Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis{2-[(4-chlorophenylimino)methyl]phenolato}iron(II)

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Received 8 May 2006
Accepted 10 May 2006

In the title mononuclear iron(II) complex, $[Fe(C_{13}H_{14}ClNO)_2]$, the Fe^{II} cation lies on a twofold rotation axis. It is four-coordinated in a tetrahedral geometry by the imino N and phenolate O atoms of the two chelating Schiff base ligands.

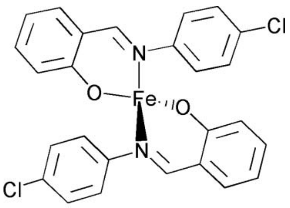
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.052
wR factor = 0.108
Data-to-parameter ratio = 15.4

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

Comment

A number of Schiff bases and their metal ion complexes have attracted considerable interest in chemistry and biology owing to their potentially beneficial biological activities which have often been related to a chelation phenomenon with trace metal ions (Dios *et al.*, 2002; Ren *et al.*, 2002; Zabinski & Toney, 2001). Schiff bases are believed to exercise their beneficial therapeutic properties in mammalian cells by inhibiting ribonucleotide reductase in the synthesis of DNA precursors (Nagarajan *et al.*, 2003). Iron complexes have been shown to be more active in cell destruction, as well as in the inhibition of DNA synthesis, than the uncomplexed Schiff bases (Taatjes *et al.*, 1997). In a continuation of our earlier reports on Schiff base complexes (Wei, 2005*a*,*b*; Wei & Wang, 2006; Zhu *et al.*, 2006), the present paper reports the synthesis and structural characterization of a mononuclear iron(II) complex with the Schiff base ligand 2-[(4-chlorophenylimino)methyl]phenolate.



(I)

In the title complex, (I), the Fe^{II} cation lies on a twofold rotation axis. It is four-coordinated in a tetrahedral geometry by the imino N and phenolate O atoms of the two chelating Schiff base ligands (Fig. 1). The Fe–ligand bond lengths (Table 1) are comparable with the corresponding values observed in other Fe–Schiff base structures (Boudalis *et al.*, 2004; Costes *et al.*, 2002; Brefuel *et al.*, 2005).

In the crystal structure, molecules are linked through weak $C-H\cdots O$ and $C-H\cdots N$ hydrogen bonds, forming columns along the *c* axis (Fig. 2 and Table 2).

Experimental

Salicylaldehyde (0.2 mmol, 24.3 mg), 4-chlorophenylamine (0.2 mmol, 25.4 mg) and $FeCl_2$ (0.1 mg, 12.7 mg) were dissolved in

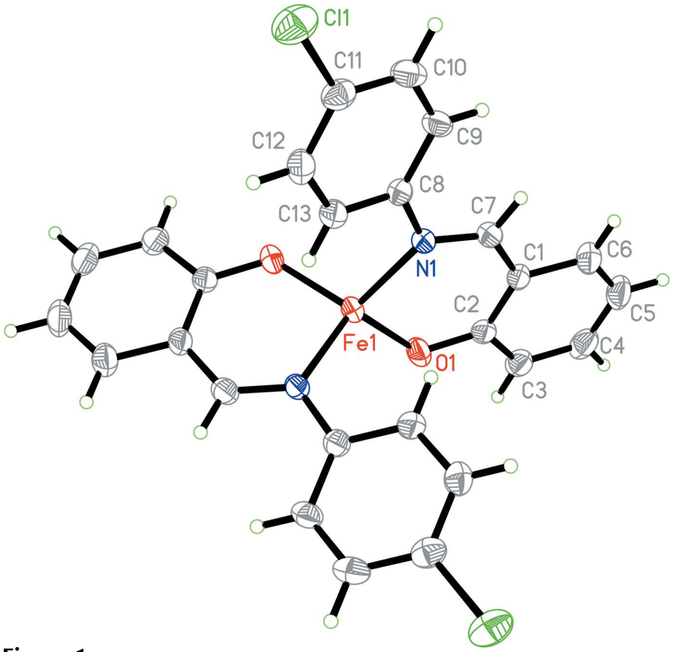


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code for unlabelled atoms: $-x, y, \frac{3}{2} - z$.]

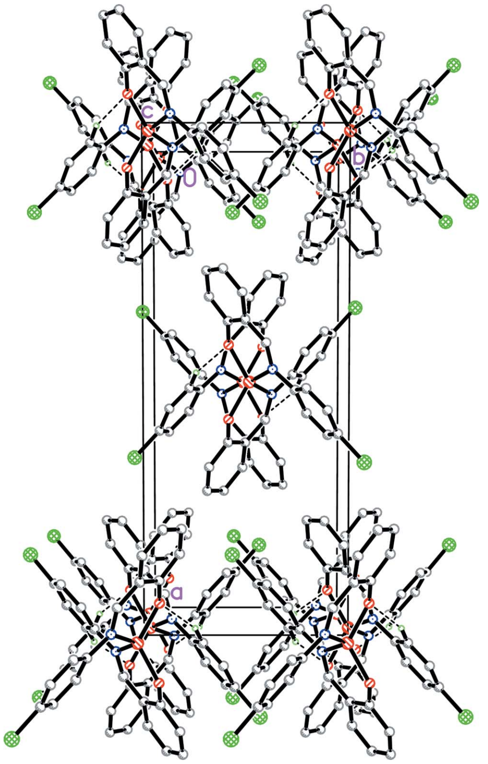


Figure 2
The crystal packing of (I), viewed along the *c* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

MeOH (30 ml). The mixture was refluxed at 340 K under argon for about 1 h, giving a clear brown solution. Deep-brown needle-shaped crystals of (I) formed after leaving the cooled solution to stand in the dark for about one week.

Crystal data

$[Fe(C_{13}H_9ClNO)_2]$
$M_r = 517.17$
Monoclinic, $C2/c$
$a = 21.870$ (5) Å
$b = 8.762$ (2) Å
$c = 11.788$ (3) Å
$\beta = 95.964$ (3)°
$V = 2246.8$ (9) Å^3
$Z = 4$
$D_x = 1.529$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.94$ mm^{-1}
$T = 298$ (2) K
Needle, brown
0.18 × 0.09 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.850$, $T_{max} = 0.921$
8075 measured reflections
2313 independent reflections
1589 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.108$
$S = 1.04$
2313 reflections
150 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.3814P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	1.894 (2)	Fe1—N1	1.996 (3)
$O1^i$—Fe1—O1	122.30 (14)	O1—Fe1—N1	96.97 (10)
O1—Fe1—$N1^i$	111.00 (9)	$N1^i$—Fe1—N1	120.39 (15)

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

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
C9—H9$\cdots$$O1^{ii}$	0.93	2.44	3.324 (3)	160
C13—H13$\cdots$$N1^i$	0.93	2.62	3.488 (3)	155

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

All the H atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

The authors acknowledge the Natural Science Foundation of Anhui Provincial Universities, People's Republic of China, for research grant No. 2005 K J019ZD.

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