Development of more labile low electron count Co(I) sources: catalytic functionalization of activated alkanes using a [$(Cp^*Co)_2$-μ-(η^4:η^4-arene)] complex

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-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 cyclohexane-d_{12} 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. $Co(acac)_2$ was purchased from Strem and sublimed prior to use. Cp*Co(acac),[2] **3**,[3] **4**,[4] **6-10**,[4] and **11**,[5] and **12**[6] were prepared according to literature procedures. Vinyltrimethylsilane was purchased from Alfa Aesar and dried over sieves prior to use. Sodium metal, potassium metal, and graphite were purchased from Aldrich and used as received. Trimethylphosphine was purchased from Strem and used as received. Potassium graphite was prepared by vigorous stirring of potassium metal and graphite under vacuum at 100 ºC for 15 minutes. Graphite powder or flakes (Aldrich) can both be used interchangeably. ^{1}H and ^{13}C NMR spectra were recorded on a Mercury Plus 300 Spectrometer operating at 300.07 MHz (^{1}H) and 75.46 MHz (^{13}C), respectively. Two-dimensional NMR spectra were recorded on an INOVA 500 MHz spectrometer operating at 499.71 MHz (^{1}H) and 125.67 MHz (^{13}C), respectively. 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.

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 150 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 (Version 6.14) 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.

Preparation of [$(Cp^*Co)_2$-μ-(η^4:η^4-benzene)] (1). A 50 mL round-bottomed flask was charged with 0.275 g (2.04 mmol) of KC_8 and approximately 10 mL of pentane. While stirring, 0.300 g (1.02 mmol) of Cp*Co(acac) was added, followed by 0.241 g (3.09 mmol) of benzene. The resulting reaction mixture was stirred vigorously for 7 hours, and the dark red solution was decanted from the KC_8 and filtered through Celite. Removal of the pentane *in vacuo* followed by recrystallization from pentane at -35 °C afforded 0.139 g (67%) of **1** as a dark red solid. Spectral data match previous reports of the complex.[7]

Preparation of [$(Cp^*Co)_2$-μ-(η^4:η^4-toluene)] (2). A 50 mL round-bottomed flask was charged with 0.276 g (2.05 mmol) of KC_8 and approximately 10 mL of pentane. While stirring, 0.301 g (1.02 mmol) of Cp*Co(acac) was added, followed by 0.282 g (3.07 mmol) of toluene. The resulting reaction mixture was stirred vigorously for 7 hours, and the dark red solution was decanted from the KC_8 and filtered through Celite. Removal of the pentane *in vacuo* followed by recrystallization from pentane at -35 °C afforded 0.152 g (71 %) of **2** as a dark red solid. Spectral

data match previous reports of the complex.[7] The complex can also be prepared using neat toluene in a similar manner with comparable isolated yields of **2**. ^{1}H NMR (cyclohexane-d_{12}): δ = 1.38 (s, 3H, toluene CH_3), 1.77 (s, 30H, Cp*), 2.67 (br, 2H, toluene), 2.78 (br, 2H, toluene), 2.91 (br, 1H, toluene). ^{13}C NMR (cyclohexane-d_{12}): δ = 11.00 (toluene CH$_3$), 26.50 (Cp*), 52.94, 55.09, 55.74 (toluene), 85.68 (Cp*).

Standard catalytic run of 4 and 6-10 using catalyst 2. A 75 mL thick walled glass vessel was charged with 0.012 g (11.8 mmol) of **2** and dissolved in approximately 2 mL of benzene, followed by addition of 0.098 g (0.56 mmol) of **5**. The reaction mixture was then stirred at 45 °C for 3h. The solvent was removed *in vacuo* and the resulting product was redissolved in pentane and filtered through Celite for further analysis by NMR spectroscopy. A similar procedure was followed for catalytic runs using **6**-**10** instead of **4** as previously described, also using 5 mol % of **2** with respect to the substrate.

The catalysis can also be performed at lower catalysts loadings for **2** (down to 2 mol%) with full conversion to products, except in the case of **9**, though additional heating is required (between 8-24 hours depending on substrate).

Note: In catalytic runs, purity of **2** and substrate are critical. Substrate must be freshly distilled from unidentified impurities which develop over the course of weeks, as observed by ^{1}H NMR spectroscopy in benzene-d_6. Also, the quality of Co(acac)$_2$ used in synthesis of Cp*Co(acac) prior to preparation of **2** is crucial. Incorrect stoichiometry between Cp*$_2$Mg and Co(acac)$_2$ leads to formation of Cp*$_2$Co which is present even after the reduction to form **2**. This impurity reduces the amount of active catalyst present and decreases the rate of catalytic turnover with substrates at lower temperatures.

Characterization of Cp*Co(η^2-H$_2$C=CHSiMe$_2$(NC$_5$H$_{10}$))(PMe$_3$) (15). A 50 mL round-bottomed flask was charged with 0.320 g (0.67 mmol) of **2**, approximately 5 mL of benzene and 0.225 g (1.33 mmol) of **4**. The resulting reaction mixture was stirred vigorously for 6 hours, followed by addition of 0.253 g (3.33 mmol) of PMe$_3$ and stirring for 12 additional hours. After removal of the benzene *in vacuo*, the compound was dissolved in pentane and filtered through Celite affording 0.302 g (52%) of **15** as a dark red oil after solvent removal. Samples for combustion analysis consistently gave lower than expected C and H contents, perhaps due to decomposition to **5** and **16**, as observed over time in solution. ^{1}H NMR (benzene-d_6): δ = 0.08 (m, 1H, -CH=CH$_2$), 0.32 (s, 3H, Si(CH_3)$_2$), 0.33 (s, 3H, Si(CH_3)$_2$), 0.90 (d, 9H, P(CH_3)$_3$), 1.25 (m, 1H, -CH=C(H *trans*)H), 1.43 (m, 4H, (CH_2CH$_2$)$_2$N), 1.56 (m, 2H, CH_2(CH$_2$CH$_2$)$_2$N), 1.61 (s, 15H, Cp*), 2.15 (br, 1H, -CH=C(H *cis*)H), 3.04 (m, 4H, N-(CH_2)$_2$). ^{13}C NMR (benzene-d_6): δ = 2.59, 3.50 (Si(CH_3)$_2$). 10.34 (Cp*), 18.60 (P(CH$_3$)$_3$), 23.69 (-CH=CH$_2$), 26.51 (CH$_2$(CH$_2$CH$_2$)$_2$N), 28.30 ((CH$_2$CH$_2$)$_2$N), 37.10 (-C(H)=CH$_2$), 47.22 (N-(CH$_2$)$_2$) 89.79 (Cp*). ^{31}P NMR (benzene-d_6): δ = 9.07.

Half life determination in the reaction between 2 and 4. A J. Young NMR tube was charged with 0.2 mL of a 0.088 M stock solution of **2**, 0.1 mL of a 0.088 M stock solution of Cp$_2$Fe, and 0.2 mL of a 0.176 M stock solution of **4**. Stock solutions were prepared using benzene-d_6, and cyclohexane-d_{12}. The reaction was then monitored at various times by ^{1}H NMR spectroscopy at ambient temperature. Half-life measurements for consumption of **4** and formation of **5** were averaged over 3 independent trials in each of the aforementioned deuterated solvents, using the

ferrocene resonance as an internal standard. Mixing of the clearly distinguishable phases of **2** and **4** was done previous to insertion of the J. Young tube into the probe.

Half life determination in the reaction between 3 and 4. A J. Young NMR tube was charged with 0.2 mL of a 0.156 M stock solution of **3**, 0.1 mL of a 0.088 M stock solution of Cp_2Fe, and 0.2 mL of a 0.156 M stock solution of **4**. Stock solutions were prepared using benzene-d_6 and cyclohexane-d_{12}. The reaction was then monitored at various times by ^{1}H NMR spectroscopy at ambient temperature. Half-life measurements for consumption of **4** and formation of **5** were averaged over two independent trials in each of the aforementioned deuterated solvents. Mixing of the clearly distinguishable phases of **3** and **4** was done previous to insertion of the J. Young tube into the probe.

Concentration dependence study in the reaction between 2 and vinyltrimethylsilane. A J. Young NMR tube was charged with 0.2 mL of a 0.044 M benzene-d_6 stock solution of **2**, 0.1 mL of a 0.088 M stock solution of Cp_2Fe, and 0.2 mL of a stock solution of vinyltrimethylsilane in benzene-d_6. Three different concentrations of vinyltrimethylsilane stock solutions were used (0.177 M, 0.352 M, and 0.528 M) corresponding to 4, 8, and 12 eq. respectively, relative to the concentration of **2**. Half-life measurements for disappearance of **2** and formation of **3** were averaged over two independent trials for each concentration, using a NMR probe that allowed recording of spectra in 1 minute intervals. Mixing of the clearly distinguishable phases of **2** and vinyltrimethylsilane was done immediately prior to insertion of the J. Young tube into the NMR probe at 25 ºC.

Computational Details.

All DFT calculations were performed using a hybrid functional [the three-parameter exchange functional of Becke (B3)[8] and the correlation functional of Lee, Yang, and Parr (LYP)][9] (B3LYP) as implemented in Gaussian 09.[10] The cobalt atom uses the effective core potential and associated basis set of Hay and Wadt (LANL2DZ)[11,12] in which the two outermost p functions were replaced by reoptimized 4p functions as suggested by Couty and Hall,[13] and an f polarization function[14] was added. All other atoms use the 6-31G(d',p') basis set.[15-17] 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** (1 of the 4 molecules in the asymmetric unit) and **11**.

Supplementary Information

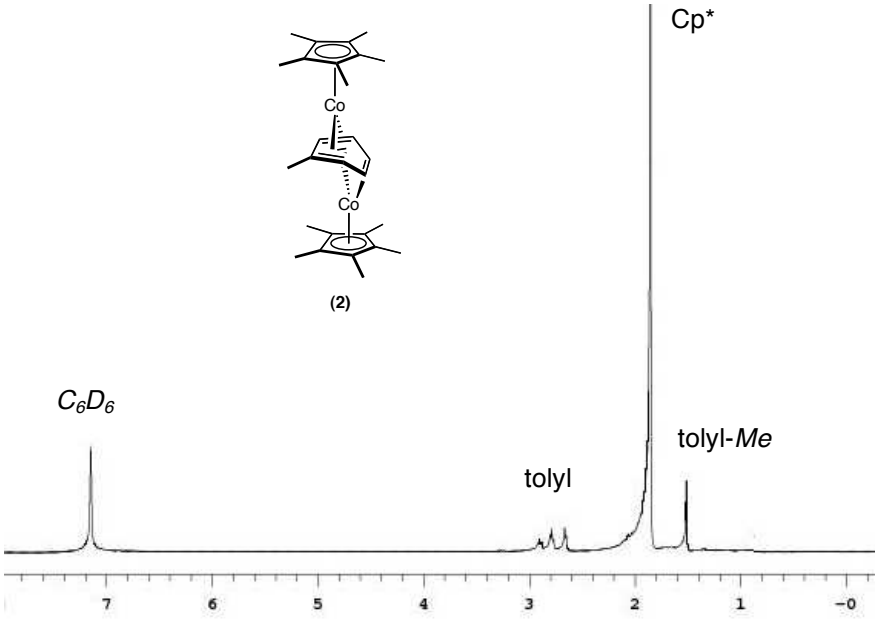

Figure S1. ^{1}H NMR spectrum of **2** in benzene-d_6.

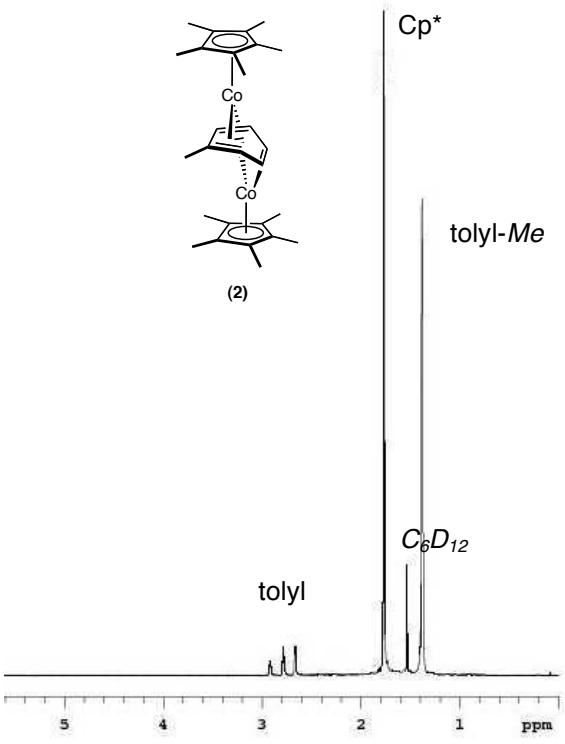

Figure S2. ^{1}H NMR spectrum of **2** in cyclohexane-d_{12}.

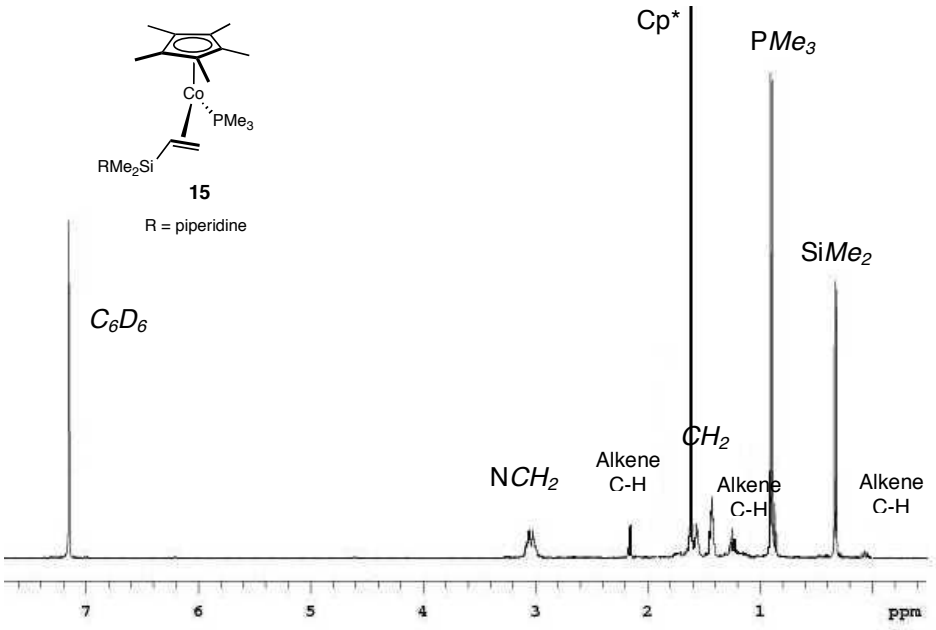

Figure S3. ^{1}H NMR spectrum of **15** in benzene-d_6.

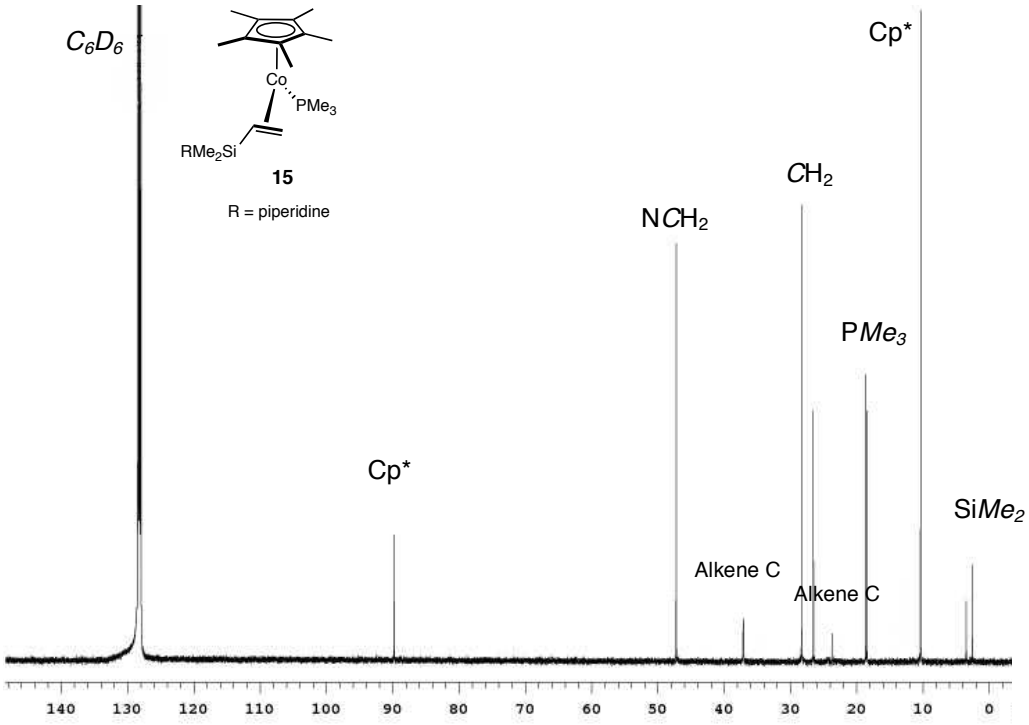

Figure S4. ^{13}C NMR spectrum of **15** in benzene-d_6.

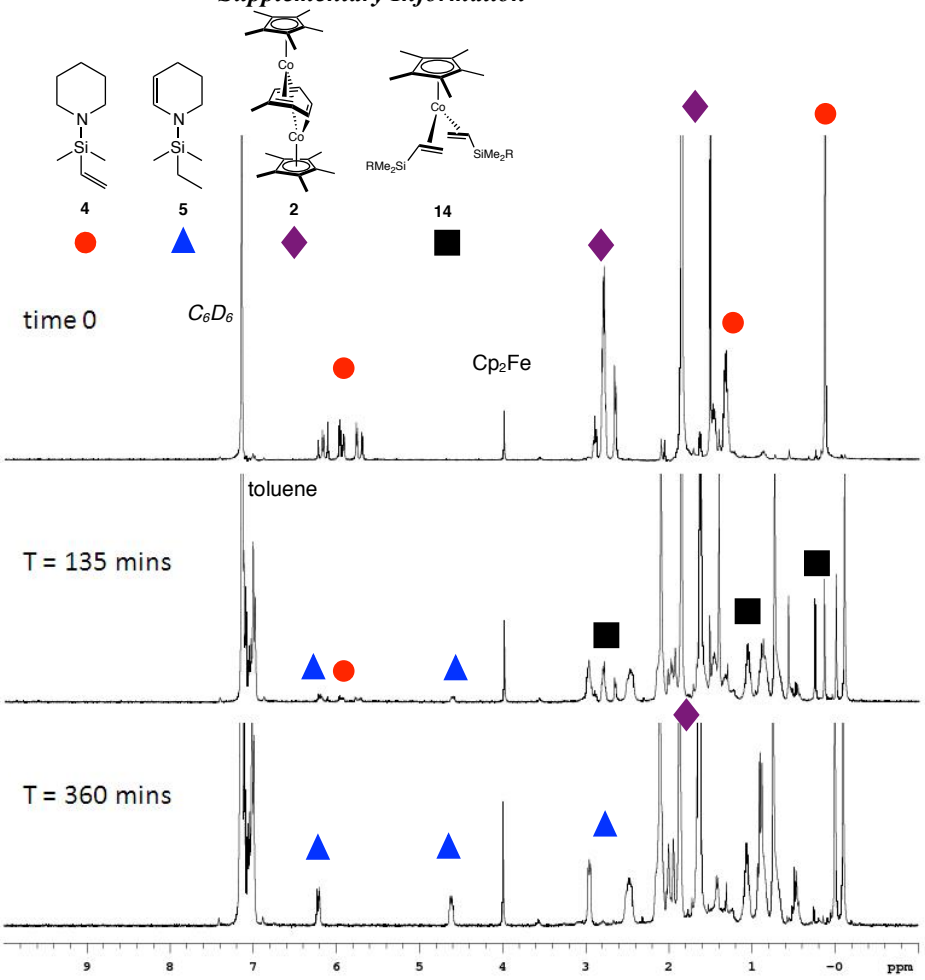

Figure S5. ^{1}H NMR spectra of stoichiometric addition of **4** to **2** in benzene-d_6 as a function of time. (Only one potential isomer of **14** is drawn.)

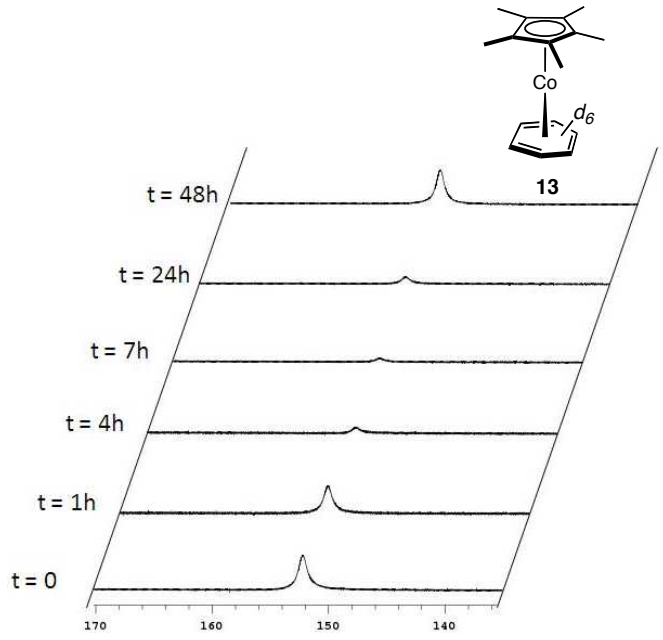

Figure S6. ^{1}H NMR spectra, indicating the change in concentration of **13**, of stoichiometric addition of **4** to **2** in benzene-d_6 at 25 ºC as a function of time.

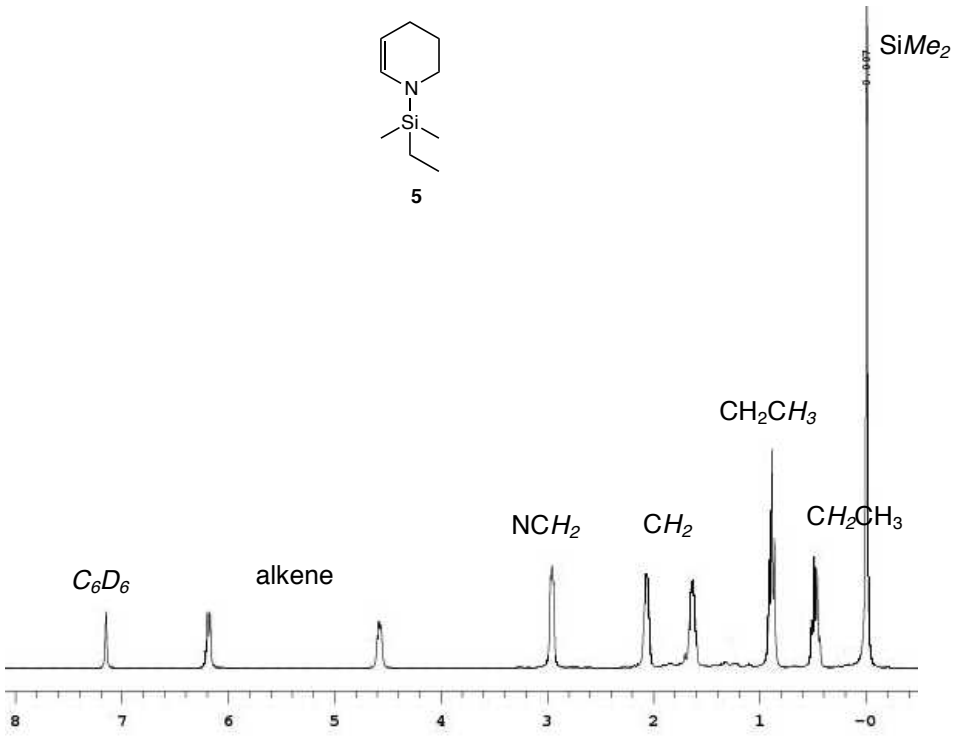

Figure S7. Representative ^{1}H NMR spectrum of catalytic conversion of **4** to **5** using 5 mol% **2** after 3 hours at 45 ºC in benzene-d_6. A trap-to-trap distillation was performed to isolate **5** from **2**.

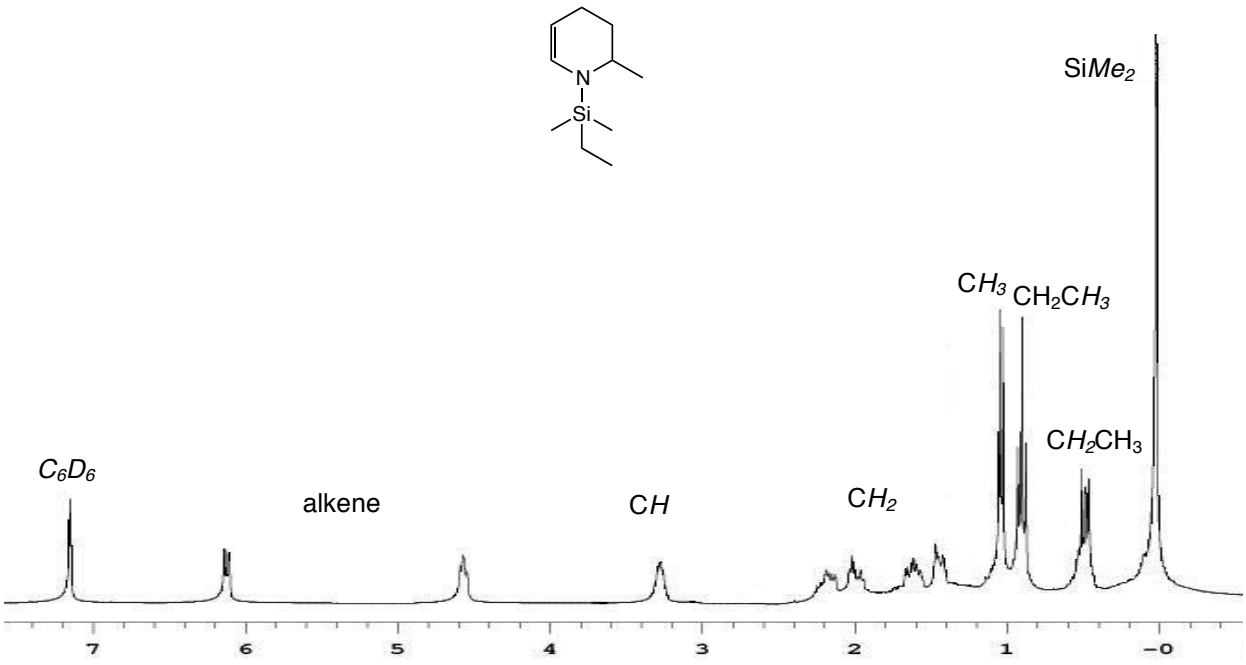

Figure S8. Representative ^{1}H NMR spectrum of catalytic conversion of **6** using 5 mol% **2** after 3 hours at 45 ºC in benzene-d_6. A trap-to-trap distillation was performed to isolate the product from **2**.

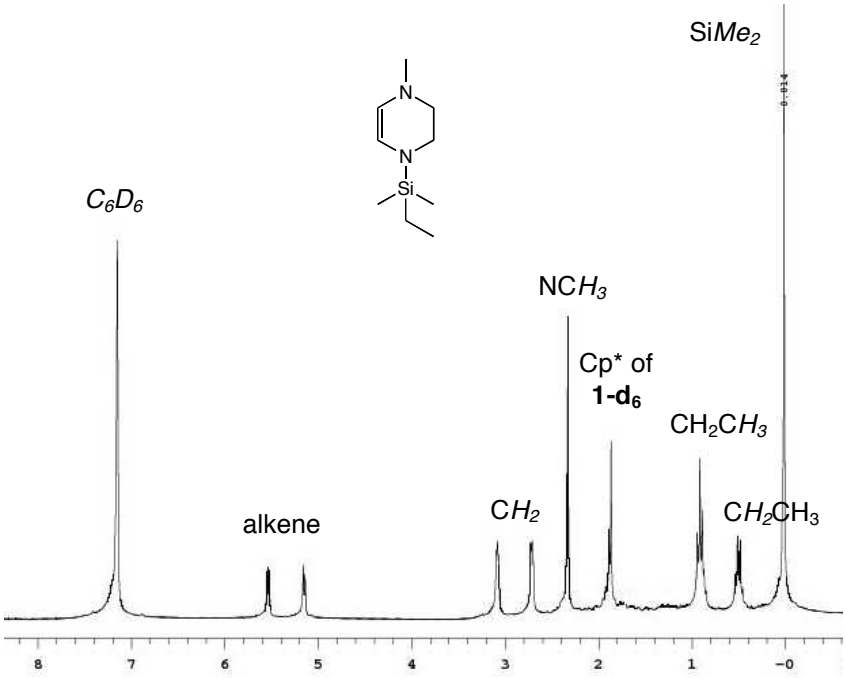

Figure S9. Representative ^{1}H NMR spectrum of catalytic conversion of **7** using 5 mol% of **2** after 7 hours at 45 ºC in benzene-d_6. No separation from catalyst was performed.

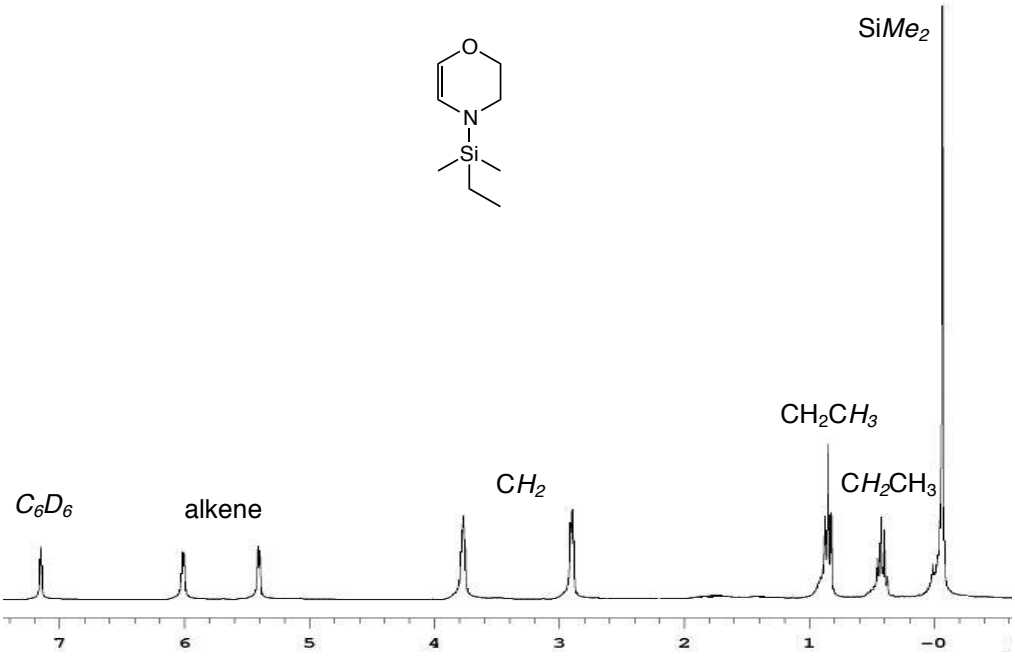

Figure S10. Representative ^{1}H NMR spectrum of catalytic conversion of **8** using 5 mol% of **2** after 7 hours at 45 ºC in benzene-d_6. N A trap-to-trap distillation was performed to isolate product from **2**.

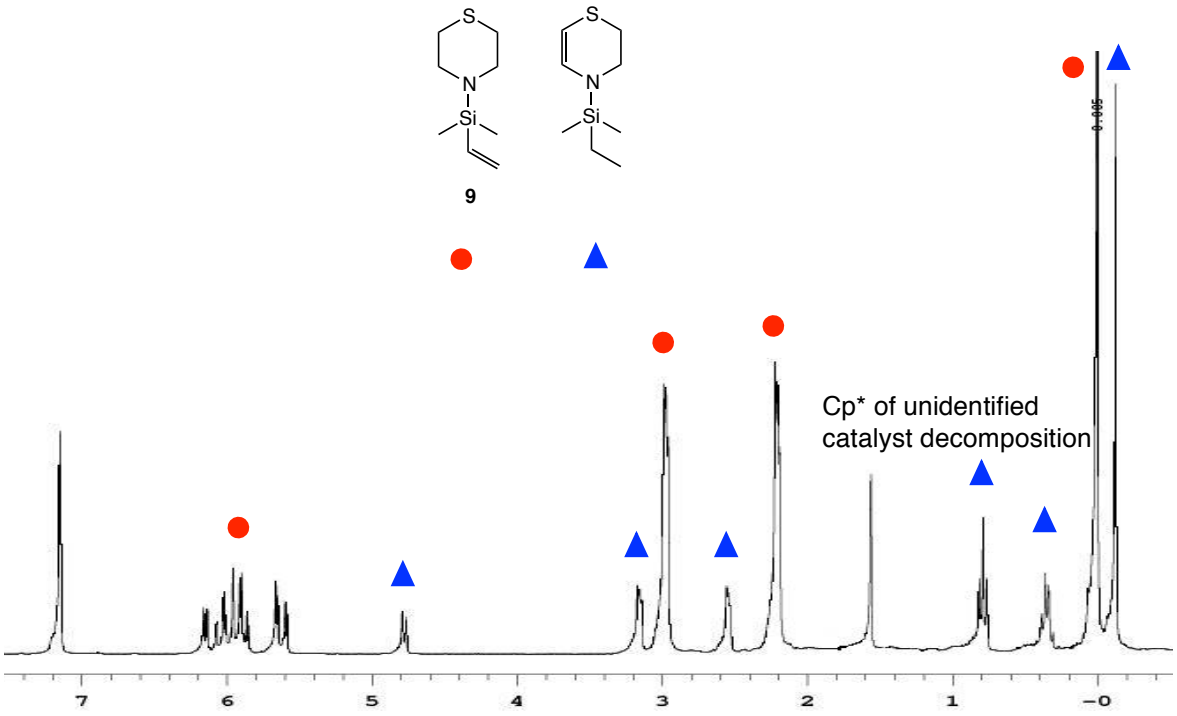

Figure S11. Representative ^{1}H NMR spectrum of catalytic conversion of **9** using 5 mol% of **2** after 48 hours at 45 ºC in benzene-d_6. Only partial conversion to product is observed.

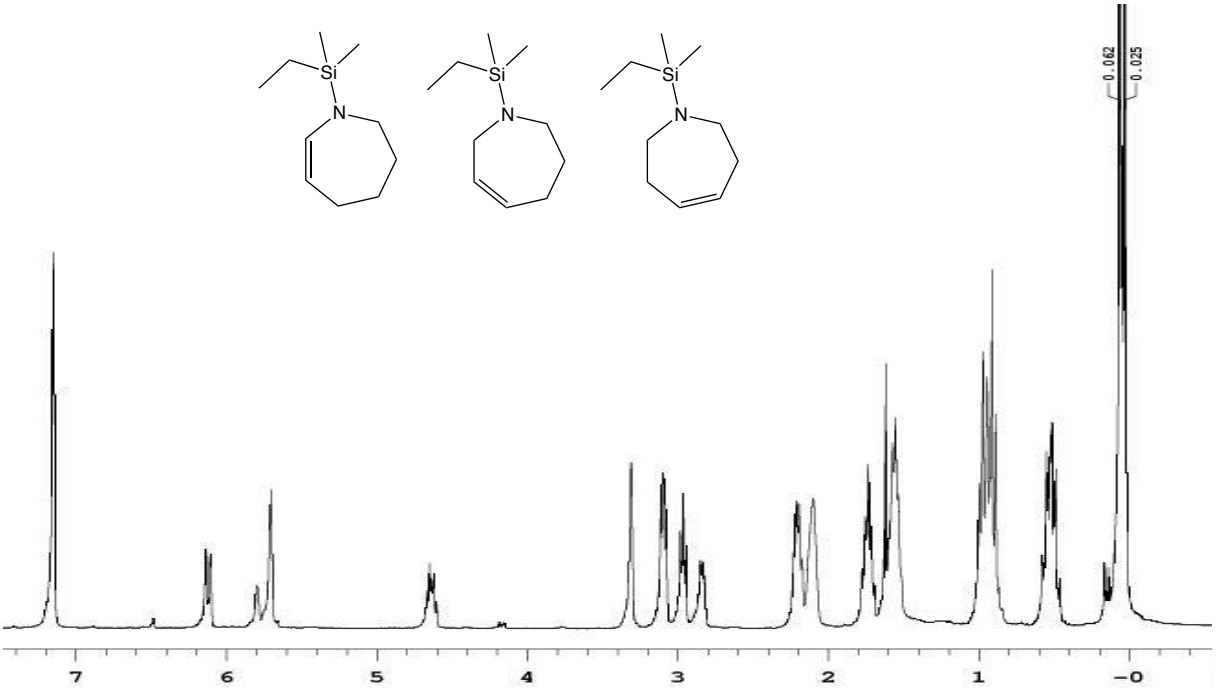

Figure S12. Representative ^{1}H NMR spectrum of catalytic conversion of **10** using 5 mol% of **2** after 3 hours at 45 ºC in benzene-d_6. Note a mixture of isomeric products are observed but no **10** remains.

Supplementary Information

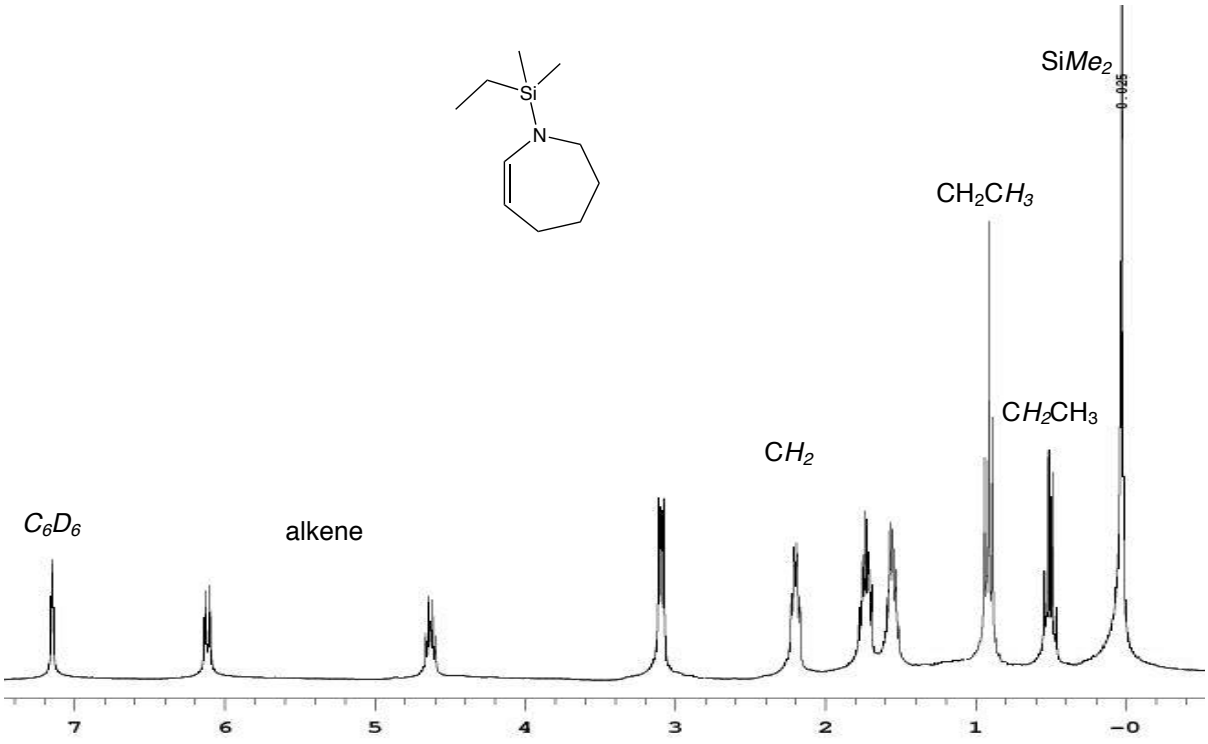

Figure S13. Representative ^{1}H NMR spectrum of catalytic conversion of **10** using 5 mol% of **2** after 9 hours at 45 ºC in benzene-d_6. Note only one isomer remains after the prolonged thermolysis.

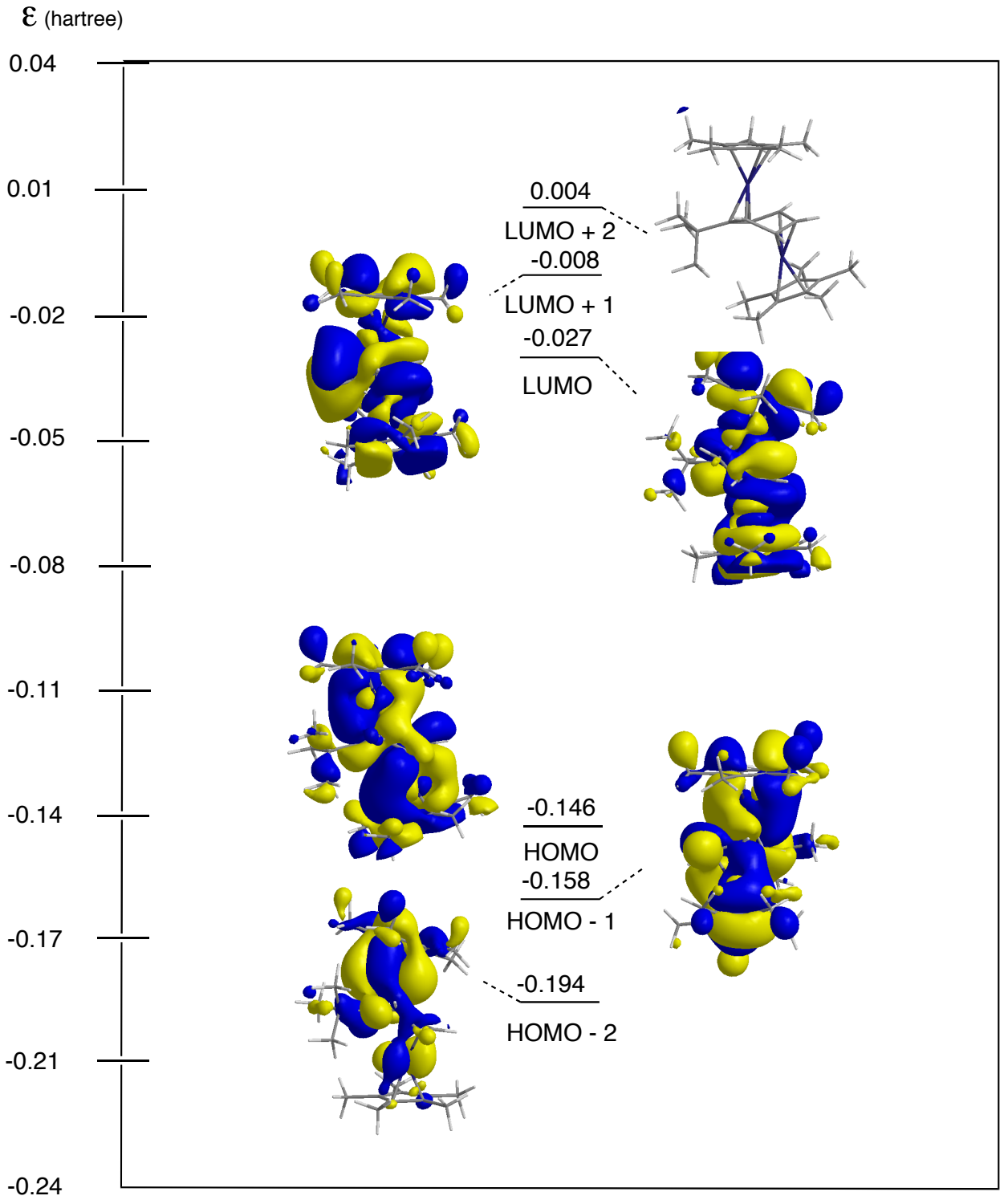

Figure S13. Frontier molecular orbital diagram of **2** as calculated using the Gaussian 09 program suite. Basis set: B3LYP, 631-G (C/H); LANL2DZ (Co). Isocontour values = 0.01.

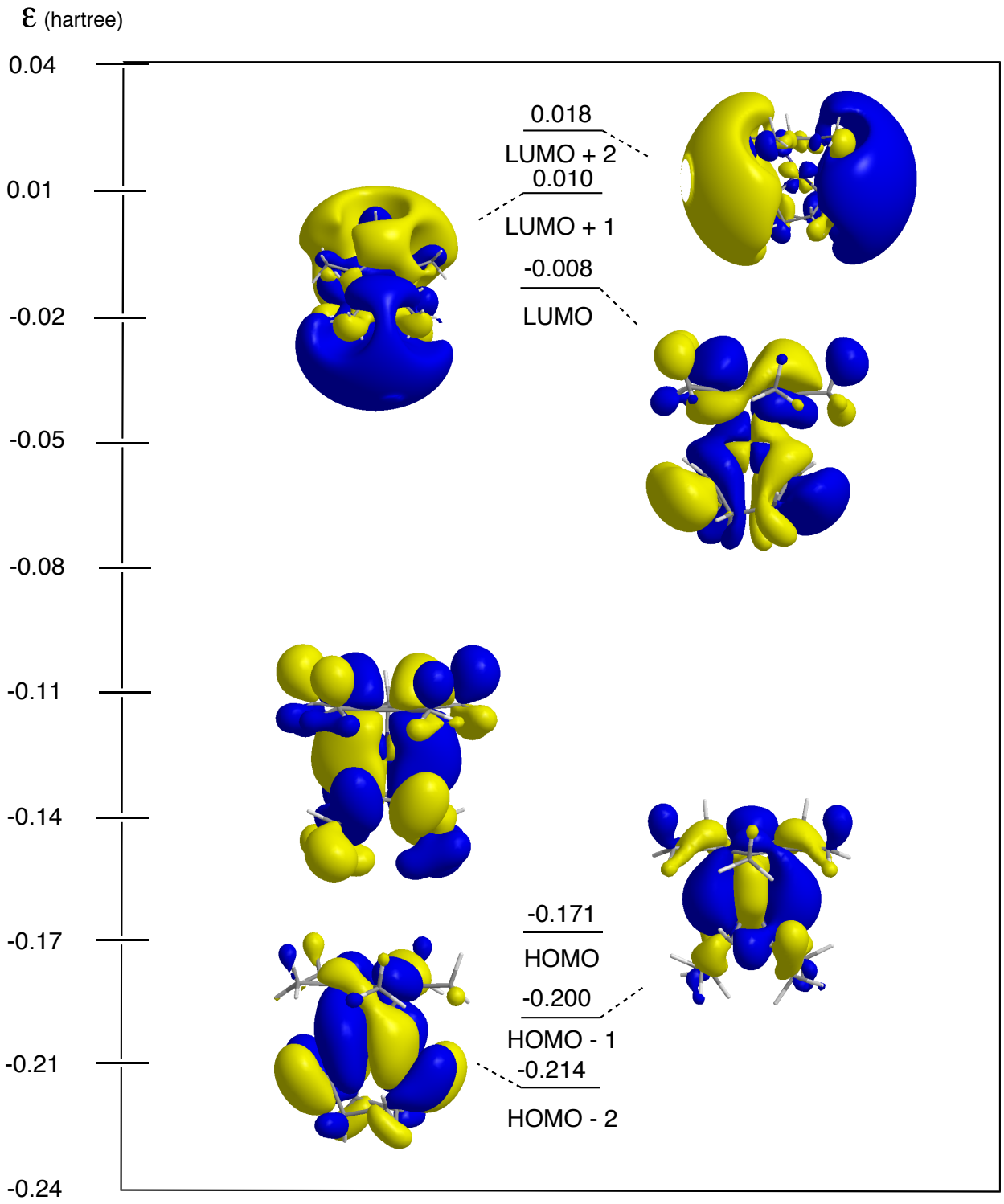

Figure S14. Frontier molecular orbital diagram of **11** as calculated using the Gaussian 09 program suite. Basis set: B3LYP, 631-G (C/H); LANL2DZ (Co). Isocontour values = 0.01.

Supplementary Information

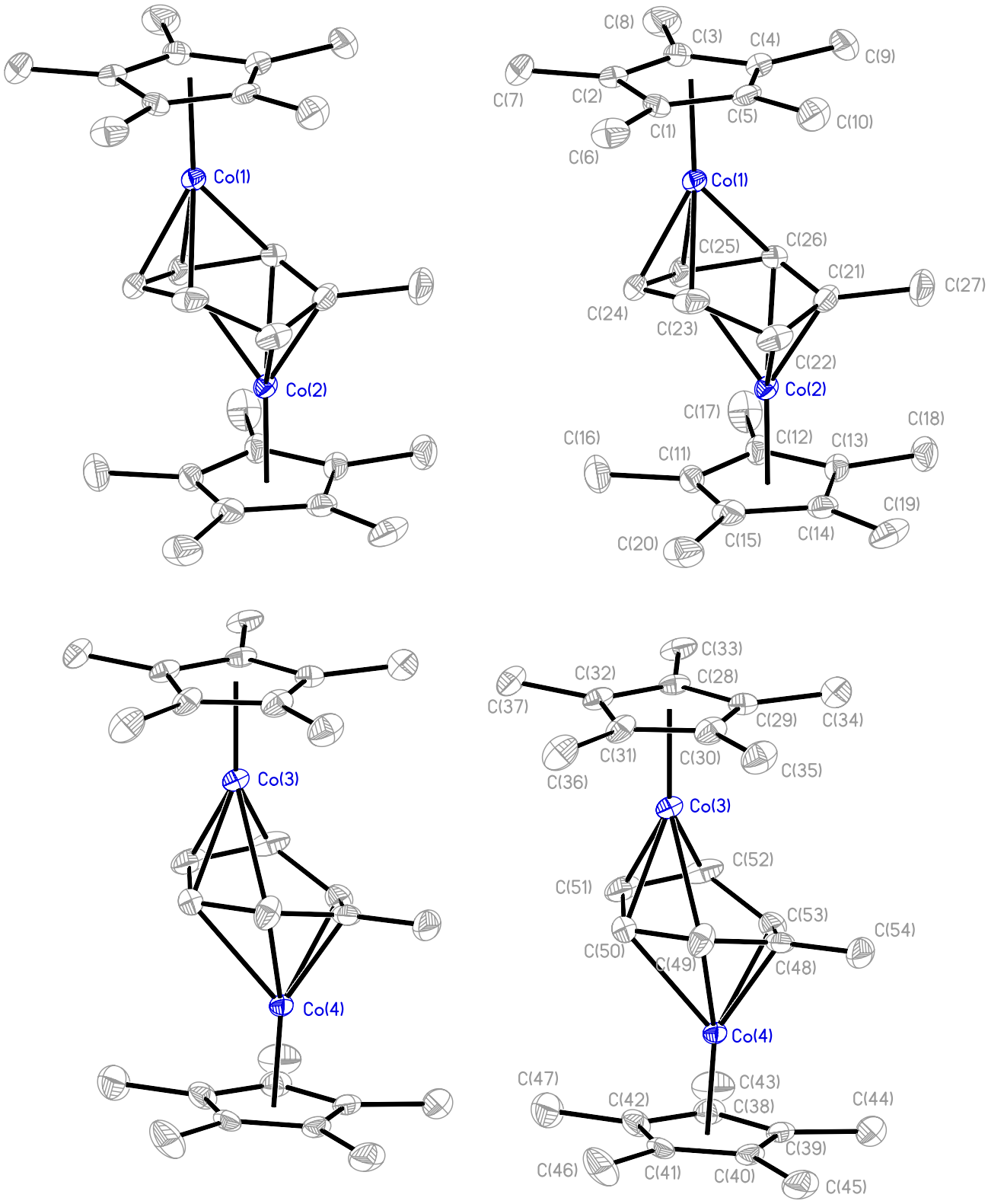

Figure S15. Molecular structures of two of the four molecules in the asymmetric unit of **2** with 30 % probability ellipsoids and full atom labeling schemes. Hydrogen atoms omitted for clarity.

Supplementary Information

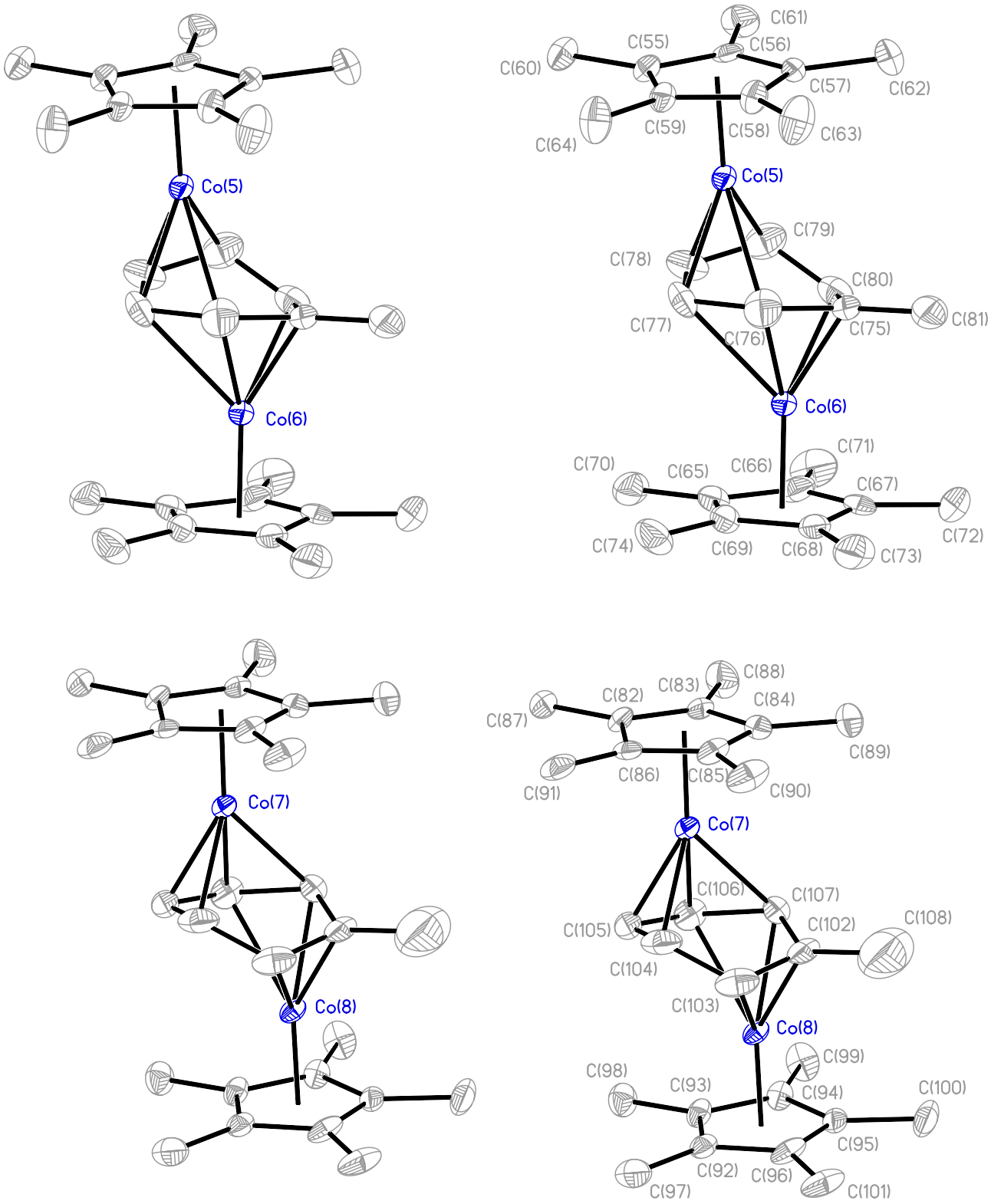

Figure S16. Molecular structures of the other two molecules in the asymmetric unit of **2** with 30 % probability ellipsoids and full atom labeling schemes. Hydrogen atoms omitted for clarity.

Supplementary Information

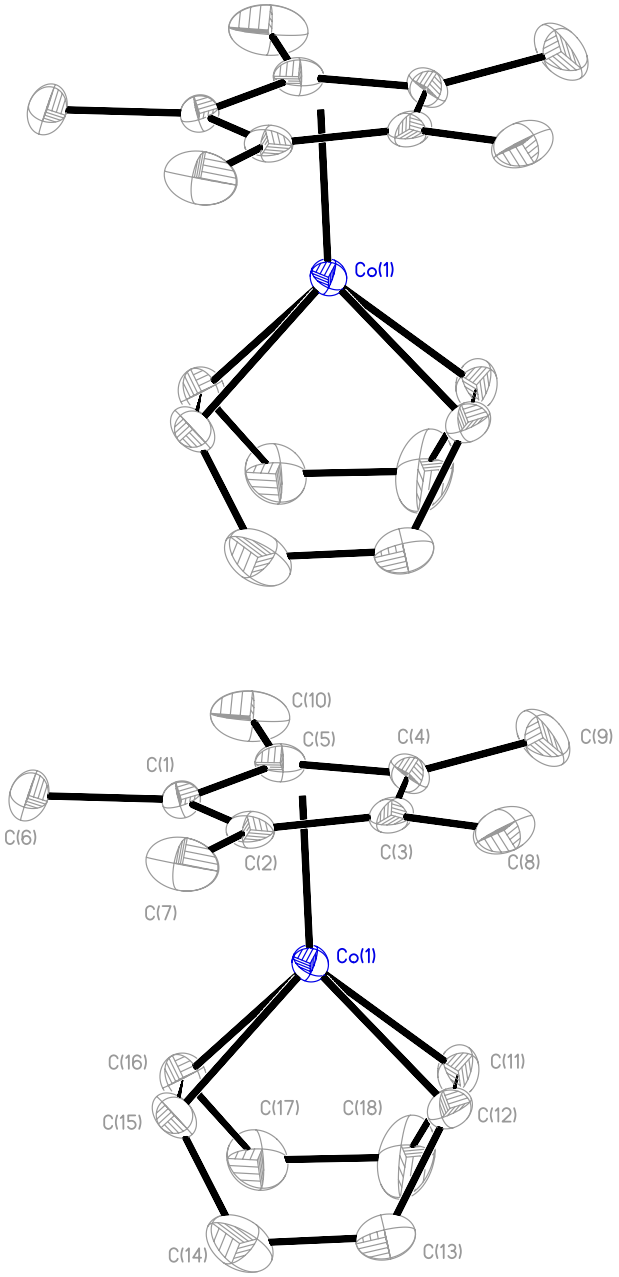

Figure S17. Molecular structure of **11** with 30 % probability ellipsoids and full atom labeling schemes. Hydrogen atoms omitted for clarity.

Supplementary Information

Table 1. Crystallographic data for complexes **2** and **11**.

Compound	**2**	**11**
Empirical formula	$C_{27}H_{38}Co_2$	$C_{18}H_{27}Co$
Formula mass	480.43	302.33
a [Å]	11.0407(11)	12.590(3)
b [Å]	13.9848(14)	9.245(2)
c [Å]	31.459(3)	14.347(3)
α [°]	89.798(10)	90
β [°]	85.884(10)	112.057(4)
γ [°]	89.751(10)	90
V [Å^3]	4844.7(8)	1547.7(6)
Z	8	4
Crystal system	Triclinic	Monoclinic
Space group	P-1	P2(1)/c
T [K]	150(2)	150(2)
$D_{calcd.}$ [g cm^{-3}]	1.317	1.297
μ [mm^{-1}]	1.380	1.094
$2\theta_{max.}$ [°]	25.67	25.68
Reflections measured	68111	14391
Reflections used (R_{int})	18288(0.0445)	2947(0.0377)
Restraints/parameters	0/1089	0/193
R_1 [$I > 2\sigma(I)$]	0.0856	0.0374
wR_2 [$I > 2\sigma(I)$]	0.1762	0.0903
$R(F_o^2)$ (all data)	0.0996	0.0494
$R_w(F_o^2)$ (all data)	0.1816	0.0973
GOF on F^2	1.213	1.012

Further crystallographic information can be found on the Cambridge Structural Database (CSD) for **2** (CCDC #: 841425) and **11** (CCDC #: 841426).

Table 2. Bond lengths [Å] and angles [°] for **2**

Co(1)-C(24)	1.930(7)
Co(1)-C(1)	2.007(7)
Co(1)-C(23)	2.051(7)
Co(1)-C(25)	2.053(7)
Co(1)-C(5)	2.066(7)
Co(1)-C(4)	2.080(7)
Co(1)-C(3)	2.086(7)
Co(1)-C(2)	2.094(7)
Co(1)-C(26)	2.254(7)
Co(2)-C(21)	1.908(7)
Co(2)-C(22)	2.047(7)
Co(2)-C(15)	2.052(7)
Co(2)-C(26)	2.056(7)
Co(2)-C(14)	2.062(7)
Co(2)-C(13)	2.071(6)
Co(2)-C(11)	2.083(7)
Co(2)-C(12)	2.086(7)
Co(2)-C(25)	2.254(7)
Co(3)-C(51)	1.917(7)
Co(3)-C(28)	2.028(6)
Co(3)-C(52)	2.031(7)
Co(3)-C(29)	2.057(7)
Co(3)-C(50)	2.069(8)
Co(3)-C(32)	2.082(7)
Co(3)-C(31)	2.093(7)
Co(3)-C(30)	2.102(7)
Co(3)-C(49)	2.320(8)
Co(4)-C(48)	1.924(7)
Co(4)-C(49)	2.037(7)
Co(4)-C(38)	2.045(7)
Co(4)-C(39)	2.046(7)
Co(4)-C(53)	2.053(7)
Co(4)-C(40)	2.075(6)
Co(4)-C(41)	2.081(6)
Co(4)-C(42)	2.089(7)
Co(4)-C(50)	2.289(8)
Co(5)-C(78)	1.966(10)
Co(5)-C(77)	2.013(9)
Co(5)-C(56)	2.042(7)
Co(5)-C(57)	2.042(7)
Co(5)-C(59)	2.074(7)
Co(5)-C(58)	2.079(8)
Co(5)-C(55)	2.096(7)
Co(5)-C(79)	2.102(9)
Co(5)-C(76)	2.273(10)
Co(6)-C(75)	1.930(8)
Co(6)-C(76)	2.026(9)
Co(6)-C(80)	2.037(9)
Co(6)-C(67)	2.039(8)
Co(6)-C(69)	2.058(7)
Co(6)-C(66)	2.063(8)
Co(6)-C(68)	2.085(7)

Co(6)-C(65)	2.098(7)
Co(6)-C(77)	2.327(10)
Co(7)-C(105)	1.938(8)
Co(7)-C(86)	2.025(7)
Co(7)-C(106)	2.040(8)
Co(7)-C(85)	2.047(7)
Co(7)-C(104)	2.066(8)
Co(7)-C(84)	2.071(7)
Co(7)-C(83)	2.083(7)
Co(7)-C(82)	2.101(7)
Co(7)-C(107)	2.276(8)
Co(8)-C(102)	1.897(7)
Co(8)-C(103)	2.039(8)
Co(8)-C(107)	2.042(8)
Co(8)-C(96)	2.053(7)
Co(8)-C(92)	2.063(7)
Co(8)-C(93)	2.071(7)
Co(8)-C(94)	2.080(7)
Co(8)-C(95)	2.083(7)
Co(8)-C(106)	2.264(8)
C(1)-C(5)	1.431(10)
C(1)-C(2)	1.436(9)
C(1)-C(6)	1.513(10)
C(2)-C(3)	1.426(10)
C(2)-C(7)	1.486(10)
C(3)-C(4)	1.424(10)
C(3)-C(8)	1.505(11)
C(4)-C(5)	1.421(10)
C(4)-C(9)	1.505(10)
C(5)-C(10)	1.497(10)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(15)	1.408(11)
C(11)-C(12)	1.435(10)
C(11)-C(16)	1.505(10)
C(12)-C(13)	1.412(9)
C(12)-C(17)	1.491(11)
C(13)-C(14)	1.420(10)
C(13)-C(18)	1.516(9)
C(14)-C(15)	1.479(10)
C(14)-C(19)	1.484(11)

C(15)-C(20)	1.495(10)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.420(11)
C(21)-C(26)	1.437(10)
C(21)-C(27)	1.509(10)
C(22)-C(23)	1.461(11)
C(22)-H(22)	0.9500
C(23)-C(24)	1.416(11)
C(23)-H(23)	0.9500
C(24)-C(25)	1.414(10)
C(24)-H(24)	0.9500
C(25)-C(26)	1.466(9)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(32)	1.418(10)
C(28)-C(29)	1.423(10)
C(28)-C(33)	1.525(10)
C(29)-C(30)	1.406(10)
C(29)-C(34)	1.531(11)
C(30)-C(31)	1.435(10)
C(30)-C(35)	1.496(10)
C(31)-C(32)	1.427(10)
C(31)-C(36)	1.513(11)
C(32)-C(37)	1.506(10)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-H(37A)	0.9800

C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-C(42)	1.410(11)
C(38)-C(39)	1.454(10)
C(38)-C(43)	1.503(11)
C(39)-C(40)	1.411(10)
C(39)-C(44)	1.504(11)
C(40)-C(41)	1.423(10)
C(40)-C(45)	1.516(10)
C(41)-C(42)	1.446(10)
C(41)-C(46)	1.496(11)
C(42)-C(47)	1.499(10)
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-C(49)	1.416(10)
C(48)-C(53)	1.423(10)
C(48)-C(54)	1.503(10)
C(49)-C(50)	1.449(10)
C(49)-H(49)	0.9500
C(50)-C(51)	1.408(12)
C(50)-H(50)	0.9500
C(51)-C(52)	1.397(12)
C(51)-H(51)	0.9500
C(52)-C(53)	1.470(10)
C(52)-H(52)	0.9500
C(53)-H(53)	0.9500
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-C(59)	1.400(10)
C(55)-C(56)	1.424(10)
C(55)-C(60)	1.483(10)
C(56)-C(57)	1.422(10)
C(56)-C(61)	1.512(10)
C(57)-C(58)	1.423(10)
C(57)-C(62)	1.522(10)
C(58)-C(59)	1.447(10)
C(58)-C(63)	1.479(11)
C(59)-C(64)	1.523(10)
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800

C(60)-H(60C)	0.9800
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-C(69)	1.421(10)
C(65)-C(66)	1.434(11)
C(65)-C(70)	1.478(11)
C(66)-C(67)	1.454(12)
C(66)-C(71)	1.504(12)
C(67)-C(68)	1.418(12)
C(67)-C(72)	1.488(12)
C(68)-C(69)	1.430(10)
C(68)-C(73)	1.507(11)
C(69)-C(74)	1.510(11)
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
C(73)-H(73A)	0.9800
C(73)-H(73B)	0.9800
C(73)-H(73C)	0.9800
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
C(75)-C(80)	1.427(13)
C(75)-C(76)	1.437(12)
C(75)-C(81)	1.469(11)
C(76)-C(77)	1.508(13)
C(76)-H(76)	0.9500
C(77)-C(78)	1.370(14)
C(77)-H(77)	0.9500
C(78)-C(79)	1.351(14)
C(78)-H(78)	0.9500
C(79)-C(80)	1.451(13)
C(79)-H(79)	0.9500
C(80)-H(80)	0.9500
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(82)-C(83)	1.428(10)

C(82)-C(86)	1.438(10)
C(82)-C(87)	1.489(10)
C(83)-C(84)	1.461(11)
C(83)-C(88)	1.503(11)
C(84)-C(85)	1.418(11)
C(84)-C(89)	1.506(11)
C(85)-C(86)	1.440(10)
C(85)-C(90)	1.508(10)
C(86)-C(91)	1.479(11)
C(87)-H(87A)	0.9800
C(87)-H(87B)	0.9800
C(87)-H(87C)	0.9800
C(88)-H(88A)	0.9800
C(88)-H(88B)	0.9800
C(88)-H(88C)	0.9800
C(89)-H(89A)	0.9800
C(89)-H(89B)	0.9800
C(89)-H(89C)	0.9800
C(90)-H(90A)	0.9800
C(90)-H(90B)	0.9800
C(90)-H(90C)	0.9800
C(91)-H(91A)	0.9800
C(91)-H(91B)	0.9800
C(91)-H(91C)	0.9800
C(92)-C(93)	1.419(10)
C(92)-C(96)	1.436(11)
C(92)-C(97)	1.493(10)
C(93)-C(94)	1.436(10)
C(93)-C(98)	1.505(10)
C(94)-C(95)	1.424(10)
C(94)-C(99)	1.497(10)
C(95)-C(96)	1.420(10)
C(95)-C(100)	1.501(10)
C(96)-C(101)	1.517(10)
C(97)-H(97A)	0.9800
C(97)-H(97B)	0.9800
C(97)-H(97C)	0.9800
C(98)-H(98A)	0.9800
C(98)-H(98B)	0.9800
C(98)-H(98C)	0.9800
C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800
C(99)-H(99C)	0.9800
C(100)-H(10D)	0.9800
C(100)-H(10E)	0.9800
C(100)-H(10F)	0.9800
C(101)-H(10G)	0.9800
C(101)-H(10H)	0.9800
C(101)-H(10I)	0.9800
C(102)-C(103)	1.416(13)
C(102)-C(107)	1.422(12)
C(102)-C(108)	1.431(17)
C(103)-C(104)	1.411(13)
C(103)-H(103)	0.9500

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C(104)-C(105)	1.387(13)
C(104)-H(104)	0.9500
C(105)-C(106)	1.424(12)
C(105)-H(105)	0.9500
C(106)-C(107)	1.469(11)
C(106)-H(106)	0.9500
C(107)-H(107)	0.9500
C(108)-H(10J)	0.9800
C(108)-H(10K)	0.9800
C(108)-H(10L)	0.9800

C(24)-Co(1)-C(1)	118.4(3)
C(24)-Co(1)-C(23)	41.6(3)
C(1)-Co(1)-C(23)	103.5(3)
C(24)-Co(1)-C(25)	41.5(3)
C(1)-Co(1)-C(25)	156.5(3)
C(23)-Co(1)-C(25)	69.2(3)
C(24)-Co(1)-C(5)	148.0(3)
C(1)-Co(1)-C(5)	41.1(3)
C(23)-Co(1)-C(5)	110.6(3)
C(25)-Co(1)-C(5)	162.2(3)
C(24)-Co(1)-C(4)	171.9(3)
C(1)-Co(1)-C(4)	68.1(3)
C(23)-Co(1)-C(4)	144.3(3)
C(25)-Co(1)-C(4)	130.9(3)
C(5)-Co(1)-C(4)	40.1(3)
C(24)-Co(1)-C(3)	135.9(3)
C(1)-Co(1)-C(3)	68.0(3)
C(23)-Co(1)-C(3)	169.4(3)
C(25)-Co(1)-C(3)	115.9(3)
C(5)-Co(1)-C(3)	67.6(3)
C(4)-Co(1)-C(3)	40.0(3)
C(24)-Co(1)-C(2)	113.8(3)
C(1)-Co(1)-C(2)	40.9(3)
C(23)-Co(1)-C(2)	129.5(3)
C(25)-Co(1)-C(2)	126.4(3)
C(5)-Co(1)-C(2)	68.4(3)
C(4)-Co(1)-C(2)	67.4(3)
C(3)-Co(1)-C(2)	39.9(3)
C(24)-Co(1)-C(26)	73.4(3)
C(1)-Co(1)-C(26)	163.4(3)
C(23)-Co(1)-C(26)	77.5(3)
C(25)-Co(1)-C(26)	39.4(3)
C(5)-Co(1)-C(26)	122.7(3)
C(4)-Co(1)-C(26)	101.2(3)
C(3)-Co(1)-C(26)	112.5(3)
C(2)-Co(1)-C(26)	148.3(3)
C(21)-Co(2)-C(22)	41.9(3)
C(21)-Co(2)-C(15)	142.2(3)
C(22)-Co(2)-C(15)	106.6(3)
C(21)-Co(2)-C(26)	42.3(3)
C(22)-Co(2)-C(26)	70.0(3)
C(15)-Co(2)-C(26)	166.3(3)
C(21)-Co(2)-C(14)	116.3(3)

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C(22)-Co(2)-C(14)	107.3(3)
C(15)-Co(2)-C(14)	42.1(3)
C(26)-Co(2)-C(14)	151.3(3)
C(21)-Co(2)-C(13)	117.4(3)
C(22)-Co(2)-C(13)	137.8(3)
C(15)-Co(2)-C(13)	68.6(3)
C(26)-Co(2)-C(13)	123.1(3)
C(14)-Co(2)-C(13)	40.2(3)
C(21)-Co(2)-C(11)	175.1(3)
C(22)-Co(2)-C(11)	136.2(3)
C(15)-Co(2)-C(11)	39.8(3)
C(26)-Co(2)-C(11)	134.3(3)
C(14)-Co(2)-C(11)	68.2(3)
C(13)-Co(2)-C(11)	67.2(3)
C(21)-Co(2)-C(12)	142.1(3)
C(22)-Co(2)-C(12)	174.4(3)
C(15)-Co(2)-C(12)	68.0(3)
C(26)-Co(2)-C(12)	115.6(3)
C(14)-Co(2)-C(12)	67.8(3)
C(13)-Co(2)-C(12)	39.7(3)
C(11)-Co(2)-C(12)	40.3(3)
C(21)-Co(2)-C(25)	73.7(3)
C(22)-Co(2)-C(25)	77.1(3)
C(15)-Co(2)-C(25)	127.3(3)
C(26)-Co(2)-C(25)	39.4(3)
C(14)-Co(2)-C(25)	169.1(3)
C(13)-Co(2)-C(25)	140.7(3)
C(11)-Co(2)-C(25)	101.6(3)
C(12)-Co(2)-C(25)	107.3(3)
C(51)-Co(3)-C(28)	120.8(3)
C(51)-Co(3)-C(52)	41.3(4)
C(28)-Co(3)-C(52)	105.6(3)
C(51)-Co(3)-C(29)	150.5(4)
C(28)-Co(3)-C(29)	40.8(3)
C(52)-Co(3)-C(29)	112.9(3)
C(51)-Co(3)-C(50)	41.1(4)
C(28)-Co(3)-C(50)	157.9(3)
C(52)-Co(3)-C(50)	69.1(4)
C(29)-Co(3)-C(50)	161.3(3)
C(51)-Co(3)-C(32)	114.0(3)
C(28)-Co(3)-C(32)	40.4(3)
C(52)-Co(3)-C(32)	129.6(3)
C(29)-Co(3)-C(32)	68.1(3)
C(50)-Co(3)-C(32)	126.1(3)
C(51)-Co(3)-C(31)	134.7(4)
C(28)-Co(3)-C(31)	67.2(3)
C(52)-Co(3)-C(31)	169.4(3)
C(29)-Co(3)-C(31)	67.2(3)
C(50)-Co(3)-C(31)	114.5(3)
C(32)-Co(3)-C(31)	40.0(3)
C(51)-Co(3)-C(30)	169.9(4)
C(28)-Co(3)-C(30)	67.2(3)
C(52)-Co(3)-C(30)	146.0(3)
C(29)-Co(3)-C(30)	39.5(3)

C(50)-Co(3)-C(30)	129.4(3)
C(32)-Co(3)-C(30)	67.4(3)
C(31)-Co(3)-C(30)	40.0(3)
C(51)-Co(3)-C(49)	71.6(3)
C(28)-Co(3)-C(49)	163.8(3)
C(52)-Co(3)-C(49)	76.6(3)
C(29)-Co(3)-C(49)	123.3(3)
C(50)-Co(3)-C(49)	38.0(3)
C(32)-Co(3)-C(49)	148.1(3)
C(31)-Co(3)-C(49)	112.6(3)
C(30)-Co(3)-C(49)	101.8(3)
C(48)-Co(4)-C(49)	41.8(3)
C(48)-Co(4)-C(38)	141.5(3)
C(49)-Co(4)-C(38)	167.6(3)
C(48)-Co(4)-C(39)	116.4(3)
C(49)-Co(4)-C(39)	150.5(3)
C(38)-Co(4)-C(39)	41.6(3)
C(48)-Co(4)-C(53)	41.8(3)
C(49)-Co(4)-C(53)	70.1(3)
C(38)-Co(4)-C(53)	106.1(3)
C(39)-Co(4)-C(53)	107.1(3)
C(48)-Co(4)-C(40)	117.4(3)
C(49)-Co(4)-C(40)	122.6(3)
C(38)-Co(4)-C(40)	68.5(3)
C(39)-Co(4)-C(40)	40.0(3)
C(53)-Co(4)-C(40)	137.3(3)
C(48)-Co(4)-C(41)	142.7(3)
C(49)-Co(4)-C(41)	115.9(3)
C(38)-Co(4)-C(41)	68.1(3)
C(39)-Co(4)-C(41)	67.7(3)
C(53)-Co(4)-C(41)	174.0(3)
C(40)-Co(4)-C(41)	40.1(3)
C(48)-Co(4)-C(42)	174.7(3)
C(49)-Co(4)-C(42)	135.3(3)
C(38)-Co(4)-C(42)	39.9(3)
C(39)-Co(4)-C(42)	68.0(3)
C(53)-Co(4)-C(42)	135.4(3)
C(40)-Co(4)-C(42)	67.7(3)
C(41)-Co(4)-C(42)	40.6(3)
C(48)-Co(4)-C(50)	72.1(3)
C(49)-Co(4)-C(50)	38.6(3)
C(38)-Co(4)-C(50)	129.5(3)
C(39)-Co(4)-C(50)	170.8(3)
C(53)-Co(4)-C(50)	76.6(3)
C(40)-Co(4)-C(50)	140.9(3)
C(41)-Co(4)-C(50)	108.1(3)
C(42)-Co(4)-C(50)	103.3(3)
C(78)-Co(5)-C(77)	40.3(4)
C(78)-Co(5)-C(56)	119.3(4)
C(77)-Co(5)-C(56)	155.8(4)
C(78)-Co(5)-C(57)	148.1(4)
C(77)-Co(5)-C(57)	163.2(3)
C(56)-Co(5)-C(57)	40.7(3)
C(78)-Co(5)-C(59)	135.5(4)

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C(77)-Co(5)-C(59)	116.1(3)
C(56)-Co(5)-C(59)	67.1(3)
C(57)-Co(5)-C(59)	68.0(3)
C(78)-Co(5)-C(58)	171.5(4)
C(77)-Co(5)-C(58)	131.5(4)
C(56)-Co(5)-C(58)	67.9(3)
C(57)-Co(5)-C(58)	40.4(3)
C(59)-Co(5)-C(58)	40.8(3)
C(78)-Co(5)-C(55)	114.4(4)
C(77)-Co(5)-C(55)	126.2(3)
C(56)-Co(5)-C(55)	40.2(3)
C(57)-Co(5)-C(55)	68.0(3)
C(59)-Co(5)-C(55)	39.2(3)
C(58)-Co(5)-C(55)	67.5(3)
C(78)-Co(5)-C(79)	38.6(4)
C(77)-Co(5)-C(79)	68.8(4)
C(56)-Co(5)-C(79)	102.1(3)
C(57)-Co(5)-C(79)	112.0(4)
C(59)-Co(5)-C(79)	164.1(3)
C(58)-Co(5)-C(79)	147.8(4)
C(55)-Co(5)-C(79)	125.1(3)
C(78)-Co(5)-C(76)	71.4(4)
C(77)-Co(5)-C(76)	40.6(3)
C(56)-Co(5)-C(76)	162.2(3)
C(57)-Co(5)-C(76)	122.6(3)
C(59)-Co(5)-C(76)	116.6(3)
C(58)-Co(5)-C(76)	103.0(3)
C(55)-Co(5)-C(76)	152.1(3)
C(79)-Co(5)-C(76)	77.3(4)
C(75)-Co(6)-C(76)	42.5(4)
C(75)-Co(6)-C(80)	42.0(4)
C(76)-Co(6)-C(80)	69.6(4)
C(75)-Co(6)-C(67)	113.9(3)
C(76)-Co(6)-C(67)	146.0(4)
C(80)-Co(6)-C(67)	110.5(4)
C(75)-Co(6)-C(69)	146.7(3)
C(76)-Co(6)-C(69)	116.5(4)
C(80)-Co(6)-C(69)	171.2(4)
C(67)-Co(6)-C(69)	68.3(3)
C(75)-Co(6)-C(66)	137.4(3)
C(76)-Co(6)-C(66)	171.6(4)
C(80)-Co(6)-C(66)	105.4(4)
C(67)-Co(6)-C(66)	41.5(3)
C(69)-Co(6)-C(66)	67.7(3)
C(75)-Co(6)-C(68)	118.7(3)
C(76)-Co(6)-C(68)	120.1(4)
C(80)-Co(6)-C(68)	143.5(4)
C(67)-Co(6)-C(68)	40.2(3)
C(69)-Co(6)-C(68)	40.4(3)
C(66)-Co(6)-C(68)	68.0(3)
C(75)-Co(6)-C(65)	173.0(3)
C(76)-Co(6)-C(65)	138.3(4)
C(80)-Co(6)-C(65)	131.2(4)
C(67)-Co(6)-C(65)	68.8(3)

C(69)-Co(6)-C(65)	40.0(3)
C(66)-Co(6)-C(65)	40.3(3)
C(68)-Co(6)-C(65)	67.6(3)
C(75)-Co(6)-C(77)	73.5(3)
C(76)-Co(6)-C(77)	39.8(4)
C(80)-Co(6)-C(77)	75.1(4)
C(67)-Co(6)-C(77)	172.6(3)
C(69)-Co(6)-C(77)	105.4(3)
C(66)-Co(6)-C(77)	133.3(3)
C(68)-Co(6)-C(77)	136.7(3)
C(65)-Co(6)-C(77)	104.0(3)
C(105)-Co(7)-C(86)	115.7(3)
C(105)-Co(7)-C(106)	41.8(3)
C(86)-Co(7)-C(106)	152.4(3)
C(105)-Co(7)-C(85)	143.6(4)
C(86)-Co(7)-C(85)	41.4(3)
C(106)-Co(7)-C(85)	165.8(3)
C(105)-Co(7)-C(104)	40.4(4)
C(86)-Co(7)-C(104)	104.6(3)
C(106)-Co(7)-C(104)	68.7(4)
C(85)-Co(7)-C(104)	108.8(4)
C(105)-Co(7)-C(84)	175.1(3)
C(86)-Co(7)-C(84)	69.2(3)
C(106)-Co(7)-C(84)	133.5(3)
C(85)-Co(7)-C(84)	40.3(3)
C(104)-Co(7)-C(84)	140.2(4)
C(105)-Co(7)-C(83)	139.2(4)
C(86)-Co(7)-C(83)	68.9(3)
C(106)-Co(7)-C(83)	115.6(3)
C(85)-Co(7)-C(83)	68.4(3)
C(104)-Co(7)-C(83)	173.1(3)
C(84)-Co(7)-C(83)	41.2(3)
C(105)-Co(7)-C(82)	115.5(3)
C(86)-Co(7)-C(82)	40.7(3)
C(106)-Co(7)-C(82)	124.4(3)
C(85)-Co(7)-C(82)	67.9(3)
C(104)-Co(7)-C(82)	133.3(3)
C(84)-Co(7)-C(82)	67.9(3)
C(83)-Co(7)-C(82)	39.9(3)
C(105)-Co(7)-C(107)	73.2(3)
C(86)-Co(7)-C(107)	168.1(3)
C(106)-Co(7)-C(107)	39.3(3)
C(85)-Co(7)-C(107)	126.8(3)
C(104)-Co(7)-C(107)	76.9(3)
C(84)-Co(7)-C(107)	101.9(3)
C(83)-Co(7)-C(107)	110.0(3)
C(82)-Co(7)-C(107)	144.5(3)
C(102)-Co(8)-C(103)	42.0(4)
C(102)-Co(8)-C(107)	42.1(4)
C(103)-Co(8)-C(107)	70.1(4)
C(102)-Co(8)-C(96)	117.5(3)
C(103)-Co(8)-C(96)	105.5(3)
C(107)-Co(8)-C(96)	154.1(3)
C(102)-Co(8)-C(92)	143.7(4)

C(103)-Co(8)-C(92)	107.0(3)
C(107)-Co(8)-C(92)	164.8(3)
C(96)-Co(8)-C(92)	40.8(3)
C(102)-Co(8)-C(93)	175.2(3)
C(103)-Co(8)-C(93)	138.6(4)
C(107)-Co(8)-C(93)	133.3(3)
C(96)-Co(8)-C(93)	67.3(3)
C(92)-Co(8)-C(93)	40.1(3)
C(102)-Co(8)-C(94)	139.8(4)
C(103)-Co(8)-C(94)	173.0(3)
C(107)-Co(8)-C(94)	115.8(3)
C(96)-Co(8)-C(94)	67.6(3)
C(92)-Co(8)-C(94)	68.4(3)
C(93)-Co(8)-C(94)	40.5(3)
C(102)-Co(8)-C(95)	116.0(3)
C(103)-Co(8)-C(95)	133.9(3)
C(107)-Co(8)-C(95)	124.9(3)
C(96)-Co(8)-C(95)	40.2(3)
C(92)-Co(8)-C(95)	68.3(3)
C(93)-Co(8)-C(95)	67.3(3)
C(94)-Co(8)-C(95)	40.0(3)
C(102)-Co(8)-C(106)	72.9(3)
C(103)-Co(8)-C(106)	75.8(3)
C(107)-Co(8)-C(106)	39.5(3)
C(96)-Co(8)-C(106)	166.3(3)
C(92)-Co(8)-C(106)	125.5(3)
C(93)-Co(8)-C(106)	102.4(3)
C(94)-Co(8)-C(106)	111.1(3)
C(95)-Co(8)-C(106)	146.0(3)
C(5)-C(1)-C(2)	109.2(6)
C(5)-C(1)-C(6)	127.3(7)
C(2)-C(1)-C(6)	123.1(6)
C(5)-C(1)-Co(1)	71.7(4)
C(2)-C(1)-Co(1)	72.8(4)
C(6)-C(1)-Co(1)	127.0(5)
C(3)-C(2)-C(1)	106.3(6)
C(3)-C(2)-C(7)	127.0(7)
C(1)-C(2)-C(7)	126.7(7)
C(3)-C(2)-Co(1)	69.7(4)
C(1)-C(2)-Co(1)	66.3(4)
C(7)-C(2)-Co(1)	129.9(5)
C(4)-C(3)-C(2)	108.8(6)
C(4)-C(3)-C(8)	126.2(7)
C(2)-C(3)-C(8)	125.0(7)
C(4)-C(3)-Co(1)	69.8(4)
C(2)-C(3)-Co(1)	70.3(4)
C(8)-C(3)-Co(1)	128.1(5)
C(5)-C(4)-C(3)	108.6(6)
C(5)-C(4)-C(9)	125.6(7)
C(3)-C(4)-C(9)	125.7(7)
C(5)-C(4)-Co(1)	69.4(4)
C(3)-C(4)-Co(1)	70.2(4)
C(9)-C(4)-Co(1)	127.8(5)
C(4)-C(5)-C(1)	106.8(6)

C(4)-C(5)-C(10)	127.7(7)
C(1)-C(5)-C(10)	125.5(7)
C(4)-C(5)-Co(1)	70.5(4)
C(1)-C(5)-Co(1)	67.2(4)
C(10)-C(5)-Co(1)	126.1(5)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(15)-C(11)-C(12)	109.0(6)
C(15)-C(11)-C(16)	125.4(7)
C(12)-C(11)-C(16)	125.6(7)
C(15)-C(11)-Co(2)	68.9(4)
C(12)-C(11)-Co(2)	70.0(4)
C(16)-C(11)-Co(2)	126.9(5)
C(13)-C(12)-C(11)	107.7(6)
C(13)-C(12)-C(17)	126.5(7)
C(11)-C(12)-C(17)	125.8(7)
C(13)-C(12)-Co(2)	69.6(4)
C(11)-C(12)-Co(2)	69.7(4)
C(17)-C(12)-Co(2)	128.2(6)
C(12)-C(13)-C(14)	109.6(6)
C(12)-C(13)-C(18)	126.1(7)
C(14)-C(13)-C(18)	124.2(7)
C(12)-C(13)-Co(2)	70.7(4)
C(14)-C(13)-Co(2)	69.5(4)
C(18)-C(13)-Co(2)	129.2(5)
C(13)-C(14)-C(15)	106.6(6)

C(13)-C(14)-C(19)	126.2(7)
C(15)-C(14)-C(19)	127.2(7)
C(13)-C(14)-Co(2)	70.3(4)
C(15)-C(14)-Co(2)	68.6(4)
C(19)-C(14)-Co(2)	124.5(5)
C(11)-C(15)-C(14)	107.1(6)
C(11)-C(15)-C(20)	127.0(8)
C(14)-C(15)-C(20)	125.8(8)
C(11)-C(15)-Co(2)	71.3(4)
C(14)-C(15)-Co(2)	69.3(4)
C(20)-C(15)-Co(2)	127.5(5)
C(11)-C(16)-H(16A)	109.5
C(11)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(11)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(12)-C(17)-H(17A)	109.5
C(12)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(12)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(15)-C(20)-H(20A)	109.5
C(15)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(26)	110.9(6)
C(22)-C(21)-C(27)	125.9(7)
C(26)-C(21)-C(27)	122.6(8)
C(22)-C(21)-Co(2)	74.3(4)
C(26)-C(21)-Co(2)	74.4(4)
C(27)-C(21)-Co(2)	126.0(5)
C(21)-C(22)-C(23)	117.9(6)
C(21)-C(22)-Co(2)	63.8(4)
C(23)-C(22)-Co(2)	105.8(5)
C(21)-C(22)-H(22)	121.0
C(23)-C(22)-H(22)	121.0
Co(2)-C(22)-H(22)	99.5
C(24)-C(23)-C(22)	117.7(6)

C(24)-C(23)-Co(1)	64.7(4)
C(22)-C(23)-Co(1)	105.5(5)
C(24)-C(23)-H(23)	121.1
C(22)-C(23)-H(23)	121.1
Co(1)-C(23)-H(23)	98.9
C(25)-C(24)-C(23)	110.8(6)
C(25)-C(24)-Co(1)	73.9(4)
C(23)-C(24)-Co(1)	73.8(4)
C(25)-C(24)-H(24)	124.6
C(23)-C(24)-H(24)	124.6
Co(1)-C(24)-H(24)	119.3
C(24)-C(25)-C(26)	121.7(7)
C(24)-C(25)-Co(1)	64.6(4)
C(26)-C(25)-Co(1)	77.7(4)
C(24)-C(25)-Co(2)	96.9(5)
C(26)-C(25)-Co(2)	63.0(4)
Co(1)-C(25)-Co(2)	117.9(3)
C(24)-C(25)-H(25)	119.2
C(26)-C(25)-H(25)	119.2
Co(1)-C(25)-H(25)	131.2
Co(2)-C(25)-H(25)	110.1
C(21)-C(26)-C(25)	119.9(7)
C(21)-C(26)-Co(2)	63.3(4)
C(25)-C(26)-Co(2)	77.6(4)
C(21)-C(26)-Co(1)	96.5(5)
C(25)-C(26)-Co(1)	62.9(4)
Co(2)-C(26)-Co(1)	117.8(3)
C(21)-C(26)-H(26)	120.1
C(25)-C(26)-H(26)	120.1
Co(2)-C(26)-H(26)	131.5
Co(1)-C(26)-H(26)	110.1
C(21)-C(27)-H(27A)	109.5
C(21)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(21)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(32)-C(28)-C(29)	109.3(6)
C(32)-C(28)-C(33)	123.7(6)
C(29)-C(28)-C(33)	126.9(7)
C(32)-C(28)-Co(3)	71.9(4)
C(29)-C(28)-Co(3)	70.7(4)
C(33)-C(28)-Co(3)	126.2(5)
C(30)-C(29)-C(28)	107.8(6)
C(30)-C(29)-C(34)	126.4(7)
C(28)-C(29)-C(34)	125.7(7)
C(30)-C(29)-Co(3)	72.0(4)
C(28)-C(29)-Co(3)	68.5(4)
C(34)-C(29)-Co(3)	127.7(5)
C(29)-C(30)-C(31)	107.9(6)
C(29)-C(30)-C(35)	127.0(7)
C(31)-C(30)-C(35)	125.1(7)
C(29)-C(30)-Co(3)	68.5(4)
C(31)-C(30)-Co(3)	69.6(4)

C(35)-C(30)-Co(3)	127.0(5)
C(32)-C(31)-C(30)	108.4(7)
C(32)-C(31)-C(36)	126.0(7)
C(30)-C(31)-C(36)	125.6(7)
C(32)-C(31)-Co(3)	69.6(4)
C(30)-C(31)-Co(3)	70.3(4)
C(36)-C(31)-Co(3)	127.3(5)
C(28)-C(32)-C(31)	106.6(6)
C(28)-C(32)-C(37)	126.4(6)
C(31)-C(32)-C(37)	126.9(7)
C(28)-C(32)-Co(3)	67.8(4)
C(31)-C(32)-Co(3)	70.4(4)
C(37)-C(32)-Co(3)	128.8(5)
C(28)-C(33)-H(33A)	109.5
C(28)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(28)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(29)-C(34)-H(34A)	109.5
C(29)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(29)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(30)-C(35)-H(35A)	109.5
C(30)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(30)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(31)-C(36)-H(36A)	109.5
C(31)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(31)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(32)-C(37)-H(37A)	109.5
C(32)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(32)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(42)-C(38)-C(39)	107.7(6)
C(42)-C(38)-C(43)	126.2(7)
C(39)-C(38)-C(43)	126.0(7)
C(42)-C(38)-Co(4)	71.8(4)
C(39)-C(38)-Co(4)	69.2(4)
C(43)-C(38)-Co(4)	126.9(5)
C(40)-C(39)-C(38)	108.0(6)
C(40)-C(39)-C(44)	126.5(7)
C(38)-C(39)-C(44)	125.5(8)
C(40)-C(39)-Co(4)	71.1(4)
C(38)-C(39)-Co(4)	69.1(4)

C(44)-C(39)-Co(4)	126.3(5)
C(39)-C(40)-C(41)	108.4(6)
C(39)-C(40)-C(45)	127.3(7)
C(41)-C(40)-C(45)	124.2(7)
C(39)-C(40)-Co(4)	68.9(4)
C(41)-C(40)-Co(4)	70.2(4)
C(45)-C(40)-Co(4)	128.9(5)
C(40)-C(41)-C(42)	107.9(6)
C(40)-C(41)-C(46)	127.6(7)
C(42)-C(41)-C(46)	124.5(7)
C(40)-C(41)-Co(4)	69.7(4)
C(42)-C(41)-Co(4)	70.0(4)
C(46)-C(41)-Co(4)	127.7(6)
C(38)-C(42)-C(41)	107.9(6)
C(38)-C(42)-C(47)	126.6(7)
C(41)-C(42)-C(47)	125.4(7)
C(38)-C(42)-Co(4)	68.4(4)
C(41)-C(42)-Co(4)	69.4(4)
C(47)-C(42)-Co(4)	126.9(6)
C(38)-C(43)-H(43A)	109.5
C(38)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(38)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(39)-C(44)-H(44A)	109.5
C(39)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(39)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(40)-C(45)-H(45A)	109.5
C(40)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(40)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(41)-C(46)-H(46A)	109.5
C(41)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(41)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(42)-C(47)-H(47A)	109.5
C(42)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(42)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(49)-C(48)-C(53)	111.8(6)
C(49)-C(48)-C(54)	121.2(7)
C(53)-C(48)-C(54)	126.7(7)
C(49)-C(48)-Co(4)	73.4(4)
C(53)-C(48)-Co(4)	74.0(4)

C(54)-C(48)-Co(4)	125.2(5)
C(48)-C(49)-C(50)	121.2(7)
C(48)-C(49)-Co(4)	64.9(4)
C(50)-C(49)-Co(4)	80.1(5)
C(48)-C(49)-Co(3)	93.3(5)
C(50)-C(49)-Co(3)	61.6(4)
Co(4)-C(49)-Co(3)	116.8(3)
C(48)-C(49)-H(49)	119.4
C(50)-C(49)-H(49)	119.4
Co(4)-C(49)-H(49)	127.4
Co(3)-C(49)-H(49)	115.2
C(51)-C(50)-C(49)	122.2(8)
C(51)-C(50)-Co(3)	63.7(4)
C(49)-C(50)-Co(3)	80.4(5)
C(51)-C(50)-Co(4)	95.5(6)
C(49)-C(50)-Co(4)	61.3(4)
Co(3)-C(50)-Co(4)	116.8(4)
C(51)-C(50)-H(50)	118.9
C(49)-C(50)-H(50)	118.9
Co(3)-C(50)-H(50)	129.1
Co(4)-C(50)-H(50)	113.4
C(52)-C(51)-C(50)	111.9(7)
C(52)-C(51)-Co(3)	73.7(5)
C(50)-C(51)-Co(3)	75.2(5)
C(52)-C(51)-H(51)	124.1
C(50)-C(51)-H(51)	124.1
Co(3)-C(51)-H(51)	118.6
C(51)-C(52)-C(53)	118.6(7)
C(51)-C(52)-Co(3)	65.0(4)
C(53)-C(52)-Co(3)	104.6(5)
C(51)-C(52)-H(52)	120.7
C(53)-C(52)-H(52)	120.7
Co(3)-C(52)-H(52)	99.6
C(48)-C(53)-C(52)	117.5(7)
C(48)-C(53)-Co(4)	64.3(4)
C(52)-C(53)-Co(4)	104.2(5)
C(48)-C(53)-H(53)	121.3
C(52)-C(53)-H(53)	121.3
Co(4)-C(53)-H(53)	100.5
C(48)-C(54)-H(54A)	109.5
C(48)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(48)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(59)-C(55)-C(56)	107.4(6)
C(59)-C(55)-C(60)	127.2(7)
C(56)-C(55)-C(60)	125.4(7)
C(59)-C(55)-Co(5)	69.6(4)
C(56)-C(55)-Co(5)	67.9(4)
C(60)-C(55)-Co(5)	129.0(5)
C(57)-C(56)-C(55)	108.9(6)
C(57)-C(56)-C(61)	126.2(7)
C(55)-C(56)-C(61)	124.9(7)

C(57)-C(56)-Co(5)	69.6(4)
C(55)-C(56)-Co(5)	71.9(4)
C(61)-C(56)-Co(5)	125.4(5)
C(56)-C(57)-C(58)	107.9(6)
C(56)-C(57)-C(62)	127.0(7)
C(58)-C(57)-C(62)	125.0(7)
C(56)-C(57)-Co(5)	69.6(4)
C(58)-C(57)-Co(5)	71.2(4)
C(62)-C(57)-Co(5)	127.4(5)
C(57)-C(58)-C(59)	106.7(6)
C(57)-C(58)-C(63)	127.2(7)
C(59)-C(58)-C(63)	126.1(7)
C(57)-C(58)-Co(5)	68.4(4)
C(59)-C(58)-Co(5)	69.5(4)
C(63)-C(58)-Co(5)	127.2(7)
C(55)-C(59)-C(58)	109.1(6)
C(55)-C(59)-C(64)	126.5(7)
C(58)-C(59)-C(64)	124.3(7)
C(55)-C(59)-Co(5)	71.2(4)
C(58)-C(59)-Co(5)	69.8(4)
C(64)-C(59)-Co(5)	128.3(6)
C(55)-C(60)-H(60A)	109.5
C(55)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(55)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(56)-C(61)-H(61A)	109.5
C(56)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(56)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(57)-C(62)-H(62A)	109.5
C(57)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(57)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(58)-C(63)-H(63A)	109.5
C(58)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(58)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
C(59)-C(64)-H(64A)	109.5
C(59)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(59)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(69)-C(65)-C(66)	107.0(7)
C(69)-C(65)-C(70)	126.3(7)
C(66)-C(65)-C(70)	126.7(8)

C(69)-C(65)-Co(6)	68.5(4)
C(66)-C(65)-Co(6)	68.5(4)
C(70)-C(65)-Co(6)	127.4(6)
C(65)-C(66)-C(67)	108.0(7)
C(65)-C(66)-C(71)	124.3(8)
C(67)-C(66)-C(71)	127.7(8)
C(65)-C(66)-Co(6)	71.2(4)
C(67)-C(66)-Co(6)	68.3(5)
C(71)-C(66)-Co(6)	127.3(6)
C(68)-C(67)-C(66)	107.7(7)
C(68)-C(67)-C(72)	125.9(9)
C(66)-C(67)-C(72)	126.2(9)
C(68)-C(67)-Co(6)	71.7(5)
C(66)-C(67)-Co(6)	70.1(4)
C(72)-C(67)-Co(6)	127.1(6)
C(67)-C(68)-C(69)	107.7(7)
C(67)-C(68)-C(73)	125.9(8)
C(69)-C(68)-C(73)	126.4(8)
C(67)-C(68)-Co(6)	68.1(4)
C(69)-C(68)-Co(6)	68.8(4)
C(73)-C(68)-Co(6)	127.8(6)
C(65)-C(69)-C(68)	109.5(7)
C(65)-C(69)-C(74)	125.3(7)
C(68)-C(69)-C(74)	125.1(7)
C(65)-C(69)-Co(6)	71.6(4)
C(68)-C(69)-Co(6)	70.8(4)
C(74)-C(69)-Co(6)	127.8(6)
C(65)-C(70)-H(70A)	109.5
C(65)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(65)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(66)-C(71)-H(71A)	109.5
C(66)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(66)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
C(67)-C(72)-H(72A)	109.5
C(67)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(67)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(68)-C(73)-H(73A)	109.5
C(68)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
C(68)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
C(69)-C(74)-H(74A)	109.5
C(69)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5

C(69)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
C(80)-C(75)-C(76)	108.2(8)
C(80)-C(75)-C(81)	124.6(8)
C(76)-C(75)-C(81)	126.9(9)
C(80)-C(75)-Co(6)	73.0(5)
C(76)-C(75)-Co(6)	72.3(5)
C(81)-C(75)-Co(6)	125.7(6)
C(75)-C(76)-C(77)	121.4(9)
C(75)-C(76)-Co(6)	65.2(5)
C(77)-C(76)-Co(6)	80.9(6)
C(75)-C(76)-Co(5)	95.0(6)
C(77)-C(76)-Co(5)	60.4(5)
Co(6)-C(76)-Co(5)	118.4(5)
C(75)-C(76)-H(76)	119.3
C(77)-C(76)-H(76)	119.3
Co(6)-C(76)-H(76)	126.2
Co(5)-C(76)-H(76)	114.6
C(78)-C(77)-C(76)	119.4(8)
C(78)-C(77)-Co(5)	68.1(5)
C(76)-C(77)-Co(5)	79.0(5)
C(78)-C(77)-Co(6)	92.0(7)
C(76)-C(77)-Co(6)	59.3(5)
Co(5)-C(77)-Co(6)	116.6(4)
C(78)-C(77)-H(77)	120.3
C(76)-C(77)-H(77)	120.3
Co(5)-C(77)-H(77)	124.0
Co(6)-C(77)-H(77)	118.1
C(79)-C(78)-C(77)	117.5(10)
C(79)-C(78)-Co(5)	76.1(6)
C(77)-C(78)-Co(5)	71.7(6)
C(79)-C(78)-H(78)	121.2
C(77)-C(78)-H(78)	121.2
Co(5)-C(78)-H(78)	122.3
C(78)-C(79)-C(80)	114.2(10)
C(78)-C(79)-Co(5)	65.3(6)
C(80)-C(79)-Co(5)	101.3(7)
C(78)-C(79)-H(79)	122.9
C(80)-C(79)-H(79)	122.9
Co(5)-C(79)-H(79)	101.8
C(75)-C(80)-C(79)	122.1(9)
C(75)-C(80)-Co(6)	65.0(5)
C(79)-C(80)-Co(6)	106.9(7)
C(75)-C(80)-H(80)	118.9
C(79)-C(80)-H(80)	118.9
Co(6)-C(80)-H(80)	97.9
C(75)-C(81)-H(81A)	109.5
C(75)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(75)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(83)-C(82)-C(86)	108.5(6)

C(83)-C(82)-C(87)	125.4(7)
C(86)-C(82)-C(87)	126.1(7)
C(83)-C(82)-Co(7)	69.4(4)
C(86)-C(82)-Co(7)	66.8(4)
C(87)-C(82)-Co(7)	127.8(5)
C(82)-C(83)-C(84)	107.5(6)
C(82)-C(83)-C(88)	127.2(7)
C(84)-C(83)-C(88)	125.3(7)
C(82)-C(83)-Co(7)	70.7(4)
C(84)-C(83)-Co(7)	69.0(4)
C(88)-C(83)-Co(7)	127.7(6)
C(85)-C(84)-C(83)	107.6(6)
C(85)-C(84)-C(89)	126.6(8)
C(83)-C(84)-C(89)	125.8(8)
C(85)-C(84)-Co(7)	69.0(4)
C(83)-C(84)-Co(7)	69.9(4)
C(89)-C(84)-Co(7)	127.6(6)
C(84)-C(85)-C(86)	108.9(7)
C(84)-C(85)-C(90)	126.1(8)
C(86)-C(85)-C(90)	124.9(8)
C(84)-C(85)-Co(7)	70.8(4)
C(86)-C(85)-Co(7)	68.5(4)
C(90)-C(85)-Co(7)	125.6(5)
C(82)-C(86)-C(85)	107.3(7)
C(82)-C(86)-C(91)	124.4(7)
C(85)-C(86)-C(91)	127.9(7)
C(82)-C(86)-Co(7)	72.5(4)
C(85)-C(86)-Co(7)	70.1(4)
C(91)-C(86)-Co(7)	128.3(5)
C(82)-C(87)-H(87A)	109.5
C(82)-C(87)-H(87B)	109.5
H(87A)-C(87)-H(87B)	109.5
C(82)-C(87)-H(87C)	109.5
H(87A)-C(87)-H(87C)	109.5
H(87B)-C(87)-H(87C)	109.5
C(83)-C(88)-H(88A)	109.5
C(83)-C(88)-H(88B)	109.5
H(88A)-C(88)-H(88B)	109.5
C(83)-C(88)-H(88C)	109.5
H(88A)-C(88)-H(88C)	109.5
H(88B)-C(88)-H(88C)	109.5
C(84)-C(89)-H(89A)	109.5
C(84)-C(89)-H(89B)	109.5
H(89A)-C(89)-H(89B)	109.5
C(84)-C(89)-H(89C)	109.5
H(89A)-C(89)-H(89C)	109.5
H(89B)-C(89)-H(89C)	109.5
C(85)-C(90)-H(90A)	109.5
C(85)-C(90)-H(90B)	109.5
H(90A)-C(90)-H(90B)	109.5
C(85)-C(90)-H(90C)	109.5
H(90A)-C(90)-H(90C)	109.5
H(90B)-C(90)-H(90C)	109.5
C(86)-C(91)-H(91A)	109.5

C(86)-C(91)-H(91B)	109.5
H(91A)-C(91)-H(91B)	109.5
C(86)-C(91)-H(91C)	109.5
H(91A)-C(91)-H(91C)	109.5
H(91B)-C(91)-H(91C)	109.5
C(93)-C(92)-C(96)	106.4(6)
C(93)-C(92)-C(97)	126.4(7)
C(96)-C(92)-C(97)	127.2(7)
C(93)-C(92)-Co(8)	70.2(4)
C(96)-C(92)-Co(8)	69.2(4)
C(97)-C(92)-Co(8)	126.9(5)
C(92)-C(93)-C(94)	109.3(6)
C(92)-C(93)-C(98)	125.9(7)
C(94)-C(93)-C(98)	124.7(7)
C(92)-C(93)-Co(8)	69.6(4)
C(94)-C(93)-Co(8)	70.1(4)
C(98)-C(93)-Co(8)	128.0(5)
C(95)-C(94)-C(93)	107.3(6)
C(95)-C(94)-C(99)	126.1(7)
C(93)-C(94)-C(99)	126.6(7)
C(95)-C(94)-Co(8)	70.1(4)
C(93)-C(94)-Co(8)	69.4(4)
C(99)-C(94)-Co(8)	128.0(6)
C(96)-C(95)-C(94)	107.8(6)
C(96)-C(95)-C(100)	125.5(7)
C(94)-C(95)-C(100)	126.6(7)
C(96)-C(95)-Co(8)	68.8(4)
C(94)-C(95)-Co(8)	69.9(4)
C(100)-C(95)-Co(8)	128.6(5)
C(95)-C(96)-C(92)	109.2(6)
C(95)-C(96)-C(101)	125.5(8)
C(92)-C(96)-C(101)	125.3(8)
C(95)-C(96)-Co(8)	71.1(4)
C(92)-C(96)-Co(8)	70.0(4)
C(101)-C(96)-Co(8)	125.2(5)
C(92)-C(97)-H(97A)	109.5
C(92)-C(97)-H(97B)	109.5
H(97A)-C(97)-H(97B)	109.5
C(92)-C(97)-H(97C)	109.5
H(97A)-C(97)-H(97C)	109.5
H(97B)-C(97)-H(97C)	109.5
C(93)-C(98)-H(98A)	109.5
C(93)-C(98)-H(98B)	109.5
H(98A)-C(98)-H(98B)	109.5
C(93)-C(98)-H(98C)	109.5
H(98A)-C(98)-H(98C)	109.5
H(98B)-C(98)-H(98C)	109.5
C(94)-C(99)-H(99A)	109.5
C(94)-C(99)-H(99B)	109.5
H(99A)-C(99)-H(99B)	109.5
C(94)-C(99)-H(99C)	109.5
H(99A)-C(99)-H(99C)	109.5
H(99B)-C(99)-H(99C)	109.5
C(95)-C(100)-H(10D)	109.5

C(95)-C(100)-H(10E)	109.5
H(10D)-C(100)-H(10E)	109.5
C(95)-C(100)-H(10F)	109.5
H(10D)-C(100)-H(10F)	109.5
H(10E)-C(100)-H(10F)	109.5
C(96)-C(101)-H(10G)	109.5
C(96)-C(101)-H(10H)	109.5
H(10G)-C(101)-H(10H)	109.5
C(96)-C(101)-H(10I)	109.5
H(10G)-C(101)-H(10I)	109.5
H(10H)-C(101)-H(10I)	109.5
C(103)-C(102)-C(107)	111.3(7)
C(103)-C(102)-C(108)	123.4(13)
C(107)-C(102)-C(108)	124.9(13)
C(103)-C(102)-Co(8)	74.4(5)
C(107)-C(102)-Co(8)	74.4(5)
C(108)-C(102)-Co(8)	124.2(8)
C(104)-C(103)-C(102)	119.2(8)
C(104)-C(103)-Co(8)	107.0(7)
C(102)-C(103)-Co(8)	63.6(4)
C(104)-C(103)-H(103)	120.4
C(102)-C(103)-H(103)	120.4
Co(8)-C(103)-H(103)	98.6
C(105)-C(104)-C(103)	118.1(8)
C(105)-C(104)-Co(7)	64.8(5)
C(103)-C(104)-Co(7)	105.2(6)
C(105)-C(104)-H(104)	121.0
C(103)-C(104)-H(104)	121.0
Co(7)-C(104)-H(104)	99.1
C(104)-C(105)-C(106)	111.1(8)
C(104)-C(105)-Co(7)	74.8(5)
C(106)-C(105)-Co(7)	72.9(5)
C(104)-C(105)-H(105)	124.4
C(106)-C(105)-H(105)	124.4
Co(7)-C(105)-H(105)	119.4
C(105)-C(106)-C(107)	121.8(8)
C(105)-C(106)-Co(7)	65.2(4)
C(107)-C(106)-Co(7)	79.0(5)
C(105)-C(106)-Co(8)	95.7(6)
C(107)-C(106)-Co(8)	62.1(4)
Co(7)-C(106)-Co(8)	118.1(4)
C(105)-C(106)-H(106)	119.1
C(107)-C(106)-H(106)	119.1
Co(7)-C(106)-H(106)	128.8
Co(8)-C(106)-H(106)	112.3
C(102)-C(107)-C(106)	118.8(7)
C(102)-C(107)-Co(8)	63.5(4)
C(106)-C(107)-Co(8)	78.4(5)
C(102)-C(107)-Co(7)	95.0(5)
C(106)-C(107)-Co(7)	61.6(4)
Co(8)-C(107)-Co(7)	117.5(4)
C(102)-C(107)-H(107)	120.6
C(106)-C(107)-H(107)	120.6
Co(8)-C(107)-H(107)	129.4

Co(7)-C(107)-H(107)	112.4
C(102)-C(108)-H(10J)	109.5
C(102)-C(108)-H(10K)	109.5
H(10J)-C(108)-H(10K)	109.5
C(102)-C(108)-H(10L)	109.5
H(10J)-C(108)-H(10L)	109.5
H(10K)-C(108)-H(10L)	109.5

Table 3. Bond lengths [Å] and angles [°] for **11**.

Co(1)-C(15)	2.006(3)
Co(1)-C(12)	2.011(3)
Co(1)-C(11)	2.017(3)
Co(1)-C(16)	2.024(3)
Co(1)-C(1)	2.065(3)
Co(1)-C(4)	2.096(3)
Co(1)-C(5)	2.096(3)
Co(1)-C(2)	2.100(3)
Co(1)-C(3)	2.104(3)
C(1)-C(5)	1.424(4)
C(1)-C(2)	1.430(4)
C(1)-C(6)	1.502(4)
C(2)-C(3)	1.406(4)
C(2)-C(7)	1.503(4)
C(3)-C(4)	1.438(4)
C(3)-C(8)	1.507(4)
C(4)-C(5)	1.400(4)
C(4)-C(9)	1.501(4)
C(5)-C(10)	1.513(4)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.380(5)
C(11)-C(18)	1.516(5)
C(11)-H(11)	0.93(3)
C(12)-C(13)	1.494(5)
C(12)-H(12)	0.99(3)
C(13)-C(14)	1.439(5)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.512(5)

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C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.389(5)
C(15)-H(15)	0.91(4)
C(16)-C(17)	1.526(5)
C(16)-H(16)	0.99(4)
C(17)-C(18)	1.465(5)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(15)-Co(1)-C(12)	84.73(13)
C(15)-Co(1)-C(11)	97.65(14)
C(12)-Co(1)-C(11)	40.08(15)
C(15)-Co(1)-C(16)	40.33(13)
C(12)-Co(1)-C(16)	98.17(13)
C(11)-Co(1)-C(16)	83.96(13)
C(15)-Co(1)-C(1)	99.02(12)
C(12)-Co(1)-C(1)	159.01(13)
C(11)-Co(1)-C(1)	156.09(14)
C(16)-Co(1)-C(1)	97.88(12)
C(15)-Co(1)-C(4)	165.31(12)
C(12)-Co(1)-C(4)	108.53(12)
C(11)-Co(1)-C(4)	96.66(13)
C(16)-Co(1)-C(4)	138.93(13)
C(1)-Co(1)-C(4)	66.34(10)
C(15)-Co(1)-C(5)	129.34(13)
C(12)-Co(1)-C(5)	145.09(13)
C(11)-Co(1)-C(5)	116.35(14)
C(16)-Co(1)-C(5)	104.54(12)
C(1)-Co(1)-C(5)	40.01(11)
C(4)-Co(1)-C(5)	39.02(11)
C(15)-Co(1)-C(2)	101.95(12)
C(12)-Co(1)-C(2)	118.86(13)
C(11)-Co(1)-C(2)	149.46(13)
C(16)-Co(1)-C(2)	125.76(12)
C(1)-Co(1)-C(2)	40.15(11)
C(4)-Co(1)-C(2)	66.45(10)
C(5)-Co(1)-C(2)	67.03(10)
C(15)-Co(1)-C(3)	134.65(13)
C(12)-Co(1)-C(3)	96.13(12)
C(11)-Co(1)-C(3)	111.90(12)
C(16)-Co(1)-C(3)	163.88(12)
C(1)-Co(1)-C(3)	66.52(10)
C(4)-Co(1)-C(3)	40.04(11)
C(5)-Co(1)-C(3)	66.57(11)
C(2)-Co(1)-C(3)	39.08(11)
C(5)-C(1)-C(2)	108.6(2)
C(5)-C(1)-C(6)	126.1(3)
C(2)-C(1)-C(6)	125.2(3)
C(5)-C(1)-Co(1)	71.18(15)
C(2)-C(1)-Co(1)	71.25(15)
C(6)-C(1)-Co(1)	127.6(2)

C(3)-C(2)-C(1)	107.4(2)
C(3)-C(2)-C(7)	127.1(3)
C(1)-C(2)-C(7)	125.4(3)
C(3)-C(2)-Co(1)	70.60(15)
C(1)-C(2)-Co(1)	68.60(14)
C(7)-C(2)-Co(1)	128.2(2)
C(2)-C(3)-C(4)	107.9(2)
C(2)-C(3)-C(8)	126.6(3)
C(4)-C(3)-C(8)	125.4(3)
C(2)-C(3)-Co(1)	70.32(15)
C(4)-C(3)-Co(1)	69.70(15)
C(8)-C(3)-Co(1)	128.6(2)
C(5)-C(4)-C(3)	108.6(2)
C(5)-C(4)-C(9)	125.9(3)
C(3)-C(4)-C(9)	125.3(3)
C(5)-C(4)-Co(1)	70.49(15)
C(3)-C(4)-Co(1)	70.26(15)
C(9)-C(4)-Co(1)	128.7(2)
C(4)-C(5)-C(1)	107.4(2)
C(4)-C(5)-C(10)	126.8(3)
C(1)-C(5)-C(10)	125.8(3)
C(4)-C(5)-Co(1)	70.49(16)
C(1)-C(5)-Co(1)	68.81(15)
C(10)-C(5)-Co(1)	127.4(2)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(2)-C(7)-H(7A)	109.5
C(2)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(2)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(3)-C(8)-H(8A)	109.5
C(3)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(3)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-C(9)-H(9A)	109.5
C(4)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(4)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5

C(12)-C(11)-C(18)	124.4(4)
C(12)-C(11)-Co(1)	69.74(18)
C(18)-C(11)-Co(1)	113.5(2)
C(12)-C(11)-H(11)	116(2)
C(18)-C(11)-H(11)	114(2)
Co(1)-C(11)-H(11)	110(2)
C(11)-C(12)-C(13)	124.7(4)
C(11)-C(12)-Co(1)	70.18(19)
C(13)-C(12)-Co(1)	112.0(2)
C(11)-C(12)-H(12)	117.0(18)
C(13)-C(12)-H(12)	113.7(18)
Co(1)-C(12)-H(12)	109.3(18)
C(14)-C(13)-C(12)	114.8(3)
C(14)-C(13)-H(13A)	108.6
C(12)-C(13)-H(13A)	108.6
C(14)-C(13)-H(13B)	108.6
C(12)-C(13)-H(13B)	108.6
H(13A)-C(13)-H(13B)	107.5
C(13)-C(14)-C(15)	115.0(3)
C(13)-C(14)-H(14A)	108.5
C(15)-C(14)-H(14A)	108.5
C(13)-C(14)-H(14B)	108.5
C(15)-C(14)-H(14B)	108.5
H(14A)-C(14)-H(14B)	107.5
C(16)-C(15)-C(14)	123.2(3)
C(16)-C(15)-Co(1)	70.52(17)
C(14)-C(15)-Co(1)	111.7(2)
C(16)-C(15)-H(15)	119(2)
C(14)-C(15)-H(15)	114(2)
Co(1)-C(15)-H(15)	107(2)
C(15)-C(16)-C(17)	124.2(3)
C(15)-C(16)-Co(1)	69.14(17)
C(17)-C(16)-Co(1)	113.3(2)
C(15)-C(16)-H(16)	123(2)
C(17)-C(16)-H(16)	108(2)
Co(1)-C(16)-H(16)	112(2)
C(18)-C(17)-C(16)	113.6(3)
C(18)-C(17)-H(17A)	108.9
C(16)-C(17)-H(17A)	108.9
C(18)-C(17)-H(17B)	108.9
C(16)-C(17)-H(17B)	108.9
H(17A)-C(17)-H(17B)	107.7
C(17)-C(18)-C(11)	114.5(3)
C(17)-C(18)-H(18A)	108.6
C(11)-C(18)-H(18A)	108.6
C(17)-C(18)-H(18B)	108.6
C(11)-C(18)-H(18B)	108.6
H(18A)-C(18)-H(18B)	107.6

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