Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[[μ-4,4′-bipyridine-bis[aquazinc(II)]]-di-μ-benzene-1,3-dicarboxylato] dihydrate]

Ling-Yun Zhang[a] and Xian-Zhong Sun[b]*

[a]Department of Technology, Guangdong Police Officers College, Guangzhou, Guangdong 510230, People's Republic of China, and [b]Department of Chemistry, Luoyang Normal University, Luoyang, Henan 471022, People's Republic of China

Correspondence e-mail: sxz1226@yahoo.com.cn

Received 27 July 2006
Accepted 23 August 2006

Key indicators

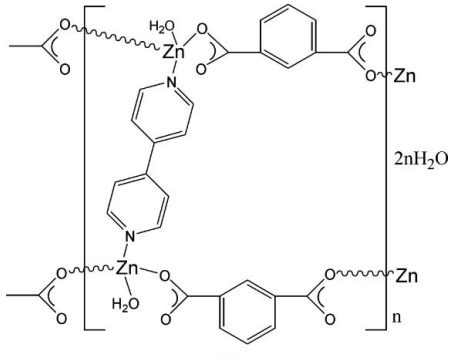
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.072
wR factor = 0.216
Data-to-parameter ratio = 13.8

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

The title one-dimensional coordination polymer, $\{[Zn_2(C_8H_4O_4)_2(C_{10}H_8N_2)(H_2O)_2]\cdot 2H_2O\}_n$, was synthesized by hydrothermal synthesis. Two asymmetric units, $C_{13}H_{10}NO_5Zn\cdot H_2O$, make up each monomer, such that the benzene-1,3-dicarboxylate ligands link Zn^{II} atoms, forming a one-dimensional linear chain, with two adjacent chains bridged by bpy ligands into a ladder running along the *b* axis. These ladders are assembled into three-dimensional networks *via* hydrogen bonds between the coordinated water and the carboxylate O atoms in adjacent ladders. Further hydrogen bonding connects uncoordinated water molecules to the coordinated water, carboxyl O atoms and other solvent water molecules.

Comment

The construction of supramolecular architectures is currently of great interest owing to their intriguing network topologies and potential functions such as adsorption, shape-selective catalysis and ion exchange, as well as for non-linear and magnetic materials (Lehn, 1995). Multicarboxylate ligands have various possible coordination modes to furnish a variety of polymeric structures with adjustable dimensions and show a great variation in functional characters (Tao *et al.*, 2000). 4,4′-Bipyridine and its analogues have been extensively utilized to bridge metal centers, leading to interesting metal-organic frameworks (Tong *et al.* 1999). We have been pursuing synthetic strategies to obtain one-dimensional coordination polymers by the use of V-shaped dicarboxylate dianions together with bipyridyl-like linkers as the principal building blocks, and report here the crystal structure of a new complex, $[Zn_2(mba)_2(bpy)(H_2O)_2]\cdot 2H_2O$ (mba is *m*-phthalate and bpy is 4,4′-bipyridine), (I).



(I)

Complex (I) consists of one-dimensional ladder-like coordination frameworks. The asymmetric unit consists of one

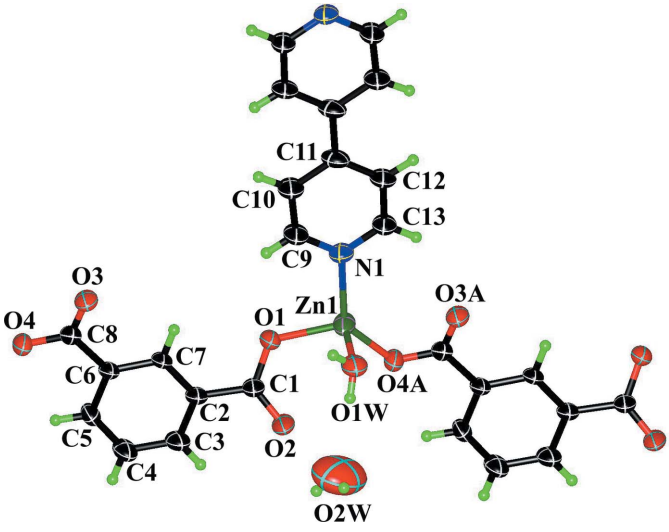


Figure 1
View of (I), showing the atom-labelling scheme and 50% probability displacement ellipsoids [symmetry code: (A) x, $1 + y$, z]. Unlabelled atoms are related to labelled atoms by the symmetry operations (x, $1 + y$, z) (atoms O1–O4/C1–C8) and ($-x$, $-y$, $1 - z$) (atoms N1/C9–C13).

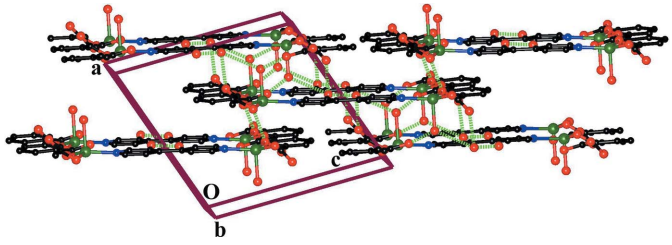


Figure 2
Packing diagram, viewed along the b axis. Dashed lines indicate hydrogen bonds. H atoms have been omitted for clarity.

Zn^{II} atom, one mpa ligand, one half 4,4′-bpy ligand, one coordinated water and one uncoordinated water molecule. As shown in Fig. 1, each Zn^{II} atom is coordinated by one N atom from a bridging 4,4′-bpy ligand, two O atoms from the carboxylate groups of two mpa ligands and one O atom from the coordinated H_2O to furnish a tetrahedral geometry (Fig. 1 and Table 1). The V-shaped mpa ligand acts in a bis-monodentate coordination mode bridging adjacent Zn^{II} atoms to form linear chains running along the b axis. Adjacent chains are connected by 4,4′-bpy ligands, forming one-dimensional ladders running along the b axis. These ladders are assembled into three-dimensional networks *via* O—H···O hydrogen bonds. The hydrogen bonds are formed by the coordinated water and the carboxyl O atom (O1W···O3 = 2.71 Å); the coordinated water and the uncoordinated water (O1W···O2W = 2.88 Å); the uncoordinated water and the carboxyl O atom [O2W···O2 = 2.62 Å and O2W···O2^{i} = 3.08 Å, symmetry code: (i) x, $1 + y$, z]; and the uncoordinated water molecules (O2W···O2W = 2.24 Å) (Fig. 2 and Table 2). Thermogravimetric analysis (TGA) shows a weight loss corresponding to the liberation of water molecules in the range of 323–413 K, and a weight loss corresponding to the liberation of the 4,4′-bpy and mpa above 675 K.

Experimental

A mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (1.0 mmol), H_2mpa (0.5 mmol), bpy (1.0 mmol), NaOH (1.0 mmol) and water (10 ml) was stirred for 15 min in air, then transferred to and sealed in a 23 ml Teflon-lined reactor, which was heated at 433 K for 5 d and then cooled to room temperature at a rate of 5 K h^{-1}. Colorless prisms were obtained, washed with deionized water and absolute ethanol (yield > 30% based on Zn). Elemental analysis (%) for $C_{13}H_{12}NO_6Zn$ calculated: C 45.44, H 3.52, N 4.08; found C 45.50, H 3.59, N 4.00.

Crystal data

$[Zn_2(C_8H_4O_4)_2(C_{10}H_8N_2)(H_2O)_2]{\cdot}2H_2O$
M_r = 343.61
Monoclinic, $P2_1/n$
a = 11.73 (1) Å
b = 9.863 (6) Å
c = 12.23 (1) Å
β = 109.07 (2)°
V = 1336 (2) Å^3
Z = 4
D_x = 1.708 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.87 mm^{-1}
T = 293 (2) K
Block, colorless
0.50 × 0.46 × 0.44 mm

Data collection

Siemens R3m diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.456, T_{max} = 0.494
(expected range = 0.406–0.440)
2757 measured reflections
2628 independent reflections
1533 reflections with $I > 2\sigma(I)$
R_{int} = 0.118
θ_{max} = 26.0°
2 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.216
S = 1.06
2628 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1095P)^2 + 1.2922P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O4^{i}	1.944 (5)	Zn1—N1	2.068 (6)
Zn1—O1	2.007 (5)	Zn1—O1W	2.130 (6)
O4^{i}—Zn1—O1	116.1 (2)	O4^{i}—Zn1—O1W	99.1 (2)
O4^{i}—Zn1—N1	135.3 (2)	O1—Zn1—O1W	99.4 (2)
O1—Zn1—N1	103.0 (2)	N1—Zn1—O1W	94.8 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O2W	0.85	2.03	2.88 (1)	179
O1W—H1WB···O3^{ii}	0.85	1.87	2.71 (1)	173
O2W—H2WB···O2	0.85	2.32	2.62 (1)	101
O2W—H2WB···O2W^{iii}	0.85	1.48	2.24 (2)	147
O2W—H2WA···O2^{iii}	0.85	2.54	3.08 (2)	122

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

H atoms bonded to C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding on their parent atoms, with U_{iso}(H) =

1.2U_{eq}(C). H atoms bonded to O atoms were located in difference maps and refined as riding on their parent atoms (O—H = 0.85 Å), with U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *R3m Software* (Siemens, 1990); cell refinement: *R3m Software*; data reduction: *R3m Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL* (Bruker, 2000); molecular graphics: *SHELXTL* and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *SHELXTL* and *OLEX*.

This work was supported by the Education Department of Henan Province.

References

Bruker (2000). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Dolomanov, O. V., Blake, A. J., Champness, N. R. & Schröder, M. (2003). *J. Appl. Cryst.* **36**, 1283–1284.
Lehn, J. M. (1995). *Supramolecular Chemistry*. Weinheim: VCH.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXS97*, University of Göttingen, Germany.
Siemens (1990). *R3m Software*. Version 4.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tao, J., Tong, M.-L., Shi, J.-X., Chen, X.-M. & Ng, S. W. (2000). *Chem. Commun.* pp. 2043–2044.
Tong, M.-L., Chen, X.-M., Ye, B.-H. & Ji, L.-N. (1999). *Angew. Chem. Int. Ed.* **38**, 2237–2240.