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A supramolecular cadmium(II) complex: (1,10-phenanthroline)-[tris(2-aminoethyl)amine]cadmium(II) dinitrate hydrate

Hao Zhang,[a] Jiwen Cai,[b] Guang Yang,[a] Gen-Qiang Xue[a] and Liang-Nian Ji[a]*

[a]Department of Chemistry, Zhongshan University, Guangzhou 510275, People's Republic of China, and [b]Instrumentation Analysis and Research Center, Zhongshan University, Guangzhou 510275, People's Republic of China
Correspondence e-mail: cesjln@zsu.edu.cn

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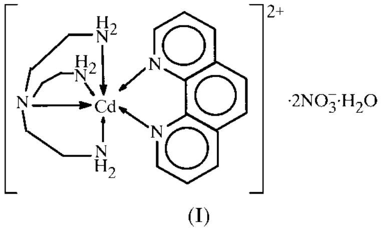
Colourless prismatic crystals of the title compound, $[Cd(tren)(phen)](NO_3)_2\cdot H_2O$ [phen = 1,10-phenanthroline, $C_{12}H_8N_2$; tren = tris(2-aminoethyl)amine, $C_6H_{18}N_4$], form from an aqueous solution of equivalent amounts of $Cd(NO_3)_2$, tren and phen. Infinite one-dimensional polymeric zigzag motifs, constructed *via* alternating hydrogen-bonding and π–π interactions, are further mediated by nitrate–amine hydrogen bonds to create three-dimensional networks.

Comment

Crystal engineering and the design of solid-state architectures are of considerable contemporary interest by virtue of the potential application of functional materials (Braga *et al.*, 1998; Hagrman *et al.*, 1999). Four main types of interactions have been exploited in the construction of supramolecular materials: (i) coordinate covalent bonds connecting metal centres and appropriate bi- or polydentate ligands (Wang *et al.*, 1999); (ii) intermolecular hydrogen bonds (Aakeröy & Beatty, 1998); (iii) π–π interactions of aromatic rings (Ning *et al.*, 1999); and (iv) charge-transfer interactions (Bailey *et al.*, 1998). Among these interactions, hydrogen bonds and π–π stacking play vital roles in molecular recognition and supramolecular chemistry. Herein, we describe a three-dimensional supramolecular cadmium(II) complex, (I), directed by alternating hydrogen-bonding and π–π interactions.



(I)

The Cd atom of (I) adopts a distorted octahedral coordination with six N atoms from tren and phen. The Cd—N distances range from 2.314 to 2.508 Å, in accordance with those values previously reported (Klüfers & Mayer, 1998).

The crystal packing of the complex reveals offset π-stacking between the phen rings with the interplane distances of about 3.50 Å, which is comparable to the phen–phen distance of 3.24–3.42 Å in the stacking of $[M(\text{phen})_2](X_2)$ (Geremia *et al.*, 1992; Ye *et al.*, 1998). Two neighboring $[Cd(\text{phen})(\text{tren})]^{2+}$ cations form a dimeric motif. Furthermore, nitates bridge the adjacent motifs by hydrogen bonds formed between nitrate and amine. Infinite one-dimensional polymeric zigzag motifs constructed *via* alternating hydrogen-bonding and π–π interactions are thus assembled (Munakata *et al.*, 1996; Tse *et al.*, 1998). These exotic supermotifs are further linked by another nitrate–amine hydrogen bond to extend into three-dimensional networks.

Experimental

The ligand tren (2 mmol) in water (5 ml) was added dropwise with stirring to $Cd(NO_3)_2$ (2 mmol) dissolved in water (15 ml) at room temperature, followed by the addition of solid phen (2 mmol). After the filtrate was allowed to stand in the air for several weeks, colourless prismatic crystals of the compound were obtained (yield 65.2%). Elemental analysis calculated for $C_{18}H_{28}CdN_8O_7$ (%): C 37.22, H 4.86, N 19.29; found: C 37.23, H 4.50, N 19.27.

Crystal data

$[Cd(C_6H_{18}N_4)(C_{12}H_8N_2)](NO_3)_2\cdot H_2O$
$M_r = 580.88$
Monoclinic, $P2_1/c$
$a = 11.385\ (2)$ Å
$b = 9.951\ (2)$ Å
$c = 20.745\ (4)$ Å
$\beta = 92.72\ (3)^\circ$
$V = 2347.6\ (8)$ Å^3
$Z = 4$
$D_x = 1.644$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4451 reflections
$\theta = 1.79$–25.68°
$\mu = 0.986$ mm^{-1}
$T = 293\ (2)$ K
Prism, colourless
0.21 × 0.13 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: empirical (Blessing, 1995)
$T_{\min} = 0.820$, $T_{\max} = 0.934$
12 068 measured reflections
4451 independent reflections
3857 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.020$
$\theta_{\max} = 25.68^\circ$
$h = -13 \rightarrow 12$
$k = -12 \rightarrow 9$
$l = -25 \rightarrow 25$
Intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.030$
$wR(F^2) = 0.087$
$S = 1.096$
4451 reflections
309 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.9055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.77$ e Å^{-3}
$\Delta\rho_{\min} = -0.61$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*C*···O5	0.90	2.28	3.142 (7)	162
N2—H2*D*···O5$^{\rm i}$	0.90	2.08	2.977 (6)	171
N3—H3*C*···O2$^{\rm ii}$	0.90	2.20	3.060 (5)	160
N3—H3*D*···O3$^{\rm iii}$	0.90	2.66	3.282 (4)	127
N4—H4*C*···O1*W*	0.90	2.28	3.088 (5)	150
N4—H4*D*···O2	0.90	2.35	3.104 (4)	142
O1*W*—H1*W*···O6$^{\rm iv}$	0.92	2.43	3.134 (7)	134
O1*W*—H2*W*···O4$^{\rm iv}$	0.88	2.38	3.188 (7)	154

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

All H atoms of organic ligands were placed in idealized positions and refined as riding atoms with isotropic displacement parameters. H atoms of the water molecule were found from the difference Fourier map and were also refined as riding atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT*+ (Bruker, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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