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Diaquabis[*N*-(2-pyridylmethyl)benzamide-κ^2N,O]cadmium(II) dinitrate

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Key indicators

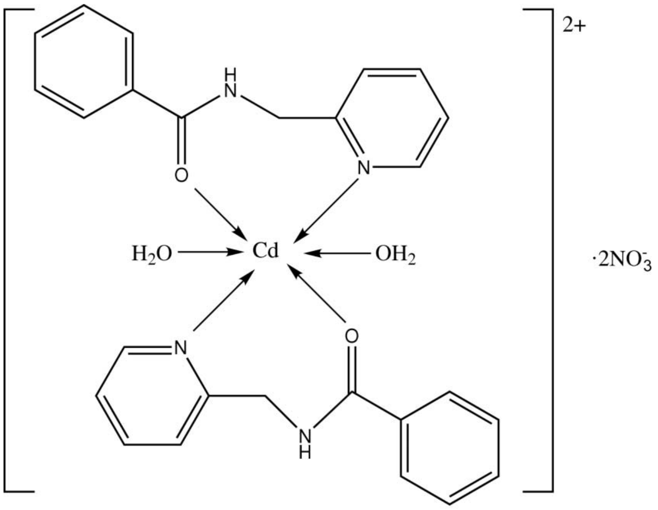
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.083
Data-to-parameter ratio = 14.3

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

In the title compound, $[Cd(C_{13}H_{12}N_2O)_2(H_2O)_2](NO_3)_2$, the Cd atom, located on a twofold rotation axis, is octahedrally coordinated by O and N atoms from two benzamide ligands, and two O atoms from water molecules also located on the twofold axis. Molecules are linked into chains along the *b* axis by O—H···O hydrogen bonds. The packing is further stabilized into a three-dimensional framework by N—H···O interaction.

Comment

It is known that some benzamide molecules with the amino-pyridine structure exhibit anti-ulcerogenic, sedative or anti-inflammatory properties (Arora *et al.*, 2005; Nielsen *et al.*, 2004). As part of our ongoing research on this type of molecule, the crystal structure of the title complex, (I), is reported.



(I)

The Cd^II atom, which is located on a twofold rotation axis, is six-coordinated by two O atoms and two N atoms from two benzamide ligands, and two O atoms from two water molecules also located on the twofold axis (Fig. 1). The geometry around the Cd atom is octahedral, and two nitrate anions lie outside the coordination sphere, balancing the charge. The amide C—N bond is known to possess a partial double-bond character due to donation of the non-bonding electron pair on the nitrogen (Fekner *et al.*, 2004). As expected, the benzamide chelate is not planar and the two aromatic rings make a dihedral angle of 60.6 (1)°.

In the crystal structure, the water molecules act as donors to form O—H···O hydrogen bonds (Table 1). These hydrogen bonds involving the nitrate anions link the ions and molecules into chains along the *b* axis (Fig. 2). The packing is further stabilized into a three-dimensional framework by N—H···O interactions (see Table 1 and Fig. 2).

Experimental

To a cold solution of 2-(2-aminomethyl)pyridine (2 ml, 19 mmol) and triethylamine (2.63 ml, 19 mmol) in dry CH_2Cl_2 (25 ml) was added dropwise a solution of benzyl chloride (2 ml, 17.2 mmol) in dry CH_2Cl_2 (15 ml). Stirring was continued at room temperature for 1 h, then at 333 K for 5 h. After filtering, the filtrate was washed with water, dried over anhydrous Na_2SO_4, and then evaporated to give *N*-(pyridin-2-ylmethyl)benzamide as a yellow oil. To a solution of the oil (0.16 g, 0.75 mmol) in ethyl acetate (10 ml) was added slowly a solution of $Cd(NO_3)_2\cdot4H_2O$ (0.12 g, 0.39 mmol) in EtOH (5 ml). The mixture was stirred for 5 h until a white solid appeared. Colourless crystals suitable for an X-ray diffraction study were obtained by slow evaporation of an EtOH solution.

Crystal data

$[Cd(C_{13}H_{12}N_2O)_2(H_2O)_2](NO_3)_2$
$M_r = 694.94$
Monoclinic, $C2/c$
$a = 15.7144$ (10) Å
$b = 9.1003$ (6) Å
$c = 21.2585$ (13) Å
$\beta = 105.547$ (1)°
$V = 2928.9$ (3) Å^3
$Z = 4$

$D_x = 1.576$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2586 reflections
$\theta = 2.6$–22.8°
$\mu = 0.81$ mm^{-1}
$T = 293$ (2) K
Needle, colourless
0.32 × 0.06 × 0.04 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.781$, $T_{max} = 0.968$
7992 measured reflections

2886 independent reflections
2549 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.0°$
$h = -18 \rightarrow 19$
$k = -11 \rightarrow 9$
$l = -26 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.083$
$S = 1.02$
2886 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 1.1414P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2^{ii}	0.843 (10)	1.96 (2)	2.783 (4)	164 (8)
O2*W*—H2*WA*···O2^{iii}	0.845 (10)	2.23 (5)	2.974 (4)	146 (8)
O2*W*—H2*WA*···O4^{iii}	0.845 (10)	2.25 (4)	3.037 (4)	156 (8)
N1—H1···O3	0.86	2.38	3.062 (4)	136
N1—H1···O4	0.86	2.31	3.089 (4)	151

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

All H atoms attached to C and N atoms were located in difference Fourier maps but introduced in calculated position and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, N—H = 0.86 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$. The H atoms for the water molecules were refined using O—H restraints of 0.85 (1) Å and $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* and *PARST* (Nardelli, 1995).

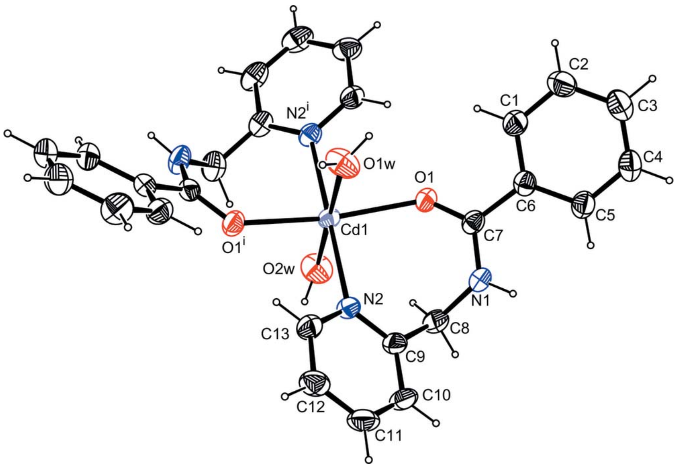


Figure 1
The structure of compound (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The nitrate anion has been omitted for clarity. [Symmetry codes: (i) $-x, y, \frac{1}{2} - z$.]

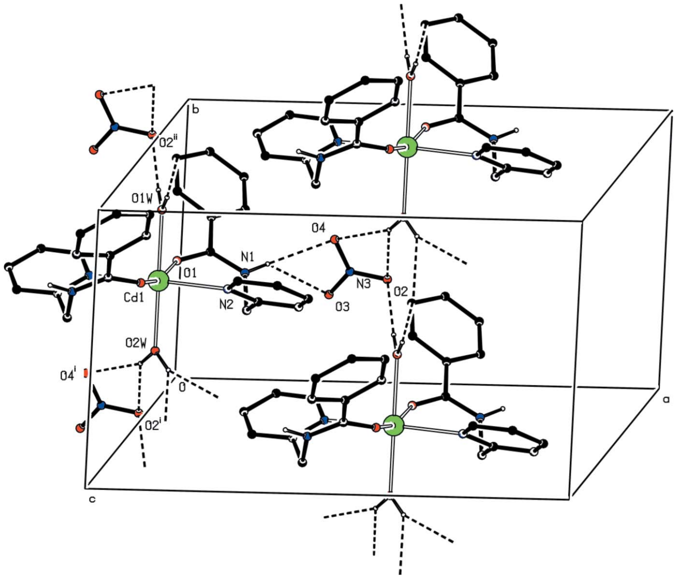


Figure 2
A view showing the O—H···O and N—H···O hydrogen bonds and the three-dimensional network. Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen-bond interactions have been omitted for clarity. [Symmetry codes: (i) $-x, y, \frac{1}{2} - z$; (ii) $x - \frac{1}{2}, \frac{1}{2} + y, z$.]

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