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Key indicators

Single-crystal X-ray study
T = 295 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.025
wR factor = 0.062
Data-to-parameter ratio = 18.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Dichloro(methanol- κO)[2-(2-pyridylmethyl-
iminomethyl)phenolato- $\kappa^3 N, N', O$]iron(III)

In the crystal structure of the methanol-coordinated mononuclear title compound, $[\text{Fe}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{O})\text{Cl}_2(\text{CH}_4\text{O})]$, the Fe^{III} atom is six-coordinate in an octahedral environment and the Cl atoms are *cis* to each other. Hydrogen bonds between the hydroxyl group of the methanol ligand and the Cl atom of an adjacent molecule lead to the formation of a chain that runs along the *b* axis of the orthorhombic unit cell.

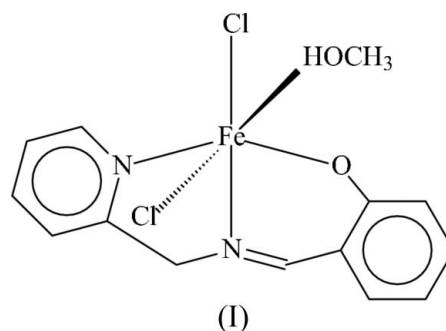
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Comment

The crystallographic literature mentions only one example of a metal derivative of the Schiff base that is derived by condensing 2-pyridylmethylamine with salicylaldehyde, (3,5-di-*t*-butylcatecholato)[*N*-(2-pyridylmethyl)salicylideneimino]oxovanadium(V) monohydrate (Baruah *et al.*, 2002). In that compound, the ligand functions as an *N, N', O*-terdentate chelate that occupies the equatorial sites of the octahedron around the metal atom. In the title iron(III) derivative, (I) (Fig. 1), the metal atom is similarly chelated by the Schiff base, and the sixth coordination site is occupied by a methanol molecule.



One Cl atom [Fe1—Cl2 2.349 (1) Å] is involved in hydrogen bonding, to furnish a chain running along the *b* axis.

Experimental

Salicylaldehyde (1.05 ml, 10 mmol) was dissolved in methanol (10 ml) and 2-aminomethylpyridine (1.08 g, 10 mmol) in methanol solution (5 ml) was added with stirring. The resulting orange solution was continuously stirred for 40 min at room temperature, and then iron(II) chloride (1.65 mg, 10 mmol) in methanol solution (20 ml) was added with stirring. The product began to crystallize from the solution almost immediately. After 1 h, the black–purple solid was filtered off, washed with methanol and air-dried. X-ray quality single crystals of (I) were grown by the vapour diffusion of diethylether into a methanol solution of the solid to yield purple crystals of the title complex. Analysis, calculated for $\text{C}_{14}\text{H}_{15}\text{Cl}_2\text{FeN}_2\text{O}_2$: C 45.40, H 4.05, N 7.57%; found: C 45.72, H 4.16, N 7.36%.

Crystal data

[Fe(C₁₃H₁₁N₂O)Cl₂(CH₄O)] $M_r = 370.03$ Orthorhombic, *Pca*2₁ $a = 19.428 (1) \text{ \AA}$ $b = 7.0016 (5) \text{ \AA}$ $c = 11.5352 (8) \text{ \AA}$ $V = 1569.13 (19) \text{ \AA}^3$ $Z = 4$ $D_x = 1.566 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation

Cell parameters from 3270

reflections

 $\theta = 2.5\text{--}25.6^\circ$ $\mu = 1.31 \text{ mm}^{-1}$ $T = 295 (2) \text{ K}$

Block, purple

 $0.26 \times 0.14 \times 0.10 \text{ mm}$

Data collection

Bruker APEX-II area-detector

diffractometer

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2004)

 $T_{\min} = 0.486$, $T_{\max} = 0.881$

9057 measured reflections

3571 independent reflections

3144 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.029$ $\theta_{\text{max}} = 27.5^\circ$ $h = -25 \rightarrow 25$ $k = -6 \rightarrow 9$ $l = -14 \rightarrow 14$

Refinement

Refinement on F^2 $R[F^2 > 2\sigma(F^2)] = 0.025$ $wR(F^2) = 0.062$ $S = 0.96$

3571 reflections

195 parameters

H atoms treated by a mixture of

independent and constrained

refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0292P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\text{max}} = 0.001$ $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$ $\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$

Absolute structure: Flack (1983),

with 1679 Friedel pairs

Flack parameter: 0.00 (1)

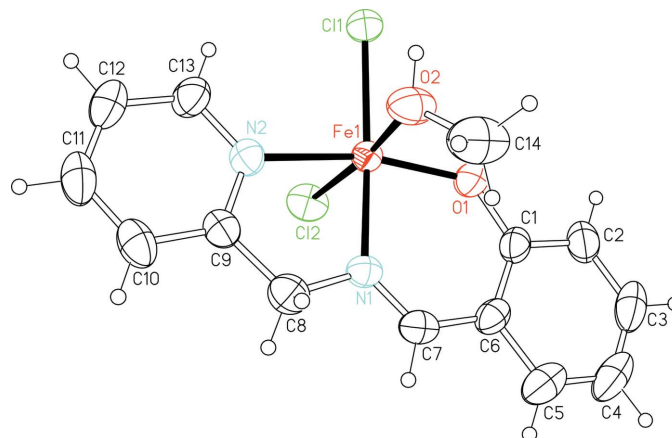


Figure 1

A plot of (I), with displacement ellipsoids drawn at the 50% probability level and H atoms shown as spheres of arbitrary radii.

The methanol H atom was located in a difference Fourier map and it was refined freely with a distance restraint of O–H = 0.85 (1) Å. C-bound H atoms were positioned geometrically, with C–H = 0.93 Å for aromatic H, 0.97 Å for methylene H and 0.96 Å for methyl H, and were treated as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. The methyl group was rotated to fit the electron density.

Table 1

Selected geometric parameters (Å, °).

Fe1–Cl1	2.292 (1)	Fe1–O2	2.206 (2)
Fe1–Cl2	2.349 (1)	Fe1–N1	2.106 (2)
Fe1–O1	1.889 (2)	Fe1–N2	2.163 (2)
Cl1–Fe1–Cl2	97.41 (3)	Cl2–Fe1–N2	87.33 (5)
Cl1–Fe1–O1	98.88 (5)	O1–Fe1–O2	91.00 (8)
Cl1–Fe1–O2	82.99 (5)	O1–Fe1–N1	87.49 (7)
Cl1–Fe1–N1	166.74 (5)	O1–Fe1–N2	163.85 (8)
Cl1–Fe1–N2	95.79 (5)	O2–Fe1–N1	85.30 (7)
Cl2–Fe1–O1	97.40 (6)	O2–Fe1–N2	84.10 (7)
Cl2–Fe1–O2	171.42 (6)	N1–Fe1–N2	76.80 (7)
Cl2–Fe1–N1	93.26 (5)		

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$O2\text{--}H2O\cdots Cl2^i$	0.84 (1)	2.51 (2)	3.295 (2)	157 (3)

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

Data collection: SMART (Bruker, 2004); cell refinement: SAINTE (Bruker, 2004); data reduction: SAINTE; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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