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Dichlorido{1-[(2-hydroxyethyl)iminomethyl]-2-naphtholato}pyridineiron(III) pyridine monosolvate

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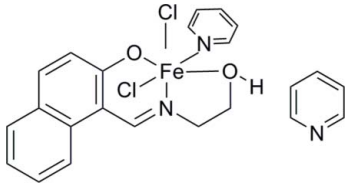
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 12.1.

In the title complex, $[Fe(C_{13}H_{12}NO_2)Cl_2(C_5H_5N)]\cdot C_5H_5N$, the iron(III) atom is six-coordinated by the N and O atoms from the Schiff base ligand, the N atom from a pyridine molecule and two chloride anions in a distorted octahedral geometry. The crystal packing is stabilized by intermolecular O—H···N hydrogen bonds and C—H···π interactions.

Related literature

For the synthesis and applications of magnetic complexes, see: Oshio *et al.* (2004); Aromí & Brechin (2006). For related structures, see: Goodwin *et al.* (2000); Qian *et al.* (2008); Hoshino *et al.* (2009).



Experimental

Crystal data

$[Fe(C_{13}H_{12}NO_2)Cl_2(C_5H_5N)]\cdot C_5H_5N$
M_r = 499.19
Monoclinic, $P2_1$
a = 7.8590 (6) Å
b = 10.0153 (11) Å
c = 14.4884 (16) Å
β = 90.123 (1)°
V = 1140.4 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 298 K
0.48 × 0.44 × 0.37 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
T_{min} = 0.666, T_{max} = 0.727
5726 measured reflections
3395 independent reflections
3143 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.00
3395 reflections
281 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), 1265 Friedel pairs
Flack parameter: 0.02 (2)

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the C4–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N3	0.82	1.81	2.617 (4)	168
C12—H12···Cg^{i}	0.93	2.71	3.594 (5)	159
C16—H16···Cg^{ii}	0.93	2.78	3.653 (6)	157

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2519).

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supporting information

Acta Cryst. (2010). E**66**, m1585 [https://doi.org/10.1107/S1600536810046623]

Dichlorido{1-[(2-hydroxyethyl)iminomethyl]-2-naphtholato}pyridineiron(III) pyridine monosolvate

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S1. Comment

The considerable current interest in magnetic complexes arises from their relevance in diverse fields ranging from bioinorganic chemistry to molecular magnetic materials (Oshio *et al.*, 2004; Aromí *et al.*, 2006). We report here the synthesis and crystal structure of the title compound.

In the title complex (Fig. 1), the tridentate Schiff base ligand is derived from the condensation of 2-hydroxy-1-naphthaldehyde and ethanolamine. The iron(III) metal centre is six-coordinate by the N and O atoms from the Schiff base ligand, the N atom from a pyridine molecule and two chloride anions in a distorted octahedral geometry. The Fe–O(alkoxo) bond length [Fe1–O1 = 2.105 (2) Å] is longer than the Fe–O(phenoxo) distance [Fe1–O2 = 1.897 (2) Å], which lies well within the range of values reported in the literature (Goodwin *et al.*, 2000; Qian *et al.*, 2008; Hoshino *et al.*, 2009). In the crystal structure, complex molecules and pyridine solvent molecules are linked into a three-dimensional network by O—H···N hydrogen bonds and C—H···π interactions (Table 1).

S2. Experimental

Ethanolamine (1 mmol, 61.08 mg) was dissolved in methanol (10 ml) and added dropwise to a methanol solution of 2-hydroxy-1-naphthaldehyde (1 mmol, 172.19 mg). The mixture was then stirred at 323 K for 2 h. Subsequently, an MeCN/Py solution "(3:1 *v*/*v*, 4 ml) of $FeCl_3.6H_2O$(1 mmol, 270.29 mg) was added dropwise and stirred for another 7 h. The resulting black solution was filtrated and was allowed to stand at room temperature for about one week, whereupon block crystals suitable for X-ray diffraction analysis were obtained.

S3. Refinement

All H atoms were placed in geometrically idealized positions and treated as riding on their parent atoms, with C—H = 0.93–0.97 Å, O—H = 0.82 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(O).

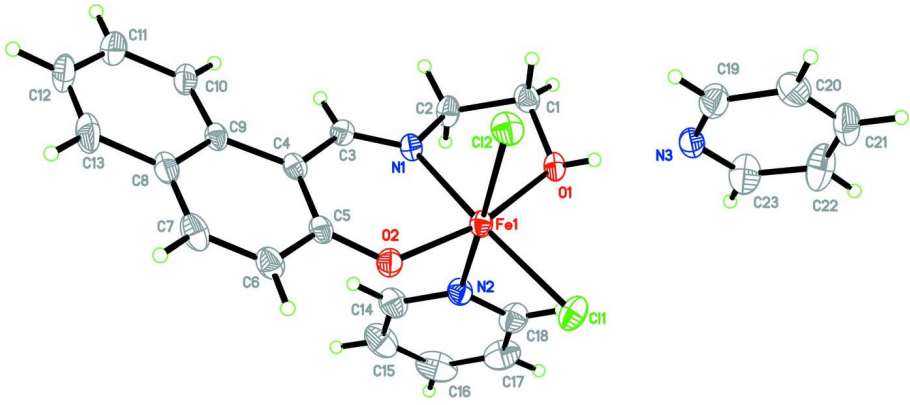

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids.

Dichlorido{1-[(2-hydroxyethyl)iminomethyl]-2-naphtholato}pyridineiron(III) pyridine monosolvate

Crystal data

$[Fe(C_{13}H_{12}NO_2)Cl_2(C_5H_5N)]\cdot C_5H_5N$
$M_r = 499.19$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 7.8590\ (6)$ Å
$b = 10.0153\ (11)$ Å
$c = 14.4884\ (16)$ Å
$\beta = 90.123\ (1)°$
$V = 1140.4\ (2)$ Å^3
$Z = 2$
$F(000) = 514$
$D_x = 1.454$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3504 reflections
$\theta = 2.5–28.0°$
$\mu = 0.92$ mm^{-1}
$T = 298$ K
Block, black
0.48 × 0.44 × 0.37 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Siemens, 1996)
$T_{min} = 0.666$, $T_{max} = 0.727$
5726 measured reflections
3395 independent reflections
3143 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.4°$
$h = -8\rightarrow9$
$k = -11\rightarrow8$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.085$
$S = 1.00$
3395 reflections
281 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.5289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Absolute structure: Flack (1983), 1265 Friedel pairs
Absolute structure parameter: 0.02 (2)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.54656 (5)	0.51232 (5)	0.28032 (3)	0.03179 (13)
Cl1	0.81839 (12)	0.59516 (12)	0.27394 (7)	0.0505 (3)
Cl2	0.61339 (13)	0.29636 (11)	0.33678 (7)	0.0486 (3)
N1	0.2862 (3)	0.4752 (3)	0.30300 (17)	0.0321 (7)
N2	0.4541 (4)	0.7190 (4)	0.2447 (2)	0.0386 (7)
N3	0.7698 (4)	0.5286 (4)	0.52783 (19)	0.0458 (8)
O1	0.5126 (3)	0.5757 (3)	0.41754 (15)	0.0374 (6)
H1	0.5968	0.5524	0.4469	0.056*
O2	0.5074 (3)	0.4537 (3)	0.15755 (16)	0.0386 (6)
C1	0.3621 (4)	0.5234 (5)	0.4608 (2)	0.0434 (9)
H1A	0.3330	0.5757	0.5149	0.052*
H1B	0.3798	0.4315	0.4796	0.052*
C2	0.2222 (4)	0.5320 (5)	0.3892 (2)	0.0409 (10)
H2A	0.1231	0.4827	0.4098	0.049*
H2B	0.1894	0.6244	0.3798	0.049*
C3	0.1855 (4)	0.4104 (4)	0.2498 (2)	0.0331 (8)
H3	0.0734	0.4006	0.2690	0.040*
C4	0.2316 (4)	0.3513 (4)	0.1627 (2)	0.0309 (8)
C5	0.3927 (4)	0.3731 (4)	0.1223 (2)	0.0334 (8)
C6	0.4347 (5)	0.3075 (5)	0.0381 (2)	0.0440 (10)
H6	0.5403	0.3227	0.0113	0.053*
C7	0.3239 (5)	0.2239 (5)	−0.0032 (2)	0.0505 (11)
H7	0.3564	0.1808	−0.0572	0.061*
C8	0.1613 (5)	0.1997 (4)	0.0327 (2)	0.0419 (10)
C9	0.1090 (5)	0.2669 (4)	0.1152 (2)	0.0330 (8)
C10	−0.0580 (5)	0.2445 (4)	0.1469 (3)	0.0431 (9)
H10	−0.0968	0.2911	0.1982	0.052*
C11	−0.1640 (6)	0.1561 (5)	0.1041 (3)	0.0566 (12)
H11	−0.2733	0.1426	0.1268	0.068*
C12	−0.1089 (6)	0.0855 (6)	0.0261 (3)	0.0632 (14)
H12	−0.1796	0.0221	−0.0011	0.076*
C13	0.0459 (6)	0.1095 (5)	−0.0094 (3)	0.0576 (12)
H13	0.0783	0.0656	−0.0631	0.069*
C14	0.3280 (5)	0.7367 (5)	0.1839 (3)	0.0496 (10)
H14	0.2786	0.6622	0.1565	0.060*
C15	0.2690 (7)	0.8615 (6)	0.1604 (3)	0.0659 (14)
H15	0.1814	0.8708	0.1177	0.079*
C16	0.3409 (7)	0.9727 (5)	0.2009 (4)	0.0731 (16)
H16	0.3043	1.0580	0.1851	0.088*
C17	0.4661 (7)	0.9548 (5)	0.2644 (4)	0.0635 (13)
H17	0.5147	1.0279	0.2940	0.076*
C18	0.5204 (5)	0.8271 (5)	0.2843 (3)	0.0509 (10)
H18	0.6071	0.8160	0.3274	0.061*
C19	0.8321 (6)	0.4104 (5)	0.5477 (3)	0.0588 (13)
H19	0.7821	0.3355	0.5211	0.071*

C20	0.9701 (7)	0.3926 (6)	0.6070 (4)	0.0650 (14)
H20	1.0113	0.3077	0.6200	0.078*
C21	1.0421 (5)	0.5014 (8)	0.6448 (3)	0.0656 (14)
H21	1.1334	0.4929	0.6852	0.079*
C22	0.9803 (7)	0.6227 (7)	0.6233 (4)	0.0805 (19)
H22	1.0306	0.6991	0.6476	0.097*
C23	0.8438 (7)	0.6334 (6)	0.5658 (4)	0.0663 (14)
H23	0.8009	0.7178	0.5527	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0295 (2)	0.0306 (3)	0.0353 (2)	0.0020 (2)	−0.00537 (16)	−0.0014 (2)
Cl1	0.0305 (4)	0.0524 (7)	0.0685 (6)	−0.0014 (4)	−0.0044 (4)	−0.0056 (5)
Cl2	0.0574 (6)	0.0332 (5)	0.0551 (6)	0.0102 (5)	−0.0071 (4)	0.0020 (4)
N1	0.0296 (14)	0.038 (2)	0.0290 (13)	0.0046 (12)	−0.0029 (11)	−0.0044 (12)
N2	0.0401 (17)	0.034 (2)	0.0420 (16)	0.0029 (15)	−0.0066 (13)	0.0025 (15)
N3	0.0476 (17)	0.046 (2)	0.0432 (16)	−0.0030 (18)	−0.0118 (13)	0.0028 (18)
O1	0.0377 (13)	0.0390 (16)	0.0354 (12)	0.0012 (11)	−0.0105 (10)	−0.0038 (11)
O2	0.0354 (13)	0.0449 (17)	0.0355 (12)	−0.0024 (11)	−0.0012 (10)	−0.0040 (11)
C1	0.0451 (18)	0.053 (3)	0.0323 (16)	0.001 (2)	0.0004 (13)	−0.005 (2)
C2	0.0336 (17)	0.051 (3)	0.0381 (17)	0.0047 (18)	−0.0013 (13)	−0.0170 (19)
C3	0.0307 (17)	0.032 (2)	0.0366 (18)	0.0043 (16)	−0.0019 (14)	0.0004 (16)
C4	0.0349 (18)	0.028 (2)	0.0294 (16)	0.0088 (15)	−0.0046 (14)	0.0009 (14)
C5	0.0358 (18)	0.033 (2)	0.0313 (17)	0.0065 (16)	−0.0076 (14)	0.0028 (15)
C6	0.0405 (19)	0.060 (3)	0.0319 (18)	0.006 (2)	0.0015 (15)	−0.0043 (19)
C7	0.060 (2)	0.060 (3)	0.0319 (19)	0.011 (2)	−0.0023 (17)	−0.014 (2)
C8	0.050 (2)	0.042 (3)	0.0339 (18)	0.002 (2)	−0.0114 (16)	−0.0019 (17)
C9	0.0387 (18)	0.029 (2)	0.0310 (16)	0.0043 (15)	−0.0086 (14)	−0.0003 (14)
C10	0.040 (2)	0.047 (3)	0.042 (2)	−0.0033 (18)	−0.0111 (16)	−0.0038 (18)
C11	0.049 (2)	0.066 (3)	0.056 (2)	−0.011 (2)	−0.016 (2)	0.001 (2)
C12	0.071 (3)	0.064 (3)	0.055 (3)	−0.020 (3)	−0.026 (2)	−0.010 (2)
C13	0.074 (3)	0.054 (3)	0.044 (2)	−0.002 (2)	−0.019 (2)	−0.018 (2)
C14	0.053 (2)	0.046 (3)	0.049 (2)	0.010 (2)	−0.0076 (19)	0.007 (2)
C15	0.070 (3)	0.069 (4)	0.058 (3)	0.027 (3)	−0.006 (2)	0.012 (3)
C16	0.094 (4)	0.047 (4)	0.078 (3)	0.028 (3)	0.015 (3)	0.021 (3)
C17	0.076 (3)	0.029 (2)	0.085 (3)	0.000 (2)	0.011 (3)	0.000 (2)
C18	0.051 (2)	0.037 (3)	0.065 (3)	−0.001 (2)	−0.0052 (19)	−0.001 (2)
C19	0.060 (3)	0.049 (3)	0.067 (3)	−0.008 (2)	−0.017 (2)	0.001 (2)
C20	0.063 (3)	0.058 (4)	0.074 (3)	0.005 (3)	−0.011 (2)	0.018 (3)
C21	0.042 (2)	0.099 (5)	0.056 (2)	0.012 (3)	−0.0130 (17)	−0.011 (3)
C22	0.061 (3)	0.091 (5)	0.089 (4)	−0.002 (3)	−0.021 (3)	−0.036 (4)
C23	0.066 (3)	0.049 (3)	0.084 (3)	0.009 (3)	−0.018 (3)	−0.012 (3)

Geometric parameters (Å, º)

Fe1—O2	1.897 (2)	C8—C13	1.417 (6)
Fe1—O1	2.105 (2)	C8—C9	1.433 (5)

Fe1—N1	2.106 (3)	C9—C10	1.409 (5)
Fe1—N2	2.254 (3)	C10—C11	1.364 (6)
Fe1—Cl1	2.2938 (10)	C10—H10	0.9300
Fe1—Cl2	2.3709 (12)	C11—C12	1.403 (7)
N1—C3	1.280 (4)	C11—H11	0.9300
N1—C2	1.462 (4)	C12—C13	1.344 (7)
N2—C18	1.331 (6)	C12—H12	0.9300
N2—C14	1.336 (5)	C13—H13	0.9300
N3—C19	1.312 (7)	C14—C15	1.375 (7)
N3—C23	1.319 (6)	C14—H14	0.9300
O1—C1	1.439 (4)	C15—C16	1.379 (8)
O1—H1	0.8200	C15—H15	0.9300
O2—C5	1.313 (4)	C16—C17	1.357 (7)
C1—C2	1.513 (4)	C16—H16	0.9300
C1—H1A	0.9700	C17—C18	1.379 (6)
C1—H1B	0.9700	C17—H17	0.9300
C2—H2A	0.9700	C18—H18	0.9300
C2—H2B	0.9700	C19—C20	1.393 (7)
C3—C4	1.440 (5)	C19—H19	0.9300
C3—H3	0.9300	C20—C21	1.344 (9)
C4—C5	1.414 (5)	C20—H20	0.9300
C4—C9	1.455 (5)	C21—C22	1.345 (9)
C5—C6	1.424 (5)	C21—H21	0.9300
C6—C7	1.348 (6)	C22—C23	1.361 (8)
C6—H6	0.9300	C22—H22	0.9300
C7—C8	1.402 (6)	C23—H23	0.9300
C7—H7	0.9300		

O2—Fe1—O1	163.37 (10)	C6—C7—H7	119.0
O2—Fe1—N1	86.33 (10)	C8—C7—H7	119.0
O1—Fe1—N1	77.32 (9)	C7—C8—C13	122.2 (4)
O2—Fe1—N2	91.01 (11)	C7—C8—C9	119.5 (3)
O1—Fe1—N2	84.14 (11)	C13—C8—C9	118.3 (4)
N1—Fe1—N2	83.39 (11)	C10—C9—C8	117.8 (3)
O2—Fe1—Cl1	102.90 (8)	C10—C9—C4	123.7 (3)
O1—Fe1—Cl1	92.81 (7)	C8—C9—C4	118.5 (3)
N1—Fe1—Cl1	167.24 (9)	C11—C10—C9	121.6 (4)
N2—Fe1—Cl1	87.61 (8)	C11—C10—H10	119.2
O2—Fe1—Cl2	94.40 (9)	C9—C10—H10	119.2
O1—Fe1—Cl2	88.73 (8)	C10—C11—C12	120.3 (4)
N1—Fe1—Cl2	90.00 (9)	C10—C11—H11	119.9
N2—Fe1—Cl2	171.18 (9)	C12—C11—H11	119.9
Cl1—Fe1—Cl2	97.95 (4)	C13—C12—C11	119.9 (4)
C3—N1—C2	119.9 (3)	C13—C12—H12	120.0
C3—N1—Fe1	126.5 (2)	C11—C12—H12	120.0
C2—N1—Fe1	113.6 (2)	C12—C13—C8	121.9 (4)
C18—N2—C14	117.8 (4)	C12—C13—H13	119.0
C18—N2—Fe1	121.5 (3)	C8—C13—H13	119.0

C14—N2—Fe1	120.7 (3)	N2—C14—C15	122.2 (5)
C19—N3—C23	117.5 (3)	N2—C14—H14	118.9
C1—O1—Fe1	114.1 (2)	C15—C14—H14	118.9
C1—O1—H1	109.5	C14—C15—C16	119.4 (4)
Fe1—O1—H1	107.4	C14—C15—H15	120.3
C5—O2—Fe1	131.7 (2)	C16—C15—H15	120.3
O1—C1—C2	106.1 (3)	C17—C16—C15	118.5 (5)
O1—C1—H1A	110.5	C17—C16—H16	120.7
C2—C1—H1A	110.5	C15—C16—H16	120.7
O1—C1—H1B	110.5	C16—C17—C18	119.2 (5)
C2—C1—H1B	110.5	C16—C17—H17	120.4
H1A—C1—H1B	108.7	C18—C17—H17	120.4
N1—C2—C1	108.3 (3)	N2—C18—C17	122.9 (4)
N1—C2—H2A	110.0	N2—C18—H18	118.6
C1—C2—H2A	110.0	C17—C18—H18	118.6
N1—C2—H2B	110.0	N3—C19—C20	122.7 (5)
C1—C2—H2B	110.0	N3—C19—H19	118.7
H2A—C2—H2B	108.4	C20—C19—H19	118.7
N1—C3—C4	125.4 (3)	C21—C20—C19	118.3 (5)
N1—C3—H3	117.3	C21—C20—H20	120.8
C4—C3—H3	117.3	C19—C20—H20	120.8
C5—C4—C3	121.8 (3)	C20—C21—C22	119.1 (4)
C5—C4—C9	119.1 (3)	C20—C21—H21	120.5
C3—C4—C9	119.1 (3)	C22—C21—H21	120.5
O2—C5—C4	123.2 (3)	C21—C22—C23	119.8 (6)
O2—C5—C6	117.2 (3)	C21—C22—H22	120.1
C4—C5—C6	119.6 (3)	C23—C22—H22	120.1
C7—C6—C5	121.1 (4)	N3—C23—C22	122.6 (5)
C7—C6—H6	119.5	N3—C23—H23	118.7
C5—C6—H6	119.5	C22—C23—H23	118.7
C6—C7—C8	122.1 (4)		

O2—Fe1—N1—C3	12.9 (3)	C3—C4—C5—O2	−4.1 (5)
O1—Fe1—N1—C3	−170.2 (3)	C9—C4—C5—O2	176.0 (3)
N2—Fe1—N1—C3	104.4 (3)	C3—C4—C5—C6	177.2 (3)
Cl1—Fe1—N1—C3	149.8 (3)	C9—C4—C5—C6	−2.8 (5)
Cl2—Fe1—N1—C3	−81.5 (3)	O2—C5—C6—C7	−179.5 (4)
O2—Fe1—N1—C2	−167.0 (3)	C4—C5—C6—C7	−0.7 (6)
O1—Fe1—N1—C2	9.8 (2)	C5—C6—C7—C8	1.7 (7)
N2—Fe1—N1—C2	−75.6 (3)	C6—C7—C8—C13	−178.5 (4)
Cl1—Fe1—N1—C2	−30.2 (5)	C6—C7—C8—C9	0.8 (7)
Cl2—Fe1—N1—C2	98.5 (3)	C7—C8—C9—C10	177.3 (4)
O2—Fe1—N2—C18	−146.3 (3)	C13—C8—C9—C10	−3.4 (5)
O1—Fe1—N2—C18	49.6 (3)	C7—C8—C9—C4	−4.2 (5)
N1—Fe1—N2—C18	127.5 (3)	C13—C8—C9—C4	175.1 (4)
Cl1—Fe1—N2—C18	−43.5 (3)	C5—C4—C9—C10	−176.5 (3)
O2—Fe1—N2—C14	34.9 (3)	C3—C4—C9—C10	3.6 (5)
O1—Fe1—N2—C14	−129.1 (3)	C5—C4—C9—C8	5.1 (5)

N1—Fe1—N2—C14	−51.3 (3)	C3—C4—C9—C8	−174.8 (3)
Cl1—Fe1—N2—C14	137.8 (3)	C8—C9—C10—C11	3.8 (6)
O2—Fe1—O1—C1	29.9 (5)	C4—C9—C10—C11	−174.6 (4)
N1—Fe1—O1—C1	19.0 (3)	C9—C10—C11—C12	−0.6 (7)
N2—Fe1—O1—C1	103.5 (3)	C10—C11—C12—C13	−3.2 (8)
Cl1—Fe1—O1—C1	−169.2 (3)	C11—C12—C13—C8	3.5 (8)
Cl2—Fe1—O1—C1	−71.3 (3)	C7—C8—C13—C12	179.1 (5)
O1—Fe1—O2—C5	−36.4 (6)	C9—C8—C13—C12	−0.2 (7)
N1—Fe1—O2—C5	−25.7 (3)	C18—N2—C14—C15	1.4 (6)
N2—Fe1—O2—C5	−109.0 (3)	Fe1—N2—C14—C15	−179.8 (3)
Cl1—Fe1—O2—C5	163.2 (3)	N2—C14—C15—C16	−0.3 (7)
Cl2—Fe1—O2—C5	64.0 (3)	C14—C15—C16—C17	−1.3 (8)
Fe1—O1—C1—C2	−42.2 (4)	C15—C16—C17—C18	1.8 (8)
C3—N1—C2—C1	145.1 (4)	C14—N2—C18—C17	−0.9 (6)
Fe1—N1—C2—C1	−34.9 (4)	Fe1—N2—C18—C17	−179.7 (3)
O1—C1—C2—N1	48.7 (5)	C16—C17—C18—N2	−0.7 (7)
C2—N1—C3—C4	179.1 (4)	C23—N3—C19—C20	0.5 (7)
Fe1—N1—C3—C4	−0.9 (5)	N3—C19—C20—C21	−0.3 (8)
N1—C3—C4—C5	−7.3 (6)	C19—C20—C21—C22	−0.8 (7)
N1—C3—C4—C9	172.6 (4)	C20—C21—C22—C23	1.7 (8)
Fe1—O2—C5—C4	25.9 (5)	C19—N3—C23—C22	0.3 (8)
Fe1—O2—C5—C6	−155.4 (3)	C21—C22—C23—N3	−1.5 (10)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C4–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N3	0.82	1.81	2.617 (4)	168
C12—H12···*Cg*^{i}	0.93	2.71	3.594 (5)	159
C16—H16···*Cg*^{ii}	0.93	2.78	3.653 (6)	157

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