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Aqua[N^1-(2-oxidobenzylideneamino)-3-aza-pentane-1,5-diamine]iron(II) chloride

Kun Chen[a]* and Jian-Hua Wang[b]

[a]School of Life Sciences, Guangzhou University, Guangzhou 510006, People's Republic of China, and [b]Bioengineering College, Chongqing University, Chongqing 400044, People's Republic of China

Correspondence e-mail: kun_chen863@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.045
wR factor = 0.122
Data-to-parameter ratio = 14.1

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

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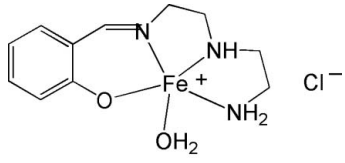
The title compound, $[Fe(C_{11}H_{18}N_3O_2)(H_2O)]Cl$, is a mononuclear iron(II) complex, consisting of one coordination cation and one uncoordinated Cl^- anion. The central metal has distorted square-pyramidal geometry. Weak intermolecular hydrogen bonds link the molecules to form two-dimensional layers parallel to the *bc* plane.

Comment

Metal complexes with Schiff base ligands form a large area in the field of coordination chemistry. Many different Schiff bases and their complexes have been reported recently (Qu *et al.*, 2005; You & Zhu, 2004*a*, 2006; You *et al.*, 2004*a*; Zhu *et al.*, 2000), including some iron(II,III) complexes (Liu *et al.*, 2004; You *et al.*, 2005, 2004*b*; You & Zhu, 2004*b*; Zhu *et al.*, 2003). We are interested in preparing mononuclear and dinuclear iron(II, III) complexes which are then assayed for their biological activity. Reported in this paper is the title mononuclear iron(II) complex, (I).



(I)

Complex (I) is a discrete mononuclear iron(II) complex, which consists of one coordinated monovalent cation and one uncoordinated Cl^- anion. In the cation, the central Fe^{II} atom is five-coordinated by one O atom and three N atoms from one Schiff base ligand, and by one O atom from a coordinated water molecule. The Fe^{II} atom has a distorted square-pyramidal geometry. The four donor atoms from the ligand constitute a well defined base plane of the polyhedron, with a mean deviation of 0.081 (6) Å. The Fe^{II} atom lies 0.178 (6) Å above the basal plane towards the water molecule. The dihedral angle between the basal plane of the square pyramid and the plane of the benzene ring is 11.9 (2)°. The bond lengths involving the central metal atom are comparable with those found in the literature (Liu *et al.*, 2004; You *et al.*, 2005, 2004*b*; You & Zhu, 2004*b*; Zhu *et al.*, 2003).

The water molecules, the Cl^- anions and the amine N atoms in the Schiff base participate in hydrogen bonds, which form two-dimensional layers parallel to the *bc* plane.

Experimental

$FeCl_2·6H_2O$ (1 mmol, 235 mg), salicylaldehyde (1 mmol, 122 mg) and diethylenetriamine (1 mmol, 103 mg) were dissolved in a mixture of

methanol and acetonitrile (20 ml, 1:1 *v*/*v*), resulting in a light-green solution. Diethyl ether was slowly diffused into this solution for 24 h, after which time large green prism crystals were precipitated. These were filtered off, washed three times with methanol and dried *in vacuo* (yield 67%). The product darkens in colour when exposed to the air for more than 2 d.

Crystal data

$[Fe(C_{11}H_{18}N_3O_2)(H_2O)]Cl$
M_r = 315.58
Monoclinic, $P2_1/c$
a = 9.059 (4) Å
b = 13.679 (5) Å
c = 10.800 (5) Å
β = 101.880 (10)°
V = 1309.6 (10) Å^3
Z = 4
D_x = 1.601 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 293 (2) K
Prism, green
0.5 × 0.4 × 0.4 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.623, T_{max} = 0.733
(expected range = 0.495–0.582)
2581 measured reflections
2425 independent reflections
2055 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.122
S = 1.08
2425 reflections
172 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 3.4826P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0127 (18)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1^{i}	0.843 (10)	1.842 (14)	2.675 (5)	169 (5)
O1W—H1WB···Cl1	0.85 (6)	2.36 (4)	3.124 (4)	151 (7)
N2—H2N···Cl1	0.90	2.36	3.253 (4)	170
N3—H3NA···Cl1^{ii}	0.99	2.39	3.340 (4)	162
N3—H3NB···O1W^{i}	0.92	2.43	3.115 (5)	131

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

All H atoms attached to C atoms were placed in geometrically calculated positions and constrained to ride on their parent atoms, with C—H = 0.96 Å. They were treated as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C). H atoms attached to O atoms were refined (Table 1).

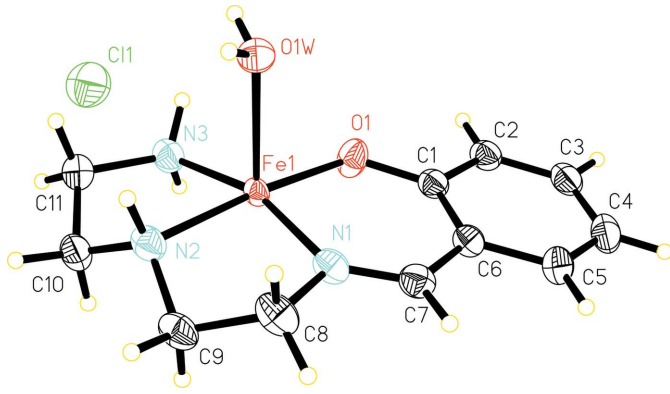


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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

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