

catena-Poly[[tetraaquacadmium(II)- μ -hexane-1,6-diamine- $\kappa^2N:N'$] terephthalate dihydrate]**Xiang-Gao Meng^a and
Zhi-Dong Lin^{b*}**^aCentral China Normal University WuHan, Wuhan, 430073, People's Republic of China, and ^bSchool of Materials Science and Technology, Wuhan Institute of Chemical Technology, Wuhan, 430073, People's Republic of China

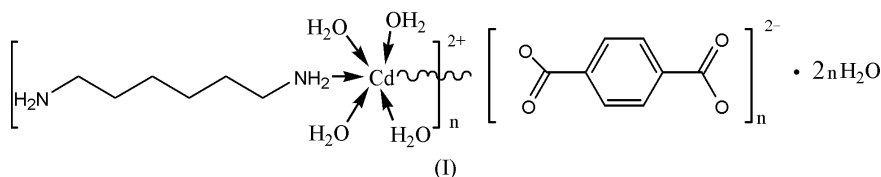
Correspondence e-mail: zhidong.lin@126.com

Key indicatorsSingle-crystal X-ray study
 $T = 293$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.036
 wR factor = 0.084
Data-to-parameter ratio = 12.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\{[Cd(C_6H_{16}N_2)(H_2O)_4](C_8H_4O_4) \cdot 2H_2O\}_n$, (I), exhibits a chain structure. The central Cd^{II} ion is coordinated by four water molecules and two N atoms derived from two 1,6-diaminohexane molecules, giving a zigzag-shaped polymeric chain with a $[Cd-N-C-C-C-C-C-N]_n$ backbone running parallel to the b axis. The two independent terephthalate anions are not coordinated to cadmium(II), acting rather as counter-ions. Each coordinated water molecule forms strong $O-H \cdots O$ hydrogen bonds with the adjacent terephthalate counter-ions, forming a three-dimensional hydrogen-bonded supramolecular architecture.

Received 3 December 2004
Accepted 23 December 2004
Online 15 January 2005**Comment**

The construction of polymers through self-assembly of cations with the appropriate multifunctional ligands has a relatively long history (Efraty *et al.*, 1980; Robl, 1987) and is still a topic of intense interest (Moore & Lee, 1994). One-, two- and three-dimensional polymers with interesting properties, such as electronic, magnetic, optical and physical, have been prepared in recent years. We report here the structure of a new cadmium(II) polymeric complex, (I).



The structure of (I) is shown in Fig. 1. The single-crystal X-ray structure analysis indicates that each Cd^{II} atom is six-coordinated by two 1,6-diaminohexane N atoms and four aqua O atoms. The coordination environment of the Cd^{II} atom is distorted octahedral, in which two N atoms of 1,6-diaminohexane occupy the axial sites. The $Cd1-N1$ bond length [2.314 (3) Å] is consistent with a mean value of 2.308 (4) Å in a similar cadmium complex containing 1,6-diaminohexane (Yuge *et al.*, 1996). The $Cd-O(H_2O)$ bond lengths range from 2.330 (5) to 2.504 (4) Å. 1,6-Diaminohexane acts as a bridging ligand, linking Cd atoms in an end-to-end coordination mode [$N1-Cd1-N1A = 167.00(16)^\circ$], generating a zigzag chain, with a $Cd \cdots Cd$ separation of 12.748 (6) Å. Compound (I) forms an infinite one-dimensional chain extending along the b axis. In the crystal structure, the 1,6-diaminohexane, the carboxylate O atoms of the terephthalate anions and a coordinated water O atom act as acceptors to form $O-H \cdots O$ and $N-H \cdots O$ hydrogen bonds (Table 1), giving a three-dimensional network.

Experimental

All reagents and solvents were used as obtained without further purification. Cd(OH)₂ (1 mmol, 146 mg), terephthalic acid (1 mmol, 166 mg) and 1,6-diaminohexane (1 mmol, 116 mg) were dissolved in an aqueous ammonia solution (10 ml, 30%), and the mixture was stirred for about 20 min at room temperature. The resulting clear colorless solution was kept in air and, after slow evaporation of the solvent over a period of a week, large colorless crystals of (I) formed at the bottom of the vessel. The crystals were isolated, washed three times with water and dried in a vacuum desiccator using anhydrous CaCl₂ (yield 57%). Analysis found: C 33.70, H 6.54, N 5.48%; calculated for C₁₄H₃₂CdN₂O₁₀: C 33.57, H 6.44, N 5.59%.

Crystal data

[Cd(C₆H₁₆N₂)(H₂O)₄](C₈H₄O₄)·2H₂O
M_r = 500.82
 Monoclinic, *P*₂₁/*m*
a = 6.4744 (16) Å
b = 23.758 (6) Å
c = 7.5236 (19) Å
 β = 108.715 (3)°
V = 1096.1 (5) Å³
Z = 2
D_x = 1.517 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 800 reflections
 θ = 2.3–25.0°
 μ = 1.05 mm⁻¹
T = 293 (2) K
 Block, colorless
 0.45 × 0.38 × 0.30 mm

Data collection

Siemens SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.631, *T_{max}* = 0.727
 5584 measured reflections
 1949 independent reflections
 1886 reflections with *I* > 2σ(*I*)
R_{int} = 0.027
 θ_{max} = 25.0°
h = -7 → 7
k = -28 → 28
l = -8 → 8

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.036
wR(*F*²) = 0.085
S = 1.22
 1949 reflections
 154 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 1.7591P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} = 0.001
 Δρ_{max} = 0.77 e Å⁻³
 Δρ_{min} = -1.44 e Å⁻³

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

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1...O7 ⁱ	0.90	2.28	3.137 (5)	159
N1—H2...O1	0.90	2.24	3.102 (5)	162
O3—H11...O7 ⁱ	0.872 (19)	1.87 (2)	2.740 (4)	173 (5)
O5—H12...O2 ⁱⁱ	0.909 (19)	2.31 (3)	3.186 (5)	161 (5)
O6—H13...O2 ⁱⁱⁱ	0.920 (19)	2.15 (2)	3.069 (5)	176 (5)
O7—H16...O1	0.91 (6)	1.88 (7)	2.773 (5)	169 (5)
O7—H15...O2 ⁱⁱ	0.78 (6)	1.94 (6)	2.713 (5)	171 (6)

Symmetry codes: (i) *x*, *y*, *z* + 1; (ii) *x* + 1, *y*, *z*; (iii) *x* + 1, *y*, *z* + 1.

The H atoms bonded to C and N atoms were constrained to ride on their parent atoms, with distances of 0.93 or 0.97 Å and 0.90 Å, respectively, and *U*_{iso}(H) = 1.2*U*_{eq}(parent atom). Atoms H11, H12, H13 and H14, bonded to O atoms, were found in a difference Fourier map and were refined with restraints on the O...H distance [0.87 (2)–0.92 (2) Å]. The deepest hole was located near to the Cd atom.

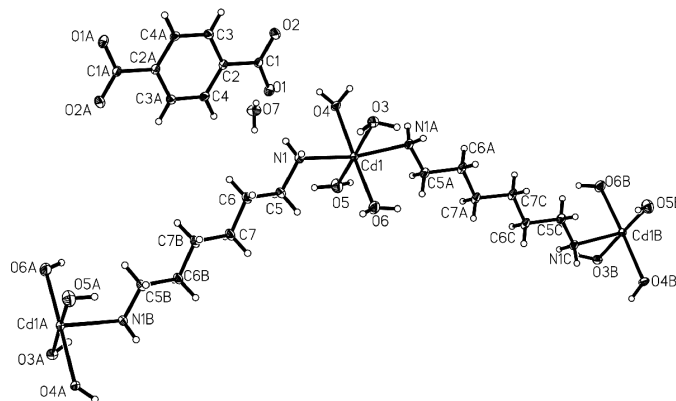


Figure 1 A fragment of the polymeric structure of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. [Symmetry codes: (A) *x*, ½ - *y*, *z*; (B) 2 - *x*, 1 - *y*, 2 - *z*; (C) 2 - *x*, ½ + *y*, 2 - *z*.]

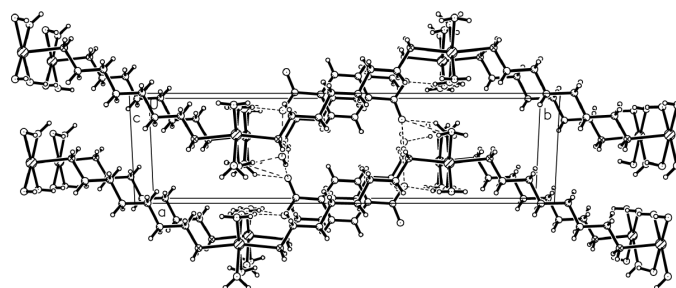


Figure 2 Perspective view of the crystal packing in the unit cell, showing the linkage of the polymeric chains by hydrogen bonding (dashed lines).

Data collection: SMART (Siemens, 1996); cell refinement: SMART; data reduction: SAINT (Siemens, 1996); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The authors thank the Education Office of Hubei Province, People's Republic of China, for research grant No. 2004D007.

References

Efraty, A., Feinstein, I., Wackerle, L. & Frolow, F. (1980). *Angew. Chem. Int. Ed. Engl.* **19**, 633–634.
 Moore, J. S. & Lee, S. (1994). *Chem. Ind. (London)*, pp. 556–560.
 Robl, C. (1987). *Mater. Res. Bull.* **22**, 1483–1491.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997a). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS, Inc., Madison, Wisconsin, USA.
 Siemens (1996). *SMART* and *SAINTE*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
 Yuge, H., Nishikiori, S. I. & Iwamoto, T. (1996). *Acta Cryst.* **C52**, 575–578.