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## Key indicators

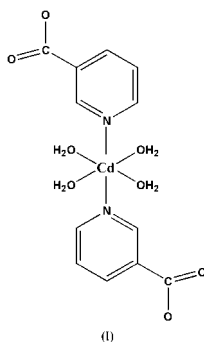
Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$   
 $R$  factor = 0.038  
 $wR$  factor = 0.095  
Data-to-parameter ratio = 8.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Tetraaqua-*trans*-bis(nicotinato- $\kappa\text{N}$ )cadmium(II)

The title compound,  $[\text{Cd}(\text{C}_6\text{H}_4\text{NO}_2)_2(\text{H}_2\text{O})_4]$ , was synthesized by the hydrothermal reaction of cadmium chloride and nicotinic acid. Crystallographic analysis reveals it to be a new nicotinic acid complex. The molecule has crystallographic  $2/m$  symmetry. The hydrogen-bonding interaction between the molecules results in a three-dimensional supramolecular structure.

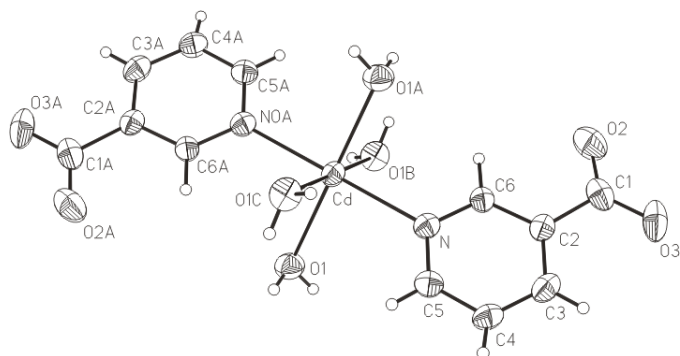
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## Comment

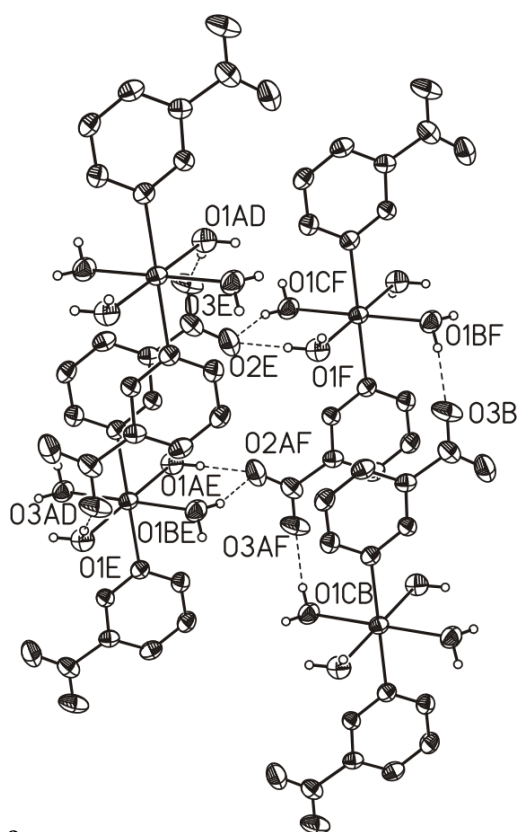
Recently, the design and syntheses of non-centrosymmetric transition metal complexes has attracted widespread attention, since it is an essential requirement for a bulk material to exhibit non-linear optical (NLO) effects. We have investigated the coordination chemistry of nicotinic acid complexes. Our interest in these systems stems from the lack of a center of symmetry in the ligand. In addition, the introduction of electronic asymmetry (push-pull effects) through the bifunctional *m*-pyridinecarboxylate group is necessary for second-order optical non-linearity. The reason that we adopted the Cd atom as the metal center is because its complexes are usually colorless, which is good for optical materials. Several nicotinic acid-transition metal complexes have been synthesized and studied, such as zinc (Lin *et al.*, 1998; Cotton *et al.*, 1991), chromium (Cotton *et al.*, 1991; Broderick *et al.*, 1986), cobalt and copper (Waizumi *et al.*, 1998), and nickel (Batten & Harris, 2001).



Here we report a new cadmium(II) complex, tetraaqua-*trans*-bis(nicotinato- $\kappa\text{N}$ )cadmium(II), (I). X-ray single-crystal diffraction analysis reveals that it is isomorphous with other transition metal dinicotinates and crystallizes in the space group  $C2/m$ . The molecule has crystallographic  $2/m$  symmetry. Each cadmium(II) center is coordinated by two N atoms from two nicotinate groups and four O atoms from four water molecules in a slightly distorted octahedral geometry. Two nicotinate groups are in *trans* positions. The Cd-N and Cd-



**Figure 1**  
View of the molecule of the title complex, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary radii. Suffix letters indicate symmetry-equivalent atoms.



**Figure 2**  
The molecular packing of the title complex. H atoms bonded to C atoms have been omitted for clarity.

O bond lengths are 2.309 (5) and 2.321 (4) Å, respectively (Table 1).

The O atom of each coordinated water molecule forms bifurcated hydrogen bonds with the carbonyl O atom of nicotinate groups (Table 2). The intermolecular hydrogen-bonding interactions thus link the molecules into a three-dimensional network, as shown in Fig. 2.

## Experimental

The hydrothermal reaction of cadmium chloride (0.05 g, 0.27 mmol) and nicotinic acid (0.04 g, 0.32 mmol) in a molar ratio of 1:1 was

carried out at 443 K for 5 d. After cooling to room temperature at 5 K h<sup>-1</sup>, colorless platelet crystals of (I) were isolated in 63% yield (based on Cd). Elemental analysis calculated for C<sub>12</sub>H<sub>16</sub>CdN<sub>2</sub>O<sub>8</sub>: C 33.62, H 3.76, N 6.53%; found: C 33.41, H 3.43, N 6.51%.

## Crystal data

[Cd(C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>4</sub>]  
*M<sub>r</sub>* = 428.68  
 Monoclinic, *C2/m*  
*a* = 14.5727 (8) Å  
*b* = 6.9988 (1) Å  
*c* = 8.5447 (5) Å  
 $\beta$  = 118.012 (3)°  
*V* = 769.39 (7) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 1.850 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 35 reflections  
 $\theta$  = 2.7–25.0°  
 $\mu$  = 1.46 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Plate, colorless  
 0.36 × 0.14 × 0.12 mm

## Data collection

Siemens SMART CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.520, *T<sub>max</sub>* = 0.839  
 1341 measured reflections

733 independent reflections  
 718 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.037  
 $\theta_{max}$  = 25.0°  
*h* = -15 → 17  
*k* = -8 → 8  
*l* = -9 → 10

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.038  
*wR* (*F*<sup>2</sup>) = 0.095  
*S* = 1.15  
 733 reflections  
 89 parameters  
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.4415P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 1.03 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.83 \text{ e \AA}^{-3}$   
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.019 (2)

**Table 1**

Selected geometric parameters (Å, °).

Cd—N	2.309 (5)	C1—O3	1.260 (9)
Cd—O1	2.321 (4)	C1—C2	1.495 (9)
C1—O2	1.254 (10)		
N—Cd—N <sup>i</sup>	180.0	O1 <sup>iii</sup> —Cd—O1	92.1 (2)
N—Cd—O1 <sup>i</sup>	88.87 (13)	O2—C1—O3	125.2 (7)
N—Cd—O1	91.13 (13)	O2—C1—C2	117.1 (6)
O1 <sup>ii</sup> —Cd—O1	87.9 (2)	O3—C1—C2	117.8 (7)

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

**Table 2**

Hydrogen-bonding 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>
O1—H1A...O2 <sup>iv</sup>	0.84 (7)	1.90 (8)	2.705 (7)	158 (?)
O1—H1B...O3 <sup>v</sup>	0.80 (8)	1.92 (8)	2.709 (5)	173 (?)

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

All H atoms were located in a difference Fourier map and refined freely [*C*—H = 0.79 (11)–1.00 (9) Å], with isotropic displacement parameters. The highest peak is 0.89 Å from the Cd center.

Data collection: SMART (Siemens, 1996); cell refinement: SMART; data reduction: SAINT (Siemens, 1996) and XPREP (Bruker, 1997); program(s) used to solve structure: SHELXTL (Siemens, 1994); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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