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Crystal structure of (η^2,η^2-cycloocta-1,5-diene)(η^5-indenyl)cobalt(I)

Phillip Jungk, Anke Spannenberg and Marko Hapke*

Leibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Strasse 29a, 18059 Rostock, Germany. *Correspondence e-mail: marko.hapke@catalysis.de

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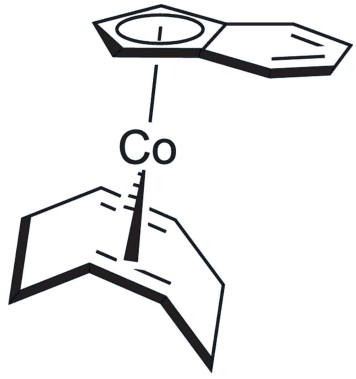
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Co(C_8H_{12})(C_9H_7)]$, was synthesized by the reaction of metallated 2-*H*-indene with $CoCl(PPh_3)_3$ and 1,5-cyclooctadiene in tetrahydrofuran/toluene. In the molecule, the Co^I atom is coordinated by the two double bonds of the 1,5-cyclooctadiene ligand and η^5-bonded to the indenyl ligand. The asymmetric unit contains two molecules of the Co^I complex with very similar conformations. In the crystal, molecules are arranged into rows parallel to [100]. Apart from dispersion forces, there are no notable intermolecular interactions in the crystal.

3D view

Chemical scheme



Structure description

The title compound (Fig. 1) is used for the formation of poly(enones) by terpolymerization of carbon monoxide with diynes and norbornadiene (Tsuda & Tsugawa, 1996) and also as catalyst in [2 + 2 + 2] cycloaddition reactions of acetylene and nitriles to form pyridine derivatives under irradiation (Heller & Oehme, 1995). It was synthesized by the reaction of metallated 2-*H*-indene with $CoCl(PPh_3)_3$ and 1,5-cyclooctadiene in tetrahydrofuran/toluene. In the molecule, the Co^I atom is coordinated by the two double bonds of the 1,5-cyclooctadiene ligand and η^5-bonded to the indenyl ligand. The asymmetric unit contains two molecules of the Co^I complex with very similar conformations. In the crystal, molecules are arranged into rows parallel to [100], Fig. 2. Apart from dispersion forces, there are no notable intermolecular interactions in the crystal.

For reported synthetic procedures of the title product by reducing the bis(η^5-indenyl) cobalt(II) complex in the presence of 1,5-cyclooctadiene and lithium, see: Salzer & Täschler (1985), and in the presence of magnesium-anthracene, see: Bönnemann *et al.* (1993). Chiral derivatives of the title compound, varying the substituent on the 1-indenyl position, were reported by Gutnov *et al.* (2004) and Heller & Oehme (1995). The

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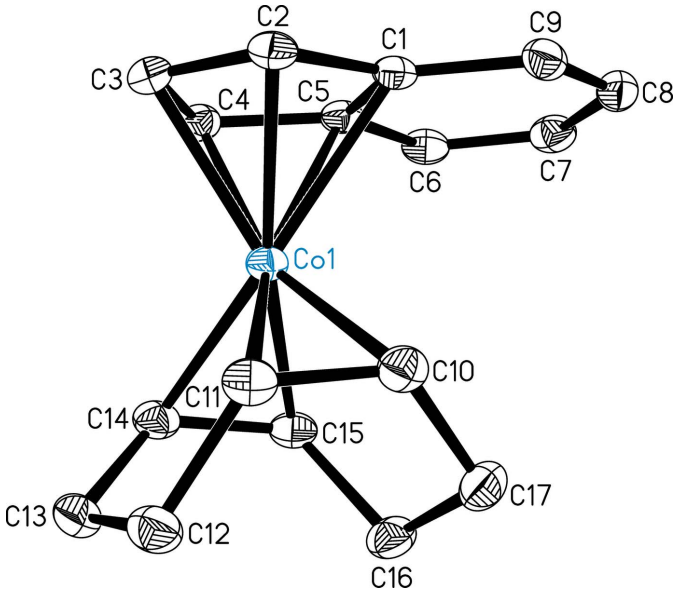

Figure 1
Molecular structure of one of the two molecules in the asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms were omitted for clarity.

structure of the Cp-analog of the title compound is reported by Ondráček *et al.* (1990). Hung-Low & Bradley (2011, 2013) report substituted indenyl derivatives.

Synthesis and crystallization

All manipulations were carried out under an argon atmosphere using standard Schlenk techniques. THF, toluene and *n*-hexane were dried over two columns with activated aluminium oxide with an Inert PureSolv MD5 solvent purification system (Innovative Technology) under argon. 2*H*-Indene (0.06 ml, 0.50 mmol) was added to a suspension of potassium hydride (20 mg, 0.50 mmol) in 5 ml THF in a Schlenk flask and stirred for 15 min at room temperature. Using a Schlenk glass adapter, solid $CoCl(PPh_3)_3$ (0.44 g, 0.50 mmol) was added, rinsed with 5 ml THF and the resulting mixture was stirred for additional 3 h. The solvent was evaporated *in vacuo* and the resulting residue was dissolved in 10 ml toluene. Finally, 1,5-cyclooctadiene (0.09 ml, 0.75 mmol) was added and the reaction mixture stirred for 6 h at 383 K and an additional 15 h at room temperature. The resulting mixture was filtered through a short column with degassed silica (2 x 3 cm) and the filtrate diluted with THF. The solvent was removed *in vacuo* and the product isolated as red crystals (0.12 g, 81%) after column chromatography under inert conditions over degassed silica with *n*-hexane as eluent. Crystals suitable for X-ray analysis were obtained by evaporation of the eluting solvent. The identity of the compound was proven by ^{1}H and ^{13}C NMR.

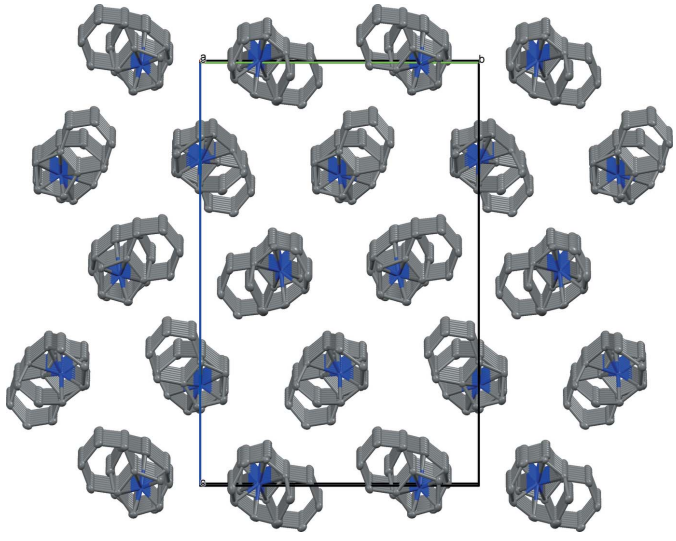

Figure 2
Crystal packing of the title compound in a view approximately along the *a* axis. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms were omitted for clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Co(C_8H_{12})(C_9H_7)]$
M_r	282.25
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	8.0307 (2), 14.4939 (3), 22.2528 (6)
β (°)	98.814 (2)
V (Å^3)	2559.55 (11)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.32
Crystal size (mm)	0.35 × 0.34 × 0.27
Data collection	
Diffractometer	Stoe IPDS II
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35986, 5024, 4307
R_{int}	0.032
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.060, 1.03
No. of reflections	5024
No. of parameters	357
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.39

Computer programs: *X-AREA* (Stoe & Cie, 2005), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *XP* in *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2006), *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

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full crystallographic data

IUCrData (2016). **1**, x160027 [doi:10.1107/S2414314616000274]

Crystal structure of (η^2,η^2-cycloocta-1,5-diene)(η^5-indenyl)cobalt(I)

Phillip Jungk, Anke Spannenberg and Marko Hapke

(η^2,η^2-Cycloocta-1,5-diene)(η^5-indenyl)cobalt(I)

Crystal data

$[Co(C_8H_{12})(C_9H_7)]$
M_r = 282.25
Monoclinic, $P2_1/n$
a = 8.0307 (2) Å
b = 14.4939 (3) Å
c = 22.2528 (6) Å
β = 98.814 (2)°
V = 2559.55 (11) Å^3
Z = 8
$F(000)$ = 1184
D_x = 1.465 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3014 reflections
θ = 1.6–27.1°
μ = 1.32 mm^{-1}
T = 150 K
Prism, red-brown
0.35 × 0.34 × 0.27 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω–scans
35986 measured reflections
5024 independent reflections
4307 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.0°, θ_{min} = 1.7°
h = −9→9
k = −17→17
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.060
S = 1.03
5024 reflections
357 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Co1	0.59531 (2)	−0.00072 (2)	0.23597 (2)	0.02402 (7)

C1	0.84516 (16)	0.06045 (10)	0.24041 (7)	0.0262 (3)
C2	0.78946 (18)	0.01032 (10)	0.18505 (7)	0.0294 (3)
H2	0.7702	0.0359	0.1453	0.035*
C3	0.76847 (18)	−0.08314 (10)	0.19994 (7)	0.0318 (3)
H3	0.7427	−0.1324	0.1719	0.038*
C4	0.79252 (18)	−0.09065 (10)	0.26417 (7)	0.0300 (3)
H4	0.7762	−0.1448	0.2866	0.036*
C5	0.84612 (18)	−0.00198 (9)	0.28988 (7)	0.0270 (3)
C6	0.88758 (18)	0.03005 (11)	0.35024 (7)	0.0320 (3)
H6	0.8853	−0.0106	0.3836	0.038*
C7	0.93101 (19)	0.12060 (11)	0.35988 (7)	0.0351 (3)
H7	0.9605	0.1425	0.4004	0.042*
C8	0.93288 (19)	0.18232 (11)	0.31084 (8)	0.0344 (3)
H8	0.9652	0.2447	0.3190	0.041*
C9	0.88928 (18)	0.15423 (10)	0.25217 (7)	0.0310 (3)
H9	0.8884	0.1967	0.2196	0.037*
C10	0.47123 (19)	0.11738 (10)	0.21129 (7)	0.0316 (3)
H10	0.547 (2)	0.1588 (12)	0.1943 (8)	0.039 (5)*
C11	0.40445 (19)	0.04573 (10)	0.17247 (7)	0.0311 (3)
H11	0.444 (2)	0.0405 (11)	0.1338 (8)	0.030 (4)*
C12	0.2365 (2)	0.00024 (11)	0.17674 (8)	0.0363 (4)
H12A	0.1815	−0.0179	0.1356	0.044*
H12B	0.1620	0.0450	0.1932	0.044*
C13	0.25913 (19)	−0.08530 (11)	0.21783 (8)	0.0362 (4)
H13A	0.1589	−0.0924	0.2384	0.043*
H13B	0.2671	−0.1408	0.1924	0.043*
C14	0.41473 (18)	−0.07912 (11)	0.26525 (7)	0.0316 (3)
H14	0.463 (2)	−0.1390 (12)	0.2795 (8)	0.035 (4)*
C15	0.45397 (19)	−0.00372 (10)	0.30418 (7)	0.0305 (3)
H15	0.526 (2)	−0.0130 (10)	0.3411 (8)	0.031 (4)*
C16	0.3418 (2)	0.08051 (11)	0.30450 (8)	0.0377 (4)
H16A	0.3503	0.1045	0.3465	0.045*
H16B	0.2231	0.0626	0.2907	0.045*
C17	0.3921 (2)	0.15631 (11)	0.26299 (8)	0.0387 (4)
H17A	0.2909	0.1924	0.2463	0.046*
H17B	0.4729	0.1987	0.2872	0.046*
Co2	0.03476 (2)	0.78868 (2)	1.00510 (2)	0.02282 (6)
C18	−0.22601 (17)	0.76375 (10)	0.96523 (7)	0.0275 (3)
C19	−0.19275 (18)	0.85687 (10)	0.98738 (7)	0.0312 (3)
H19	−0.2044	0.9113	0.9633	0.037*
C20	−0.14008 (19)	0.85315 (11)	1.05075 (7)	0.0325 (3)
H20	−0.1194	0.9047	1.0772	0.039*
C21	−0.12338 (19)	0.75916 (11)	1.06809 (7)	0.0313 (3)
H21	−0.0803	0.7369	1.1076	0.038*
C22	−0.18288 (17)	0.70295 (10)	1.01557 (7)	0.0279 (3)
C23	−0.19716 (19)	0.60644 (10)	1.00634 (8)	0.0346 (3)
H23	−0.1673	0.5649	1.0392	0.041*
C24	−0.2546 (2)	0.57421 (11)	0.94931 (8)	0.0384 (4)

H24	−0.2671	0.5096	0.9430	0.046*
C25	−0.29577 (19)	0.63447 (11)	0.89959 (8)	0.0373 (4)
H25	−0.3344	0.6096	0.8604	0.045*
C26	−0.28128 (19)	0.72780 (11)	0.90658 (7)	0.0329 (3)
H26	−0.3078	0.7678	0.8726	0.040*
C27	0.1724 (2)	0.87766 (11)	0.96298 (8)	0.0365 (4)
H27	0.108 (2)	0.9323 (13)	0.9565 (9)	0.048 (5)*
C28	0.1180 (2)	0.80406 (12)	0.92464 (8)	0.0365 (4)
H28	0.026 (3)	0.8137 (13)	0.8947 (9)	0.050 (5)*
C29	0.2226 (2)	0.72263 (13)	0.91177 (8)	0.0458 (4)
H29A	0.3078	0.7431	0.8868	0.055*
H29B	0.1491	0.6767	0.8878	0.055*
C30	0.3114 (2)	0.67713 (12)	0.96903 (8)	0.0415 (4)
H30A	0.4269	0.7024	0.9789	0.050*
H30B	0.3206	0.6100	0.9619	0.050*
C31	0.21792 (19)	0.69281 (11)	1.02245 (7)	0.0310 (3)
H31	0.166 (2)	0.6412 (12)	1.0364 (8)	0.037 (5)*
C32	0.25222 (19)	0.76667 (11)	1.06207 (7)	0.0329 (3)
H32	0.226 (2)	0.7578 (11)	1.1021 (8)	0.037 (5)*
C33	0.3829 (2)	0.83998 (13)	1.05601 (9)	0.0458 (4)
H33A	0.4962	0.8113	1.0622	0.055*
H33B	0.3806	0.8870	1.0882	0.055*
C34	0.3530 (2)	0.88699 (12)	0.99418 (10)	0.0466 (4)
H34A	0.3814	0.9533	0.9994	0.056*
H34B	0.4290	0.8596	0.9679	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02222 (10)	0.02618 (11)	0.02454 (11)	0.00065 (7)	0.00640 (8)	0.00204 (7)
C1	0.0193 (6)	0.0305 (7)	0.0301 (8)	0.0012 (5)	0.0078 (6)	0.0028 (6)
C2	0.0257 (7)	0.0364 (8)	0.0280 (8)	−0.0009 (6)	0.0099 (6)	0.0023 (6)
C3	0.0288 (7)	0.0330 (8)	0.0363 (9)	0.0009 (6)	0.0134 (6)	−0.0057 (6)
C4	0.0267 (7)	0.0265 (7)	0.0382 (9)	0.0039 (6)	0.0095 (6)	0.0043 (6)
C5	0.0197 (7)	0.0306 (7)	0.0312 (8)	0.0039 (5)	0.0058 (6)	0.0030 (6)
C6	0.0250 (7)	0.0430 (8)	0.0281 (8)	0.0037 (6)	0.0047 (6)	0.0061 (7)
C7	0.0253 (7)	0.0472 (9)	0.0320 (8)	0.0022 (6)	0.0016 (6)	−0.0080 (7)
C8	0.0261 (7)	0.0315 (8)	0.0454 (10)	0.0004 (6)	0.0052 (7)	−0.0062 (7)
C9	0.0248 (7)	0.0296 (7)	0.0389 (9)	0.0001 (5)	0.0056 (6)	0.0043 (6)
C10	0.0282 (7)	0.0299 (7)	0.0363 (9)	0.0044 (6)	0.0033 (6)	0.0074 (6)
C11	0.0281 (7)	0.0370 (8)	0.0277 (8)	0.0035 (6)	0.0027 (6)	0.0057 (6)
C12	0.0268 (8)	0.0455 (9)	0.0357 (9)	−0.0011 (6)	0.0020 (7)	−0.0023 (7)
C13	0.0290 (8)	0.0397 (9)	0.0413 (9)	−0.0066 (6)	0.0097 (7)	−0.0036 (7)
C14	0.0278 (7)	0.0331 (8)	0.0363 (9)	−0.0015 (6)	0.0124 (6)	0.0057 (7)
C15	0.0261 (7)	0.0395 (9)	0.0277 (8)	0.0010 (6)	0.0101 (6)	0.0034 (6)
C16	0.0345 (8)	0.0444 (9)	0.0364 (9)	0.0045 (7)	0.0117 (7)	−0.0083 (7)
C17	0.0378 (9)	0.0326 (8)	0.0453 (10)	0.0075 (6)	0.0056 (7)	−0.0045 (7)
Co2	0.02156 (10)	0.02390 (10)	0.02391 (11)	0.00029 (7)	0.00638 (7)	0.00126 (7)

C18	0.0190 (7)	0.0306 (7)	0.0334 (8)	0.0017 (5)	0.0061 (6)	0.0031 (6)
C19	0.0257 (7)	0.0280 (7)	0.0412 (9)	0.0051 (6)	0.0088 (6)	0.0018 (6)
C20	0.0285 (7)	0.0333 (8)	0.0384 (9)	0.0004 (6)	0.0139 (6)	−0.0072 (7)
C21	0.0279 (7)	0.0411 (8)	0.0265 (8)	−0.0033 (6)	0.0098 (6)	0.0012 (6)
C22	0.0218 (7)	0.0325 (7)	0.0310 (8)	−0.0015 (5)	0.0088 (6)	0.0026 (6)
C23	0.0314 (8)	0.0318 (8)	0.0412 (9)	−0.0033 (6)	0.0077 (7)	0.0082 (7)
C24	0.0339 (8)	0.0289 (8)	0.0529 (10)	−0.0047 (6)	0.0082 (7)	−0.0059 (7)
C25	0.0296 (8)	0.0454 (9)	0.0369 (9)	−0.0038 (7)	0.0050 (7)	−0.0092 (7)
C26	0.0258 (7)	0.0401 (8)	0.0323 (8)	0.0005 (6)	0.0024 (6)	0.0033 (7)
C27	0.0313 (8)	0.0332 (8)	0.0473 (10)	−0.0007 (6)	0.0135 (7)	0.0131 (7)
C28	0.0328 (8)	0.0501 (10)	0.0283 (8)	0.0003 (7)	0.0107 (7)	0.0117 (7)
C29	0.0470 (10)	0.0585 (11)	0.0359 (9)	−0.0013 (8)	0.0193 (8)	−0.0079 (8)
C30	0.0398 (9)	0.0423 (9)	0.0444 (10)	0.0100 (7)	0.0132 (8)	−0.0062 (8)
C31	0.0278 (7)	0.0300 (8)	0.0356 (9)	0.0054 (6)	0.0066 (6)	0.0040 (6)
C32	0.0252 (7)	0.0458 (9)	0.0269 (8)	0.0016 (6)	0.0020 (6)	0.0006 (7)
C33	0.0305 (8)	0.0565 (11)	0.0496 (11)	−0.0103 (7)	0.0041 (7)	−0.0130 (9)
C34	0.0336 (9)	0.0368 (9)	0.0710 (13)	−0.0109 (7)	0.0135 (8)	0.0023 (8)

Geometric parameters (Å, º)

Co1—C10	2.0142 (14)	Co2—C28	2.0169 (16)
Co1—C14	2.0269 (14)	Co2—C31	2.0173 (15)
Co1—C15	2.0304 (15)	Co2—C32	2.0199 (16)
Co1—C11	2.0336 (15)	Co2—C27	2.0200 (15)
Co1—C2	2.0693 (14)	Co2—C19	2.0615 (14)
Co1—C4	2.0727 (14)	Co2—C21	2.0751 (15)
Co1—C3	2.0844 (14)	Co2—C20	2.0770 (14)
Co1—C5	2.1808 (15)	Co2—C18	2.1757 (14)
Co1—C1	2.1820 (13)	Co2—C22	2.1859 (14)
C1—C9	1.419 (2)	C18—C26	1.412 (2)
C1—C5	1.424 (2)	C18—C22	1.426 (2)
C1—C2	1.441 (2)	C18—C19	1.448 (2)
C2—C3	1.411 (2)	C19—C20	1.410 (2)
C2—H2	0.9500	C19—H19	0.9500
C3—C4	1.417 (2)	C20—C21	1.417 (2)
C3—H3	0.9500	C20—H20	0.9500
C4—C5	1.445 (2)	C21—C22	1.445 (2)
C4—H4	0.9500	C21—H21	0.9500
C5—C6	1.412 (2)	C22—C23	1.416 (2)
C6—C7	1.366 (2)	C23—C24	1.365 (2)
C6—H6	0.9500	C23—H23	0.9500
C7—C8	1.413 (2)	C24—C25	1.408 (2)
C7—H7	0.9500	C24—H24	0.9500
C8—C9	1.361 (2)	C25—C26	1.365 (2)
C8—H8	0.9500	C25—H25	0.9500
C9—H9	0.9500	C26—H26	0.9500
C10—C11	1.404 (2)	C27—C28	1.394 (2)
C10—C17	1.506 (2)	C27—C34	1.515 (2)

C10—H10	0.974 (18)	C27—H27	0.945 (19)
C11—C12	1.518 (2)	C28—C29	1.502 (2)
C11—H11	0.964 (17)	C28—H28	0.93 (2)
C12—C13	1.535 (2)	C29—C30	1.513 (3)
C12—H12A	0.9900	C29—H29A	0.9900
C12—H12B	0.9900	C29—H29B	0.9900
C13—C14	1.510 (2)	C30—C31	1.517 (2)
C13—H13A	0.9900	C30—H30A	0.9900
C13—H13B	0.9900	C30—H30B	0.9900
C14—C15	1.400 (2)	C31—C32	1.387 (2)
C14—H14	0.984 (17)	C31—H31	0.934 (18)
C15—C16	1.518 (2)	C32—C33	1.514 (2)
C15—H15	0.939 (18)	C32—H32	0.957 (18)
C16—C17	1.529 (2)	C33—C34	1.521 (3)
C16—H16A	0.9900	C33—H33A	0.9900
C16—H16B	0.9900	C33—H33B	0.9900
C17—H17A	0.9900	C34—H34A	0.9900
C17—H17B	0.9900	C34—H34B	0.9900

C10—Co1—C14	102.45 (6)	C28—Co2—C31	85.13 (7)
C10—Co1—C15	84.96 (6)	C28—Co2—C32	101.68 (7)
C14—Co1—C15	40.37 (6)	C31—Co2—C32	40.20 (7)
C10—Co1—C11	40.58 (6)	C28—Co2—C27	40.40 (7)
C14—Co1—C11	84.77 (6)	C31—Co2—C27	95.39 (7)
C15—Co1—C11	94.50 (6)	C32—Co2—C27	84.84 (7)
C10—Co1—C2	99.66 (6)	C28—Co2—C19	100.47 (7)
C14—Co1—C2	148.83 (6)	C31—Co2—C19	164.95 (6)
C15—Co1—C2	164.90 (6)	C32—Co2—C19	148.37 (7)
C11—Co1—C2	98.33 (6)	C27—Co2—C19	97.88 (6)
C10—Co1—C4	160.07 (6)	C28—Co2—C21	160.50 (7)
C14—Co1—C4	95.81 (6)	C31—Co2—C21	103.44 (6)
C15—Co1—C4	104.41 (6)	C32—Co2—C21	95.93 (6)
C11—Co1—C4	151.42 (6)	C27—Co2—C21	151.64 (7)
C2—Co1—C4	67.02 (6)	C19—Co2—C21	67.16 (6)
C10—Co1—C3	135.52 (6)	C28—Co2—C20	136.49 (7)
C14—Co1—C3	110.78 (6)	C31—Co2—C20	138.07 (7)
C15—Co1—C3	139.25 (6)	C32—Co2—C20	110.38 (7)
C11—Co1—C3	113.50 (6)	C27—Co2—C20	113.49 (7)
C2—Co1—C3	39.71 (6)	C19—Co2—C20	39.83 (6)
C4—Co1—C3	39.85 (6)	C21—Co2—C20	39.90 (6)
C10—Co1—C5	122.26 (6)	C28—Co2—C18	94.90 (6)
C14—Co1—C5	117.67 (6)	C31—Co2—C18	126.28 (6)
C15—Co1—C5	99.41 (6)	C32—Co2—C18	156.24 (6)
C11—Co1—C5	156.82 (6)	C27—Co2—C18	118.53 (6)
C2—Co1—C5	65.92 (6)	C19—Co2—C18	39.84 (6)
C4—Co1—C5	39.62 (5)	C21—Co2—C18	65.84 (6)
C3—Co1—C5	65.95 (6)	C20—Co2—C18	66.02 (6)
C10—Co1—C1	94.59 (6)	C28—Co2—C22	122.44 (7)

C14—Co1—C1	155.71 (6)	C31—Co2—C22	99.18 (6)
C15—Co1—C1	126.18 (6)	C32—Co2—C22	118.15 (6)
C11—Co1—C1	119.14 (6)	C27—Co2—C22	156.30 (7)
C2—Co1—C1	39.52 (6)	C19—Co2—C22	65.99 (6)
C4—Co1—C1	65.62 (5)	C21—Co2—C22	39.53 (6)
C3—Co1—C1	65.62 (6)	C20—Co2—C22	65.93 (6)
C5—Co1—C1	38.10 (5)	C18—Co2—C22	38.16 (5)
C9—C1—C5	119.64 (14)	C26—C18—C22	120.14 (14)
C9—C1—C2	132.58 (14)	C26—C18—C19	132.39 (14)
C5—C1—C2	107.74 (13)	C22—C18—C19	107.39 (13)
C9—C1—Co1	126.84 (10)	C26—C18—Co2	125.78 (10)
C5—C1—Co1	70.90 (8)	C22—C18—Co2	71.31 (8)
C2—C1—Co1	66.02 (8)	C19—C18—Co2	65.83 (8)
C3—C2—C1	108.41 (13)	C20—C19—C18	108.45 (13)
C3—C2—Co1	70.72 (8)	C20—C19—Co2	70.68 (8)
C1—C2—Co1	74.46 (8)	C18—C19—Co2	74.34 (8)
C3—C2—H2	125.8	C20—C19—H19	125.8
C1—C2—H2	125.8	C18—C19—H19	125.8
Co1—C2—H2	120.7	Co2—C19—H19	120.9
C2—C3—C4	107.94 (13)	C19—C20—C21	108.09 (13)
C2—C3—Co1	69.57 (8)	C19—C20—Co2	69.49 (8)
C4—C3—Co1	69.63 (8)	C21—C20—Co2	69.98 (8)
C2—C3—H3	126.0	C19—C20—H20	126.0
C4—C3—H3	126.0	C21—C20—H20	126.0
Co1—C3—H3	126.3	Co2—C20—H20	126.1
C3—C4—C5	108.50 (13)	C20—C21—C22	108.44 (14)
C3—C4—Co1	70.52 (8)	C20—C21—Co2	70.12 (8)
C5—C4—Co1	74.22 (8)	C22—C21—Co2	74.37 (8)
C3—C4—H4	125.8	C20—C21—H21	125.8
C5—C4—H4	125.8	C22—C21—H21	125.8
Co1—C4—H4	121.2	Co2—C21—H21	121.4
C6—C5—C1	119.93 (13)	C23—C22—C18	119.49 (14)
C6—C5—C4	132.96 (14)	C23—C22—C21	133.15 (14)
C1—C5—C4	107.04 (13)	C18—C22—C21	107.30 (13)
C6—C5—Co1	125.72 (10)	C23—C22—Co2	126.47 (10)
C1—C5—Co1	71.00 (8)	C18—C22—Co2	70.54 (8)
C4—C5—Co1	66.15 (8)	C21—C22—Co2	66.10 (8)
C7—C6—C5	118.85 (15)	C24—C23—C22	118.78 (15)
C7—C6—H6	120.6	C24—C23—H23	120.6
C5—C6—H6	120.6	C22—C23—H23	120.6
C6—C7—C8	121.30 (15)	C23—C24—C25	121.56 (15)
C6—C7—H7	119.3	C23—C24—H24	119.2
C8—C7—H7	119.3	C25—C24—H24	119.2
C9—C8—C7	121.32 (14)	C26—C25—C24	121.30 (15)
C9—C8—H8	119.3	C26—C25—H25	119.3
C7—C8—H8	119.3	C24—C25—H25	119.3
C8—C9—C1	118.93 (14)	C25—C26—C18	118.71 (15)
C8—C9—H9	120.5	C25—C26—H26	120.6

C1—C9—H9	120.5	C18—C26—H26	120.6
C11—C10—C17	125.52 (14)	C28—C27—C34	122.49 (15)
C11—C10—Co1	70.45 (8)	C28—C27—Co2	69.68 (9)
C17—C10—Co1	111.05 (11)	C34—C27—Co2	113.45 (11)
C11—C10—H10	114.9 (10)	C28—C27—H27	115.8 (12)
C17—C10—H10	115.4 (10)	C34—C27—H27	117.2 (12)
Co1—C10—H10	108.4 (10)	Co2—C27—H27	106.4 (11)
C10—C11—C12	122.84 (14)	C27—C28—C29	125.88 (16)
C10—C11—Co1	68.97 (8)	C27—C28—Co2	69.92 (9)
C12—C11—Co1	113.28 (11)	C29—C28—Co2	110.72 (11)
C10—C11—H11	117.5 (10)	C27—C28—H28	117.8 (12)
C12—C11—H11	116.0 (10)	C29—C28—H28	112.9 (12)
Co1—C11—H11	106.2 (10)	Co2—C28—H28	108.5 (12)
C11—C12—C13	111.27 (13)	C28—C29—C30	112.79 (14)
C11—C12—H12A	109.4	C28—C29—H29A	109.0
C13—C12—H12A	109.4	C30—C29—H29A	109.0
C11—C12—H12B	109.4	C28—C29—H29B	109.0
C13—C12—H12B	109.4	C30—C29—H29B	109.0
H12A—C12—H12B	108.0	H29A—C29—H29B	107.8
C14—C13—C12	112.24 (13)	C29—C30—C31	111.63 (13)
C14—C13—H13A	109.2	C29—C30—H30A	109.3
C12—C13—H13A	109.2	C31—C30—H30A	109.3
C14—C13—H13B	109.2	C29—C30—H30B	109.3
C12—C13—H13B	109.2	C31—C30—H30B	109.3
H13A—C13—H13B	107.9	H30A—C30—H30B	108.0
C15—C14—C13	124.23 (14)	C32—C31—C30	122.65 (15)
C15—C14—Co1	69.95 (8)	C32—C31—Co2	70.00 (9)
C13—C14—Co1	111.40 (10)	C30—C31—Co2	112.77 (11)
C15—C14—H14	116.6 (10)	C32—C31—H31	117.5 (11)
C13—C14—H14	114.7 (10)	C30—C31—H31	116.2 (11)
Co1—C14—H14	109.3 (10)	Co2—C31—H31	105.4 (11)
C14—C15—C16	123.58 (15)	C31—C32—C33	123.91 (15)
C14—C15—Co1	69.68 (8)	C31—C32—Co2	69.80 (9)
C16—C15—Co1	112.73 (10)	C33—C32—Co2	112.20 (12)
C14—C15—H15	118.6 (10)	C31—C32—H32	115.9 (10)
C16—C15—H15	113.5 (10)	C33—C32—H32	115.7 (11)
Co1—C15—H15	108.4 (11)	Co2—C32—H32	108.1 (11)
C15—C16—C17	111.29 (13)	C32—C33—C34	112.29 (14)
C15—C16—H16A	109.4	C32—C33—H33A	109.1
C17—C16—H16A	109.4	C34—C33—H33A	109.1
C15—C16—H16B	109.4	C32—C33—H33B	109.1
C17—C16—H16B	109.4	C34—C33—H33B	109.1
H16A—C16—H16B	108.0	H33A—C33—H33B	107.9
C10—C17—C16	111.94 (13)	C27—C34—C33	112.45 (13)
C10—C17—H17A	109.2	C27—C34—H34A	109.1
C16—C17—H17A	109.2	C33—C34—H34A	109.1
C10—C17—H17B	109.2	C27—C34—H34B	109.1
C16—C17—H17B	109.2	C33—C34—H34B	109.1

H17A—C17—H17B	107.9	H34A—C34—H34B	107.8