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**Key indicators**

Single-crystal X-ray study  
 T = 298 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.012 \text{ \AA}$   
 R factor = 0.086  
 wR factor = 0.224  
 Data-to-parameter ratio = 13.6

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

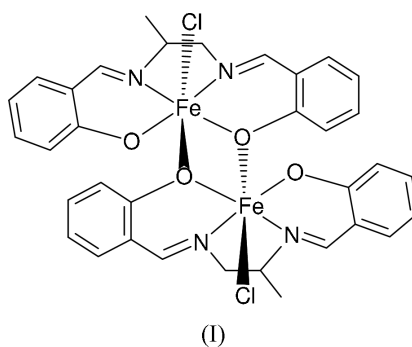
**A dinuclear Schiff base iron(III) complex with  
 the ligand *N,N'*-bis(2-oxidophenylmethylene-  
 imino)propane-1,2-diamine**

The centrosymmetric title compound, bis[ $\mu$ -*N,N'*-bis( $\mu$ -2-oxidophenylmethyleneimino)propane-1,2-diaminato(3-)]-iron(III),  $[\text{Fe}_2(\text{C}_{17}\text{H}_{16}\text{ClN}_2\text{O}_2)_2]$ , is a dinuclear iron(III) complex. Each  $\text{Fe}^{\text{III}}$  atom is six-coordinated by two N atoms and three O atoms from two Schiff base ligands, and one Cl atom, giving an approximately octahedral coordination environment.

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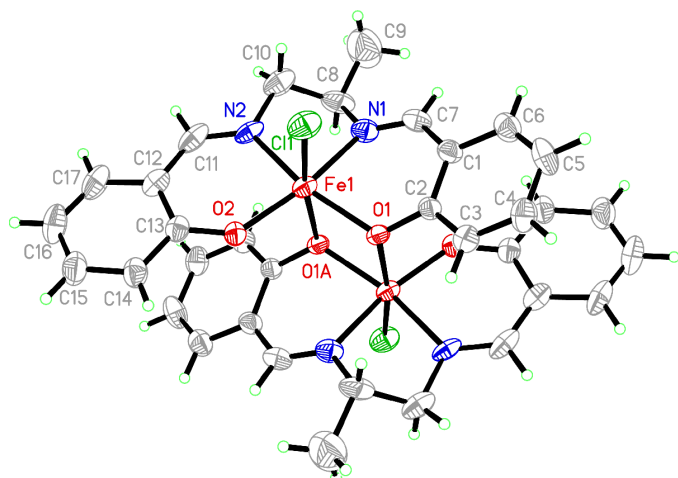
**Comment**

Investigations into the magnetic properties of molecular-based materials containing a polynuclear assembly have become a fascinating subject in the field of condensed matter physics and materials chemistry (Dalai *et al.*, 2002; Bhaduri *et al.*, 2003). Much attention has been focused on coordination complexes with novel magnetic properties, which may have potentially useful applications in materials science (Ray *et al.*, 2003). The prime strategy for designing these molecular materials is using a suitable bridging ligand, which determines the nature of the magnetic interactions (Koner *et al.*, 2003). Recently, we have reported a few Schiff base complexes (You, Lin *et al.*, 2003; You, Xiong *et al.*, 2004; You, Chen *et al.*, 2004). As an extension of our work on the structural characterization of Schiff base complexes, the title dinuclear iron(III) complex, (I), is reported here



The asymmetric unit consists of one-half of (I), with the other half generated by a crystallographic inversion centre (Fig. 1). The two  $\text{Fe}^{\text{III}}$  ions of the dinuclear complex are bridged by two  $\mu$ - $\text{O}^-$  (phenolate O atoms) ions. The octahedral coordination of each  $\text{Fe}^{\text{III}}$  ion is completed by a tetra-Schiff base ligand and a terminal  $\text{Cl}^-$  ion. The two  $\text{Cl}^-$  ligands are exactly *trans* about the  $\text{Fe} \cdots \text{Fe}$  vector, due to the inversion centre.

The longer  $\text{Fe1}-\text{O1}(-x, 1-y, 1-z)$  bond (Table 1), compared with the  $\text{Fe1}-\text{O1}$  bond, is indicative of a greater



**Figure 1**

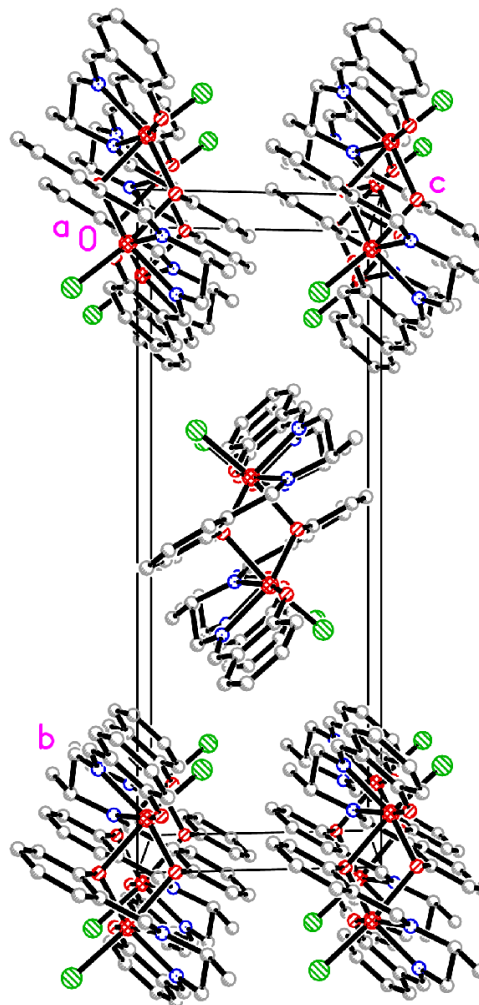
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Atom O1A is generated by the symmetry operation  $(-x, 1 - y, 1 - z)$ .

*trans* influence of the  $\text{Cl}^-$  compared to the Schiff base N atom. The Fe1—Cl1 bond is a little longer than the corresponding distance of 2.254 (2) Å observed in another iron(III) complex (Abrahams *et al.*, 1996). The Fe1—O2 bond is a little shorter than the corresponding distance of 1.926 (6) Å observed in a similar Schiff base iron(III) complex (You, Zhu & Liu, 2004). The Fe1—O1 bond is much longer than Fe1—O2, due to coordination of atom O1 to atom Fe1 $(-x, 1 - y, 1 - z)$ . The average Fe—N(imine) bond length of 2.100 (6) Å is a little less than the corresponding value of 2.138 (7) Å observed in the same complex (You, Zhu & Liu, 2004).

The three *trans* angles at the  $\text{Fe}^{\text{III}}$  atom lie in the range 159.5 (2)–171.27 (13)° (Table 1). The other angles subtended at the  $\text{Fe}^{\text{III}}$  atom are close to 90°, varying from 76.10 (19) to 107.90 (19)°, indicating a somewhat distorted octahedral geometry of the  $\text{Fe}^{\text{III}}$  atom. The  $\text{Fe}^{\text{III}}$  atom is 0.182 (3) Å out of the plane defined by the four chelating atoms, N1/N2/O2/O1. Atoms C8 and C10 deviate from the Fe1/N1/N2 plane by 0.413 (12) and  $-0.234$  (12) Å, respectively. The dihedral angle between the two benzene rings is 24.6 (3)°. As a result of the centre of symmetry, the  $\text{Fe}_2\text{O}_2$  core of (I) is perfectly planar.

## Experimental

Salicylaldehyde and 1,2-diaminopropane were obtained commercially and were used without further purification. Salicylaldehyde (0.2 mmol, 24.2 mg) and 1,2-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in ethanol (10 ml). The mixture was stirred for 1 h to give a clear yellow solution of *L* (0.1 mmol), where *L* is (2-oxido-phenylmethyleneimino)propane-1,2-diamine. To this solution of *L* was added an ethanol solution (10 ml) of  $\text{FeCl}_3 \cdot \text{H}_2\text{O}$  (0.1 mmol, 18.0 mg) with stirring. After keeping the resulting solution in air for 12 d, brown block-shaped crystals of (I) were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using anhydrous  $\text{CaCl}_2$  (yield 81.2%). Analysis, found: C 54.5, H 4.5, N 7.3%; calculated for  $\text{C}_{34}\text{H}_{32}\text{Cl}_2\text{Fe}_2\text{N}_4\text{O}_4$ : C 54.9, H 4.3, N 7.5%.



**Figure 2**

The crystal packing of (I), viewed along the *a* axis. All H atoms have been omitted for clarity.

### Crystal data

$[\text{Fe}_2(\text{C}_{17}\text{H}_{16}\text{ClN}_2\text{O}_2)_2]$   
 $M_r = 743.24$   
 Monoclinic,  $P2_1/c$   
 $a = 10.937$  (8) Å  
 $b = 20.406$  (14) Å  
 $c = 7.484$  (5) Å  
 $\beta = 101.864$  (11)°  
 $V = 1635$  (2) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.510$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 2307 reflections  
 $\theta = 2.2$ – $22.3$ °  
 $\mu = 1.10$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Block, brown  
 $0.28 \times 0.22 \times 0.14$  mm

### Data collection

Siemens SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.749$ ,  $T_{\text{max}} = 0.862$   
 8018 measured reflections

2838 independent reflections  
 1515 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.176$   
 $\theta_{\text{max}} = 25.0$ °  
 $h = -13 \rightarrow 12$   
 $k = -24 \rightarrow 23$   
 $l = -8 \rightarrow 6$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.086$   
 $wR(F^2) = 0.224$   
 $S = 0.94$   
 2838 reflections  
 209 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.1021P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 1.30$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.61$  e Å<sup>-3</sup>

**Table 1**  
Selected geometric parameters (Å, °).

Fe1—O2	1.886 (5)	Fe1—O1 <sup>i</sup>	2.205 (4)
Fe1—O1	1.977 (4)	Fe1—Cl1	2.306 (2)
Fe1—N2	2.089 (6)	O1—Fe1 <sup>i</sup>	2.205 (4)
Fe1—N1	2.111 (6)		
O2—Fe1—O1	107.90 (19)	N2—Fe1—O1 <sup>i</sup>	91.81 (19)
O2—Fe1—N2	87.7 (2)	N1—Fe1—O1 <sup>i</sup>	85.0 (2)
O1—Fe1—N2	159.5 (2)	O2—Fe1—Cl1	96.35 (15)
O2—Fe1—N1	163.3 (2)	O1—Fe1—Cl1	95.31 (14)
O1—Fe1—N1	85.0 (2)	N2—Fe1—Cl1	95.95 (17)
N2—Fe1—N1	77.4 (3)	N1—Fe1—Cl1	92.83 (18)
O2—Fe1—O1 <sup>i</sup>	87.92 (18)	O1 <sup>i</sup> —Fe1—Cl1	171.27 (13)
O1—Fe1—O1 <sup>i</sup>	76.10 (19)		

Symmetry code: (i)  $-x, 1 - y, 1 - z$ .

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5$  times  $U_{\text{eq}}(\text{C})$ . An unassigned maximum residual density of  $1.30 \text{ e } \text{Å}^{-3}$  was observed  $0.64 \text{ Å}$  from atom H10A. The minimum residual density was observed  $1.10 \text{ Å}$  from atom Fe1. The value of  $R_{\text{int}}$ , 0.176, is probably due to the poor diffraction quality of the crystal.

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

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