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#### Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å  
 $R$  factor = 0.090  
 $wR$  factor = 0.244  
Data-to-parameter ratio = 16.8

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

## Dichloro(dimethylformamide)[2-hydroxy-5-nitro-*N*-(8-quinolyl)salicylaldiminato]iron(III)

In the title complex,  $[\text{FeCl}_2(\text{C}_3\text{H}_7\text{NO})(\text{C}_{16}\text{H}_{10}\text{N}_3\text{O}_3)(\text{C}_3\text{H}_7\text{NO})]$ , the  $\text{Fe}^{\text{III}}$  ion is in an octahedral environment, with the equatorial plane being defined by the two N and one O atoms of the tridentate ligand 2-hydroxy-5-nitro-*N*-(8-quinolyl)salicylaldimine, and a chlorine, the octahedron being completed by the other chlorine and a dimethylformamide (DMF) O atom in axial positions. Non-classical hydrogen bonds between 8-aminoquinolyl C—H groups and nitro O and Cl atoms of neighbouring molecules generate a layered hydrogen-bonded network.

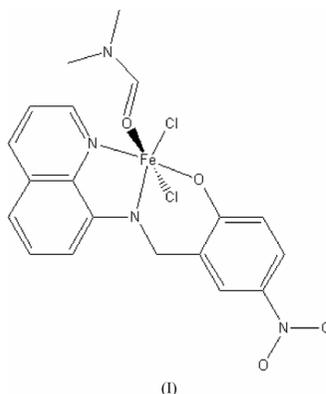
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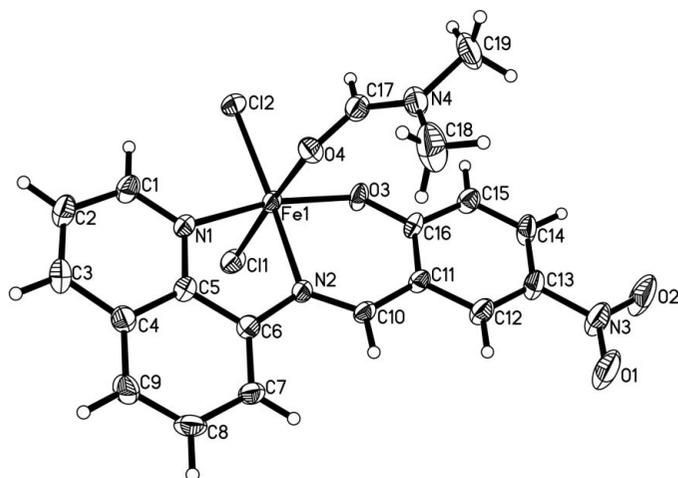
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#### Comment

A great deal of work has been reported on the synthesis and characterization of different types of Schiff-base complexes of transition and non-transition elements. Schiff bases usually have variable donation sites; they can be bidentate, tridentate or tetradentate, forming mono- or polynuclear complexes (Fatima & Tareq, 2000). Owing to the high affinity of iron(III) for phenols and naphthols, a vast number of complexes has been reported for iron with Schiff bases derived from salicylaldehyde or hydroxynaphthaldehyde. However, less is known about reactions of such Schiff-base complexes with dithiocarbamate, thiocyanate and quinolate anions. Interest in transition-metal complexes of these anions still continues, not only due to the interesting structural and bonding modes they possess but also due to their varied industrial applications. In a continuation of our interest in studying the reaction of transition metals with nitrogen-donor ligands, the present work describes the formation and characterization of the iron(III) complex, (I), with the Schiff-base ligand 2-hydroxy-5-nitro-*N*-(8-quinolyl)salicylaldimine (L), which is tridentate.



The structure described here shows (I) to be a mononuclear species (Fig. 1 and Table 1). The  $\text{Fe}^{\text{III}}$  ion is in an octahedral environment, with the equatorial plane being defined by the 8-quinolyl atoms N1 and N2, atom O3 of the hydroxyl group of



**Figure 1**  
Displacement ellipsoid plot of (I) with ellipsoids at the 30% probability level.

ligand L and atom Cl2; the octahedron is completed by Cl1 and atom O4 of DMF in axial positions.

Hydrogen bonds between 8-aminoquinoyl C—H groups and nitro O and Cl atoms of neighbouring molecules generate a layered hydrogen-bonded network (Fig. 2 and Table 2). The non-classical hydrogen-bonding interactions produce a three-dimensional framework with channels. Along the *b* axis, there are channels with a width of 4.32 Å and a height of 10.41 Å.

## Experimental

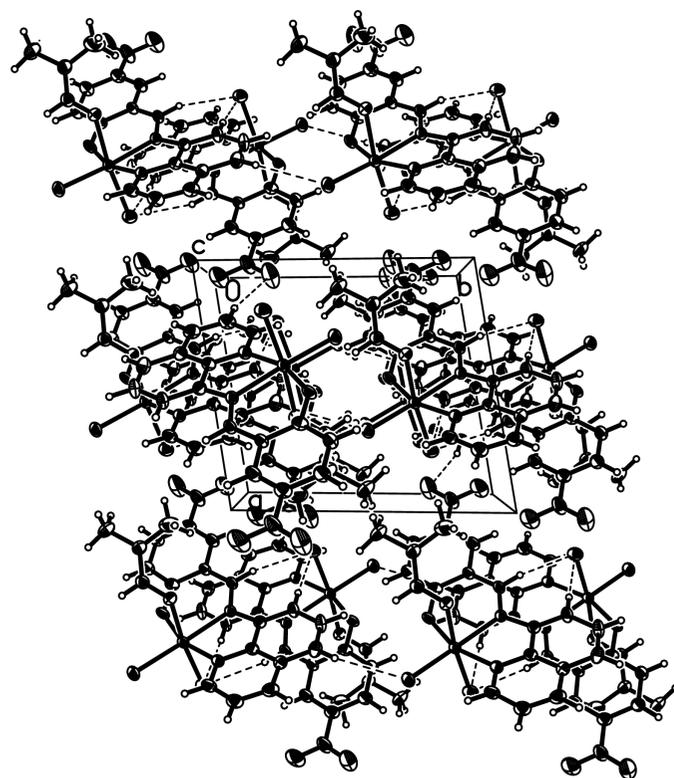
The ligand 2-hydroxy-5-nitro-*N*-(8-quinoyl)salicylalimine, L, was prepared as follows: 0.01 mol of each of 8-aminoquinoline and 5-nitrosalicylaldehyde were dissolved in 50 ml of methanol, and the mixture was refluxed for 4 h. The cooled solution was mixed with 1.35 g of FeCl<sub>3</sub>·6H<sub>2</sub>O (0.005 mol) in 50 ml of methanol and the resulting solution was stirred overnight. The solid which formed was collected and showed poor solubility in normal organic solvents. Black needle-shaped crystals of (I) suitable for X-ray analysis were prepared by diffusing ethyl ether into a dimethylformamide solution of the complex for about a week.

### Crystal data

[FeCl <sub>2</sub> (C <sub>16</sub> H <sub>10</sub> N <sub>3</sub> O <sub>3</sub> )(C <sub>3</sub> H <sub>7</sub> NO)]	<i>Z</i> = 2
<i>M<sub>r</sub></i> = 492.12	<i>D<sub>x</sub></i> = 1.597 Mg m <sup>-3</sup>
Triclinic, <i>P</i> 1	Mo <i>K</i> α radiation
<i>a</i> = 9.205 (2) Å	Cell parameters from 742 reflections
<i>b</i> = 10.372 (2) Å	$\theta$ = 5.1–46.3°
<i>c</i> = 10.989 (2) Å	$\mu$ = 1.03 mm <sup>-1</sup>
$\alpha$ = 81.831 (4)°	<i>T</i> = 293 (2) K
$\beta$ = 87.033 (4)°	Needle, black
$\gamma$ = 80.405 (4)°	0.20 × 0.10 × 0.10 mm
<i>V</i> = 1023.6 (4) Å <sup>3</sup>	

### Data collection

Bruker CCD area-detector diffractometer	4582 independent reflections
$\varphi$ and $\omega$ scans	2740 reflections with <i>I</i> > 2σ( <i>I</i> )
Absorption correction: refined from $\Delta F$ (SHELXA; Sheldrick, 1990)	<i>R</i> <sub>int</sub> = 0.111
<i>T</i> <sub>min</sub> = 0.816, <i>T</i> <sub>max</sub> = 0.908	$\theta$ <sub>max</sub> = 28.1°
6454 measured reflections	<i>h</i> = -12 → 12
	<i>k</i> = -7 → 13
	<i>l</i> = -14 → 13



**Figure 2**  
Packing diagram of the unit cell of (I).

### Refinement

Refinement on <i>F</i> <sup>2</sup>	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.090$	$w = 1/[\sigma^2(F_o^2) + (0.1404P)^2]$
$wR(F^2) = 0.244$	where $P = (F_o^2 + 2F_c^2)/3$
<i>S</i> = 0.95	( $\Delta/\sigma$ ) <sub>max</sub> < 0.001
4582 reflections	$\Delta\rho_{\text{max}} = 0.64 \text{ e \AA}^{-3}$
273 parameters	$\Delta\rho_{\text{min}} = -0.66 \text{ e \AA}^{-3}$

**Table 1**

Selected interatomic distances (Å).

Fe1—O3	1.927 (4)	Fe1—N2	2.162 (4)
Fe1—N1	2.147 (4)	Fe1—Cl2	2.2858 (16)
Fe1—O4	2.160 (4)	Fe1—Cl1	2.3116 (18)

**Table 2**

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C1—H1...Cl2	0.93	2.76	3.359 (6)	123
C2—H2...O2 <sup>i</sup>	0.93	2.58	3.478 (10)	164
C7—H7...Cl1 <sup>ii</sup>	0.93	2.79	3.719 (7)	174
C9—H9...Cl2 <sup>iii</sup>	0.93	2.81	3.645 (6)	149

Symmetry codes: (i) 1 + *x*, *y*, 1 + *z*; (ii) 1 - *x*, 2 - *y*, 1 - *z*; (iii) *x*, 1 + *y*, *z*.

The positions of all H atoms were fixed geometrically and distances to H atoms were set by the program.

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT (Bruker, 1997); program(s) used to solve

structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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