

Liang Wang, Guang-Bo Che* and
Chun-Bo LiuDepartment of Chemistry, Jilin Normal
University, Siping 136000, People's Republic of
ChinaCorrespondence e-mail:
guangbochejl@yahoo.com

Key indicators

Single-crystal X-ray study
 $T = 292\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
 R factor = 0.074
 wR factor = 0.193
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.A new Zn^{II} coordination polymer with
intermolecular $\pi-\pi$ interactions: catena-
poly[[aqua(dipyrido[3,2-*a*:2',3'-*c*]phenazine)-
zinc(II)]- μ -benzene-1,4-dicarboxylato]

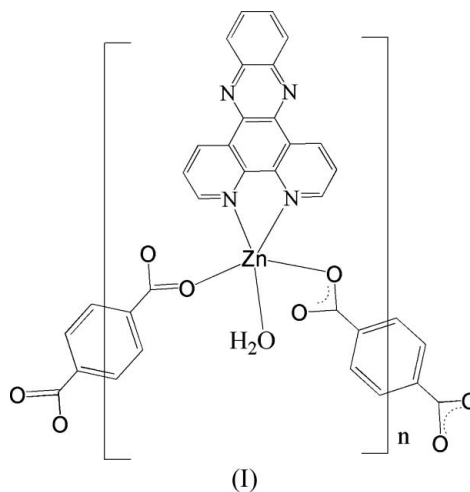
In the title compound, $[\text{Zn}(1,4\text{-BDC})(L)]_n$, where 1,4-BDC is the benzene-1,4-dicarboxylate dianion, $\text{C}_7\text{H}_3\text{O}_4\text{N}^{2-}$, and L is dipyrido[3,2-*a*:2',3'-*c*]phenazine, $\text{C}_{18}\text{H}_{10}\text{N}_4$, each Zn^{II} atom is five-coordinated by two N atoms (from one dipyrido[3,2-*a*:2',3'-*c*]phenazine ligand) and three O atoms (from two monodentate benzene-1,4-dicarboxylate ligands and one water molecule). The Zn^{II} atoms are bridged by benzene-1,4-dicarboxylate ligands, forming a one-dimensional chain structure. Neighboring one-dimensional chains interact through $\pi-\pi$ contacts, leading to a two-dimensional supramolecular structure, and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds complete the structure.

Received 6 July 2006

Accepted 22 August 2006

Comment

Studies on metal dicarboxylato complexes with heteroaromatic N -donor chelating ligands are of special interest (Che, Liu, Cui & Li, 2006). 1,10-Phenanthroline (phen) and its derivatives are important ligands with numerous uses in the construction of metal-organic complexes (Che, Xu & Liu, 2006). Supramolecular architectures containing the dipyrido[3,2-*a*:2',3'-*c*]phenazine (L) ligand have received considerably less attention. We selected benzene-1,4-dicarboxylic acid (1,4- H_2BDC) as a linker and L as a secondary ligand, forming a new coordination polymer, $[\text{Zn}(1,4\text{-BDC})(L)]_n$ (I), which is reported here.



In (I), each Zn^{II} atom is five-coordinated by three O atoms from two different BDC ligands and one water molecule, and two N atoms from one L ligand. The coordination environment is intermediate between square pyramidal and trigonal-

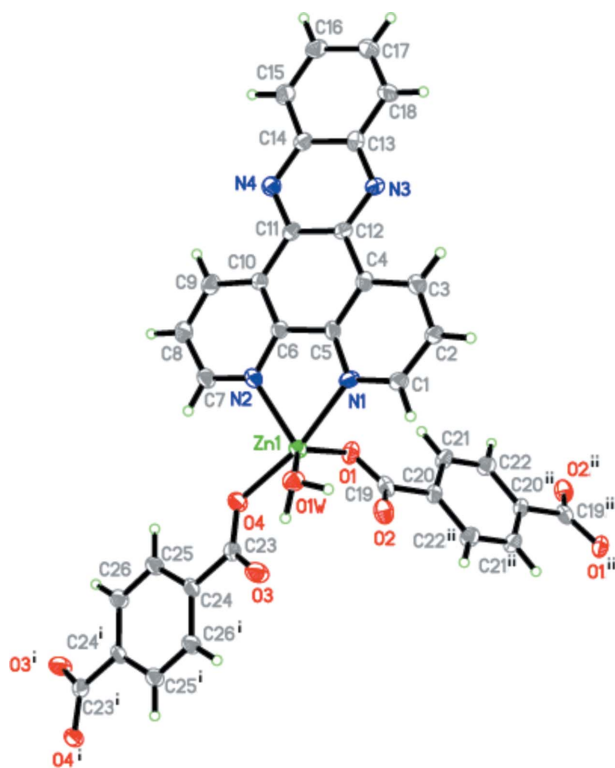


Figure 1
View of the local coordination of compound (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) $1 - x, 1 - y, -z$; (ii) $2 - x, -y, -z$.]

bipyramidal ($\tau = 0.51$; Addison *et al.*, 1984), but will be discussed in terms of a distorted trigonal-bipyramidal coordination (Fig. 1). Atoms O1*W*, O1 and N2 form the equatorial plane, whereas N1 and O4 occupy the axial positions, with Zn1–N1 and Zn1–O4 distances of 2.179 (4) and 2.036 (4) Å, respectively (Table 1). Neighbouring Zn^{II} atoms are bridged by 1,4-BDC ligands, forming a single-chain structure (Fig. 2).

Neighbouring single chains are connected through π – π interactions between *L* ligands with a π – π stacking distance of *ca.* 3.54 Å, resulting in a two-dimensional supramolecular structure (Fig. 3). Clearly, the aromatic–aromatic interactions help to stabilize and influence the structure of (I). O–H...O hydrogen bonds involving the water molecules as donors and carboxylate O atoms as acceptors (Table 2) complete the structure of (I).

Experimental

Ligand *L* was synthesized according to the literature method of Dickeson & Summers (1970). A methanol solution (15 ml) of *L* (0.5 mmol) was added slowly to an aqueous solution (12 ml) of ZnCl₂·H₂O (0.5 mmol) and 1,4-H₂BDC (0.5 mmol) with stirring. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for several days, yielding colorless crystals of (I) (31% yield based on Zn).

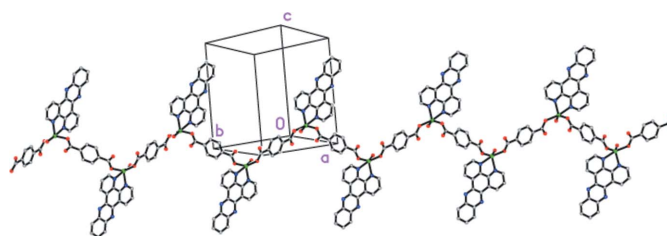


Figure 2
View of the one-dimensional chain structure of (I). H atoms have been omitted.

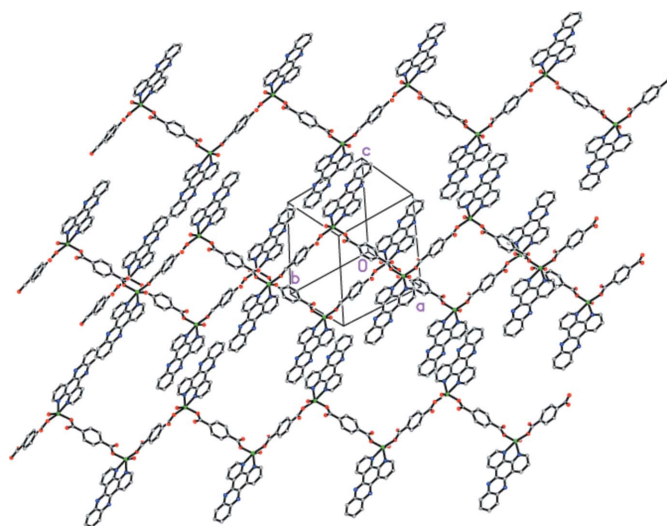


Figure 3
View of the two-dimensional superamolecular structure of (I) built up via π – π interactions. H atoms have been omitted.

Crystal data

[Zn(C₇H₃NO₄)(C₁₈H₁₀N₄)]
 $M_r = 529.80$
 Monoclinic, $P2_1/n$
 $a = 10.389$ (2) Å
 $b = 14.007$ (3) Å
 $c = 15.023$ (3) Å
 $\beta = 94.61$ (3)°
 $V = 2179.0$ (8) Å³

$Z = 4$
 $D_x = 1.615$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.18$ mm⁻¹
 $T = 292$ (2) K
 Block, colorless
 $0.27 \times 0.24 \times 0.21$ mm

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.721, T_{\max} = 0.785$

19770 measured reflections
 4919 independent reflections
 2633 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.125$
 $\theta_{\max} = 27.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.074$
 $wR(F^2) = 0.193$
 $S = 1.01$
 4919 reflections
 333 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0937P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.97$ e Å⁻³
 $\Delta\rho_{\min} = -0.66$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—O4	2.036 (4)	Zn1—N2	2.131 (5)
Zn1—O1W	2.040 (4)	Zn1—N1	2.179 (4)
Zn1—O1	2.062 (4)		
O4—Zn1—O1W	89.92 (17)	O1—Zn1—N2	98.23 (18)
O4—Zn1—O1	101.96 (16)	O4—Zn1—N1	167.79 (17)
O1W—Zn1—O1	137.19 (17)	O1W—Zn1—N1	89.28 (17)
O4—Zn1—N2	93.60 (16)	O1—Zn1—N1	86.81 (16)
O1W—Zn1—N2	122.17 (18)	N2—Zn1—N1	76.58 (16)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—HW12...O2 ⁱ	0.92 (2)	1.83 (3)	2.719 (6)	162 (8)
O1W—HW11...O3	0.92 (4)	1.69 (3)	2.567 (6)	159 (5)

Symmetry code: (i) $-x + 1, -y, -z$.

All H atoms on C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atoms

of water molecules were located in difference Fourier maps and their positions and U_{iso} values were freely refined.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

The authors thank Jilin Normal University for supporting this work.

References

- Addison, A. A., Rao, T. N., Reedijk, J., van Rijn, J. & Verschoor, G. C. (1984). *J. Chem. Soc. Dalton Trans.* pp. 1349–1356.
- Che, G.-B., Liu, C.-B., Cui, Y.-C. & Li, C.-B. (2006). *Acta Cryst.* **E62**, m1362–m1364.
- Che, G.-B., Xu, Z.-L. & Liu, C.-B. (2006). *Acta Cryst.* **E62**, m1370–m1372.
- Dickeson, J. E. & Summers, L. A. (1970). *Aust. J. Chem.* **23**, 1023–1027.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.