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Diaqua(benzimidazole)(nitrato-*κO*)(1,10-phenanthroline)cadmium(II) nitrate

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In the crystal structure of the title compound, [Cd(NO_3)($C_7H_6N_2$)($C_{12}H_8N_2$)(H_2O)$_2$]NO_3, the phenanthroline-chelated Cd atom is bonded to the benzimidazole, two water molecules and a monodentate nitrate group in a six-coordinate octahedral geometry. The cation interacts with the nitrate anion to form a three-dimensional hydrogen-bonding network.

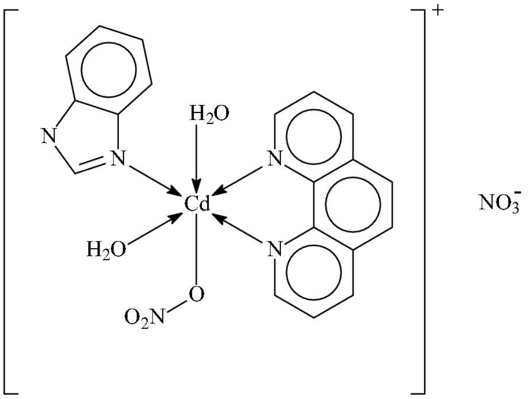
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.008 Å
R factor = 0.046
wR factor = 0.137
Data-to-parameter ratio = 15.1

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

Comment

Cadmium salts, such as cadmium carboxylates, yield adducts with 1,10-phenanthroline in which the heterocycle binds in the typical chelating mode, and a number of such complexes can be found in the Cambridge Structural Database (Version 5.26; Allen, 2002). Cadmium nitrate affords only two complexes, (nitrato-κ^2O,O')(nitrato-*κO*)bis(1,10-phenanthroline)-cadmium (Shi *et al.*, 2004) and di(nitrato-κ^2O,O')bis(1,10-phenanthroline) (Tadjarodi *et al.*, 2001), probably because the two ligands present severe crowding around the metal atom.



(I)

The present study used a hydrothermal method to synthesize a cadmium nitrate adduct with both 1,10-phenanthroline and benzimidazole as donor ligands. Monodentate benzimidazole has been used to bind to, for example, cadmium succinate (Liu & Xu, 2004*a*), cadmium phthalate (Liu & Xu, 2004*b*) and the cadmium derivative of pentaazapentacycloheptacosatridecaene (Sessler *et al.*, 1989). The synthesis yielded diaqua(benzimidazole)(nitrato-*κO*)(1,10-phenanthroline)cadmium(II) nitrate, (I), in which the nitrate anion interacts indirectly with the Cd atom through the coordinated water molecules. In this mixed-ligand compound, the Cd atom in the cation exists in an octahedral environment; the donor atoms of the ligands and a water molecule comprise a square around it. The second water molecule and the O atom of the monodentate nitrate group occupy the other two positions

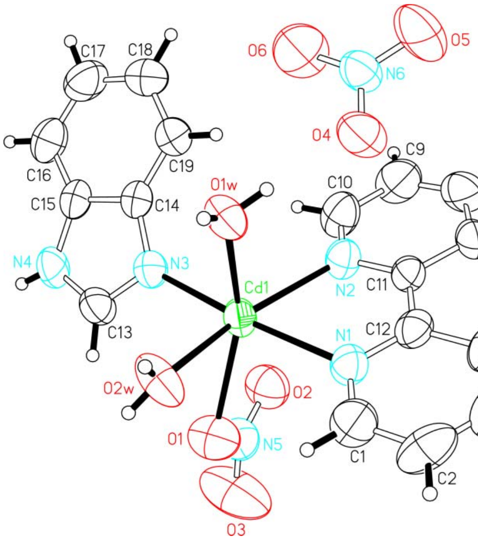


Figure 1
ORTEPII plot (Johnson, 1976) of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radii.

(Fig. 1). The cation and anion interact through H atoms to furnish a tightly held three-dimensional network (Table 2).

Experimental

The title compound was synthesized hydrothermally from cadmium nitrate dihydrate (1 mmol, 0.27 g), 1,10-phenanthroline (2 mmol, 0.36 g), benzimidazole (2 mmol, 0.24 g) and water (20 ml). The reagents were heated in a 30 ml Teflon-lined stainless steel Parr bomb at 426 K for 5 d. The bomb was slowly cooled to room temperature to yield colourless crystals that were collected and washed with water.

Crystal data

$[Cd(NO_3)(C_7H_6N_2)(C_{12}H_8N_2)(H_2O)_2]NO_3$
$M_r = 570.79$
Monoclinic, $P2_1/n$
$a = 7.5119$ (4) Å
$b = 16.9551$ (9) Å
$c = 17.1127$ (9) Å
$\beta = 90.821$ (1)°
$V = 2179.3$ (2) Å^3
$Z = 4$
$D_x = 1.740$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5541 reflections
$\theta = 2.4$–26.8°
$\mu = 1.06$ mm^{-1}
$T = 295$ (2) K
Block, colourless
0.32 × 0.24 × 0.21 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.336$, $T_{max} = 0.808$
13 046 measured reflections
4878 independent reflections
4191 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$
$h = -8 \rightarrow 9$
$k = -19 \rightarrow 21$
$l = -17 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.137$
$S = 1.13$
4878 reflections
322 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 2.947P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.85$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.405 (4)	Cd1—N1	2.343 (4)
Cd1—O1*w*	2.345 (4)	Cd1—N2	2.348 (4)
Cd1—O2*w*	2.316 (3)	Cd1—N3	2.246 (4)
O1—Cd1—O1*w*	151.9 (1)	O1*w*—Cd1—N3	90.0 (1)
O1—Cd1—O2*w*	71.7 (1)	O2*w*—Cd1—N1	90.3 (2)
O1—Cd1—N1	89.9 (2)	O2*w*—Cd1—N2	158.7 (2)
O1—Cd1—N2	117.2 (1)	O2*w*—Cd1—N3	96.1 (2)
O1—Cd1—N3	92.0 (2)	N1—Cd1—N2	71.2 (1)
O1*w*—Cd1—O2*w*	80.2 (1)	N1—Cd1—N3	173.6 (1)
O1*w*—Cd1—N1	91.2 (1)	N2—Cd1—N3	102.6 (1)
O1*w*—Cd1—N2	89.7 (1)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O4	0.848 (10)	1.873 (13)	2.717 (5)	173 (5)
O1*w*—H1*w*2···O2^{i}	0.849 (10)	1.975 (12)	2.824 (5)	179 (6)
O2*w*—H2*w*1···O6^{ii}	0.843 (10)	1.96 (2)	2.775 (5)	163 (5)
O2*w*—H2*w*2···O3^{i}	0.844 (10)	1.883 (15)	2.721 (6)	172 (7)
N4—H4n···O4^{iii}	0.848 (10)	2.03 (3)	2.789 (5)	149 (5)

Symmetry codes: (i) $1 + x, y, z$; (ii) $\frac{3}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$; (iii) $x - \frac{1}{2}, \frac{3}{2} - y, \frac{1}{2} + z$.

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) values tied to the U_{eq} of the parent atoms by a factor of 1.2. The water and amino H atoms were located in difference Fourier maps and were refined, with distance restraints of O—H = N—H = 0.85 (1) Å and H···H = 1.39 (1) Å; their displacement parameters could not be satisfactorily refined and were instead similarly tied.

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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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (2002). *SADABS, SAINT, SMART* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Liu, B.-X. & Xu, D.-J. (2004*a*). *Acta Cryst.* C**60**, m39–m41.
Liu, B.-X. & Xu, D.-J. (2004*b*). *Acta Cryst.* C**60**, m183–m185.
Sessler, J. L., Murai, T. & Lynch, V. (1989). *Inorg. Chem.* **28**, 1333–1341.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shi, X., Zhu, G.-S., Fang, Q.-R., Wu, G., Tian, G., Wang, R.-W., Zhang, D.-L., Xue, M. & Qiu, S.-L. (2004). *Eur. J. Inorg. Chem.* pp. 185–191.
Tadjarodi, A., Taeb, A. & Ng, S. W. (2001). *Main Group Met. Chem.* **24**, 805–806.

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