Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Poly[bis(μ_3-pyridine-2-carboxylato)iron(II)]

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Received 29 September 2006
Accepted 12 December 2006

The title compound, $[Fe(C_6(CH_4N_4O_2)_2]_n$, has been prepared by a hydrothermal reaction of iron(II) chloride and pyridine-2-carboxylic acid. The asymmetric unit contains one Fe^{II} atom and two pyridine-2-carboxylate anions. The Fe^{II} atoms are linked *via* bridging pyridine-2-carboxylate, yielding a layered structure. The coordination geometry about the Fe atom is distorted octahedral.

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.036
wR factor = 0.122
Data-to-parameter ratio = 11.0

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

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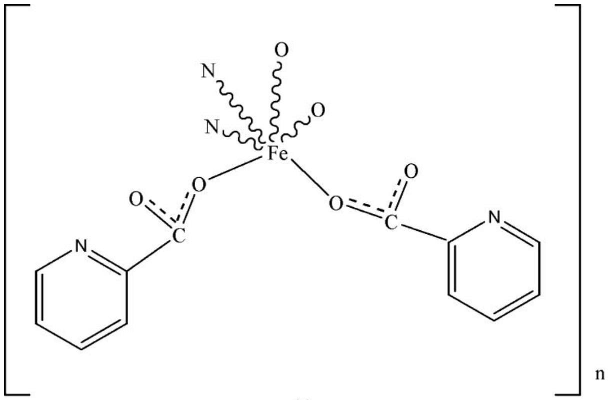
Comment

In recent years, carboxylic acids have been widely used as polydentate ligands, which can coordinate to transition or rare earth metal ions yielding complexes with interesting properties that are useful in materials science (Church & Halvorson, 1959; Chung *et al.*, 1971) and in biological systems (Okabe & Oya, 2000; Serre *et al.*, 2005; Pocker & Fong, 1980; Scapin *et al.*, 1997). For example, Kim *et al.* (2001) focused on the syntheses of transition metal complexes containing benzenecarboxylate and rigid aromatic pyridine ligands in order to study their electronic conductivity and magnetic properties. The importance of transition metal–dicarboxylate complexes in materials science and biological systems prompted us to pursue synthetic strategies for these compounds, using pyridine-2-carboxylate as a polydentate ligand. In this paper, we report the synthesis and X-ray crystallographic analysis of the title compound, [Fe(pyridine-2-carboxylate)$_2$]$_n$, (I).



(I)

The Fe(II) atom is six-coordinate, chelated by four O atoms and two N atoms from four pyridine-2-carboxylate anions (Fig. 1). The coordination about the Fe atom is distorted octahedral (Table 1).

Two iron atoms are linked *via* two O atoms, forming a four-membered Fe—O—Fe—O ring (Fig. 1). These rings are further linked by pyridine-2-carboxylate, forming a layered structure with two-dimensional sheets in the *bc* plane (Fig. 2).

Experimental

All chemicals were used as purchased from Shanghai Chemical Ltd Co. Ltd. A mixture of iron(II) chloride (0.5 mmol), potassium hydroxide (0.5 mmol), pyridine-2-carboxylic acid (0.5 mmol) and H_2O (8 ml) in a 25 ml Teflon-lined stainless steel autoclave was kept at 413 K for 2 d, and then cooled to room temperature. Red, block-shaped crystals of (I) were obtained in a yield of 10%. Anal. Calc. for $C_{12}H_8FeN_2NO_4$: C 48.04, H 2.69, N 9.34, Fe 18.61%; Found: C 47.78, H 2.73, N 9.36, Fe 18.56%.

Crystal data

$[Fe(C_6H_4NO_2)_2]$
$M_r = 300.05$
Monoclinic, $P2_1/c$
$a = 10.221$ (4) Å
$b = 10.912$ (4) Å
$c = 10.221$ (4) Å
$\beta = 108.000$ (1)°
$V = 1084.2$ (7) Å^3
$Z = 4$
$D_x = 1.838$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.40$ mm^{-1}
$T = 298$ (2) K
Block, red
0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: none
5317 measured reflections
1899 independent reflections
1754 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 25.0$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.122$
$S = 1.00$
1899 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0853P)^2 + 1.7322P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.64$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.74$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.009 (2)

Table 1
Selected bond lengths (Å).

Fe—O3	2.119 (2)	Fe—O1$^{\rm ii}$	2.228 (2)
Fe—O1	2.144 (2)	Fe—N1$^{\rm ii}$	2.291 (3)
Fe—O4$^{\rm i}$	2.219 (2)	Fe—N2$^{\rm i}$	2.313 (3)

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, -y+1, -z+1$.

H atoms were located in difference maps and were refined riding on the respective carrier atom with C—H=0.82–0.96 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier atom).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

The authors thank the Chinese Natural Science Foundation (grant No. 20501011) and Liaocheng University (grant No. 31801) for financial support. In addition, we thank Professor Jianmin Dou for his help.

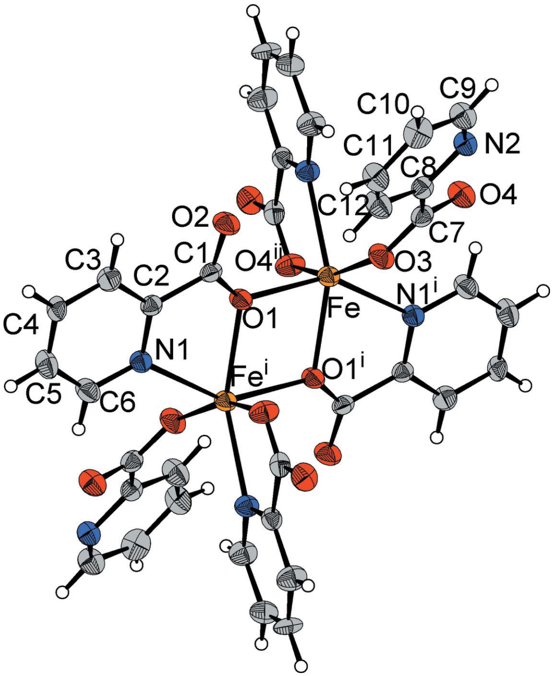


Figure 1
TPart of the polymeric structure of (I), with displacement ellipsoids drawn at the 50% probability level. Symmetry codes are as in Table 1.

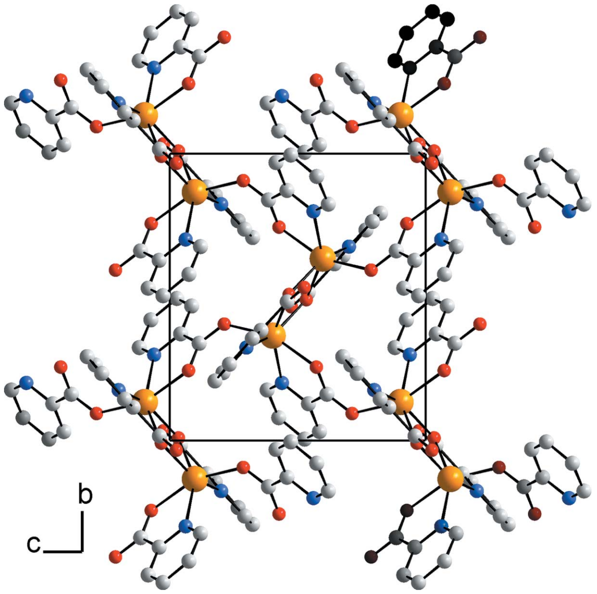


Figure 2
The two-dimensional layer structure of (I). H atoms have been omitted.

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