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Bis[(*E*)-4-chloro-2-(2-furylmethyliminomethyl)phenolato]iron(II)

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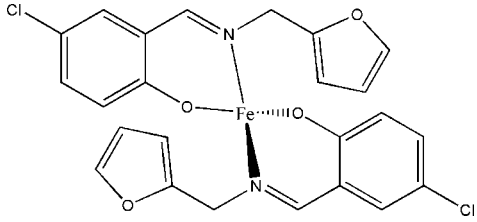
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.021 Å; R factor = 0.061; wR factor = 0.203; data-to-parameter ratio = 8.4.

The Fe atom of the title compound, $[Fe(C_{12}H_9ClNO_2)_2]$, lies on a crystallographic twofold rotation axis. The Fe^{II} atom is four-coordinated in a tetrahedral geometry by the O and N atoms of the two Schiff base ligands. The O atom of the furan substituent in the ligand unit is not involved in coordination to the Fe atom.

Related literature

For related structures, see: Chen & Wang (2006); Chen *et al.* (2007); Ran *et al.* (2006); Ye *et al.* (2007); Zhu *et al.* (2003).



Experimental

Crystal data

$[Fe(C_{12}H_9ClNO_2)_2]$
M_r = 525.15
Monoclinic, $C2$
a = 22.550 (4) Å
b = 4.6270 (6) Å
c = 13.822 (3) Å
β = 127.73 (3)°
V = 1140.6 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 298 (2) K
0.21 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.829, T_{max} = 0.836
1314 measured reflections
1262 independent reflections
973 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.203
S = 1.06
1262 reflections
151 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983), with no Friedel pairs
Flack parameter: −0.02 (9)

Table 1
Selected geometric parameters (Å, °).

Fe1—O1	1.888 (8)	Fe1—N1	1.992 (8)
O1—Fe1—O1^{i}	124.0 (6)	O1—Fe1—N1^{i}	113.5 (3)
O1—Fe1—N1	95.2 (3)	N1—Fe1—N1^{i}	117.3 (5)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: SJ2505).

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supporting information

Acta Cryst. (2008). E**64**, m844 [doi:10.1107/S1600536808015559]

Bis[(*E*)-4-chloro-2-(2-furylmethyliminomethyl)phenolato]iron(II)

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S1. Comment

As part of our ongoing interest in the structure of iron complexes (Zhu *et al.*, 2003), we report herein the crystal structure of the title compound, a new mononuclear iron(II) complex, (I), Fig. 1, derived from the Schiff base ligand 4-chloro-2-[(furan-2-ylmethylimino)methyl]phenol.

Compound (I) possesses crystallographic two-fold symmetry. The Fe^{II} atom in (I) is four-coordinate in a tetrahedral geometry, binding to the O and N atoms of two Schiff base ligands. The O atom of the furan substituent in the ligand lies well away from the coordination sphere of the Fe atom. The coordinate bond values (Table 1) are comparable to values observed in other iron(II) complexes (Chen & Wang, 2006; Chen *et al.*, 2007; Ran *et al.*, 2006; Ye *et al.*, 2007).

S2. Experimental

5-Chlorosalicylaldehyde (62.4 mg, 0.2 mmol), furan-2-ylmethylamine (19.4 mg, 0.2 mmol), and $FeCl_2$ (12.6 mg, 0.1 mmol) were dissolved in methanol (30 ml). The mixture was stirred for 30 min at room temperature. The resulting solution was kept still in air for a few days, yielding brown crystals.

S3. Refinement

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) set at 1.2U_{eq}(C).

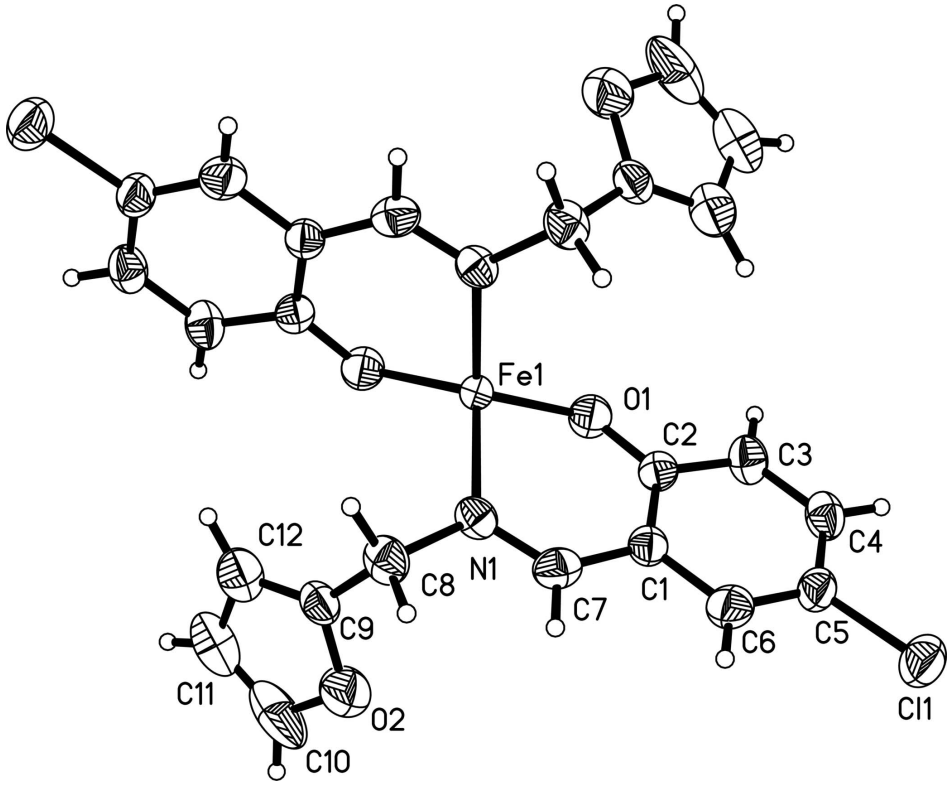

Figure 1

The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. Numbered atoms are related to un-numbered atoms by the symmetry code 1-x, y, 1-z.

Bis[(E)-4-chloro-2-(2-furylmethyliminomethyl)phenolato]iron(II)

Crystal data

$[Fe(C_{12}H_9ClNO_2)_2]$
$M_r = 525.15$
Monoclinic, *C*2
Hall symbol: C 2y
$a = 22.550\ (4)$ Å
$b = 4.6270\ (6)$ Å
$c = 13.822\ (3)$ Å
$\beta = 127.73\ (3)°$
$V = 1140.6\ (4)$ Å^3
$Z = 2$
$F(000) = 536$
$D_x = 1.529$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 823 reflections
$\theta = 2.4–26.2°$
$\mu = 0.93$ mm^{-1}
$T = 298$ K
Block, brown
0.21 × 0.21 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.829$, $T_{max} = 0.836$
1314 measured reflections
1262 independent reflections
973 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
$h = -21\rightarrow27$
$k = -5\rightarrow0$
$l = -17\rightarrow0$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.203$
$S = 1.06$
1262 reflections
151 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
$w = 1/[\sigma^2(F_o^2) + (0.1149P)^2 + 2.2051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.011 (3)
Absolute structure: Flack (1983), 0 Friedel pairs
Absolute structure parameter: −0.02 (9)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.5000	0.5044 (3)	0.5000	0.0419 (6)
Cl1	0.87863 (17)	0.7649 (11)	1.0179 (3)	0.0929 (13)
N1	0.5246 (5)	0.728 (2)	0.6435 (8)	0.055 (2)
O1	0.5933 (4)	0.313 (2)	0.5865 (7)	0.067 (2)
O2	0.4619 (6)	0.600 (3)	0.7844 (9)	0.102 (4)
C1	0.6584 (5)	0.630 (3)	0.7611 (9)	0.053 (2)
C2	0.6554 (5)	0.419 (2)	0.6848 (9)	0.053 (3)
C3	0.7253 (6)	0.309 (3)	0.7192 (11)	0.069 (3)
H3	0.7250	0.1686	0.6709	0.083*
C4	0.7929 (6)	0.406 (3)	0.8218 (11)	0.068 (3)
H4	0.8377	0.3317	0.8429	0.081*
C5	0.7933 (6)	0.620 (3)	0.8943 (10)	0.065 (3)
C6	0.7284 (6)	0.737 (3)	0.8663 (10)	0.070 (3)
H6	0.7300	0.8824	0.9145	0.084*
C7	0.5937 (6)	0.759 (3)	0.7390 (10)	0.066 (3)
H7	0.6021	0.8786	0.8003	0.079*
C8	0.4677 (6)	0.890 (3)	0.6455 (11)	0.067 (3)
H8A	0.4926	1.0336	0.7100	0.080*
H8B	0.4329	0.9882	0.5681	0.080*
C9	0.4259 (6)	0.683 (3)	0.6671 (10)	0.061 (3)
C10	0.4146 (12)	0.427 (6)	0.786 (2)	0.137 (10)
H10	0.4242	0.3498	0.8560	0.164*

C11	0.3509 (10)	0.381 (4)	0.6710 (18)	0.105 (6)
H11	0.3109	0.2606	0.6466	0.126*
C12	0.3594 (7)	0.555 (4)	0.5982 (13)	0.087 (5)
H12	0.3238	0.5781	0.5141	0.104*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0384 (9)	0.0462 (11)	0.0399 (9)	0.000	0.0233 (7)	0.000
Cl1	0.0661 (17)	0.122 (3)	0.0664 (18)	−0.012 (2)	0.0279 (15)	0.017 (2)
N1	0.062 (5)	0.047 (5)	0.065 (5)	0.000 (5)	0.044 (4)	−0.005 (4)
O1	0.065 (4)	0.068 (6)	0.066 (4)	−0.001 (4)	0.040 (4)	−0.017 (4)
O2	0.093 (6)	0.136 (12)	0.089 (6)	0.016 (7)	0.062 (5)	0.022 (7)
C1	0.052 (5)	0.054 (6)	0.053 (5)	0.001 (5)	0.032 (5)	0.006 (5)
C2	0.053 (5)	0.050 (8)	0.053 (5)	0.005 (5)	0.031 (5)	0.009 (5)
C3	0.061 (6)	0.062 (8)	0.088 (8)	−0.007 (6)	0.048 (6)	−0.008 (7)
C4	0.056 (6)	0.070 (9)	0.081 (7)	0.012 (6)	0.043 (6)	0.019 (7)
C5	0.048 (6)	0.081 (9)	0.055 (6)	0.001 (6)	0.026 (5)	0.013 (6)
C6	0.071 (7)	0.077 (9)	0.059 (6)	−0.001 (7)	0.038 (6)	0.010 (7)
C7	0.074 (7)	0.067 (8)	0.054 (6)	−0.004 (7)	0.038 (6)	0.002 (6)
C8	0.070 (7)	0.059 (7)	0.079 (7)	0.019 (6)	0.049 (6)	0.009 (6)
C9	0.061 (6)	0.067 (8)	0.070 (7)	0.011 (6)	0.048 (6)	0.005 (6)
C10	0.161 (17)	0.15 (3)	0.199 (19)	0.037 (18)	0.158 (17)	0.06 (2)
C11	0.112 (12)	0.085 (11)	0.167 (17)	0.000 (11)	0.110 (13)	−0.004 (13)
C12	0.080 (8)	0.088 (14)	0.102 (9)	−0.001 (9)	0.061 (8)	−0.007 (9)

Geometric parameters (Å, º)

Fe1—O1	1.888 (8)	C3—H3	0.9300
Fe1—O1^{i}	1.888 (8)	C4—C5	1.402 (17)
Fe1—N1	1.992 (8)	C4—H4	0.9300
Fe1—N1^{i}	1.992 (8)	C5—C6	1.377 (16)
Cl1—C5	1.746 (12)	C6—H6	0.9300
N1—C7	1.294 (13)	C7—H7	0.9300
N1—C8	1.499 (12)	C8—C9	1.493 (16)
O1—C2	1.310 (12)	C8—H8A	0.9700
O2—C10	1.34 (2)	C8—H8B	0.9700
O2—C9	1.352 (14)	C9—C12	1.328 (18)
C1—C2	1.411 (14)	C10—C11	1.35 (2)
C1—C7	1.424 (15)	C10—H10	0.9300
C1—C6	1.429 (15)	C11—C12	1.39 (2)
C2—C3	1.431 (15)	C11—H11	0.9300
C3—C4	1.374 (16)	C12—H12	0.9300
O1—Fe1—O1^{i}	124.0 (6)	C4—C5—Cl1	119.4 (9)
O1—Fe1—N1	95.2 (3)	C5—C6—C1	118.1 (13)
O1^{i}—Fe1—N1	113.5 (3)	C5—C6—H6	121.0
O1—Fe1—N1^{i}	113.5 (3)	C1—C6—H6	121.0

O1^{i}—Fe1—N1^{i}	95.2 (3)	N1—C7—C1	127.6 (11)
N1—Fe1—N1^{i}	117.3 (5)	N1—C7—H7	116.2
C7—N1—C8	115.9 (9)	C1—C7—H7	116.2
C7—N1—Fe1	120.0 (8)	C9—C8—N1	109.7 (10)
C8—N1—Fe1	123.9 (7)	C9—C8—H8A	109.7
C2—O1—Fe1	123.4 (7)	N1—C8—H8A	109.7
C10—O2—C9	106.7 (14)	C9—C8—H8B	109.7
C2—C1—C7	123.7 (10)	N1—C8—H8B	109.7
C2—C1—C6	121.3 (10)	H8A—C8—H8B	108.2
C7—C1—C6	115.0 (11)	C12—C9—O2	108.5 (12)
O1—C2—C1	124.5 (9)	C12—C9—C8	135.8 (12)
O1—C2—C3	118.3 (10)	O2—C9—C8	115.7 (11)
C1—C2—C3	117.3 (9)	O2—C10—C11	111.3 (16)
C4—C3—C2	121.8 (12)	O2—C10—H10	124.4
C4—C3—H3	119.1	C11—C10—H10	124.4
C2—C3—H3	119.1	C10—C11—C12	103.7 (16)
C3—C4—C5	119.1 (10)	C10—C11—H11	128.2
C3—C4—H4	120.5	C12—C11—H11	128.2
C5—C4—H4	120.5	C9—C12—C11	109.7 (14)
C6—C5—C4	122.4 (11)	C9—C12—H12	125.2
C6—C5—Cl1	117.9 (11)	C11—C12—H12	125.2

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