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μ-4,4′-Bipyridine-κ^2N:N'-bis[triaqua(pyridine-2,4-dicarboxylato-κ^2N,O^2)zinc(II)] dihydrate

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Key indicators

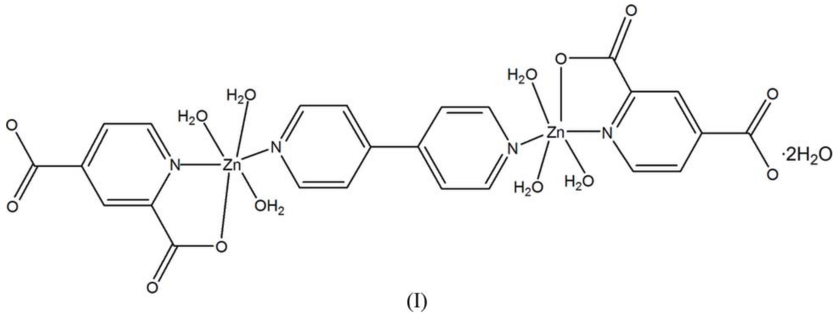
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.036
wR factor = 0.061
Data-to-parameter ratio = 13.8

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

In the centrosymmetric title compound, $[Zn_2(C_7H_3NO_4)_2(C_{10}H_8N_2)(H_2O)_6]\cdot 2H_2O$, each Zn^{II} atom is six-coordinated in an octahedral geometry by one N atom of 4,4′-bipyridine (bpy), one N atom and one O atom of pyridine-2,4-dicarboxylate (pydc) and three water molecules. The crystal structure features O—H···O hydrogen bonds between carboxylate groups and water molecules, and π–π stacking interactions between the bpy and pydc molecules.

Comment

Metal–organic complexes show a variety of supramolecular architectures (Eddaoudi *et al.*, 2001). These metal–organic network structures depend on judicious selections of metal centers and organic ligands that may provide desirable coordination covalent bonds, hydrogen-bonding linkages or π–π interactions for the construction of new supramolecular complexes. The 4,4′-bipyridine (bpy) ligand is a common linker in the construction of metal–organic frameworks, and a wide range of coordination polymers have been generated with it. Pyridinedicarboxylic acids, which can serve as bifunctional ligands, have been utilized to build coordination networks (Zhang & Chen, 2003; Wang *et al.*, 2004; Gu *et al.*, 2004). In this work, we employed pyridine-2,4-dicarboxylate (pydc) and bpy ligands, generating a new dinuclear compound, $[Zn_2(pydc)_2(bpy)(H_2O)_6]\cdot 2H_2O$, (I), under hydrothermal conditions.



(I)

In (I), each Zn^{II} atom is six-coordinated in an octahedral geometry by one N atom from the bpy ligand, one N atom and one O atom from the pydc ligand, and three water molecules (Fig. 1). The compound is binuclear, bridged by a bpy ligand across a center of inversion. π–π Interactions between the bpy and pydc molecules, with a shortest atom-to-atom distance of 3.621 (4) Å between C3 and C10(1 + x, y, z), lead to the formation of a one-dimensional chain structure. The supramolecular bands are linked into a three-dimensional network by O—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

Compound (I) was prepared from a mixture of $Zn(NO_3)_2·6H_2O$ (0.149 g, 0.5 mmol), H_2pydc (0.083 g, 0.5 mmol), bpy (0.078 g, 0.5 mmol) and H_2O (18 ml) in a 30 ml Teflon-lined autoclave under autogenous pressure at 433 K for 5 d. After cooling to room temperature, colorless needle-shaped crystals suitable for X-ray structure analysis were obtained. Analysis calculated for $C_{24}H_{30}N_4O_{16}Zn_2$: C 37.9, H 4.0, N 7.4%; found: C 37.7, H 3.8, N 7.3%.

Crystal data

$[Zn_2(C_7H_3NO_4)_2(C_{10}H_8N_2)(H_2O)_6]·2H_2O$
M_r = 761.26
Monoclinic, $P2_1/c$
a = 10.023 (2) Å
b = 13.941 (3) Å
c = 11.239 (2) Å
β = 106.478 (3)°
V = 1505.9 (5) Å^3
Z = 2
D_x = 1.679 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 292 (2) K
Needle, colorless
0.43 × 0.07 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.860, T_{max} = 0.899
8056 measured reflections
2985 independent reflections
1979 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.061
S = 0.83
2985 reflections
216 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2)]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H12···O2^{i}	0.80	1.81	2.599 (3)	169
O5—H13···O4^{ii}	0.83	1.94	2.744 (3)	165
O6—H11···O1^{iii}	0.78	2.06	2.827 (3)	168
O6—H10···O3^{iv}	0.99	1.73	2.719 (3)	175
O7—H8···O8^{i}	0.92	1.94	2.808 (3)	157
O7—H9···O8^{v}	1.00	1.74	2.735 (3)	171
O8—H1W···O5	0.73	2.17	2.889 (4)	173
O8—H2W···O4^{vi}	0.94	1.75	2.689 (4)	174

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

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms of water molecules were located in a difference Fourier map and refined as riding in their as-found relative positions, with individual isotropic displacement parameters.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

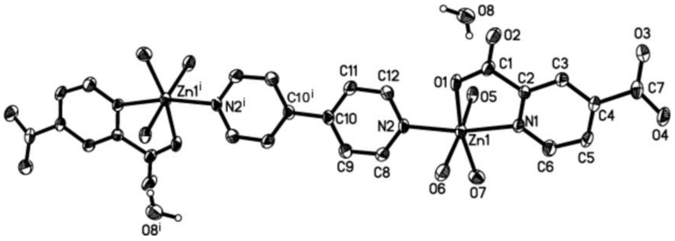


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted except for those of the uncoordinated water molecules. [Symmetry code: (i) $-x, 2-y, -z$.]

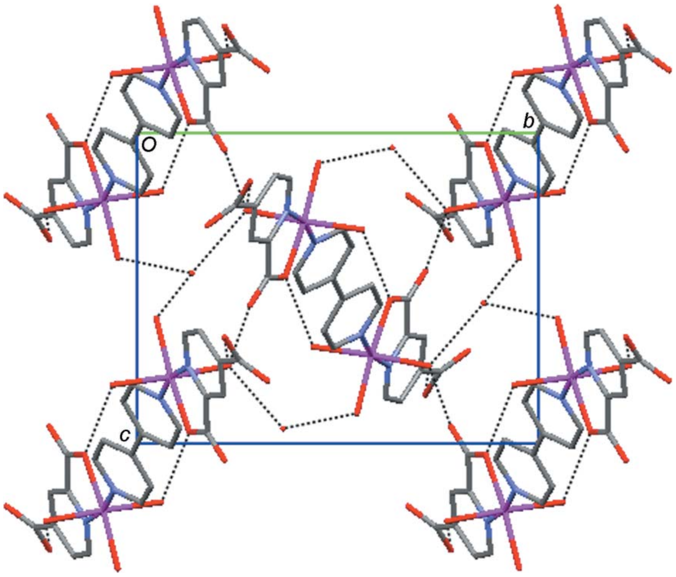


Figure 2
A view of crystal packing along the a axis. Dashed lines indicate hydrogen bonds. H atoms have been omitted for clarity.

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