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Diaquabis[5-(pyrazin-2-yl)tetrazolato]iron(II)

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Key indicators

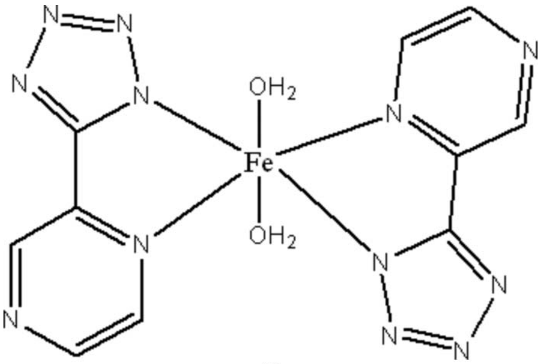
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.076
Data-to-parameter ratio = 13.7

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

The title complex, $[Fe(C_5H_3N_3)_2(H_2O)_2]$, has a crystallographically imposed inversion centre. The Fe^{II} atom is coordinated by four N atoms from two 5-(pyrazin-2-yl)tetrazolate ligands and the O atoms from two water molecules in a distorted octahedral geometry. The packing is governed by intramolecular O—H···N hydrogen bonds.

Comment

There is a growing interest in the design, synthesis, characterization and properties of supramolecular networks formed by functionalized organic molecules as bridges between metal centres (Rizk *et al.*, 2005; Eddaoudi *et al.*, 2001). The literature on tetrazoles is expanding rapidly, since tetrazoles play an important role as ligands in coordination chemistry. Since Franke *et al.* (1982) synthesized N1-substituted tetrazoles as ligands of iron(II) spin-crossover compounds in the beginning of the 1980s, many homologous alkyl-substituted ligands have been prepared. Recently, 5-substituted 1*H*-tetrazoles have been synthesized by a facile approach (Demko & Sharpless, 2001*a*,*b*). In the general reaction, tetrazoles are prepared by the addition of azide to nitriles in water with the aid of a Lewis acid such as Zn^{2+}. In this paper, we report the crystal structure of a new Fe mononuclear complex, (I), obtained under hydrothermal conditions by reaction of 2-cyanopyrazine, NaN_3 and $FeCl_2$ as Lewis acid.



(I)

In (I), the Fe^{II} atom, which occupies a crystallographically imposed centre of symmetry, is coordinated by four N atoms from two 5-(pyrazin-2-yl)tetrazolate ligands and by the O atoms from two water molecules (Fig. 1) in a distorted octahedral geometry (Table 1). In each ligand, the pyrazinyl and tetrazolyl rings are almost coplanar, making a dihedral angle of 2.36 (8)°. Intermolecular O—H···N hydrogen bonds (Table 2) stabilize the crystal structure (Fig. 2).

Experimental

Hydrothermal treatment of $FeCl_2$ (1.0 mmol, 0.126 g), 2-cyanopyrazine (1 mmol, 0.105 g), NaN_3 (1 mmol, 0.065 g) and water (3 ml) over 50 h at 422 K yielded red prismatic crystals (yield: 45%).

Crystal data

$[Fe(C_5H_3N_3)_2(H_2O)_2]$
$M_r = 386.15$
Monoclinic, $P2_1/n$
$a = 6.0326\ (5)$ Å
$b = 11.4804\ (7)$ Å
$c = 10.8416\ (7)$ Å
$\beta = 105.454\ (5)^\circ$
$V = 723.71\ (9)$ Å^3
$Z = 2$
$D_x = 1.772$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.08$ mm^{-1}
$T = 293\ (2)$ K
Prism, red
$0.25 \times 0.20 \times 0.18$ mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.774$, $T_{max} = 0.829$
5759 measured reflections
1679 independent reflections
1270 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.7^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.076$
$S = 1.02$
1679 reflections
123 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0289P)^2 + 0.2572P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	2.0742 (18)	Fe1—N1	2.2424 (17)
Fe1—N3	2.1715 (17)		
O1—Fe1—O1^i	180	O1^i—Fe1—N1	89.95 (7)
O1—Fe1—N3^i	91.89 (7)	N3^i—Fe1—N1	103.34 (6)
O1^i—Fe1—N3^i	88.11 (7)	N3—Fe1—N1	76.66 (6)
N3^i—Fe1—N3	180	N1—Fe1—N1^i	180
O1—Fe1—N1	90.05 (7)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H3$W\cdots$N6^{ii}	0.80 (3)	1.94 (3)	2.730 (3)	170 (3)
O1—H2$W\cdots$N4^{iii}	0.79 (3)	2.01 (3)	2.794 (3)	167 (3)

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

Water H atoms were located in a difference Fourier map and were refined isotropically. Other H atoms were placed in calculated positions (C—H = 0.93Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$

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, 1998); software used to prepare material for publication: *SHELXTL*.

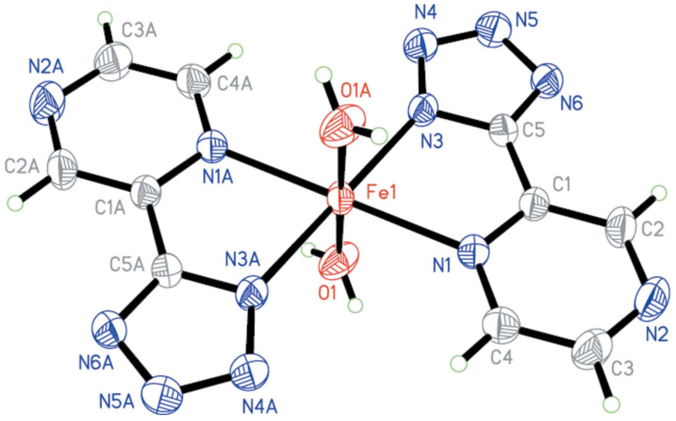


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Non-H atoms are drawn as 50% probability displacement ellipsoids. [Symmetry code: (A) $2-x, -y, 1-z$.]

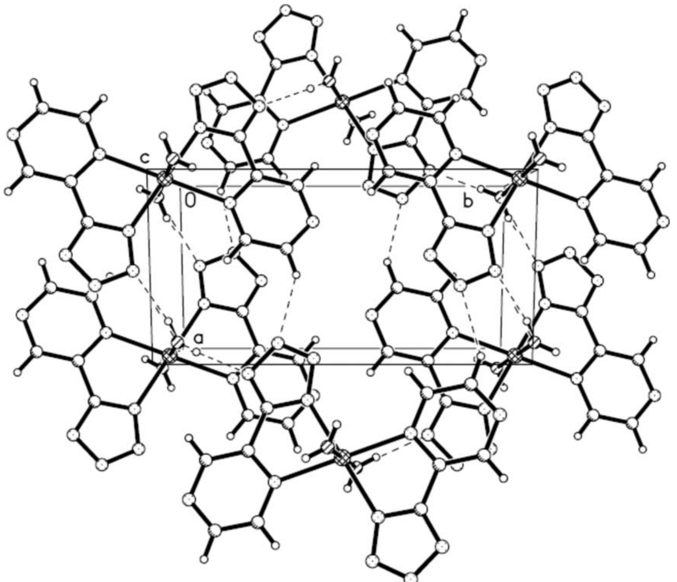


Figure 2
Packing diagram of the title complex, viewed along the c axis. Hydrogen bonds are shown as dashed lines.

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