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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.044  
 $wR$  factor = 0.098  
Data-to-parameter ratio = 15.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**catena-Poly[[aqua(2,2'-bipyridine- $\kappa^2\text{N},\text{N}'$ )zinc(II)]-  
 $\mu$ -4-carboxylatophenoxyacetato- $\kappa^3\text{O},\text{O}':\text{O}''$ ]**

In the title coordination polymer,  $[\text{Zn}(\text{C}_9\text{H}_6\text{O}_5)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]_n$ , the  $\text{Zn}^{\text{II}}$  ion displays a distorted octahedral coordination configuration, defined by two N atoms from the 2,2'-bipyridine ligand, three carboxylate O atoms from two 4-carboxylatophenoxyacetate dianions and one water molecule. Adjacent  $\text{Zn}^{\text{II}}$  atoms are linked by carboxylate groups into zigzag chains with a  $\text{Zn} \cdots \text{Zn}$  separation of 9.710 (3) Å across the chains. Intermolecular hydrogen bonds serve to assemble the chains into a double-chain structure.

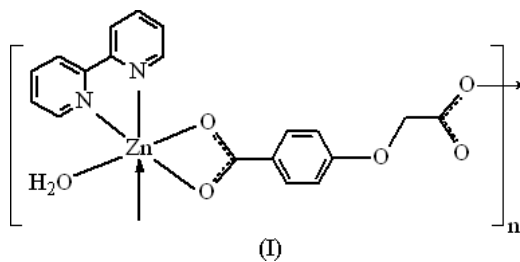
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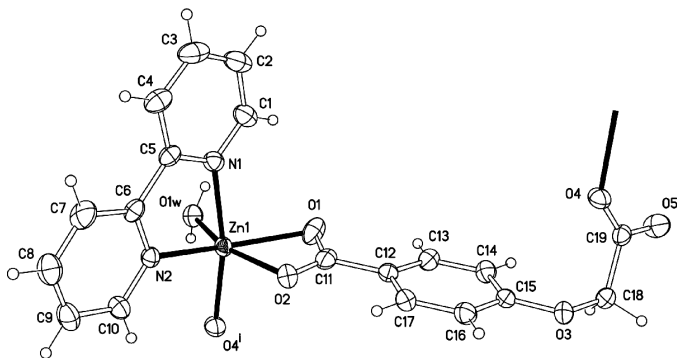
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## Comment

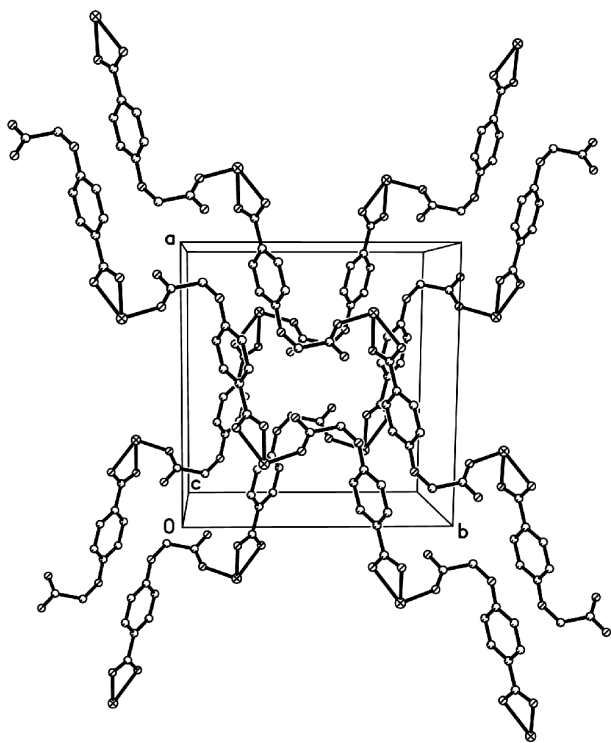
4-Carboxyphenoxyacetic acid (4-cpoaH<sub>2</sub>), which is a biologically active compound and widely used in agriculture, is a good candidate for the construction of supramolecular systems. It is a bifunctional ligand that not only is capable of binding to metal centers with versatile binding modes but also forms classical hydrogen bonds as both donor and acceptor. As a contribution to this field, we have recently reported the structures of mononuclear  $\text{Mg}^{\text{II}}$  and  $\text{Cu}^{\text{II}}$  complexes (Gao, Li *et al.*, 2004; Gao, Yue *et al.*, 2004), and one one-dimensional  $\text{Mn}^{\text{II}}$  polymer, in which the  $\text{Mn}^{\text{II}}$  ion exists in a distorted pentagonal bipyramidal coordination environment and the 4-cpoa<sup>2-</sup> group acts as a tetradentate bridging ligand (Gu *et al.*, 2004). In order to gain further insight into the metal-binding modes of the 4-cpoa<sup>2-</sup> ligand, we have now introduced the  $\text{Zn}^{\text{II}}$  ion and 2,2'-bipy molecule into the coordination system of the 4-cpoa<sup>2-</sup> ligand, producing the title coordination polymer,  $[\text{Zn}(4\text{-cpoa})(2,2'\text{-bipy})(\text{H}_2\text{O})]_n$  (I).



As depicted in Fig. 1, the  $\text{Zn}^{\text{II}}$  center is in a distorted octahedral coordination defined by two N atoms from 2,2'-bipy ligand, three carboxylate O atoms from two 4-cpoa<sup>2-</sup> groups and one water molecule. The  $\text{Zn}-\text{O}4^i$  distance [2.070 (2) Å; symmetry code: (i)  $x + \frac{1}{2}, y + \frac{1}{2}, z$ ] is significantly shorter than the  $\text{Zn}-\text{O}1$  and  $\text{Zn}-\text{O}2$  distances [2.210 (2)–2.221 (3) Å]. Atoms O1, O2, N2 and O1W constitute the equatorial plane, with an r.m.s. deviation of 0.12 (3) Å, the Zn atom being displaced from the plane by 0.13 (4) Å. Atoms N1 and O4<sup>i</sup> occupy the apical sites. The small bite angle of the



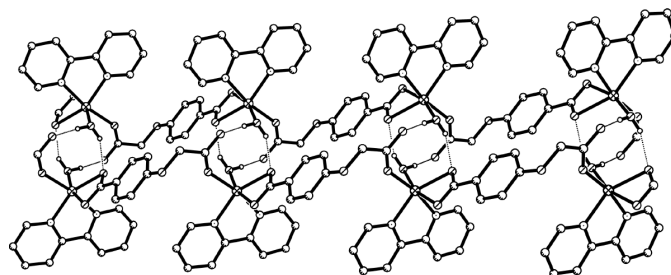
**Figure 1**  
The repeat unit of (I), showing 30% probability ellipsoids and the atomic labeling. The symmetry code is as given in Table 1.



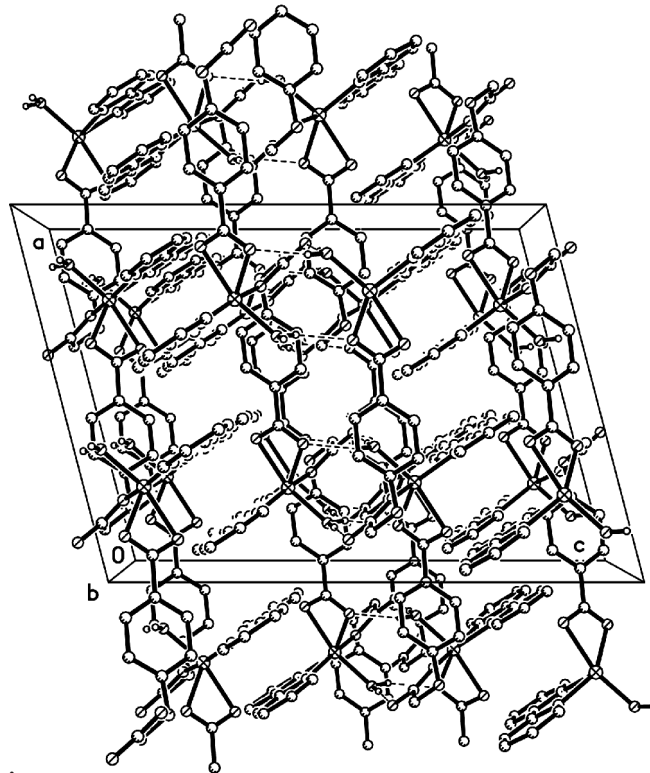
**Figure 2**  
The zigzag chains of (I) running along two distinct directions. The 2,2'-bipyridine molecules and H atoms have been omitted for clarity.

carboxylate group [ $O1-Zn-O2 = 59.30(9)^\circ$ ] indicates the main distortion of the octahedral geometry. The two C—O bond distances of each carboxylate group are almost identical, suggesting electron delocalization (Table 1). The carboxylate group  $O1-C11-O2$  and the attached benzene ring are nearly coplanar, while the oxyacetate group is twisted out of the benzene ring plane.

Adjacent  $Zn^{II}$  atoms are joined by the  $4-cpoa^{2-}$  groups through monodentate and bidentate chelation, forming zigzag chains along  $[110]$  and  $[\bar{1}10]$ . The  $Zn \cdots Zn$  separation across the chain is  $9.710(3) \text{ \AA}$  (see Fig. 2). Two adjacent chains are further interlinked through hydrogen bonds between the coordinated water molecule and O atoms of carboxylate groups (Table 2), leading to a double-chain structural motif, as



**Figure 3**  
The double-chain structure of (I) constructed by hydrogen bonds (dashed lines). H atoms attached to C have been omitted for clarity.



**Figure 4**  
Packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms attached to C have been omitted for clarity.

illustrated in Fig. 3. The terminal 2,2'-bipy ligands are located at both sides of the double chain. Furthermore, these chains are stacked in an offset manner through  $\pi$ - $\pi$  stacking interactions between 2,2'-bipy ligands [centroid-centroid distance =  $3.553(3) \text{ \AA}$ ]; in this way, a two-dimensional supramolecular network is constructed, as shown in Fig. 4.

## Experimental

The title complex was synthesized by the addition of zinc diacetate dihydrate (4.40 g, 20 mmol), and 2,2'-bipyridine (3.12 g, 20 mmol) to a hot aqueous solution of 4-carboxyphenoxyacetic acid (3.92 g, 20 mmol); the pH was then adjusted to 6 with 0.2 M NaOH. The solution was allowed to evaporate at room temperature, and colorless prismatic crystals of (I) were obtained over a period of several days. Elemental analysis calculated: C 52.62, H 3.72, N 6.46%; found: C 52.75, H 3.66, N 6.50%.

Crystal data

[Zn(C<sub>9</sub>H<sub>6</sub>O<sub>5</sub>)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)]  
*M<sub>r</sub>* = 433.73  
 Monoclinic, *C*<sub>2</sub>/*c*  
*a* = 14.234 (3) Å  
*b* = 13.210 (3) Å  
*c* = 19.522 (4) Å  
 β = 104.56 (3)°  
*V* = 3552.9 (14) Å<sup>3</sup>  
*Z* = 8

*D<sub>x</sub>* = 1.622 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 14284 reflections  
 θ = 3.3–27.4°  
 μ = 1.42 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Prism, colorless  
 0.34 × 0.25 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer  
 ω scans  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
*T<sub>min</sub>* = 0.643, *T<sub>max</sub>* = 0.794  
 16561 measured reflections

4067 independent reflections  
 2998 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.053  
 θ<sub>max</sub> = 27.5°  
*h* = -18 → 17  
*k* = -16 → 17  
*l* = -25 → 25

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.044  
*wR* (*F*<sup>2</sup>) = 0.099  
*S* = 1.03  
 4067 reflections  
 259 parameters  
 H atoms treated by a mixture of independent and constrained refinement

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0464*P*)<sup>2</sup> + 3.0155*P*]  
 where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3  
 (Δ/σ)<sub>max</sub> = 0.001  
 Δρ<sub>max</sub> = 0.44 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.30 e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Zn1–N1	2.191 (2)	Zn1–O1W	2.032 (2)
Zn1–N2	2.096 (2)	O1–C11	1.258 (4)
Zn1–O1	2.210 (2)	O2–C11	1.255 (4)
Zn1–O2	2.221 (3)	O4–C19	1.254 (3)
Zn1–O4 <sup>i</sup>	2.070 (2)	O5–C19	1.246 (4)
N1–Zn1–O1	90.13 (9)	O4 <sup>i</sup> –Zn1–O1	101.94 (9)
N1–Zn1–O2	92.87 (9)	O4 <sup>i</sup> –Zn1–O2	91.45 (9)
N2–Zn1–N1	76.43 (9)	O1W–Zn1–N1	88.78 (9)
N2–Zn1–O1	149.76 (9)	O1W–Zn1–N2	104.94 (9)
N2–Zn1–O2	93.96 (9)	O1W–Zn1–O1	101.67 (9)
O1–Zn1–O2	59.30 (9)	O1W–Zn1–O2	160.87 (9)
O4 <sup>i</sup> –Zn1–N1	167.74 (9)	O1W–Zn1–O4 <sup>i</sup>	90.88 (9)
O4 <sup>i</sup> –Zn1–N2	91.83 (9)		
N1–C5–C6–N2	-1.4 (3)	C15–O3–C18–C19	74.7 (3)
O1–C11–C12–C13	-6.9 (4)	C18–O3–C15–C14	0.9 (4)

Symmetry code: (i) ½ + *x*, ½ + *y*, *z*.

Table 2

Hydrogen-bonding 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–H1W1···O1 <sup>ii</sup>	0.84 (3)	2.04 (2)	2.726 (3)	139 (3)
O1W–H1W2···O5 <sup>iii</sup>	0.85 (3)	1.75 (3)	2.596 (3)	176 (4)

Symmetry codes: (ii) ½ – *x*, ½ – *y*, 1 – *z*; (iii) 1 – *x*, –*y*, 1 – *z*.

H atoms attached to C were placed in calculated positions [*C*–H = 0.93 or 0.97 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C)] and refined using the riding-model approximation. The H atoms of the water molecule were located in a difference Fourier map and refined with O–H distance restraints of 0.85 (1) Å and with *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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