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Bis(μ-2-carboxylatoethylphosphonato)-bis[aqua(2,2′-bipyridine)zinc(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.026
wR factor = 0.063
Data-to-parameter ratio = 18.0

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

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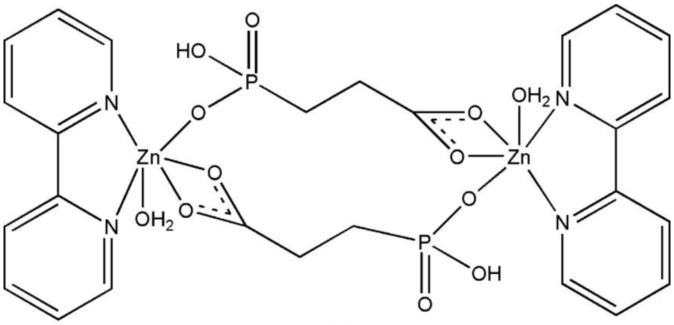
The title compound, $[Zn_2(HO_3PCH_2CH_2COO)_2(C_{10}H_8N_2)_2(H_2O)_2]$, was synthesized by the hydrothermal method. Two zinc ions are linked by two 2-carboxyethylphosphonic acid ligands to form a dimer. These dimers are located on inversion centres and are further interlinked by hydrogen bonds and π–π stacking interactions to form a three-dimensional supramolecular structure.

Comment

In recent years, the chemistry of metal phosphonates has been a research field of rapid expansion, mainly due to their potential application in the areas of catalysis, ion exchange, proton conductivity, intercalation chemistry, photochemistry and materials chemistry (Clearfield 1998). Various kinds of phosphonate ligands have been used (Cheetham *et al.*, 1999; Stock *et al.*, 2000; Serpaggi *et al.*, 1999; Ying *et al.*, 2006). Among these, there are many studies on metal phosphonates which contain carboxylate functional groups (Ayyappan *et al.*, 1999; Gómez-Alcantara *et al.*, 2006; Zhang *et al.*, 2003, 2005). These compounds exhibit various kinds of structure. For example, $[Mn(O_3PCH_2CH_2COOH)]H_2O$ exhibits a two-dimensional layer structure (Gómez-Alcantara *et al.*, 2006). $Pb_3(O_2CCH_2CH_2PO_3)_2$ exhibits a three-dimensional open framework (Ayyappan *et al.*, 1999). However, as far as we are aware, there are only a few reports on metal carboxyalkylphosphonates that contain second ligands (Drumel *et al.*, 1996; Zhang *et al.*, 2003, 2005). As part of a study of the effect of the second ligands on the structure of the metal carboxyalkylphosphonates, we report the synthesis and crystal structure of the title compound, (I).



(I)

The centrosymmetric title compound contains one zinc(II) ion, one doubly deprotonated 2-carboxyethylphosphonic acid ligand, one 2,2′-bipyridine group and one aqua ligand in its asymmetric unit. As shown in Fig. 1, the zinc(II) ion is sixcoordinated by one phosphonate O atom, one water molecule, two carboxylate O atoms and two N atoms from a 2,2′-bipyridine ligand (Table 1). The two zinc(II) ions are linked by two 2-carboxyethylphosphonic acid ligands to form a dimer. These dimers are further interlinked by hydrogen bonds and π–π interactions to form a three-dimensional supramolecular structure (Fig. 2). The hydrogen bonds are formed between the water molecules and the O atoms of the 2-carboxyethylphosphonate ligand (Table 2).

Experimental

A mixture of zinc(II) acetate (0.5 mmol, 0.011 g), 2-carboxyethylphosphonic acid (0.5 mmol, 0.078 g) and 2,2′-bipyridine (0.50 mmol, 0.078 g) in 10 ml of distilled water was sealed in an autoclave equipped with a Teflon liner (20 ml) and then heated at 453 K for 5 d. Crystals of the title compound were obtained.

Crystal data

$[Zn_2(C_3H_5O_5P)_2(C_{10}H_8N_2)_2(H_2O)_2]$
$M_r = 783.22$
Orthorhombic, *Pbca*
$a = 8.6344$ (3) Å
$b = 17.7484$ (6) Å
$c = 20.5928$ (7) Å
$V = 3155.78$ (19) Å^3
$Z = 4$
$D_x = 1.648$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.69$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.37 × 0.28 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.574$, $T_{max} = 0.701$
22393 measured reflections
3885 independent reflections
2606 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.063$
$S = 0.85$
3885 reflections
216 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.9939 (12)	P1—O1	1.4950 (13)
Zn1—O6	2.0384 (14)	P1—O3	1.5048 (13)
Zn1—N2	2.1274 (15)	P1—O2	1.5682 (13)
Zn1—O5	2.1643 (13)	O4—C11	1.246 (2)
Zn1—N1	2.1911 (15)	O5—C11	1.266 (2)
Zn1—O4	2.2734 (14)		
O1—Zn1—O6	94.72 (5)	N2—Zn1—N1	75.49 (6)
O1—Zn1—N2	90.95 (6)	O5—Zn1—N1	90.31 (5)
O6—Zn1—N2	107.89 (6)	O1—Zn1—O4	94.80 (5)
O1—Zn1—O5	102.53 (5)	O6—Zn1—O4	154.03 (6)
O6—Zn1—O5	95.47 (5)	N2—Zn1—O4	96.05 (5)
N2—Zn1—O5	152.01 (5)	O5—Zn1—O4	58.85 (5)
O1—Zn1—N1	166.38 (6)	N1—Zn1—O4	87.94 (5)
O6—Zn1—N1	88.45 (6)		

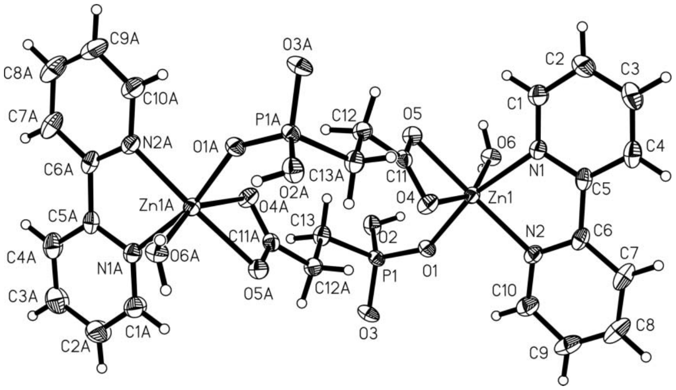


Figure 1
The molecular structure of the title compound with 30% probability displacement ellipsoids. [Symmetry code: (A) $-x$, $-y$, $-z + 1$.]

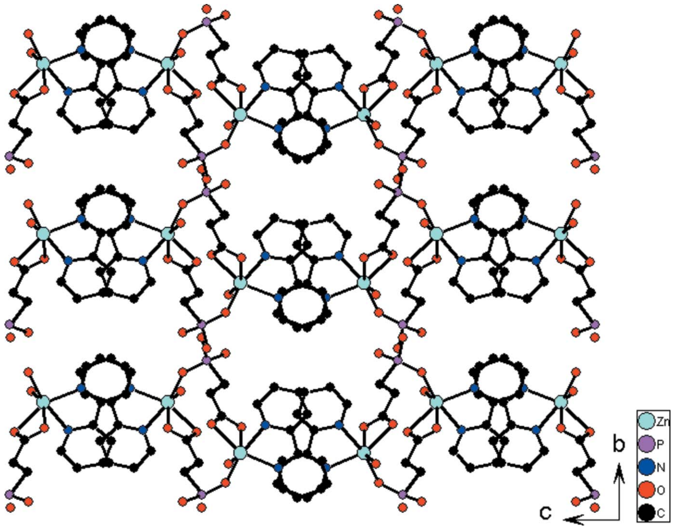


Figure 2
Projection of the title compound along the *a* axis. Hydrogen atoms are omitted for clarity.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O6—H611$\cdots$O5^{i}	0.854 (18)	1.858 (18)	2.7114 (19)	178 (3)
O6—H612$\cdots$O3^{ii}	0.857 (17)	1.820 (18)	2.6638 (18)	168 (2)
O2—H22$\cdots$O3^{ii}	0.82	1.72	2.5294 (18)	169

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

All the C-bound H atoms and the H atoms from the PO_3H group were positioned geometrically, with C—H = 0.93–0.97 Å and O—H = 0.82 Å, and refined in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$. The H atoms of the water molecule were found in a difference Fourier map and refined with the distance restraint O—H = 0.85 Å(3) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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