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**Key indicators**

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(C-C)$  = 0.017 Å  
 R factor = 0.063  
 wR factor = 0.142  
 Data-to-parameter ratio = 11.8

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

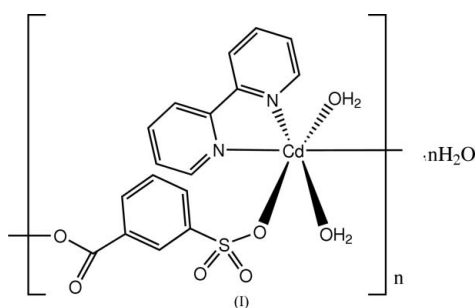
**catena-Poly[[[*cis*-diaqua(2,2'-bipyridine)-  
 cadmium(II)]- $\mu$ -3-sulfonatobenzoato]  
 monohydrate]**

The title complex,  $\{[Cd(C_7H_4O_5S)(C_{10}H_8N_2)(H_2O)_2] \cdot H_2O\}_n$ , which was obtained by hydrothermal synthesis, forms a one-dimensional zigzag chain. The coordination polyhedron of the Cd<sup>II</sup> atom is a distorted octahedron completed by four O atoms from two water molecules and two 3-sulfonatobenzoate ligands, and two N atoms from 2,2'-bipyridine. O—H...O hydrogen bonds give rise to a three-dimensional network.

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**Comment**

Recently, sulfobenzoate metal complexes have received much attention owing to their interesting coordination modes and structural topologies (Fan & Zhu, 2005; Ma *et al.*, 2005). The 4-sulfobenzoate (4-sb)/cadmium(II)/2,2'-bipyridine system under hydrothermal conditions produced a one-dimensional polymer containing a box unit,  $[Cd_2(4-sb)_2(2,2'-bipy)_2(H_2O)_2]_n$ , (II) (Yuan *et al.*, 2001), in which the carboxylate group acts in a chelating-bridging mode. We present here the cadmium(II) complex with the 3-sulfobenzoate (3-sb) ligand, (I), which forms a one-dimensional zigzag chain and is isostructural with the zinc(II) complex (Li *et al.*, 2005). The copper(II) complex with 3-sb and 2,2'-bipyridine has also been reported (Miao *et al.*, 2005).



The Cd<sup>II</sup> atom in (I) has an octahedral geometry defined by two O atoms from two water molecules, two N atoms from 2,2'-bipyridine and two O-atom donors from two 3-sb ligands (Fig. 1 and Table 1). The coordination geometry of (I) is different from that of (II), in which the Cd<sup>II</sup> atom adopts a seven-coordinate geometry. The Cd—O(carboxylate), Cd—N, and Cd—O(sulfonate) distances in (I) are slightly shorter than those of (II). The dihedral angle between the planes of the 3-sb ring and its carboxylate group is 11.5 (16)° and the dihedral angle between the two rings of the 2,2'-bipyridine ligand is 5.5 (6)°. The C7—O5 bond length [1.267 (14) Å] in (I) is longer than the C7—O4 distance [1.219 (15) Å], suggesting the more keto character for the C7—O4 bond. There is a hydrogen bond between the coordinated water molecule and

the uncoordinated carboxylate atom O4. The 3-sb ligands, *cis*-arranged around each Cd<sup>II</sup> atom, bridge the Cd<sup>II</sup> atoms and lead to a one-dimensional zigzag chain (Fig. 2), in which the Cd<sup>II</sup>–Cd<sup>II</sup> separation by 3-sb is 8.4860 (17) Å. Extensive O–H···O hydrogen bonds between the chains generate a three-dimensional hydrogen-bonding architecture (Table 2), which enhances the stability of the structure.

## Experimental

A mixture of Cd(CH<sub>3</sub>COO)<sub>2</sub>·2H<sub>2</sub>O (0.266 g, 1 mmol), sodium hydrogen 3-sulfobenzoate (0.225 g, 1 mmol), 2,2'-bipyridine (0.158 g, 1 mmol) and water (15 ml) was sealed in a 30 ml stainless steel reactor with a Teflon liner, then heated at 423 K for 31 h. After cooling, the clear solution was set aside at room temperature for 4 d. Colorless needle-shaped crystals of (I) were formed and these were filtered off.

### Crystal data

[Cd(C<sub>7</sub>H<sub>4</sub>O<sub>5</sub>S)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)·(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>·H<sub>2</sub>O  
*M<sub>r</sub>* = 522.79  
 Monoclinic, *Cc*  
*a* = 8.0131 (16) Å  
*b* = 29.833 (6) Å  
*c* = 8.4860 (17) Å  
 $\beta$  = 110.914 (3)°  
*V* = 1895.0 (7) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.832 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 1377 reflections  
 $\theta$  = 2.7–20.6°  
 $\mu$  = 1.31 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Needle, colorless  
 0.19 × 0.04 × 0.03 mm

### Data collection

Bruker APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2002)  
*T<sub>min</sub>* = 0.789, *T<sub>max</sub>* = 0.962  
 6663 measured reflections

3294 independent reflections  
 2603 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.055  
 $\theta_{\max}$  = 25.1°  
*h* = -9 → 9  
*k* = -35 → 35  
*l* = -10 → 10

### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.063  
*wR*(*F*<sup>2</sup>) = 0.142  
*S* = 0.99  
 3294 reflections  
 280 parameters  
 H atoms treated by a mixture of independent and constrained refinement

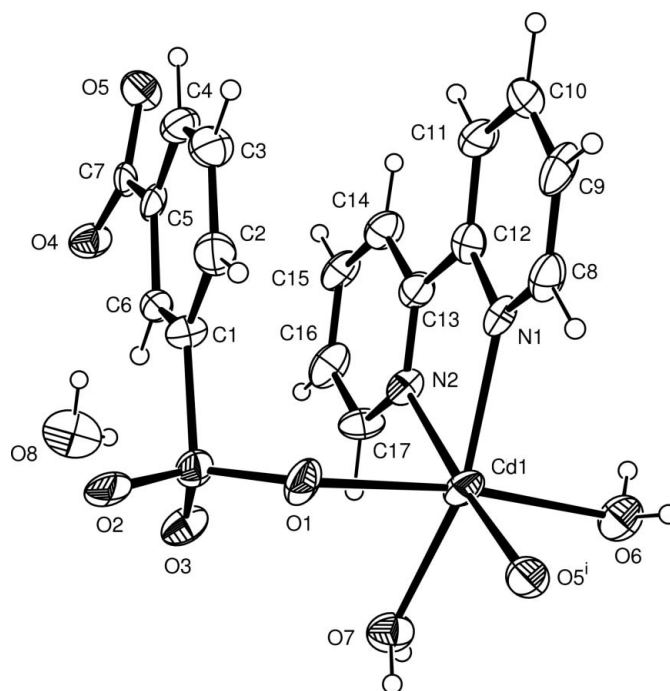
$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.98 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.90 \text{ e } \text{Å}^{-3}$   
 Absolute structure: Flack (1983),  
 1606 Friedel pairs  
 Flack parameter: -0.01 (6)

**Table 1**

Selected geometric parameters (Å, °).

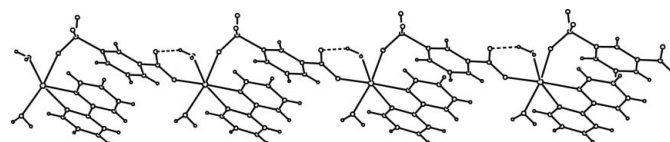
Cd1–O1	2.346 (8)	Cd1–O7	2.287 (8)
Cd1–O5 <sup>i</sup>	2.174 (8)	Cd1–N1	2.256 (9)
Cd1–O6	2.347 (9)	Cd1–N2	2.307 (9)
O5 <sup>i</sup> –Cd1–N1	102.5 (3)	O7–Cd1–O1	84.1 (3)
O5 <sup>i</sup> –Cd1–O7	93.7 (3)	N2–Cd1–O1	96.4 (3)
N1–Cd1–O7	162.3 (3)	O5 <sup>i</sup> –Cd1–O6	89.7 (3)
O5 <sup>i</sup> –Cd1–N2	174.0 (3)	N1–Cd1–O6	95.1 (3)
N1–Cd1–N2	71.5 (3)	O7–Cd1–O6	91.9 (3)
O7–Cd1–N2	92.1 (3)	N2–Cd1–O6	91.7 (3)
O5 <sup>i</sup> –Cd1–O1	82.6 (3)	O1–Cd1–O6	171.2 (3)
N1–Cd1–O1	90.9 (3)		

Symmetry code: (i) *x* + 1, *y*, *z* + 1.



**Figure 1**

ORTEP-3 (Farrugia, 1997) diagram of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 40% probability level [symmetry code: (i) 1 + *x*, *y*, 1 + *z*].



**Figure 2**

A view of the one-dimensional zigzag chain of (I). Hydrogen bonds are drawn as dashed lines and solvent molecules have been omitted for clarity.

**Table 2**

Hydrogen-bond 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>
O6–H6A···O8 <sup>ii</sup>	0.85 (5)	1.84 (3)	2.669 (13)	166 (12)
O6–H6B···O3 <sup>ii</sup>	0.86 (8)	1.99 (5)	2.747 (12)	149 (9)
O7–H7A···O4 <sup>i</sup>	0.85 (4)	1.90 (5)	2.655 (11)	149 (9)
O7–H7B···O8 <sup>iii</sup>	0.85 (3)	2.48 (10)	3.073 (13)	128 (10)
O8–H8A···O4	0.85 (11)	1.97 (7)	2.761 (13)	154 (15)
O8–H8B···O6 <sup>iv</sup>	0.85 (10)	2.35 (9)	3.185 (13)	168 (14)

Symmetry codes: (i) *x* + 1, *y*, *z* + 1; (ii) *x* + 1, *y*, *z*; (iii) *x* + 1, -*y* + 2, *z* + ½; (iv) *x* - 1, -*y* + 2, *z* - ½.

All H atoms bonded to C atoms were positioned geometrically and treated as riding, with C–H distances of 0.93 Å and *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C). The water H atoms were located in a difference Fourier map and refined with a distance restraint of O–H = 0.85 (1) Å and with fixed *U<sub>iso</sub>*(H) of 0.08 Å<sup>2</sup>.

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: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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