Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Poly[diaqua[μ-1,2-bis(4-pyridyl)ethene-κ^2N:N']-tetrakis(μ-isonicotinato-κ^2N:O)dicadmium(II)]

Ju-Hsiou Liao* and Chien-De Ho

Department of Chemistry and Biochemistry, National Chung Cheng University, 160 San-Hsing, Min-Hsiung, Chia-Yi 621, Taiwan

Correspondence e-mail: chejhl@ccu.edu.tw

Received 31 October 2003
Accepted 3 November 2003
Online 17 January 2004

Key indicators

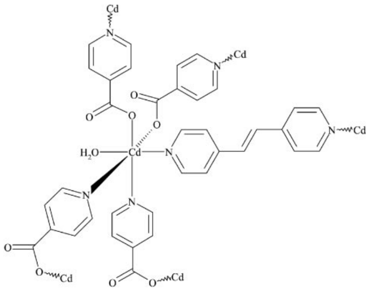
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.023
wR factor = 0.058
Data-to-parameter ratio = 12.3

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

In the title compound, $[Cd_2(C_6H_4NO_2)_4(C_{12}H_{10}N_2)(H_2O)_2]$, the Cd^{II} atom, the water O atom and the bridging *trans*-1,2-bis(4-pyridyl)ethene ligand are located on a mirror plane. An inversion center is located at the mid-point of the ethene link. Each Cd^{II} atom is in an octahedral environment, coordinated by one water molecule, one *trans*-1,2-bis(4-pyridyl)ethene molecule and four isonicotinate anions. This forms an interpenetrated framework composed of bilayered cuboidal motifs.

Comment

The design of extended frameworks by linking metal centers with multidentate ligands has attracted much attention (Eddaoudi *et al.*, 2001). Rational modification and substitution of functional organic ligands may provide a way to fine-tune the properties of materials. Isonicotinates (Evans & Lin, 2001) and *trans*-1,2-bis(4-pyridyl)ethene (Lu & Babb, 2001) have been used as rigid building blocks to construct various coordination polymers with interesting crystal structures. The reaction of isonicotinic acid, *trans*-1,2-bis(4-pyridyl)ethene, and Cd^{II} resulted in the formation of the title compound, (I) (Fig. 1), which is isomorphous with [Cd$_2$(isonicotinate)$_4$[*trans*-1,2-bis(4-pyridyl)ethane](H$_2$O)$_2$] (Fu *et al.*, 2001).



(I)

The crystal structure of (I) is composed of bilayered cuboidal motifs, interpenetrating one another (Fig. 2). Each Cd^{2+} ion is coordinated by one H_2O, one *trans*-1,2-bis(4-pyridyl)ethene and four isonicotinates. The Cd^{II} atom, the water O atom and the bridging *trans*-1,2-bis(4-pyridyl)ethene ligand are located on a mirror plane. A crystallographic inversion center is located at the mid-point of the ethene link. In the isonicotinate, the carboxylate group and the pyridyl ring are not coplanar, with a dihedral angle of 20.7 (2)°. The Cd—O1(water) distance, 2.354 (2) Å, is slightly longer than that of Cd—O2(carboxylate) [2.3191 (16) Å]. Hydrogen bonding is observed between the coordinated water molecule and the nearby carboxylate atom O3.

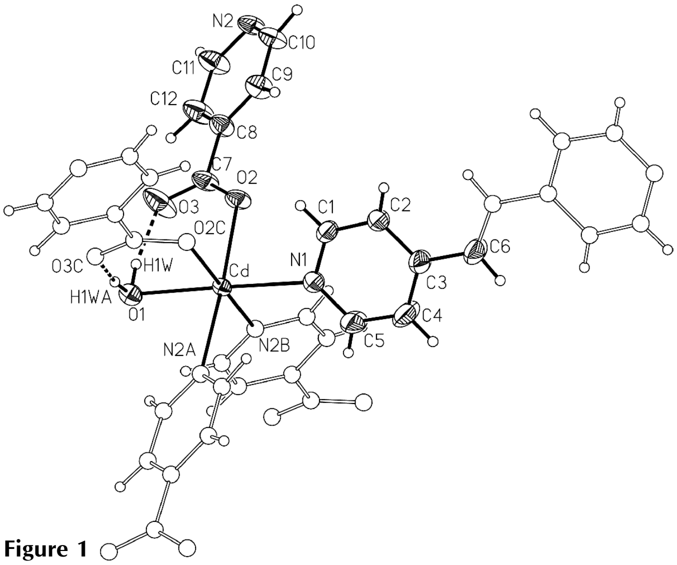


Figure 1
The structure and labeling scheme of (I), showing 50% probability displacement ellipsoids for the asymmetric unit. Symmetry-generated atoms are shown as spheres.

Experimental

$Cd(NO_3)_2{\cdot}4H_2O$ (0.154 g, 0.5 mmol) was dissolved in distilled water (5 ml), and a mixture of isonicotinic acid (0.123 g, 1 mmol) and *trans*-1,2-bis(4-pyridyl)ethene (0.182 g, 1 mmol) was dissolved in distilled water (10 ml) at 353 K. The two solutions were mixed and sealed in a 30 ml test tube, forming a cloudy solution with pH = 4.53. The solution was kept at 353 K for a week until numerous large colorless parallelepiped crystals were observed. The final pH value was 4.01. The crystals (0.127 g, 54.5% yield, based on Cd) were collected after filtration and several washings with distilled water and acetone.

Crystal data

$[Cd_2(C_6H_4NO_2)_4(C_{12}H_{10}N_2)(H_2O)_2]$
$M_r = 465.74$
Monoclinic, $C2/m$
$a = 12.6311\ (19)$ Å
$b = 14.6070\ (19)$ Å
$c = 11.1428\ (15)$ Å
$\beta = 112.94\ (2)^\circ$
$V = 1893.3\ (5)$ Å^3
$Z = 4$
$D_x = 1.634$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 12.3–12.5^\circ$
$\mu = 1.19$ mm^{-1}
$T = 298\ (2)$ K
Parallelepiped, colorless
0.50 × 0.30 × 0.20 mm

Data collection

Bruker $P4$ diffractometer
$\theta/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.588$, $T_{\max} = 0.797$
3920 measured reflections
1737 independent reflections
1647 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.039$
$\theta_{\max} = 25.0^\circ$
$h = -11 \rightarrow 14$
$k = -16 \rightarrow 11$
$l = -13 \rightarrow 13$
3 standard reflections every 97 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.058$
$S = 1.21$
1737 reflections
141 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 1.2195P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.65$ e Å^{-3}
$\Delta\rho_{\min} = -0.60$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0045 (3)

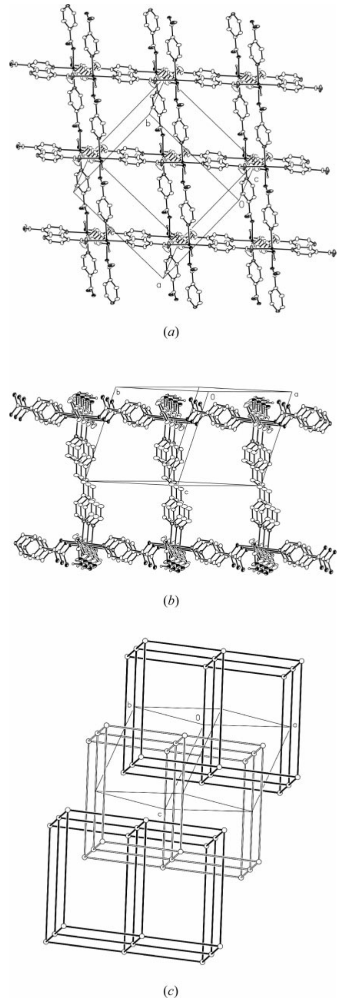

(*a*)
(*b*)
(*c*)

Figure 2
The bilayered network of (I), showing (a) a top view, (*b*) a side view and (*c*) a schematic drawing of three interpenetrating motifs.

Table 1
Selected geometric parameters (Å, °).

Cd—O2$^{\rm i}$	2.3191 (16)	Cd—N2$^{\rm ii}$	2.360 (2)
Cd—O2	2.3191 (16)	Cd—N2$^{\rm iii}$	2.360 (2)
Cd—N1	2.349 (3)	C6—C6$^{\rm iv}$	1.310 (8)
Cd—O1	2.354 (2)		
O2$^{\rm i}$—Cd—O2	90.50 (9)	N1—Cd—N2$^{\rm ii}$	93.23 (7)
O2$^{\rm i}$—Cd—N1	88.84 (7)	O1—Cd—N2$^{\rm ii}$	85.85 (7)
O2—Cd—N1	88.84 (7)	O2$^{\rm i}$—Cd—N2$^{\rm iii}$	86.85 (7)
O2$^{\rm i}$—Cd—O1	92.12 (6)	O2—Cd—N2$^{\rm iii}$	176.60 (7)
O2—Cd—O1	92.12 (6)	N1—Cd—N2$^{\rm iii}$	93.23 (7)
N1—Cd—O1	178.63 (9)	O1—Cd—N2$^{\rm iii}$	85.85 (7)
O2$^{\rm i}$—Cd—N2$^{\rm ii}$	176.60 (7)	N2$^{\rm ii}$—Cd—N2$^{\rm iii}$	95.71 (11)
O2—Cd—N2$^{\rm ii}$	86.85 (7)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$W\cdots$O3	0.86 (3)	1.77 (3)	2.615 (2)	170 (3)

Water atom H1*W* was refined freely. All other H atoms were treated as riding on their parent atoms [C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)].

Data collection: *XSCANS* (Bruker, 1992); cell refinement: *XSCANS*; data reduction: *XPREP* in *SHELXTL* (Bruker, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL*; software used to prepare material for publication: *XCIF* in *SHELXTL*.

JHL thanks the National Science Council of Taiwan for financial support.

References

Bruker (1992). *XSCANS Users Manual*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1994). *SHELXTL*. Version 5. Bruker AXS Inc., Madison, Wisconsin, USA.

Eddaoudi, M., Moler, D. B., Li, H., Chen, B., Reineke, T. M., O'Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.

Evans, O. R. & Lin, W. (2001). *Chem. Mater.* **13**, 3009–3017.

Fu, Z.-Y., Wu, X.-T., Dai, J.-C., Wu, L.-M., Cui, C.-P. & Hu, S.-M. (2001). *Chem. Commun.* pp. 1856–1857.

Lu, J. Y. & Babb, A. M. (2001). *Inorg. Chem.* **40**, 3261–3261.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.