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catena-Poly[[bis(pyridine-κN)iron(II)]-μ-oxalato-κ^2O,O':κ^2O'',O''']

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Key indicators

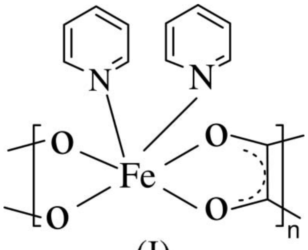
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.094
Data-to-parameter ratio = 24.2

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

The title compound, [$Fe(C_2O_4)(C_5H_5N)_2$], was synthesized *via* unexpected oxidation of (*S*,*S*)-tartaric acid under solvothermal conditions. The Fe^{II} atom reveals octahedral coordination involving two N atoms of pyridine and two oxalate groups acting as tetradentate bridging ligands between two Fe^{II} centres. The Fe^{II} coordination polyhedra are connected into one-dimensional zigzag chains linked by *exo*-tetradentate oxalate groups.

Comment

The hydro- or solvothermal method provides a rich source of new materials, both in traditional inorganic framework systems and, more recently, in the development of metal–organic frameworks (Cheetham *et al.*, 1999). These systems are synthetically complex and although some tailoring has now been introduced, particularly in metal–organic frameworks (Li *et al.*, 1999; Yao *et al.*, 2007), it is often not possible to predict the products of a new solvothermal reaction with certainty (Evans & Lin, 2001). In this paper, we report our unexpected finding of the synthesis of the title new ferrous oxalate coordination polymer, (I), *via* facile oxidation of *S*,*S*-tartaric acid to oxalic acid under solvothermal conditions.



(I)

The asymmetric unit of (I) contains one Fe atom, an oxalate group and two coordinated pyridine molecules (Fig. 1). The Fe centre exhibits distorted octahedral geometry, coordinated by four O atoms of two oxalate ligands and two pyridine N atoms in a *cis*-arrangement. The Fe—O distances range from 2.0822 (14) to 2.1858 (15) Å, while the O—Fe—O angles show distortions particularly as a result of chelation (Table 1). The *exo*-tetradentate oxalate groups link adjacent Fe centres to form one-dimensional zigzag chains (Fig. 2).

Experimental

The title compound was prepared by a solvothermal reaction of *S*,*S*-tartaric acid (0.031 g), H_3BO_3 (0.013 g), $FeCl_3\cdot6H_2O$ (0.054 g) and KOH (0.012 g) using a pyridine–water (1:2 *v*/*v*) solvent mixture. The

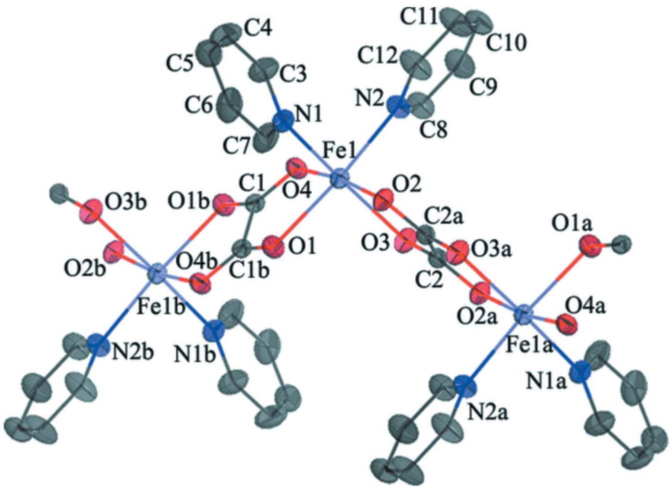


Figure 1
Part of the polymeric structure of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted. [Symmetry codes: (a) $2 - x, 1 - y, -z$; (b) $1 - x, 1 - y, -z$.]

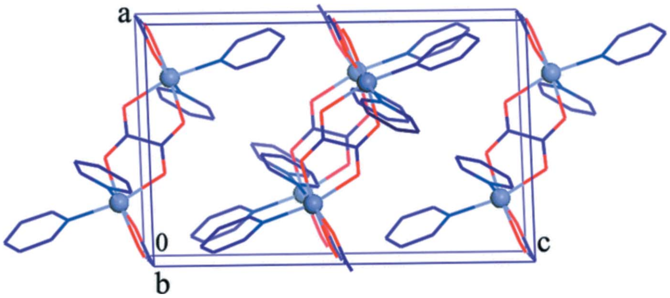


Figure 2
The crystal packing of (I). H atoms have been omitted.

mixture was sealed in a Pyrex glass tube filled to *ca* 10% capacity, placed in a stainless steel autoclave and heated at 393 K for 6 d. After cooling to ambient temperature, the product was washed with ethanol and yellow block crystals of (I) were obtained.

Crystal data

$[Fe(C_2O_4)(C_5H_5N)_2]$
$M_r = 302.07$
Monoclinic, $P2_1/c$
$a = 9.714$ (6) Å
$b = 8.895$ (6) Å
$c = 15.359$ (10) Å
$\beta = 91.688$ (7)°
$V = 1326.5$ (14) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.15$ mm^{-1}
$T = 273$ (2) K
0.30 × 0.22 × 0.19 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: none
12351 measured reflections
4354 independent reflections
3281 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.094$
$S = 1.04$
4354 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.33$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O4	2.0822 (14)	Fe1—O3	2.1858 (15)
Fe1—O2	2.0898 (14)	Fe1—N2	2.1926 (18)
Fe1—O1	2.1832 (15)	Fe1—N1	2.2017 (19)
O4—Fe1—O2	172.52 (4)	O4—Fe1—O3	96.85 (6)
O4—Fe1—O1	77.73 (6)	O2—Fe1—O3	77.57 (5)
O2—Fe1—O1	97.30 (6)	O1—Fe1—O3	91.53 (5)

H atoms were positioned geometrically, with C—H = 0.93 Å, and allowed to ride during subsequent refinement, with $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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