Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Poly[bis(μ-3-pyridinecarboxylato-$\kappa^3N,O:O'$)cadmium(II)]

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Received 25 April 2005
Accepted 9 May 2005
Online 14 May 2005

Key indicators

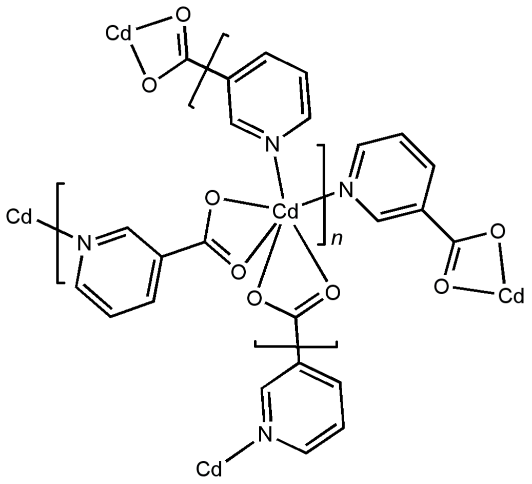
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.037
wR factor = 0.130
Data-to-parameter ratio = 13.2

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

The title compound, $[\mathrm{Cd(C_6H_4NO_2)_2}]_n$, is a two-dimensional coordination polymer, which consists of Cd^{II} atoms and bridging nicotinate anions. The Cd atom is coordinated in a highly distorted $\mathrm{CdO_4N_2}$ octahedron by two chelating carboxylate groups and two *cis* pyridyl groups.

Comment

3- and 4-pyridinecarboxylates and their derivatives are good bridging ligands in the construction of two- and three-dimensional functional metal-organic frameworks (Evans & Lin, 2002; Lu, 2003; Tong *et al.*, 2003; Wang *et al.*, 2003). The title complex, (I), was obtained unexpectedly in an attempt to prepare a bimetallic coordination network with nicotinic acid (3-pyridinecarboxylic acid).



(I)

The structure of (I) is a two-dimensional coordination network, which is parallel to the ($\bar{1}$01) plane (Fig. 1). The Cd^{II} atom, which is located in a general position, is coordinated by four O atoms from two chelating carboxylate groups and two pyridyl N atoms. The Cd1—N [2.316 (5) and 2.321 (5) Å] and Cd1—O [2.271 (4)–2.476 (4) Å] bond lengths are similar to those found in poly[(μ_3-nicotinato)(μ-nicotinato)cadmium(II)] [Cd—N = 2.310 (5) and 2.321 (5) Å, and Cd—O = 2.270 (4)–2.640 (4) Å] (Evans & Lin, 2001; Lu & Kohler, 2002), those found in poly[tetrakis(μ-nicotinato-N,O,O')-bis(μ-nicotinato-N,O)tetraaquatricadmium(II)] [Cd—N = 2.326 (5) and 2.395 (4) Å, and Cd—O = 2.269 (4)–2.539 (5) Å] (Chen, 2003), and those in poly[bis(μ-nicotinato-N,O,O')-aquacadmium(II)] [Cd—N 2.307 (2) and 2.353 (2) Å, and Cd—O = 2.276 (2)–2.639 (3) Å] (Clegg *et al.*, 1995). The angular distortions of the coordination octahedron are caused

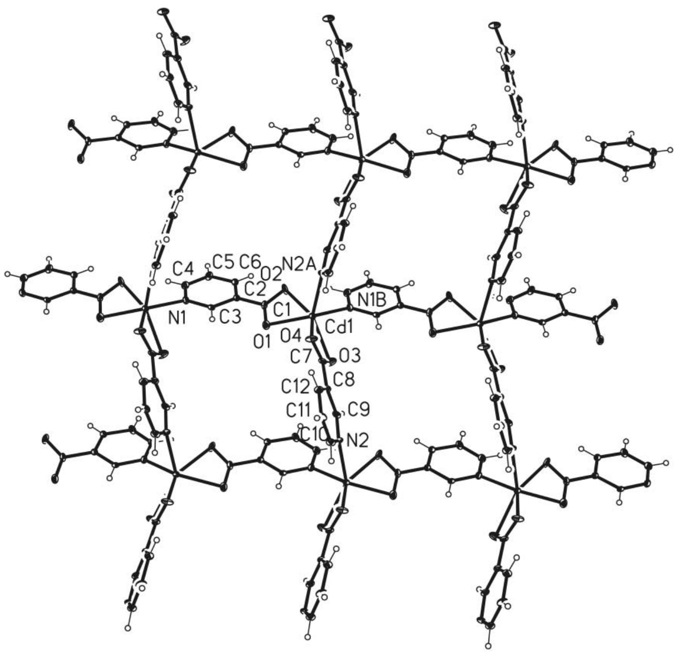


Figure 1
ORTEPII (Johnson, 1976) drawing of the extended two-dimensional layered structure of (I), with the atom-labeling scheme. Displacement ellipsoids are plotted at the 40% probability level. [Symmetry codes: (A) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (B) $x, 1+y, z$.]

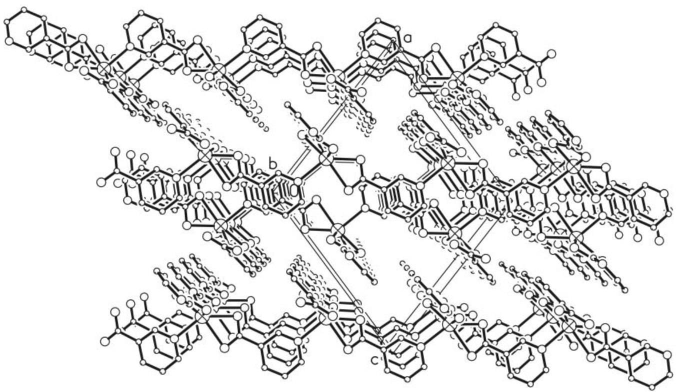


Figure 2
Perspective view of the molecular packing of (I).

by the chelate formation, the chelate bite angles O1—Cd1—O2 and O3—Cd1—O4 being 55.21 (15) and 56.05 (16)°, respectively.

The coordination structure of (I) is similar to that of poly[bis(μ-nicotinato)zinc(II)] (Evans & Lin, 2001); however, their crystal packings are quite different. The former is monoclinic $P2_1/n$, while the latter is tetragonal $P4_32_12$. In (I), the extensive interlayer π–π stackings between the pyridyl rings of the nicotinate ligands play an important role in consolidating their crystal architectures (Fig. 2). There are two kinds of π–π stackings; one is face-to-face stacking interactions between the N1/C2–C6 pyridyl ring and its symmetry-related counterpart at $(2-x, -1-y, 1-z)$, the distance between the centroids being 3.644 Å; the other type is offset π stacking interactions between the pyridyl N2/C8—C12 ring and its symmetry-related counterpart at $(2-x, -y, 2-z)$, with an interplanar distance of 3.546 Å (the center-to-center distance is 4.307 Å).

Experimental

To a methanol–water solution (4/1 *v*/*v*, 10 ml) of cadmium nitrate tetrahydrate (0.154 g, 0.5 mmol) and europium(III) nitrate hexahydrate (0.112 g, 0.25 mmol), a solution of nicotinic acid (0.123 g, 1.0 mmol) in MeOH (5 ml) was added slowly with stirring for 30 min at 333 K. The solution was adjusted to pH > 4 by addition of dilute NaOH solution. Colorless block-shaped crystals of (I) were deposited within two weeks in *ca* 60% yield.

Crystal data

$[Zn(C_6H_4NO_2)_2]$
$M_r = 356.60$
Monoclinic, $P2_1/n$
$a = 12.454$ (5) Å
$b = 7.807$ (2) Å
$c = 12.825$ (5) Å
$\beta = 105.269$ (5)°
$V = 1203.0$ (7) Å^3
$Z = 4$

$D_x = 1.969$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4560 reflections
$\theta = 3.1$–26.0°
$\mu = 1.83$ mm^{-1}
$T = 293$ (2) K
Polyhedron, colorless
0.22 × 0.16 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{\min} = 0.696$, $T_{\max} = 0.803$
5157 measured reflections

2278 independent reflections
2123 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 26.0°$
$h = -15 \rightarrow 15$
$k = -9 \rightarrow 9$
$l = -9 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.130$
$S = 1.21$
2278 reflections
172 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 5.4598P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.03$ e Å^{-3}
$\Delta\rho_{\min} = -0.68$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.271 (4)	Cd1—O3	2.324 (4)
Cd1—N2^{i}	2.316 (5)	Cd1—O4	2.414 (5)
Cd1—N1^{ii}	2.321 (5)	Cd1—O2	2.476 (4)
O1—Cd1—N2^{i}	117.64 (18)	N1^{ii}—Cd1—O4	130.15 (16)
O1—Cd1—N1^{ii}	127.80 (16)	O3—Cd1—O4	56.05 (16)
N2^{i}—Cd1—N1^{ii}	90.39 (18)	O1—Cd1—O2	55.21 (15)
O1—Cd1—O3	102.28 (19)	N2^{i}—Cd1—O2	90.25 (17)
N2^{i}—Cd1—O3	127.78 (18)	N1^{ii}—Cd1—O2	84.00 (15)
N1^{ii}—Cd1—O3	90.32 (18)	O3—Cd1—O2	141.66 (18)
O1—Cd1—O4	97.13 (16)	O4—Cd1—O2	145.50 (16)
N2^{i}—Cd1—O4	85.42 (16)		

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

The H atoms were included in geometrically calculated positions and constrained to ride at a distance of 0.93 Å from their parent C atoms with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The highest peak is located near the mid-point of C3 and O1. It is not geometrically reasonable to be assigned as the aromatic proton of C3.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 1998); software used to prepare material for publication: *SHELXL97*.

We thank the Foundation for the Item of Education Office of Guangdong Province (No. z03065) for generously supporting this work.

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