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Diazidobis(1,7-phenanthroline)zinc(II)

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Key indicators

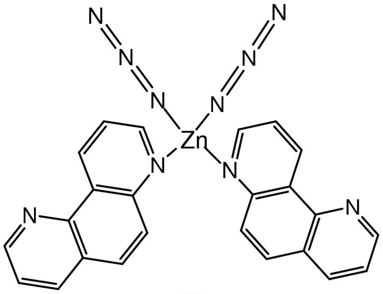
Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.123
Data-to-parameter ratio = 20.2

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

The title complex, $[Zn(N_3)_2(C_{12}H_8N_2)_2]$, possesses C_2 symmetry. The Zn^{2+} ion has a distorted tetrahedral coordination environment and is coordinated by two N atoms from two 1,7-phenanthroline ligands and by two N atoms of end-on-coordinated azides. In the crystal structure, the molecules stack up the *c* axis *via* π–π interactions between the 1,7-phenanthroline ligands.

Comment

The synthesis of new organic–inorganic hybrid compounds is a relatively new research area that has developed rapidly (Ciurtin *et al.*, 2001). A large number of complexes with azido ligands, from dimers to three-dimensional networks, have been structurally and magnetically characterized in recent years (Monfort *et al.*, 2000). Azido-bridged complexes have attracted considerable attention due to their structural diversity (Li *et al.*, 2002). They may coordinate as $\mu_{1,3}$-N_3 (end-to-end, EE) or $\mu_{1,1}$-N_3 (end-on, EO), or in even more exotic modes, such as $\mu_{1,1,3}$-N_3 or $\mu_{1,1,1}$-N_3 (Goher *et al.*, 2000; Ribas *et al.*, 1994). Recently, we have synthesized the title compound, (I), and its structure is reported here.



(I)

The molecular structure of (I) is illustrated in Fig. 1 and selected bond distances and angles are given in Table 1. The Zn^{2+} ion is situated on a twofold axis and assumes a distorted tetrahedral geometry. It is coordinated by two terminal N atoms of two N_3^- ligands, and by two N atoms of two 1,7-phenanthroline ligands. Non-linear coordination of the N_3^- ligands to the Zn^{2+} centre is apparent from the Zn1—N1—N2 bond angles of 115.8 (2)°. The bond distances and angles in the 1,7-phenanthroline ligands are normal. They are nearly planar, with the largest deviation of any atom from the 1,7-phen mean-plane being 0.0162 Å for C9. The dihedral angle of the two phenanthroline ligands, which coordinate to the Zn^{2+} ion, is 80.56 (2)°.

The three-dimensional crystal structure of (I) can be regarded as being constructed *via* π–π stacking interactions, as

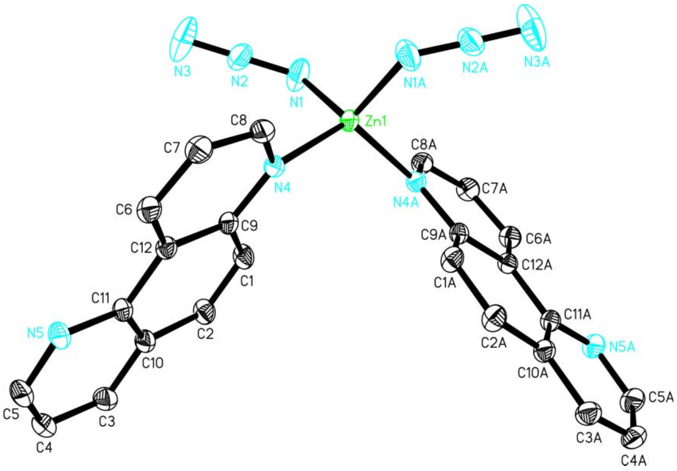


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and 30% probability displacement ellipsoids. [Symmetry code: (A) $\frac{1}{2} - x, y, 1 - z$.]

shown in Fig. 2. The interacting 1,7-phenanthroline ligands are nearly parallel to one another and are separated by a distance of *ca* 3.36 Å.

Experimental

To an aqueous solution (5 ml) of $Zn(OAc)_2 \cdot H_2O$ (219.22 mg, 1 mmol) was added 1,7-phenanthroline (182.22 mg, 1 mmol) dissolved in methanol (5 ml). This mixture was then added to an aqueous solution (10 ml) of NaN_3 (130.03 mg, 2 mmol). The resulting clear solution was left to stand undisturbed at room temperature. After two weeks, X-ray quality crystals of (I) were obtained by slow evaporation. These were filtered, washed with water and air dried. The yield was 55%. Analysis calculated for $C_{24}H_{16}N_{10}Zn$: C 56.68, H 3.17, N 27.56%; found: C 56.36, H 3.56, N 27.21%. IR (KBr disk): $\mu(N{=}N{=}N)$ 2072 cm^{-1}.

Crystal data

$[Zn(N_3)_2(C_{12}H_8N_2)_2]$
$M_r = 509.84$
Orthorhombic, *Ibca*
$a = 13.7823$ (13) Å
$b = 17.5908$ (17) Å
$c = 18.1368$ (18) Å
$V = 4397.1$ (7) Å^3
$Z = 8$
$D_x = 1.540$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 18 030 reflections
$\theta = 2.3$–30.0°
$\mu = 1.15$ mm^{-1}
$T = 223$ (2) K
Polyhedron, colourless
0.26 × 0.22 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.748$, $T_{max} = 0.812$
18 030 measured reflections
3214 independent reflections
2346 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 30.0°$
$h = -19 \rightarrow 16$
$k = -24 \rightarrow 24$
$l = -25 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.123$
$S = 1.02$
3214 reflections
159 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 1.193P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

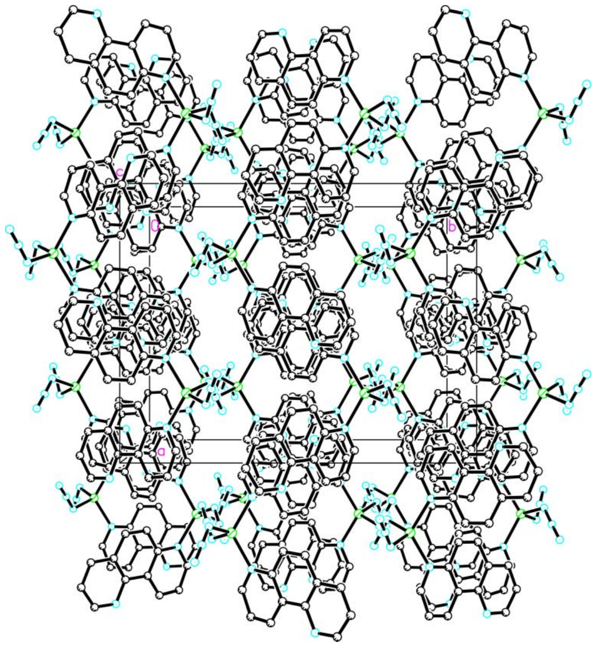


Figure 2
The crystal packing of (I), viewed along the *c* axis.

Table 1
Selected geometric parameters (Å, °).

Zn1—N1^i	1.954 (2)	N4—C8	1.329 (3)
Zn1—N4	2.0403 (16)	N4—C9	1.367 (2)
N1—N2	1.179 (3)	N5—C5	1.319 (3)
N2—N3	1.138 (3)	N5—C11	1.357 (2)
N1^i—Zn1—N1	115.98 (15)	N3—N2—N1	177.4 (3)
N1^i—Zn1—N4	101.76 (8)	C8—N4—C9	118.58 (17)
N1—Zn1—N4	108.41 (8)	C8—N4—Zn1	116.33 (13)
N4—Zn1—N4^i	121.29 (9)	C9—N4—Zn1	124.61 (13)
N2—N1—Zn1	122.60 (18)		

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

H atoms were placed in calculated positions and treated as riding, with C—H = 0.94 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXTL*.

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