

1,4-Diferrocenylbutane-1,4-dione

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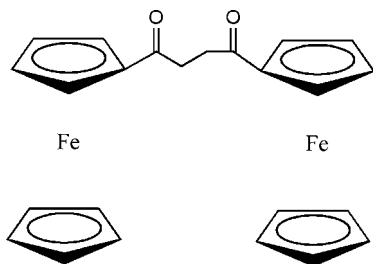
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.036; wR factor = 0.076; data-to-parameter ratio = 14.2.

In the crystal structure of the title compound, $[\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_{14}\text{H}_{12}\text{O}_2)]$, each carbonyl group is coplanar with the adjacent cyclopentadienyl ring, thus maximizing the π -orbital overlap and electronic interactions between the groups. In the crystal structure, there are inter- and intramolecular $\text{C}-\text{H}\cdots\text{O}$ contacts.

Related literature

For related literature, see: Brown *et al.* (2005); Chidsey *et al.* (1990); Creager & Rowe (1997); Gemici (2005); Hickman *et al.* (1991); Kealy & Pauson (1951); Miller *et al.* (1988); Navarro *et al.* (2005); Nicolosi *et al.* (1994); Okochi *et al.* (2005); Pugh *et al.* (2006); Sawamura & Ito (1992); Togni & Hayashi (1995).



Experimental

Crystal data

$[\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_{14}\text{H}_{12}\text{O}_2)]$	$V = 1931.2$ (2) Å ³
$M_r = 454.12$	$Z = 4$
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
$a = 10.4175$ (7) Å	$\mu = 1.52$ mm ⁻¹
$b = 18.5954$ (10) Å	$T = 298$ (2) K
$c = 9.9690$ (6) Å	$0.45 \times 0.33 \times 0.08$ mm

Data collection

Stoe IPDS2 diffractometer	11622 measured reflections
Absorption correction: integration ($X\text{-RED32}$; Stoe & Cie, 2002)	3612 independent reflections
$T_{\min} = 0.525$, $T_{\max} = 0.899$	2941 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.0383$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$	H-atom parameters not refined
$wR(F^2) = 0.075$	$\Delta\rho_{\text{max}} = 0.36$ e Å ⁻³
$S = 1.01$	$\Delta\rho_{\text{min}} = -0.22$ e Å ⁻³
3612 reflections	Absolute structure: Flack (1983),
254 parameters	1418 Freidel pairs
1 restraint	Flack parameter: 0.01 (2)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C12}-\text{H12B}\cdots\text{O1}^i$	0.97	2.51	3.448 (5)	164
$\text{C13}-\text{H13B}\cdots\text{O2}^i$	0.97	2.55	3.400 (6)	147
$\text{C23}-\text{H23}\cdots\text{O1}$	0.93	2.60	3.499 (5)	164
$\text{C10}-\text{H10}\cdots\text{O2}$	0.93	2.58	3.457 (6)	157

Symmetry code: (i) $-x + \frac{1}{2}, y, z + \frac{1}{2}$.

Data collection: *X-Area* (Stoe & Cie, 2002); cell refinement: *X-Area*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PUBLICIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2537).

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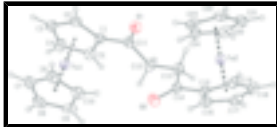
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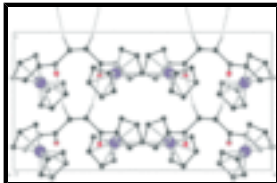
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