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# *catena*-Poly[[[di-$\mu$-acetato-1$\kappa^2$*O*:2$\kappa^2$*O*′-bis[(acetato-$\kappa^2$*O*,*O*′)cadmium(II)]]-di-$\mu$-4,4′-bipyridine-1$\kappa$*N*:1′$\kappa$*N*′;2$\kappa$*N*:2′$\kappa$*N*′] monohydrate]

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The title compound, $\{[Cd_2(CH_3COO)_4(C_{10}H_8N_2)_2]\cdot H_2O\}_n$, is a new metal-organic framework structure. The cadmium(II) ion has a distorted octahedral geometry. One of the acetate anions is coordinated to the metal atom in a bidentate chelating mode, whereas the other two anions act as bridges between adjacent $Cd^{II}$ ions. The bipyridine ligands link the cadmium(II) ions, forming a ribbon structure. There is a centre of symmetry midway between the Cd atoms and a twofold rotation axis relating the pyridyl rings, and the water molecule also lies on a twofold rotation axis.

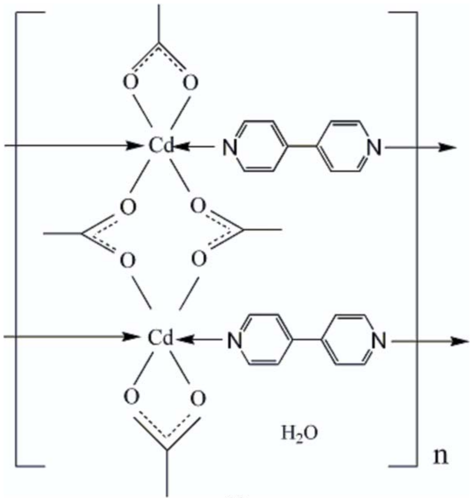
**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean $\sigma$(C–C) = 0.004 Å
*R* factor = 0.026
*wR* factor = 0.066
Data-to-parameter ratio = 16.2

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

## Comment

The construction of metal-organic frameworks (MOFs) is currently receiving considerable attention owing to their potential properties as functional solid materials, as well as their fascinating framework structures (Evans & Lin, 2002; Lu *et al.*, 2001; Li *et al.*, 1999). New materials spur new technologies (Snurr *et al.*, 2004), and these compounds can be potentially useful in gas storage, as molecular sieves, in size- and shape-selective catalysis, in magnetism, in opto-electronic devices, and so on (Eddaoudi *et al.*, 2002; Kitaura *et al.*, 2003; Moulton & Zaworotko, 2001; Millange *et al.*, 2002). These MOF structures can be rapidly, accurately and efficiently synthesized from relatively simple subunits, where the metal ions, multidentate organic ligands, and coordinating bonds are the parameters for directing the self-assembly process. Our studies on the complexation of cadmium(II) salts with 4,4′-bipyridine (bpy) has led to the formation of the title compound, (I).



(I)

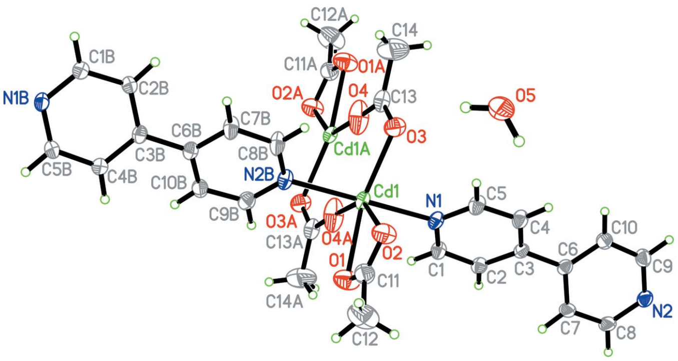


**Figure 1**

A view of part of the polymeric structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. The suffices A and B denote atoms related by the symmetry operators ($\frac{1}{2} - x$, $\frac{1}{2} - y$, $1 - z$) and ($\frac{1}{2} + x$, $\frac{1}{2} - y$, $\frac{1}{2} + z$), respectively.

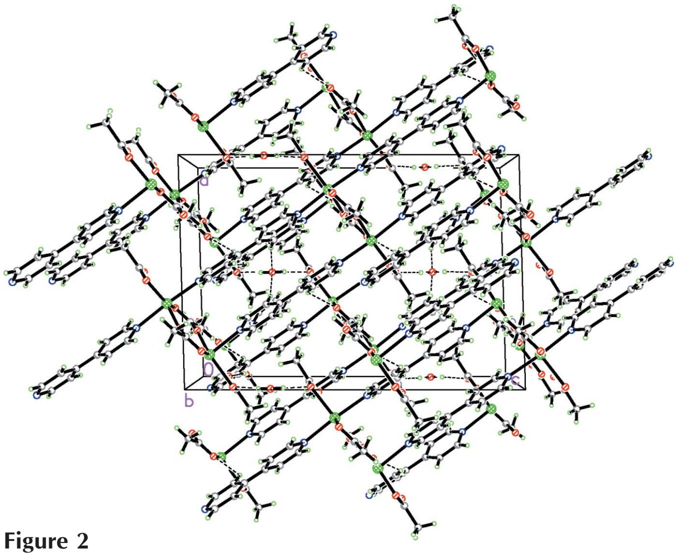


**Figure 2**

The polymeric structure of compound (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

A part of the polymeric structure of compound (I) is shown in Fig. 1, and selected bond distances and angles are listed in Table 1. There is a centre of symmetry midway between the Cd atoms and a twofold rotation axis relating the pyridyl rings, and the water molecule also lies on a twofold rotation axis. Each Cd$^{II}$ centre is six-coordinated by two N atoms (N1 and N2*B*) from two bpy ligands and four O atoms (O1,O2,O3 and O4*A*) from three acetate anions, forming a distorted octahedron. One of the acetate anions is coordinated to the metal atom in a bidentate chelating mode, while the other two anions act as bridges between adjacent Cd$^{II}$ ions. The bpy ligands link the cadmium(II) ions, forming a ribbon structure. Adjacent ribbons are interconnected by O—H···O hydrogen-bonding interactions (Table 2), forming a two-dimensional network (Fig. 2).

## Experimental

Compound (I) was obtained by a hydrothermal reaction. The starting materials, $Cd(OAc)_2 \cdot 4H_2O$ (0.533 g, 2 mmol), 4,4′-bipyridine (0.192 g, 1 mmol) and deionized water (10 ml) were mixed. The resulting suspension was stirred for 1 h, then sealed in a 20 ml stainless-steel bomb with a Teflon liner and heated at 453 K for 4 d. The autoclave was then cooled at 6 K $h^{-1}$ to 373 K. This temperature was maintained for 12 h, and then the system was cooled to room temperature at the same cooling rate. Colourless crystals of (I) were obtained and washed with water.

*Crystal data*

$[Cd_2(C_2H_3O_2)_4(C_{10}H_8N_2)_2] \cdot H_2O$
$M_r = 791.36$
Monoclinic, $C2/c$
$a = 13.5069$ (16) Å
$b = 11.8393$ (14) Å
$c = 19.570$ (2) Å
$\beta = 91.595$ (2)°
$V = 3128.3$ (6) Å$^3$
$Z = 4$

$D_x = 1.680$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 4745 reflections
$\theta = 2.3$–26.3°
$\mu = 1.42$ mm$^{-1}$
$T = 294$ (2) K
Block, colourless
0.22 × 0.18 × 0.12 mm

*Data collection*

Bruker SMART 1000 CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.651$, $T_{max} = 0.844$
8593 measured reflections

3179 independent reflections
2644 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.3°$
$h = -16 \rightarrow 15$
$k = -14 \rightarrow 14$
$l = -24 \rightarrow 16$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.066$
$S = 1.13$
3179 reflections
196 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 1.454P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.39$ e Å$^{-3}$
$\Delta\rho_{min} = -0.57$ e Å$^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cd1—O4$^i$ | 2.296 (2) | Cd1—N1 | 2.338 (2) |
| Cd1—O3 | 2.323 (2) | Cd1—O1 | 2.364 (2) |
| Cd1—N2$^{ii}$ | 2.329 (2) | Cd1—O2 | 2.396 (2) |
| | | | |
| O4$^i$—Cd1—O3 | 124.35 (10) | N2$^{ii}$—Cd1—O1 | 88.22 (9) |
| O4$^i$—Cd1—N2$^{ii}$ | 88.56 (8) | N1—Cd1—O1 | 93.10 (9) |
| O3—Cd1—N2$^{ii}$ | 93.13 (8) | O4$^i$—Cd1—O2 | 146.60 (11) |
| O4$^i$—Cd1—N1 | 87.01 (8) | O3—Cd1—O2 | 88.90 (8) |
| O3—Cd1—N1 | 88.45 (8) | N2$^{ii}$—Cd1—O2 | 93.09 (9) |
| N2$^{ii}$—Cd1—N1 | 175.43 (8) | N1—Cd1—O2 | 91.23 (9) |
| O4$^i$—Cd1—O1 | 92.50 (12) | O1—Cd1—O2 | 54.26 (7) |
| O3—Cd1—O1 | 143.14 (8) | | |

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

**Table 2**

Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O5—H5*A*···O2$^{iii}$ | 0.84 | 2.02 | 2.848 (3) | 172 |

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

Atom H5*A* was located in a difference map and allowed to ride on O5 with O5—H5*A* = 0.84 Å and $U_{iso}(H) = 1.2U_{eq}(O5)$. The remaining H atoms were placed in calculated positions and constrained to ride on their parent C atoms with C—H distances in the range 0.93–0.96 Å

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and $U_{iso}$(H) set at $1.5U_{eq}$(C) for methyl H atoms and $1.2U_{eq}$(C) for other H atoms. The $U^{ij}$ components of atom C14 were restrained to approximate isotropic behaviour.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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, 2000); software used to prepare material for publication: *SHELXTL*.

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