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catena-Poly[[aqua(nitrato-κ^2O,O')(1,10-phenanthroline)cadmium(II)]-μ-nitrato-κ^2O:O']

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.024
wR factor = 0.058
Data-to-parameter ratio = 11.5

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

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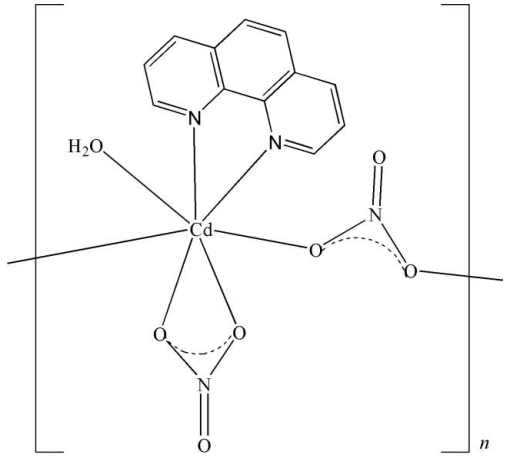
In the title compound, $[Cd(NO_3)_2(C_{12}H_8N_2)(H_2O)]_n$, each Cd^{II} ion is surrounded by two N atoms from a 1,10-phenanthroline ligand, and five O atoms from a water molecule and three nitrate anions, with two in bridging mode and one in chelating mode, forming a seven-coordinate CdO_5N_2 environment. Each cadmium(II) center is bridged to two others by two nitrate anions to produce a zigzag chain structure along the [010] direction. O—H···O hydrogen-bonding interactions link adjacent chains into a two-dimensional network parallel to (001).

Comment

Cadmium nitrate yields adducts with 1,10-phenanthroline in which the heterocycle binds in the typical chelating mode, and two such complexes, *viz*. (nitrato-κ^2O,O')(nitrato-κO)bis(1,10-phenanthroline)cadmium and di(nitrato-κ^2O,O')bis(1,10-phenanthroline)cadmium, have been reported (Shi *et al.*, 2004; Tadjarodi *et al.*, 2001). The present study used a hydrothermal method for synthesizing a new cadmium nitrate adduct with 1,10-phenanthroline by adjusting the molar ratio of cadmium nitrate and 1,10-phenanthroline, yielding *catena*-poly-[[aqua(nitrato-κ^2O,O')(1,10-phenanthroline)cadmium(II)]-μ-nitrato-κ^2O:O'], (I).



(I)

The asymmetric unit of (I) consists of a Cd ion in a seven-coordinate environment, one coordinated water molecule, one chelating nitrate anion, one bridging nitrate anion and one chelating 1,10-phenanthroline. Each Cd center is bridged to two others by two nitrate anions to produce a zigzag chain structure generated by the twofold screw axis along the [010] direction, with a Cd1···Cd1($-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$) separation of 5.6461 (3) Å (Fig. 1 and Table 1). In the crystal structure,

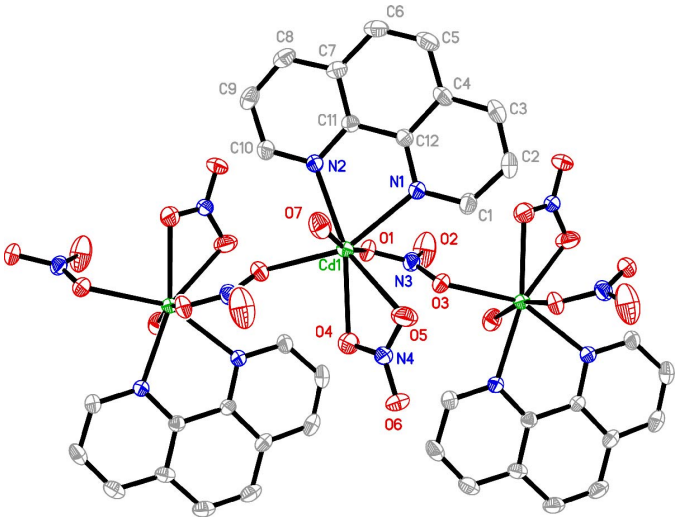


Figure 1
The zigzag chain of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. All H atoms have been omitted for clarity.

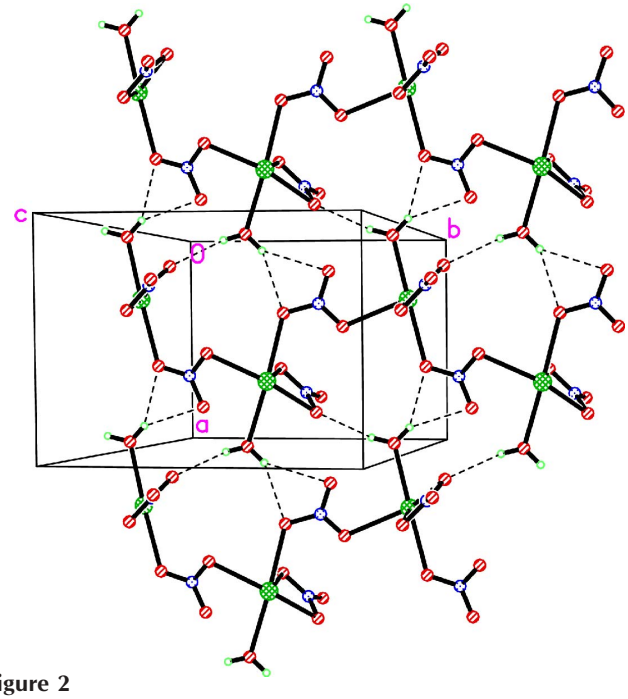


Figure 2
The grid network formed by hydrogen-bonding interactions, which are shown as dashed lines. The 1,10-phenanthroline ligands have been omitted for clarity.

adjacent chains interact *via* intermolecular O—H···O hydrogen bonds to form a two-dimensional grid network parallel to (001) (Fig. 2 and Table 2). The hydrogen-bonding pattern, as shown in Fig. 2, contains the graph-set motif $R_2^2(10)$ (Etter, 1990; Grell *et al.*, 2000).

Experimental

The title compound was synthesized hydrothermally from cadmium nitrate dihydrate (1 mmol, 0.27 g), 1,10-phenanthroline (1 mmol, 0.18 g) and water (20 ml). The reagents were heated in a 30 ml Teflon-lined stainless steel Parr bomb at 424 K for 4 d. The bomb was cooled slowly to room temperature to yield colorless crystals that were collected and washed with water.

Crystal data

$[Cd(NO_3)_2(C_{12}H_8N_2)(H_2O)]$
M_r = 434.64
Monoclinic, $P2_1/c$
a = 7.2499 (4) Å
b = 9.4445 (6) Å
c = 20.8273 (12) Å
β = 93.159 (1)°
V = 1423.91 (15) Å^3
Z = 4
D_x = 2.027 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4283 reflections
θ = 2.4–25.2°
μ = 1.58 mm^{-1}
T = 298 (2) K
Block, colorless
0.34 × 0.22 × 0.21 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.655, T_{max} = 0.720
7349 measured reflections
2566 independent reflections
2348 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.2°
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 9$
$l = -22 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.059
S = 1.07
2566 reflections
224 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2 + 0.9061P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0137 (5)

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.337 (2)	Cd1—O1	2.412 (2)
Cd1—O7	2.337 (2)	Cd1—O3^{i}	2.453 (2)
Cd1—N2	2.346 (2)	Cd1—O5	2.499 (2)
Cd1—O4	2.390 (2)	Cd1···Cd1^{i}	5.6461 (3)
N1—Cd1—O7	86.66 (8)	N2—Cd1—O4	157.08 (7)
N1—Cd1—N2	71.52 (7)	N1—Cd1—O1	85.69 (8)
O7—Cd1—N2	80.62 (8)	O7—Cd1—O1	166.55 (8)
N1—Cd1—O4	127.77 (7)	N2—Cd1—O1	86.46 (7)
O7—Cd1—O4	110.09 (9)	O4—Cd1—O1	83.33 (8)

Symmetry code: (i) $1-x, y-\frac{1}{2}, \frac{1}{2}-z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O1^{ii}	0.807 (16)	2.28 (2)	3.017 (3)	153 (2)
O7—H7A···O2^{ii}	0.807 (16)	2.366 (16)	3.105 (4)	153 (2)
O7—H7B···O5^{iii}	0.811 (16)	2.128 (18)	2.929 (3)	169 (3)
O7—H7B···O2^{i}	0.811 (16)	2.60 (3)	3.008 (4)	113 (2)

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

The aromatic H atoms were placed at calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C). The water H atoms were located in difference Fourier maps and were refined with distance restraints of O—H = 0.82 (2) Å and H···H = 1.39(1) Å and with U_{iso}(H) = 1.2U_{eq}(O).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXL97*.

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