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4,5-Bis(ferrocenylmethylthio)-1,3-dithiol-2-one

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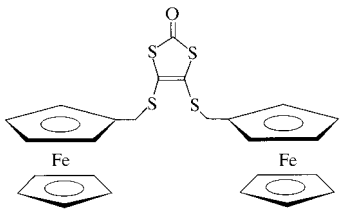
In the compound 4,5-bis(ferrocenylmethylthio)-1,3-dithiol-2-one, $[Fe_2(C_5H_5)_2(C_{15}H_{12}OS_4)]$, the values of the geometric parameters of the ferrocene and 1,3-dithiol-2-one (dmio) moieties are within normal ranges. The dmio group is essentially planar. There are no short S···S contacts.

Comment

Examination of the title structure, (I), with *PLATON* (Spek, 1999) showed that there were no solvent-accessible voids in the crystal lattice.



(I)

Experimental

The title compound was prepared from (chloromethyl)ferrocene and $[NEt_4]_2[Zn(dmio)_2]$ and was recrystallized from dichloromethane/petroleum ether (333–353 K) producing orange crystals (m.p. 97–99°C).

Crystal data

$[Fe_2(C_5H_5)_2(C_{15}H_{12}OS_4)]$	D_x = 1.608 Mg m^{-3}
M_r = 578.37	Mo Kα radiation
Monoclinic, $P2_1/n$	Cell parameters from 4915 reflections
a = 11.953 (2) Å	θ = 2.02–28.26°
b = 18.433 (4) Å	μ = 1.580 mm^{-1}
c = 11.954 (2) Å	T = 150.0 (1) K
β = 114.86 (3)°	Plate, orange
V = 2389.8 (8) Å^3	0.40 × 0.35 × 0.10 mm
Z = 4	

Data collection

KappaCCD diffractometer	2658 reflections with $I > 2\sigma(I)$
φ and ω scans with κ offset scans	R_{int} = 0.0738
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)	θ_{max} = 28.26°
T_{min} = 0.571, T_{max} = 0.901	$h = -15 \rightarrow 13$
34055 measured reflections	$k = -17 \rightarrow 24$
5785 independent reflections	$l = -13 \rightarrow 15$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.056	$w = 1/[\sigma^2(F_o^2) + (0.0660P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.148	$(\Delta/\sigma)_{max}$ = 0.004
S = 0.947	$\Delta\rho_{max}$ = 0.654 e Å^{-3}
5785 reflections	$\Delta\rho_{min}$ = −0.615 e Å^{-3}
289 parameters	

The title compound crystallized in the monoclinic system; space group $P2_1/n$ from the systematic absences. H atoms were treated as riding atoms with C—H distances in the range 0.93–0.97 Å.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL*97 and *WordPerfect* macro *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC, X-ray Crystallographic Service, University of Southampton, using an Enraf–Nonius KappaCCD diffractometer. The authors thank the staff for all there help and advice.

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