

Bis(η^5 -pentamethylcyclopentadienyl)-cobalt(II)

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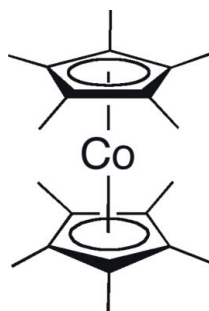
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.031; wR factor = 0.089; data-to-parameter ratio = 28.4.

The crystal structure of the title compound, decamethylcobaltocene, $[\text{Co}(\text{C}_{10}\text{H}_{15})_2]$, has been determined. High-quality single crystals were grown from a cold saturated hexamethyldisiloxane solution. The structure is related to the manganese and iron analogs. The molecule has D_{5d} symmetry, with the Co atom in a crystallographic $2/m$ position. The cobalt-centroid(C_5) distance is 1.71 Å and the centroid(C_5)-Co-centroid(C_5) angle is 180° , by symmetry.

Related literature

For the synthesis of the title compound and its electrochemical and magnetic properties, see: Robbins *et al.* (1982). For its formal potential and use as a reducing agent, see: Connelly & Geiger (1996). For the isotopic manganese and iron structures, see: Struchkov *et al.* (1978); Freyburg *et al.* (1979); Augart *et al.* (1991); Arrais *et al.* (2003).



Experimental

Crystal data

$[\text{Co}(\text{C}_{10}\text{H}_{15})_2]$	$V = 1737.0$ (3) Å ³
$M_r = 329.37$	$Z = 4$
Orthorhombic, $Cmca$	Mo $K\alpha$ radiation
$a = 15.0848$ (16) Å	$\mu = 0.98$ mm ⁻¹
$b = 11.5031$ (12) Å	$T = 100$ K
$c = 10.0105$ (10) Å	$0.28 \times 0.28 \times 0.14$ mm

Data collection

Bruker APEXII CCD diffractometer	19672 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2008a)	2386 independent reflections
$T_{\min} = 0.771$, $T_{\max} = 0.875$	1903 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$	84 parameters
$wR(F^2) = 0.089$	All H-atom parameters refined
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.70$ e Å ⁻³
2386 reflections	$\Delta\rho_{\text{min}} = -0.74$ e Å ⁻³

Table 1

Selected bond lengths (Å).

Co1—C1	2.0914 (12)	C1—C4	1.4961 (18)
Co1—C3	2.0956 (8)	C2—C3	1.4231 (12)
Co1—C2	2.1113 (8)	C2—C5	1.4935 (14)
C1—C2	1.4304 (12)	C3—C6	1.4950 (13)

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008b); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008b); molecular graphics: SHELXTL (Sheldrick, 2008b); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2590).

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supplementary materials

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Comment

The structure of (I) has been conspicuously absent from the literature, despite its being a widely used reducing agent (Connelly & Geiger, 1996). Robbins and co-workers referred to a structural determination in 1982 (Robbins *et al.*, 1982), specifically its D_{5d} symmetry and its similarity to the manganese analog. However, no structural data were presented. Attempts to grow single crystals from toluene and hexane, the latter from which Robbins reported having grown crystals, resulted in very poor quality specimens that were unsuitable for X-ray diffraction experiments. A cold (-38 °C) saturated hexamethyldisiloxane solution of (I) afforded excellent crystals that resulted in a high quality structural determination.

The structure is isomorphous to that of decamethylferrocene (refcodes DMFERR, Struchkov *et al.*, 1978, DMFERR01, Freyburg *et al.*, 1979, DMFERR02, Arrais *et al.*, 2003) and the low temperature polymorph of decamethylmanganocene (refcodes DMCPMN01 and DMCPMN02, Augart *et al.*, 1991), for which the metal atoms are in crystallographic $2/m$ positions.

Experimental

All operations were performed under an inert atmosphere (dinitrogen). Hexamethyldisiloxane was stirred over CaH_2 and vacuum transferred from sodium benzophenone ketyl. (I) was purchased from Sigma-Aldrich and used as is. Hexamethyldisiloxane (1 ml) was added to (I) (10 mg, 30 μmol), most of which dissolved over the course of a few hours at room temperature. After filtration through Celite, the filtrate was stored at -38 °C, resulting in dark yellow-brown crystals of (I) after a few hours.

Refinement

Hydrogen atoms were found from the difference Fourier map and refined independently from their respective carbon atoms with individual isotropic displacement parameters.

Figures

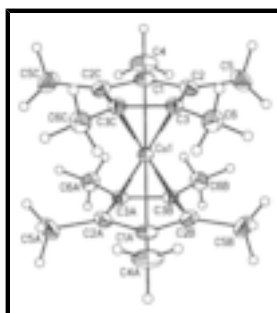


Fig. 1. A displacement ellipsoid (50% probability) drawing of (I). The cobalt atom is in a crystallographic $2/m$ position.

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Crystal data

[Co(C ₁₀ H ₁₅) ₂]	$F_{000} = 708$
$M_r = 329.37$	$D_x = 1.259 \text{ Mg m}^{-3}$
Orthorhombic, $Cmca$	Mo $K\alpha$ radiation
Hall symbol: -C 2bc 2	$\lambda = 0.71073 \text{ \AA}$
$a = 15.0848 (16) \text{ \AA}$	Cell parameters from 4000 reflections
$b = 11.5031 (12) \text{ \AA}$	$\theta = 3.0\text{--}37.5^\circ$
$c = 10.0105 (10) \text{ \AA}$	$\mu = 0.98 \text{ mm}^{-1}$
$V = 1737.0 (3) \text{ \AA}^3$	$T = 100 \text{ K}$
$Z = 4$	Block, dark yellow-brown
	$0.28 \times 0.28 \times 0.14 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer	2386 independent reflections
Radiation source: fine-focus sealed tube	1903 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.046$
$T = 100 \text{ K}$	$\theta_{\text{max}} = 38.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.7^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2008a)	$h = -25 \rightarrow 25$
$T_{\text{min}} = 0.771$, $T_{\text{max}} = 0.875$	$k = -19 \rightarrow 19$
19672 measured reflections	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	All H-atom parameters refined
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2 + 0.2743P]$
$S = 1.07$	where $P = (F_o^2 + 2F_c^2)/3$
2386 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
84 parameters	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.74 \text{ e \AA}^{-3}$
	Extinction correction: none

Special details

Experimental. The crystal was examined under N₂ and affixed to the end of a glass capillary with viscous oil, which protected the crystal during transfer to the cold stream.

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) etc. and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.0000	0.0000	0.01533 (7)
C1	0.0000	-0.17732 (10)	0.04617 (12)	0.0228 (2)
C2	-0.07677 (6)	-0.12416 (7)	0.10364 (8)	0.02149 (15)
C3	-0.04749 (5)	-0.03551 (7)	0.19244 (8)	0.01843 (13)
C4	0.0000	-0.27361 (12)	-0.05429 (14)	0.0348 (3)
H4A	0.0000	-0.352 (3)	-0.013 (2)	0.045 (8)*
H4B	-0.0486 (10)	-0.2711 (18)	-0.1133 (16)	0.063 (5)*
C5	-0.17089 (8)	-0.15651 (11)	0.07606 (12)	0.0340 (2)
H5A	-0.1798 (16)	-0.184 (2)	-0.0134 (18)	0.053 (6)*
H5B	-0.2119 (12)	-0.0926 (16)	0.0778 (19)	0.059 (5)*
H5C	-0.1896 (11)	-0.2189 (15)	0.1358 (16)	0.047 (4)*
C6	-0.10544 (7)	0.04079 (10)	0.27607 (9)	0.02731 (18)
H6A	-0.1134 (15)	0.0057 (13)	0.360 (3)	0.045 (6)*
H6B	-0.1638 (11)	0.0562 (13)	0.2287 (15)	0.039 (4)*
H6C	-0.0774 (11)	0.1158 (14)	0.2912 (14)	0.037 (4)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01811 (10)	0.01380 (9)	0.01409 (9)	0.000	0.000	-0.00032 (6)
C1	0.0353 (6)	0.0161 (4)	0.0170 (4)	0.000	0.000	-0.0004 (4)
C2	0.0245 (3)	0.0202 (3)	0.0198 (3)	-0.0054 (3)	-0.0013 (3)	0.0016 (3)
C3	0.0205 (3)	0.0180 (3)	0.0168 (3)	0.0002 (3)	0.0014 (2)	0.0006 (2)
C4	0.0653 (11)	0.0183 (5)	0.0206 (5)	0.000	0.000	-0.0029 (4)
C5	0.0290 (4)	0.0371 (5)	0.0359 (5)	-0.0147 (4)	-0.0069 (4)	0.0063 (4)
C6	0.0293 (4)	0.0292 (4)	0.0234 (4)	0.0056 (4)	0.0068 (3)	-0.0005 (3)

Geometric parameters (\AA , $^\circ$)

Co1—C1 ⁱ	2.0914 (12)	C2—C3	1.4231 (12)
Co1—C1	2.0914 (12)	C2—C5	1.4935 (14)
Co1—C3 ⁱⁱ	2.0955 (8)	C3—C3 ⁱⁱ	1.4328 (17)
Co1—C3	2.0956 (8)	C3—C6	1.4950 (13)
Co1—C3 ⁱ	2.0956 (8)	C4—H4A	0.99 (3)
Co1—C3 ⁱⁱⁱ	2.0956 (8)	C4—H4B	0.942 (16)

supplementary materials

Co1—C2 ⁱⁱⁱ	2.1113 (8)	C5—H5A	0.960 (18)
Co1—C2	2.1113 (8)	C5—H5B	0.962 (18)
Co1—C2 ⁱⁱ	2.1113 (8)	C5—H5C	0.976 (17)
Co1—C2 ⁱ	2.1113 (8)	C6—H6A	0.94 (2)
C1—C2	1.4304 (12)	C6—H6B	1.016 (16)
C1—C2 ⁱⁱ	1.4304 (12)	C6—H6C	0.973 (16)
C1—C4	1.4961 (18)		
C1 ⁱ —Co1—C1	180.0	C3—Co1—C2 ⁱ	140.46 (3)
C1 ⁱ —Co1—C3 ⁱⁱ	113.16 (4)	C3 ⁱ —Co1—C2 ⁱ	39.54 (3)
C1—Co1—C3 ⁱⁱ	66.84 (4)	C3 ⁱⁱⁱ —Co1—C2 ⁱ	66.67 (3)
C1 ⁱ —Co1—C3	113.16 (4)	C2 ⁱⁱⁱ —Co1—C2 ⁱ	66.53 (5)
C1—Co1—C3	66.84 (4)	C2—Co1—C2 ⁱ	180.0
C3 ⁱⁱ —Co1—C3	39.98 (5)	C2 ⁱⁱ —Co1—C2 ⁱ	113.47 (5)
C1 ⁱ —Co1—C3 ⁱ	66.84 (4)	C2—C1—C2 ⁱⁱ	108.12 (10)
C1—Co1—C3 ⁱ	113.16 (4)	C2—C1—C4	125.94 (5)
C3 ⁱⁱ —Co1—C3 ⁱ	140.02 (5)	C2 ⁱⁱ —C1—C4	125.93 (5)
C3—Co1—C3 ⁱ	180.0	C2—C1—Co1	70.85 (6)
C1 ⁱ —Co1—C3 ⁱⁱⁱ	66.84 (4)	C2 ⁱⁱ —C1—Co1	70.85 (6)
C1—Co1—C3 ⁱⁱⁱ	113.16 (4)	C4—C1—Co1	124.99 (9)
C3 ⁱⁱ —Co1—C3 ⁱⁱⁱ	180.0	C3—C2—C1	107.84 (8)
C3—Co1—C3 ⁱⁱⁱ	140.02 (5)	C3—C2—C5	126.09 (9)
C3 ⁱ —Co1—C3 ⁱⁱⁱ	39.98 (5)	C1—C2—C5	126.07 (9)
C1 ⁱ —Co1—C2 ⁱⁱⁱ	39.79 (3)	C3—C2—Co1	69.63 (5)
C1—Co1—C2 ⁱⁱⁱ	140.21 (3)	C1—C2—Co1	69.36 (6)
C3 ⁱⁱ —Co1—C2 ⁱⁱⁱ	140.46 (3)	C5—C2—Co1	126.81 (7)
C3—Co1—C2 ⁱⁱⁱ	113.34 (3)	C2—C3—C3 ⁱⁱ	108.08 (5)
C3 ⁱ —Co1—C2 ⁱⁱⁱ	66.66 (3)	C2—C3—C6	126.09 (8)
C3 ⁱⁱⁱ —Co1—C2 ⁱⁱⁱ	39.54 (3)	C3 ⁱⁱ —C3—C6	125.78 (5)
C1 ⁱ —Co1—C2	140.21 (3)	C2—C3—Co1	70.82 (5)
C1—Co1—C2	39.79 (3)	C3 ⁱⁱ —C3—Co1	70.01 (2)
C3 ⁱⁱ —Co1—C2	66.67 (3)	C6—C3—Co1	126.88 (6)
C3—Co1—C2	39.54 (3)	C1—C4—H4A	112.8 (13)
C3 ⁱ —Co1—C2	140.46 (3)	C1—C4—H4B	113.5 (11)
C3 ⁱⁱⁱ —Co1—C2	113.33 (3)	H4A—C4—H4B	107.0 (15)
C2 ⁱⁱⁱ —Co1—C2	113.47 (5)	C2—C5—H5A	112.8 (15)
C1 ⁱ —Co1—C2 ⁱⁱ	140.21 (3)	C2—C5—H5B	114.7 (11)
C1—Co1—C2 ⁱⁱ	39.79 (3)	H5A—C5—H5B	100.5 (18)
C3 ⁱⁱ —Co1—C2 ⁱⁱ	39.54 (3)	C2—C5—H5C	110.1 (9)
C3—Co1—C2 ⁱⁱ	66.67 (3)	H5A—C5—H5C	106.7 (16)
C3 ⁱ —Co1—C2 ⁱⁱ	113.33 (3)	H5B—C5—H5C	111.4 (14)
C3 ⁱⁱⁱ —Co1—C2 ⁱⁱ	140.46 (3)	C3—C6—H6A	109.0 (11)

C2 ⁱⁱⁱ —Co1—C2 ⁱⁱ	180.0	C3—C6—H6B	110.4 (9)
C2—Co1—C2 ⁱⁱ	66.53 (5)	H6A—C6—H6B	112.4 (16)
C1 ⁱ —Co1—C2 ⁱ	39.79 (3)	C3—C6—H6C	110.7 (9)
C1—Co1—C2 ⁱ	140.21 (3)	H6A—C6—H6C	107.2 (15)
C3 ⁱⁱ —Co1—C2 ⁱ	113.33 (3)	H6B—C6—H6C	107.2 (13)
C1 ⁱ —Co1—C1—C2	22.38 (12)	C2 ⁱⁱⁱ —Co1—C2—C1	141.96 (6)
C3 ⁱⁱ —Co1—C1—C2	80.81 (6)	C2 ⁱⁱ —Co1—C2—C1	-38.04 (6)
C3—Co1—C1—C2	37.16 (5)	C2 ⁱ —Co1—C2—C1	-59.99 (6)
C3 ⁱ —Co1—C1—C2	-142.84 (5)	C1 ⁱ —Co1—C2—C5	59.74 (11)
C3 ⁱⁱⁱ —Co1—C1—C2	-99.18 (6)	C1—Co1—C2—C5	-120.26 (11)
C2 ⁱⁱⁱ —Co1—C1—C2	-62.03 (10)	C3 ⁱⁱ —Co1—C2—C5	158.44 (10)
C2 ⁱⁱ —Co1—C1—C2	117.97 (10)	C3—Co1—C2—C5	120.46 (11)
C2 ⁱ —Co1—C1—C2	180.0	C3 ⁱ —Co1—C2—C5	-59.54 (11)
C1 ⁱ —Co1—C1—C2 ⁱⁱ	-95.59 (13)	C3 ⁱⁱⁱ —Co1—C2—C5	-21.56 (10)
C3 ⁱⁱ —Co1—C1—C2 ⁱⁱ	-37.16 (5)	C2 ⁱⁱⁱ —Co1—C2—C5	21.70 (8)
C3—Co1—C1—C2 ⁱⁱ	-80.82 (6)	C2 ⁱⁱ —Co1—C2—C5	-158.30 (8)
C3 ⁱ —Co1—C1—C2 ⁱⁱ	99.18 (6)	C2 ⁱ —Co1—C2—C5	179.75 (9)
C3 ⁱⁱⁱ —Co1—C1—C2 ⁱⁱ	142.84 (5)	C1—C2—C3—C3 ⁱⁱ	-1.34 (8)
C2 ⁱⁱⁱ —Co1—C1—C2 ⁱⁱ	180.0	C5—C2—C3—C3 ⁱⁱ	178.27 (8)
C2—Co1—C1—C2 ⁱⁱ	-117.97 (10)	Co1—C2—C3—C3 ⁱⁱ	-60.38 (2)
C2 ⁱ —Co1—C1—C2 ⁱⁱ	62.03 (10)	C1—C2—C3—C6	-178.77 (9)
C1 ⁱ —Co1—C1—C4	143.40 (12)	C5—C2—C3—C6	0.85 (14)
C3 ⁱⁱ —Co1—C1—C4	-158.17 (3)	Co1—C2—C3—C6	122.20 (9)
C3—Co1—C1—C4	158.17 (3)	C1—C2—C3—Co1	59.04 (7)
C3 ⁱ —Co1—C1—C4	-21.83 (3)	C5—C2—C3—Co1	-121.35 (9)
C3 ⁱⁱⁱ —Co1—C1—C4	21.83 (3)	C1 ⁱ —Co1—C3—C2	142.61 (5)
C2 ⁱⁱⁱ —Co1—C1—C4	58.98 (5)	C1—Co1—C3—C2	-37.39 (5)
C2—Co1—C1—C4	121.01 (5)	C3 ⁱⁱ —Co1—C3—C2	-118.44 (5)
C2 ⁱⁱ —Co1—C1—C4	-121.01 (5)	C3 ⁱ —Co1—C3—C2	-112.12 (6)
C2 ⁱ —Co1—C1—C4	-58.99 (5)	C3 ⁱⁱⁱ —Co1—C3—C2	61.56 (5)
C2 ⁱⁱ —C1—C2—C3	2.17 (13)	C2 ⁱⁱⁱ —Co1—C3—C2	99.14 (7)
C4—C1—C2—C3	-179.08 (11)	C2 ⁱⁱ —Co1—C3—C2	-80.87 (7)
Co1—C1—C2—C3	-59.21 (6)	C2 ⁱ —Co1—C3—C2	180.0
C2 ⁱⁱ —C1—C2—C5	-177.44 (7)	C1 ⁱ —Co1—C3—C3 ⁱⁱ	-98.952 (19)
C4—C1—C2—C5	1.30 (17)	C1—Co1—C3—C3 ⁱⁱ	81.049 (19)
Co1—C1—C2—C5	121.18 (9)	C3 ⁱ —Co1—C3—C3 ⁱⁱ	6.32 (2)
C2 ⁱⁱ —C1—C2—Co1	61.38 (8)	C3 ⁱⁱⁱ —Co1—C3—C3 ⁱⁱ	180.0
C4—C1—C2—Co1	-119.87 (12)	C2 ⁱⁱⁱ —Co1—C3—C3 ⁱⁱ	-142.43 (3)
C1 ⁱ —Co1—C2—C3	-60.72 (8)	C2—Co1—C3—C3 ⁱⁱ	118.44 (5)
C1—Co1—C2—C3	119.28 (8)	C2 ⁱⁱ —Co1—C3—C3 ⁱⁱ	37.57 (3)
C3 ⁱⁱ —Co1—C2—C3	37.98 (5)	C2 ⁱ —Co1—C3—C3 ⁱⁱ	-61.56 (5)

supplementary materials

C3 ⁱ —Co1—C2—C3	180.0	C1 ⁱ —Co1—C3—C6	21.37 (9)
C3 ⁱⁱⁱ —Co1—C2—C3	-142.02 (5)	C1—Co1—C3—C6	-158.63 (9)
C2 ⁱⁱⁱ —Co1—C2—C3	-98.77 (5)	C3 ⁱⁱ —Co1—C3—C6	120.32 (8)
C2 ⁱⁱ —Co1—C2—C3	81.24 (5)	C3 ⁱ —Co1—C3—C6	126.64 (8)
C2 ⁱ —Co1—C2—C3	59.29 (5)	C3 ⁱⁱⁱ —Co1—C3—C6	-59.68 (8)
C1 ⁱ —Co1—C2—C1	180.0	C2 ⁱⁱⁱ —Co1—C3—C6	-22.11 (9)
C3 ⁱⁱ —Co1—C2—C1	-81.30 (6)	C2—Co1—C3—C6	-121.24 (10)
C3—Co1—C2—C1	-119.28 (8)	C2 ⁱⁱ —Co1—C3—C6	157.89 (9)
C3 ⁱ —Co1—C2—C1	60.72 (8)	C2 ⁱ —Co1—C3—C6	58.76 (10)
C3 ⁱⁱⁱ —Co1—C2—C1	98.70 (6)		

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, y, z$; (iii) $x, -y, -z$.

Fig. 1

