

**catena-Poly[[aqua(1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)]- $\mu$ -5-[4-(hydroxymethyl)benzyloxy]isophthalato- $\kappa^3O^1,O^1':O^3$ -[aqua(1,10-phenanthroline- $\kappa^2N,N'$ )zinc(II)]- $\mu$ -5-[4-(hydroxymethyl)benzyloxy]isophthalato- $\kappa^2O^1:O^3$ ]**

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Received 23 July 2007

Accepted 20 September 2007

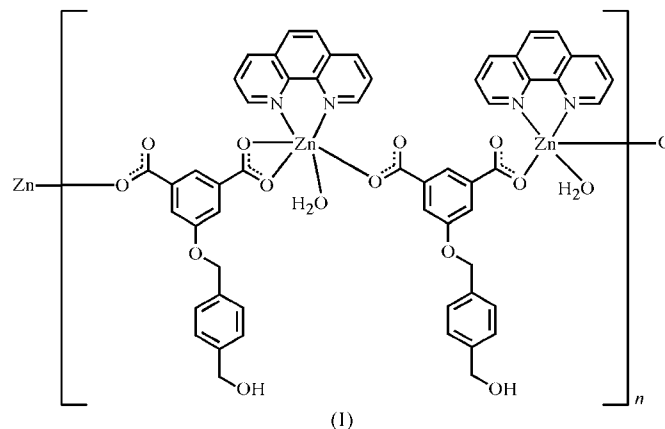
Online 13 October 2007

The title compound,  $[Zn_2(C_{16}H_{12}O_6)_2(C_{12}H_8N_2)_2(H_2O)_2]_n$ , consists of linear chains formed through 5-[4-(hydroxymethyl)benzyloxy]isophthalate (mabobdc) ligands linking five- and six-coordinated  $Zn^{II}$  ions. The linear chains are linked into a bilayer network *via* O—H...O hydrogen bonds. Adjacent bilayer structures are further linked with each other *via* C—H...O hydrogen bonds and  $\pi$ – $\pi$  and C—H... $\pi$  interactions to give a three-dimensional supramolecular framework. The results demonstrate the coordination and supramolecular chemistry of the mabobdc ligand.

### Comment

Considerable progress has been made recently on the crystal engineering of supramolecular architectures organized and sustained by means of coordinate covalent supramolecular contacts (such as hydrogen bonds and  $\pi$ – $\pi$  interactions), aurophilicity interactions, and so on (Colacio *et al.*, 2002; Roesky & Andruh, 2003; Guilera & Steed, 1999). As an excellent building block in the design and construction of supramolecular polymers, 1,10-phenanthroline (1,10-phen) is relatively well known. Multicarboxylate ligands are good candidates for the construction of hydrogen-bonding networks. 5-[4-(Hydroxymethyl)benzyloxy]isophthalic acid ( $H_2$ mabobdc) not only has two rigid carboxyl groups but also one flexible hydroxyl group. Thus, the mabobdc ligand may be a suitable ligand not only in the construction of coordination compounds but also in the construction of supramolecular networks. We report here the novel title Zn supramolecular complex,  $[Zn_2(mabobdc)_2(1,10\text{-phen})_2(H_2O)_2]_n$ , (I), which is

the first example of the coordination and supramolecular chemistry of the mabobdc ligand (Cambridge Structural Database, Version 5.28; Allen, 2002).

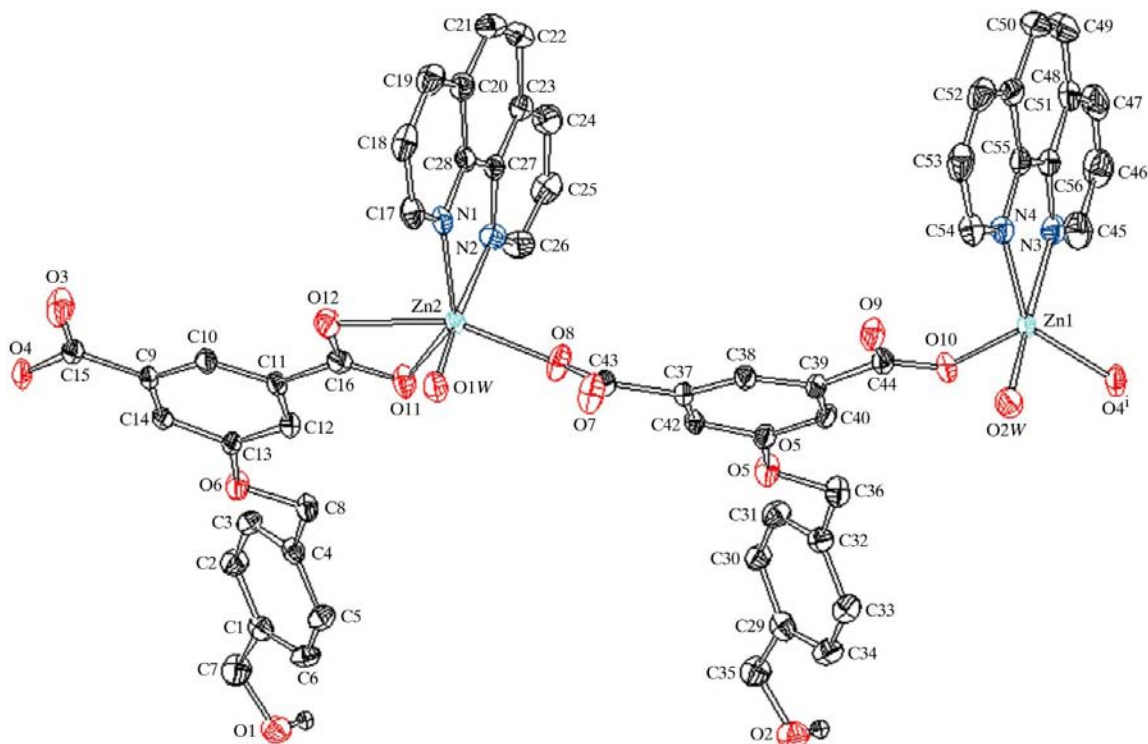


There are two crystallographically independent mabobdc ligands in (I) (Fig. 1). One of these acts as a bidentate bridging ligand linking atoms Zn1 and Zn2 in a monodentate mode, while the other ligand bridges atoms Zn1 and Zn2 in monodentate and chelate fashions, respectively. The mabobdc ligands thus connect the  $Zn^{II}$  centres to form a novel metal–organic chain in which 1,10-phen molecules act as terminal chelating ligands. Atom Zn1 has a distorted trigonal–bipyramidal coordination, with the equatorial plane defined by atom N4 from a 1,10-phen ligand and two O atoms [O10 and O4 ( $x, 1 - y, z$ )] from two monodentate carboxylate groups of two mabobdc ligands. Atom N3 from the 1,10-phen ligand and water atom O2W occupy the apical positions (Table 1). Atom Zn2 has distorted octahedral coordination, with the basal plane consisting of the 1,10-phen atoms N1 and N2, atom O11 from one chelating carboxylate group of a mabobdc ligand and water atom O1W. The apical sites are occupied by atoms O8 and O12 of two mabobdc ligands (Table 1).

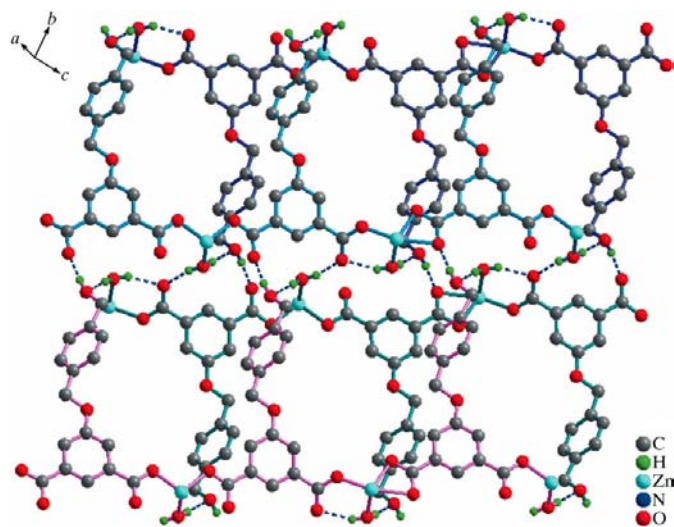
In (I), the Zn–O bond distances lie in the range 2.012 (5)–2.315 (5) Å, which is greater than that in  $\{[Zn_3\{5\text{-}(\text{carboxylatomethoxy})\text{isophthalate}\}_2(\text{phen})_3\cdot 2H_2O\}_n$ , (II) [Zn–O = 2.083 (3)–2.268 (7) Å; Cao *et al.*, 2004]. The Zn–N bond lengths are in the range 2.119 (5)–2.215 (5) Å, which is longer than those reported in (II) [Zn–N = 2.098 (4)–2.112 (6) Å; Cao *et al.*, 2004].

The chains of (I) are linked by O—H...O hydrogen bonds consisting of two different hydroxy and two different carboxylate O atoms (O1—H1...O12<sup>ii</sup> and O2—H2A...O9<sup>ii</sup>; all symmetry codes as in Table 2), resulting in monolayer sheets (Fig. 2 and Table 2). These sheets are further linked into bilayer structures *via* three O—H...O hydrogen bonds (O1W—H1D...O1<sup>iii</sup>, O2W—H2C...O2<sup>iv</sup> and O2W—H2D...O7<sup>v</sup>), as shown in Fig. 2; details are given in Table 2.

The hydrogen-bonded bilayer structures are further linked by C—H...O hydrogen bonds and  $\pi$ – $\pi$  and C—H... $\pi$  interactions. Three C—H...O hydrogen bonds (Table 2) are formed by C—H groups of 1,10-phen ligands. The principal centroid-to-centroid interactions include  $Cg1...Cg2 = 3.477$  (4) Å [ $Cg1$  is the centroid of the N1/C17–C20/C28 ring and  $Cg2$  is the centroid of the C51–C54/N4/C55 ring at ( $2 - x,$



**Figure 1**  
Part of the structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are plotted at the 30% probability level. Most H atoms have been omitted for clarity. [Symmetry code: (i)  $x, 1 + y, 1 + z$ .]



**Figure 2**  
A view of (I), showing how the O—H...O hydrogen bonds contribute to the construction of the  $[Zn_2(mabobdc)_2(1,10\text{-phen})_2(H_2O)_2]_n$  two-dimensional bilayer network, with hydrogen bonds shown as dashed lines. 1,10-Phen ligands have been omitted for clarity.

$3 - y, 1 - z]$  and  $Cg3 \cdots Cg3^* = 3.711(4) \text{ \AA}$  [ $Cg3$  is the centroid of the C9–C14 ring and  $Cg3^*$  is the centroid of the same ring at  $(1 - x, 1 - y, -z)$ ]. The principal C—H... $\pi$  interactions are as detailed in Table 2. These interactions serve to generate a three-dimensional supramolecular framework.

## Experimental

The  $H_2mabobdc$  ligand was isolated as a by-product from the reaction of *p*-xylylene dibromide with dimethyl 5-hydroxyisophthalate. A mixture of  $Zn(CH_3CO_2)_2 \cdot 2H_2O$  (0.3 mmol),  $H_2mabobdc$  (0.3 mmol), 1,10-phen (0.3 mmol),  $K_2CO_3$  (0.45 mmol) and water (10 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor and heated at 433 K for 3 d. On completion of the reaction, the reactor was cooled slowly to room temperature and the mixture was filtered, giving yellow single crystals of (I) suitable for X-ray analysis.

### Crystal data

$[Zn_2(C_{16}H_{12}O_6)_2(C_{12}H_8N_2)_2(H_2O)_2]$   $\gamma = 103.8860(10)^\circ$   
 $M_r = 1127.73$   $V = 2383.82(10) \text{ \AA}^3$   
 Triclinic,  $P\bar{1}$   $Z = 2$   
 $a = 10.6016(2) \text{ \AA}$  Mo  $K\alpha$  radiation  
 $b = 12.2791(3) \text{ \AA}$   $\mu = 1.08 \text{ mm}^{-1}$   
 $c = 19.6827(5) \text{ \AA}$   $T = 263(2) \text{ K}$   
 $\alpha = 105.2220(10)^\circ$   $0.30 \times 0.20 \times 0.10 \text{ mm}$   
 $\beta = 92.6320(10)^\circ$

### Data collection

Siemens SMART 1K CCD area-detector diffractometer 12481 measured reflections  
 8350 independent reflections  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996) 6518 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.036$   
 $T_{min} = 0.773, T_{max} = 0.899$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.080$   
 $wR(F^2) = 0.200$   
 $S = 1.08$   
 8350 reflections  
 693 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{max} = 0.60 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.69 \text{ e \AA}^{-3}$

**Table 1**  
Selected bond lengths (Å).

Zn1—O10	2.012 (5)	Zn2—O11	2.102 (5)
Zn1—O4 <sup>i</sup>	2.013 (5)	Zn2—O1W	2.126 (5)
Zn1—N4	2.119 (5)	Zn2—N1	2.129 (6)
Zn1—O2W	2.145 (5)	Zn2—N2	2.201 (6)
Zn1—N3	2.215 (6)	Zn2—O12	2.315 (5)
Zn2—O8	2.018 (5)		

Symmetry code: (i)  $x, y + 1, z + 1$ .**Table 2**  
Hydrogen-bond geometry (Å, °).

Cg1, Cg2 and Cg4 are the centroids of the N1/C17–C20/C28, C51–C54/N4/C55 and C29–C34 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ O12 <sup>ii</sup>	0.82	1.99	2.796 (7)	167
O2—H2A $\cdots$ O9 <sup>ii</sup>	0.82	1.87	2.665 (8)	165
O1W—H1C $\cdots$ O7	0.82	2.05	2.776 (7)	147
O1W—H1D $\cdots$ O1 <sup>iii</sup>	1.02 (10)	1.80 (10)	2.797 (7)	164 (8)
O2W—H2C $\cdots$ O2 <sup>iv</sup>	0.82	2.06	2.876 (8)	179
O2W—H2D $\cdots$ O7 <sup>v</sup>	0.86 (10)	2.05 (10)	2.870 (8)	160 (10)
C3—H3 $\cdots$ O12 <sup>vi</sup>	0.93	2.58	3.460 (9)	158
C19—H19 $\cdots$ O3 <sup>vii</sup>	0.93	2.42	3.150 (9)	135
C45—H45 $\cdots$ O11 <sup>viii</sup>	0.93	2.51	3.176 (10)	128
C2—H2B $\cdots$ Cg1 <sup>vi</sup>	0.93	2.75	3.558 (8)	146
C30—H30 $\cdots$ Cg2 <sup>viii</sup>	0.93	2.78	3.604 (8)	149
C24—H24 $\cdots$ Cg4 <sup>ix</sup>	0.93	2.81	3.609 (8)	145
C53—H53 $\cdots$ Cg4 <sup>x</sup>	0.93	2.69	3.400 (8)	134

Symmetry codes: (ii)  $x - 1, y - 1, z$ ; (iii)  $-x, -y + 1, -z$ ; (iv)  $-x, -y + 2, -z + 1$ ; (v)  $-x + 1, -y + 3, -z + 1$ ; (vi)  $-x + 1, -y + 1, -z$ ; (vii)  $-x + 2, -y + 2, -z$ ; (viii)  $-x + 1, -y + 2, -z + 1$ ; (ix)  $x + 1, y, z$ ; (x)  $x + 1, y + 1, z$ .

H atoms bonded to C atoms were positioned geometrically and treated as riding, with aromatic C—H = 0.93 Å and aliphatic C—H = 0.97 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . H atoms bonded to O atoms were positioned geometrically and treated as riding, with O—H =

0.82 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ , except for the two H atoms on the water molecules, which were located in a difference Fourier map and refined freely.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Version 2.1c; Bergerhoff *et al.*, 1996); software used to prepare material for publication: *SHELXTL* (Siemens, 1996).

The authors acknowledge financial support from the Natural Science Foundation of Fujian Province (grant No. 2006F3042), the Education Office of the Science Research Foundation of Fujian Province (grant No. JB06073) and the Undergraduate Students' Extracurricular Technology Project of Fujian Normal University (grant No. BKL2007032).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FG3050). Services for accessing these data are described at the back of the journal.

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