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catena-Poly[[[diaqua(2-sulfonatobenzoato-κ²O:O′)zinc(II)]-μ₂-1,3-di-4-pyridylpropane-κ²N:N′] N,N-dimethylformamide solvate]

In the title compound, $[Zn(C_7H_4O_5S)(C_{13}H_{14}N_2)(H_2O)_2]\cdot C_3H_7NO$, the Zn^{II} atom is coordinated by two N atoms from two 1,3-di-4-pyridylpropane molecules, two O atoms from one 2-sulfonatobenzoate dianion and two aqua O atoms, in a distorted octahedral geometry. The 2-sulfonatobenzoate dianions function as chelating ligands and the 1,3-di-4-pyridylpropane as a μ_2-bridging ligand, forming a chain. O—H···O hydrogen bonds link neighbouring chains into a three-dimensional network.

Comment

2-Sulfobenzoic acid (*o*-H$_2$sb), a ligand with a combination of one sulfonic group and one carboxyl group, is a good ligand for the preparation of metal–organic coordination polymers (Li & Yang, 2004; Xiao, 2005; Xiao, Shi & Cheng, 2005; Su *et al.*, 2005; Zhang *et al.*, 2005). The flexible ligand 1,3-di-4-pyridylpropane (dpp) can rotate freely to coordinate to two metal ions (Li, Cao *et al.*, 2004; Xiao, Wang *et al.*, 2005). In this work, we used both *o*-H$_2$sb and dpp to construct the title compound, $[Zn(dpp)(o\text{-}sb)(H_2O)_2]_n \cdot nDMF$, (I) (DMF is dimethylformamide).

(I)
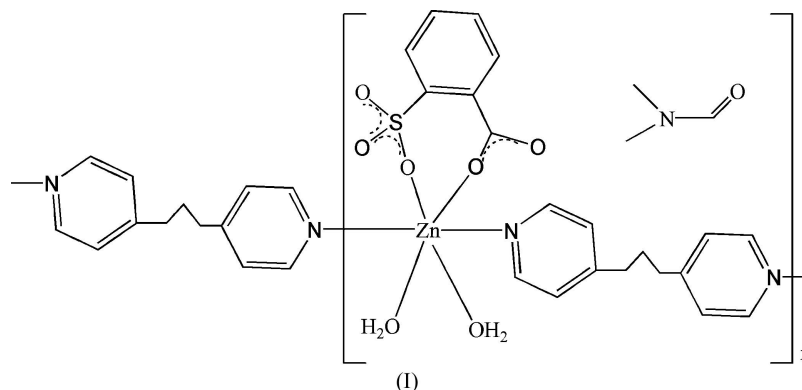
In compound (I), the Zn^{II} atom is in a distorted octahedral geometry, coordinated by two aqua O atoms, two O atoms of a 2-sulfonatobenzoate dianion and two N atoms of two 1,3-di-4-pyridylpropane molecules (Fig. 1 and Table 1). The *o*-sb ligand chelates to the Zn^{II} centre, forming a seven-membered ring. The dihedral angle between the planes of the *o*-sb ring and its carboxylate group is 115.6 (3)°, which is much larger than in the complex $[Ni(o\text{-}sb)(bpe)(H_2O)_2]_n \cdot 0.25nH_2O$ [bpe is 1,2-bis(4-pyridyl)ethylene; Xiao, Li & Hu, 2005]. The C1—O1 bond [1.268 (5) Å] is longer than the C1—O2 distance [1.230 (5) Å]. The 1,3-di-4-pyridylpropane ligands function as μ_2-bridging ligands, forming a chain (Fig. 2).
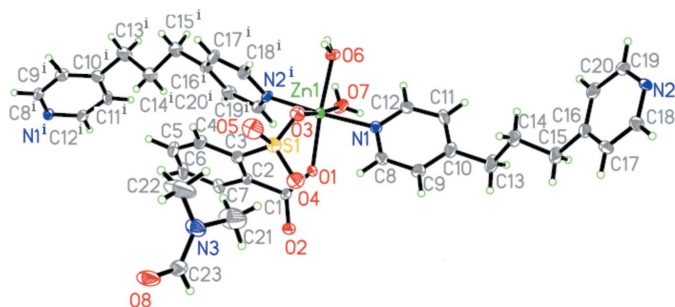
Figure 1
The coordination environment of the Zn^{II} atom in (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [Symmetry code: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$.]

The stability of the solid-state structure of (I) is significantly enhanced by hydrogen-bonding interactions (Table 2). The voids in this structure are filled by *N,N*-dimethylformamide solvent molecules, which are linked by hydrogen bonds.

Experimental

An aqueous solution (10 ml) of $Zn(CH_3CO_2)_2 \cdot 2H_2O$ (0.20 mmol, 0.051 g) was added slowly to an *N,N*-dimethylformamide solution (10 ml) of 1,3-di-4-pyridylpropane (0.20 mmol, 0.040 g) and 2-sulfobenzoic acid (0.20 mmol, 0.041 g). Colourless crystals of (I) suitable for X-ray analysis were obtained by leaving the solution at room temperature for three weeks.

Crystal data

$[Zn(C_7H_4O_5S)(C_{13}H_{14}N_2)(H_2O)_2] \cdot C_3H_7NO$	$Z = 8$
$M_r = 572.95$	$D_x = 1.464$ Mg m^{-3}
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 16.933$ (4) Å	$\mu = 1.08$ mm^{-1}
$b = 10.918$ (3) Å	$T = 298$ (2) K
$c = 28.116$ (6) Å	Prism, colourless
$V = 5198$ (2) Å^3	$0.32 \times 0.18 \times 0.16$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	26390 measured reflections
φ and ω scans	4736 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	4326 reflections with $I > 2\sigma(I)$
$T_{min} = 0.725, T_{max} = 0.847$	$R_{int} = 0.050$
	$\theta_{max} = 25.3°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 10.3016P]$
$R[F^2 > 2\sigma(F^2)] = 0.072$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.141$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.35$	$\Delta\rho_{max} = 0.68$ e Å^{-3}
4736 reflections	$\Delta\rho_{min} = -0.41$ e Å^{-3}
327 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.075 (3)	Zn1—O3	2.128 (3)
Zn1—O7	2.099 (3)	Zn1—N1	2.142 (4)
Zn1—O6	2.118 (3)	Zn1—N2^i	2.161 (3)
O1—Zn1—O7	92.54 (13)	O6—Zn1—N1	88.65 (13)
O1—Zn1—O6	175.51 (11)	O3—Zn1—N1	90.10 (13)
O7—Zn1—O6	86.65 (13)	O1—Zn1—N2^i	95.92 (13)
O1—Zn1—O3	93.43 (12)	O7—Zn1—N2^i	85.50 (14)
O7—Zn1—O3	173.88 (13)	O6—Zn1—N2^i	88.42 (13)
O6—Zn1—O3	87.50 (13)	O3—Zn1—N2^i	92.52 (14)
O1—Zn1—N1	86.96 (13)	N1—Zn1—N2^i	175.98 (14)
O7—Zn1—N1	91.58 (13)		

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

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O6—H6A$\cdots$O1^{ii}	0.82	2.04	2.860 (4)	175
O6—H6B$\cdots$O8^{iii}	0.82	1.89	2.707 (5)	176
O7—H7A$\cdots$O2^{ii}	0.82	1.83	2.637 (5)	168
O7—H7B$\cdots$O8^{iv}	0.82	1.85	2.667 (5)	171

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

H atoms were placed in calculated positions and refined using a riding-model approximation, with C—H distances ranging from 0.93 to 0.97 Å for H atoms bonded to C and O—H distances of 0.82 Å. U_{iso}(H) values were set to $1.2U_{eq}$(C,O) or 1.5(C$_{methyl}$). The methyl groups were allowed to rotate but not to tip.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXT*L (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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