Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaquabis(2-methoxymethyl-1*H*-benzimidazole-κN^3)cadmium(II)]-μ-terephthalato-$\kappa^2 O:O'$]

Long-Fei Zu, Yong Wang, Zhong-Min Su,* Kui-Zhan Shao and Ya-Hui Zhao

Institute of Functional Materials Chemistry, Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail: zmsu@nenu.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.064
Data-to-parameter ratio = 15.9

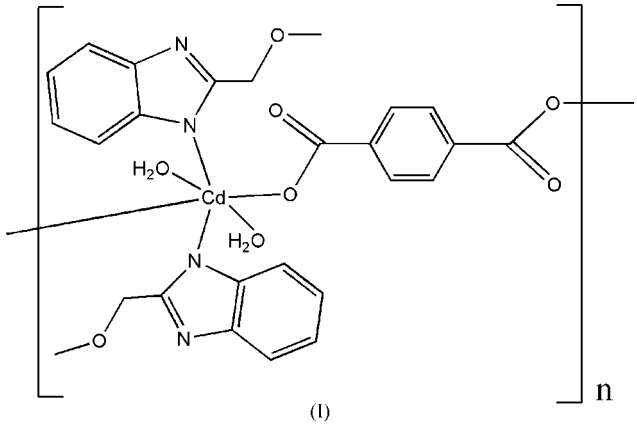
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 13 December 2006
Accepted 14 December 2006

The structure of $[Cd(C_8H_4O_4)(C_9H_{10}N_2O)_2(H_2O)_2]_n$, consists of linear chains with terephthalate anions bridging the Cd atoms. The Cd atom exists in an octahedral coordination environment, coordinated by two water O atoms, two N atoms of the benzimidazole ligands and two terephthalate O atoms. The Cd atom and the terephthalate group both lie on inversion centers. Interchain hydrogen bonds form a three-dimensional supramolecular framework.

Comment

Carboxylic acids such as terephthalic acid are used in the synthesis of metal–organic frameworks (Anokhina *et al.*, 2005; Barthelet *et al.*, 2004; Li *et al.*, 1998 Wang *et al.*, 2005; Williams *et al.*, 2005). We have reported two coordination polymers of terephthalic acid (Xu *et al.*, 2004; Wang *et al.*, 2006). The reports are now extended to the present study, which has 2-methoxymethyl-1*H*-benzoimidazole as a neutral *N*-donor. The title complex, (I), was synthesized hydrothermally.



(I)

The Cd atom exists in an octahedral environment, coordinated by two carboxylate O atoms from two terephthalate dianions, two N atoms from two benzimidazoles and two water molecules (Fig. 1). The Cd atom and the terephthalate group both lie on inversion centers. The Cd—N and Cd—O distances are similar to those in a related compound (Liu *et al.*, 2004). The dianaion functions in a bridging mode, linking adjacent metal atoms into a linear chain (Fig. 2). Intermolecular hydrogen bonds (Table 2) link the chains into a three-dimensional supramolecular framework.

Experimental

A mixture of cadmium(II) acetate dihydrate (0.080 g), terephthalic acid (0.050 g), sodium hydroxide (0.024 g), 2-methoxymethyl-1*H*-

benzimidazole (0.049 g) and water (10 ml) was stirred for 20 min. The mixture was then transferred to a 23 ml Teflon-lined reactor. The mixture was heated to 443 K and maintained at that temperature for 3 d; it was then cooled to room temperature at a rate of 5 K h^{-1}. Colorless block-shaped crystals were obtained; these were washed with water and then dried (yield: *ca* 80%, based on Cd). Elemental analysis found: C 48.91, H 4.49, N 8.96%; calculated: C 49.03, H 4.43, N 8.80%.

Crystal data

$C_{26}H_{28}CdN_4O_8$
M_r = 636.92
Triclinic, $P\overline{1}$
a = 7.622 (5) Å
b = 8.714 (5) Å
c = 11.082 (5) Å
α = 94.120 (5)°
β = 103.502 (5)°
γ = 111.320 (5)°
V = 656.7 (6) Å^3
Z = 1
D_x = 1.611 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 293 (2) K
Block, colorless
0.22 × 0.19 × 0.17 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.829, T_{max} = 0.864
4086 measured reflections
2957 independent reflections
2888 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.064
S = 1.05
2957 reflections
186 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0261P)^2 + 0.3405P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.280 (2)	Cd1—O3*W*	2.359 (2)
Cd1—O1	2.3183 (18)		
N1—Cd1—O1	88.26 (6)	O1—Cd1—O3*W*	94.20 (7)
N1—Cd1—O3*W*	92.80 (7)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.12	2.939 (3)	159
O3*W*—H3*B*···O2^{ii}	0.862 (10)	1.863 (12)	2.709 (3)	167 (3)
O3*W*—H3*A*···O2^{iii}	0.857 (10)	2.056 (16)	2.864 (3)	157 (3)

Symmetry codes: (i) $-x, -y-1, -z$; (ii) $-x, -y, -z$; (iii) $x-1, y, z$.

H atoms were initially located in difference maps, but were subsequently introduced in calculated positions and treated as riding, with C—H = 0.93 (CH), 0.96 (CH_3) or 0.97 Å (CH_2), and N—H = 0.86 Å. Water H atoms were refined using restraints [O—H = 0.85 (1) Å and H···H = 1.39 (2) Å]. All H atoms were allocated displacement parameters related to those of their parent atoms [U_{iso}(H) = 1.2U_{eq}(C or N) or 1.5U_{eq}(O or methyl C)].

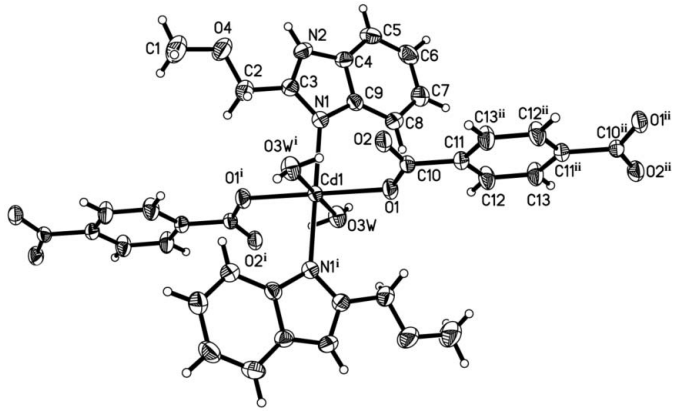


Figure 1
Part of the polymeric structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x, -y, -z$; (ii) $1-x, -y, 1-z$.]

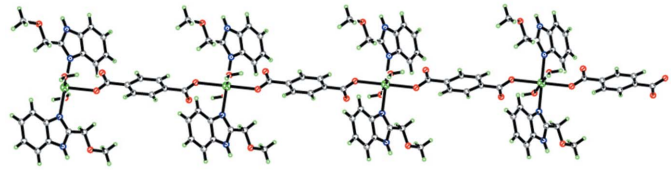


Figure 2
The chain structure of (I).

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

We gratefully acknowledge financial support from the National Natural Science Foundation of China (project Nos 20573016 and 20373009).

References

Anokhina, E. R., Vougo-Zanda, M., Wang, X. Q. & Jacobson, A. J. (2005). *J. Am. Chem. Soc.* **127**, 15000–15001.
Barthelet, K., Marrot, J., Ferey, G. & Riou, D. (2004). *Chem. Commun.* pp. 520–521.
Bruker. (2004). *APEX2* (Version 1.08), *SAINT* (Version 7.03) and *SADABS* (Version 2.11). Bruker AXS Inc., Madison, Wisconsin, USA.
Li, H. L., Daivis, C. E., Groy, T. L., Kelley, D. G. & Yaghi, O. M. (1998). *J. Am. Chem. Soc.* **120**, 2186–2187.
Liu, B.-X., Su, J.-R. & Xu, D.-J. (2004). *Acta Cryst.* C**60**, m183–m185.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, X. L., Qin, C., Wang, E. B., Su, Z. M., Xu, L. & Batten, S. R. (2005). *Chem. Commun.* pp. 4789–4791.
Wang, Y., Su, Z.-M., Hao, X.-R., Shao, K.-Z. & Zhao, Y.-H. (2006). *Acta Cryst.* E**62**, m322–m324.
Williams, C. A., Blake, A. J., Hubberstey, P. & Schroder, M. (2005). *Chem. Commun.* pp. 5435–5437.
Xu, H. B., Su, Z. M., Shao, K. Z., Zhao, Y. H., Xing, Y., Liang, Y. C., Zhang, H. J. & Zhu, D. X. (2004). *Inorg. Chem. Commun.* **7**, 260–263.