metal-organic compounds

[2,2'-(2,6,9,13-Tetraazatetradeca-1,13-diene-1,14-diyl)diphenolato]iron(III) chloride

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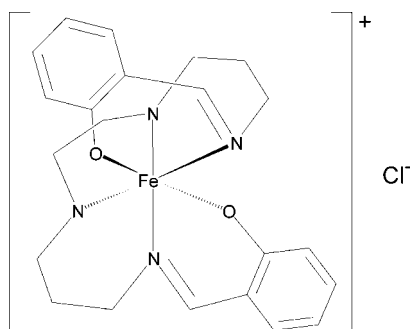Correspondence e-mail: rbutcher99@yahoo.com

The structure of the title compound, [Fe(C$_{22}$H$_{28}$N$_4$O$_2$)]Cl {also known as [N,N'-bis[3-(salicylideneamino)propyl]ethane-1,2-diamine]iron(III) chloride}, has crystallographic symmetry with both the Fe and Cl atoms lying on twofold axes. The structure adopts a conformation where the phenolate O atoms are *trans*. The geometry about the Fe center is distorted octahedral due to the restrictions imposed by the bite angles of the chelate rings. The structure displays N—H$\cdots$Cl hydrogen bonding.

Related literature

For related literature, see: Bera *et al.* (2005); Boinnard *et al.* (1994); Das Sarma & Bailar (1955); Dorbes *et al.* (2005); Dwyer & Lions (1947); Floquet *et al.* (2004); Gultneh *et al.* (2006); Harpstrite *et al.* (2003); Hayami *et al.* (1997); Ito *et al.* (1983); Maeda *et al.* (1991); McPartlin *et al.* (1978); Nishida *et al.* (1987); Salmon *et al.* (1999); Sinn *et al.* (1978); Yisgedu *et al.* (2007); Butcher *et al.* (2007); Zhu *et al.* (2002).

Experimental

Crystal data

[Fe(C$_{22}$H$_{28}$N$_4$O$_2$)]Cl	V = 2144.2 (7) Å^3
M_r = 471.78	Z = 4
Orthorhombic, $Pccn$	Mo $K\alpha$ radiation
a = 7.5156 (15) Å	μ = 0.86 mm^{-1}
b = 16.161 (3) Å	T = 293 (2) K
c = 17.654 (4) Å	0.47 × 0.35 × 0.27 mm

Data collection

Bruker P4 diffractometer	1873 independent reflections
Absorption correction: ψ scans	1284 reflections with $I > 2\sigma(I)$
(North *et al.*, 1968)	3 standard reflections
T_{min} = 0.576, T_{max} = 0.731	every 97 reflections
(expected range = 0.626–0.794)	intensity decay: none
1873 measured reflections	

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040	154 parameters
$wR(F^2)$ = 0.114	H-atom parameters constrained
S = 1.05	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
1873 reflections	$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe—O1	1.882 (2)	Fe—N2	2.018 (3)
Fe—N1	1.957 (3)		
O1—Fe—O1^i	174.73 (15)	N1—Fe—N2^i	173.15 (13)
O1—Fe—N1	89.62 (12)	O1—Fe—N2	91.18 (12)
O1^i—Fe—N1	93.97 (12)	N1—Fe—N2	90.19 (13)
N1—Fe—N1^i	94.36 (17)	N2^i—Fe—N2	85.8 (2)
O1—Fe—N2^i	84.96 (12)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots$A	D—H	H$\cdots$A	$D\cdots$A	D—H$\cdots$A
N2—H2N$\cdots$Cl	0.75 (4)	2.70 (4)	3.241 (3)	131 (4)

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2016).

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supplementary materials

[2,2'-(2,6,9,13-Tetraazatetradeca-1,13-diene-1,14-diyl)diphenolato]iron(III) chloride

R. J. Butcher, M. Pourian and J. P. Jasinski

Comment

Metal complexes of linear hexadentate ligands have fascinated inorganic chemists since their first report in 1947 (Dwyer & Lions, 1947). The first such report of a Fe complex of a linear FeN_4O_2 ligand (*i.e.* a ligand in which all the N and O donor atoms are linked in a straight chain with no branching) derived from the Schiff base condensation of salicylaldehyde and triethylenetetraamine was in 1955 (Das Sarma & Bailar, 1955). However, this interest lapsed for several years until the discovery that such complexes exhibited spin-crossover magnetic behavior (Sinn *et al.*, 1978). Hexadentate linear FeN_4O_2 ligands derived from the Schiff base condensation of salicylaldehyde and linear tetramines can be characterized by the number of linking carbon atoms in the tetramine backbone (see Scheme 1). The structures of Fe complexes of Sal222 (Sinn *et al.*, 1978; Hayami *et al.*, 1997; Floquet *et al.*, 2004; Dorbes *et al.*, 2005; Bera *et al.*, 2005; Nishida *et al.*, 1987; Salmon *et al.*, 1999; McPartlin *et al.*, 1978; Maeda *et al.*, 1991; Boinnard *et al.*, 1994), Sal232 (Hayami *et al.*, 1997), Sal323 (Hayami *et al.*, 1997; Ito *et al.*, 1983), and Sal333 (Ito *et al.*, 1983) have been reported. When chelating to Fe, as the number of carbon atoms in the tetramine backbone increases from 6 to 9, the conformation adopted by the ligand changes from a *cis*-FeN_4O_2 to a *trans*-FeN_4O_2 arrangement for the phenolic O donors. All structurally characterized Fe complexes with Sal222 have adopted the *cis*-FeN_4O_2 conformation while all those with either Sal323 or Sal333 have adopted the *trans*-FeN_4O_2 conformation. Further, it has been observed that the angles subtended at the Fe center reflect the magnetic properties of the compound (Hayami *et al.*, 1997; Nishida *et al.*, 1987) with low-spin compounds having angles closer to 90° and 180°. While several structures containing the 323 backbone have been structurally characterized, there is no report of a structure containing a chloride anion. There is a report of an isomorphous and isostructural Mn derivative (Zhu *et al.*, 2002).

In the structure of I both the Fe of the cation and Cl anion lie on crystallographic 2 fold axes. The cation has adopted a conformation in which the phenolic O donors are *trans* to each other. The *cis* and *trans* bond angles subtended at the Fe center range from 84.96 (12) to 94.36 (17)° and 173.15 (13) to 174.73 (15)° respectively, indicating that the Fe is low spin. The Fe—O (1.882 (2) Å) and Fe—N bond lengths [1.957 (3)and 2.018 (3) Å] also reflect this.

Experimental

To 4.0 g (20 mmol) of 1,5,8,12-tetraazadodecane in 15 ml of ethanol was added 6.0 g (40 mmol) of salicylaldehyde in 10 ml of ethanol drop-wise. The deep yellow solution was left to stir for half an hour and a crystalline product resulted (H~2~*L*). To 0.85 g of H~2~*L* dissolved in 10.0 ml of methanol was added 0.58 g of $FeCl_3.xH2O$. The solution became violet and a red-purple solid precipitated. This was stirred overnight, the solid filtered, washed with methanol and dried. Crystallization was effected by slow evaporation of a DMF solution of the complex.

Refinement

The H atoms were idealized with C—H distances of 0.93 (aromatic C—H), and 0.97 (CH~2~) \%A and Uĩso~(H) = 1.2U~eq~(C). The amine H atoms were refined isotropically.
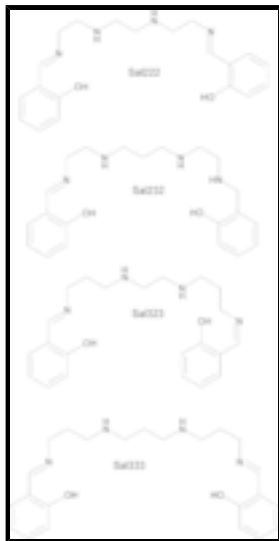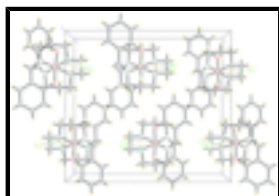
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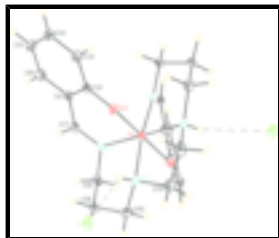
Fig. 1. The cation with numbering scheme used. Ellipsoids are drawn at the 20% probabilty level.

Fig. 2. The packing arrangement viewed down the *a* axis showing the N—H···Cl hydrogen bonding interactions.

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Crystal data

$[Fe(C_{22}H_{28}N_4O_2)]Cl$	$D_x = 1.461$ Mg m^{-3}
$M_r = 471.78$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Orthorhombic, *Pccn*	Cell parameters from 52 reflections
$a = 7.5156 (15)$ Å	$\theta = 2.5–27.6º$
$b = 16.161 (3)$ Å	$\mu = 0.86$ mm^{-1}
$c = 17.654 (4)$ Å	$T = 293 (2)$ K
$V = 2144.2 (7)$ Å^3	Prism, black
$Z = 4$	$0.47 \times 0.35 \times 0.27$ mm
$F_{000} = 988$	

Data collection

Bruker P4 diffractometer	$R_{int} = 0.0000$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.0°$
Monochromator: graphite	$\theta_{min} = 2.3°$
$T = 293(2)$ K	$h = 0 \rightarrow 8$
ω scans	$k = 0 \rightarrow 19$
Absorption correction: ψ scans (North *et al.*, 1968)	$l = 0 \rightarrow 20$
$T_{min} = 0.576$, $T_{max} = 0.731$	3 standard reflections
1873 measured reflections	every 97 reflections
1873 independent reflections	intensity decay: none
1284 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H-atom parameters constrained
$wR(F^2) = 0.114$	$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 2.7631P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
1873 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 > 2sigma(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	$U_{iso}*/U_{eq}$
Fe	0.2500	0.2500	0.45616 (4)	0.0252 (2)
Cl	−0.2500	0.2500	0.64500 (8)	0.0477 (4)
O1	0.1430 (3)	0.35514 (14)	0.46105 (14)	0.0328 (6)

N1	0.0734 (4)	0.21620 (19)	0.38082 (17)	0.0290 (7)
N2	0.0916 (4)	0.2076 (2)	0.53991 (19)	0.0321 (8)
H2N	0.018 (5)	0.239 (3)	0.543 (2)	0.036 (12)*
C1	0.0179 (5)	0.3553 (2)	0.3355 (2)	0.0306 (8)
C2	0.0830 (5)	0.3955 (2)	0.4010 (2)	0.0304 (9)
C3	0.0817 (5)	0.4824 (2)	0.4026 (3)	0.0387 (10)
H3A	0.1254	0.5100	0.4450	0.027 (10)*
C4	0.0173 (6)	0.5272 (3)	0.3428 (3)	0.0458 (11)
H4A	0.0212	0.5847	0.3443	0.053 (13)*
C5	−0.0538 (6)	0.4877 (3)	0.2800 (3)	0.0500 (12)
H5A	−0.1004	0.5185	0.2402	0.073 (16)*
C6	−0.0553 (6)	0.4032 (3)	0.2768 (2)	0.0426 (10)
H6A	−0.1055	0.3769	0.2351	0.039 (11)*
C7	−0.0010 (5)	0.2664 (2)	0.3343 (2)	0.0314 (9)
H7A	−0.0729	0.2437	0.2968	0.032 (9)*
C8	−0.0042 (5)	0.1322 (2)	0.3848 (2)	0.0365 (10)
H8A	0.0898	0.0912	0.3824	0.034 (11)*
H8B	−0.0833	0.1235	0.3422	0.034 (11)*
C9	−0.1069 (5)	0.1228 (2)	0.4585 (2)	0.0436 (11)
H9A	−0.1953	0.1664	0.4614	0.042 (11)*
H9B	−0.1697	0.0703	0.4575	0.051 (12)*
C10	0.0070 (6)	0.1259 (2)	0.5292 (2)	0.0420 (10)
H10A	−0.0664	0.1135	0.5730	0.072 (16)*
H10B	0.0987	0.0838	0.5259	0.048 (12)*
C11	0.1977 (5)	0.2105 (3)	0.6102 (2)	0.0455 (11)
H11A	0.2777	0.1634	0.6124	0.063 (14)*
H11B	0.1199	0.2085	0.6540	0.057 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe	0.0230 (3)	0.0250 (3)	0.0277 (4)	0.0014 (3)	0.000	0.000
Cl	0.0391 (7)	0.0573 (9)	0.0468 (8)	0.0180 (8)	0.000	0.000
O1	0.0354 (15)	0.0276 (13)	0.0353 (15)	0.0095 (11)	−0.0071 (12)	−0.0031 (11)
N1	0.0256 (17)	0.0286 (15)	0.0327 (17)	−0.0019 (13)	0.0018 (14)	−0.0032 (13)
N2	0.0294 (18)	0.0321 (18)	0.0349 (19)	0.0075 (15)	0.0068 (15)	0.0045 (15)
C1	0.025 (2)	0.037 (2)	0.030 (2)	0.0020 (17)	0.0002 (16)	0.0018 (16)
C2	0.022 (2)	0.030 (2)	0.039 (2)	0.0037 (16)	0.0028 (16)	−0.0007 (17)
C3	0.035 (2)	0.028 (2)	0.053 (3)	0.0043 (18)	0.000 (2)	−0.0046 (19)
C4	0.039 (2)	0.034 (2)	0.064 (3)	0.0079 (19)	0.007 (2)	0.011 (2)
C5	0.047 (3)	0.050 (3)	0.053 (3)	0.008 (2)	0.001 (2)	0.023 (2)
C6	0.036 (2)	0.059 (3)	0.033 (2)	0.001 (2)	0.0002 (19)	0.005 (2)
C7	0.0231 (17)	0.044 (2)	0.0272 (18)	0.0008 (16)	−0.0020 (16)	−0.0080 (17)
C8	0.028 (2)	0.034 (2)	0.047 (2)	−0.0030 (17)	−0.0037 (18)	−0.0104 (18)
C9	0.032 (2)	0.030 (2)	0.069 (3)	−0.0091 (17)	0.011 (2)	−0.005 (2)
C10	0.045 (2)	0.031 (2)	0.049 (3)	0.0005 (19)	0.014 (2)	0.0071 (19)
C11	0.035 (2)	0.075 (3)	0.027 (2)	0.011 (2)	0.0061 (17)	0.0108 (19)

Geometric parameters (Å, °)

Fe—O1	1.882 (2)	C4—C5	1.387 (6)
Fe—O1^i	1.882 (2)	C4—H4A	0.9300
Fe—N1	1.957 (3)	C5—C6	1.367 (6)
Fe—N1^i	1.957 (3)	C5—H5A	0.9300
Fe—N2^i	2.018 (3)	C6—H6A	0.9300
Fe—N2	2.018 (3)	C7—H7A	0.9300
O1—C2	1.323 (4)	C8—C9	1.520 (5)
N1—C7	1.283 (5)	C8—H8A	0.9700
N1—C8	1.479 (5)	C8—H8B	0.9700
N2—C11	1.476 (5)	C9—C10	1.515 (6)
N2—C10	1.478 (5)	C9—H9A	0.9700
N2—H2N	0.75 (4)	C9—H9B	0.9700
C1—C6	1.406 (5)	C10—H10A	0.9700
C1—C2	1.414 (5)	C10—H10B	0.9700
C1—C7	1.443 (5)	C11—C11^i	1.500 (9)
C2—C3	1.406 (5)	C11—H11A	0.9700
C3—C4	1.369 (6)	C11—H11B	0.9700
C3—H3A	0.9300		
O1—Fe—O1^i	174.73 (15)	C3—C4—H4A	119.7
O1—Fe—N1	89.62 (12)	C5—C4—H4A	119.7
O1^i—Fe—N1	93.97 (12)	C6—C5—C4	119.8 (4)
O1—Fe—N1^i	93.97 (12)	C6—C5—H5A	120.1
O1^i—Fe—N1^i	89.62 (12)	C4—C5—H5A	120.1
N1—Fe—N1^i	94.36 (17)	C5—C6—C1	121.1 (4)
O1—Fe—N2^i	84.96 (12)	C5—C6—H6A	119.5
O1^i—Fe—N2^i	91.18 (12)	C1—C6—H6A	119.5
N1—Fe—N2^i	173.15 (13)	N1—C7—C1	125.2 (3)
N1^i—Fe—N2^i	90.19 (13)	N1—C7—H7A	117.4
O1—Fe—N2	91.18 (12)	C1—C7—H7A	117.4
O1^i—Fe—N2	84.96 (12)	N1—C8—C9	109.5 (3)
N1—Fe—N2	90.19 (13)	N1—C8—H8A	109.8
N1^i—Fe—N2	173.15 (13)	C9—C8—H8A	109.8
N2^i—Fe—N2	85.8 (2)	N1—C8—H8B	109.8
C2—O1—Fe	123.6 (2)	C9—C8—H8B	109.8
C7—N1—C8	116.1 (3)	H8A—C8—H8B	108.2
C7—N1—Fe	123.7 (3)	C10—C9—C8	114.5 (3)
C8—N1—Fe	119.4 (2)	C10—C9—H9A	108.6
C11—N2—C10	111.6 (3)	C8—C9—H9A	108.6
C11—N2—Fe	106.7 (2)	C10—C9—H9B	108.6
C10—N2—Fe	117.6 (3)	C8—C9—H9B	108.6
C11—N2—H2N	108 (3)	H9A—C9—H9B	107.6
C10—N2—H2N	107 (3)	N2—C10—C9	112.2 (3)
Fe—N2—H2N	106 (3)	N2—C10—H10A	109.2

C6—C1—C2	119.1 (4)	C9—C10—H10A	109.2
C6—C1—C7	119.8 (4)	N2—C10—H10B	109.2
C2—C1—C7	120.2 (3)	C9—C10—H10B	109.2
O1—C2—C3	118.6 (3)	H10A—C10—H10B	107.9
O1—C2—C1	123.1 (3)	N2—C11—C11^i	108.0 (3)
C3—C2—C1	118.2 (4)	N2—C11—H11A	110.1
C4—C3—C2	121.0 (4)	C11^i—C11—H11A	110.1
C4—C3—H3A	119.5	N2—C11—H11B	110.1
C2—C3—H3A	119.5	C11^i—C11—H11B	110.1
C3—C4—C5	120.6 (4)	H11A—C11—H11B	108.4
O1^i—Fe—O1—C2	−173.3 (3)	Fe—O1—C2—C3	−151.3 (3)
N1—Fe—O1—C2	−40.4 (3)	Fe—O1—C2—C1	29.5 (5)
N1^i—Fe—O1—C2	53.9 (3)	C6—C1—C2—O1	175.3 (3)
N2^i—Fe—O1—C2	143.8 (3)	C7—C1—C2—O1	5.7 (5)
N2—Fe—O1—C2	−130.6 (3)	C6—C1—C2—C3	−3.9 (5)
O1—Fe—N1—C7	29.5 (3)	C7—C1—C2—C3	−173.4 (4)
O1^i—Fe—N1—C7	−154.4 (3)	O1—C2—C3—C4	−178.4 (4)
N1^i—Fe—N1—C7	−64.4 (3)	C1—C2—C3—C4	0.8 (6)
N2^i—Fe—N1—C7	67.0 (12)	C2—C3—C4—C5	2.1 (6)
N2—Fe—N1—C7	120.7 (3)	C3—C4—C5—C6	−1.8 (7)
O1—Fe—N1—C8	−139.4 (3)	C4—C5—C6—C1	−1.4 (7)
O1^i—Fe—N1—C8	36.8 (3)	C2—C1—C6—C5	4.3 (6)
N1^i—Fe—N1—C8	126.7 (3)	C7—C1—C6—C5	173.9 (4)
N2^i—Fe—N1—C8	−101.8 (11)	C8—N1—C7—C1	162.0 (4)
N2—Fe—N1—C8	−48.2 (3)	Fe—N1—C7—C1	−7.2 (5)
O1—Fe—N2—C11	−99.5 (3)	C6—C1—C7—N1	173.4 (4)
O1^i—Fe—N2—C11	76.9 (3)	C2—C1—C7—N1	−17.1 (6)
N1—Fe—N2—C11	170.9 (3)	C7—N1—C8—C9	−106.7 (4)
N1^i—Fe—N2—C11	39.2 (12)	Fe—N1—C8—C9	63.0 (4)
N2^i—Fe—N2—C11	−14.7 (2)	N1—C8—C9—C10	−65.7 (4)
O1—Fe—N2—C10	134.3 (3)	C11—N2—C10—C9	178.3 (3)
O1^i—Fe—N2—C10	−49.2 (3)	Fe—N2—C10—C9	−58.0 (4)
N1—Fe—N2—C10	44.7 (3)	C8—C9—C10—N2	65.0 (4)
N1^i—Fe—N2—C10	−86.9 (12)	C10—N2—C11—C11^i	170.8 (4)
N2^i—Fe—N2—C10	−140.8 (3)	Fe—N2—C11—C11^i	41.1 (4)

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

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N2—H2N⋯Cl	0.75 (4)	2.70 (4)	3.241 (3)	131 (4)

Fig. 1

Fig. 2

Fig. 3

Sal222

Sal232

Sal323

Sal333