

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

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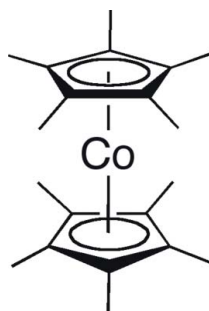
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.001$ Å; R factor = 0.031; wR factor = 0.089; data-to-parameter ratio = 28.4.

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).

References

- Arrais, A., Diana, E., Gobetto, R., Milanesio, M., Viterbo, D. & Stanghellini, P. L. (2003). *Eur. J. Inorg. Chem.* pp. 1186–1192.
- Augart, N., Boese, R. & Schmid, G. (1991). *Z. Anorg. Allg. Chem.* **595**, 27–34.
- Bruker (2008). SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2009). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.
- Connelly, N. G. & Geiger, W. E. (1996). *Chem. Rev.* **96**, 877–910.
- Freyburg, D. P., Robbins, J. L., Raymond, K. N. & Smart, J. C. (1979). *J. Am. Chem. Soc.* **101**, 892–897.
- Robbins, J. L., Edelstein, N., Spencer, B. & Smart, J. C. (1982). *J. Am. Chem. Soc.* **104**, 1882–1893.
- Sheldrick, G. M. (2008a). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008b). *Acta Cryst. A* **64**, 112–122.
- Struchkov, Yu. T., Andrianov, V. G., Sal'nikova, T. N., Lyatifov, I. R. & Materikova, R. B. (1978). *J. Organomet. Chem.* **145**, 213–223.

