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Bis[2-(aminomethyl)pyridine-κ^2*N*,*N*′]dinitratoiron(II)

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Key indicators

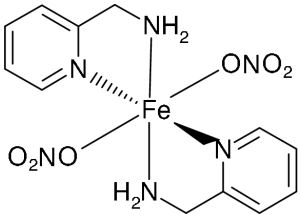
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.077
wR factor = 0.179
Data-to-parameter ratio = 13.9

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

The title compound, $[Fe(NO_3)_2(C_6H_8N_2)_2]$, is a mononuclear centrosymmetric iron(II) complex. The Fe^{II} ion is coordinated by four N atoms from two 2-aminomethylpyridine ligands and two O atoms from two nitrate anions. The six atoms around the metal constitute a slightly distorted octahedral geometry. In the crystal structure, the molecules are held together by intermolecular N—H···O hydrogen bonds, forming a three-dimensional network.

Comment

Transition metal compounds have been of great interest for many years (Yamada, 1999). These compounds play an important role in coordination chemistry. As an extension of work on the structural characterization of Fe compounds, the crystal structure of the title compound, (I), is reported here.



(I)

Compound (I) (Fig. 1) is a mononuclear iron(II) complex. The Fe atom, lying on an inversion centre, has an octahedral geometry, coordinated by two 2-aminomethylpyridine ligands and two nitrate anions. The 2-aminomethylpyridine ligand acts as a bidentate ligand and coordinates to the Fe atom through the two N atoms. The nitrate anion is a monodentate ligand and coordinates to the metal *via* one O atom. The three *trans* angles at Fe are, by symmetry, exactly 180°; the other angles are close to 90°, varying from 79.6 (2) to 100.4 (2)° (Table 1), which indicates a slightly distorted octahedral geometry around the Fe atom. The Fe1—N1 bond length [2.128 (6) Å] is longer than the value of 1.998 (2) Å observed in one other Fe^{II} compound (Munro & Ntshangase, 2003). The Fe1—N2 bond length [2.076 (5) Å] is comparable wth the value of 2.029 (2) Å observed in another Fe^{II} compound (Kobeissi *et al.*, 2002).

Atom N2 deviates by 0.503 (8) Å from the mean plane defined by atoms C1—C5 and N1. The dihedral angle between the pyridine ring and the nitrate plane is 96.4 (6)°.

In the crystal structure of (I), the molecules are held together by intermolecular N—H···O hydrogen bonds, forming a three-dimensional network (Table 2 and Fig. 2).

Experimental

2-Aminomethylpyridine (0.1 mmol, 10.8 mg), $FeCl_2\cdot2H_2O$ (0.1 mmol, 16.3 mg) and $NaNO_3$ (0.1 mmol, 8.5 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h at room temperature and then filtered. After allowing the brown filtrate to stand in air for 11 d, brown block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$[Fe(NO_3)_2(C_6H_8N_2)_2]$
$M_r = 396.16$
Monoclinic, $P2_1/c$
$a = 8.781$ (2) Å
$b = 8.845$ (2) Å
$c = 10.171$ (2) Å
$\beta = 101.34$ (3)°
$V = 774.5$ (3) Å^3
$Z = 2$
$D_x = 1.699$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 462 reflections
$\theta = 2.4$–20.7°
$\mu = 1.02$ mm^{-1}
$T = 293$ (2) K
Block, brown
0.22 × 0.18 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.807$, $T_{max} = 0.887$
3482 measured reflections
1596 independent reflections
900 reflections with $I > 2\sigma(I)$
$R_{int} = 0.098$
$\theta_{max} = 26.5$°
$h = -11 \rightarrow 5$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.077$
$wR(F^2) = 0.179$
$S = 0.95$
1596 reflections
115 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.87$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—N2	2.076 (5)	Fe1—O1	2.297 (4)
Fe1—N1	2.128 (6)		
$N2^i$—Fe1—N2	180.	N2—Fe1—O1	94.20 (18)
N2—Fe1—$N1^i$	100.4 (2)	$N1^i$—Fe1—O1	91.19 (19)
N2—Fe1—N1	79.6 (2)	N1—Fe1—O1	88.81 (19)
$N1^i$—Fe1—N1	180	O1—Fe1—$O1^i$	180
$N2^i$—Fe1—O1	85.80 (18)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···$O2^i$	0.90	2.65	3.338 (8)	134
N2—H2B···$O1^i$	0.90	2.43	3.139 (7)	135
N2—H2B···O3	0.90	2.42	2.976 (7)	120
N2—H2A···$O3^{ii}$	0.90	2.24	3.130 (7)	171

Symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $2 - x, y - \frac{1}{2}, \frac{5}{2} - z$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and N—H distances of 0.90 Å and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

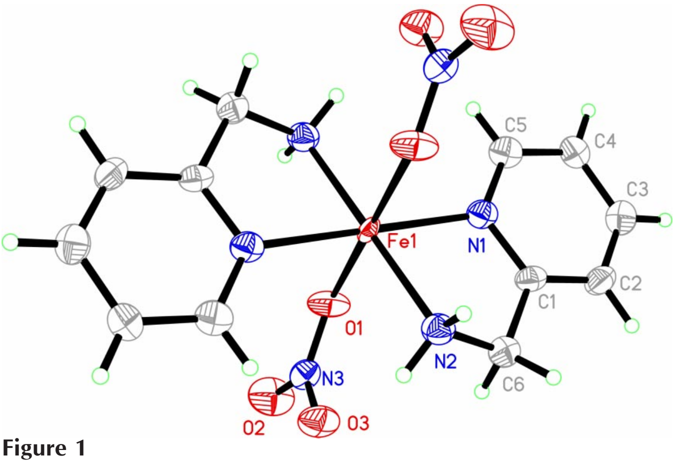


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by $2 - x, -y, 2 - z$.

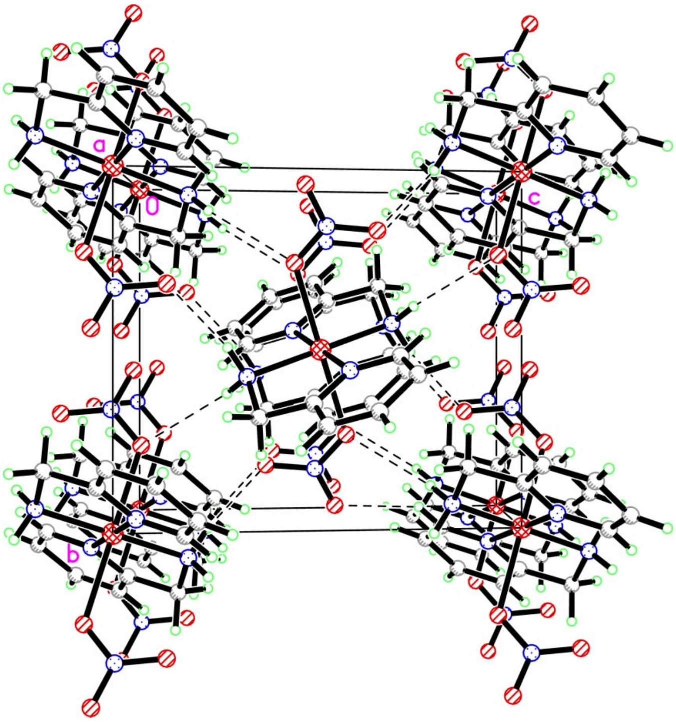


Figure 2
The crystal packing of (I), viewed along the a axis. Dashed lines indicate hydrogen bonds.

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

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