Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(quinolin-8-olato-κ^2N,O)iron(III) methanol solvate

Guang Chen

Department of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China

Correspondence e-mail: qufuchenguang@163.com

Received 13 November 2006
Accepted 14 November 2006

The title compound, $[Fe(C_9H_6NO)_3]\cdot CH_3OH$, consists of a mononuclear $[Fe(C_9H_6NO)_3]$ complex molecule and a methanol solvent molecule. The Fe^{III} ion is coordinated by three N atoms and three O atoms from three quinolin-8-olate ligands. The six atoms around the metal form a slightly distorted octahedral geometry.

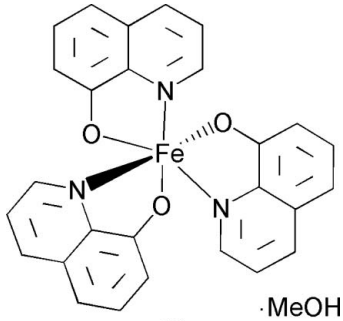
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.144
Data-to-parameter ratio = 17.0

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

Comment

Recently, we have reported the structures of a number of transition metal complexes (Chen *et al.*, 2004*a*,*b*, 2005). As an extension of our work on the structural characterization of iron compounds, the title mononuclear iron(III) compound, (I), is reported here.



(I)

The structure of (I) (Fig. 1) consists of a mononuclear $[Fe(C_9H_6NO)_3]$ complex molecule and a methanol solvent molecule. The Fe^{III} ion is coordinated by three N atoms and three O atoms from three quinolin-8-olate ligands. The three *trans* angles at Fe range from 168.64 (8) to 171.16 (8)° (Table 1); the other angles range from 79.51 (7) to 95.50 (8)°, indicating a distorted octahedral geometry about the Fe atom. The Fe—N and Fe—O bond lengths are typical and comparable with the values in other iron complexes (Zibaseresht *et al.*, 2006; Onggo *et al.*, 2005; Bakir *et al.*, 2005). The methanol molecule is linked to the complex through the intermolecular O4—H4···O1 hydrogen bond (Table 2).

Experimental

Quinolin-8-ol (1.0 mmol, 145.1 mg) and $Fe(NO_3)_3\cdot 9H_2O$ (0.5 mmol, 202.0 mg) were dissolved in a methanol solution (50 ml). The mixture was stirred for 1 h at room temperature and then filtered. After allowing the brown filtrate to stand in air for two weeks, brown block-shaped crystals were formed.

Crystal data

$[Fe(C_9H_6NO)_3]\cdot CH_4O$
M_r = 520.34
Monoclinic, $P2_1/n$
a = 10.868 (1) Å
b = 13.246 (1) Å
c = 17.288 (1) Å
β = 97.729 (1)°
V = 2466.1 (3) Å^3
Z = 4
D_x = 1.401 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.65 mm^{-1}
T = 298 (2) K
Block, brown
0.23 × 0.22 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.865, T_{max} = 0.886
14542 measured reflections
5575 independent reflections
4441 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.144
S = 1.03
5575 reflections
327 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.076P)^2 + 1.6804P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O2	1.908 (2)	Fe1—N2	2.054 (2)
Fe1—O3	1.915 (2)	Fe1—N1	2.237 (2)
Fe1—O1	1.921 (2)	Fe1—N3	2.272 (2)
O2—Fe1—O3	92.84 (7)	O1—Fe1—N1	79.60 (8)
O2—Fe1—O1	170.18 (8)	N2—Fe1—N1	94.59 (8)
O3—Fe1—O1	95.50 (8)	O2—Fe1—N3	94.21 (8)
O2—Fe1—N2	82.26 (7)	O3—Fe1—N3	79.51 (7)
O3—Fe1—N2	171.16 (8)	O1—Fe1—N3	92.40 (8)
O1—Fe1—N2	90.10 (8)	N2—Fe1—N3	93.46 (8)
O2—Fe1—N1	94.81 (8)	N1—Fe1—N3	168.64 (8)
O3—Fe1—N1	93.15 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O1	0.82	2.04	2.814 (4)	158

All H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93–0.96 Å and O—H = 0.82 Å. They were treated as riding atoms, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C,O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

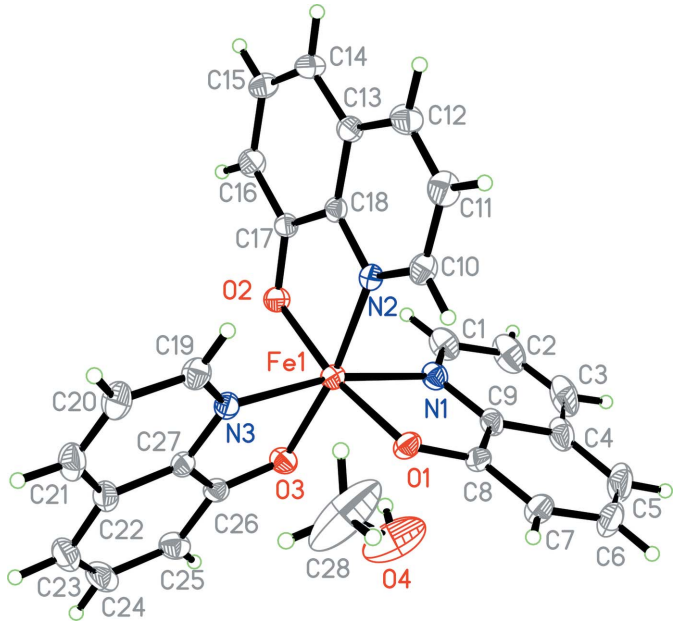


Figure 1
The molecular structure of the title compound, (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

The author thanks the Qufu Normal University for research grant No. xj03005.

References

Bakir, M., Dasgupta, T. P., Dutta, S. K., Ngah, N. & Yamin, B. M. (2005). *Acta Cryst.* E**61**, m1464–m1466.
Chen, G., Bai, Z.-P. & Qu, S.-J. (2005). *Acta Cryst.* E**61**, m2718–m2719.
Chen, G., Sun, Y.-X., Sun, M. & Qi, W. (2004*a*). *Acta Cryst.* E**60**, m1547–m1549.
Chen, G., Sun, Y.-X., Sun, M. & Qi, W. (2004*b*). *Acta Cryst.* E**60**, m1550–m1551.
Onggo, D., Mimin, A., Yamin, B. M. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m387–m388.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Zibaseresht, R., Robinson, W. T. & Hartshorn, R. M. (2006). *Acta Cryst.* E**62**, m1150–m1153.