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Infinite hydrogen-bonded chains in tris(1,10-phenanthroline)zinc(II) nitrate bis(glutaric acid) dihydrate

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Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.003 Å
Disorder in solvent or counterion
R factor = 0.036
wR factor = 0.065
Data-to-parameter ratio = 15.2

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

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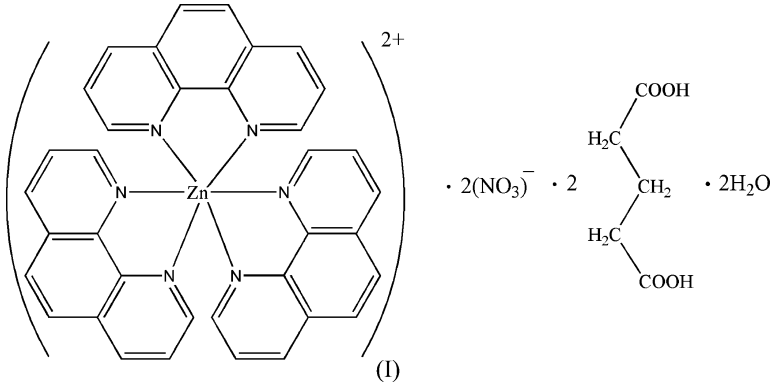
The cation of the title complex, $[Zn(C_{12}H_8N_2)_3](NO_3)_2\cdot 2C_5H_8O_4\cdot 2H_2O$, contains a six-coordinate Zn atom with a distorted octahedral geometry, with three 1,10-phenanthroline molecules as bidentate ligands, and lies on a twofold rotation axis. The asymmetric unit also contains an uncoordinated nitrate anion, a glutaric acid molecule and a water molecule. The anions and neutral molecules of the crystal structure are connected together by O—H···O hydrogen bonds, forming infinite chains, and the complex cations are located between the chains.

Comment

A number of Zn^{II} complexes with one (Zhang & Janiak, 2001), two (Moghimi *et al.*, 2005; Zhu *et al.*, 2005; Yang *et al.*, 2003) and three (Moghimi *et al.*, 2005; Wei *et al.*, 2004; Ejsmont *et al.*, 2002) 1,10-phenanthroline ligands have been prepared and structurally characterized previously. The above complexes, with neutral ligands, have counter-ions. The structure of the title compound, (I), contains a cationic complex, $[Zn(C_{12}H_8N_2)_3]^{2+}$, accompanied by two nitrate anions for charge balance.



(I)

As shown in Fig. 1, the complex cation has twofold rotation symmetry. This cation has appeared in the literature with different counter-ions such as perchlorate (Wei *et al.*, 2004), dichromate (Ejsmont *et al.*, 2002), hydrogen bis(pyridine-2,6-dicarboxylate) and nitrate (Moghimi *et al.*, 2005). The central Zn atom in (I) is coordinated by six N atoms from three bidentate 1,10-phenanthroline ligands. All Zn—N bond distances are almost equal and in good agreement with the previous reports. The geometry of the complex is distorted octahedral. The deviations from ideal octahedral bond angles (Table 1) are a consequence of chelate ring formation. However, larger deviations were observed in the previous reports (Wei *et al.*, 2004; Ejsmont *et al.*, 2002). Twofold disorder is observed for O6 and O7 of the nitrate anion. The

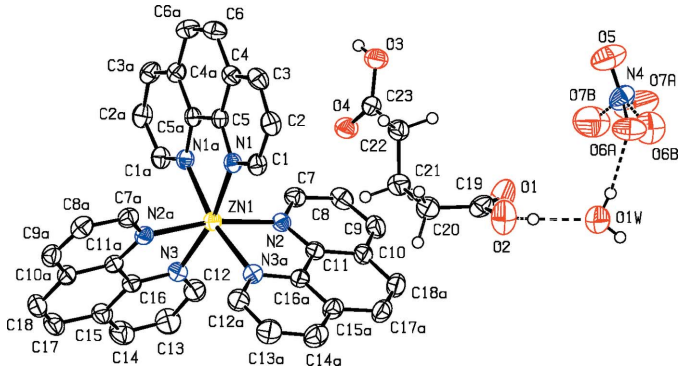


Figure 1
The molecular structure of compound (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probabilty level. Both disorder components of the anion are shown. Dashed lines represent hydrogen bonds. [Symmetry code: (*a*) $-x, y, \frac{1}{2}-z$.]

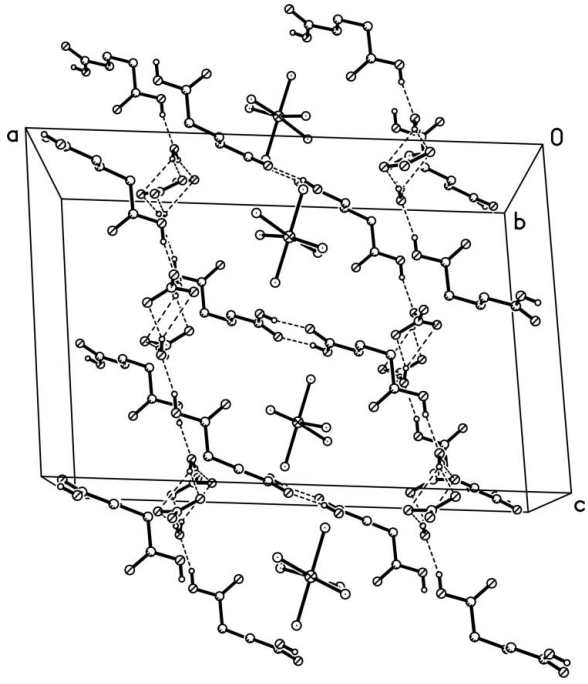


Figure 2
Crystal packing of compound (I), showing hydrogen-bonded (dashed lines) chains. The complex cations are shown as ZnN_6 fragments for clarity, located between the chains.

presence of nitrate ions as well as uncoordinated glutaric acid and water molecules leads to the most important characteristic of the complex, the presence of strong hydrogen-bonding interactions, with O···O distances ranging from 2.598 (2) to 2.952 (11) Å (Table 2). The O atoms of the nitrate ions, the glutaric acid molecules and the water molecules are involved in hydrogen bonds. Each glutaric acid molecule is connected to another acid molecule through two equivalent hydrogen bonds, forming an eight-membered ring of two carboxylic acid groups (Fig. 2). The other carboxyl group of glutaric acid forms a hydrogen bond with a water molecule (Fig. 1 and Table 2). The water molecule acts as a bridge, connecting the glutaric acid molecule to the nitrate anion and forming a hydrogen-bonded chain, as shown in Fig. 2.

Experimental

An aqueous solution containing $Zn(NO_3)_2{\cdot}4H_2O$, 1,10-phenanthroline and glutaric acid in a 1:2:2 molar ratio was refluxed for 2 h. Crystals were obtained after two weeks at room temperature.

Crystal data

$[Zn(C_{12}H_8N_2)_3](NO_3)_2{\cdot}2C_5H_8O_4{\cdot}2H_2O$
$M_r = 1030.28$
Monoclinic, $C2/c$
$a = 21.923$ (4) Å
$b = 14.532$ (3) Å
$c = 14.820$ (3) Å
$\beta = 95.351$ (14)°
$V = 4700.9$ (15) Å^3
$Z = 4$
$D_x = 1.456$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
$\theta = 8$–14°
$\mu = 0.60$ mm^{-1}
$T = 193$ (2) K
Prism, orange
0.2 × 0.15 × 0.1 mm

Data collection

Rebuilt Syntex P2$_1$/Siemens P3 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: none
5202 measured reflections
5067 independent reflections
3736 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.0°$
$h = -11 \rightarrow 28$
$k = -14 \rightarrow 18$
$l = -18 \rightarrow 18$
2 standard reflections
every 98 reflections
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.066$
$S = 0.99$
5067 reflections
334 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.004P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.1478 (16)	Zn1—N2	2.1683 (15)
Zn1—N3	2.1572 (16)		
N1—Zn1—N1^{i}	77.90 (8)	N3—Zn1—N2^{i}	77.40 (6)
N1—Zn1—N3^{i}	93.11 (6)	N1—Zn1—N2	93.73 (5)
N1—Zn1—N3	167.83 (6)	N3—Zn1—N2	95.20 (6)
N3^{i}—Zn1—N3	96.90 (9)	N2^{i}—Zn1—N2	168.96 (8)
N1—Zn1—N2^{i}	94.85 (6)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1*W*	0.82	1.80	2.598 (2)	166
O3—H3···O4^{ii}	0.82	1.84	2.649 (2)	171
O1*W*—H1*W*1···O6*B*^{iii}	0.82	2.04	2.774 (11)	149
O1*W*—H1*W*1···O7*A*^{iii}	0.82	2.09	2.869 (3)	160
O1*W*—H1*W*2···O6*A*	0.82	2.00	2.795 (3)	163
O1*W*—H1*W*2···O6*B*	0.82	2.13	2.952 (11)	175
O1*W*—H1*W*2···O7*B*	0.82	2.17	2.776 (9)	131

Symmetry codes: (ii) $-x, -y+2, -z+1$; (iii) $-x-\frac{1}{2}, -y+\frac{3}{2}, -z+2$.

H atoms attached to O atoms were found in a difference Fourier synthesis; others were placed in geometrically calculated positions. All were refined using a riding model, with O—H = 0.82 Å, C—H = 0.95 or 0.99 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(O)$.

Data collection: *P3/PC* (Siemens, 1989); cell refinement: *P3/PC*; data reduction: *P3/PC*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure:

SHELXTL; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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