Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Tris(2,2′-bipyridyl-*N*,*N*′)iron(II) diperchlorate

Stuart R. Batten *et al.*

Electronic paper
This paper is published electronically. It meets the data-validation criteria for publication in Acta Crystallographica Section C. The submission has been checked by a Section C Co-editor though the text in the 'Comments' section is the responsibility of the authors.

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Tris(2,2′-bipyridyl-*N*,*N*′)iron(II) diperchlorate

Stuart R. Batten,* Keith S. Murray and Nathan J. Sinclair

Department of Chemistry, PO Box 23, Monash University 3800, Australia
Correspondence e-mail: stuart.batten@sci.monash.edu.au

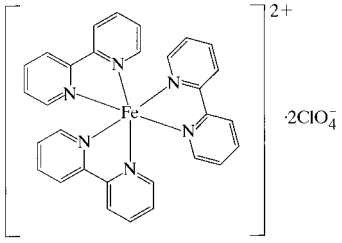
Received 5 June 2000
Accepted 26 June 2000

Data validation number: IUC0000176

The title compound, $[Fe(C_{10}H_8N_2)_3](ClO_4)_2$, is isomorphous with the Zn^{II} and Ru^{II} analogues. A twofold axis passes through the metal atom and the midpoint of the C—C bond joining the two pyridine rings of one of the bipyridyl ligands.

Comment

The structure of $[Fe(bipy)_3](ClO_4)_2$, (I), is isomorphous with the related Ru^{II} (Harrowfield & Sobolev, 1994; Krausz *et al.*, 1995) and Zn^{II} (Chen *et al.*, 1995; Klement *et al.*, 1995; Krausz *et al.*, 1995) analogues. A twofold axis passes through the



(I)

metal and the midpoint of the C—C bond joining the two pyridine rings of one of the bipyridine ligands. Thus, the asymmetric unit contains one metal on a special position, one perchlorate, and one and a half bipyridyl ligands.

Experimental

Crystals of (I) were obtained inadvertently by slow evaporation of an ethanolic solution containing $[Fe(bpm)_2(H_2O)_2](ClO_4)_2$ [bpm is bis(1-pyrazolyl)methane], 2,2′-bipyridine and sodium dicyanamide (yield 75%); satisfactory elemental analysis obtained.

Crystal data

$[Fe(C_{10}H_8N_2)_3](ClO_4)_2$
M_r = 723.30
Monoclinic, $C2/c$
a = 17.0545 (10) Å
b = 10.5812 (6) Å
c = 15.9456 (7) Å
β = 91.332 (6)°
V = 2876.7 (3) Å^3
Z = 4
D_x = 1.670 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10435 reflections
θ = 3.39–28.26°
μ = 0.776 mm^{-1}
T = 150 (2) K
Cube, dark red
0.5 × 0.5 × 0.38 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
5238 measured reflections
3049 independent reflections
1935 reflections with $I > 2\sigma(I)$
R_{int} = 0.1396
θ_{max} = 28.26°
$h = -22 \rightarrow 10$
$k = -11 \rightarrow 13$
$l = -19 \rightarrow 19$
Intensity decay: <1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.137
S = 1.061
3049 reflections
213 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 1.9714P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.655 e Å^{-3}
$\Delta\rho_{min}$ = −0.410 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—N21	1.953 (3)	Cl1—O2	1.431 (3)
Fe1—N12	1.970 (3)	Cl1—O1	1.443 (3)
Fe1—N11	1.972 (3)	Cl1—O3	1.444 (4)
Cl1—O4	1.424 (3)		
N21—Fe1—N21^i	82.01 (18)	N12—Fe1—N11	81.18 (13)
N21—Fe1—N12	96.12 (12)	N12^i—Fe1—N11	93.43 (13)
N21^i—Fe1—N12	173.55 (13)	N21—Fe1—N11^i	92.72 (12)
N21—Fe1—N12^i	173.55 (13)	N21^i—Fe1—N11^i	92.82 (13)
N21^i—Fe1—N12^i	96.12 (12)	N12—Fe1—N11^i	93.43 (13)
N12—Fe1—N12^i	86.40 (18)	N12^i—Fe1—N11^i	81.18 (12)
N21—Fe1—N11	92.82 (13)	N11—Fe1—N11^i	172.65 (18)
N21^i—Fe1—N11	92.72 (12)		

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO–SMN*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The receipt of an ARC Postdoctoral Fellowship (to SRB) is gratefully acknowledged. This work was also supported by grants from the Australian Research Council (ARC Large and Small Grants) to KSM.

References

Chen, X.-M., Wang, R.-Q. & Yu, X.-L. (1995). *Acta Cryst.* C**51**, 1545–1547.
Harrowfield, J. M. & Sobolev, A. N. (1994). *Aust. J. Chem.* **47**, 763–767.
Hooft, R. (1998). *COLLECT Software*. Nonius BV, Delft, The Netherlands.
Klement, U., Trumbach, D. & Yersin, H. (1995). *Z. Kristallogr.* **210**, 228–228.
Krausz, E., Riesen, H. & Rae, A. D. (1995). *Aust. J. Chem.* **48**, 929–954.
Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307–326.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.