

Aquadibenzoato(2,2'-bipyridine)cadmium(II)  
monohydrateLong-Guan Zhu<sup>a\*</sup> and  
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## Key indicators

Single-crystal X-ray study

T = 295 K

Mean  $\sigma(C-C) = 0.007 \text{ \AA}$ 

R factor = 0.034

wR factor = 0.085

Data-to-parameter ratio = 12.7

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

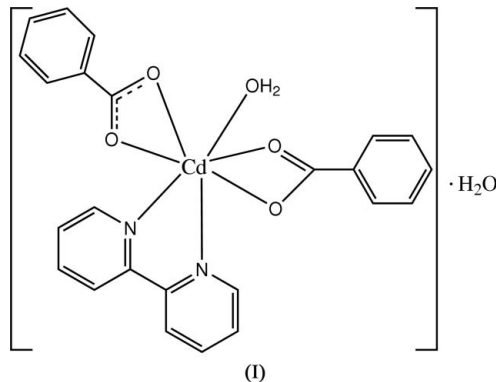
The monomeric title complex,  $[\text{Cd}(\text{C}_7\text{H}_5\text{O}_2)_2(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$ , contains a seven-coordinate  $\text{Cd}^{\text{II}}$  atom and the  $\text{CdO}_5\text{N}_2$  polyhedron is irregular. Hydrogen bonds between water molecules and carboxylate groups give rise to a one-dimensional extended architecture.

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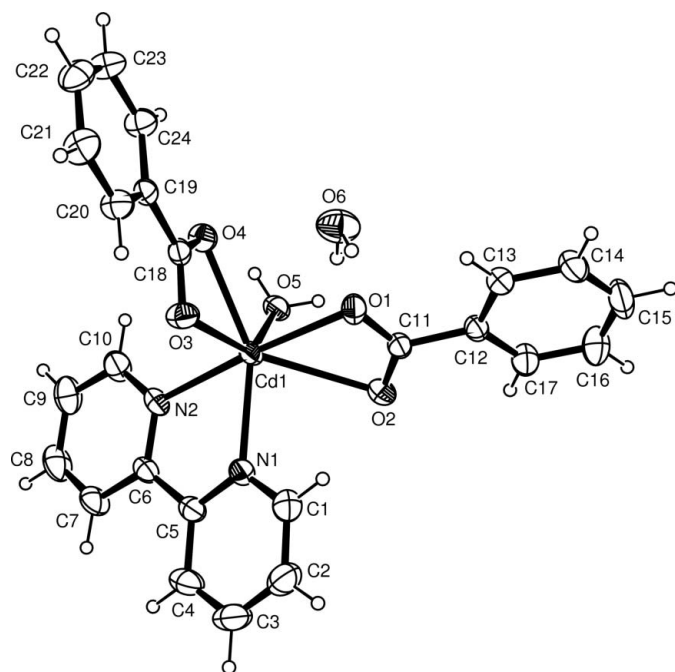
## Comment

In the past decade, numerous 1,4-benzenedicarboxylate (bdc) metal complexes have been prepared due to their potential applications as functional materials (Yaghi *et al.*, 2003; Chisholm, 2003; Xiao & Zhu, 2003). Very recently, some 4-substituted benzoate complexes have been prepared to expand the scope of bdc-like complexes (Zhang *et al.*, 2005). We selected a new ligand, 4-carboxybenzeneboronic acid (Hcbba), to prepare bdc-like complexes. Hcbba was unexpectedly converted to the benzoate anion under hydrothermal conditions. We present here the structure of the resulting mixed-ligand cadmium(II) title complex, (I).



The  $\text{Cd}^{\text{II}}$  atom in (I) adopts an irregular seven-coordinate polyhedral geometry defined by four O atoms from two bidentate benzoate ligands, two N atoms from a 2,2'-bipyridine molecule and one water molecule O atom (Fig. 1 and Table 1). The Cd—O (except Cd1—O2) and Cd—N bond lengths are in the normal ranges found in related Cd complexes (Zhu *et al.*, 2003; Yuan *et al.*, 2001). The polyhedral geometry in (I) is similar to that of the seven-coordinate  $\text{Cd}^{\text{II}}$  atom in  $[\text{Cd}_3(\text{C}_4\text{H}_4\text{N})_2(\text{C}_7\text{H}_5\text{O}_2)_6]_n$  (Liu, 2005), in which one Cd—O bond is also substantially longer than the others. It is notable that for the C11 benzoate ion in (I), the two carboxylate C—O bond lengths are distinctly different, while for the C18 group the two corresponding bonds are almost the same length.

The extended structure of (I) is built up from one-dimensional hydrogen-bonded chains between water molecules and



**Figure 1**  
View of (I), showing 40% displacement ellipsoids (arbitrary spheres for the H atoms).

carboxylate groups (Fig. 2 and Table 2). In the chain, there are no significant  $\pi$ - $\pi$  interactions between benzene or pyridine rings, while between chains,  $\pi$ - $\pi$  interactions involving the pyridine rings [at  $(x, y, z)$  and  $(-x, 2 - y, 1 - z)$ ] with a centroid separation of 3.790 Å occur.

## Experimental

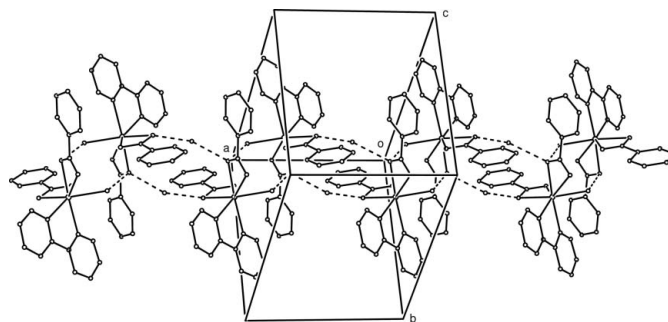
A mixture of  $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$  (0.129 g, 0.48 mmol), 4-carboxybenzeneboronic acid (0.079 g, 0.48 mmol), 2,2'-bipyridine (0.080 g, 0.51 mmol) and water (15 ml) was sealed in a 30 ml Teflon-lined stainless steel reactor and heated at 423 K for 96 h. After cooling, colorless plate-shaped crystals of (I) were recovered by filtration.

### Crystal data

|  |   |
|--|---|
| $[\text{Cd}(\text{C}_7\text{H}_5\text{O}_2)_2(\text{C}_{10}\text{H}_8\text{N}_2) \cdot (\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$ | $Z = 2$                                   |
| $M_r = 546.84$   | $D_x = 1.596 \text{ Mg m}^{-3}$           |
| Triclinic, $P\bar{1}$  | Mo $K\alpha$ radiation                    |
| $a = 9.9605$ (7) Å   | Cell parameters from 3421 reflections     |
| $b = 10.9160$ (7) Å  | $\theta = 2.8$ – $25.1^\circ$             |
| $c = 11.8547$ (8) Å  | $\mu = 1.00 \text{ mm}^{-1}$              |
| $\alpha = 116.101$ (1)°  | $T = 295$ (2) K                           |
| $\beta = 98.348$ (1)°  | Plate, colorless                          |
| $\gamma = 91.999$ (1)°   | $0.31 \times 0.19 \times 0.14 \text{ mm}$ |
| $V = 1138.14$ (13) Å <sup>3</sup>  |   |

### Data collection

|  |  |
|--|--|
| Bruker SMART APEX area-detector diffractometer           | 3938 independent reflections           |
| $\varphi$ and $\omega$ scans                             | 3691 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2002) | $R_{\text{int}} = 0.017$               |
| $T_{\text{min}} = 0.746$ , $T_{\text{max}} = 0.872$      | $\theta_{\text{max}} = 25.0^\circ$     |
| 5981 measured reflections                                | $h = -10 \rightarrow 11$               |
|  | $k = -12 \rightarrow 12$               |
|  | $l = -14 \rightarrow 10$               |



**Figure 2**  
A view of the one-dimensional hydrogen-bonded chain in (I). The O...O contacts of the hydrogen bonds are drawn as dashed lines and H atoms are omitted for clarity.

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.085$   
 $S = 1.07$   
 3938 reflections  
 310 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 0.8309P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} = 0.001$$

$$\Delta\rho_{\text{max}} = 0.73 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{Å}^{-3}$$

**Table 1**

Selected bond lengths (Å).

|        |           |        |           |
|--------|-----------|--------|-----------|
| Cd1—O1 | 2.275 (2) | Cd1—N2 | 2.327 (3) |
| Cd1—O2 | 2.681 (3) | C11—O1 | 1.279 (4) |
| Cd1—O3 | 2.408 (3) | C11—O2 | 1.234 (4) |
| Cd1—O4 | 2.394 (2) | C18—O3 | 1.259 (4) |
| Cd1—O5 | 2.330 (3) | C18—O4 | 1.254 (4) |
| Cd1—N1 | 2.326 (3) |        |           |

**Table 2**

Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$            | $D-H$      | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---------------------------|------------|--------------|--------------|----------------|
| O5—H5A...O4 <sup>i</sup>  | 0.84 (3)   | 1.998 (19)   | 2.765 (3)    | 151 (3)        |
| O5—H5B...O1 <sup>i</sup>  | 0.839 (10) | 2.08 (2)     | 2.829 (4)    | 149 (3)        |
| O6—H6A...O1               | 0.86 (3)   | 2.15 (3)     | 2.975 (4)    | 163 (3)        |
| O6—H6B...O3 <sup>ii</sup> | 0.855 (10) | 1.985 (12)   | 2.837 (4)    | 174 (4)        |

Symmetry codes: (i)  $-x, -y + 1, -z + 1$ ; (ii)  $-x + 1, -y + 1, -z + 1$ .

All H atoms bonded to the C atoms were positioned geometrically and refined as riding, with  $C-H = 0.93$  Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The water H atoms were located in a difference Fourier map and refined with an O—H distance restraint [0.85 (1) Å] and with  $U_{\text{iso}}(\text{H}) = 0.05$  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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