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catena-Poly[[aqua(pyrazine-2-carboxylato)-iron(II)]-μ-pyrazine-2-carboxylato]

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The title compound, $[Fe(C_{10}H_6N_4O_4)_2(H_2O)]_n$, has been prepared from an aqueous solution of iron(II) chloride and pyrazine-2-carboxylic acid. The asymmetric unit contains one Fe^{II}, two pyrazine-2-carboxylate anions and one aqua ligand. The Fe^{II} atoms are linked *via* bridging pyrazine-2-carboxylate ligands, leading to a polymeric structure with zigzag-chains extending parallel to the *b* axis. The coordination of the Fe atom is distorted octahedral.

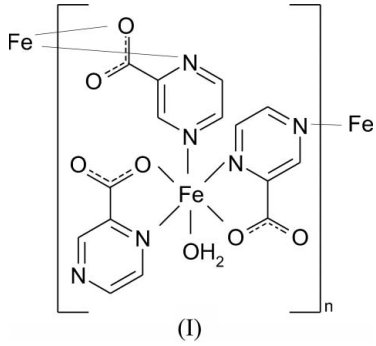
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.067
Data-to-parameter ratio = 12.6

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

Comment

In recent years, carboxylic acids have been widely used as polydentate ligands, which can coordinate to transition or rare earth 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 aromatic carboxylate and rigid aromatic pyridine ligands in order to study their electronic conductivity and magnetic properties. The importance of transition metal dicarboxylate complexes motivated us to pursue synthetic strategies for these compounds, using pyrazine-2-carboxylate as a polydentate ligand. Here we report the synthesis and X-ray crystal structure analysis of the title compound, (I).



(I)

The Fe atom is coordinated in a bidentate fashion by two O and two N atoms from two independent pyrazine-2-carboxylate anions. The distorted octahedral coordination is completed by another N atom from a third pyrazine-2-carboxylate ligand, and by the O atom of a water molecule (Fig. 1). The Fe—N bond lengths range from 2.081 (2) to 2.125 (2) Å and are slightly longer than the Fe—O bond lengths, which range from 2.028 (2) to 2.0594 (19) Å.

The pyrazine-2-carboxylate ligand that binds with one of the pyrazine N atoms to one Fe atom coordinates to a

neighboring Fe atom *via* the second pyrazine N atom and one O atom of the carboxylate group. This arrangement leads to a polymeric structure with zigzag chains extending parallel to the *b* axis (Fig. 2). Medium–strong hydrogen bonding between the water molecules (Table 2) additionally stabilizes the structure.

Experimental

A mixture of iron(II) chloride (0.5 mmol), potassium hydroxide (0.5 mmol) and pyrazine-2-carboxylic acid (0.5 mmol) in 30 ml H_2O was stirred for 1 h and filtered under the protection of a nitrogen atmosphere. The filtrate was then cooled in an ice box. Colorless block-shaped crystals of (I) were obtained in a yield of 10%. Analysis calculated for $C_{10}H_8FeN_4O_5$: C 37.53, H 2.52, N 17.51, Fe 17.45%; found: C 37.51, H 2.53, N 17.49, Fe 17.47%.

Crystal data

$[Fe(C_5H_3N_2O_2)_2(H_2O)]$	$Z = 4$
$M_r = 320.05$	$D_x = 1.853$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 7.7905$ (15) Å	$\mu = 1.34$ mm^{-1}
$b = 9.8787$ (19) Å	$T = 298$ (2) K
$c = 14.909$ (3) Å	Block, colorless
$V = 1147.4$ (4) Å^3	0.10 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer	2370 independent reflections
φ and ω scans	2215 reflections with $I > 2\sigma(I)$
6291 measured reflections	$R_{int} = 0.026$
	$\theta_{max} = 26.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.028$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.067$	$\Delta\rho_{max} = 0.92$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -0.22$ e Å^{-3}
2370 reflections	Absolute structure: Flack (1983), 987 Friedel pairs
188 parameters	Flack parameter: 0.453 (18)
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected bond lengths (Å).

Fe1—O1	2.028 (2)	Fe1—N2	2.081 (2)
Fe1—O3	2.035 (2)	Fe1—N1	2.097 (2)
Fe1—O5	2.0594 (19)	Fe1—N4	2.125 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O1^{i}	0.887 (18)	1.874 (18)	2.759 (3)	176 (4)
O5—H2W···O3^{ii}	0.899 (18)	1.814 (19)	2.686 (3)	163 (4)

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

The structure was refined from an inversion-twinned crystal with a twin ratio close to 1:1. The H atoms of the water molecule were located in difference density maps and were refined with distance restraints of H···H = 1.38 (2) and O—H = 0.88 (2) Å, and with a fixed U_{iso} value of 0.80 Å^2. All other H atoms were placed in calculated positions, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

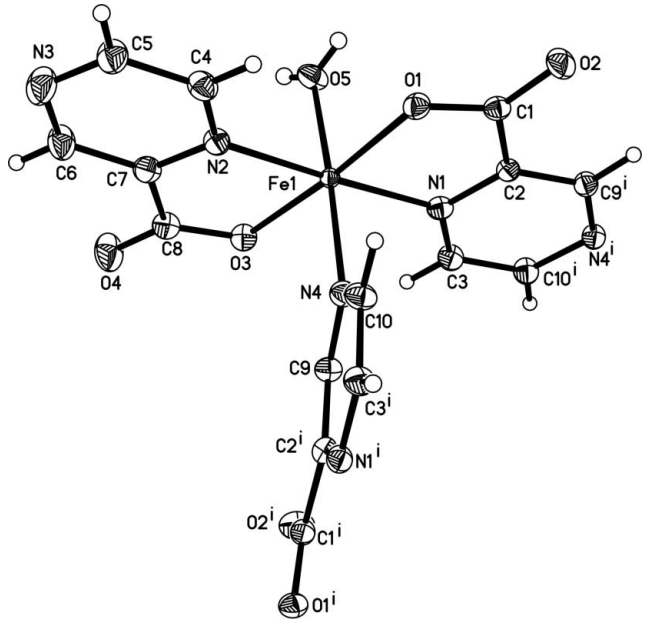


Figure 1
Part of the polymeric structure of (I), drawn with 30% probability displacement ellipsoids. [Symmetry code: (i) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$.]

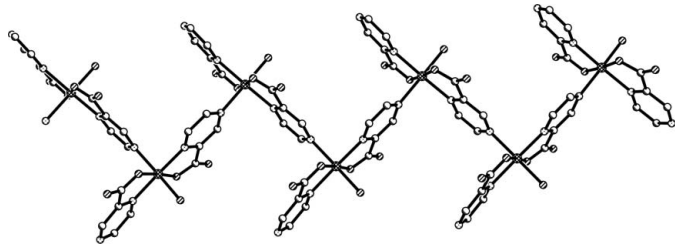


Figure 2
The zigzag chains extending parallel to the *b* axis. H atoms have been omitted for clarity.

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*.

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