

Bis[dicarbonyl(cyclopentadienyl)ferrio]mercury(II)

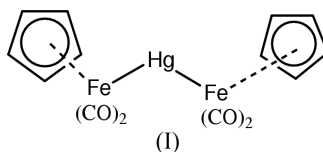
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Key indicators

Single-crystal X-ray study
 $T = 203$ K
Mean $\sigma(\text{C}-\text{C}) = 0.014$ Å
 R factor = 0.037
 wR factor = 0.100
Data-to-parameter ratio = 17.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Crystals of $\text{Hg}[\text{Fe}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]_2$ contain discrete molecules with crystallographically imposed twofold symmetry, $\text{Hg}-\text{Fe}$ 2.5546 (10) Å and an $\text{Fe}-\text{Hg}-\text{Fe}$ angle of $156.34(6)^\circ$, the most acute yet found for a simple $\text{Hg}[\text{ML}_n]_2$ species.

Comment

Well separated molecules of $\text{Hg}[\text{Fe}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]_2$ lie on a twofold axis, with two $\text{Fe}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)$ groups attached to the Hg atom by $\text{Fe}-\text{Hg}$ bonds. The most interesting parameter is the $\text{Fe}-\text{Hg}-\text{Fe}$ angle of $156.34(6)^\circ$. Related compounds, such as $\text{Hg}[\text{Fe}(\text{CO})_2(\text{NO})(\text{PET}_3)]_2$ (Stephens, 1972), $\text{Hg}[\text{Fe}(\text{CO})_4(\text{COOMe})_2]$ (Mauro *et al.*, 1994) and $\text{Hg}[\text{Fe}(\text{CO})_3(\text{NO})\{\text{Si}(\text{OMe})_3\}(\text{dppm})_2]$ [dppm is bis(diphenylphosphino)methane; Braunstein *et al.*, 1992], have essentially linear $\text{Fe}-\text{Hg}-\text{Fe}$ groupings. Similarly, $\text{Hg}[\text{Mn}(\text{CO})_5]_2$ (Flörke & Haupt, 1992) and $\text{Hg}[\text{Co}(\text{CO})_4]_2$ (Sheldrick & Simpson, 1968) have bond angles of 180° about the Hg atom. The $\text{Hg}-\text{Fe}$ bond length of 2.5546 (10) Å is similar to those in other examples.

Experimental

Crystals of $\text{Hg}[\text{Fe}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]_2$ were isolated in low yield from a reaction involving $\text{Na}[\text{Fe}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]$ formed by reducing the dimer $[\text{Fe}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]_2$ with sodium amalgam. Better syntheses are available (King, 1963). Crystals were obtained from a cooled CH_2Cl_2 solution.

Crystal data

$[\text{HgFe}_2(\text{C}_5\text{H}_5)_2(\text{CO})_4]$
 $M_r = 554.51$
 Tetragonal, $P4_32_12$
 $a = 11.6756(1)$ Å
 $c = 10.5030(1)$ Å
 $V = 1431.77(2)$ Å³
 $Z = 4$
 $D_x = 2.572$ Mg m⁻³

Mo $K\alpha$ radiation
 Cell parameters from 1726 reflections
 $\theta = 2-28^\circ$
 $\mu = 12.71$ mm⁻¹
 $T = 203(2)$ K
 Prism, brown
 $0.58 \times 0.48 \times 0.36$ mm

Data collection

Siemens SMART CCD diffractometer
 ω and φ scans
 Absorption correction: multi-scan (Blessing, 1995)
 $T_{\min} = 0.003$, $T_{\max} = 0.011$
 3323 measured reflections

1726 independent reflections
 1687 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\text{max}} = 28.3^\circ$
 $h = -15 \rightarrow 15$
 $k = 0 \rightarrow 15$
 $l = 0 \rightarrow 13$

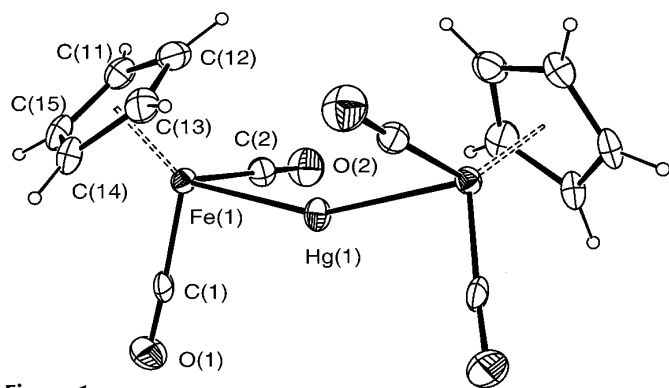


Figure 1
The structure of $\text{Hg}[\text{Fe}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]_2$ with ellipsoids drawn at the 50% probability level (Farrugia, 1997).

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.100$
 $S = 1.09$
 1726 reflections
 97 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 16.5365P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.72 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -2.49 \text{ e } \text{\AA}^{-3}$

The structure was refined as a 0.66:0.34 racemic twin. H atoms were placed in calculated positions, with $U_{\text{iso}} = 1.2U_{\text{eq}}$ of the associated C atom.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SADABS* (Sheldrick, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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