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cis-Dichlorobis(1,10-phenanthroline)iron(II)

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
R factor = 0.067
wR factor = 0.149
Data-to-parameter ratio = 17.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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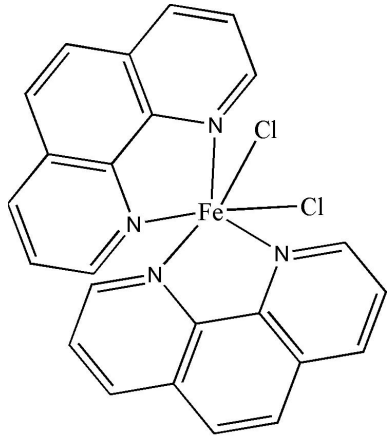
In the title compound, *cis*-$[FeCl_2(C_{12}H_8N_2)_2]$, the Fe atom has a distorted octahedral coordination composed of four N atoms from two phenanthroline groups and two Cl atoms. The crystal packing is stabilized by weak π–π stacking of neighboring phenanthroline groups.

Comment

The title compound, *cis*-$[Fe(phen)_2Cl_2]$, (I) (phen is 1,10-phenanthroline), was previously reported by Baker & Bobonich (1963), and its magnetic behavior has been studied (König *et al.*, 1967). However, its crystal structure has not yet been reported. *cis*-$[Fe(phen)_2Cl_2]$, was unexpectedly obtained while attempting to prepare $[Fe(terephth)(phen)(H_2O)]$ (terephth is terephthalate). The Fe^{II} atom has a distorted octahedral coordination composed of a pair of phen groups and two Cl atoms. The Cl1—Fe1—Cl2 angle is 100.09 (4)°. The crystal packing of (I) is stabilized by extended π–π stacking of the conjugated phen ring systems, characterized by interplanar distances in the range 3.404 (6)–3.608 (6) Å. (see Fig.2).



(I)

Experimental

The title compound was prepared from a mixture of $FeCl_3$, terephthalic acid, 1,10-phenanthroline (monohydrated), NaOH and EtOH with a molar ratio of 1:2:1:2:206. The mixture was stirred for 2 h, sealed in a 15 ml Teflon-lined stainless steel bomb, kept at 413 K for 96 h, and then cooled slowly to ambient temperature. The resulting black–red crystals of (I) were filtered and washed with acetone.

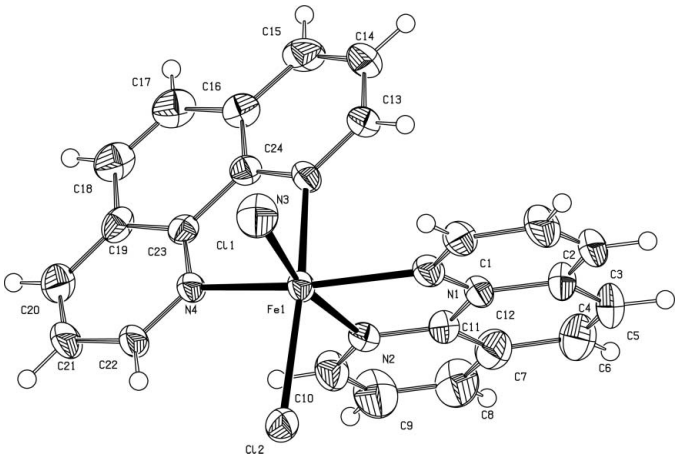


Figure 1
View of the title complex, showing the labeling of the non-H atoms and 50% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radii.

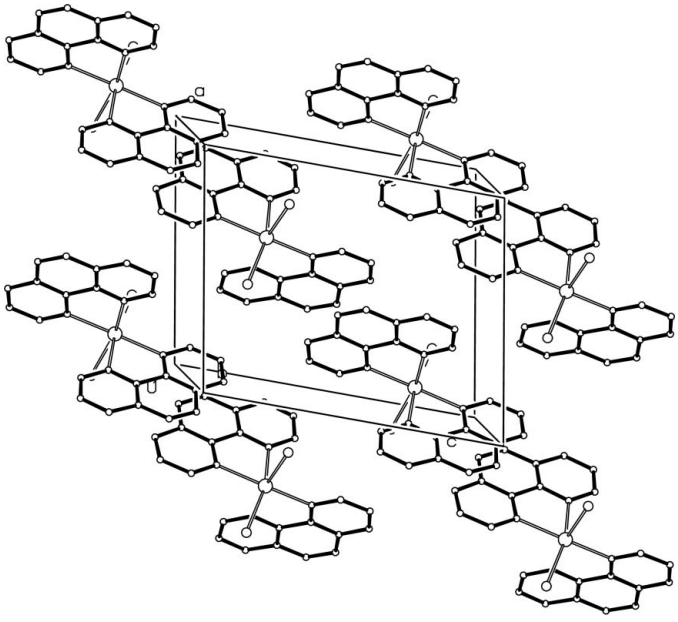


Figure 2
A view of the π–π stacking. H atoms have been omitted.

Crystal data

$[FeCl_2(C_{12}H_8N_2)_2]$	D_x = 1.533 Mg m^{-3}
M_r = 487.16	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3005 reflections
a = 10.1699 (18) Å	θ = 2.7–25.1°
b = 16.883 (3) Å	μ = 0.99 mm^{-1}
c = 12.490 (2) Å	T = 292 (2) K
β = 100.126 (3)°	Block, black–red
V = 2111.1 (6) Å^3	0.40 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	4760 independent reflections
φ and ω scans	3251 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	R_{int} = 0.060
T_{min} = 0.693, T_{max} = 0.908	θ_{max} = 27.5°
13352 measured reflections	$h = -10 \rightarrow 13$
	$k = -21 \rightarrow 21$
	$l = -15 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.7354P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.067	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.149	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
S = 1.08	$\Delta\rho_{min}$ = −0.69 e Å^{-3}
4760 reflections	
280 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Fe1—N4	2.179 (3)	Fe1—N2	2.276 (3)
Fe1—N1	2.179 (3)	Fe1—Cl1	2.3604 (12)
Fe1—N3	2.246 (3)	Fe1—Cl2	2.4696 (11)
N4—Fe1—N1	156.32 (12)	N3—Fe1—Cl1	93.85 (8)
N4—Fe1—N3	74.47 (11)	N2—Fe1—Cl1	168.52 (8)
N1—Fe1—N3	87.65 (11)	N4—Fe1—Cl2	93.00 (8)
N4—Fe1—N2	87.49 (11)	N1—Fe1—Cl2	100.72 (9)
N1—Fe1—N2	73.94 (11)	N3—Fe1—Cl2	162.77 (8)
N3—Fe1—N2	79.90 (11)	N2—Fe1—Cl2	87.91 (8)
N4—Fe1—Cl1	100.19 (9)	Cl1—Fe1—Cl2	100.09 (4)
N1—Fe1—Cl1	96.32 (9)		

H atoms were placed in calculated positions and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) and C–H distances of 0.93 Å.

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

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