metal-organic papers

[1,2-Bis(1H-pyrrol-2-ylmethyleneamino)-ethane-$\kappa^4 N$]iron(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.047
wR factor = 0.126
Data-to-parameter ratio = 12.9

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

In the title compound, [Fe($C_{12}H_{12}N_4$)], the metal atom is four-coordinated by four N atoms from the Schiff base ligand in an approximately square-planar configuration. The Fe—N distances are in the range 1.833 (3)–1.876 (3) Å.

Comment

Transition metal compounds have been of great interest for many years. They are very important in the development of coordination chemistry. As an extension of work on the structural characterization of Fe compounds, we report here the crystal structure of a new mononuclear iron(II) compound, (I).

(I)
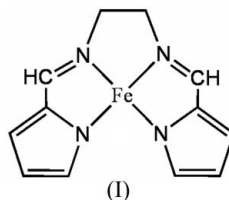
Compound (I) is an electronically neutral mononuclear Fe[II] complex (Fig. 1). The Fe[II] ion in the compound is four-coordinated by four N atoms from a Schiff base ligand, in a slightly distorted square-planar geometry. The Fe1—N1 and Fe1—N2 bond distances are longer than the Fe1—N3 and Fe1—N4 bond distances. The N4—Fe1—N3 angle is smaller than the N2—Fe1—N1 angle (Table 1). The molecules are stacked along the a axis.

Experimental

Ethylenediamine (1 mmol, 60 mg) and pyrrole-2-aldehyde (2 mmol, 95 mg) were dissolved in methanol (25 ml). The mixture was stirred at 333 K for 30 min to give a brown solution. The solution was cooled to room temperature, and $FeCl_2 \cdot 4H_2O$ (1 mmol, 198 mg) and NaOAc (1.3 g) were added with stirring. The mixture was stirred for 12 h at room temperature and filtered. The resulting precipitate was collected and dissolved in a mixture of diethyl ether and acetonitrile (1:1 v/v). The solution was allowed to stand in air for 3 d, and brown crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

[Fe($C_{12}H_{12}N_4$)]	V = 574.3 (4) Å³
M_r = 268.11	Z = 2
Triclinic, $P\bar{1}$	D_x = 1.550 Mg m⁻³
a = 6.923 (3) Å	Mo $K\alpha$ radiation
b = 8.828 (3) Å	μ = 1.29 mm⁻¹
c = 10.512 (4) Å	T = 293 (2) K
α = 114.634 (4)°	Block, brown
β = 92.149 (4)°	0.68 × 0.52 × 0.33 mm
γ = 98.351 (4)°	

Data collection

Siemens SMART CCD area-detector diffractometer	2960 measured reflections
	1988 independent reflections
φ and ω scans	1740 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.028$
	$\theta_{max} = 25.0°$
$T_{min} = 0.473$, $T_{max} = 0.675$	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0909P)^2]$
$wR(F^2) = 0.127$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
1988 reflections	$\Delta\rho_{max} = 0.83$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.76$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1—N4	1.833 (3)	Fe1—N2	1.876 (3)
Fe1—N3	1.841 (3)	Fe1—N1	1.876 (3)
N4—Fe1—N3	84.53 (15)	N4—Fe1—N1	168.68 (14)
N4—Fe1—N2	84.67 (14)	N3—Fe1—N1	84.43 (14)
N3—Fe1—N2	169.07 (13)	N2—Fe1—N1	106.43 (15)

H atoms were included in calculated positions [C—H = 0.93 or 0.97 Å] and refined using a riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics:

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: *SHELXL97*.

References

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