

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(2,2'-Biquinoline- κ^2N,N')dichlorido-iron(II)

Narjes Rahimi, Nasser Safari,* Vahid Amani and Hamid Reza Khavasi

Department of Chemistry, Shahid Beheshti University, G. C., Evin, Tehran 1983963113, Iran

Correspondence e-mail: n-safari@cc.sbu.ac.ir

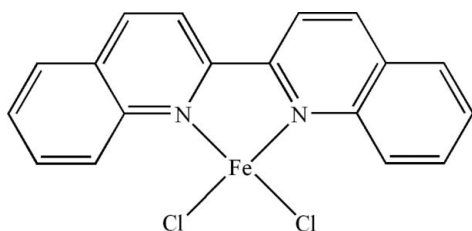
Received 8 October 2009; accepted 10 October 2009

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.037; wR factor = 0.093; data-to-parameter ratio = 20.8.

In the title compound, $[\text{FeCl}_2(\text{C}_{18}\text{H}_{12}\text{N}_2)]$, the Fe^{II} atom is four-coordinated in a distorted tetrahedral arrangement by an N,N' -bidentate 2,2'-biquinoline ligand and two chloride ions. In the crystal, there are extensive π - π contacts between the pyridine rings [centroid-centroid distances = 3.7611 (3), 3.7603 (4), 3.5292 (4), 3.5336 (5) and 3.6656 (4) Å].

Related literature

For related structures, see: Amani *et al.* (2009); Amani, Safari & Khavasi (2007); Amani, Safari, Khavasi & Mirzaei (2007); Chan & Baird (2004); Gibson *et al.* (2002); Handley *et al.* (2001); Khavasi *et al.* (2007, 2008). For bond-length data, see: Figgis *et al.* (1983); Kulkarni *et al.* (1998).



Experimental

Crystal data

$[\text{FeCl}_2(\text{C}_{18}\text{H}_{12}\text{N}_2)]$
 $M_r = 383.05$
 Monoclinic, $P2_1/n$
 $a = 7.9777$ (6) Å
 $b = 12.2268$ (11) Å

$c = 16.9904$ (12) Å
 $\beta = 102.899$ (6)°
 $V = 1615.5$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 1.26$ mm⁻¹
 $T = 298$ K

0.45 × 0.43 × 0.31 mm

Data collection

Stoe IPDS II diffractometer
 Absorption correction: numerical
 (*X-SHAPE*; Stoe & Cie, 2005)
 $T_{\text{min}} = 0.577$, $T_{\text{max}} = 0.681$

13058 measured reflections
 4323 independent reflections
 3739 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.093$
 $S = 1.06$
 4323 reflections

208 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.52$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.44$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Fe1—N1	2.1051 (14)	Fe1—Cl2	2.2265 (6)
Fe1—N2	2.1008 (15)	Fe1—Cl1	2.2341 (7)
N2—Fe1—N1	78.06 (6)		

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

We are grateful to the Shahid Beheshti University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5133).

References

- Amani, V., Safari, N. & Khavasi, H. R. (2007). *Polyhedron*, **26**, 4257–4262.
 Amani, V., Safari, N., Khavasi, H. R. & Mirzaei, P. (2007). *Polyhedron*, **26**, 4908–4914.
 Amani, V., Safari, N., Notash, B. & Khavasi, H. R. (2009). *J. Coord. Chem.* **62**, 1939–1950.
 Chan, B. C. K. & Baird, M. C. (2004). *Inorg. Chim. Acta*, **357**, 2776–2782.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Figgis, B. N., Patrick, J. M., Reynolds, P. A., Skelton, B. W., White, A. H. & Healy, P. C. (1983). *Aust. J. Chem.* **36**, 2043–2055.
 Gibson, V. C., Reilly, R. K., Reed, W., Wass, D. F., White, A. J. P. & Williams, D. J. (2002). *Chem. Commun.* pp. 1850–1851.
 Handley, D. A., Hitchcock, P. B., Lee, T. H. & Leigh, G. J. (2001). *Inorg. Chim. Acta*, **314**, 14–21.
 Khavasi, H. R., Amani, V. & Safari, N. (2007). *Z. Kristallogr. New Cryst. Struct.* **222**, 155–156.
 Khavasi, H. R., Amani, V. & Safari, N. (2008). *Z. Kristallogr. New Cryst. Struct.* **223**, 41–42.
 Kulkarni, P., Padhye, S. & Sinn, E. (1998). *Polyhedron*, **17**, 2623–2626.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Stoe & Cie (2005). *X-AREA*, *X-SHAPE* and *X-RED*. Stoe & Cie, Darmstadt, Germany.

supplementary materials

Acta Cryst. (2009). E65, m1370 [doi:10.1107/S1600536809041439]

(2,2'-Biquinoline- κ^2N,N')dichloridoiron(II)

N. Rahimi, N. Safari, V. Amani and H. R. Khavasi

Comment

Recently, we reported the synthesis and crystal structure of iron (III) hetero-ligand complexes such as [Fe(bipy)Cl₄][bipy.H], (II), [Fe(5,5'-dmbpy)₂Cl₂][FeCl₄], (III), (Amani, Safari & Khavasi 2007), [Fe(phen)Cl₃(CH₃OH)].CH₃OH, (IV), (Khavasi *et al.*, 2007), [Fe(bipy)Cl₃(DMSO)], (V) and [Fe(phen)Cl₃(DMSO)], (VI), (Amani, Safari, khavasi & Mirzaei, 2007), [Fe(phen)Cl₄][phen.H], (VII), (Khavasi *et al.*, 2008), [Fe(4,4'-dmbpy)Cl₄][4,4'-dmbpy.H], (VIII) and [Fe(4,4'-dmbpy)Cl₃(DMSO)], (IX), (Amani *et al.*, 2009) [where bipy is 2,2'-bipyridine, 5,5'-dmbpy is 5,5'-dimethyl-2,2'-bipyridine, phen is 1,10-phenanthroline, DMSO is dimethyl sulfoxide and 4,4'-dmbpy is 4,4'-dimethyl-2,2'-bipyridine].

There are several Fe^{II} complexes, with formula, [FeCl₂(N—N)], such as [FeCl₂(6,6'-dmbpy)], (X), (Chan & Baird 2004), [FeCl₂(BDP)], (XI), (Handley *et al.*, 2001) and [FeCl₂(DEI)], (XII), (Gibson *et al.*, 2002) [where 6,6'-dmbpy is 6, 6'-dimethyl-2, 2'-bipyridine, BDP is 1,3-bis(dimethylamino) propane and DEI is *N,N'*-dicyclohexyl-1,2-ethanedimine] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound (I).

In the molecule of the title compound, (I), (Fig. 1), the Fe^{II} atom is four-coordinated in distorted tetrahedral configurations by two N atoms from one 2, 2'-biquinoline and two terminal Cl atoms. The Fe—Cl and Fe—N bond lengths and angles (Table 1) are within normal range (X). In this complex, Fe—N average distance is 2.1029 (15) Å and the Fe—Cl average bond distance is 2.2303 (6) Å. The Fe—N average bond distances in high-spin Fe^{II} and Fe^{III} phenanthroline and bipyridine complexes are around 2.2 Å. However, low-spin Fe^{II} and Fe^{III} complexes, the Fe—N distances less than 2 Å were reported (Figgis *et al.*, 1983; Kulkarni *et al.*, 1998). Therefore, in the molecule of the title compound, the Fe—N bond distance is unambiguously high-spin Fe^{II}. It seems substitution in the 6 position of bipyridine is crucial to stabilize Fe^{II} high-spin *versus* (Fe^{II}) especially low-spin. Also, biquinoline result in auto reduce of Fe^{III} to Fe^{II}.

The π - π contacts between the pyridine rings, Cg2ⁱ...Cg2ⁱ, Cg2ⁱ...Cg4ⁱ, Cg3ⁱⁱ...Cg3ⁱⁱ, Cg3ⁱⁱ...Cg5ⁱ, Cg4ⁱⁱ...Cg4ⁱⁱ and Cg5ⁱⁱ...Cg3ⁱⁱ [symmetry cods: (i) 1-X, 1-Y, 1-Z, (ii) 1-X,-Y,1-Z, where Cg2, Cg3, Cg4 and Cg5 are centroids of the rings (N1/C1/C6—C9), (N2/C10—C13/C18), (C1—C6) and (C13—C18), respectively] further stabilize the structure, with centroid-centroid distance of 3.7611 (3), 3.7603 (4), 3.5292 (4), 3.5336 (5) and 3.6656 (4) Å, respectively. It seems this π - π stacking is effective in the stabilization of the crystal structure (Fig. 2).

Experimental

A solution of 2,2'-biquinoline (0.20 g, 0.78 mmol) in methanol (6 ml) and chloroform (2 ml) was added to a solution of FeCl₃.6H₂O (0.07 g, 0.26 mmol) in methanol (6 ml) and chloroform (2 ml) and the resulting yellow solution was stirred for

supplementary materials

15 min at room temperature. This solution was left to evaporate slowly at room temperature. After two weeks, red blocks of (I) were isolated (yield 0.07 g, 70.3%).

Refinement

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}$.

Figures

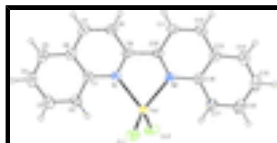


Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at the 30% probability level.

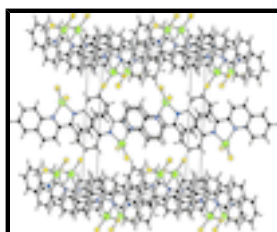


Fig. 2. Unit-cell packing diagram for (I).

(2,2'-Biquinoline- κ^2N,N')dichloridoiron(II)

Crystal data

[FeCl₂(C₁₈H₁₂N₂)]

$M_r = 383.05$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 7.9777$ (6) Å

$b = 12.2268$ (11) Å

$c = 16.9904$ (12) Å

$\beta = 102.899$ (6)°

$V = 1615.5$ (2) Å³

$Z = 4$

$F_{000} = 776$

$D_x = 1.575$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1323 reflections

$\theta = 2.1$ – 29.3 °

$\mu = 1.26$ mm⁻¹

$T = 298$ K

Block, red

$0.45 \times 0.43 \times 0.31$ mm

Data collection

Stoe IPDS II
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 0.15 mm pixels mm⁻¹

$T = 298$ K

rotation method scans

Absorption correction: numerical

4323 independent reflections

3739 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\text{max}} = 29.3$ °

$\theta_{\text{min}} = 2.1$ °

$h = -10 \rightarrow 10$

$k = -16 \rightarrow 16$

(X-SHAPE; Stoe & Cie, 2005)

$T_{\min} = 0.577$, $T_{\max} = 0.681$

$l = -23 \rightarrow 21$

13058 measured reflections

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.037$

H-atom parameters constrained

$wR(F^2) = 0.093$

$$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.7232P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.06$

$(\Delta/\sigma)_{\max} = 0.007$

4323 reflections

$\Delta\rho_{\max} = 0.52 \text{ e } \text{\AA}^{-3}$

208 parameters

$\Delta\rho_{\min} = -0.44 \text{ e } \text{\AA}^{-3}$

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2274 (2)	0.95885 (14)	0.02892 (11)	0.0367 (3)
C2	0.3108 (3)	1.01753 (16)	0.09821 (13)	0.0462 (4)
H2	0.3097	0.9909	0.1494	0.055*
C3	0.3929 (3)	1.11314 (18)	0.09004 (15)	0.0546 (5)
H3	0.4477	1.1515	0.1359	0.066*
C4	0.3959 (3)	1.15461 (17)	0.01308 (17)	0.0571 (6)
H4	0.4536	1.2196	0.0086	0.069*
C5	0.3157 (3)	1.10094 (17)	-0.05409 (15)	0.0520 (5)
H5	0.3174	1.1297	-0.1046	0.062*
C6	0.2289 (2)	1.00112 (15)	-0.04852 (12)	0.0417 (4)
C7	0.1447 (3)	0.94060 (17)	-0.11614 (12)	0.0475 (4)
H7	0.1447	0.9656	-0.1678	0.057*
C8	0.0630 (3)	0.84538 (16)	-0.10617 (11)	0.0438 (4)
H8	0.0069	0.8052	-0.1508	0.053*
C9	0.0647 (2)	0.80865 (14)	-0.02736 (10)	0.0352 (3)

supplementary materials

C10	-0.0289 (2)	0.70846 (13)	-0.01190 (10)	0.0352 (3)
C11	-0.1412 (3)	0.65279 (15)	-0.07475 (11)	0.0426 (4)
H11	-0.1539	0.6755	-0.1280	0.051*
C12	-0.2310 (2)	0.56528 (16)	-0.05670 (12)	0.0459 (4)
H12	-0.3060	0.5280	-0.0977	0.055*
C13	-0.2108 (2)	0.53109 (15)	0.02390 (12)	0.0423 (4)
C14	-0.2993 (3)	0.44022 (17)	0.04699 (16)	0.0550 (5)
H14	-0.3764	0.4011	0.0080	0.066*
C15	-0.2720 (3)	0.4098 (2)	0.12585 (17)	0.0637 (6)
H15	-0.3316	0.3506	0.1404	0.076*
C16	-0.1546 (4)	0.4673 (2)	0.18538 (16)	0.0652 (6)
H16	-0.1362	0.4450	0.2390	0.078*
C17	-0.0666 (3)	0.55570 (18)	0.16561 (13)	0.0544 (5)
H17	0.0105	0.5933	0.2056	0.065*
C18	-0.0937 (2)	0.58938 (15)	0.08446 (11)	0.0398 (4)
N1	0.14684 (19)	0.86245 (11)	0.03785 (8)	0.0349 (3)
N2	-0.00420 (19)	0.67763 (12)	0.06478 (8)	0.0361 (3)
Fe1	0.17508 (4)	0.77276 (2)	0.145770 (14)	0.04109 (9)
Cl1	0.43989 (8)	0.70190 (6)	0.17323 (4)	0.06732 (17)
Cl2	0.05960 (9)	0.84372 (5)	0.24216 (3)	0.06434 (17)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0346 (8)	0.0354 (8)	0.0411 (9)	0.0060 (7)	0.0107 (7)	0.0011 (6)
C2	0.0462 (10)	0.0451 (10)	0.0478 (10)	-0.0023 (8)	0.0114 (8)	-0.0066 (8)
C3	0.0477 (11)	0.0463 (10)	0.0710 (14)	-0.0045 (9)	0.0156 (10)	-0.0112 (10)
C4	0.0507 (12)	0.0392 (10)	0.0878 (17)	-0.0023 (9)	0.0289 (12)	0.0013 (10)
C5	0.0519 (11)	0.0429 (10)	0.0679 (13)	0.0073 (9)	0.0278 (10)	0.0135 (9)
C6	0.0409 (9)	0.0401 (9)	0.0479 (10)	0.0089 (7)	0.0177 (8)	0.0062 (7)
C7	0.0558 (11)	0.0511 (11)	0.0372 (9)	0.0099 (9)	0.0142 (8)	0.0113 (8)
C8	0.0535 (11)	0.0459 (9)	0.0307 (8)	0.0044 (8)	0.0066 (7)	0.0020 (7)
C9	0.0385 (8)	0.0362 (8)	0.0302 (7)	0.0073 (7)	0.0062 (6)	0.0016 (6)
C10	0.0360 (8)	0.0359 (8)	0.0319 (7)	0.0055 (6)	0.0041 (6)	-0.0021 (6)
C11	0.0446 (10)	0.0443 (9)	0.0341 (8)	0.0052 (8)	-0.0018 (7)	-0.0032 (7)
C12	0.0391 (9)	0.0438 (9)	0.0492 (10)	0.0022 (8)	-0.0017 (8)	-0.0082 (8)
C13	0.0357 (9)	0.0388 (9)	0.0537 (11)	0.0023 (7)	0.0127 (8)	-0.0036 (8)
C14	0.0449 (11)	0.0452 (10)	0.0780 (15)	-0.0050 (9)	0.0205 (10)	-0.0055 (10)
C15	0.0647 (14)	0.0508 (12)	0.0867 (18)	-0.0081 (11)	0.0409 (13)	0.0016 (11)
C16	0.0862 (18)	0.0610 (13)	0.0585 (13)	-0.0056 (13)	0.0374 (13)	0.0073 (11)
C17	0.0693 (14)	0.0544 (12)	0.0433 (10)	-0.0083 (10)	0.0204 (10)	0.0008 (9)
C18	0.0411 (9)	0.0383 (8)	0.0422 (9)	0.0008 (7)	0.0138 (7)	-0.0006 (7)
N1	0.0383 (7)	0.0352 (7)	0.0310 (6)	0.0033 (6)	0.0074 (5)	0.0004 (5)
N2	0.0398 (7)	0.0372 (7)	0.0308 (6)	0.0008 (6)	0.0070 (5)	-0.0009 (5)
Fe1	0.04860 (17)	0.04469 (15)	0.02751 (13)	-0.00218 (11)	0.00321 (10)	0.00021 (10)
Cl1	0.0545 (3)	0.0818 (4)	0.0594 (3)	0.0111 (3)	-0.0006 (2)	0.0081 (3)
Cl2	0.0820 (4)	0.0767 (4)	0.0333 (2)	0.0170 (3)	0.0107 (2)	-0.0042 (2)

Geometric parameters (Å, °)

C1—N1	1.367 (2)	C11—C12	1.360 (3)
C1—C2	1.412 (3)	C11—H11	0.9300
C1—C6	1.416 (3)	C12—C13	1.406 (3)
C2—C3	1.362 (3)	C12—H12	0.9300
C2—H2	0.9300	C13—C18	1.418 (3)
C3—C4	1.407 (4)	C13—C14	1.418 (3)
C3—H3	0.9300	C14—C15	1.360 (4)
C4—C5	1.348 (3)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.404 (4)
C5—C6	1.417 (3)	C15—H15	0.9300
C5—H5	0.9300	C16—C17	1.371 (3)
C6—C7	1.405 (3)	C16—H16	0.9300
C7—C8	1.363 (3)	C17—C18	1.409 (3)
C7—H7	0.9300	C17—H17	0.9300
C8—C9	1.409 (2)	C18—N2	1.376 (2)
C8—H8	0.9300	Fe1—N1	2.1051 (14)
C9—N1	1.329 (2)	Fe1—N2	2.1008 (15)
C9—C10	1.488 (2)	Fe1—C12	2.2265 (6)
C10—N2	1.328 (2)	Fe1—C11	2.2341 (7)
C10—C11	1.407 (2)		
N1—C1—C2	119.43 (16)	C11—C12—C13	120.10 (17)
N1—C1—C6	121.30 (16)	C11—C12—H12	119.9
C2—C1—C6	119.27 (17)	C13—C12—H12	119.9
C3—C2—C1	119.9 (2)	C12—C13—C18	118.12 (17)
C3—C2—H2	120.0	C12—C13—C14	123.11 (19)
C1—C2—H2	120.0	C18—C13—C14	118.76 (19)
C2—C3—C4	120.8 (2)	C15—C14—C13	120.4 (2)
C2—C3—H3	119.6	C15—C14—H14	119.8
C4—C3—H3	119.6	C13—C14—H14	119.8
C5—C4—C3	120.5 (2)	C14—C15—C16	120.5 (2)
C5—C4—H4	119.7	C14—C15—H15	119.8
C3—C4—H4	119.7	C16—C15—H15	119.8
C4—C5—C6	120.6 (2)	C17—C16—C15	120.9 (2)
C4—C5—H5	119.7	C17—C16—H16	119.5
C6—C5—H5	119.7	C15—C16—H16	119.5
C7—C6—C1	117.76 (17)	C16—C17—C18	119.7 (2)
C7—C6—C5	123.42 (19)	C16—C17—H17	120.2
C1—C6—C5	118.83 (19)	C18—C17—H17	120.2
C8—C7—C6	120.19 (17)	N2—C18—C17	119.52 (17)
C8—C7—H7	119.9	N2—C18—C13	120.76 (16)
C6—C7—H7	119.9	C17—C18—C13	119.71 (18)
C7—C8—C9	119.12 (18)	C9—N1—C1	119.39 (15)
C7—C8—H8	120.4	C9—N1—Fe1	113.92 (11)
C9—C8—H8	120.4	C1—N1—Fe1	125.75 (11)
N1—C9—C8	122.20 (17)	C10—N2—C18	119.32 (15)
N1—C9—C10	115.71 (14)	C10—N2—Fe1	114.56 (12)

supplementary materials

C8—C9—C10	122.08 (16)	C18—N2—Fe1	126.12 (12)
N2—C10—C11	122.49 (17)	N2—Fe1—N1	78.06 (6)
N2—C10—C9	115.87 (14)	N2—Fe1—Cl2	111.38 (5)
C11—C10—C9	121.60 (15)	N1—Fe1—Cl2	117.15 (4)
C12—C11—C10	119.19 (17)	N2—Fe1—Cl1	113.32 (5)
C12—C11—H11	120.4	N1—Fe1—Cl1	107.24 (5)
C10—C11—H11	120.4	Cl2—Fe1—Cl1	121.65 (3)
N1—C1—C2—C3	179.35 (18)	C12—C13—C18—N2	0.7 (3)
C6—C1—C2—C3	-0.6 (3)	C14—C13—C18—N2	179.59 (17)
C1—C2—C3—C4	0.0 (3)	C12—C13—C18—C17	-178.33 (19)
C2—C3—C4—C5	0.7 (3)	C14—C13—C18—C17	0.5 (3)
C3—C4—C5—C6	-0.8 (3)	C8—C9—N1—C1	2.5 (3)
N1—C1—C6—C7	0.0 (3)	C10—C9—N1—C1	-176.11 (14)
C2—C1—C6—C7	179.98 (17)	C8—C9—N1—Fe1	-167.08 (14)
N1—C1—C6—C5	-179.45 (16)	C10—C9—N1—Fe1	14.32 (19)
C2—C1—C6—C5	0.5 (3)	C2—C1—N1—C9	178.34 (17)
C4—C5—C6—C7	-179.2 (2)	C6—C1—N1—C9	-1.7 (2)
C4—C5—C6—C1	0.2 (3)	C2—C1—N1—Fe1	-13.4 (2)
C1—C6—C7—C8	0.9 (3)	C6—C1—N1—Fe1	166.54 (13)
C5—C6—C7—C8	-179.67 (19)	C11—C10—N2—C18	-1.3 (3)
C6—C7—C8—C9	-0.2 (3)	C9—C10—N2—C18	176.38 (15)
C7—C8—C9—N1	-1.6 (3)	C11—C10—N2—Fe1	178.50 (13)
C7—C8—C9—C10	176.93 (17)	C9—C10—N2—Fe1	-3.78 (19)
N1—C9—C10—N2	-7.2 (2)	C17—C18—N2—C10	179.36 (18)
C8—C9—C10—N2	174.23 (17)	C13—C18—N2—C10	0.3 (3)
N1—C9—C10—C11	170.57 (16)	C17—C18—N2—Fe1	-0.4 (3)
C8—C9—C10—C11	-8.0 (3)	C13—C18—N2—Fe1	-179.52 (13)
N2—C10—C11—C12	1.3 (3)	C10—N2—Fe1—N1	8.54 (12)
C9—C10—C11—C12	-176.28 (17)	C18—N2—Fe1—N1	-171.64 (15)
C10—C11—C12—C13	-0.2 (3)	C10—N2—Fe1—Cl2	123.25 (12)
C11—C12—C13—C18	-0.8 (3)	C18—N2—Fe1—Cl2	-56.93 (15)
C11—C12—C13—C14	-179.55 (19)	C10—N2—Fe1—Cl1	-95.27 (12)
C12—C13—C14—C15	178.8 (2)	C18—N2—Fe1—Cl1	84.55 (14)
C18—C13—C14—C15	0.0 (3)	C9—N1—Fe1—N2	-12.47 (12)
C13—C14—C15—C16	-0.7 (4)	C1—N1—Fe1—N2	178.74 (14)
C14—C15—C16—C17	0.8 (4)	C9—N1—Fe1—Cl2	-120.54 (11)
C15—C16—C17—C18	-0.3 (4)	C1—N1—Fe1—Cl2	70.66 (14)
C16—C17—C18—N2	-179.5 (2)	C9—N1—Fe1—Cl1	98.51 (12)
C16—C17—C18—C13	-0.4 (3)	C1—N1—Fe1—Cl1	-70.28 (14)

Fig. 1

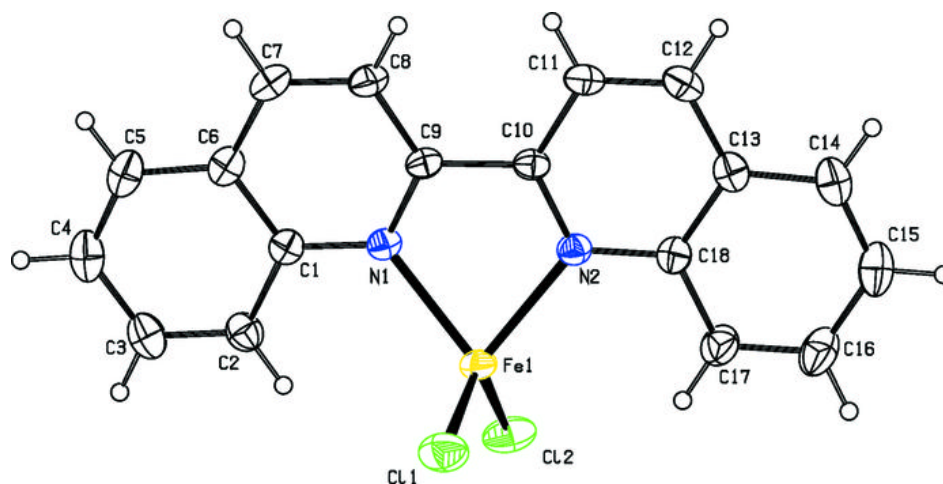


Fig. 2

