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Bis(2,2′-bipyridine-*N*,*N*′)dicyanoiron(III) nitrate

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Key indicators

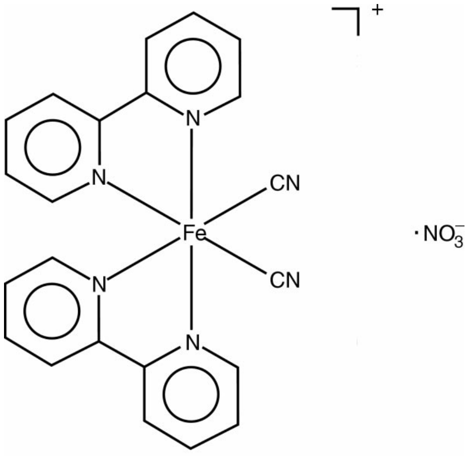
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.031
wR factor = 0.038
Data-to-parameter ratio = 14.3

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

The Fe atom of the title compound, $[Fe(bipy)_2(CN)_2](NO_3)$ (bipy is 2,2′-bipyridine, $C_{10}H_8N_2$), is octahedrally coordinated to the N atoms of the bipyridines and to the C atoms of the cyanide groups which are *cis* to each other. The Fe—C distances are 1.922 (3) and 1.923 (2) Å, and the Fe—N bonds *trans* to CN are 1.972 (2) and 1.973 (2) Å and are longer than those *cis* to the CN groups, *viz*. 1.955 (2) and 1.962 (2) Å. The bipyridine groups are close to being planar, with N—C—C—N torsion angles of −2.4 (3) and 1.6 (3)°, and bite angles of 81.43 (8) and 81.74 (8)°.

Comment

During an investigation of reactions between iron diimine complexes and the hexacyanoferrate anion, we prepared the title compound, $[Fe(bipy)_2(CN)_2](NO_3)$ (bipy is 2,2′-bipyridine), (I), and determined its crystal structure (Fig. 1).



(I)

The Fe atom is octahedrally coordinated to the N atoms of the bipyridines and to the C atoms of the cyanide groups, which are *cis* to each other. The Fe—C distances (Table 1) are 1.922 (3) and 1.923 (2) Å, and the Fe—N bonds *trans* to CN are 1.972 (2) and 1.973 (2) Å and are longer than those *cis* to the CN groups, *viz*. 1.955 (2) and 1.962 (2) Å. The bipyridine groups are close to being planar, with N—C—C—N torsion angles of −2.4 (3) and 1.6 (3)°, and bite angles of 81.43 (8) and 81.74 (8)°. The bond distances are very similar to those found for the corresponding perchlorate complex (Lu *et al.*, 1988), *i.e.* Fe—C 1.928 (7) and 1.931 (7) Å, Fe—N(*trans* to CN) 1.993 (5) and 1.988 (5) Å, and Fe—N(*cis* to CN) 1.955 (4) and 1.972 (4) Å. The two compounds have the same space group and very similar cell dimensions.

Experimental

The title compound was prepared as described by Schilt (1960).

Crystal data

$[Fe(C_{10}H_8N_2)_2(CN)_2](NO_3)$
$M_r = 482.28$
Orthorhombic, $P2_12_12_1$
$a = 10.7902 (6)$ Å
$b = 11.7031 (6)$ Å
$c = 16.1857 (9)$ Å
$V = 2043.9 (1)$ Å^3
$Z = 4$
$D_x = 1.567$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 8263 reflections
$\theta = 2.1–29.8°$
$\mu = 0.78$ mm^{-1}
$T = 120$ K
Block, red
0.40 × 0.34 × 0.34 mm

Data collection

Siemens SMART CCD diffractometer
ω rotation scans with narrow frames
Absorption correction: by integration (*XPREP*; Siemens, 1995)
$T_{\min} = 0.718$, $T_{\max} = 0.836$
19 837 measured reflections

5807 independent reflections
4302 reflections with $I > 3\sigma(I)$
$R_{\rm int} = 0.058$
$\theta_{\max} = 29.8°$
$h = -14 \rightarrow 15$
$k = -15 \rightarrow 14$
$l = -19 \rightarrow 21$

Refinement

Refinement on F
$R = 0.031$
$wR = 0.038$
$S = 1.20$
4302 reflections
300 parameters
H-atom parameters constrained
$w = 1/\{[\sigma_{cs}(F^2) + 1.03F^2]^{1/2} - |F|\}^2$
$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.80 (8)$ e Å^{-3}
$\Delta\rho_{\min} = -0.64 (8)$ e Å^{-3}
Extinction correction: B—C type 1, Lorentzian isotropic (Becker & Coppens, 1974)
Extinction coefficient: 24 (8)
Rogers parameter = 1.02 (3); 1815 Friedel pairs (84%)

Table 1
Selected geometric parameters (Å, °).

Fe—C21	1.923 (2)	Fe—N2	1.972 (2)
Fe—C22	1.922 (3)	Fe—N3	1.973 (2)
Fe—N1	1.962 (2)	Fe—N4	1.955 (2)
C21—Fe—C22	85.8 (1)	N3—Fe—C21	93.15 (9)
N4—Fe—C22	95.89 (9)	N1—Fe—N4	176.87 (8)
N1—Fe—C22	86.07 (9)	N2—Fe—N4	96.05 (8)
N2—Fe—C22	91.66 (9)	N3—Fe—N4	81.74 (8)
N3—Fe—C22	177.47 (9)	N1—Fe—N2	81.43 (8)
N4—Fe—C21	85.86 (9)	N1—Fe—N3	96.34 (8)
N1—Fe—C21	96.74 (9)	N2—Fe—N3	89.49 (8)
N2—Fe—C21	176.95 (9)		

H atoms were kept in calculated positions (C—H = 0.95 Å) with $U_{\rm iso} = 1.2U_{\rm eq}$ for the atom to which they are attached.

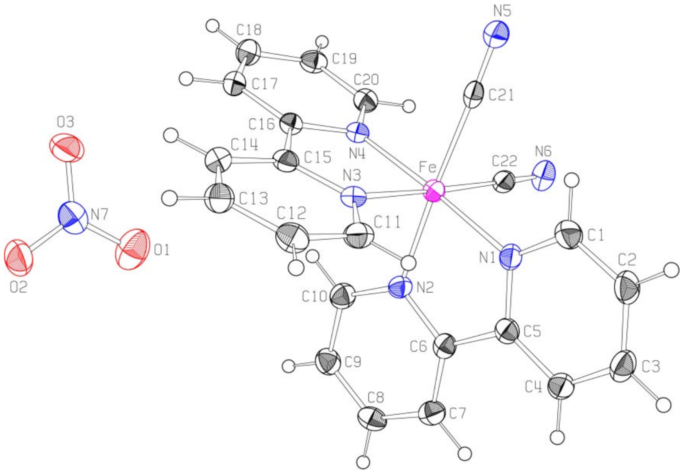


Figure 1
View of $[Fe(bipy)_2(CN)_2](NO_3)$ showing the labelling of the non-H atoms. Displacement ellipsoids are shown at 50% probability level and H atoms are drawn as small circles of arbitrary radius.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1997) and *KRYSTAL* (Hazell, 1995); program(s) used to refine structure: modified *ORFLS* (Busing *et al.*, 1962) and *KRYSTAL*; molecular graphics: *ORTEP*III (Burnett & Johnson, 1996) and *KRYSTAL*; software used to prepare material for publication: *KRYSTAL*.

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