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Key indicators

Single-crystal X-ray study
T = 203 K
Mean σ(C–C) = 0.014 Å
R factor = 0.037
wR factor = 0.100
Data-to-parameter ratio = 17.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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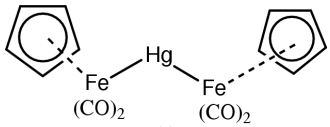
Crystals of $Hg[Fe(CO)_2(\eta^5\text{–}C_5H_5)]_2$ contain discrete molecules with crystallographically imposed twofold symmetry, Hg—Fe 2.5546 (10) Å and an Fe—Hg—Fe angle of 156.34 (6)°, the most acute yet found for a simple $Hg[ML_n]_2$ species.

Comment

Well separated molecules of $Hg[Fe(CO)_2(\eta^5\text{–}C_5H_5)]_2$ lie on a twofold axis, with two $Fe(CO)_2(\eta^5\text{–}C_5H_5)$ groups attached to the Hg atom by Fe—Hg bonds. The most interesting parameter is the Fe—Hg—Fe angle of 156.34 (6)°. Related compounds, such as $Hg[Fe(CO)_2(NO)(PEt_3)]_2$ (Stephens, 1972), $Hg[Fe(CO)_4(COOMe)]_2$ (Mauro *et al.*, 1994) and $Hg[Fe(CO)_3(NO)\{Si(OMe)_3\}(dppm)]_2$ [dppm is bis(diphenylphosphino)methane; Braunstein *et al.*, 1992], have essentially linear Fe—Hg—Fe groupings. Similarly, $Hg[Mn(CO)_5]_2$ (Flörke & Haupt, 1992) and $Hg[Co(CO)_4]_2$ (Sheldrick & Simpson, 1968) have bond angles of 180° about the Hg atom. The Hg—Fe bond length of 2.5546 (10) Å is similar to those in other examples.



(I)

Experimental

Crystals of $Hg[Fe(CO)_2(\eta^5\text{–}C_5H_5)]_2$ were isolated in low yield from a reaction involving $Na[Fe(CO)_2(\eta^5\text{–}C_5H_5)]$ formed by reducing the dimer $[Fe(CO)_2(\eta^5\text{–}C_5H_5)]_2$ with sodium amalgam. Better syntheses are available (King, 1963). Crystals were obtained from a cooled CH_2Cl_2 solution.

Crystal data

$[HgFe_2(C_5H_5)_2(CO)_4]$
M_r = 554.51
Tetragonal, $P4_32_12$
a = 11.6756 (1) Å
c = 10.5030 (1) Å
V = 1431.77 (2) Å^3
Z = 4
D_x = 2.572 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1726 reflections
θ = 2–28°
μ = 12.71 mm^{-1}
T = 203 (2) K
Prism, brown
0.58 × 0.48 × 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_{int} = 0.029
θ_{max} = 28.3°
$h = -15 \rightarrow 15$
$k = 0 \rightarrow 15$
$l = 0 \rightarrow 13$

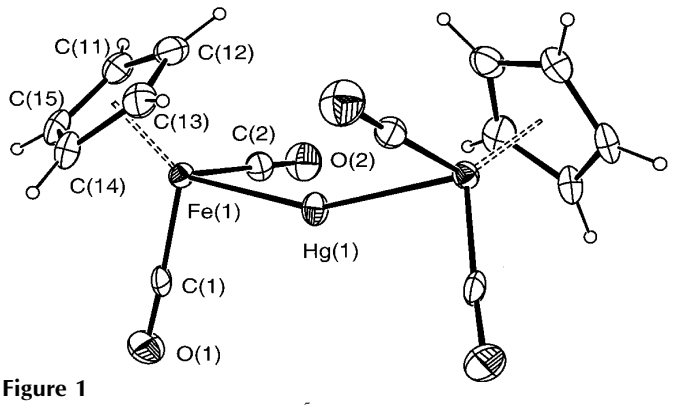


Figure 1
The structure of $Hg[Fe(CO)_2(\eta^5\text{–}C_5H_5)]_2$ with ellipsoids drawn at the 50% probability level (Farrugia, 1997).

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 16.5365P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.100$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.09$	$\Delta\rho_{max} = 1.72$ e Å^{-3}
1726 reflections	$\Delta\rho_{min} = -2.49$ e Å^{-3}
97 parameters	
H-atom parameters constrained	

The structure was refined as a 0.66:0.34 racemic twin. H atoms were placed in calculated positions, with $U_{iso} = 1.2U_{eq}$ 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: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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