

**{1,1'-[Propane-1,3-diylbis(nitrilomethylidyne)]-
di-2-naphtholato}iron(II)**

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The title mononuclear iron(II) compound, $[\text{Fe}(\text{C}_{25}\text{H}_{20}\text{N}_2\text{O}_2)]$, possesses C_s symmetry with the Fe atom located on a mirror plane. The metal atom is four-coordinated by two N atoms and two O atoms from the Schiff base ligand in an approximately square-planar configuration.

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Key indicators

Single-crystal X-ray study

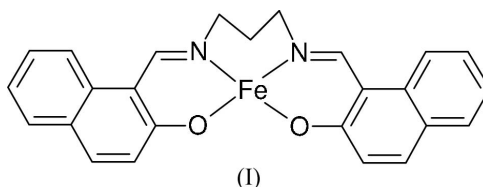
 $T = 273 \text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$ R factor = 0.040 wR factor = 0.096

Data-to-parameter ratio = 15.0

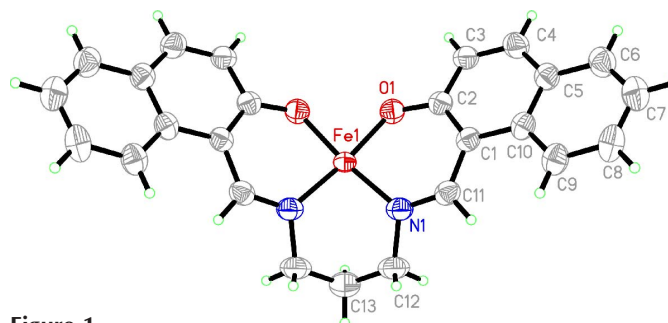
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Comment

Compounds containing Schiff base ligands have been of interest for a long time (Archer & Wang, 1990; Chang *et al.*, 1998). These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). As an extension of the work on the structural characterization of the Schiff base iron complexes, we report here the crystal structure of a new mononuclear iron(II) compound, (I).



The molecular structure of compound (I), a mononuclear Fe^{II} compound possessing C_s symmetry, is illustrated in Fig. 1. Selected bond distances and angles are given in Table 1. The central Fe atom, located on a mirror plane, is in an approximately square-planar configuration and is four-coordinated by two O atoms and two N atoms from the Schiff base ligand. The four coordinating atoms around the Fe atom are perfectly coplanar; the Fe atom lies $0.023(2) \text{ \AA}$ above this plane. The FeO_2N_2 coordination has a slightly distorted square-planar

**Figure 1**

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the reflection symmetry operator $(2 - x, y, z)$.

configuration, both *trans*-O—Fe—N angles being 173.87 (11)°.

In the crystal structure the molecules stack along the twofold screw axis parallel to the *c* axis (Fig. 2).

Experimental

2-Hydroxy-1-naphthaldehyde (0.2 mmol, 34.3 mg) and 1,3-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in methanol (15 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added an aqueous solution (10 ml) of FeSO₄·7H₂O (0.1 mmol, 27.8 mg) with stirring. The mixture was stirred for about 20 min at room temperature and filtered. The filtrate was allowed to stand in air for 5 d, after which time brown block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using anhydrous CaCl₂. Analysis found: C 68.5, H 4.6, N 6.5%; calculated for C₂₅H₂₀FeN₂O₂: C 68.8, H 4.6, N 6.4%.

Crystal data

[Fe(C ₂₅ H ₂₀ N ₂ O ₂)]	Mo K α radiation
<i>M_r</i> = 436.28	Cell parameters from 1687 reflections
Orthorhombic, <i>Cmc</i> 2 ₁	θ = 2.5–22.7°
<i>a</i> = 30.514 (3) Å	μ = 0.78 mm ⁻¹
<i>b</i> = 8.436 (2) Å	<i>T</i> = 273 (2) K
<i>c</i> = 7.742 (2) Å	Block, brown
<i>V</i> = 1992.9 (7) Å ³	0.32 × 0.26 × 0.22 mm
<i>Z</i> = 4	
<i>D_x</i> = 1.454 Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	2090 independent reflections
ω scans	1722 reflections with <i>I</i> > 2 σ (<i>I</i>)
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	<i>R</i> _{int} = 0.034
<i>T</i> _{min} = 0.788, <i>T</i> _{max} = 0.847	θ _{max} = 26.5°
5567 measured reflections	<i>h</i> = -28 → 38
	<i>k</i> = -9 → 10
	<i>l</i> = -9 → 9

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.096$	(Δ/σ) _{max} < 0.001
<i>S</i> = 1.00	$\Delta\rho_{max} = 0.32 \text{ e \AA}^{-3}$
2090 reflections	$\Delta\rho_{min} = -0.28 \text{ e \AA}^{-3}$
139 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	953 Friedel pairs
	Flack parameter = -0.05 (3)

Table 1

Selected geometric parameters (Å, °).

Fe1—O1	1.840 (2)	Fe1—N1	1.861 (3)
O1—Fe1—O1 ¹	82.66 (15)	O1—Fe1—N1	91.35 (12)
O1—Fe1—N1 ¹	173.87 (11)	N1 ¹ —Fe1—N1	94.60 (18)

Symmetry code: (i) 2 - *x*, *y*, *z*.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with *U*_{iso}(H) = 1.2*U*_{eq}(C).

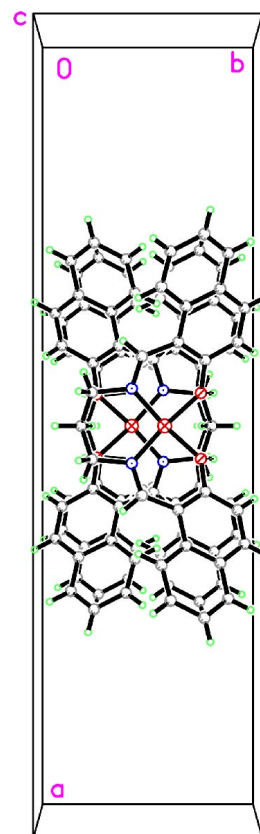


Figure 2

Part of the crystal packing of (I), viewed along the *c* axis.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; 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*.

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