Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis(ethylenediammonium) tris(pyridine-2,6-dicarboxylato-κ^3O,O',N)cadmium(II) hexahydrate

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Received 23 August 2004
Accepted 1 September 2004
Online 4 September 2004

In the title complex, $(C_2H_{10}N_2)_2[Cd(C_7H_3NO_4)_3]\cdot 6H_2O$, the Cd^{II} atom is nine-coordinated by three pyridine-2,6-dicarboxylate ligands *via* six O atoms and three N atoms in a distorted tricapped trigonal prismatic structure. A crystallographic twofold rotation axis passes through the Cd atom and three atoms of one pyridine ring, *viz*. N, the C in the *p*-position and its attached H atom. The pyridine-2,6-dicarboxylate ligands, ethylenediammonium cations and uncoordinated water molecules contribute to the formation of intermolecular hydrogen bonds, forming a three-dimensional network.

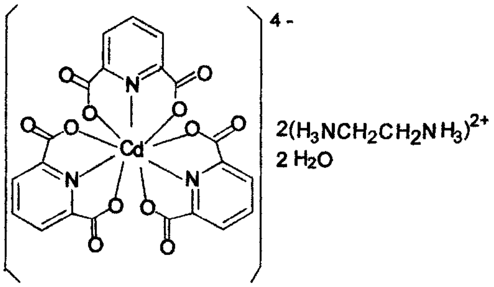
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.028
wR factor = 0.067
Data-to-parameter ratio = 12.5

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

Comment

The title compound, (I), consists of a $[Cd(C_7H_3NO_4)_3]^{4-}$ anion, two $(H_3NCH_2CH_2NH_3)^{2+}$ cations and six uncoordinated water molecules. The Cd^{II} atom is nine-coordinated by three pyridine-2,6-dicarboxylate ligands [denoted by L_1, L_2 and L_1^{i}; symmetry code: (i) $2-x, y, \frac{1}{2}-z$], *via* six O atoms and three N atoms (Fig. 1). The coordination geometry around Cd corresponds to a distorted tricapped trigonal prism, with the capping positions occupied by atom N2 of L_2, O1 of L_1 and O1^{i} of L_1^{i}.



(I)

A crystallographic twofold rotation axis passes through the Cd atom and three atoms of ligand *L*2, *viz*. N2, C11 and its attached H atom H5. In the ninefold coordination, there are three unique Cd—O distances and two unique Cd—N distances; these are Cd1—O1 = 2.5408 (15) Å, Cd1—O3 = 2.5225 (15) Å, Cd1—O5 = 2.5671 (15) Å, Cd1—N1 = 2.4194 (17) Å and Cd1—N2 = 2.397 (2) Å. The dihedral angles between the two pyridine rings of L_1 and L_2, L_1 and L_1^{i}, L_2 and L_1^{i} are 83.0 (6), 91.5 (6) and 97.0 (6)°, respectively.

All NH groups of the cation and all OH groups of uncoordinated water molecules, together with all O atoms of the pyridine-2,6-dicarboxylate ligands, contribute to the formation of intermolecular N—H···O and O—H···O hydrogen bonds, forming a three-dimensional network (Table 1 and Fig. 2).

Experimental

$Cd(NO_3)_2 \cdot 6H_2O$ (1 mmol) was dissolved in distilled water (20 ml). To this solution was added dropwise, at 333 K, an aqueous mixture (30 ml) of L_1 (2 mmol) and ethylenediamine (2 mmol). The mixture was stirred for 4 h and part of the solvent was evaporated in a rotary vacuum evaporator. The resulting solution was filtered and allowed to stand in air for about 1.5 months. Large colourless block-like crystals of (I) were obtained. Analysis calculated for $C_{25}H_{41}CdN_7O_{18}$: C 35.74, H 4.92, N 11.67%; found: C 35.58, H 4.81, N 11.55%.

Crystal data

$(C_2H_{10}N_2)_2[Cd(C_7H_3NO_4)_3] \cdot 6H_2O$
$M_r = 840.05$
Orthorhombic, *Pbcn*
$a = 16.250$ (3) Å
$b = 10.0614$ (15) Å
$c = 20.021$ (3) Å
$V = 3273.4$ (9) Å^3
$Z = 4$
$D_x = 1.705$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 5899 reflections
$\theta = 2.4$–$26.6°$
$\mu = 0.76$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.40 × 0.30 × 0.15 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.751$, $T_{max} = 0.895$
19 430 measured reflections

3930 independent reflections
2680 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 28.3°$
$h = -21 \rightarrow 20$
$k = -13 \rightarrow 12$
$l = -23 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.067$
$S = 0.95$
3930 reflections
314 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.46$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N3-H6\cdots O8^{i}$	0.95 (3)	1.86 (3)	2.801 (3)	168 (2)
$N3-H7\cdots O1^{ii}$	0.91 (3)	1.92 (3)	2.823 (3)	176 (2)
$N3-H8\cdots O7^{iii}$	0.88 (3)	2.01 (3)	2.852 (3)	160 (2)
$N4-H13\cdots O9^{iv}$	0.88 (3)	2.31 (3)	2.912 (3)	126 (2)
$N4-H14\cdots O6^{v}$	0.83 (3)	1.98 (3)	2.779 (3)	162 (3)
$N4-H15\cdots O1^{ii}$	0.83 (3)	2.37 (3)	3.126 (3)	151 (2)
$O7-H16\cdots O2^{v}$	0.864 (10)	1.875 (12)	2.723 (3)	167 (3)
$O7-H17\cdots O6^{ii}$	0.867 (10)	2.150 (18)	2.940 (2)	151 (3)
$O8-H18\cdots O4^{vi}$	0.874 (10)	1.972 (13)	2.819 (2)	163 (3)
$O8-H19\cdots O3^{vii}$	0.876 (10)	1.804 (13)	2.661 (2)	165 (3)
$O9-H20\cdots O7^{viii}$	0.861 (10)	2.060 (11)	2.919 (3)	175 (3)
$O9-H21\cdots O5^{vii}$	0.872 (10)	1.972 (13)	2.810 (2)	161 (3)

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

The water O—H distances were restrained to 0.90 (1) Å and the U_{iso}(H) values were allowed to refine. The amine H atoms were located in a difference Fourier synthesis and refined isotropically. All other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and $U_{iso}(H) = xU_{eq}(C)$, with x in the range 0.8–1.4.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

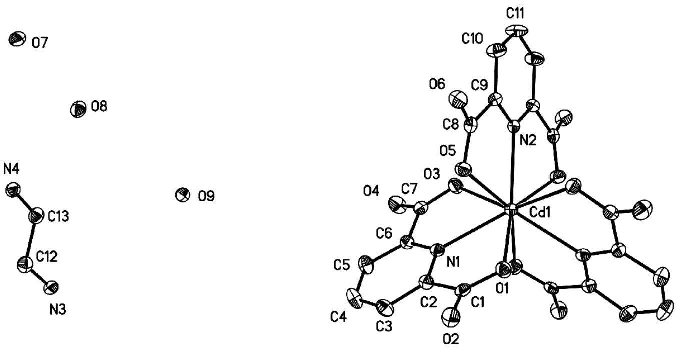


Figure 1
The structure of (I). Atoms of the asymmetric unit are labelled. Unlabelled atoms are related to their corresponding labelled atoms by $(2 - x, y, \frac{1}{2} - z)$. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

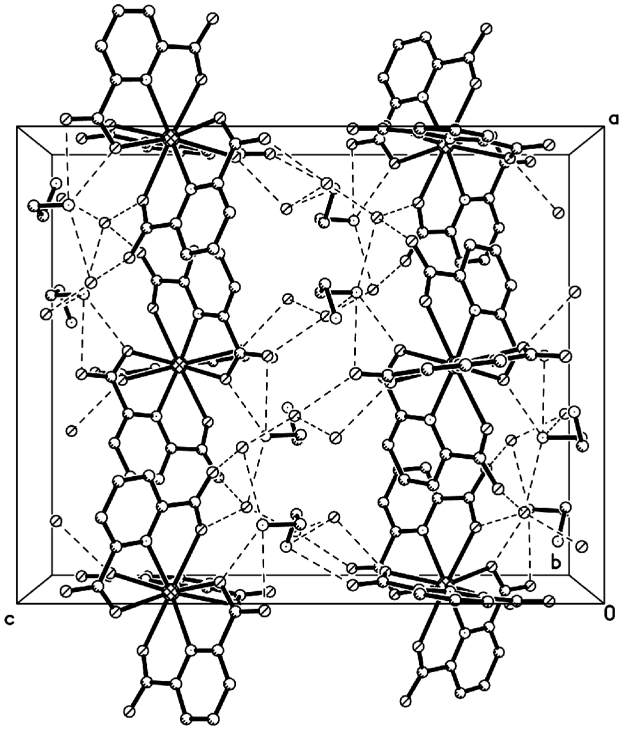


Figure 2
The crystal packing of (I), showing the O—H···O and N—H···O hydrogen-bond interactions as dashed lines. H atoms have been omitted for clarity.

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Acta Cryst. (2004). E**60**, m1372–m1373 Fu *et al.* • $(C_2H_{10}N_2)_2[Cd(C_7H_3NO_4)_3] \cdot 6H_2O$ **m1373**