Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Tetraaquabis(pyridine-3-carboxylato-*κN*)iron(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.007 Å
R factor = 0.052
wR factor = 0.139
Data-to-parameter ratio = 11.7

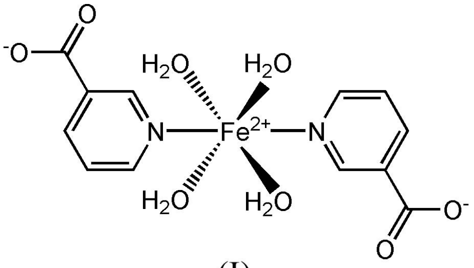
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 July 2005
Accepted 9 August 2005
Online 17 August 2005

Pyridine-3-carboxylic acid (nicH) reacts with iron(II) chloride tetrahydrate in a methanol–water mixture to form the title compound, $[Fe(C_6H_4NO_2)_2(H_2O)_4]$. The Fe^{II} atom is in a slightly distorted octahedral coordination. The crystal structure is stabilized by O—H···O hydrogen bonds involving all the water H atoms and the carboxylate groups.

Comment

Pyridinecarboxylates and their derivatives are useful ligands in the construction of one- to three-dimensional functional metal–organic frameworks (Evans & Lin, 2002; Lu, 2003; Tong *et al.*, 2003, 2004, 2005; Wang *et al.*, 2003). The title complex, (I), was obtained in an attempt to prepare a multidimensional coordination network.



(I)

In the structure of (I), the Fe^{II} atom, which occupies a special position of 2/*m* symmetry, is coordinated by four aqua ligands and two pyridyl N atoms from two pyridine-3-carboxylate (nic) ligands (Fig. 1). The Fe1—O [2.210 (3) Å]

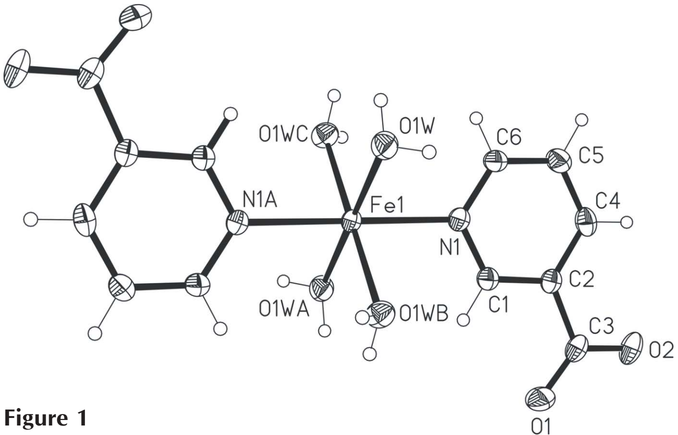


Figure 1
ORTEPII plot (Johnson, 1976) of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are plotted at the 40% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (*A*) *x*, −*y*, *z*; (*B*) −*x*, *y*, −*z*; (*C*) −*x*, −*y*, −*z*.]

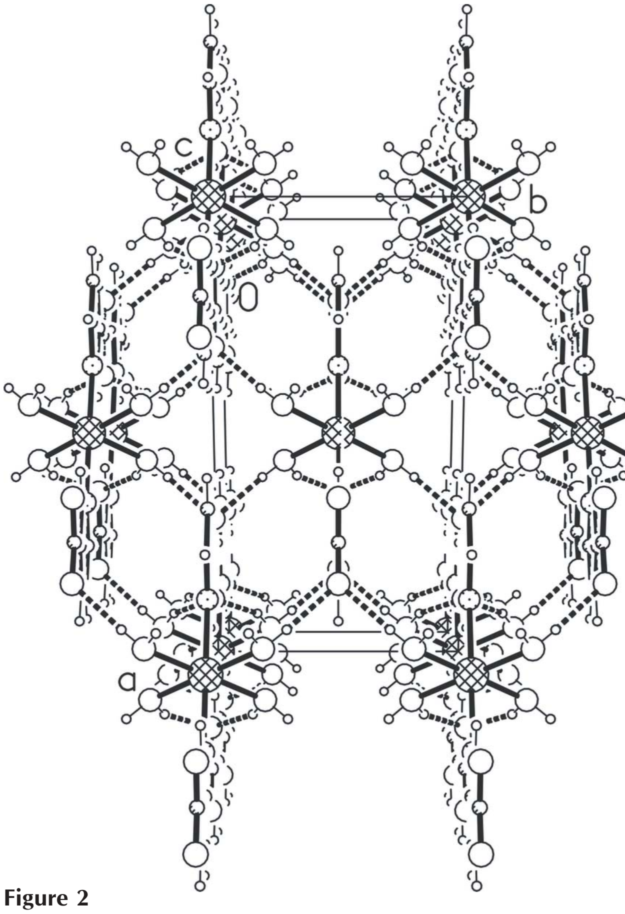


Figure 2
Perspective view of the molecular packing of (I).

and Fe1—N [2.135 (2) Å] bond lengths are similar to those found in tetraaquabis(pyridine-4-carboxylato-*κN*)iron(II) [Fe—N = 2.202 (2) Å and Fe—O = 2.125 (2) and 2.136 (2) Å; Liu *et al.*, 1999]. The Fe^{II} atom, the pyridyl rings and the carboxylate groups are coplanar. The structure of (I) is isostructural with that of *trans*-tetraaquabis(pyridine-3-carboxylato-*κN*)chromium(II) (Cotton *et al.*, 1991), *trans*-tetraaquabis(pyridine-3-carboxylato-*κN*)cobalt(II) (Anagnostopoulos *et al.*, 1969), *trans*-tetraaquabis(pyridine-3-carboxylato-*κN*)nickel(II) (Batten & Harris, 2001), *trans*-tetraaquabis(pyridine-3-carboxylato-*κN*)zinc(II) (Cingi *et al.*, 1971), and *trans*-tetraaquabis(pyridine-3-carboxylato-*κN*)cadmium(II) (Zhou *et al.*, 2003). The extensive intermolecular O—H···O hydrogen bonds [O···O = 2.696 (4)–2.713 (3) Å] between the carboxylate groups and the aqua ligands play an important role in consolidating the crystal architecture (Fig. 2).

Experimental

To a methanol–water solution (5:1 *v*/*v*), 10 ml) of iron(II) chloride tetrahydrate (0.100 g, 0.5 mmol), a solution of pyridine-3-carboxylic acid (0.123 g, 1.0 mmol) in MeOH (5 ml) was added slowly, with stirring, over a period of 10 min at ambient temperature. Red block-shaped crystals were deposited within 2 d in *ca* 45% yield.

Crystal data

$[Fe(C_6H_4NO_2)_2(H_2O)_4]$
$M_r = 372.12$
Monoclinic, $C2/m$
$a = 14.235$ (4) Å
$b = 6.901$ (2) Å
$c = 8.538$ (3) Å
$\beta = 118.12$ (1)°
$V = 739.7$ (4) Å^3
$Z = 2$

$D_x = 1.671$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 680 reflections
$\theta = 3.3$–27.5°
$\mu = 1.06$ mm^{-1}
$T = 293$ (2) K
Block, red
0.32 × 0.26 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{min} = 0.704$, $T_{max} = 0.821$
2628 measured reflections

886 independent reflections
770 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 27.5°$
$h = -18 \rightarrow 13$
$k = -7 \rightarrow 8$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.139$
$S = 1.03$
886 reflections
76 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.097P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.72$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O1*W*	2.135 (2)	Fe1—N1	2.210 (3)
O1W^{i}—Fe1—O1*W*	90.59 (14)	O1*W*—Fe1—N1	90.21 (9)
O1*W*—Fe1—O1W^{ii}	89.41 (14)	C5—C6—H6	118.3
O1*W*—Fe1—N1^{iii}	89.79 (9)		

Symmetry codes: (i) $x, -y, z$; (ii) $-x, y, -z$; (iii) $-x, -y, -z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1^{iv}	0.85 (1)	1.88 (1)	2.696 (4)	161 (4)
O1*W*—H1*WB*···O2^{v}	0.85 (1)	1.87 (1)	2.713 (3)	174 (4)

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

The pyridyl H atoms were included in geometrically calculated positions and constrained to ride, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The aqua H atoms were located in difference Fourier maps and refined with isotropic displacement parameters subject to the restraint O—H = 0.85 (1) Å.

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

The authors thank the Foundation for the Items of Education Office of Guangdong Province (No, z03065) for generously supporting this work.

Acta Cryst. (2005). E**61**, m1782–m1784 Liang *et al.* • $[Fe(C_6H_4NO_2)_2(H_2O)_4]$ **m1783**

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