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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C)$ = 0.008 Å
 R factor = 0.046
 wR factor = 0.103
 Data-to-parameter ratio = 13.6

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

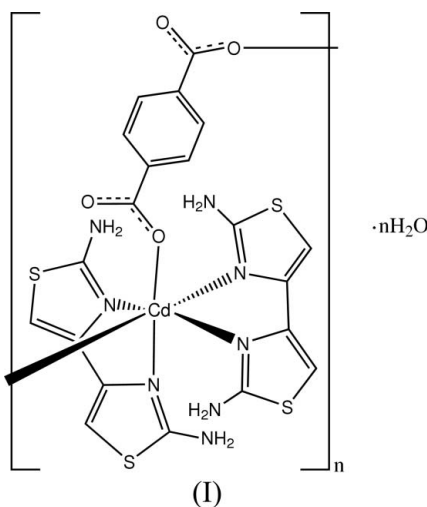
catena-Poly[[[bis(2,2'-diamino-4,4'-bi-1,3-thiazole- κ^2N,N')cadmium(II)]- μ -terephthalato- $\kappa^2O:O'$] monohydrate]

In the crystal structure of the title compound, $\{[Cd(C_8H_4O_4)(C_6H_6N_4S_2)_2] \cdot H_2O\}_n$, the Cd^{II} ion is located on a twofold axis, and is coordinated by two diaminobithiazole ligands and two terephthalate dianions in a distorted octahedral geometry. The terephthalate dianion, located on an inversion centre, bridges the Cd^{II} ions to form polymeric chains.

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Comment

Metal complexes of 2,2'-diamino-4,4'-bi-1,3-thiazole (DABT) have shown potential application in some fields, for example, a Co^{II} complex and an Ni^{II} complex with the DABT ligand have been found to be effective inhibitors of DNA synthesis in tumour cells (Waring, 1981; Fisher *et al.*, 1985). As part of a series of structural investigations of metal complexes with DABT, we present here the crystal structure of the title Cd^{II} complex, (I).



A segment of the polymeric complex structure of (I) is shown in Fig. 1. The Cd^{II} ion is located on a twofold axis, and is coordinated by two DABT and two terephthalate dianions in a distorted octahedral geometry (Table 1). The terephthalate dianion, located on an inversion centre, bridges the Cd^{II} ions to form polymeric chains.

The two thiazole rings of the DABT ligand are twisted relative to each other with a dihedral angle of 14.7 (3)°. This compares with 17.23 (7)° found in $[Cr(C_4H_5NO_4)(DABT)(H_2O)]Cl \cdot H_2O$ (Liu *et al.*, 2004), but is different from the value of 2.60 (10)° found in $[Mn(C_8H_4O_4)(DABT)(H_2O)_2] \cdot 2H_2O$ (Liu *et al.*, 2006). The C1–C4 bond distance of 1.469 (7) Å shows a typical single bond between two *sp*²-hybrid C atoms.

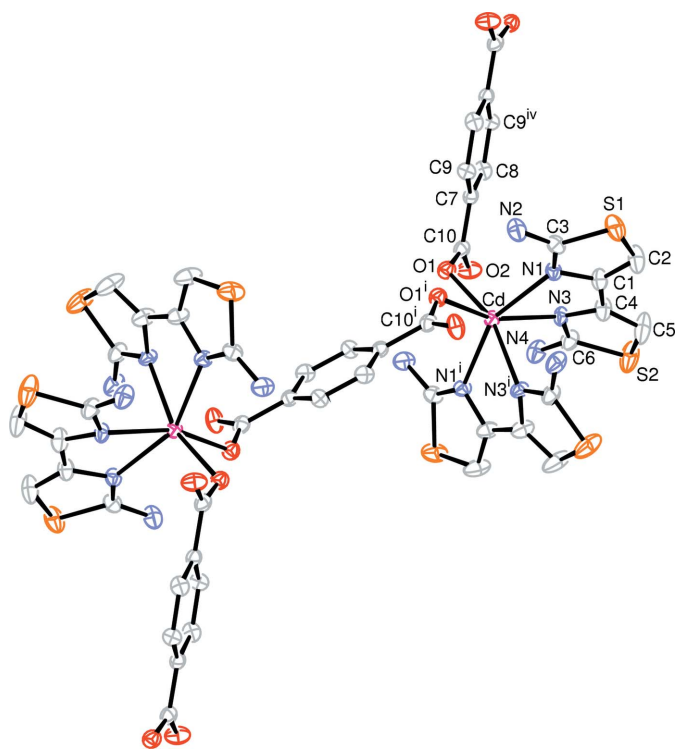


Figure 1

A segment of the polymeric structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). The solvent water molecule and the H atoms have been omitted for clarity. [Symmetry codes: (i) $1 - x, y, -z + \frac{1}{2}$; (iv) $\frac{3}{2} - x, \frac{3}{2} - y, 1 - z$].

An extensive hydrogen-bonding network occurs in the crystal structure of (I) (Table 2). Intra- and interchain N—H···O hydrogen bonding helps to stabilize the crystal structure. The solvent water molecule, located on a twofold axis, is hydrogen bonded with the complex.

Experimental

An aqueous solution (20 ml) containing DABT (1 mmol) and CdCl₂ (1 mmol) was mixed with an aqueous solution (10 ml) of terephthalic acid (1 mmol) and NaOH (2 mmol). The mixture was refluxed for 5 h. The solution was filtered after cooling to room temperature. Yellow single crystals of (I) were obtained from the filtrate after 10 d.

Crystal data

[Cd(C₈H₄O₄)(C₆H₆N₄S₂)₂]₂·H₂O
M_r = 691.06
 Monoclinic, C2/c
a = 9.4657 (14) Å
b = 16.749 (3) Å
c = 17.181 (3) Å
 β = 101.714 (2)°
V = 2667.2 (8) Å³

Z = 4
D_x = 1.721 Mg m⁻³
 Mo *K*α radiation
 μ = 1.18 mm⁻¹
T = 295 (2) K
 Prism, yellow
 0.25 × 0.16 × 0.13 mm

Data collection

Bruker APEXII diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
T_{min} = 0.780, *T_{max}* = 0.860

6709 measured reflections
 2359 independent reflections
 1755 reflections with *I* > 2σ(*I*)
R_{int} = 0.065
 θ_{\max} = 25.0°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.046
wR(*F*²) = 0.103
S = 1.01
 2359 reflections
 174 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.67 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.98 \text{ e } \text{Å}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick, 1997)
 Extinction coefficient: 0.0015 (3)

Table 1

Selected geometric parameters (Å, °).

Cd—O1	2.286 (3)	Cd—N3	2.389 (4)
Cd—N1	2.376 (4)		
O1—Cd—O1 ⁱ	84.95 (18)	N1—Cd—N3 ⁱ	90.98 (14)
O1—Cd—N1 ⁱ	90.66 (13)	O1—Cd—N3	94.13 (13)
O1—Cd—N1	108.73 (13)	N1—Cd—N3	70.92 (14)
N1 ⁱ —Cd—N1	153.9 (2)	N3 ⁱ —Cd—N3	93.2 (2)
O1—Cd—N3 ⁱ	160.27 (13)		

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

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1W—H1W···O1	0.90	2.04	2.893 (6)	158
N2—H2A···O1 ⁱ	0.87	2.27	3.093 (6)	158
N2—H2B···O2 ⁱⁱ	0.89	2.08	2.905 (6)	153
N4—H4A···O1W ⁱⁱⁱ	0.85	2.27	2.946 (6)	137
N4—H4B···O2	0.85	2.14	2.960 (6)	162

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

Amino and water H atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with *U*_{iso}(H) = 1.5*U*_{eq}(O,N). Other H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

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