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Tris(1,10-phenanthroline-κ^2N,N')zinc(II) bis(perchlorate) ethanol solvate monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.013 Å
R factor = 0.085
wR factor = 0.168
Data-to-parameter ratio = 12.8

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

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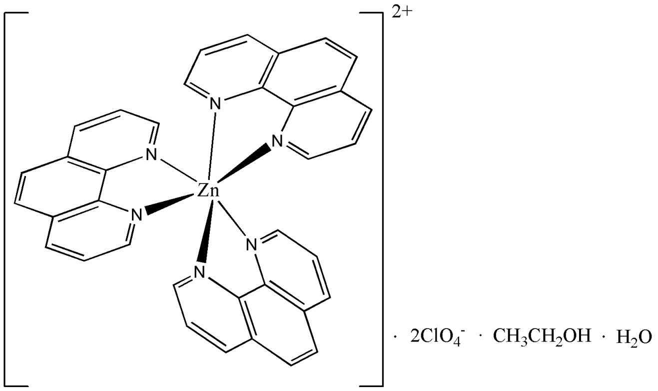
The title compound, $[Zn(C_{12}H_8N_2)_3](ClO_4)_2\cdot C_2H_6O\cdot H_2O$, was crystallized from an aqueous ethanol (1:1) solution of $Zn(ClO_4)_2\cdot 6H_2O$ and 1,10-phenanthroline. The Zn atom is six-coordinated by six N atoms from three 1,10-phenanthroline ligands, with a slightly distorted octahedral geometry.

Comment

The interaction of polypyridyl transition metal complexes with DNA has attracted considerable interest. Most attention has focused upon complexes that are capable of binding to DNA in an intercalation mode. To date, complexes of Ru^{2+}, Rh^{3+} (Watson *et al.*, 1999; Kane-Maguire & Langford, 2001), Co^{3+} (Zhang *et al.*, 2001) and Cr^{3+} (Barker *et al.*, 2001) have been reported. We are interested in related complexes containing zinc because of its ability to adopt coordination numbers of 4, 5 and 6 and to change its coordination geometry comparatively easily. In this paper, we report the synthesis and structure of the title compound, (I).



(I)

The structure of the cation and the crystal packing of (I) are illustrated in Figs. 1 and 2, respectively. Selected geometric parameters are listed in Table 1. The asymmetric unit of (I) contains one $[Zn(phen)_3]^{2+}$ cation (phen is 1,10-phenanthroline), two $[ClO_4]^-$ anions, an ethanol molecule and a water molecule. The bite angles of the three phen ligands are 77.1 (2), 76.7 (2) and 76.6 (2)° for N1—Zn1—N2, N3—Zn1—N4 and N5—Zn1—N6, respectively; these are similar to corresponding values in related systems (Ejsmont *et al.*, 2002). The nominal *trans* octahedral angles are all very similar: N1—Zn1—N4, N2—Zn1—N5 and N3—Zn1—N6 are 163.66 (18), 166.27 (19) and 169.3 (2)°, respectively. The three phen ligands, phen1 (N1/N2/C1—C12), phen2 (N3/N4/C13—C24) and phen3 (N5/N6/C25—C36), are almost planar, with

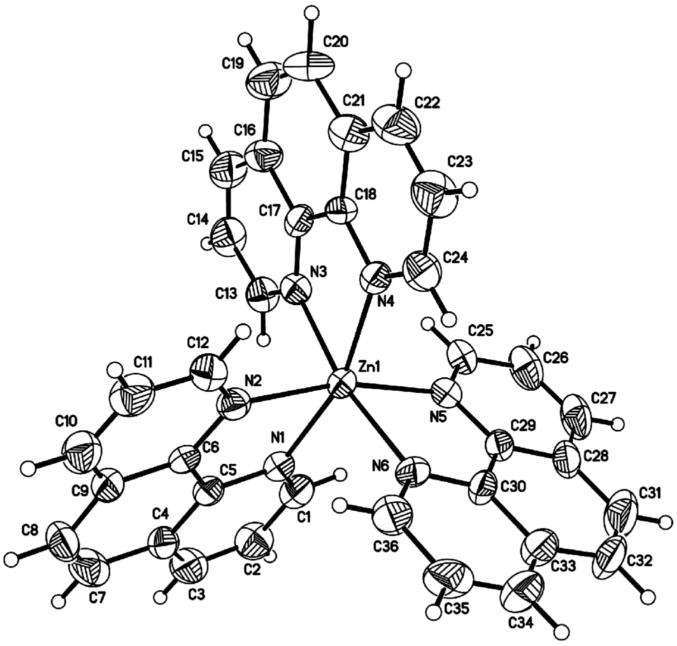


Figure 1
The structure of the complex cation in (I) (30% probability ellipsoids; H atoms are shown as small spheres of arbitrary radii).

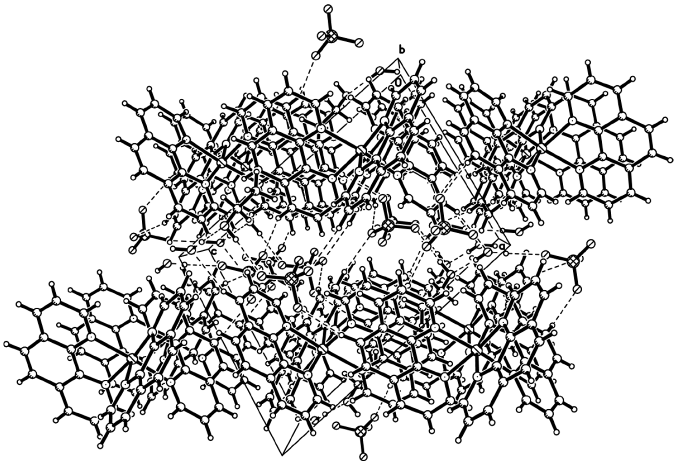


Figure 2
Packing diagram of (I). Hydrogen bonds are shown as dashed lines.

respective r.m.s. deviations from their mean planes of 0.0141, 0.0302 and 0.0132 Å, respectively. The dihedral angle between phen1 and phen2 is 89.94 (9)°, with corresponding values of 75.63 (9)° for phen2 and phen3, and 85.78 (8)° for phen1 and phen3.

Experimental

$Zn(ClO_4)_2 \cdot 6H_2O$ (1 mmol, 0.371 g) and $C_{12}H_8N_2 \cdot H_2O$ (3 mmol, 0.594 g) were dissolved in a 1:1 ethanol–water solution (10 ml). The reaction mixture was refluxed for 30 min and cooled to room temperature. Colorless crystals of (I) suitable for X-ray crystallography were obtained after about a month by slow evaporation of the solvent.

Crystal data

$[Zn(C_{12}H_8N_2)_3](ClO_4)_2 \cdot C_2H_6O \cdot H_2O$
$M_r = 868.97$
Triclinic, $P\overline{1}$
$a = 11.313$ (2) Å
$b = 12.907$ (3) Å
$c = 14.483$ (3) Å
$\alpha = 83.049$ (3)°
$\beta = 76.301$ (3)°
$\gamma = 68.085$ (3)°
$V = 1905.0$ (7) Å^3
$Z = 2$
$D_x = 1.515$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1357 reflections
$\theta = 2.8$–18.8°
$\mu = 0.85$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.784$, $T_{max} = 0.920$
9332 measured reflections
6568 independent reflections
3678 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$
$h = -13 \rightarrow 13$
$k = -15 \rightarrow 12$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.085$
$wR(F^2) = 0.168$
$S = 1.00$
6568 reflections
515 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N4	2.142 (5)	Zn1—N2	2.166 (5)
Zn1—N5	2.154 (5)	Zn1—N6	2.178 (5)
Zn1—N1	2.162 (5)	Zn1—N3	2.179 (5)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O10—H10A⋯O5^{i}	0.81	2.15	2.947 (14)	170
O9—H9A⋯O10^{i}	0.89	1.89	2.78 (2)	178
O9—H9B⋯O2^{ii}	0.88	1.91	2.788 (17)	178

Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $-x, 1 - y, 2 - z$.

H atoms on oxygen were located in difference Fourier maps and refined as riding in their as-found relative positions. H atoms on carbon were placed in idealized positions, with C—H = 0.93 (CH), 0.97 (CH_2) or 0.96 Å (CH_3), and constrained to ride on their carrier atoms. The isotropic displacement parameters of the H atoms were fixed at $1.2U_{eq}$ (CH and CH_2) and $1.5U_{eq}$ (CH_3, OH and H_2O) of their carrier atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL/PC*.

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