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Key indicators

Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.042
 wR factor = 0.127
Data-to-parameter ratio = 12.2

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

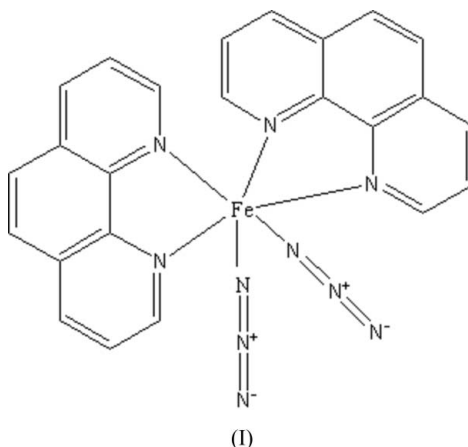
Diazidobis(1,10-phenanthroline)iron(II)

The solution reaction of Fe^{II} with 1,10-phenanthroline and NaN_3 affords the title complex, $[\text{Fe}(\text{N}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)_2]$. In this complex, the central atom adopts a six-coordinate octahedral geometry, with monodentate azide ligands occupying the *cis* sites and two phenanthroline ligands occupying the other four sites, forming a *cis* isomer.

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Comment

1,10-Phenanthroline complexes have been studied extensively with respect to geometrical isomerism. Most of them are *trans* isomers (Sun *et al.*, 2006; Phuengphai *et al.*, 2006). Azide compounds have been known for a long time and are still an area of great interest for several important reasons. One of them is their various coordination modes (Ribas *et al.*, 1999; Nayak *et al.*, 2005). The azide anion can act as a monodentate ligand, as well as a bridging ligand, adopting end-on and end-to-end modes, generating complexes with structures ranging from mononuclear to three-dimensional (Monfort *et al.*, 2001; Wang *et al.*, 2004; Pan *et al.*, 1999). We report here a new *cis*-coordinated compound, $[\text{Fe}(\text{N}_3)_2(\text{phen})_2]$, (I).



As shown in Fig. 1, the Fe^{II} atom is coordinated by six N atoms, of which four are from phen ligands and the other two are from *cis*-azide groups. The two phen planes are nearly perpendicular to one another, with a dihedral angle of 79.8° . The azide anion acts as a monodentate ligand (Kim *et al.*, 2002; Chun *et al.*, 2000). The packing of complex (I) is shown in Fig. 2.

Experimental

Complex (I) was synthesized in a solution reaction. NaN_3 (0.2 mmol) dissolved in 2 ml water was added to 5 ml aqueous solution of

FeSO₄·7H₂O (0.1 mmol) with stirring. An ethanol solution (5 ml) of phen (0.2 mmol) was then added to the solution and the mixture was stirred for 4 h. The mixture was filtered and the resulting clear solution was allowed to stand at room temperature to evaporate slowly. After one week, single crystals of (I) suitable for X-ray diffraction were obtained.

Crystal data

[Fe(N₃)₂(C₁₂H₈N₂)₂]

M_r = 500.32

Triclinic, *P* $\bar{1}$

a = 8.1824 (2) Å

b = 11.1341 (2) Å

c = 12.6788 (2) Å

α = 83.344 (1)°

β = 81.844 (1)°

γ = 73.451 (1)°

V = 1092.56 (4) Å³

Z = 2

D_x = 1.521 Mg m⁻³

Mo *K*α radiation

μ = 0.73 mm⁻¹

T = 273 (2) K

Block, red

0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.811, *T_{max}* = 0.868

12819 measured reflections

3845 independent reflections

3348 reflections with *I* > 2σ(*I*)

R_{int} = 0.026

θ_{\max} = 25.0°

Refinement

Refinement on *F*²

R[*F*² > 2σ(*F*²)] = 0.042

wR(*F*²) = 0.128

S = 1.09

3845 reflections

316 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2$

+ 0.6391*P*]

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

(Δ/σ)_{max} = 0.001

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

$\Delta\rho_{\min} = -0.36 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Fe1—N5	2.160 (3)	Fe1—N1	2.321 (2)
Fe1—N8	2.195 (3)	N5—N6	1.160 (4)
Fe1—N2	2.257 (2)	N6—N7	1.147 (4)
Fe1—N4	2.272 (2)	N8—N9	1.034 (4)
Fe1—N3	2.316 (2)	N9—N10	1.214 (6)
N5—Fe1—N8	95.38 (12)	N5—Fe1—N1	86.26 (10)
N5—Fe1—N2	101.59 (11)	N8—Fe1—N1	166.15 (9)
N8—Fe1—N2	93.88 (10)	N2—Fe1—N1	72.34 (8)
N5—Fe1—N4	94.66 (10)	N4—Fe1—N1	91.35 (8)
N8—Fe1—N4	102.20 (9)	N3—Fe1—N1	90.05 (8)
N2—Fe1—N4	155.95 (9)	N6—N5—Fe1	131.8 (2)
N5—Fe1—N3	166.42 (10)	N7—N6—N5	178.2 (3)
N8—Fe1—N3	91.33 (10)	N9—N8—Fe1	126.0 (3)
N4—Fe1—N3	72.34 (8)	N8—N9—N10	176.5 (5)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: *APEX2* (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* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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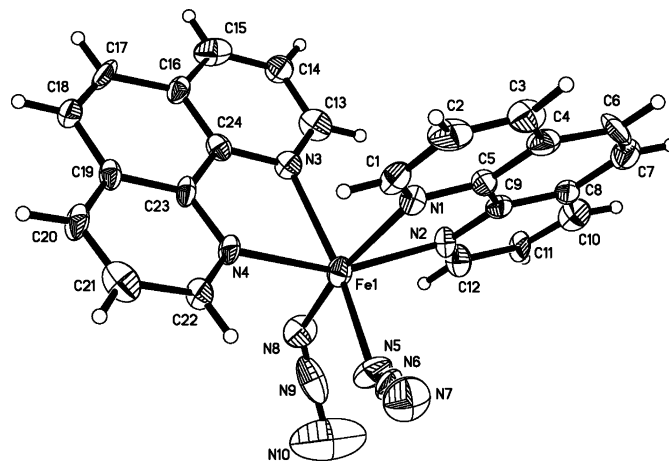


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

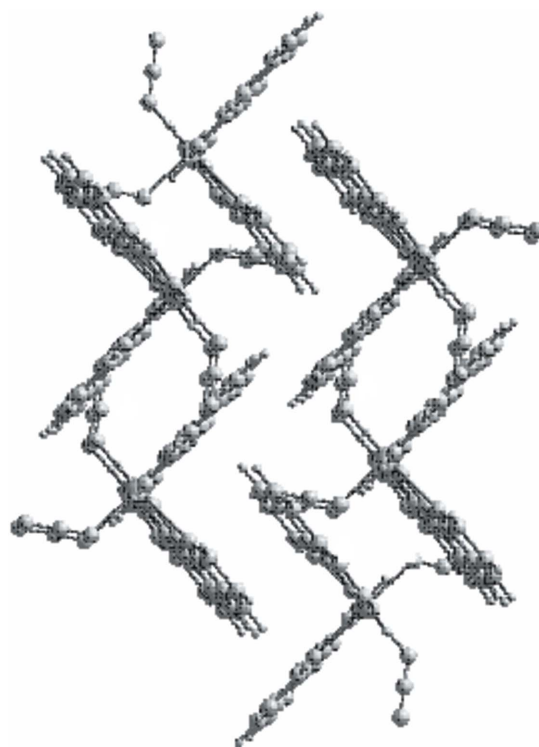


Figure 2

A packing diagram of complex (I).

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