithium aluminum hydride and approximately 5 mL of hexanes was added on a benchtop. The vessel was sealed, and underwent three freeze-pump-thaw cycles using liquid nitrogen. Methanol-d_1 (0.104 g, 3.16 mmol) in a J. Young NMR tube was then vacuum transferred into the frozen vessel and the reaction mixture was allowed to warm to ambient temperature behind a blast shield and stirred for an additional 45 minutes at ambient temperature. A J. Young NMR tube, charged with 0.025 g (0.043 mmol) of **2** dissolved in 0.5 mL of benzene-d_6, was then frozen, evacuated, and the H-D gas generated in the vessel was opened on a Schlenk line containing the open J. Young tube, permitting transfer of H-D gas into the tube. Upon warming to ambient temperature, the tube was shaken for 30 minutes. ^{1}H NMR spectra indicate partial conversion (~40%) to **2-^{c}(HD)**, but the broadness of the hydride resonance prevented determination of the H-D coupling constant. Integration of the hydride peak with respect to other resonances in the molecule are consistent with incorporation of one deuterium atom per H-D incorporated.

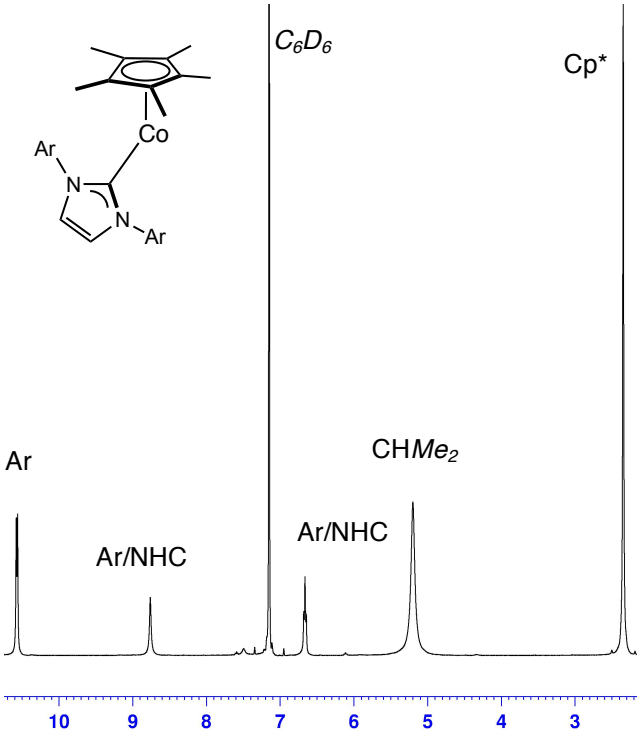


Figure S1. ^{1}H NMR spectrum of **2** in benzene-d_6 (400 MHz).

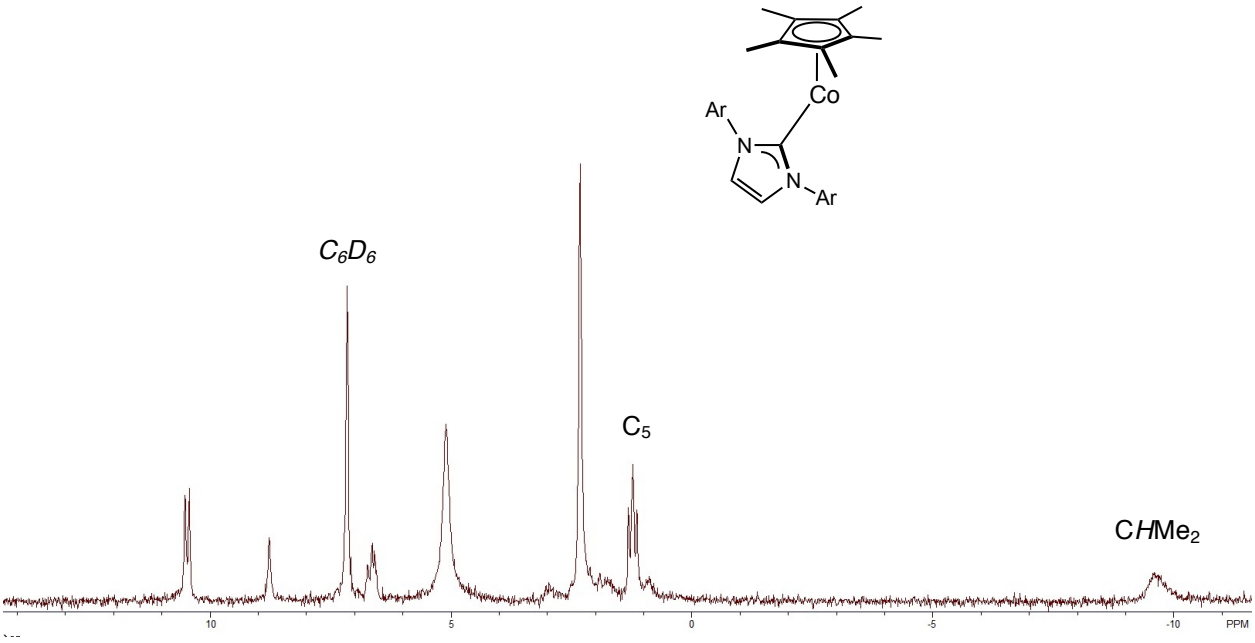


Figure S2. ^{1}H NMR spectrum of **2** in benzene-d_6 (90 MHz).

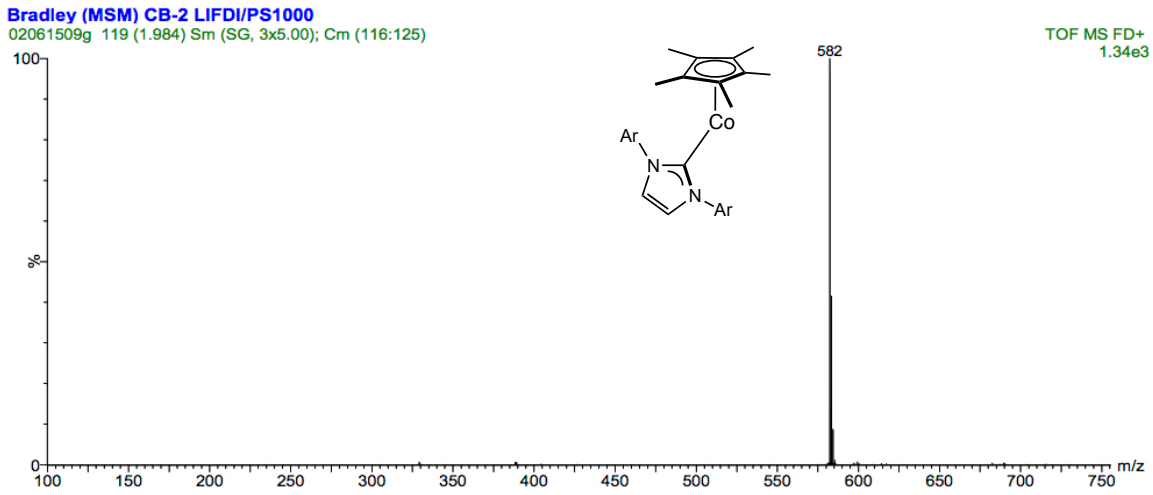


Figure S3. LIFDI mass spectrum of **2** in toluene.

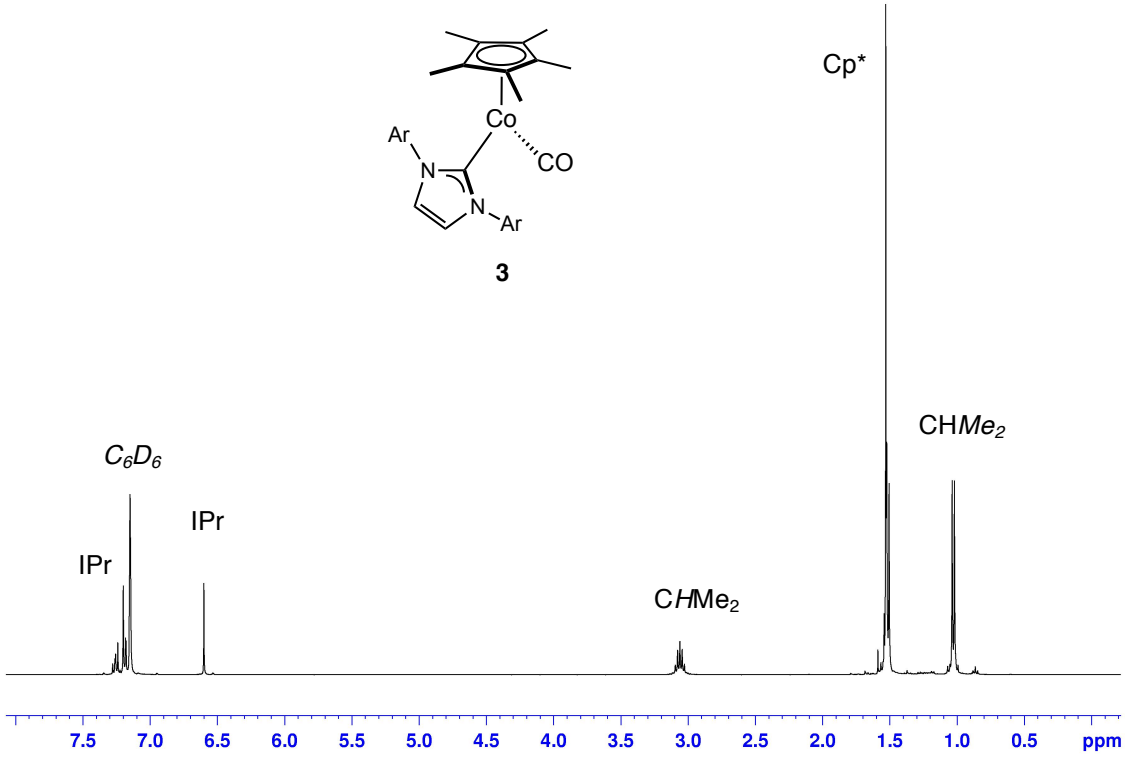


Figure S4. ^{1}H NMR spectrum of **3** in benzene-d_6.

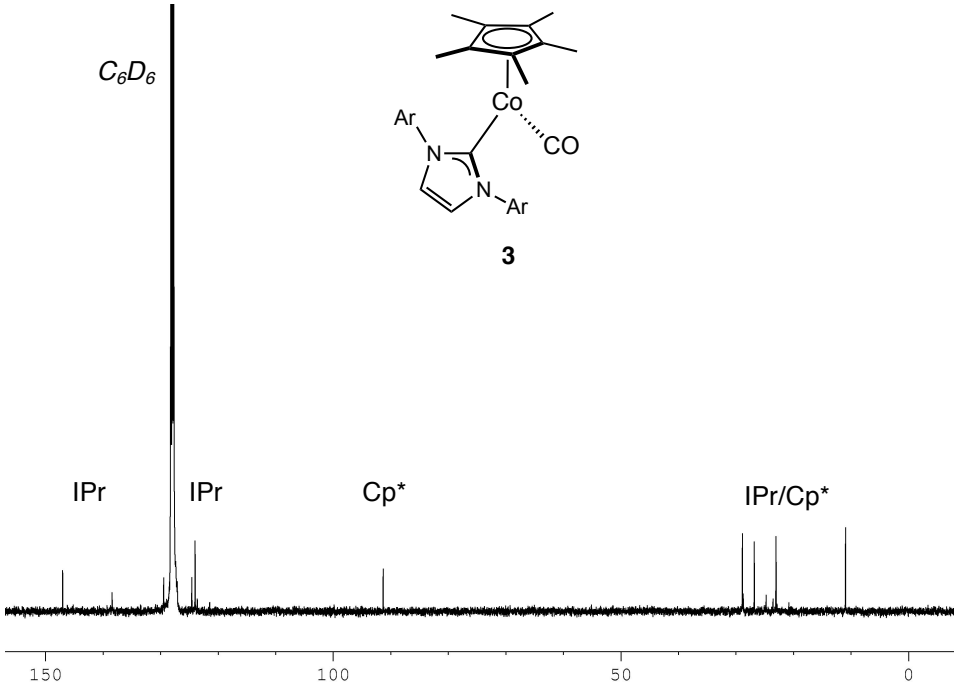


Figure S5. ^{13}C NMR spectrum of **3** in benzene-d_6.

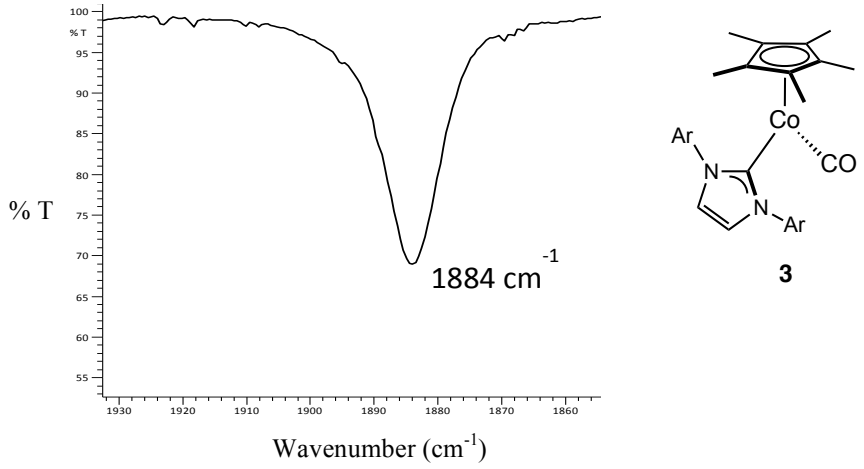


Figure S6. CO stretching region of the spectrum of **3** in ether.

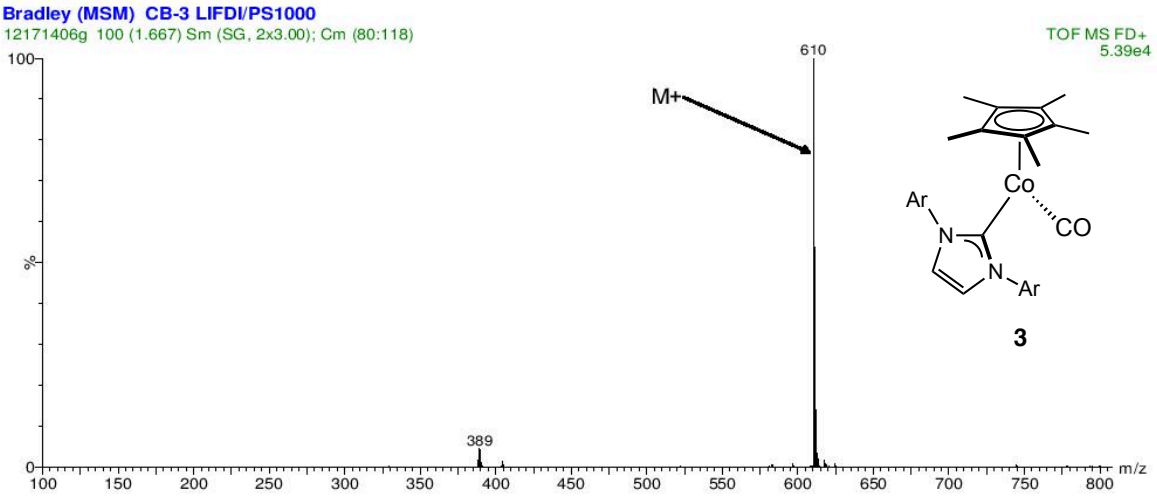


Figure S7. LIFDI mass spectrum of **3** in toluene.

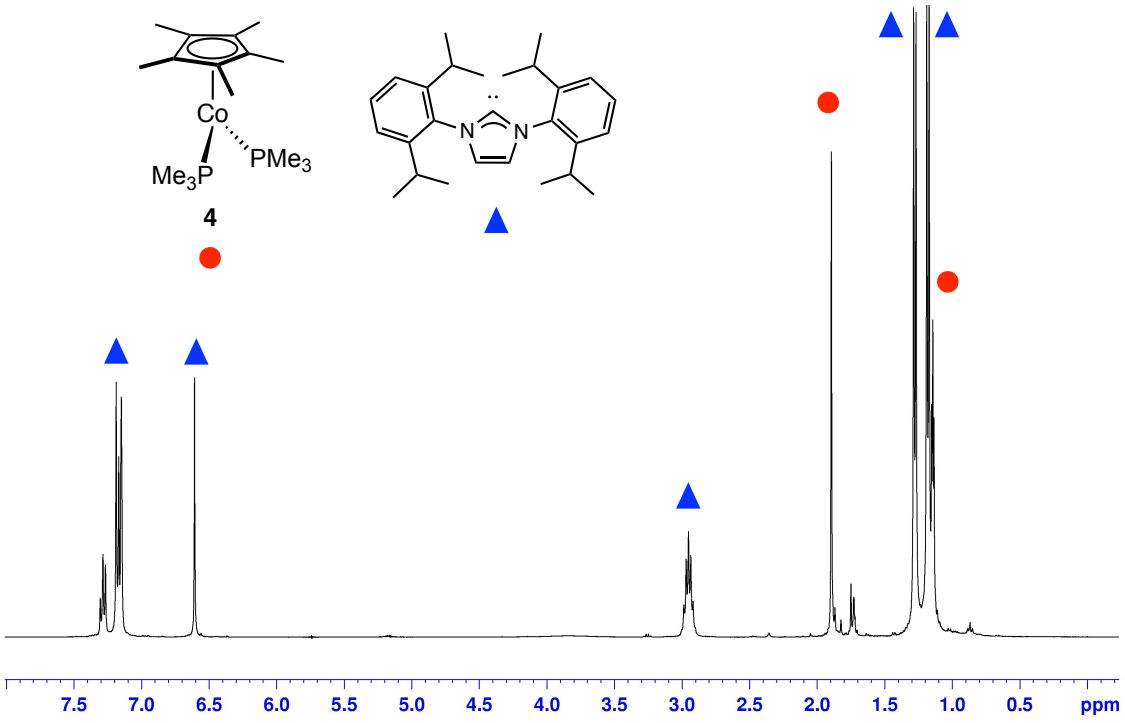


Figure S8. ^{1}H NMR spectrum of the reaction of **2** with PMe_3 overnight at 65 ºC in benzene-d_6.

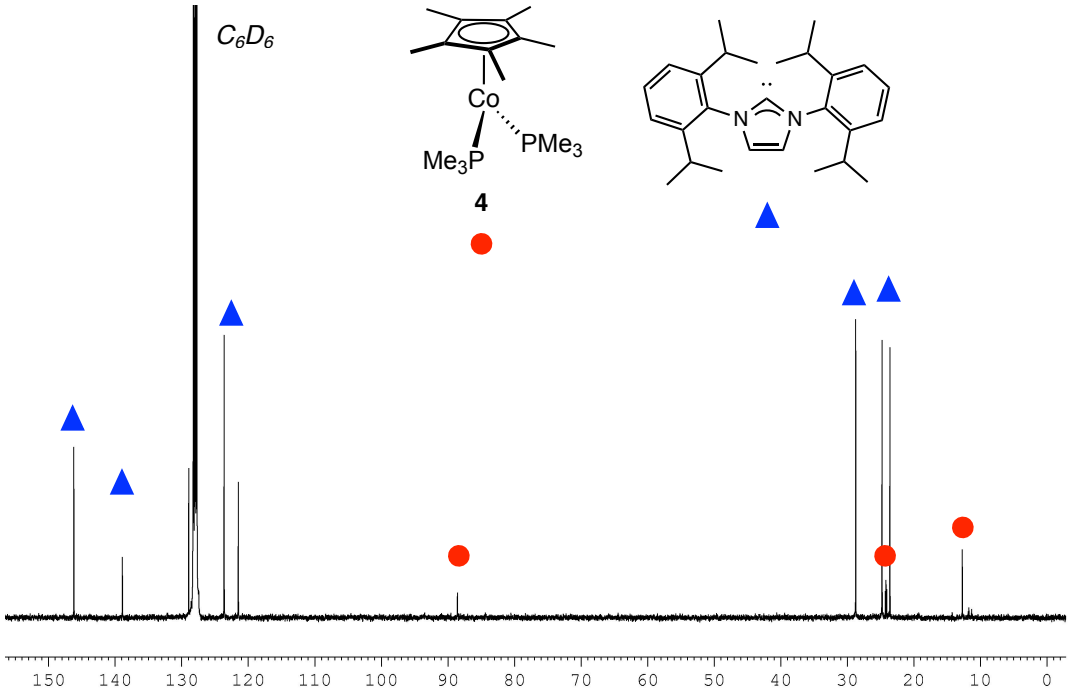


Figure S9. ^{13}C NMR spectrum of the reaction of **2** with PMe_3 overnight at 65 ºC in benzene-d_6.

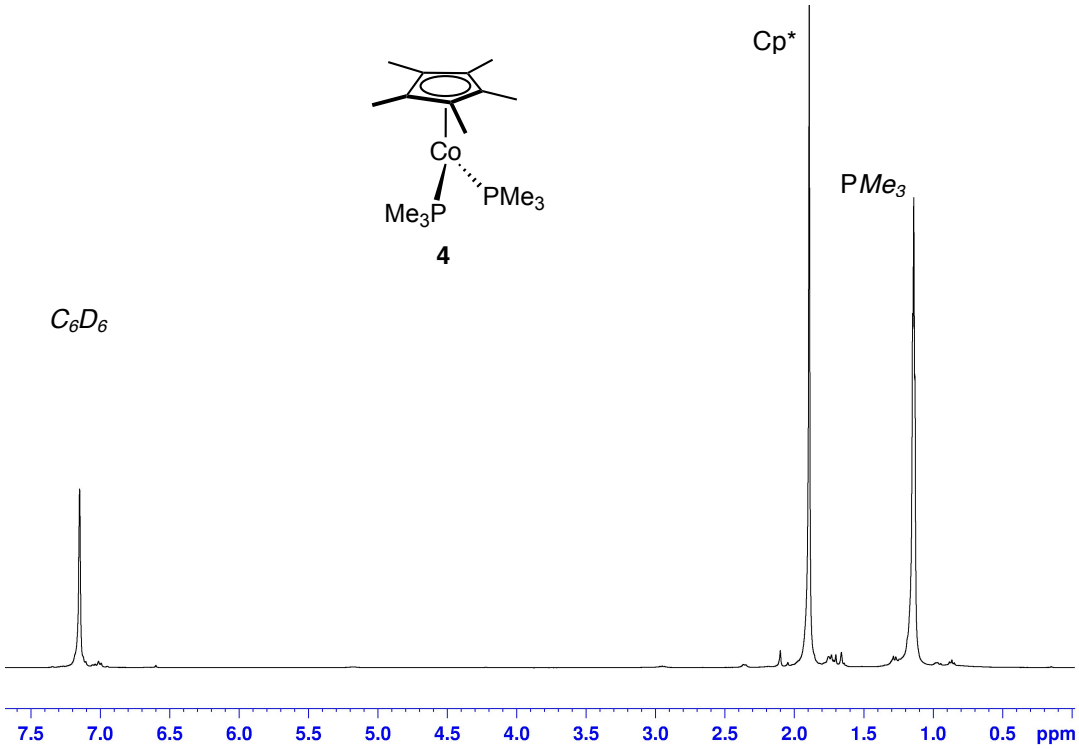


Figure S10. ^{1}H NMR spectrum of independently prepared **4** in benzene-d_6.

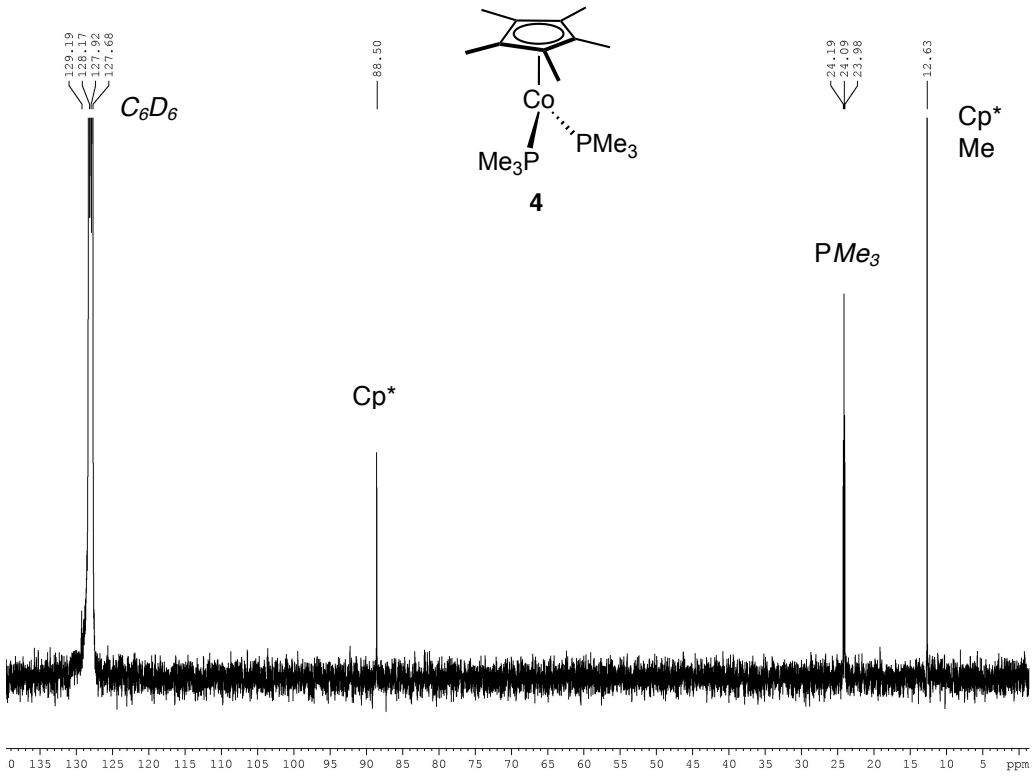


Figure S11. ^{13}C NMR spectrum of independently prepared **4** in benzene-d_6.

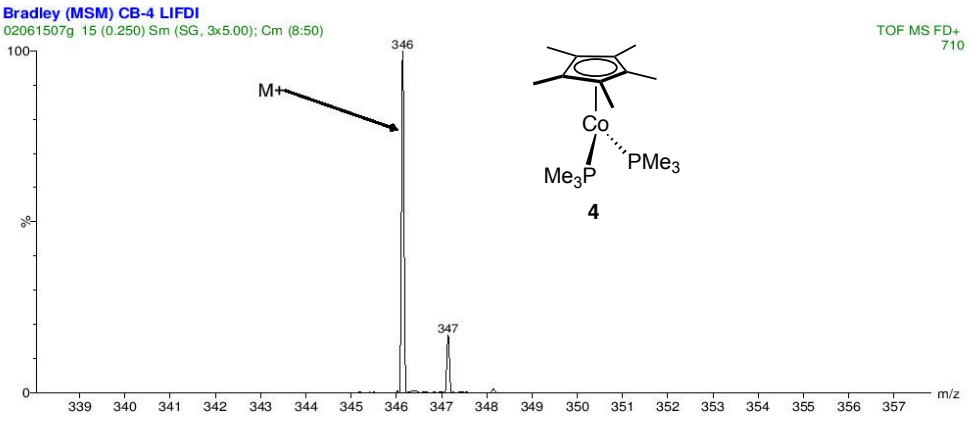


Figure S12. LIFDI mass spectra of the reaction of **2** with excess PMe_3 overnight at 65 ºC in toluene.

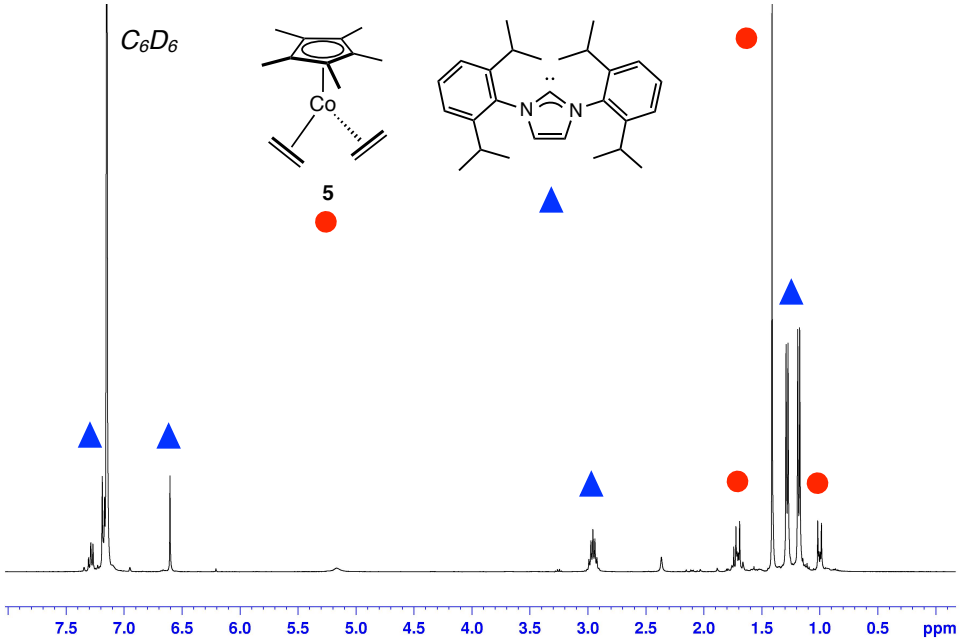


Figure S13. ^{1}H NMR spectrum of the reaction of **2** with excess ethylene at 25 ºC in benzene-d_6.

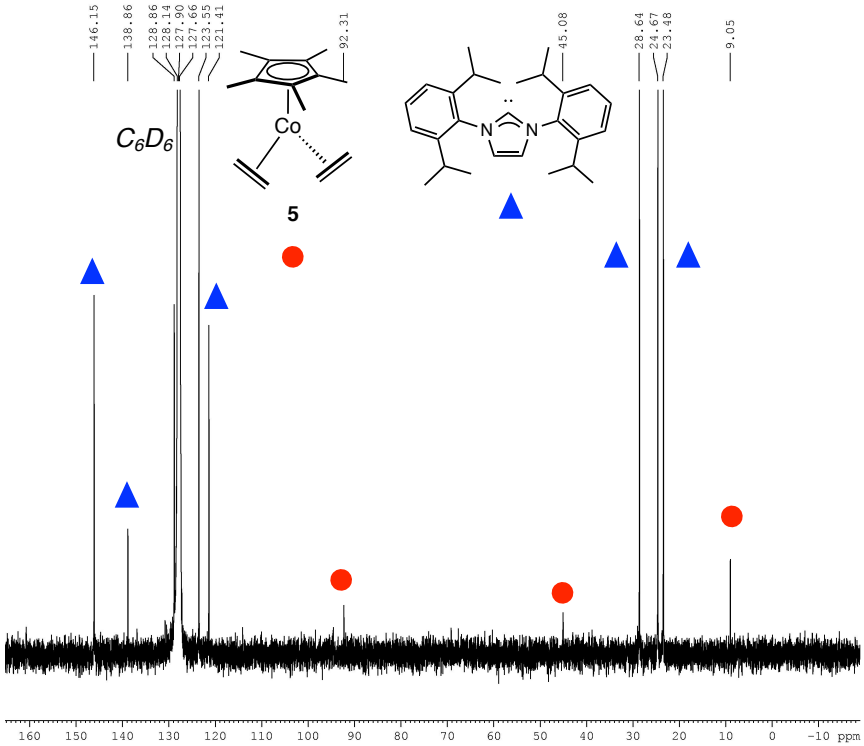


Figure S14. ^{13}C NMR spectrum of the reaction of **2** with excess ethylene at 25 ºC in benzene-d_6.

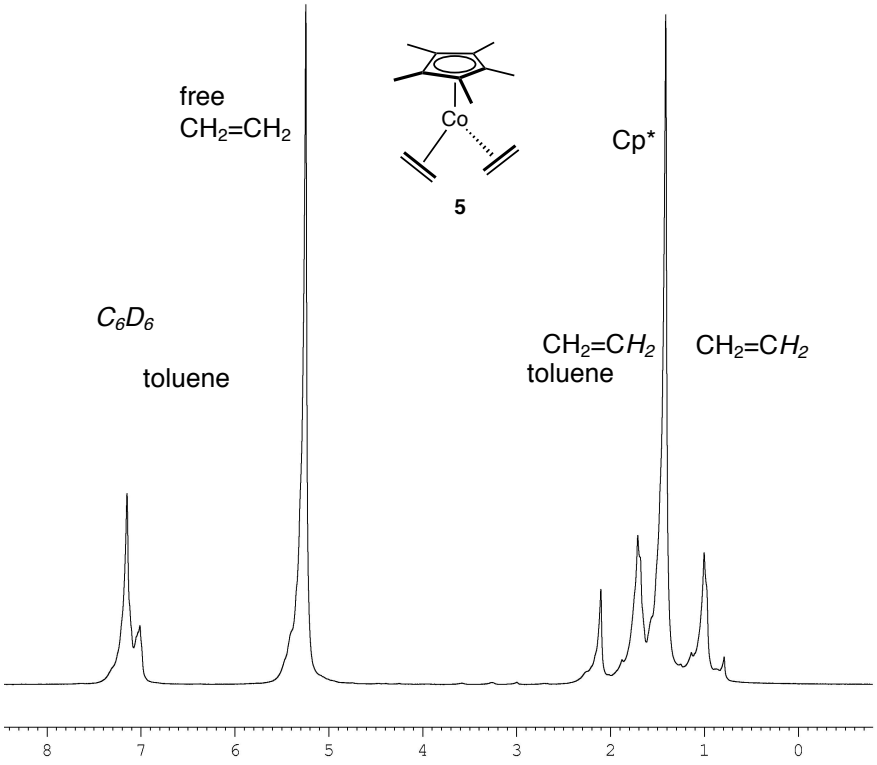


Figure S15. ^{1}H NMR spectrum of independently prepared **5** in benzene-d_6 (under excess ethylene).

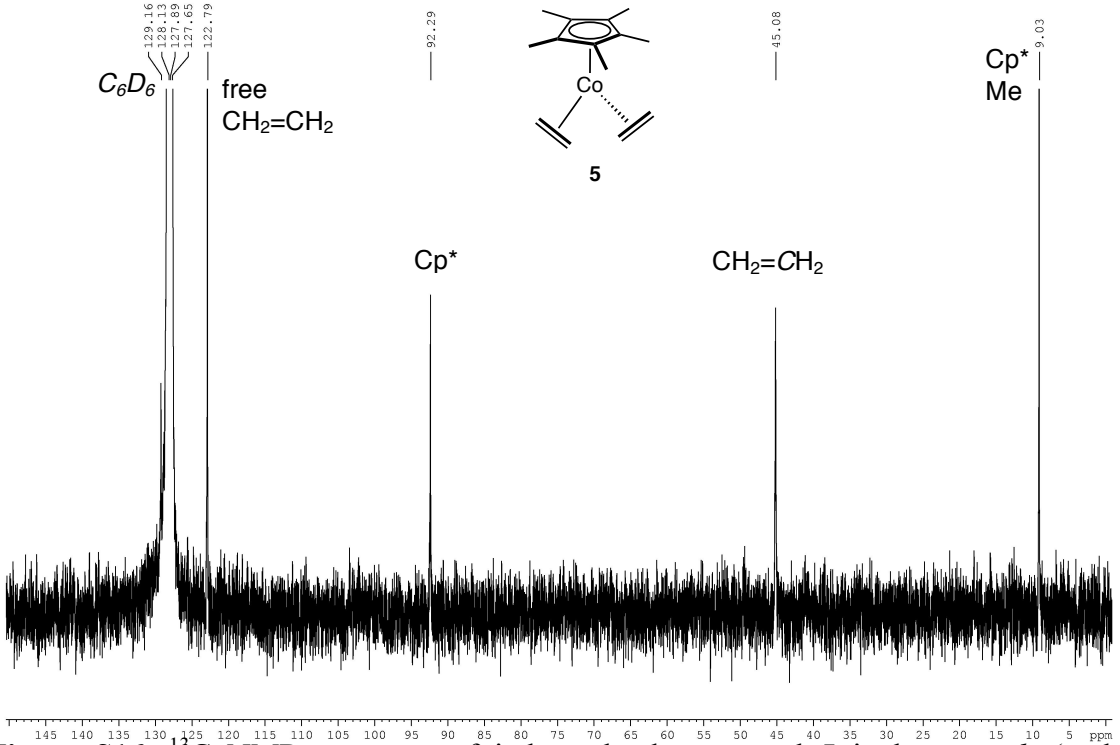


Figure S16. ^{13}C NMR spectrum of independently prepared **5** in benzene-d_6 (under excess ethylene).

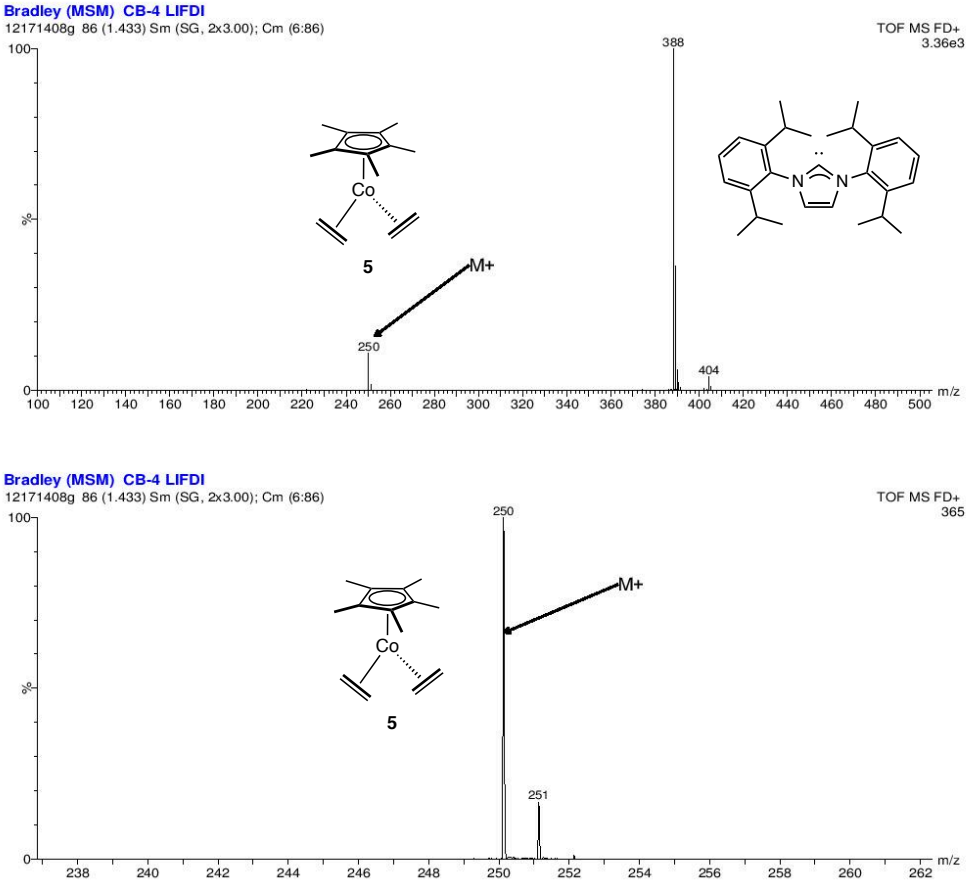


Figure S17. LIFDI mass spectrum of the reaction of **2** with excess ethylene at 65 ºC in toluene.

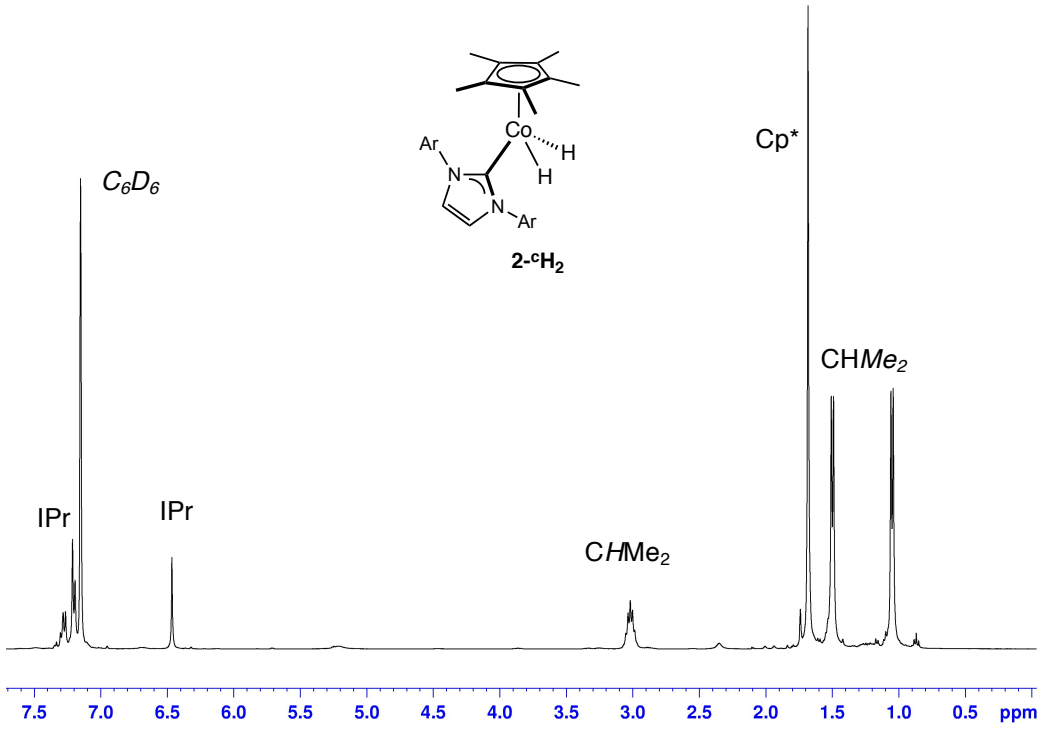


Figure S18. ^{1}H NMR spectrum of **2-^{c}H$_2$** (under excess H_2) in benzene-d_6.

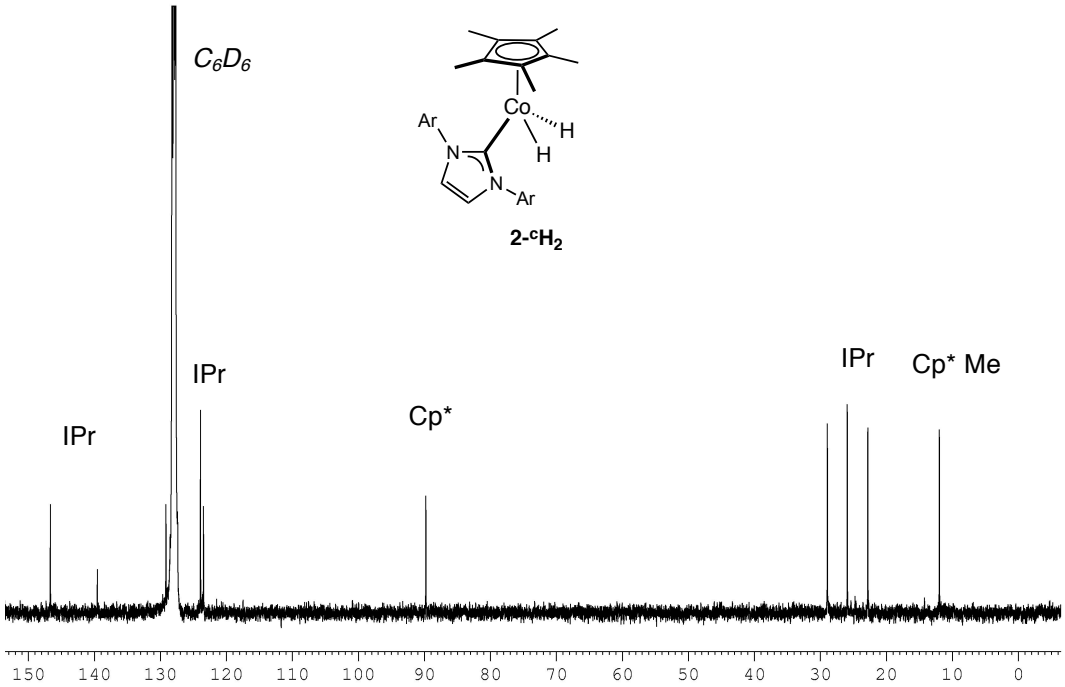


Figure S19. ^{13}C NMR spectrum of **2-^{c}H$_2$** (under excess H_2) in benzene-d_6.

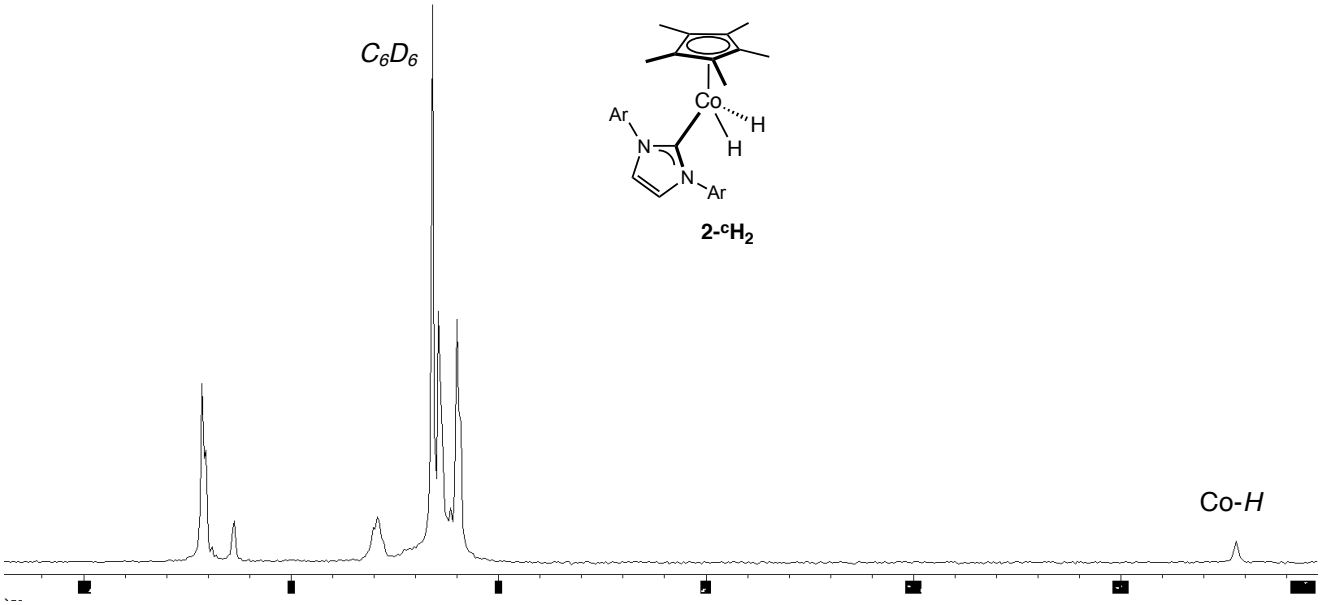


Figure S20. ^{1}H NMR spectrum of **2-^{c}H$_2$** (under excess H_2) in benzene-d_6 (90 MHz).

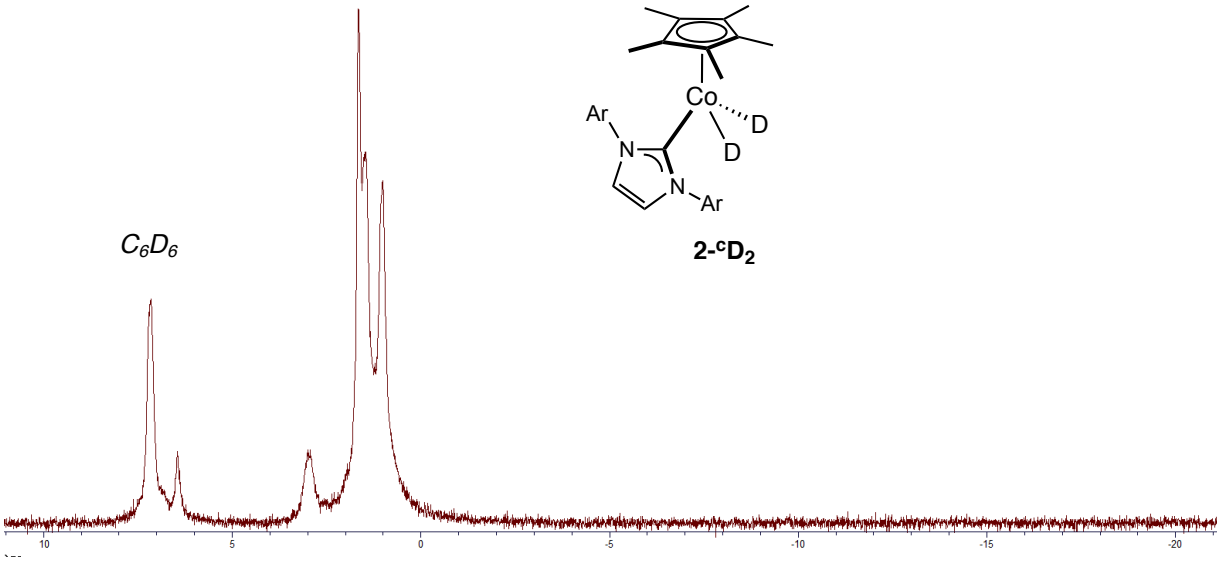


Figure S21. ^{1}H NMR spectrum of **2-^{c}D$_2$** (under excess D_2) in benzene-d_6 (90 MHz).

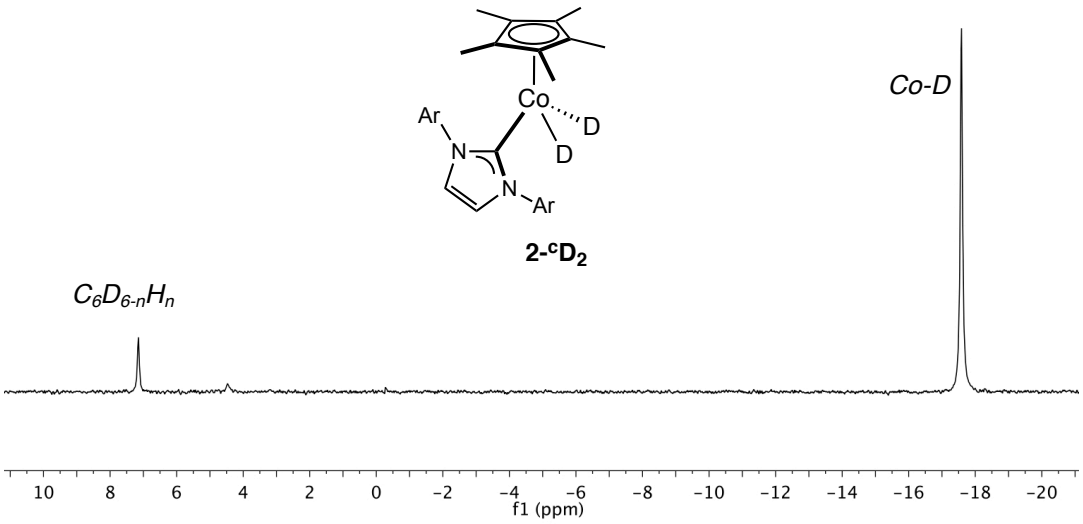


Figure S22. ^{2}H NMR spectrum of **2-^{c}D$_2$** (under excess D_2) in benzene.

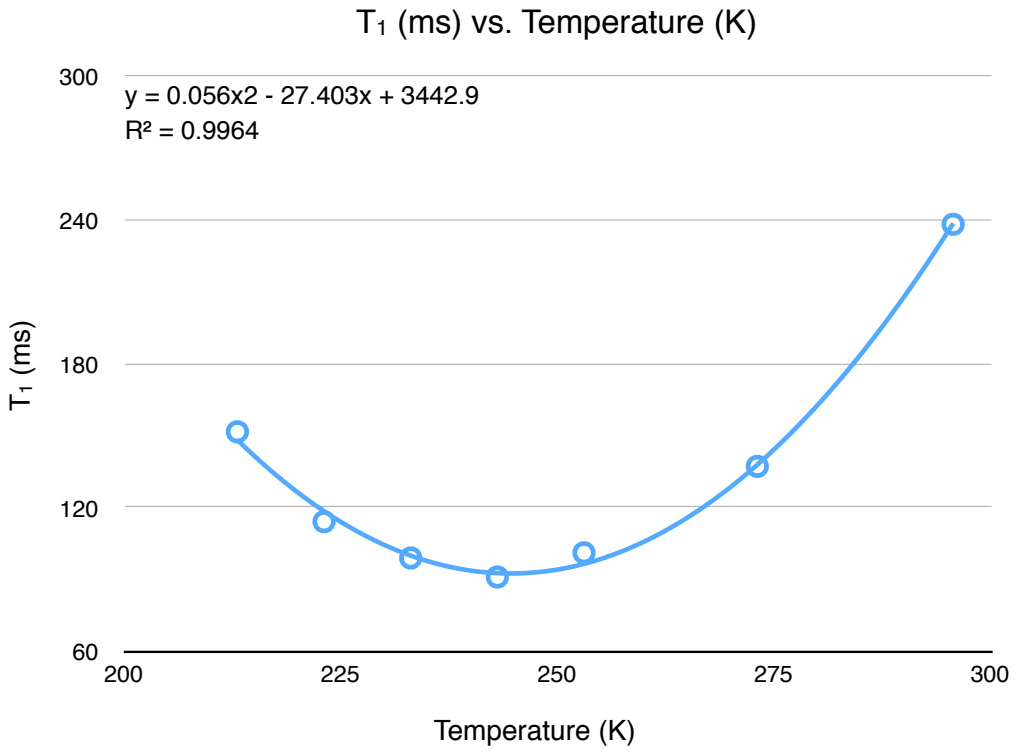


Figure S23. Plot of T_1(min) versus temperature for **2-^{c}H$_2$**.

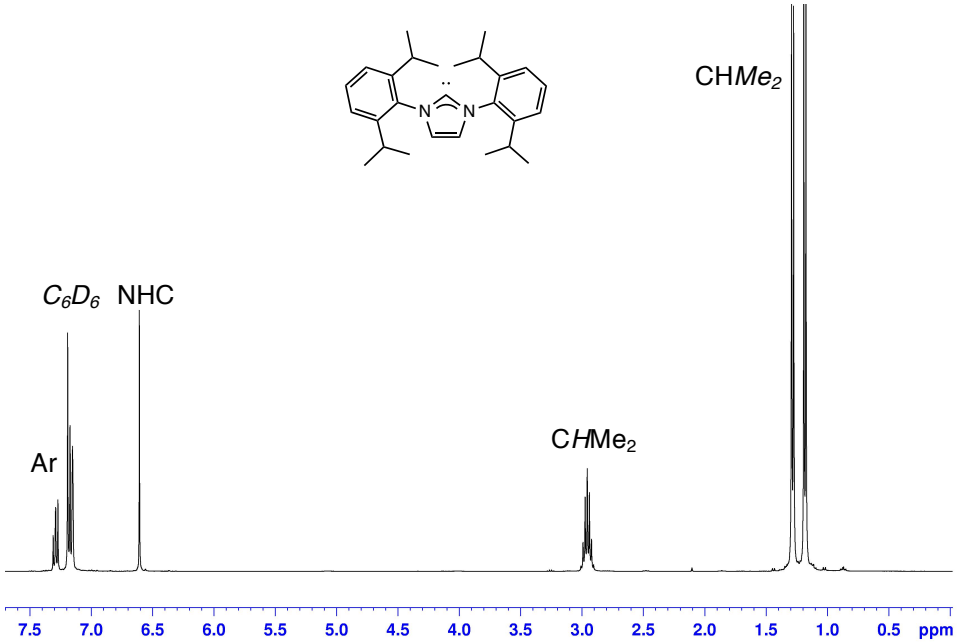


Figure S24. ^{1}H NMR spectrum of IPr in benzene-d_6.

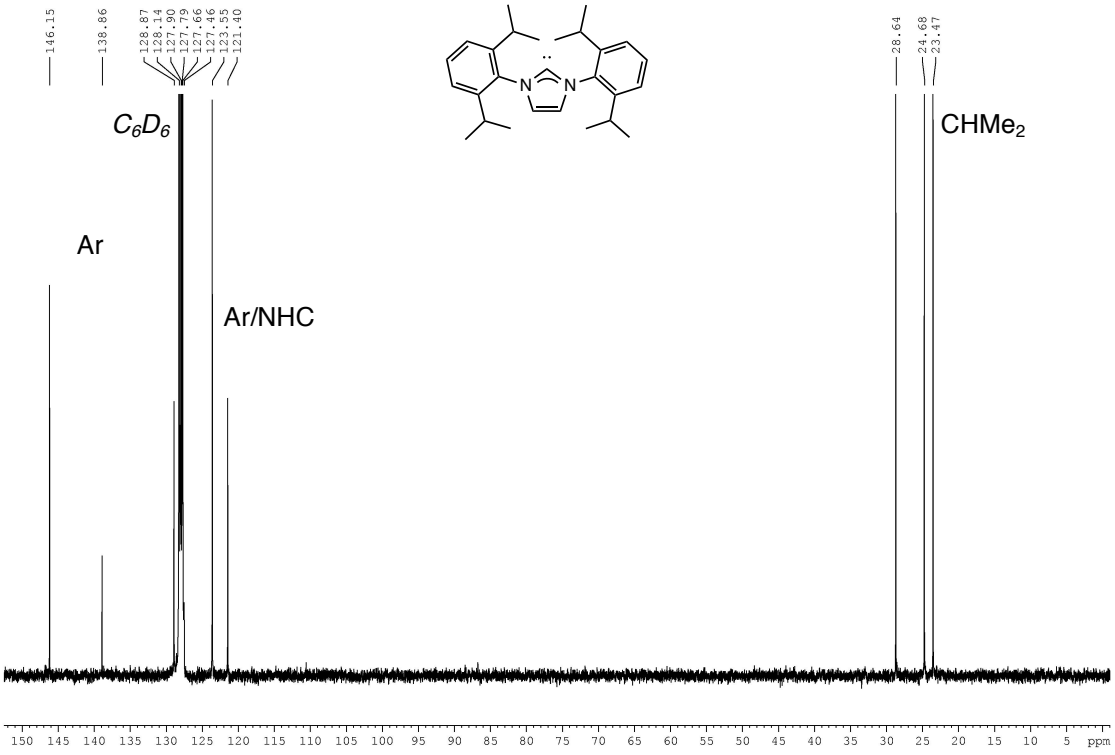
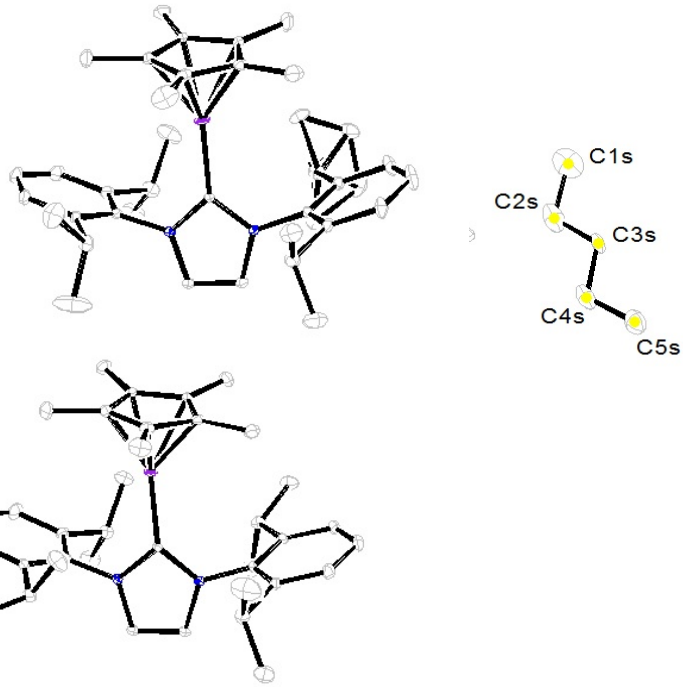


Figure S25. ^{13}C NMR spectrum of IPr in benzene-d_6.

a)



b)

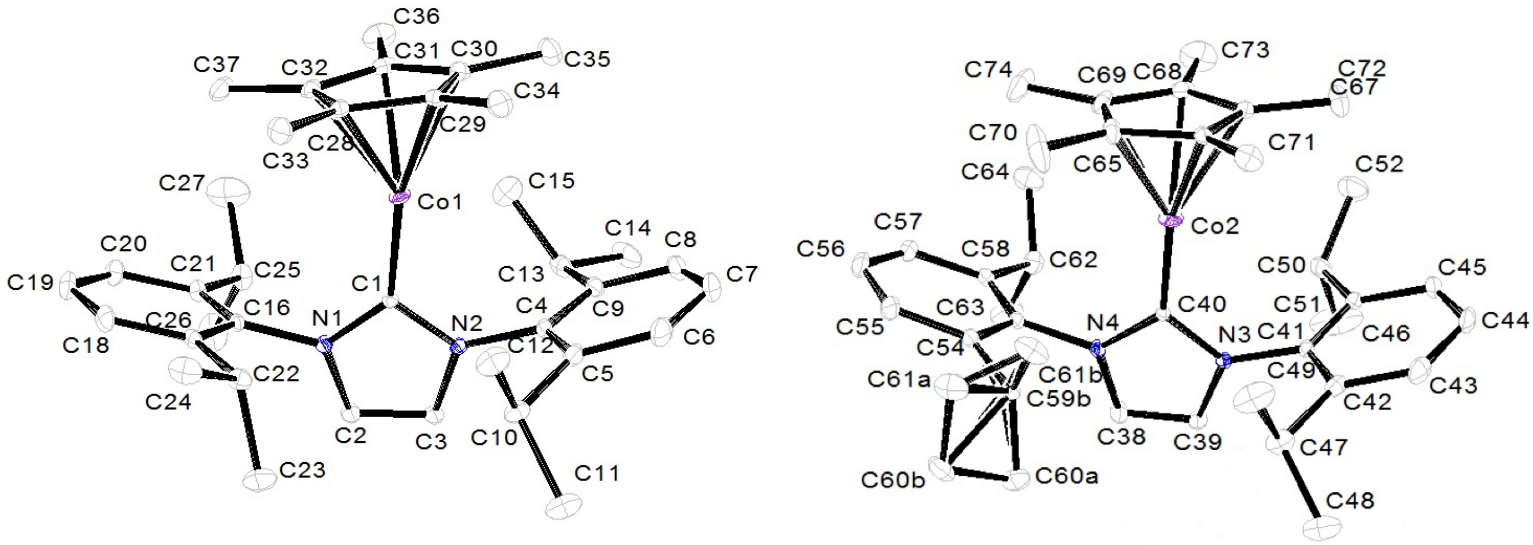


Figure S26. a) Full depiction of the asymmetric unit cell (including a molecule of pentane solvent) with 30 % probability ellipsoids. b) Full atom labeling schemes for the two molecules of **2** in the asymmetric unit. Hydrogen atoms omitted for clarity. The disorder in the isopropyl group of the second molecule in the asymmetric unit could not be modeled sufficiently.

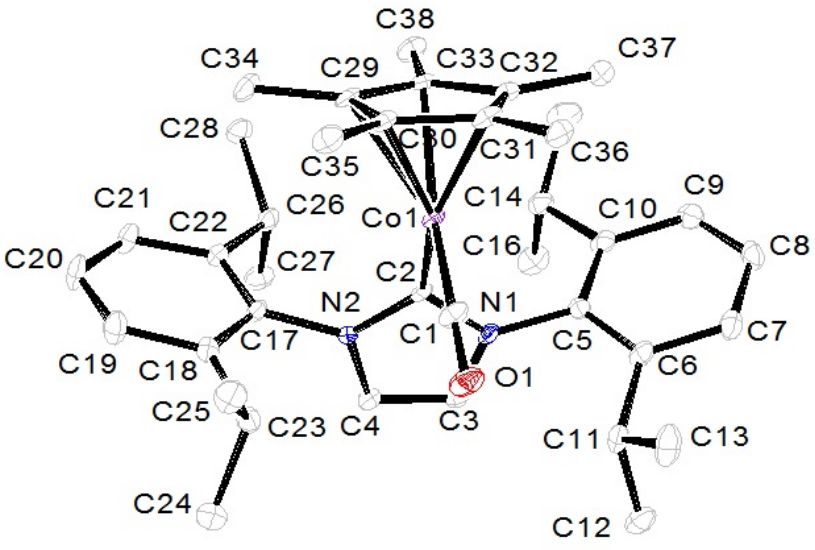


Figure S27. Molecular structure of **3** with 30 % probability ellipsoids and full atom labeling schemes. Hydrogen atoms omitted for clarity.

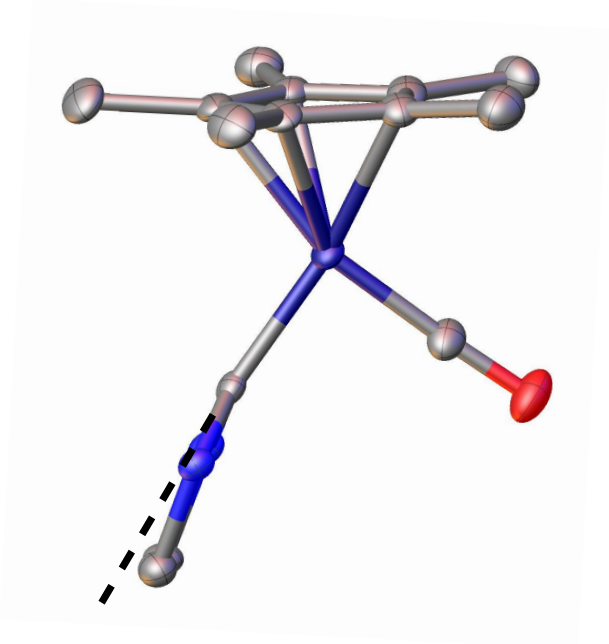


Figure S28. Alternative view of **3** with 30 % probability ellipsoids to highlight the Co(1)-C(2)-$NHC_{centroid}$ angle. Aryl substituents are omitted for clarity.

Table 1. Crystallographic data for complexes **2** and **3**.

Compound	**2**	**3**
Empirical formula	$2C_{37}H_{51}N_2Co \bullet C_5H_{12}$	$C_{38}H_{51}N_2O_1Co$
Formula mass	1237.60	610.74
a [Å]	17.6630(4)	23.5831(6)
b [Å]	18.6473(6)	17.9998(5)
c [Å]	23.0752(8)	16.1483(4)
α [°]	90	90
β [°]	107.032(1)	90
γ [°]	90	90
V [Å^3]	7266.9(4)	6854.8(3)
Z	4	8
Crystal system	Monoclinic	Orthorhombic
Space group	P2(1)/c	Aba2
T [K]	100	100
$D_{calcd.}$ [g cm^{-3}]	1.126	1.184
μ [mm^{-1}]	0.50	4.14
$\theta_{max.}$ [°]	32.1	66.7
Reflections measured	251891	19214
Reflections used (R_{int})	18424(0.057)	4633(0.093)
Restraints/parameters	0/836	1/417
R_1 [$I > 2\sigma(I)$]	0.054	0.052
wR_2 [$I > 2\sigma(I)$]	0.154	0.128

Further crystallographic information can be found on the Cambridge Structural Database (CSD) for **2** (CCDC #: 1416208) and **3** (CCDC #: 1416209).

Data Collection Details for 2.

Computing details. Cell refinement: Bruker *SAINT*; data reduction: Bruker *SAINT*; program(s) used to solve structure: *SIR* 92 (Giacavazzo, 1993); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2014); molecular graphics: *ORTEP* 3 (Farraguia, 1997).

Data collection

BRUKER APEX2 CCD diffractometer	18424 reflections with $I > 2s(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.057$
Phi and w Scans scans	$q_{max} = 32.1°$, $q_{min} = 2.2°$
Absorption correction: multi-scan *SADABS* V2008/1 (Bruker AXS)	$h = -26 \rightarrow 26$
$T_{min} = 0.688$, $T_{max} = 0.746$	$k = -27 \rightarrow 27$
251891 measured reflections	$l = -32 \rightarrow 34$
25350 independent reflections	

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2s(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.154$	$w = 1/[s^2(F_o^2) + (0.0692P)^2 + 9.6888P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.95$	$(D/s)_{max} = 0.002$
25350 reflections	$Dñ_{max} = 1.84$ e Å^{-3}
836 parameters	$Dñ_{min} = -0.91$ e Å^{-3}

Additional Details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 2. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **2**.

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.11641 (9)	0.69046 (8)	0.16901 (7)	0.0115 (2)	
C1S	0.6188 (3)	0.0276 (2)	0.5527 (2)	0.0904 (13)	
H1S1	0.5994	0.0551	0.5150	0.136*	
H1S2	0.6066	-0.0233	0.5444	0.136*	
H1S3	0.5929	0.0449	0.5823	0.136*	
C2	-0.01699 (9)	0.67577 (9)	0.14945 (8)	0.0180 (3)	
H2	-0.0670 (12)	0.6629 (3)	0.15497 (15)	0.022*	
C2S	0.7068 (2)	0.03713 (15)	0.57784 (17)	0.0628 (9)	
H2S1	0.7327	0.0205	0.5476	0.075*	
H2S2	0.7190	0.0887	0.5855	0.075*	
C3	-0.00544 (9)	0.70732 (9)	0.10008 (8)	0.0179 (3)	
H3	-0.0460 (10)	0.7212 (3)	0.0631 (9)	0.021*	
C3S	0.73779 (13)	-0.00210 (11)	0.63304 (10)	0.0312 (5)	
H3S1	0.7240	-0.0534	0.6253	0.037*	
H3S2	0.7120	0.0153	0.6632	0.037*	
C4	0.11570 (9)	0.73977 (9)	0.06988 (7)	0.0155 (3)	
C4S	0.82180 (18)	0.00420 (15)	0.65824 (14)	0.0503 (7)	
H4S1	0.8361	0.0551	0.6676	0.060*	
H4S2	0.8482	-0.0125	0.6283	0.060*	
C5	0.14662 (10)	0.68730 (10)	0.03981 (8)	0.0203 (3)	
C5S	0.84954 (19)	-0.03961 (18)	0.71481 (15)	0.0576 (8)	
H5S1	0.9071	-0.0349	0.7316	0.086*	
H5S2	0.8238	-0.0226	0.7445	0.086*	
H5S3	0.8359	-0.0901	0.7053	0.086*	
C6	0.18952 (13)	0.71102 (13)	0.00097 (9)	0.0314 (4)	
H6	0.2126 (7)	0.6774 (10)	-0.0189 (6)	0.038*	
C7	0.19811 (14)	0.78333 (14)	-0.00826 (10)	0.0355 (5)	
H7	0.2256 (10)	0.7973 (5)	-0.0322 (8)	0.043*	
C8	0.16350 (12)	0.83426 (12)	0.02019 (9)	0.0297 (4)	
H8	0.16866 (18)	0.8862 (14)	0.0117 (2)	0.036*	
C9	0.12180 (10)	0.81391 (9)	0.06027 (8)	0.0201 (3)	
C10	0.13280 (11)	0.60754 (10)	0.04638 (8)	0.0222 (3)	
H10	0.1002 (9)	0.60257 (16)	0.0728 (7)	0.027*	
C11	0.08751 (14)	0.57476 (13)	-0.01512 (10)	0.0352 (5)	

H11A	0.0373	0.6003	-0.0317	0.053*	
H11B	0.0769	0.5240	-0.0097	0.053*	
H11C	0.1195	0.5791	-0.0432	0.053*	
C12	0.20995 (13)	0.56688 (12)	0.07510 (10)	0.0318 (4)	
H12A	0.2443	0.5703	0.0487	0.048*	
H12B	0.1980	0.5164	0.0803	0.048*	
H12C	0.2369	0.5879	0.1147	0.048*	
C13	0.08462 (11)	0.86868 (9)	0.09230 (9)	0.0246 (4)	
H13	0.0336 (13)	0.8497 (5)	0.09308 (9)	0.030*	
C14	0.06939 (13)	0.94143 (11)	0.06004 (12)	0.0369 (5)	
H14A	0.1201	0.9641	0.0618	0.055*	
H14B	0.0398	0.9723	0.0801	0.055*	
H14C	0.0386	0.9344	0.0176	0.055*	
C15	0.13472 (16)	0.87976 (11)	0.15826 (10)	0.0379 (5)	
H15A	0.1450	0.8333	0.1789	0.057*	
H15B	0.1060	0.9107	0.1790	0.057*	
H15C	0.1851	0.9024	0.1591	0.057*	
C16	0.06864 (9)	0.63221 (8)	0.24935 (7)	0.0133 (3)	
C17	0.09725 (9)	0.56122 (8)	0.25844 (7)	0.0152 (3)	
C18	0.10466 (11)	0.53063 (9)	0.31505 (8)	0.0227 (3)	
H18	0.1239 (5)	0.4834 (13)	0.3228 (2)	0.027*	
C19	0.08432 (12)	0.56843 (11)	0.36017 (9)	0.0262 (4)	
H19	0.08966 (19)	0.5461 (6)	0.3987 (10)	0.031*	
C20	0.05643 (11)	0.63802 (10)	0.35003 (8)	0.0238 (4)	
H20	0.0429 (4)	0.6635 (7)	0.3814 (8)	0.029*	
C21	0.04789 (10)	0.67136 (9)	0.29413 (8)	0.0173 (3)	
C22	0.11769 (10)	0.51927 (9)	0.20849 (8)	0.0195 (3)	
H22	0.1482 (8)	0.5506 (8)	0.1903 (5)	0.023*	
C23	0.04306 (13)	0.49679 (11)	0.15836 (10)	0.0311 (4)	
H23A	0.0102	0.4661	0.1756	0.047*	
H23B	0.0584	0.4704	0.1269	0.047*	
H23C	0.0130	0.5396	0.1406	0.047*	
C24	0.16781 (12)	0.45239 (10)	0.23145 (10)	0.0290 (4)	
H24A	0.2145	0.4657	0.2647	0.043*	
H24B	0.1847	0.4313	0.1983	0.043*	
H24C	0.1363	0.4173	0.2460	0.043*	
C25	0.01647 (12)	0.74762 (9)	0.28411 (9)	0.0242 (4)	

H25	0.02022 (16)	0.7632 (5)	0.2495 (11)	0.029*	
C26	-0.06914 (15)	0.75013 (15)	0.28369 (14)	0.0477 (7)	
H26A	-0.1004	0.7175	0.2525	0.072*	
H26B	-0.0893	0.7991	0.2749	0.072*	
H26C	-0.0732	0.7354	0.3234	0.072*	
C27	0.0645 (2)	0.79786 (14)	0.33556 (17)	0.0620 (9)	
H27A	0.0589	0.7815	0.3745	0.093*	
H27B	0.0444	0.8470	0.3276	0.093*	
H27C	0.1205	0.7968	0.3370	0.093*	
C28	0.33304 (9)	0.64412 (9)	0.25993 (7)	0.0169 (3)	
C29	0.35302 (9)	0.68308 (9)	0.21279 (7)	0.0157 (3)	
C30	0.33498 (10)	0.75704 (9)	0.21825 (8)	0.0190 (3)	
C31	0.30446 (10)	0.76392 (10)	0.26894 (8)	0.0208 (3)	
C32	0.30282 (9)	0.69410 (10)	0.29449 (7)	0.0191 (3)	
C33	0.34872 (12)	0.56596 (10)	0.27354 (10)	0.0282 (4)	
H33A	0.4051	0.5589	0.2946	0.042*	
H33B	0.3343	0.5387	0.2356	0.042*	
H33C	0.3171	0.5492	0.2994	0.042*	
C34	0.39369 (11)	0.65385 (11)	0.16906 (9)	0.0254 (4)	
H34A	0.3683	0.6732	0.1285	0.038*	
H34B	0.3897	0.6014	0.1680	0.038*	
H34C	0.4496	0.6679	0.1821	0.038*	
C35	0.34958 (13)	0.81584 (11)	0.17808 (10)	0.0302 (4)	
H35A	0.3297	0.8614	0.1890	0.045*	
H35B	0.3220	0.8045	0.1357	0.045*	
H35C	0.4065	0.8199	0.1834	0.045*	
C36	0.28441 (14)	0.83263 (13)	0.29525 (11)	0.0365 (5)	
H36A	0.3265	0.8442	0.3324	0.055*	
H36B	0.2342	0.8269	0.3047	0.055*	
H36C	0.2796	0.8715	0.2658	0.055*	
C37	0.27644 (11)	0.67831 (13)	0.34946 (8)	0.0304 (4)	
H37A	0.2645	0.6271	0.3505	0.046*	
H37B	0.2289	0.7064	0.3477	0.046*	
H37C	0.3187	0.6912	0.3861	0.046*	
C38	0.49488 (10)	0.66273 (12)	0.40439 (8)	0.0261 (4)	
H38	0.4456 (13)	0.6447 (5)	0.40957 (16)	0.031*	
C39	0.50487 (10)	0.69167 (10)	0.35350 (8)	0.0223 (3)	

H39	0.4673 (11)	0.6981 (2)	0.3176 (10)	0.027*	
C40	0.62519 (9)	0.69307 (8)	0.42609 (7)	0.0117 (3)	
C41	0.62233 (9)	0.73791 (9)	0.32521 (7)	0.0146 (3)	
C42	0.65646 (10)	0.68945 (10)	0.29374 (8)	0.0213 (3)	
C43	0.69634 (12)	0.71867 (13)	0.25501 (9)	0.0301 (4)	
H43	0.7207 (7)	0.6872 (9)	0.2328 (6)	0.036*	
C44	0.70117 (12)	0.79188 (13)	0.24821 (9)	0.0307 (4)	
H44	0.7275 (9)	0.8095 (6)	0.2235 (8)	0.037*	
C45	0.66566 (11)	0.83858 (11)	0.27916 (8)	0.0252 (4)	
H45	0.66896 (14)	0.8913 (14)	0.27322 (17)	0.030*	
C46	0.62527 (10)	0.81246 (9)	0.31862 (7)	0.0175 (3)	
C47	0.65219 (13)	0.60880 (11)	0.30173 (9)	0.0282 (4)	
H47	0.6158 (11)	0.6001 (3)	0.3234 (6)	0.034*	
C48	0.62245 (16)	0.56946 (13)	0.24068 (12)	0.0433 (6)	
H48A	0.5707	0.5887	0.2178	0.065*	
H48B	0.6175	0.5181	0.2479	0.065*	
H48C	0.6602	0.5765	0.2174	0.065*	
C49	0.73207 (16)	0.57888 (14)	0.33883 (12)	0.0463 (6)	
H49A	0.7716	0.5878	0.3174	0.069*	
H49B	0.7274	0.5271	0.3444	0.069*	
H49C	0.7486	0.6025	0.3785	0.069*	
C50	0.58521 (12)	0.86282 (10)	0.35224 (9)	0.0246 (4)	
H50	0.58170 (15)	0.8388 (7)	0.3880 (10)	0.030*	
C51	0.50237 (17)	0.8799 (2)	0.31386 (18)	0.0745 (12)	
H51A	0.5046	0.9096	0.2794	0.112*	
H51B	0.4744	0.9059	0.3383	0.112*	
H51C	0.4742	0.8352	0.2989	0.112*	
C52	0.63054 (18)	0.93285 (13)	0.37156 (13)	0.0481 (6)	
H52A	0.6275	0.9620	0.3356	0.072*	
H52B	0.6861	0.9221	0.3927	0.072*	
H52C	0.6071	0.9593	0.3987	0.072*	
C53	0.58289 (9)	0.63767 (9)	0.50908 (7)	0.0171 (3)	
C54	0.61856 (10)	0.57007 (9)	0.52424 (8)	0.0202 (3)	
C55	0.63234 (14)	0.54738 (11)	0.58409 (9)	0.0318 (4)	
H55	0.6578 (8)	0.5021 (13)	0.5965 (4)	0.038*	
C56	0.60988 (16)	0.58921 (11)	0.62577 (9)	0.0385 (5)	
H56	0.6199 (3)	0.5719 (5)	0.6677 (13)	0.046*	

C57	0.57346 (13)	0.65514 (11)	0.60945 (9)	0.0289 (4)	
H57	0.5578 (5)	0.6827 (8)	0.6384 (8)	0.035*	
C58	0.55979 (10)	0.68105 (9)	0.55050 (8)	0.0200 (3)	
C62	0.51939 (12)	0.75337 (11)	0.53270 (9)	0.0259 (4)	
H62	0.52473 (19)	0.7663 (4)	0.4949 (11)	0.031*	
C63	0.43082 (13)	0.74750 (16)	0.52666 (12)	0.0427 (6)	
H63A	0.4067	0.7110	0.4964	0.064*	
H63B	0.4052	0.7939	0.5139	0.064*	
H63C	0.4240	0.7339	0.5658	0.064*	
C64	0.55715 (14)	0.81271 (12)	0.57851 (12)	0.0372 (5)	
H64A	0.5517	0.8004	0.6184	0.056*	
H64B	0.5304	0.8584	0.5649	0.056*	
H64C	0.6134	0.8171	0.5814	0.056*	
C65	0.84135 (10)	0.67803 (11)	0.53357 (9)	0.0254 (4)	
C66	0.86090 (9)	0.70413 (9)	0.48138 (7)	0.0161 (3)	
C67	0.83439 (9)	0.77694 (9)	0.47153 (7)	0.0166 (3)	
C68	0.79924 (10)	0.79590 (10)	0.51779 (8)	0.0225 (3)	
C69	0.80375 (10)	0.73467 (13)	0.55604 (8)	0.0269 (4)	
C70	0.86228 (15)	0.60542 (17)	0.56275 (15)	0.0568 (9)	
H70A	0.9109	0.6092	0.5966	0.085*	
H70B	0.8705	0.5714	0.5328	0.085*	
H70C	0.8190	0.5885	0.5778	0.085*	
C71	0.90703 (11)	0.66510 (11)	0.44588 (10)	0.0271 (4)	
H71A	0.9630	0.6784	0.4611	0.041*	
H71B	0.8866	0.6781	0.4030	0.041*	
H71C	0.9015	0.6133	0.4504	0.041*	
C72	0.84746 (13)	0.82535 (11)	0.42325 (10)	0.0310 (4)	
H72A	0.8157	0.8690	0.4207	0.047*	
H72B	0.8315	0.8005	0.3841	0.047*	
H72C	0.9036	0.8382	0.4334	0.047*	
C73	0.76925 (16)	0.86830 (14)	0.52740 (14)	0.0478 (6)	
H73A	0.8140	0.8993	0.5478	0.072*	
H73B	0.7334	0.8640	0.5526	0.072*	
H73C	0.7406	0.8893	0.4881	0.072*	
C74	0.77816 (14)	0.72947 (19)	0.61253 (10)	0.0492 (7)	
H74A	0.7427	0.6883	0.6093	0.074*	
H74B	0.7503	0.7735	0.6174	0.074*	

H74C	0.8248	0.7233	0.6477	0.074*	
N1	0.05734 (7)	0.66534 (7)	0.19086 (6)	0.0128 (2)	
N2	0.07570 (8)	0.71593 (7)	0.11264 (6)	0.0132 (2)	
N3	0.58423 (8)	0.70945 (7)	0.36744 (6)	0.0139 (2)	
N4	0.56836 (8)	0.66354 (8)	0.44799 (6)	0.0156 (3)	
Co1	0.23126 (2)	0.69181 (2)	0.20140 (2)	0.01746 (6)	
Co2	0.73787 (2)	0.70617 (2)	0.46470 (2)	0.02238 (6)	
C60A	0.56731 (19)	0.49420 (16)	0.43244 (14)	0.0290 (7)	0.666 (4)
H60A	0.5842	0.4631	0.4043	0.044*	0.666 (4)
H60B	0.5345	0.4667	0.4521	0.044*	0.666 (4)
H60C	0.5365	0.5344	0.4101	0.044*	0.666 (4)
C61A	0.6948 (2)	0.46357 (17)	0.50743 (17)	0.0354 (8)	0.666 (4)
H61A	0.7405	0.4842	0.5379	0.053*	0.666 (4)
H61B	0.6683	0.4289	0.5269	0.053*	0.666 (4)
H61C	0.7127	0.4393	0.4761	0.053*	0.666 (4)
C59A	0.6381 (6)	0.5220 (6)	0.4791 (4)	0.0259 (19)	0.666 (4)
H59A	0.6665	0.5528	0.4567	0.031*	0.666 (4)
C60B	0.6084 (4)	0.4405 (3)	0.4783 (3)	0.0323 (15)	0.334 (4)
H60D	0.5518	0.4424	0.4750	0.048*	0.334 (4)
H60E	0.6160	0.4118	0.4448	0.048*	0.334 (4)
H60F	0.6373	0.4184	0.5170	0.048*	0.334 (4)
C61B	0.7275 (3)	0.5141 (3)	0.4801 (3)	0.0314 (15)	0.334 (4)
H61D	0.7325	0.4848	0.4462	0.047*	0.334 (4)
H61E	0.7524	0.5609	0.4792	0.047*	0.334 (4)
H61F	0.7537	0.4899	0.5184	0.047*	0.334 (4)
C59B	0.6427 (10)	0.5244 (9)	0.4748 (7)	0.014 (3)*	0.334 (4)
H59B	0.6156	0.5449	0.4339	0.017*	0.334 (4)

Table 3. Atomic displacement parameters (Å^2) for **2**.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0107 (6)	0.0106 (6)	0.0122 (6)	0.0008 (5)	0.0018 (5)	0.0006 (5)
C1S	0.090 (3)	0.067 (2)	0.125 (4)	-0.002 (2)	0.047 (3)	-0.019 (2)
C2	0.0108 (7)	0.0213 (8)	0.0203 (8)	0.0011 (5)	0.0022 (6)	0.0058 (6)
C2S	0.084 (2)	0.0340 (13)	0.091 (2)	-0.0082 (14)	0.059 (2)	-0.0163 (14)
C3	0.0103 (6)	0.0217 (8)	0.0188 (7)	0.0008 (5)	0.0000 (6)	0.0051 (6)
C3S	0.0431 (11)	0.0220 (9)	0.0410 (12)	-0.0100 (8)	0.0319 (10)	-0.0096 (8)
C4	0.0124 (6)	0.0202 (7)	0.0123 (6)	-0.0002 (5)	0.0009 (5)	0.0051 (5)
C4S	0.0605 (17)	0.0393 (13)	0.0666 (18)	-0.0164 (12)	0.0429 (15)	-0.0159 (12)
C5	0.0186 (7)	0.0271 (8)	0.0145 (7)	0.0000 (6)	0.0037 (6)	0.0002 (6)
C5S	0.0597 (18)	0.0629 (18)	0.0607 (18)	-0.0112 (15)	0.0342 (15)	-0.0135 (15)
C6	0.0296 (10)	0.0471 (12)	0.0210 (9)	-0.0023 (9)	0.0130 (8)	-0.0013 (8)
C7	0.0341 (11)	0.0524 (13)	0.0243 (10)	-0.0106 (10)	0.0152 (8)	0.0063 (9)
C8	0.0275 (9)	0.0336 (10)	0.0270 (9)	-0.0085 (8)	0.0061 (8)	0.0121 (8)
C9	0.0158 (7)	0.0217 (8)	0.0199 (8)	-0.0021 (6)	0.0007 (6)	0.0082 (6)
C10	0.0217 (8)	0.0252 (8)	0.0184 (8)	0.0018 (6)	0.0037 (6)	-0.0053 (6)
C11	0.0336 (11)	0.0376 (11)	0.0281 (10)	0.0014 (9)	-0.0008 (8)	-0.0123 (9)
C12	0.0289 (10)	0.0326 (10)	0.0298 (10)	0.0086 (8)	0.0023 (8)	-0.0035 (8)
C13	0.0215 (8)	0.0157 (7)	0.0348 (10)	0.0003 (6)	0.0052 (7)	0.0071 (7)
C14	0.0288 (10)	0.0192 (9)	0.0562 (14)	-0.0002 (7)	0.0025 (9)	0.0148 (9)
C15	0.0537 (14)	0.0213 (9)	0.0343 (11)	0.0074 (9)	0.0062 (10)	-0.0021 (8)
C16	0.0127 (6)	0.0127 (6)	0.0144 (7)	0.0002 (5)	0.0038 (5)	0.0033 (5)
C17	0.0144 (7)	0.0114 (6)	0.0192 (7)	0.0007 (5)	0.0042 (6)	0.0015 (5)
C18	0.0255 (8)	0.0160 (7)	0.0262 (9)	0.0046 (6)	0.0071 (7)	0.0085 (6)
C19	0.0305 (9)	0.0289 (9)	0.0209 (8)	0.0039 (7)	0.0099 (7)	0.0104 (7)
C20	0.0282 (9)	0.0273 (9)	0.0194 (8)	0.0035 (7)	0.0122 (7)	0.0023 (7)
C21	0.0194 (7)	0.0154 (7)	0.0192 (7)	0.0021 (6)	0.0092 (6)	0.0016 (6)
C22	0.0209 (8)	0.0131 (7)	0.0244 (8)	0.0007 (6)	0.0067 (6)	-0.0034 (6)
C23	0.0305 (10)	0.0247 (9)	0.0323 (10)	-0.0001 (7)	0.0004 (8)	-0.0101 (8)
C24	0.0251 (9)	0.0159 (8)	0.0435 (11)	0.0054 (7)	0.0063 (8)	-0.0044 (7)
C25	0.0320 (9)	0.0164 (7)	0.0283 (9)	0.0079 (7)	0.0152 (8)	0.0016 (7)
C26	0.0406 (13)	0.0444 (14)	0.0642 (17)	0.0235 (11)	0.0247 (12)	0.0190 (12)
C27	0.0580 (18)	0.0300 (13)	0.086 (2)	0.0071 (12)	0.0028 (17)	-0.0157 (13)
C28	0.0110 (6)	0.0212 (7)	0.0163 (7)	-0.0011 (5)	0.0006 (5)	0.0032 (6)
C29	0.0108 (6)	0.0198 (7)	0.0155 (7)	-0.0006 (5)	0.0022 (5)	0.0004 (6)

C30	0.0160 (7)	0.0195 (7)	0.0200 (8)	-0.0024 (6)	0.0030 (6)	0.0001 (6)
C31	0.0162 (7)	0.0244 (8)	0.0191 (8)	0.0002 (6)	0.0011 (6)	-0.0056 (6)
C32	0.0114 (7)	0.0312 (9)	0.0129 (7)	-0.0008 (6)	0.0008 (5)	0.0002 (6)
C33	0.0266 (9)	0.0233 (9)	0.0310 (10)	0.0008 (7)	0.0029 (8)	0.0094 (7)
C34	0.0217 (8)	0.0313 (9)	0.0263 (9)	0.0010 (7)	0.0122 (7)	-0.0017 (7)
C35	0.0328 (10)	0.0241 (9)	0.0339 (11)	-0.0043 (8)	0.0103 (8)	0.0068 (8)
C36	0.0366 (11)	0.0353 (11)	0.0351 (11)	0.0055 (9)	0.0069 (9)	-0.0154 (9)
C37	0.0196 (8)	0.0566 (13)	0.0145 (8)	-0.0006 (8)	0.0043 (6)	0.0022 (8)
C38	0.0116 (7)	0.0420 (11)	0.0216 (8)	-0.0071 (7)	0.0002 (6)	0.0101 (8)
C39	0.0113 (7)	0.0335 (9)	0.0180 (8)	-0.0053 (6)	-0.0022 (6)	0.0064 (7)
C40	0.0107 (6)	0.0119 (6)	0.0120 (6)	-0.0008 (5)	0.0028 (5)	0.0001 (5)
C41	0.0123 (6)	0.0196 (7)	0.0112 (6)	-0.0017 (5)	0.0022 (5)	0.0023 (5)
C42	0.0187 (8)	0.0280 (9)	0.0168 (7)	0.0025 (6)	0.0049 (6)	-0.0018 (6)
C43	0.0253 (9)	0.0473 (12)	0.0212 (9)	0.0010 (8)	0.0122 (7)	-0.0035 (8)
C44	0.0270 (9)	0.0506 (13)	0.0173 (8)	-0.0083 (9)	0.0109 (7)	0.0043 (8)
C45	0.0260 (9)	0.0308 (9)	0.0182 (8)	-0.0086 (7)	0.0054 (7)	0.0063 (7)
C46	0.0169 (7)	0.0206 (7)	0.0140 (7)	-0.0034 (6)	0.0030 (6)	0.0020 (6)
C47	0.0303 (10)	0.0238 (9)	0.0298 (10)	0.0071 (7)	0.0076 (8)	-0.0051 (7)
C48	0.0419 (13)	0.0364 (12)	0.0416 (13)	0.0028 (10)	-0.0036 (10)	-0.0126 (10)
C49	0.0472 (14)	0.0394 (13)	0.0417 (13)	0.0191 (11)	-0.0035 (11)	-0.0100 (10)
C50	0.0307 (9)	0.0167 (8)	0.0278 (9)	-0.0022 (7)	0.0105 (7)	-0.0004 (7)
C51	0.0358 (14)	0.078 (2)	0.091 (3)	0.0257 (15)	-0.0095 (15)	-0.044 (2)
C52	0.0622 (17)	0.0324 (12)	0.0530 (15)	-0.0177 (11)	0.0219 (13)	-0.0143 (11)
C53	0.0140 (7)	0.0208 (7)	0.0152 (7)	-0.0060 (6)	0.0024 (5)	0.0043 (6)
C54	0.0199 (8)	0.0193 (7)	0.0190 (8)	-0.0053 (6)	0.0019 (6)	0.0038 (6)
C55	0.0491 (13)	0.0187 (8)	0.0222 (9)	-0.0050 (8)	0.0018 (8)	0.0065 (7)
C56	0.0696 (16)	0.0254 (10)	0.0161 (9)	-0.0104 (10)	0.0059 (9)	0.0046 (7)
C57	0.0437 (12)	0.0257 (9)	0.0166 (8)	-0.0089 (8)	0.0079 (8)	-0.0004 (7)
C58	0.0196 (8)	0.0216 (8)	0.0183 (8)	-0.0066 (6)	0.0047 (6)	0.0019 (6)
C62	0.0252 (9)	0.0297 (9)	0.0245 (9)	0.0046 (7)	0.0102 (7)	0.0033 (7)
C63	0.0245 (10)	0.0619 (16)	0.0407 (13)	0.0047 (10)	0.0080 (9)	-0.0119 (11)
C64	0.0345 (11)	0.0253 (10)	0.0512 (14)	0.0006 (8)	0.0116 (10)	-0.0044 (9)
C65	0.0121 (7)	0.0377 (10)	0.0251 (9)	-0.0018 (7)	0.0034 (6)	0.0157 (8)
C66	0.0112 (6)	0.0189 (7)	0.0163 (7)	-0.0021 (5)	0.0010 (5)	0.0024 (6)
C67	0.0143 (7)	0.0185 (7)	0.0159 (7)	-0.0035 (5)	0.0029 (5)	0.0007 (6)
C68	0.0161 (7)	0.0307 (9)	0.0200 (8)	-0.0046 (6)	0.0045 (6)	-0.0078 (7)
C69	0.0136 (7)	0.0545 (12)	0.0119 (7)	-0.0047 (7)	0.0023 (6)	0.0031 (7)

C70	0.0343 (12)	0.0649 (18)	0.076 (2)	0.0137 (12)	0.0239 (13)	0.0537 (16)
C71	0.0210 (8)	0.0264 (9)	0.0352 (10)	0.0021 (7)	0.0100 (8)	-0.0018 (8)
C72	0.0327 (10)	0.0284 (9)	0.0367 (11)	0.0032 (8)	0.0174 (9)	0.0137 (8)
C73	0.0473 (14)	0.0416 (13)	0.0610 (17)	0.0021 (11)	0.0260 (13)	-0.0229 (12)
C74	0.0251 (10)	0.106 (2)	0.0174 (9)	-0.0021 (12)	0.0079 (8)	0.0075 (12)
N1	0.0108 (5)	0.0135 (6)	0.0135 (6)	0.0012 (4)	0.0029 (4)	0.0024 (4)
N2	0.0106 (5)	0.0146 (6)	0.0128 (6)	0.0001 (4)	0.0010 (4)	0.0027 (5)
N3	0.0104 (5)	0.0177 (6)	0.0121 (6)	-0.0017 (4)	0.0009 (4)	0.0018 (5)
N4	0.0103 (5)	0.0206 (6)	0.0149 (6)	-0.0030 (5)	0.0020 (5)	0.0041 (5)
Co1	0.00895 (9)	0.02817 (12)	0.01336 (10)	0.00000 (8)	0.00028 (7)	-0.00070 (8)
Co2	0.00976 (10)	0.03224 (14)	0.02195 (12)	-0.00529 (9)	-0.00034 (8)	-0.00220 (10)
C60A	0.0324 (15)	0.0258 (14)	0.0269 (15)	0.0008 (11)	0.0057 (12)	-0.0073 (11)
C61A	0.0302 (16)	0.0221 (14)	0.048 (2)	0.0061 (11)	0.0023 (14)	-0.0031 (13)
C59A	0.022 (2)	0.027 (2)	0.033 (3)	0.0012 (13)	0.0157 (18)	0.0118 (16)
C60B	0.042 (4)	0.024 (3)	0.039 (3)	-0.014 (2)	0.024 (3)	-0.008 (2)
C61B	0.022 (3)	0.023 (3)	0.054 (4)	0.000 (2)	0.019 (3)	-0.007 (3)

Table 4. Geometric parameters (Å, º) for **2**.

C1—N1	1.3677 (19)	C38—C39	1.350 (3)
C1—N2	1.3734 (19)	C38—N4	1.390 (2)
C1—Co1	1.9458 (15)	C39—N3	1.384 (2)
C1S—C2S	1.502 (6)	C40—N4	1.3650 (19)
C2—C3	1.350 (2)	C40—N3	1.3691 (19)
C2—N1	1.393 (2)	C40—Co2	1.9432 (15)
C2S—C3S	1.431 (4)	C41—C42	1.401 (2)
C3—N2	1.386 (2)	C41—C46	1.401 (2)
C3S—C4S	1.431 (4)	C41—N3	1.438 (2)
C4—C5	1.400 (2)	C42—C43	1.400 (3)
C4—C9	1.409 (2)	C42—C47	1.520 (3)
C4—N2	1.442 (2)	C43—C44	1.380 (3)
C4S—C5S	1.496 (5)	C44—C45	1.387 (3)
C5—C6	1.404 (3)	C45—C46	1.398 (2)
C5—C10	1.522 (3)	C46—C50	1.519 (3)
C6—C7	1.380 (3)	C47—C49	1.526 (3)
C7—C8	1.393 (3)	C47—C48	1.538 (3)
C8—C9	1.393 (3)	C50—C51	1.506 (3)
C9—C13	1.518 (3)	C50—C52	1.528 (3)
C10—C12	1.530 (3)	C53—C58	1.401 (3)
C10—C11	1.537 (3)	C53—C54	1.407 (2)
C13—C14	1.533 (3)	C53—N4	1.440 (2)
C13—C15	1.534 (3)	C54—C55	1.396 (3)
C16—C21	1.399 (2)	C54—C59A	1.489 (10)
C16—C17	1.410 (2)	C54—C59B	1.579 (17)
C16—N1	1.4440 (19)	C55—C56	1.384 (3)
C17—C18	1.396 (2)	C56—C57	1.388 (3)
C17—C22	1.521 (2)	C57—C58	1.396 (2)
C18—C19	1.389 (3)	C58—C62	1.525 (3)
C19—C20	1.384 (3)	C62—C63	1.533 (3)
C20—C21	1.400 (2)	C62—C64	1.541 (3)
C21—C25	1.519 (2)	C65—C69	1.424 (3)
C22—C24	1.531 (2)	C65—C66	1.432 (2)
C22—C23	1.536 (3)	C65—C70	1.509 (3)
C25—C26	1.510 (3)	C65—Co2	2.1072 (18)
C25—C27	1.555 (4)	C66—C67	1.432 (2)

C28—C32	1.428 (2)	C66—C71	1.502 (3)
C28—C29	1.435 (2)	C66—Co2	2.0933 (16)
C28—C33	1.500 (2)	C67—C68	1.428 (2)
C28—Co1	2.1034 (16)	C67—C72	1.503 (2)
C29—C30	1.429 (2)	C67—Co2	2.1250 (16)
C29—C34	1.502 (2)	C68—C69	1.431 (3)
C29—Co1	2.0953 (16)	C68—C73	1.490 (3)
C30—C31	1.430 (2)	C68—Co2	2.1674 (18)
C30—C35	1.506 (3)	C69—C74	1.503 (3)
C30—Co1	2.1378 (17)	C69—Co2	2.1544 (18)
C31—C32	1.433 (3)	C60A—C59A	1.484 (10)
C31—C36	1.504 (3)	C61A—C59A	1.495 (11)
C31—Co1	2.1744 (17)	C60B—C59B	1.689 (17)
C32—C37	1.503 (2)	C61B—C59B	1.479 (19)
C32—Co1	2.1503 (16)		
N1—C1—N2	102.90 (12)	C46—C50—C52	113.24 (18)
N1—C1—Co1	133.22 (11)	C58—C53—C54	123.12 (15)
N2—C1—Co1	123.85 (11)	C58—C53—N4	118.05 (15)
C3—C2—N1	107.14 (14)	C54—C53—N4	118.83 (15)
C3S—C2S—C1S	111.5 (3)	C55—C54—C53	116.96 (17)
C2—C3—N2	106.07 (14)	C55—C54—C59A	120.1 (4)
C2S—C3S—C4S	113.6 (2)	C53—C54—C59A	122.9 (4)
C5—C4—C9	123.28 (16)	C55—C54—C59B	123.1 (7)
C5—C4—N2	117.66 (14)	C53—C54—C59B	120.0 (7)
C9—C4—N2	119.06 (15)	C56—C55—C54	120.96 (19)
C3S—C4S—C5S	110.2 (2)	C55—C56—C57	121.01 (18)
C4—C5—C6	117.27 (18)	C56—C57—C58	120.35 (19)
C4—C5—C10	122.45 (15)	C57—C58—C53	117.57 (17)
C6—C5—C10	120.25 (17)	C57—C58—C62	120.15 (17)
C7—C6—C5	120.7 (2)	C53—C58—C62	122.26 (15)
C6—C7—C8	120.66 (19)	C58—C62—C63	110.24 (18)
C7—C8—C9	121.14 (19)	C58—C62—C64	112.08 (17)
C8—C9—C4	116.83 (18)	C63—C62—C64	109.80 (18)
C8—C9—C13	121.88 (17)	C69—C65—C66	107.89 (16)
C4—C9—C13	121.29 (15)	C69—C65—C70	125.6 (2)
C5—C10—C12	112.27 (16)	C66—C65—C70	126.3 (2)

C5—C10—C11	110.61 (16)	C69—C65—Co2	72.29 (10)
C12—C10—C11	111.07 (16)	C66—C65—Co2	69.55 (9)
C9—C13—C14	113.47 (18)	C70—C65—Co2	127.22 (17)
C9—C13—C15	111.57 (16)	C65—C66—C67	107.91 (15)
C14—C13—C15	109.32 (17)	C65—C66—C71	126.66 (16)
C21—C16—C17	122.68 (14)	C67—C66—C71	125.24 (15)
C21—C16—N1	118.21 (13)	C65—C66—Co2	70.59 (9)
C17—C16—N1	119.07 (14)	C67—C66—Co2	71.35 (9)
C18—C17—C16	116.99 (15)	C71—C66—Co2	127.47 (12)
C18—C17—C22	121.38 (14)	C68—C67—C66	108.03 (15)
C16—C17—C22	121.62 (14)	C68—C67—C72	126.88 (17)
C19—C18—C17	121.35 (16)	C66—C67—C72	124.95 (16)
C20—C19—C18	120.43 (17)	C68—C67—Co2	72.19 (10)
C19—C20—C21	120.63 (17)	C66—C67—Co2	68.96 (9)
C16—C21—C20	117.91 (15)	C72—C67—Co2	127.73 (13)
C16—C21—C25	122.62 (15)	C67—C68—C69	107.80 (16)
C20—C21—C25	119.47 (15)	C67—C68—C73	125.94 (19)
C17—C22—C24	113.47 (15)	C69—C68—C73	126.10 (19)
C17—C22—C23	111.68 (15)	C67—C68—Co2	68.97 (9)
C24—C22—C23	108.66 (15)	C69—C68—Co2	70.17 (11)
C26—C25—C21	110.52 (17)	C73—C68—Co2	130.00 (15)
C26—C25—C27	107.9 (2)	C65—C69—C68	108.36 (15)
C21—C25—C27	110.77 (18)	C65—C69—C74	124.0 (2)
C32—C28—C29	107.94 (15)	C68—C69—C74	127.6 (2)
C32—C28—C33	126.42 (16)	C65—C69—Co2	68.70 (11)
C29—C28—C33	125.40 (16)	C68—C69—Co2	71.16 (10)
C32—C28—Co1	72.17 (9)	C74—C69—Co2	128.26 (14)
C29—C28—Co1	69.70 (9)	C1—N1—C2	111.52 (13)
C33—C28—Co1	128.03 (12)	C1—N1—C16	125.42 (13)
C30—C29—C28	108.12 (14)	C2—N1—C16	123.06 (13)
C30—C29—C34	124.90 (15)	C1—N2—C3	112.36 (13)
C28—C29—C34	126.69 (16)	C1—N2—C4	121.94 (13)
C30—C29—Co1	71.88 (9)	C3—N2—C4	125.22 (13)
C28—C29—Co1	70.32 (9)	C40—N3—C39	112.49 (13)
C34—C29—Co1	128.26 (12)	C40—N3—C41	122.37 (13)
C29—C30—C31	107.80 (15)	C39—N3—C41	125.04 (13)
C29—C30—C35	124.44 (16)	C40—N4—C38	111.62 (13)

C31—C30—C35	127.72 (17)	C40—N4—C53	123.92 (13)
C29—C30—Co1	68.67 (9)	C38—N4—C53	124.45 (14)
C31—C30—Co1	72.02 (10)	C1—Co1—C29	164.48 (6)
C35—C30—Co1	126.47 (13)	C1—Co1—C28	147.14 (6)
C30—C31—C32	108.24 (15)	C29—Co1—C28	39.98 (6)
C30—C31—C36	126.61 (18)	C1—Co1—C30	144.96 (6)
C32—C31—C36	124.92 (18)	C29—Co1—C30	39.45 (6)
C30—C31—Co1	69.25 (9)	C28—Co1—C30	66.30 (6)
C32—C31—Co1	69.74 (9)	C1—Co1—C32	128.73 (6)
C36—C31—Co1	130.95 (13)	C29—Co1—C32	66.09 (6)
C28—C32—C31	107.89 (15)	C28—Co1—C32	39.21 (7)
C28—C32—C37	127.05 (17)	C30—Co1—C32	65.50 (7)
C31—C32—C37	125.02 (17)	C1—Co1—C31	128.13 (6)
C28—C32—Co1	68.63 (9)	C29—Co1—C31	65.49 (6)
C31—C32—Co1	71.56 (9)	C28—Co1—C31	65.43 (7)
C37—C32—Co1	127.05 (12)	C30—Co1—C31	38.72 (7)
C39—C38—N4	107.03 (15)	C32—Co1—C31	38.70 (7)
C38—C39—N3	105.97 (15)	C40—Co2—C66	161.94 (7)
N4—C40—N3	102.88 (12)	C40—Co2—C65	149.34 (7)
N4—C40—Co2	130.27 (11)	C66—Co2—C65	39.86 (6)
N3—C40—Co2	126.80 (11)	C40—Co2—C67	143.49 (6)
C42—C41—C46	123.24 (15)	C66—Co2—C67	39.69 (6)
C42—C41—N3	118.10 (15)	C65—Co2—C67	66.35 (7)
C46—C41—N3	118.64 (14)	C40—Co2—C69	131.82 (7)
C43—C42—C41	116.94 (18)	C66—Co2—C69	65.82 (7)
C43—C42—C47	120.98 (17)	C65—Co2—C69	39.01 (8)
C41—C42—C47	122.07 (16)	C67—Co2—C69	65.33 (7)
C44—C43—C42	121.14 (19)	C40—Co2—C68	129.18 (7)
C43—C44—C45	120.67 (18)	C66—Co2—C68	65.78 (7)
C44—C45—C46	120.69 (18)	C65—Co2—C68	65.56 (8)
C45—C46—C41	117.29 (16)	C67—Co2—C68	38.84 (7)
C45—C46—C50	121.34 (16)	C69—Co2—C68	38.67 (8)
C41—C46—C50	121.36 (15)	C60A—C59A—C54	113.6 (7)
C42—C47—C49	111.06 (19)	C60A—C59A—C61A	112.1 (7)
C42—C47—C48	112.13 (18)	C54—C59A—C61A	113.3 (6)
C49—C47—C48	110.55 (18)	C61B—C59B—C54	119.4 (10)
C51—C50—C46	110.37 (18)	C61B—C59B—C60B	104.2 (11)

C51—C50—C52	109.1 (2)	C54—C59B—C60B	106.8 (10)
N1—C2—C3—N2	-0.43 (19)	C58—C53—C54—C59A	175.8 (4)
C1S—C2S—C3S—C4S	178.9 (3)	N4—C53—C54—C59A	-3.5 (5)
C2S—C3S—C4S—C5S	-178.7 (2)	C58—C53—C54—C59B	179.9 (7)
C9—C4—C5—C6	3.8 (3)	N4—C53—C54—C59B	0.6 (7)
N2—C4—C5—C6	-176.32 (15)	C53—C54—C55—C56	1.5 (3)
C9—C4—C5—C10	-174.15 (16)	C59A—C54—C55—C56	-175.7 (5)
N2—C4—C5—C10	5.8 (2)	C59B—C54—C55—C56	-179.8 (7)
C4—C5—C6—C7	-2.1 (3)	C54—C55—C56—C57	-0.4 (4)
C10—C5—C6—C7	175.87 (19)	C55—C56—C57—C58	-0.9 (3)
C5—C6—C7—C8	-0.8 (3)	C56—C57—C58—C53	1.0 (3)
C6—C7—C8—C9	2.3 (3)	C56—C57—C58—C62	179.7 (2)
C7—C8—C9—C4	-0.7 (3)	C54—C53—C58—C57	0.2 (3)
C7—C8—C9—C13	179.18 (19)	N4—C53—C58—C57	179.40 (15)
C5—C4—C9—C8	-2.4 (2)	C54—C53—C58—C62	-178.48 (16)
N2—C4—C9—C8	177.71 (15)	N4—C53—C58—C62	0.8 (2)
C5—C4—C9—C13	177.72 (16)	C57—C58—C62—C63	-73.6 (2)
N2—C4—C9—C13	-2.2 (2)	C53—C58—C62—C63	105.0 (2)
C4—C5—C10—C12	-117.09 (19)	C57—C58—C62—C64	49.0 (2)
C6—C5—C10—C12	65.1 (2)	C53—C58—C62—C64	-132.37 (19)
C4—C5—C10—C11	118.23 (19)	C69—C65—C66—C67	-0.56 (19)
C6—C5—C10—C11	-59.6 (2)	C70—C65—C66—C67	-176.2 (2)
C8—C9—C13—C14	22.0 (2)	Co2—C65—C66—C67	61.95 (11)

C4—C9—C13—C14	-158.08 (17)	C69—C65—C66—C71	174.69 (16)
C8—C9—C13—C15	-102.0 (2)	C70—C65—C66—C71	-1.0 (3)
C4—C9—C13—C15	77.9 (2)	Co2—C65—C66—C71	-122.80 (17)
C21—C16—C17—C18	-0.2 (2)	C69—C65—C66—Co2	-62.51 (12)
N1—C16—C17—C18	-177.88 (15)	C70—C65—C66—Co2	121.8 (2)
C21—C16—C17—C22	178.64 (15)	C65—C66—C67—C68	0.50 (18)
N1—C16—C17—C22	1.0 (2)	C71—C66—C67—C68	-174.83 (16)
C16—C17—C18—C19	0.3 (3)	Co2—C66—C67—C68	61.97 (11)
C22—C17—C18—C19	-178.55 (17)	C65—C66—C67—C72	176.45 (17)
C17—C18—C19—C20	-0.4 (3)	C71—C66—C67—C72	1.1 (3)
C18—C19—C20—C21	0.3 (3)	Co2—C66—C67—C72	-122.08 (18)
C17—C16—C21—C20	0.2 (2)	C65—C66—C67—Co2	-61.47 (11)
N1—C16—C21—C20	177.84 (15)	C71—C66—C67—Co2	123.20 (17)
C17—C16—C21—C25	-179.51 (16)	C66—C67—C68—C69	-0.26 (19)
N1—C16—C21—C25	-1.8 (2)	C72—C67—C68—C69	-176.10 (17)
C19—C20—C21—C16	-0.2 (3)	Co2—C67—C68—C69	59.67 (12)
C19—C20—C21—C25	179.50 (18)	C66—C67—C68—C73	175.20 (19)
C18—C17—C22—C24	-16.7 (2)	C72—C67—C68—C73	-0.6 (3)
C16—C17—C22—C24	164.47 (15)	Co2—C67—C68—C73	-124.9 (2)
C18—C17—C22—C23	106.52 (19)	C66—C67—C68—Co2	-59.92 (11)
C16—C17—C22—C23	-72.3 (2)	C72—C67—C68—Co2	124.23 (18)
C16—C21—C25—C26	112.4 (2)	C66—C65—C69—C68	0.4 (2)

C20—C21—C25—C26	-67.2 (2)	C70—C65—C69—C68	176.1 (2)
C16—C21—C25—C27	-128.0 (2)	Co2—C65—C69—C68	-60.35 (12)
C20—C21—C25—C27	52.3 (3)	C66—C65—C69—C74	-176.65 (18)
C32—C28—C29—C30	-0.10 (18)	C70—C65—C69—C74	-0.9 (3)
C33—C28—C29—C30	-174.79 (16)	Co2—C65—C69—C74	122.59 (19)
Co1—C28—C29—C30	62.31 (11)	C66—C65—C69—Co2	60.75 (12)
C32—C28—C29—C34	173.97 (16)	C70—C65—C69—Co2	-123.5 (2)
C33—C28—C29—C34	-0.7 (3)	C67—C68—C69—C65	-0.1 (2)
Co1—C28—C29—C34	-123.61 (17)	C73—C68—C69—C65	-175.5 (2)
C32—C28—C29—Co1	-62.42 (11)	Co2—C68—C69—C65	58.82 (13)
C33—C28—C29—Co1	122.89 (17)	C67—C68—C69—C74	176.83 (18)
C28—C29—C30—C31	0.43 (18)	C73—C68—C69—C74	1.4 (3)
C34—C29—C30—C31	-173.78 (16)	Co2—C68—C69—C74	-124.3 (2)
Co1—C29—C30—C31	61.75 (12)	C67—C68—C69—Co2	-58.91 (12)
C28—C29—C30—C35	178.29 (16)	C73—C68—C69—Co2	125.6 (2)
C34—C29—C30—C35	4.1 (3)	N2—C1—N1—C2	-0.57 (17)
Co1—C29—C30—C35	-120.40 (17)	Co1—C1—N1—C2	-178.77 (12)
C28—C29—C30—Co1	-61.32 (11)	N2—C1—N1—C16	179.67 (14)
C34—C29—C30—Co1	124.48 (16)	Co1—C1—N1—C16	1.5 (2)
C29—C30—C31—C32	-0.60 (19)	C3—C2—N1—C1	0.65 (19)
C35—C30—C31—C32	-178.36 (17)	C3—C2—N1—C16	-179.58 (14)
Co1—C30—C31—C32	59.02 (12)	C21—C16—N1—C1	107.24 (18)

C29—C30—C31—C36	174.11 (17)	C17—C16—N1—C1	-75.0 (2)
C35—C30—C31—C36	-3.6 (3)	C21—C16—N1—C2	-72.5 (2)
Co1—C30—C31—C36	-126.27 (19)	C17—C16—N1—C2	105.25 (18)
C29—C30—C31—Co1	-59.61 (11)	N1—C1—N2—C3	0.29 (17)
C35—C30—C31—Co1	122.62 (19)	Co1—C1—N2—C3	178.72 (11)
C29—C28—C32—C31	-0.26 (18)	N1—C1—N2—C4	-172.20 (13)
C33—C28—C32—C31	174.36 (16)	Co1—C1—N2—C4	6.2 (2)
Co1—C28—C32—C31	-61.10 (11)	C2—C3—N2—C1	0.09 (19)
C29—C28—C32—C37	-178.15 (16)	C2—C3—N2—C4	172.29 (15)
C33—C28—C32—C37	-3.5 (3)	C5—C4—N2—C1	75.36 (19)
Co1—C28—C32—C37	121.01 (17)	C9—C4—N2—C1	-104.71 (17)
C29—C28—C32—Co1	60.84 (11)	C5—C4—N2—C3	-96.14 (19)
C33—C28—C32—Co1	-124.54 (17)	C9—C4—N2—C3	83.8 (2)
C30—C31—C32—C28	0.53 (18)	N4—C40—N3—C39	0.69 (18)
C36—C31—C32—C28	-174.29 (17)	Co2—C40—N3—C39	178.25 (13)
Co1—C31—C32—C28	59.25 (11)	N4—C40—N3—C41	-175.79 (14)
C30—C31—C32—C37	178.47 (16)	Co2—C40—N3—C41	1.8 (2)
C36—C31—C32—C37	3.7 (3)	C38—C39—N3—C40	-0.4 (2)
Co1—C31—C32—C37	-122.81 (17)	C38—C39—N3—C41	175.97 (17)
C30—C31—C32—Co1	-58.72 (12)	C42—C41—N3—C40	84.85 (19)
C36—C31—C32—Co1	126.46 (18)	C46—C41—N3—C40	-93.59 (18)
N4—C38—C39—N3	-0.1 (2)	C42—C41—N3—C39	-91.2 (2)
C46—C41—C42—	1.2 (3)	C46—C41—N3—C39	90.4 (2)

C43			
N3—C41—C42—C43	-177.13 (15)	N3—C40—N4—C38	-0.73 (19)
C46—C41—C42—C47	-179.88 (16)	Co2—C40—N4—C38	-178.17 (14)
N3—C41—C42—C47	1.8 (2)	N3—C40—N4—C53	-179.74 (15)
C41—C42—C43—C44	-0.3 (3)	Co2—C40—N4—C53	2.8 (2)
C47—C42—C43—C44	-179.20 (19)	C39—C38—N4—C40	0.5 (2)
C42—C43—C44—C45	-0.8 (3)	C39—C38—N4—C53	179.52 (17)
C43—C44—C45—C46	1.0 (3)	C58—C53—N4—C40	101.81 (19)
C44—C45—C46—C41	-0.1 (3)	C54—C53—N4—C40	-78.9 (2)
C44—C45—C46—C50	-179.23 (17)	C58—C53—N4—C38	-77.1 (2)
C42—C41—C46—C45	-1.0 (2)	C54—C53—N4—C38	102.2 (2)
N3—C41—C46—C45	177.32 (14)	C55—C54—C59A—C60A	110.4 (6)
C42—C41—C46—C50	178.10 (16)	C53—C54—C59A—C60A	-66.7 (7)
N3—C41—C46—C50	-3.6 (2)	C59B—C54—C59A—C60A	-117 (14)
C43—C42—C47—C49	72.5 (2)	C55—C54—C59A—C61A	-18.9 (8)
C41—C42—C47—C49	-106.3 (2)	C53—C54—C59A—C61A	164.0 (4)
C43—C42—C47—C48	-51.7 (3)	C59B—C54—C59A—C61A	113 (14)
C41—C42—C47—C48	129.5 (2)	C55—C54—C59B—C61B	-68.5 (13)
C45—C46—C50—C51	86.8 (3)	C53—C54—C59B—C61B	110.2 (12)
C41—C46—C50—C51	-92.3 (3)	C59A—C54—C59B—C61B	-119 (14)
C45—C46—C50—C52	-35.8 (3)	C55—C54—C59B—C60B	49.2 (12)
C41—C46—C50—C52	145.12 (19)	C53—C54—C59B—C60B	-132.2 (7)
C58—C53—C54—C55	-1.4 (3)	C59A—C54—C59B—C60B	-1 (13)
N4—C53—C54—C55	179.34 (16)		

Data Collection Details for 3.

Computing details

Cell refinement: Bruker *SAINT*; data reduction: Bruker *SAINT*; program(s) used to solve structure: *SIR* 92 (Giacavazzo, 1993); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2014); molecular graphics: *ORTEP* 3 (Farraguia, 1997).

Data collection

BRUKER APEX2 CCD diffractometer	4633 reflections with $I > 2s(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.093$
Phi and w Scans scans	$q_{max} = 66.7°$, $q_{min} = 3.8°$
Absorption correction: multi-scan *SADABS* V2008/1 (Bruker AXS)	$h = -28 \rightarrow 26$
$T_{min} = 0.484$, $T_{max} = 0.753$	$k = -16 \rightarrow 21$
19214 measured reflections	$l = -18 \rightarrow 18$
5364 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	Only H-atom coordinates refined
$R[F^2 > 2s(F^2)] = 0.052$	$w = 1/[s^2(F_o^2) + (0.0733P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.128$	$(D/s)_{max} = 0.001$
$S = 1.00$	$Dñ_{max} = 0.36$ e Å^{-3}
5364 reflections	$Dñ_{min} = -0.45$ e Å^{-3}
417 parameters	Absolute structure: Classical Flack method preferred over Parsons because s.u. lower.
1 restraint	Flack parameter: -0.001 (6)

Special Details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 5. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) for **3**.

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.69932 (17)	0.8261 (2)	0.4536 (4)	0.0251 (11)
C2	0.65912 (17)	0.7230 (2)	0.5419 (3)	0.0166 (10)
C3	0.71437 (18)	0.6632 (3)	0.6376 (3)	0.0196 (10)
H3	0.7404 (19)	0.635 (2)	0.6586 (15)	0.024*
C4	0.67877 (18)	0.7077 (3)	0.6799 (3)	0.0220 (10)
H4	0.6771 (2)	0.7149 (5)	0.746 (4)	0.026*
C5	0.72783 (18)	0.6276 (3)	0.4905 (3)	0.0199 (10)
C6	0.77976 (17)	0.6496 (3)	0.4574 (3)	0.0237 (11)
C7	0.8029 (2)	0.6058 (3)	0.3936 (4)	0.0288 (12)
H7	0.839 (2)	0.6203 (10)	0.3678 (18)	0.035*
C8	0.7755 (2)	0.5428 (3)	0.3670 (4)	0.0309 (12)
H8	0.7913 (13)	0.514 (2)	0.323 (4)	0.037*
C9	0.7260 (2)	0.5199 (3)	0.4028 (4)	0.0303 (12)
H9	0.7063 (13)	0.471 (3)	0.3819 (14)	0.036*
C10	0.70085 (18)	0.5611 (3)	0.4673 (3)	0.0246 (12)
C11	0.81310 (19)	0.7147 (3)	0.4912 (4)	0.0251 (11)
H11	0.7889 (19)	0.744 (2)	0.519 (2)	0.030*
C12	0.85753 (18)	0.6869 (3)	0.5531 (4)	0.0341 (13)
H12A	0.8805 (16)	0.7357 (19)	0.581 (2)	0.051*
H12B	0.8888 (16)	0.650 (2)	0.5202 (14)	0.051*
H12C	0.8359 (9)	0.654 (2)	0.604 (3)	0.051*
C13	0.8413 (2)	0.7612 (3)	0.4227 (4)	0.0398 (17)
H13A	0.8628 (18)	0.807 (3)	0.4498 (13)	0.060*
H13B	0.8097 (14)	0.781 (2)	0.381 (3)	0.060*
H13C	0.871 (2)	0.7277 (16)	0.390 (2)	0.060*
C14	0.6482 (2)	0.5318 (3)	0.5105 (4)	0.0279 (12)
H14	0.6260 (16)	0.573 (3)	0.5258 (12)	0.034*
C15	0.6113 (2)	0.4804 (3)	0.4575 (5)	0.0404 (15)
H15A	0.571 (2)	0.472 (2)	0.4878 (19)	0.061*
H15B	0.6326 (13)	0.428 (3)	0.450 (3)	0.061*
H15C	0.6044 (17)	0.5055 (16)	0.398 (3)	0.061*
C16	0.6645 (2)	0.4898 (3)	0.5900 (4)	0.0391 (14)
H16A	0.6295 (16)	0.472 (2)	0.619 (2)	0.059*

H16B	0.6860 (19)	0.5237 (17)	0.627 (2)	0.059*
H16C	0.6886 (19)	0.446 (2)	0.5754 (8)	0.059*
C17	0.59758 (18)	0.7882 (3)	0.6458 (3)	0.0198 (10)
C18	0.60508 (18)	0.8652 (3)	0.6529 (3)	0.0242 (11)
C19	0.5590 (2)	0.9073 (3)	0.6807 (4)	0.0331 (12)
H19	0.5621 (3)	0.956 (4)	0.6836 (5)	0.040*
C20	0.5083 (2)	0.8734 (3)	0.7039 (4)	0.0361 (14)
H20	0.477 (2)	0.904 (2)	0.7247 (15)	0.043*
C21	0.5023 (2)	0.7976 (3)	0.6979 (4)	0.0305 (13)
H21	0.466 (3)	0.7739 (17)	0.7155 (13)	0.037*
C22	0.54661 (18)	0.7532 (3)	0.6672 (3)	0.0226 (11)
C23	0.66122 (19)	0.9037 (3)	0.6363 (4)	0.0253 (11)
H23	0.6854 (17)	0.869 (2)	0.6115 (18)	0.030*
C24	0.6883 (2)	0.9283 (3)	0.7185 (4)	0.0367 (13)
H24A	0.7263 (18)	0.952 (2)	0.7072 (7)	0.055*
H24B	0.6935 (16)	0.884 (2)	0.7555 (19)	0.055*
H24C	0.6629 (14)	0.965 (2)	0.7467 (18)	0.055*
C25	0.6551 (2)	0.9693 (3)	0.5779 (4)	0.0346 (13)
H25A	0.6360 (18)	0.9518 (9)	0.523 (3)	0.052*
H25B	0.6950 (17)	0.9909 (18)	0.565 (2)	0.052*
H25C	0.6303 (18)	1.010 (2)	0.6056 (15)	0.052*
C26	0.53934 (18)	0.6693 (3)	0.6625 (3)	0.0241 (11)
H26	0.5657 (18)	0.6503 (13)	0.621 (3)	0.029*
C27	0.5533 (2)	0.6326 (3)	0.7462 (4)	0.0322 (12)
H27A	0.5484 (16)	0.581 (2)	0.7419 (8)	0.048*
H27B	0.5290 (16)	0.6513 (18)	0.7869 (19)	0.048*
H27C	0.5908 (18)	0.6431 (19)	0.7606 (14)	0.048*
C28	0.47925 (19)	0.6459 (3)	0.6369 (4)	0.0289 (11)
H28A	0.4787 (4)	0.596 (2)	0.626 (3)	0.043*
H28B	0.4687 (9)	0.672 (2)	0.591 (3)	0.043*
H28C	0.4546 (12)	0.656 (2)	0.679 (2)	0.043*
C29	0.55400 (17)	0.7935 (3)	0.4095 (3)	0.0220 (10)
C30	0.59068 (17)	0.8392 (3)	0.3645 (3)	0.0213 (10)
C31	0.62798 (19)	0.7918 (3)	0.3157 (4)	0.0245 (11)
C32	0.61330 (18)	0.7166 (3)	0.3326 (3)	0.0194 (10)
C33	0.56871 (17)	0.7181 (3)	0.3915 (3)	0.0203 (10)
C34	0.50590 (18)	0.8192 (3)	0.4653 (4)	0.0298 (13)

H34A	0.4979 (12)	0.7805 (19)	0.507 (2)	0.045*
H34B	0.4716 (16)	0.828 (2)	0.4316 (15)	0.045*
H34C	0.5170 (8)	0.866 (2)	0.494 (2)	0.045*
C35	0.5893 (2)	0.9223 (3)	0.3595 (4)	0.0294 (11)
H35A	0.6247 (16)	0.9403 (9)	0.366 (3)	0.044*
H35B	0.5668 (17)	0.9403 (9)	0.400 (2)	0.044*
H35C	0.5754 (17)	0.9361 (7)	0.310 (2)	0.044*
C36	0.67170 (19)	0.8182 (3)	0.2551 (3)	0.0275 (12)
H36A	0.6862 (14)	0.861 (2)	0.2726 (15)	0.041*
H36B	0.6557 (8)	0.825 (2)	0.206 (2)	0.041*
H36C	0.6990 (16)	0.7847 (18)	0.2509 (19)	0.041*
C37	0.63852 (18)	0.6499 (3)	0.2899 (4)	0.0267 (11)
H37A	0.6363 (15)	0.6080 (19)	0.3256 (18)	0.040*
H37B	0.6771 (17)	0.6596 (9)	0.277 (2)	0.040*
H37C	0.6181 (14)	0.6401 (14)	0.240 (2)	0.040*
C38	0.53562 (19)	0.6518 (3)	0.4221 (4)	0.0285 (13)
H38A	0.5332 (14)	0.6533 (12)	0.485 (3)	0.043*
H38B	0.5555 (12)	0.6042 (19)	0.404 (2)	0.043*
H38C	0.4958 (17)	0.6530 (13)	0.398 (2)	0.043*
N1	0.70181 (13)	0.6716 (2)	0.5546 (3)	0.0180 (8)
N2	0.64486 (14)	0.7424 (2)	0.6222 (3)	0.0161 (8)
Co1	0.64098 (2)	0.77223 (3)	0.44103 (6)	0.0168 (2)
O1	0.73870 (13)	0.86527 (19)	0.4603 (3)	0.0337 (10)

Table 6. Atomic displacement parameters (Å^2) for **3**.

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0178 (19)	0.022 (2)	0.035 (3)	0.0016 (16)	-0.003 (2)	0.007 (2)
C2	0.0092 (18)	0.016 (2)	0.025 (3)	-0.0025 (14)	-0.0013 (17)	0.0023 (17)
C3	0.0170 (19)	0.025 (2)	0.017 (3)	0.0035 (17)	-0.0056 (18)	0.0014 (19)
C4	0.017 (2)	0.025 (3)	0.024 (3)	0.0001 (17)	-0.0009 (18)	0.002 (2)
C5	0.021 (2)	0.021 (2)	0.018 (3)	0.0067 (16)	-0.0036 (18)	0.0010 (19)
C6	0.020 (2)	0.021 (2)	0.030 (3)	0.0070 (16)	-0.003 (2)	0.004 (2)
C7	0.026 (2)	0.034 (3)	0.026 (3)	0.011 (2)	0.005 (2)	0.003 (2)
C8	0.036 (3)	0.031 (3)	0.026 (3)	0.017 (2)	-0.003 (2)	-0.007 (2)
C9	0.032 (3)	0.024 (3)	0.035 (3)	0.011 (2)	-0.010 (2)	-0.005 (2)
C10	0.021 (2)	0.021 (2)	0.032 (4)	0.0073 (17)	-0.0076 (18)	0.002 (2)
C11	0.020 (2)	0.025 (3)	0.030 (3)	0.0030 (18)	0.008 (2)	-0.001 (2)
C12	0.020 (2)	0.037 (3)	0.046 (4)	-0.0048 (19)	0.000 (2)	0.001 (3)
C13	0.039 (3)	0.027 (3)	0.053 (5)	0.000 (2)	0.023 (3)	0.003 (2)
C14	0.024 (2)	0.023 (3)	0.037 (4)	0.0037 (19)	-0.005 (2)	-0.002 (2)
C15	0.035 (3)	0.024 (3)	0.062 (5)	-0.008 (2)	-0.011 (3)	0.001 (3)
C16	0.034 (3)	0.034 (3)	0.049 (4)	-0.005 (2)	0.001 (3)	0.007 (3)
C17	0.0132 (19)	0.026 (2)	0.020 (3)	0.0035 (16)	0.0006 (17)	-0.0002 (19)
C18	0.021 (2)	0.025 (2)	0.027 (3)	0.0019 (18)	0.0011 (19)	-0.004 (2)
C19	0.031 (2)	0.023 (3)	0.045 (4)	0.004 (2)	0.009 (2)	-0.004 (2)
C20	0.026 (3)	0.033 (3)	0.049 (4)	0.013 (2)	0.012 (2)	-0.004 (3)
C21	0.018 (2)	0.035 (3)	0.039 (4)	0.0039 (19)	0.010 (2)	0.002 (2)
C22	0.018 (2)	0.026 (3)	0.024 (3)	0.0011 (18)	-0.0001 (18)	-0.002 (2)
C23	0.024 (2)	0.023 (3)	0.029 (3)	-0.0007 (19)	0.002 (2)	-0.006 (2)
C24	0.032 (2)	0.037 (3)	0.041 (4)	-0.001 (2)	-0.005 (2)	-0.010 (3)
C25	0.033 (2)	0.027 (3)	0.044 (4)	-0.004 (2)	0.002 (2)	0.002 (2)
C26	0.0142 (19)	0.028 (3)	0.030 (3)	-0.0012 (18)	0.0049 (19)	-0.001 (2)
C27	0.026 (2)	0.041 (3)	0.029 (3)	-0.004 (2)	-0.002 (2)	0.007 (2)
C28	0.018 (2)	0.036 (3)	0.033 (3)	-0.0062 (19)	0.003 (2)	0.001 (2)
C29	0.0099 (19)	0.031 (3)	0.026 (3)	0.0027 (18)	-0.0054 (17)	0.003 (2)
C30	0.0143 (18)	0.027 (2)	0.023 (3)	0.0024 (17)	-0.0051 (17)	0.003 (2)
C31	0.0139 (19)	0.028 (3)	0.032 (3)	0.0003 (17)	-0.0054 (19)	0.008 (2)
C32	0.016 (2)	0.022 (2)	0.020 (3)	-0.0001 (16)	-0.0060 (18)	0.0026 (19)
C33	0.013 (2)	0.027 (3)	0.020 (3)	-0.0041 (17)	-0.0071 (18)	0.0039 (19)
C34	0.0135 (19)	0.041 (3)	0.035 (4)	0.0036 (18)	0.0041 (19)	0.004 (2)

C35	0.025 (2)	0.027 (3)	0.036 (3)	0.0011 (19)	-0.005 (2)	0.004 (2)
C36	0.019 (2)	0.043 (3)	0.020 (3)	-0.002 (2)	0.0034 (19)	0.007 (2)
C37	0.022 (2)	0.031 (3)	0.027 (3)	0.0033 (18)	-0.001 (2)	-0.001 (2)
C38	0.018 (2)	0.034 (3)	0.034 (4)	-0.0058 (19)	0.0002 (19)	0.007 (2)
N1	0.0121 (15)	0.0158 (19)	0.026 (3)	0.0021 (13)	-0.0023 (14)	-0.0012 (16)
N2	0.0138 (17)	0.0185 (19)	0.016 (2)	0.0003 (13)	-0.0011 (14)	-0.0027 (15)
Co1	0.0096 (3)	0.0187 (4)	0.0222 (4)	-0.0001 (2)	-0.0018 (3)	0.0018 (3)
O1	0.0210 (16)	0.0259 (18)	0.054 (3)	-0.0066 (13)	-0.0038 (15)	0.0017 (17)

Table 7. Geometric parameters (Å, º)

C1—O1	1.171 (5)	C18—C23	1.519 (7)
C1—Co1	1.695 (4)	C19—C20	1.394 (8)
C2—N1	1.383 (6)	C20—C21	1.374 (8)
C2—N2	1.385 (7)	C21—C22	1.407 (7)
C2—Co1	1.902 (5)	C22—C26	1.521 (7)
C3—C4	1.346 (7)	C23—C25	1.517 (8)
C3—N1	1.381 (7)	C23—C24	1.538 (8)
C4—N2	1.377 (6)	C26—C28	1.535 (6)
C5—C6	1.394 (7)	C26—C27	1.540 (8)
C5—C10	1.407 (7)	C29—C30	1.397 (7)
C5—N1	1.441 (6)	C29—C33	1.431 (7)
C6—C7	1.409 (8)	C29—C34	1.521 (7)
C6—C11	1.513 (7)	C29—Co1	2.148 (4)
C7—C8	1.374 (8)	C30—C31	1.457 (7)
C8—C9	1.366 (8)	C30—C35	1.498 (7)
C9—C10	1.409 (8)	C30—Co1	2.094 (5)
C10—C14	1.519 (7)	C31—C32	1.423 (7)
C11—C12	1.533 (8)	C31—C36	1.499 (7)
C11—C13	1.538 (8)	C31—Co1	2.077 (6)
C14—C15	1.532 (8)	C32—C33	1.419 (7)
C14—C16	1.538 (9)	C32—C37	1.506 (7)
C17—C22	1.401 (7)	C32—Co1	2.121 (5)
C17—C18	1.402 (7)	C33—C38	1.509 (7)
C17—N2	1.438 (6)	C33—Co1	2.120 (4)
C18—C19	1.399 (7)		
O1—C1—Co1	177.5 (5)	C31—C30—C35	124.6 (5)
N1—C2—N2	101.9 (4)	C29—C30—Co1	72.9 (3)
N1—C2—Co1	127.1 (4)	C31—C30—Co1	68.9 (3)
N2—C2—Co1	129.0 (3)	C35—C30—Co1	128.3 (3)
C4—C3—N1	107.0 (4)	C32—C31—C30	107.8 (4)
C3—C4—N2	106.8 (5)	C32—C31—C36	126.5 (5)
C6—C5—C10	122.5 (4)	C30—C31—C36	125.6 (5)
C6—C5—N1	119.6 (4)	C32—C31—Co1	71.8 (3)
C10—C5—N1	117.8 (4)	C30—C31—Co1	70.2 (3)
C5—C6—C7	117.5 (4)	C36—C31—Co1	126.0 (3)

C5—C6—C11	122.6 (5)	C33—C32—C31	106.9 (4)
C7—C6—C11	119.8 (4)	C33—C32—C37	127.9 (4)
C8—C7—C6	120.5 (5)	C31—C32—C37	125.0 (5)
C9—C8—C7	121.2 (5)	C33—C32—Co1	70.4 (3)
C8—C9—C10	121.0 (5)	C31—C32—Co1	68.6 (3)
C5—C10—C9	117.0 (5)	C37—C32—Co1	129.2 (3)
C5—C10—C14	122.9 (5)	C32—C33—C29	109.5 (4)
C9—C10—C14	120.1 (5)	C32—C33—C38	126.0 (4)
C6—C11—C12	109.7 (4)	C29—C33—C38	124.0 (4)
C6—C11—C13	112.8 (5)	C32—C33—Co1	70.5 (2)
C12—C11—C13	110.6 (4)	C29—C33—Co1	71.5 (2)
C10—C14—C15	114.6 (5)	C38—C33—Co1	131.0 (3)
C10—C14—C16	110.4 (4)	C3—N1—C2	112.0 (4)
C15—C14—C16	108.1 (5)	C3—N1—C5	123.1 (4)
C22—C17—C18	122.2 (4)	C2—N1—C5	124.8 (4)
C22—C17—N2	118.2 (4)	C4—N2—C2	112.2 (4)
C18—C17—N2	119.4 (4)	C4—N2—C17	122.1 (4)
C19—C18—C17	117.7 (4)	C2—N2—C17	125.5 (4)
C19—C18—C23	119.1 (5)	C1—Co1—C2	89.0 (2)
C17—C18—C23	123.2 (4)	C1—Co1—C31	98.0 (2)
C20—C19—C18	121.0 (5)	C2—Co1—C31	161.1 (2)
C21—C20—C19	120.3 (5)	C1—Co1—C30	101.6 (2)
C20—C21—C22	120.8 (5)	C2—Co1—C30	154.2 (2)
C17—C22—C21	117.9 (5)	C31—Co1—C30	40.9 (2)
C17—C22—C26	122.1 (4)	C1—Co1—C33	163.8 (3)
C21—C22—C26	119.9 (4)	C2—Co1—C33	106.81 (18)
C25—C23—C18	112.5 (4)	C31—Co1—C33	65.90 (19)
C25—C23—C24	110.6 (5)	C30—Co1—C33	65.59 (18)
C18—C23—C24	109.9 (5)	C1—Co1—C32	128.2 (3)
C22—C26—C28	112.9 (4)	C2—Co1—C32	123.80 (18)
C22—C26—C27	110.9 (5)	C31—Co1—C32	39.61 (19)
C28—C26—C27	108.4 (4)	C30—Co1—C32	67.04 (19)
C30—C29—C33	107.6 (4)	C33—Co1—C32	39.09 (19)
C30—C29—C34	126.2 (5)	C1—Co1—C29	134.5 (2)
C33—C29—C34	126.1 (5)	C2—Co1—C29	120.05 (19)
C30—C29—Co1	68.7 (2)	C31—Co1—C29	66.28 (19)
C33—C29—Co1	69.3 (2)	C30—Co1—C29	38.42 (19)

C34—C29—Co1	128.7 (4)	C33—Co1—C29	39.18 (19)
C29—C30—C31	108.1 (4)	C32—Co1—C29	66.07 (18)
C29—C30—C35	127.0 (5)		
N1—C3—C4—N2	0.2 (5)	C29—C30—C31—C32	-0.4 (5)
C10—C5—C6—C7	5.3 (7)	C35—C30—C31—C32	-174.9 (4)
N1—C5—C6—C7	-178.7 (4)	Co1—C30—C31—C32	62.4 (3)
C10—C5—C6—C11	-170.5 (4)	C29—C30—C31—C36	176.5 (5)
N1—C5—C6—C11	5.5 (7)	C35—C30—C31—C36	2.0 (8)
C5—C6—C7—C8	-1.5 (7)	Co1—C30—C31—C36	-120.7 (5)
C11—C6—C7—C8	174.4 (5)	C29—C30—C31—Co1	-62.7 (3)
C6—C7—C8—C9	-1.7 (8)	C35—C30—C31—Co1	122.7 (5)
C7—C8—C9—C10	1.2 (8)	C30—C31—C32—C33	-1.0 (5)
C6—C5—C10—C9	-5.7 (7)	C36—C31—C32—C33	-177.9 (5)
N1—C5—C10—C9	178.2 (4)	Co1—C31—C32—C33	60.3 (3)
C6—C5—C10—C14	172.2 (4)	C30—C31—C32—C37	175.0 (4)
N1—C5—C10—C14	-4.0 (7)	C36—C31—C32—C37	-1.9 (8)
C8—C9—C10—C5	2.4 (7)	Co1—C31—C32—C37	-123.7 (5)
C8—C9—C10—C14	-175.5 (5)	C30—C31—C32—Co1	-61.3 (3)
C5—C6—C11—C12	95.5 (5)	C36—C31—C32—Co1	121.8 (5)
C7—C6—C11—C12	-80.2 (6)	C31—C32—C33—C29	2.0 (5)
C5—C6—C11—C13	-140.8 (5)	C37—C32—C33—C29	-173.9 (5)
C7—C6—C11—C13	43.5 (6)	Co1—C32—C33—C29	61.1 (3)
C5—C10—C14—C15	155.3 (5)	C31—C32—C33—C38	173.9 (4)

C9—C10—C14—C15	-26.9 (6)	C37—C32—C33—C38	-2.1 (8)
C5—C10—C14—C16	-82.3 (6)	Co1—C32—C33—C38	-127.1 (5)
C9—C10—C14—C16	95.5 (6)	C31—C32—C33—Co1	-59.1 (3)
C22—C17—C18—C19	-1.5 (8)	C37—C32—C33—Co1	125.0 (5)
N2—C17—C18—C19	-176.3 (5)	C30—C29—C33—C32	-2.3 (5)
C22—C17—C18—C23	175.2 (5)	C34—C29—C33—C32	175.9 (5)
N2—C17—C18—C23	0.5 (8)	Co1—C29—C33—C32	-60.5 (3)
C17—C18—C19—C20	2.8 (9)	C30—C29—C33—C38	-174.3 (4)
C23—C18—C19—C20	-174.1 (6)	C34—C29—C33—C38	3.9 (8)
C18—C19—C20—C21	-1.6 (10)	Co1—C29—C33—C38	127.5 (5)
C19—C20—C21—C22	-1.0 (10)	C30—C29—C33—Co1	58.2 (3)
C18—C17—C22—C21	-0.9 (8)	C34—C29—C33—Co1	-123.6 (5)
N2—C17—C22—C21	173.9 (5)	C4—C3—N1—C2	1.7 (5)
C18—C17—C22—C26	-177.6 (5)	C4—C3—N1—C5	-174.3 (4)
N2—C17—C22—C26	-2.8 (8)	N2—C2—N1—C3	-2.8 (5)
C20—C21—C22—C17	2.2 (9)	Co1—C2—N1—C3	162.2 (3)
C20—C21—C22—C26	179.0 (6)	N2—C2—N1—C5	173.1 (4)
C19—C18—C23—C25	-53.4 (7)	Co1—C2—N1—C5	-22.0 (6)
C17—C18—C23—C25	129.9 (6)	C6—C5—N1—C3	-85.7 (6)
C19—C18—C23—C24	70.4 (7)	C10—C5—N1—C3	90.6 (5)
C17—C18—C23—C24	-106.3 (6)	C6—C5—N1—C2	98.9 (5)
C17—C22—C26—C28	-145.4 (5)	C10—C5—N1—C2	-84.8 (6)
C21—C22—C26—C28	38.0 (7)	C3—C4—N2—C2	-2.1 (5)

C17—C22—C26—C27	92.7 (6)	C3—C4—N2—C17	173.2 (4)
C21—C22—C26—C27	-83.9 (6)	N1—C2—N2—C4	2.9 (5)
C33—C29—C30—C31	1.6 (5)	Co1—C2—N2—C4	-161.6 (3)
C34—C29—C30—C31	-176.6 (5)	N1—C2—N2—C17	-172.2 (4)
Co1—C29—C30—C31	60.2 (3)	Co1—C2—N2—C17	23.3 (6)
C33—C29—C30—C35	176.0 (5)	C22—C17—N2—C4	-80.5 (6)
C34—C29—C30—C35	-2.2 (8)	C18—C17—N2—C4	94.5 (6)
Co1—C29—C30—C35	-125.4 (5)	C22—C17—N2—C2	94.2 (6)
C33—C29—C30—Co1	-58.6 (3)	C18—C17—N2—C2	-90.9 (6)
C34—C29—C30—Co1	123.2 (5)		

Computational Details.

All DFT calculations were performed using the OLYP hybrid functional as implemented in Gaussian 09.[6] The cobalt atom uses the effective core potential and associated basis set of Hay and Wadt (LANL2DZ)[7,8] in which the two outermost p functions were replaced by reoptimized 4p functions as suggested by Couty and Hall,[9] and an f polarization function[10] was added. All other atoms use the 6-31G(d',p') basis set.[11-13] Unless otherwise noted, all geometries are fully optimized and confirmed as minima or n-order saddle points by analytical frequency calculations at the same level. Coordinates for the geometry minimizations were taken from the X-ray coordinates of **2**.

Linear versus bent geometries

The optimization of the singlet and triplet states of the 'bent' geometries was initiated from the three-dimensional structure determined for **2** by our x-ray diffraction studies. The 'linear' starting geometries were generated by adjustment of the 'bent' structure such that the Cp(centroid)-Co-C(carbene) angle was 180.0 degrees. All structures were allowed to fully optimize with geometric constraints.

Optimized 'bent' singlet structure

C	-1.303236	0.726635	-2.456649
N	-1.477279	0.413374	-1.100946
C	-0.239930	0.169586	-0.460308
N	0.666526	0.348918	-1.535002
C	0.027247	0.688579	-2.722841
C	-2.808970	0.254810	-0.566370
C	-3.401511	-1.044336	-0.607336
C	-4.710196	-1.197074	-0.118511
C	-5.423833	-0.111926	0.394526
C	-4.844160	1.154499	0.386861
C	-3.543505	1.385331	-0.113260
C	2.088123	0.175181	-1.383056
C	2.907322	1.317612	-1.147329
C	4.294044	1.109533	-1.010802
C	4.851237	-0.166569	-1.118130
C	4.037248	-1.267032	-1.401015
C	2.644099	-1.127081	-1.551098
Co	0.619348	-0.182584	1.144728
C	1.695516	0.233835	2.956014
C	0.357393	0.707427	3.034183
C	-0.507300	-0.444275	2.758358
C	0.325318	-1.644076	2.628258
C	1.675617	-1.205494	2.703359
C	2.354446	2.745881	-1.168845
C	1.805978	-2.318392	-2.026961
C	-2.689115	-2.252301	-1.229026
C	-3.144263	2.874418	-0.169527
C	-2.934228	-3.580118	-0.480770

H	-1.612747	-2.055194	-1.180324
C	-3.076879	-2.419299	-2.719145
H	0.570006	0.866969	-3.642408
C	2.803798	3.609069	0.027162
H	1.263769	2.676593	-1.113154
C	2.706352	3.442383	-2.506301
H	4.495781	-2.246786	-1.531328
H	0.753115	-2.055625	-1.882514
C	2.052093	-3.618456	-1.235675
C	2.020547	-2.553040	-3.542455
C	-0.094728	2.060131	3.515286
H	-5.180810	-2.179075	-0.138961
H	-5.414718	2.003746	0.767508
C	-1.995568	-0.455852	2.965025
H	4.949536	1.962699	-0.837379
C	2.911487	-2.064077	2.636838
C	-0.158702	-3.068360	2.641223
C	2.953670	1.022482	3.206616
C	-1.659756	3.265792	-0.073666
H	-3.631132	3.314173	0.716237
C	-3.798414	3.555782	-1.399245
H	-2.143112	0.943253	-3.103002
H	-2.223105	-0.635193	4.030735
H	-2.461927	0.495574	2.689406
H	-2.491779	-1.243933	2.390418
H	-0.155265	2.090875	4.618222
H	0.588372	2.862595	3.207605
H	-1.090203	2.318604	3.136204
H	3.385059	0.765577	4.189467
H	3.732175	0.820017	2.458561
H	2.769393	2.102755	3.210485
H	3.365156	-2.177950	3.636367
H	2.693089	-3.072283	2.266298
H	3.684483	-1.634020	1.985261
H	-0.226511	-3.456955	3.673697
H	-1.155411	-3.166894	2.199248
H	0.508520	-3.741580	2.088003
H	5.929533	-0.300635	-1.010453
H	2.312690	4.591868	-0.016917
H	2.528406	3.136845	0.975665
H	3.887567	3.790410	0.036478
H	2.245115	4.439621	-2.551314
H	3.792021	3.571161	-2.620940
H	2.348971	2.869426	-3.372102
H	1.359682	-4.400463	-1.579578
H	3.070018	-4.010310	-1.369447

H	1.881556	-3.464726	-0.165063
H	1.365020	-3.359835	-3.901559
H	1.795462	-1.653280	-4.129958
H	3.058003	-2.842656	-3.762464
H	-6.432222	-0.252578	0.788034
H	-1.590398	4.332286	0.187155
H	-1.124771	2.690487	0.686490
H	-1.137011	3.130809	-1.026413
H	-3.636567	4.642962	-1.361558
H	-3.362042	3.189456	-2.338622
H	-4.880873	3.376858	-1.440139
H	-2.249005	-4.351219	-0.860491
H	-2.762637	-3.482260	0.596952
H	-3.954318	-3.962629	-0.625442
H	-2.538469	-3.270632	-3.161204
H	-4.153945	-2.612533	-2.828260
H	-2.834071	-1.529895	-3.311883

Optimized 'bent' triplet structure

C	0.665624	2.759101	0.604530
N	1.085810	1.479492	0.251481
C	0.013614	0.593496	0.107845
N	-1.083318	1.419733	0.387658
C	-0.691097	2.722376	0.688751
C	2.491097	1.131077	0.214103
C	3.083194	0.639993	1.413453
C	4.444819	0.291998	1.385955
C	5.206382	0.441049	0.225628
C	4.618539	0.981562	-0.917105
C	3.260153	1.362073	-0.957821
C	-2.478315	1.027616	0.447006
C	-3.321333	1.302838	-0.664528
C	-4.684489	0.973451	-0.547451
C	-5.200071	0.405711	0.618742
C	-4.359186	0.172147	1.708528
C	-2.988227	0.484195	1.658283
Co	-0.023582	-1.334466	-0.235135
C	-1.083411	-2.919877	-1.229108
C	-0.174851	-2.359656	-2.196795
C	1.166292	-2.509890	-1.686943
C	1.091750	-3.164876	-0.409588
C	-0.305148	-3.421630	-0.121843
C	-2.819765	1.984201	-1.941977
C	-2.131742	0.304407	2.915723
C	2.328250	0.562246	2.745825
C	2.826166	2.058723	-2.263196

C	2.371652	-0.837833	3.392196
H	1.274625	0.782112	2.549116
C	2.837020	1.646740	3.725613
H	-1.404013	3.495767	0.942140
C	-3.289813	1.282567	-3.233750
H	-1.725814	1.930074	-1.934873
C	-3.217103	3.479836	-1.971377
H	-4.779109	-0.245842	2.622844
H	-1.082647	0.394128	2.615514
C	-2.282764	-1.086227	3.566937
C	-2.418695	1.427199	3.941288
C	-0.531638	-1.907172	-3.587950
H	4.917622	-0.093161	2.289150
H	5.226339	1.122716	-1.812580
C	2.432455	-2.225244	-2.449501
H	-5.355815	1.171014	-1.382452
C	-0.832167	-4.231893	1.035536
C	2.269266	-3.667444	0.385143
C	-2.572095	-3.080789	-1.397568
C	1.377492	1.893145	-2.755251
H	3.460269	1.594396	-3.034868
C	3.221585	3.557049	-2.230031
H	1.362615	3.569558	0.773144
H	2.736439	-3.100206	-3.051746
H	2.317990	-1.387316	-3.148526
H	3.272044	-1.986448	-1.785979
H	-0.392626	-2.724103	-4.318528
H	-1.578871	-1.593132	-3.665205
H	0.086780	-1.068166	-3.932788
H	-2.820205	-4.035570	-1.893907
H	-3.099493	-3.073454	-0.434712
H	-3.008318	-2.279501	-2.006771
H	-0.815933	-5.312918	0.809727
H	-0.237884	-4.089934	1.948645
H	-1.870991	-3.975166	1.280316
H	2.641043	-4.627647	-0.014458
H	3.111711	-2.963892	0.367484
H	2.012393	-3.843996	1.437442
H	-6.261068	0.157591	0.683441
H	-2.784128	1.724213	-4.104140
H	-3.054647	0.213126	-3.215548
H	-4.370499	1.389227	-3.401102
H	-2.808614	3.967551	-2.868381
H	-4.309300	3.602161	-1.993305
H	-2.841395	4.025102	-1.096317
H	-1.572342	-1.187468	4.399952

H	-3.287294	-1.252038	3.979821
H	-2.073864	-1.885870	2.847250
H	-1.760304	1.325274	4.816271
H	-2.252360	2.423883	3.511645
H	-3.457298	1.388880	4.299252
H	6.259012	0.152649	0.216978
H	1.331000	2.157358	-3.821956
H	1.020475	0.866484	-2.638457
H	0.682390	2.556507	-2.229468
H	3.051642	4.017092	-3.214443
H	2.622509	4.115499	-1.497631
H	4.280035	3.694347	-1.972001
H	1.778647	-0.843902	4.318294
H	1.954398	-1.592213	2.716292
H	3.391919	-1.145677	3.658739
H	2.239921	1.638551	4.649166
H	3.886579	1.482437	4.007107
H	2.765092	2.652326	3.289260

Optimized 'linear' singlet structure

C	0.821357	-2.348829	1.410432
N	1.185633	-1.161900	0.773051
C	0.059401	-0.455110	0.289155
N	-0.997509	-1.296988	0.703655
C	-0.531497	-2.430535	1.373726
C	2.574522	-0.832193	0.551684
C	3.193014	-1.301060	-0.646236
C	4.548489	-1.004332	-0.861026
C	5.287617	-0.278329	0.073132
C	4.683356	0.118832	1.263070
C	3.330950	-0.162243	1.554849
C	-2.405801	-1.123958	0.423263
C	-3.242246	-0.510235	1.398105
C	-4.611313	-0.382979	1.102081
C	-5.146996	-0.861690	-0.094743
C	-4.320857	-1.509861	-1.012894
C	-2.943346	-1.667921	-0.775943
Co	-0.134874	1.268552	-0.574039
C	-1.184617	2.638871	-1.711574
C	-0.858742	3.233648	-0.401753
C	0.549825	3.282486	-0.267154
C	1.098199	2.620997	-1.446646
C	0.028730	2.345203	-2.395427
C	-2.721416	-0.061062	2.766998
C	-2.113600	-2.479167	-1.773136
C	2.465281	-2.203056	-1.648140

C	2.919914	0.193874	2.998445
C	2.762069	-1.869010	-3.124261
H	1.390409	-2.056876	-1.502139
C	2.787757	-3.692066	-1.374881
H	-1.202844	-3.192204	1.746280
C	-3.305957	1.282535	3.248911
H	-1.638449	0.075054	2.672626
C	-2.972798	-1.146878	3.841856
H	-4.755128	-1.914960	-1.926812
H	-1.070214	-2.440287	-1.446374
C	-2.160722	-1.892159	-3.198508
C	-2.532651	-3.966978	-1.765241
C	-1.852403	3.811601	0.570057
H	5.037419	-1.354894	-1.768809
H	5.276962	0.650568	2.008763
C	1.325523	3.958434	0.826028
H	-5.274163	0.087883	1.826525
C	0.200628	1.932621	-3.830400
C	2.565083	2.503222	-1.752979
C	-2.574051	2.514811	-2.273387
C	1.477425	0.632357	3.298191
H	3.550782	1.062845	3.243915
C	3.356526	-0.932633	3.968660
H	1.554962	-3.025480	1.827595
H	1.497103	5.023441	0.588846
H	0.797617	3.924016	1.787836
H	2.312753	3.503348	0.976243
H	-1.912594	4.909126	0.465582
H	-2.864513	3.423958	0.406881
H	-1.576532	3.602006	1.611228
H	-2.847071	3.426806	-2.831206
H	-2.666359	1.668705	-2.964690
H	-3.330217	2.378542	-1.490257
H	0.393817	2.805518	-4.479887
H	1.042295	1.242791	-3.966015
H	-0.694297	1.433799	-4.222574
H	2.928484	3.436666	-2.219301
H	3.164646	2.334888	-0.852195
H	2.779908	1.689977	-2.452690
H	-6.212947	-0.749801	-0.299875
H	-2.766054	1.620324	4.144666
H	-3.215694	2.064149	2.487475
H	-4.365672	1.203027	3.528268
H	-2.563615	-0.826081	4.810681
H	-4.048959	-1.326725	3.976187
H	-2.503947	-2.103673	3.585765

H	-1.526545	-2.483680	-3.873992
H	-3.176855	-1.895754	-3.617194
H	-1.788458	-0.862350	-3.201052
H	-1.876324	-4.550190	-2.427169
H	-2.462764	-4.399992	-0.758170
H	-3.564373	-4.107484	-2.116190
H	6.336368	-0.043771	-0.115812
H	1.459205	1.148965	4.269173
H	1.087985	1.312720	2.534662
H	0.794510	-0.219969	3.372008
H	3.211042	-0.612698	5.010744
H	2.763204	-1.844482	3.817333
H	4.414953	-1.194542	3.840125
H	2.103685	-2.459050	-3.776680
H	2.585995	-0.810227	-3.343108
H	3.794668	-2.108888	-3.413474
H	2.233375	-4.338308	-2.070863
H	3.859372	-3.895985	-1.511117
H	2.517863	-3.992697	-0.355530

Optimized 'linear' triplet structure

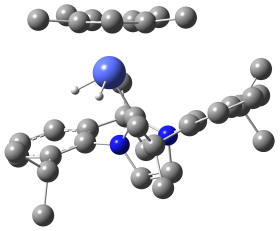
C	0.644996	-2.801507	0.546878
N	1.068074	-1.492114	0.355699
C	-0.001213	-0.624125	0.145948
N	-1.096806	-1.480330	0.221181
C	-0.712131	-2.796795	0.460317
C	2.473902	-1.148374	0.267250
C	3.085929	-1.222458	-1.015565
C	4.451006	-0.908394	-1.116881
C	5.191042	-0.535877	0.004363
C	4.579631	-0.512672	1.255679
C	3.220341	-0.839996	1.435773
C	-2.490668	-1.128993	0.019882
C	-3.310573	-0.878915	1.151976
C	-4.665268	-0.582904	0.921798
C	-5.195078	-0.553809	-0.368633
C	-4.379496	-0.847134	-1.461415
C	-3.016727	-1.151478	-1.297793
Co	0.004921	1.374944	-0.106834
C	-0.995125	3.171254	-0.651934
C	-0.564089	3.254865	0.720225
C	0.871032	3.153077	0.760087
C	1.336478	3.009169	-0.597671
C	0.192164	3.019601	-1.465768
C	-2.799707	-0.986545	2.590414
C	-2.190635	-1.557136	-2.520538

C	2.345081	-1.713536	-2.263024
C	2.776754	-0.921967	2.908294
C	2.544465	-0.803291	-3.491017
H	1.273819	-1.707985	-2.042628
C	2.739629	-3.171918	-2.593934
H	-1.429824	-3.602085	0.539058
C	-3.198870	0.212194	3.474894
H	-1.706681	-1.001756	2.554049
C	-3.259871	-2.312056	3.241805
H	-4.811149	-0.855275	-2.461356
H	-1.146906	-1.649778	-2.204123
C	-2.217890	-0.497759	-3.639813
C	-2.631839	-2.940339	-3.050993
C	-1.444531	3.567081	1.899410
H	4.941806	-0.958262	-2.087581
H	5.172517	-0.252832	2.133591
C	1.741500	3.356300	1.973801
H	-5.318424	-0.380437	1.769281
C	0.237065	3.060581	-2.970812
C	2.778204	3.024023	-1.031067
C	-2.403188	3.368577	-1.153040
C	1.323228	-0.583414	3.275412
H	3.396110	-0.164233	3.412406
C	3.187434	-2.284965	3.518640
H	1.339184	-3.613606	0.714951
H	2.022240	4.416853	2.102280
H	1.237410	3.050186	2.899299
H	2.678197	2.787636	1.909819
H	-1.473972	4.652554	2.092604
H	-2.480386	3.246493	1.734561
H	-1.091154	3.088333	2.821995
H	-2.636041	4.436341	-1.311477
H	-2.573736	2.862329	-2.111518
H	-3.150444	2.978733	-0.449884
H	0.366014	4.093977	-3.335202
H	1.067781	2.473237	-3.380031
H	-0.685611	2.680054	-3.425416
H	3.154882	4.056864	-1.131630
H	3.430366	2.513655	-0.312146
H	2.925066	2.537137	-2.002058
H	-6.249603	-0.320633	-0.520461
H	-2.705845	0.134217	4.453849
H	-2.898452	1.161568	3.021533
H	-4.280558	0.250883	3.661893
H	-2.848235	-2.403594	4.256718
H	-4.354797	-2.358410	3.319833

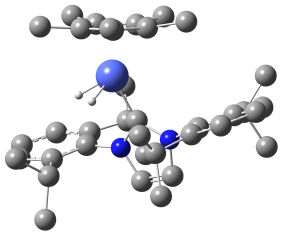
H	-2.931909	-3.188277	2.668058
H	-1.559005	-0.802129	-4.465023
H	-3.222981	-0.359232	-4.059935
H	-1.868078	0.469454	-3.265577
H	-1.989073	-3.254587	-3.885266
H	-2.571330	-3.710919	-2.271311
H	-3.667062	-2.921077	-3.417808
H	6.246715	-0.280532	-0.094378
H	1.266578	-0.386387	4.355759
H	0.959349	0.299002	2.740823
H	0.644014	-1.414181	3.064519
H	3.019472	-2.281627	4.604890
H	2.594736	-3.107273	3.096874
H	4.247299	-2.507799	3.340616
H	1.913465	-1.149421	-4.321500
H	2.263819	0.228868	-3.261494
H	3.581994	-0.805587	-3.851474
H	2.166275	-3.539644	-3.456701
H	3.806468	-3.251610	-2.843668
H	2.546050	-3.847783	-1.750936

Dihydride and dihydrogen complex geometries

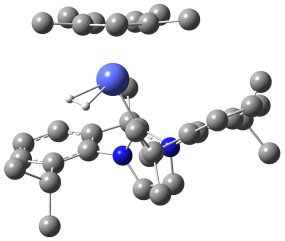
The dihydride or dihydrogen moieties were manually added to the structure of **2** that was determined by X-ray diffraction to generate the starting structures for geometry optimization. Attempts were made to optimize each structure as a singlet state and a triplet state. The dihydride complex starting structure had Co-H bond distances of 1.5 Å and an H-H distance of 2.5 Å. The compressed dihydride complex starting structure had Co-H bond distances of 1.5 Å and a locked H-H distance of 1.38 Å. The dihydrogen complex starting structure had Co-H bond distances of 1.8 Å and an H-H distance of 0.8 Å. All structures were allowed to fully optimize with geometric constraints. Stable minima were obtained for the singlet structure of the dihydride, the singlet and triplet structures of the compressed dihydride, and the triplet structure of the η^2-dihydrogen complex.



2-H_2 (singlet)



2-(^{c}H_2) (singlet)



2-(η^2-H_2) (triplet)

Complex	Calculated Energy (atomic units, au)	Relative Energy (kcal/mol)
2-H_2 (singlet)	-1696.01843440	0.00
2-^{c}H_2 (singlet)[a]	-1696.01442988	2.50
2-^{c}H_2 (triplet)[a]	-1695.99297040	16.00
2-(η^2-H_2) (triplet)[b]	-1695.97685341	26.10

[a]The H-H distance was frozen at 1.38 Å. [b] A singlet energy minimum for the dihydrogen complex could not be located.

Table 8. Optimised structures and calculated total energies for Cp*Co(IPr)H_2, compressed Cp*Co(IPr)H_2 and Cp*Co(IPr)(η^2-H_2). Computational details: Gaussian 09, OLYP exchange/correlation functionals with LANL2TZ+F on Co and 6-31g(d',p') on all other atoms.

Optimized singlet CoH_2 dihydride structure

Co	0.172114	-1.171396	-0.797206
H	1.525908	-1.217262	-0.324656
H	0.009929	-1.889525	0.456314
C	0.055317	0.302241	0.360125
C	0.737339	1.808147	1.996237
C	-0.617716	1.814059	1.994297
H	1.445701	2.349435	2.608359
H	-1.321560	2.355649	2.610374
C	-2.455927	0.708938	0.828440
C	-3.201179	1.646859	0.059102
C	-3.092679	-0.322887	1.572709
C	-4.595886	1.470510	-0.012757
C	-4.488790	-0.450272	1.449185
C	-5.234031	0.425862	0.657747
H	-5.195153	2.168163	-0.596488
H	-5.004985	-1.235143	2.000730
H	-6.316629	0.308284	0.581702
C	2.562622	0.724688	0.782550
C	3.259202	-0.233576	1.567857
C	3.242765	1.606777	-0.101425
C	4.653010	-0.326542	1.401957
C	4.637288	1.462987	-0.221459
C	5.337620	0.503396	0.512635
H	5.213143	-1.055439	1.987218
H	5.188314	2.120712	-0.892544
H	6.419900	0.413564	0.402286
C	0.524730	-2.799624	-2.010519
C	-0.904665	-2.713203	-1.805757
C	0.941377	-1.599436	-2.705921
C	-1.365984	-1.469314	-2.339249
C	-0.215986	-0.771078	-2.883502
N	1.143391	0.916656	1.007674
N	-1.033290	0.923020	1.005020
C	-2.566073	2.872111	-0.613864
C	-2.747464	4.141376	0.255367
C	-3.095714	3.155362	-2.036883
H	-1.489161	2.681856	-0.700903
H	-2.313286	4.028054	1.254988
H	-2.260291	5.004085	-0.221731
H	-3.811824	4.385568	0.380458
H	-3.054524	2.270837	-2.681215
H	-4.133738	3.514887	-2.030960
H	-2.489929	3.942016	-2.508340
C	2.528862	2.729268	-0.864296
C	3.017609	2.900318	-2.318454

C	2.644804	4.079075	-0.114537
H	1.465470	2.466045	-0.913995
H	3.027804	1.948029	-2.859985
H	2.351754	3.589463	-2.856837
H	4.028314	3.327775	-2.372423
H	2.226487	4.027962	0.897426
H	3.694487	4.394006	-0.027094
H	2.103793	4.867441	-0.658114
C	-2.339438	-1.208771	2.571434
C	-2.742277	-2.696251	2.520570
C	-2.502058	-0.662680	4.011234
H	-1.276939	-1.165449	2.312065
H	-2.655893	-3.099755	1.507158
H	-2.076654	-3.280443	3.171767
H	-3.767930	-2.869730	2.875095
H	-2.153006	0.373305	4.101935
H	-3.553064	-0.689815	4.332822
H	-1.920332	-1.272214	4.717978
C	2.566291	-1.121436	2.605914
C	2.905684	-0.666200	4.044588
C	2.871985	-2.622249	2.413401
H	1.486151	-1.006588	2.470162
H	2.643475	0.386992	4.212155
H	2.350465	-1.268985	4.777928
H	3.976770	-0.779651	4.264347
H	2.610671	-2.945510	1.399729
H	3.928900	-2.863169	2.593330
H	2.278816	-3.217992	3.122285
C	2.316526	-1.359784	-3.269907
H	2.421884	-1.842996	-4.256251
H	2.525221	-0.294161	-3.408439
H	3.102251	-1.762537	-2.620037
C	-0.274279	0.500145	-3.687493
H	0.709743	0.970712	-3.784279
H	-0.638444	0.299625	-4.709763
H	-0.949024	1.241124	-3.245983
C	-2.806900	-1.092560	-2.546056
H	-3.449901	-1.430924	-1.726221
H	-2.941917	-0.011545	-2.637075
H	-3.196176	-1.544648	-3.475346
C	-1.774349	-3.829322	-1.291356
H	-2.019319	-4.530527	-2.107224
H	-1.280537	-4.408995	-0.502685
H	-2.724236	-3.459008	-0.890492
C	1.384943	-4.001288	-1.722544
H	1.365709	-4.714523	-2.564475

H	2.432133	-3.722397	-1.555242
H	1.044034	-4.540544	-0.830326

Optimized singlet compressed CoH_2 dihydride structure (H-H frozen at 1.38 A)

Co	0.202463	-1.195849	-0.776284
H	1.471950	-1.347932	-0.148265
H	0.368246	-1.896556	0.472420
C	0.046717	0.306090	0.352032
C	0.717069	1.861191	1.948999
C	-0.637867	1.864598	1.937894
H	1.419809	2.424164	2.547943
H	-1.346076	2.420714	2.535744
C	-2.468325	0.705068	0.817954
C	-3.240744	1.630914	0.060886
C	-3.077230	-0.335573	1.573824
C	-4.635339	1.441849	0.023657
C	-4.474477	-0.475898	1.484034
C	-5.247498	0.394065	0.712467
H	-5.254370	2.131923	-0.548363
H	-4.969722	-1.266569	2.046143
H	-6.330619	0.267163	0.664276
C	2.551062	0.758981	0.760843
C	3.265813	-0.159518	1.577254
C	3.215437	1.613152	-0.162661
C	4.658584	-0.248322	1.399362
C	4.609516	1.474989	-0.292785
C	5.326120	0.549642	0.469100
H	5.231684	-0.947597	2.007627
H	5.147684	2.110448	-0.994894
H	6.407623	0.463254	0.349061
C	0.566668	-2.816735	-1.990193
C	-0.862232	-2.777411	-1.753052
C	0.938445	-1.615290	-2.706143
C	-1.364681	-1.547455	-2.270430
C	-0.242057	-0.816445	-2.844689
N	1.130742	0.942429	0.988723
N	-1.046588	0.943287	0.973168
C	-2.635014	2.852899	-0.644721
C	-2.826776	4.138954	0.196926
C	-3.188087	3.093112	-2.067199
H	-1.556193	2.678648	-0.741644
H	-2.379075	4.056764	1.193708
H	-2.359694	4.997970	-0.306170
H	-3.893369	4.369146	0.329369
H	-3.140209	2.194078	-2.690922
H	-4.232039	3.434827	-2.055442

H	-2.602246	3.878355	-2.565489
C	2.486035	2.704607	-0.955720
C	2.976906	2.850239	-2.411896
C	2.579372	4.074232	-0.239311
H	1.427338	2.422777	-1.002392
H	3.011909	1.885636	-2.929618
H	2.297283	3.510126	-2.969332
H	3.977230	3.300637	-2.473048
H	2.158134	4.043049	0.772052
H	3.624308	4.406037	-0.156999
H	2.029299	4.840596	-0.804839
C	-2.288534	-1.221060	2.545210
C	-2.716959	-2.702385	2.534499
C	-2.368933	-0.657495	3.985035
H	-1.240871	-1.199773	2.228045
H	-2.704247	-3.117378	1.521907
H	-2.018904	-3.291246	3.146348
H	-3.719357	-2.857626	2.957461
H	-1.997679	0.372538	4.047099
H	-3.403364	-0.663458	4.357900
H	-1.763680	-1.270361	4.668875
C	2.594873	-1.005461	2.664651
C	2.920062	-0.458173	4.074687
C	2.942332	-2.506596	2.565502
H	1.511732	-0.925294	2.525016
H	2.622463	0.593041	4.183475
H	2.386823	-1.036672	4.843076
H	3.994847	-0.522414	4.295880
H	2.718115	-2.898662	1.566874
H	3.999945	-2.708119	2.784333
H	2.347823	-3.076289	3.294215
C	2.290544	-1.350231	-3.312214
H	2.391437	-1.863351	-4.284219
H	2.457993	-0.283679	-3.492924
H	3.106614	-1.702227	-2.669569
C	-0.360940	0.449020	-3.650788
H	0.608075	0.939376	-3.791727
H	-0.764597	0.234975	-4.655420
H	-1.031874	1.178111	-3.185143
C	-2.816223	-1.197127	-2.446399
H	-3.446364	-1.613694	-1.652862
H	-2.982715	-0.116892	-2.455478
H	-3.195880	-1.590124	-3.406139
C	-1.680448	-3.923786	-1.221458
H	-1.880313	-4.658917	-2.019996
H	-1.169558	-4.458371	-0.411425

H	-2.653210	-3.593203	-0.841139
C	1.469213	-3.988944	-1.706749
H	1.449059	-4.713240	-2.538637
H	2.512136	-3.677849	-1.570960
H	1.166672	-4.527109	-0.799810

Optimized triplet compressed CoH_2 dihydride structure (H-H frozen at 1.38 A)

Co	-0.025007	1.475208	-0.262968
H	-0.711418	1.890149	1.016532
H	0.667703	1.841775	1.025571
C	-0.001273	-0.593893	0.283509
C	-0.678790	-2.404518	1.556771
C	0.679215	-2.403240	1.556692
H	-1.385351	-3.074044	2.028766
H	1.387028	-3.071343	2.028830
C	2.492124	-1.068653	0.545962
C	3.114593	-1.679835	-0.578078
C	3.234038	-0.331955	1.508479
C	4.497472	-1.482035	-0.744855
C	4.614076	-0.171230	1.281829
C	5.240206	-0.728456	0.166074
H	5.005096	-1.933829	-1.595978
H	5.210734	0.391183	1.999117
H	6.312081	-0.589026	0.013941
C	-2.494066	-1.072306	0.546113
C	-3.238314	-0.343067	1.512622
C	-3.114190	-1.677124	-0.582670
C	-4.619196	-0.187097	1.287803
C	-4.497813	-1.483193	-0.748012
C	-5.243538	-0.739882	0.168954
H	-5.217719	0.368832	2.008542
H	-5.003703	-1.930412	-1.602538
H	-6.316104	-0.604184	0.018340
C	-0.676454	3.621982	-1.020859
C	0.745036	3.580835	-1.028499
C	-1.162009	2.536771	-1.844136
C	1.160018	2.474111	-1.861188
C	-0.021758	1.865414	-2.418034
N	-1.083026	-1.317677	0.781390
N	1.081557	-1.315519	0.781445
C	2.360063	-2.595076	-1.550016
C	2.539052	-4.083003	-1.161210
C	2.746010	-2.389374	-3.030349
H	1.293457	-2.358022	-1.463909
H	2.196706	-4.284967	-0.139274
H	1.962516	-4.728748	-1.839515

H	3.593734	-4.385853	-1.226464
H	2.698847	-1.334627	-3.324292
H	3.757382	-2.755371	-3.254155
H	2.054775	-2.949252	-3.676037
C	-2.355593	-2.580515	-1.562344
C	-2.754919	-2.374160	-3.038891
C	-2.514072	-4.071907	-1.177756
H	-1.291419	-2.330481	-1.482910
H	-2.732872	-1.316669	-3.325561
H	-2.055324	-2.914112	-3.692387
H	-3.759308	-2.761286	-3.258889
H	-2.158776	-4.274404	-0.160412
H	-3.566021	-4.385898	-1.233505
H	-1.937565	-4.708455	-1.864746
C	2.617317	0.218014	2.799017
C	3.000686	1.685836	3.082828
C	2.979190	-0.677966	4.008019
H	1.528378	0.197004	2.681282
H	2.764004	2.328600	2.227700
H	2.433117	2.056495	3.948175
H	4.066637	1.804173	3.321831
H	2.661324	-1.718225	3.860916
H	4.063032	-0.686136	4.191665
H	2.489438	-0.305584	4.919395
C	-2.622481	0.206515	2.803755
C	-2.975831	-0.694841	4.011237
C	-3.015638	1.670959	3.092240
H	-1.533677	0.193501	2.683405
H	-2.650580	-1.732402	3.861526
H	-2.487504	-0.320867	4.922721
H	-4.059320	-0.711302	4.196447
H	-2.788629	2.316870	2.236712
H	-4.081135	1.780495	3.337374
H	-2.446139	2.044525	3.955050
C	-2.603661	2.317679	-2.223029
H	-2.891494	2.950361	-3.080469
H	-2.803316	1.278342	-2.506642
H	-3.286123	2.561162	-1.399130
C	-0.053100	0.879739	-3.554397
H	-1.003790	0.337884	-3.600450
H	0.071724	1.389038	-4.526050
H	0.743677	0.130771	-3.480947
C	2.580140	2.183231	-2.268976
H	3.288709	2.351019	-1.448307
H	2.708305	1.146298	-2.597419
H	2.894056	2.830258	-3.106535

C	1.660271	4.539401	-0.316274
H	1.870878	5.428227	-0.934834
H	1.225539	4.900327	0.625367
H	2.627371	4.080812	-0.075006
C	-1.526122	4.628477	-0.293776
H	-1.662112	5.545828	-0.891093
H	-2.527652	4.238016	-0.074866
H	-1.077845	4.931493	0.662083

Optimized triplet Co(η^2-H_2) dihydrogen structure

C	-0.216665	1.348472	-0.329305
H	-0.763632	2.088950	1.316854
H	-0.038767	1.880934	1.512038
C	0.003379	-0.511221	0.336573
C	-0.647918	-2.468098	1.404014
C	0.708927	-2.448048	1.398249
H	-1.342413	-3.196305	1.800367
H	1.427818	-3.150515	1.797053
C	2.504153	-0.983744	0.563086
C	3.184097	-1.576089	-0.536016
C	3.190579	-0.237599	1.557046
C	4.564484	-1.333562	-0.655332
C	4.571132	-0.030924	1.380394
C	5.250868	-0.559931	0.281979
H	5.115076	-1.769299	-1.487896
H	5.126432	0.539290	2.123681
H	6.322183	-0.387116	0.167608
C	-2.483093	-1.070481	0.525298
C	-3.255882	-0.421185	1.526028
C	-3.077912	-1.606344	-0.650771
C	-4.635403	-0.271276	1.292208
C	-4.462713	-1.428151	-0.821322
C	-5.234093	-0.759590	0.130532
H	-5.253660	0.223836	2.039603
H	-4.948462	-1.828987	-1.709472
H	-6.306832	-0.634877	-0.025314
C	-0.629079	3.455703	-0.859269
C	0.804361	3.326767	-0.842774
C	-1.139971	2.569978	-1.873620
C	1.178538	2.386840	-1.861831
C	-0.015662	1.933048	-2.517520
N	-1.072651	-1.308540	0.760395
N	1.097775	-1.276650	0.749015
C	2.497845	-2.527757	-1.523031
C	2.843894	-4.000875	-1.197163

C	2.814689	-2.225618	-3.002214
H	1.415542	-2.410249	-1.398948
H	2.567848	-4.271352	-0.170751
H	2.308617	-4.680048	-1.876039
H	3.919822	-4.192763	-1.313126
H	2.592872	-1.184477	-3.256953
H	3.866302	-2.418424	-3.253529
H	2.206494	-2.869428	-3.652893
C	-2.288429	-2.421632	-1.681056
C	-2.644164	-2.082001	-3.143857
C	-2.454268	-3.940612	-1.433964
H	-1.228439	-2.177597	-1.549204
H	-2.604269	-1.003540	-3.327052
H	-1.929862	-2.566334	-3.823740
H	-3.644457	-2.437255	-3.425327
H	-2.140291	-4.231223	-0.424137
H	-3.501185	-4.251077	-1.559544
H	-1.847935	-4.514363	-2.149502
C	2.511325	0.255985	2.838540
C	2.841612	1.721863	3.186891
C	2.844520	-0.674716	4.029185
H	1.428990	0.203093	2.677828
H	2.629642	2.388875	2.345403
H	2.233691	2.049317	4.041991
H	3.893511	1.857384	3.472492
H	2.548842	-1.712921	3.830868
H	3.920773	-0.673076	4.251614
H	2.315881	-0.343884	4.934594
C	-2.669172	0.043233	2.863394
C	-2.976813	-0.976610	3.985825
C	-3.135865	1.455112	3.278184
H	-1.580226	0.084553	2.752650
H	-2.582469	-1.973449	3.751443
H	-2.523049	-0.652761	4.933350
H	-4.058577	-1.077476	4.150454
H	-2.977517	2.185618	2.476257
H	-4.199610	1.479595	3.550415
H	-2.571893	1.791951	4.158957
C	-2.577526	2.487546	-2.320751
H	-2.802159	3.234167	-3.101912
H	-2.821970	1.503118	-2.737131
H	-3.277749	2.666173	-1.494443
C	-0.066586	1.122569	-3.785282
H	-1.057457	0.688499	-3.958665
H	0.160864	1.745094	-4.668552
H	0.653384	0.294456	-3.790174

C	2.591742	2.120471	-2.306628
H	3.279366	1.980585	-1.462966
H	2.663280	1.226556	-2.934942
H	2.982974	2.960747	-2.906176
C	1.751072	4.181162	-0.042406
H	1.925022	5.156545	-0.529703
H	1.369806	4.398874	0.964956
H	2.733974	3.707363	0.072710
C	-1.428889	4.455434	-0.064648
H	-1.435920	5.444601	-0.553448
H	-2.477504	4.150604	0.050669
H	-1.021328	4.607719	0.945224

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