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catena-Poly[[{2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}iron(III)]-μ-azido]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.046
wR factor = 0.116
Data-to-parameter ratio = 14.1

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

In the title polymeric complex, $\{[Fe(C_{17}H_{16}N_2O_2)(N_3)]\}_n$, the Fe^{III} atom assumes a slightly distorted octahedral geometry, formed by one Schiff base and two azide ligands. The azide anion bridges the Fe^{III} atoms through terminal N atoms, forming zigzag polymeric chains.

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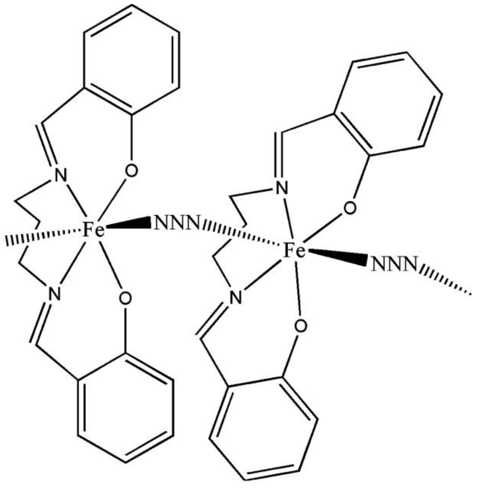
Comment

Iron(III) complexes have been shown to be active in cell destruction, as well as in the inhibition of DNA synthesis (Saha *et al.*, 2002; Bera *et al.*, 1999). In order to develop further the coordination chemistry of such iron(III) complexes, we have synthesized an azide-bridged iron(III) complex, (I), based on the Schiff base ligand *N*,*N*′-propylene-bis(salicylideneimine).



(I)

The molecular structure of the title complex, (I), is shown in Fig. 1, and selected bond distances and angles are given in Table 1. The Schiff base coordinates to the metal atom, Fe1, in the equatorial plane *via* the four donor atoms O1, N1, N2 and O2. The azide anion acts as a bridge coordinating to the Fe1 atoms in the axial positions *via* the two terminal N atoms, N3 and N5.

In the crystal structure of (I), the azide anions bridge the Fe^{III} atoms, forming zigzag polymeric chains which lie parallel to the *c* axis (Fig. 2).

Experimental

Salicylaldehyde (0.5 mmol, 61.1 mg) and propane-1,3-diamine (0.5 mmol, 36.9 mg) were stirred in 50 ml of methanol in a 100 ml beaker. After *ca* 1 h, 175.0 mg of $Fe(NO_3)_3 \cdot 6H_2O$ (0.5 mmol) in a 20 ml methanol and 32.5 mg of NaN_3 (0.5 mmol) in a 10 ml aqueous solution were added and the stirring continued for another 1 h. The solution was then filtered and the filtrate kept at room temperature for about a week, after which brown rhombic crystals were deposited.

Crystal data

$[Fe(C_{17}H_{16}N_2O_2)(N_3)]$
$M_r = 378.20$
Orthorhombic, $Pna2_1$
$a = 11.927$ (2) Å
$b = 11.927$ (1) Å
$c = 11.228$ (2) Å
$V = 1597.2$ (4) Å^3
$Z = 4$
$D_x = 1.573$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 3123 reflections
$\theta = 2.3$–25.4°
$\mu = 0.97$ mm^{-1}
$T = 298$ (2) K
Rhombic, brown
0.30 × 0.23 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.760$, $T_{\max} = 0.869$
9128 measured reflections

3176 independent reflections
2847 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 27.0^\circ$
$h = -15 \rightarrow 15$
$k = -15 \rightarrow 13$
$l = -14 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.116$
$S = 1.06$
3176 reflections
226 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0742P)^2 + 0.1094P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.76$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ e Å^{-3}
Absolute structure: Flack (1983), 1345 Friedel pairs
Flack parameter: 0.05 (2)

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	1.892 (2)	Fe1—N2	2.054 (3)
Fe1—O2	1.876 (2)	Fe1—N3	2.323 (4)
Fe1—N1	2.019 (3)	Fe1—N5^{i}	2.353 (3)
O2—Fe1—O1	85.71 (11)	N1—Fe1—N3	89.94 (13)
O2—Fe1—N1	173.59 (11)	N2—Fe1—N3	81.28 (12)
O1—Fe1—N1	88.40 (11)	O2—Fe1—N5^{i}	94.05 (13)
O2—Fe1—N2	91.56 (11)	O1—Fe1—N5^{i}	93.06 (13)
O1—Fe1—N2	175.35 (13)	N1—Fe1—N5^{i}	88.77 (12)
N1—Fe1—N2	94.49 (12)	N2—Fe1—N5^{i}	83.37 (12)
O2—Fe1—N3	88.87 (14)	N3—Fe1—N5^{i}	164.45 (12)
O1—Fe1—N3	102.40 (13)		

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

H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93–0.97 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. he cell lengths *a* and *b* are almost identical, within 1σ, but no additional symmetry could be found using the *ADDSYMM* routine in *PLATON* (Spek, 2003).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

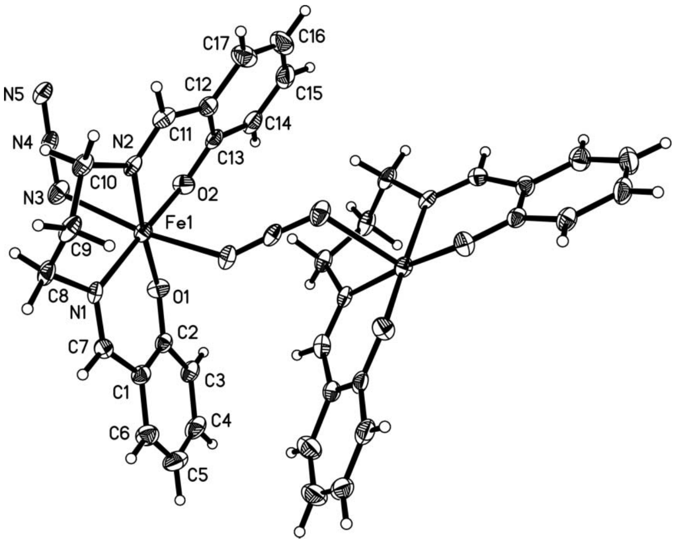


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. A second monomer unit, related by the symmetry operation $1-x, -y, z-\frac{1}{2}$, is also shown to complete the coordination of Fe1

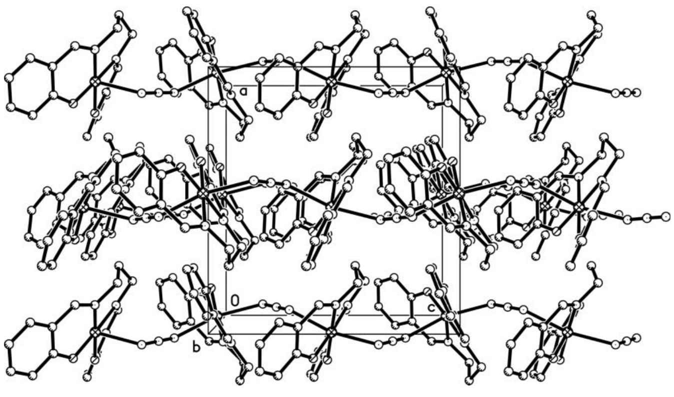


Figure 2
The packing of (I), viewed along the *b* axis.

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