APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2003; **17**: 647–649
DOI:10.1002/aoc.459

Crystallographic report

Crystal structure of a three-dimensional coordination polymer, $[Cd(Hbtc)(H_2O)]_n$ (btc = 1,2,4-benzenetricarboxylate)

Pei-Qing Zheng, La-Sheng Long*, Rong-Bin Huang and Lan-Sun Zheng

Department of Chemistry and State Key Laboratory for Physical Chemistry of Solid Surface, Xiamen University, Xiamen 361005, People's Republic of China

Received 3 February 2003; Revised 7 February 2003; Accepted 11 February 2003

The three-dimensional coordination polymer $[Cd(Hbtc)(H_2O)]_n$ (1) (btc = 1,2,4-benzenetricarboxylate) has been synthesized by hydrothermal reaction of cadmium(II) ions and 1,2,4-benzenetricarboxylic acid anhydride in which the cadmium(II) center is coordinated by one water molecule and five separated Hbtc ligands that define a distorted octahedral geometry. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: cadmium; 1,2,4-benzenetricarboxylate; crystal structure; coordination polymer

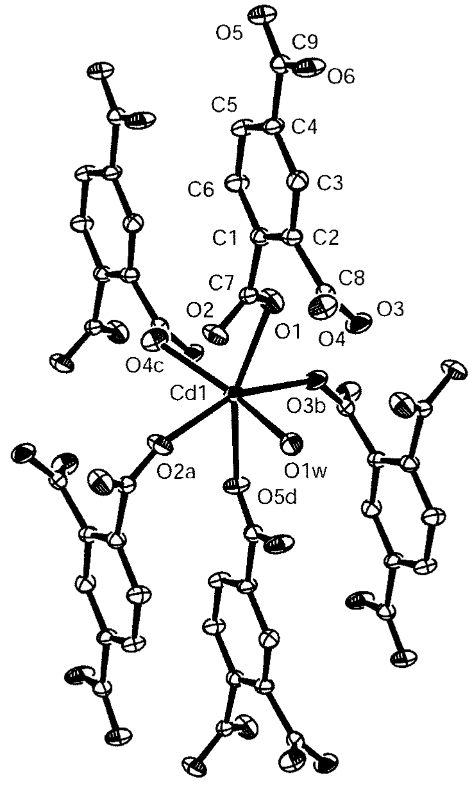

Figure 1. ORTEP plot showing the coordination environment of the cadmium atom at the 50% probability level. Hydrogen atoms were omitted for clarity. Key geometry parameters: Cd1–O1 2.358(3), Cd1–O1w 2.395(3), Cd1–O3b 2.337(3), Cd1–O2d 2.361(3), Cd1–O4a 2.262(3), Cd1–O5c 2.342(3) Å; O1–Cd1–O1w 91.35(10), O3b–Cd1–O1w 92.19(11), O3b–Cd1–O1 75.45(10), O4a–Cd1–O3b 117.34(10), O4a–Cd1–O5c 114.79(10), O3b–Cd1–O5c 81.23(10), O4a–Cd1–O1 81.52(11), O5c–Cd1–O1 156.01(10), O4a–Cd1–O2d 78.52(10), O3b–Cd1–O2d 159.62(10), O5c–Cd1–O2d 80.27(10), O1–Cd1–O2d 121.70(9), O4a–Cd1–O1w 146.24(10), O5c–Cd1–O1w 83.95(10), O2d–Cd1–O1w 77.43(10), C7–O1–Cd1 100.1(2)°. Symmetry operation: a = $x, y-1, z$; b = $-x+1, -y+1, -z$; c = $x, y-1, z+1$; d = $-x, -y+1, -z$.

---

*Correspondence to: La-Sheng Long, Department of Chemistry and State Key Laboratory for Physical Chemistry of Solid Surface, Xiamen University, Xiamen 361005, People's Republic of China.
E-mail: lslong@jingxian.xmu.edu.cn

Contract/grant sponsor: National Science Foundation of China; Contract/grant number: 20271044; 20273052.
Contract/grant sponsor: NSF of Fujian Province; Contract/grant number: E0110001.

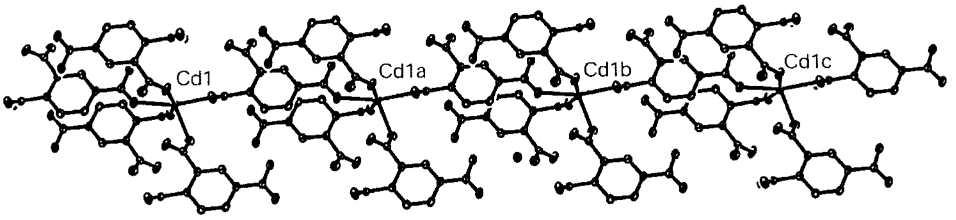

Figure 2. Perspective view of the one-dimensional cadmium chain of **1**.

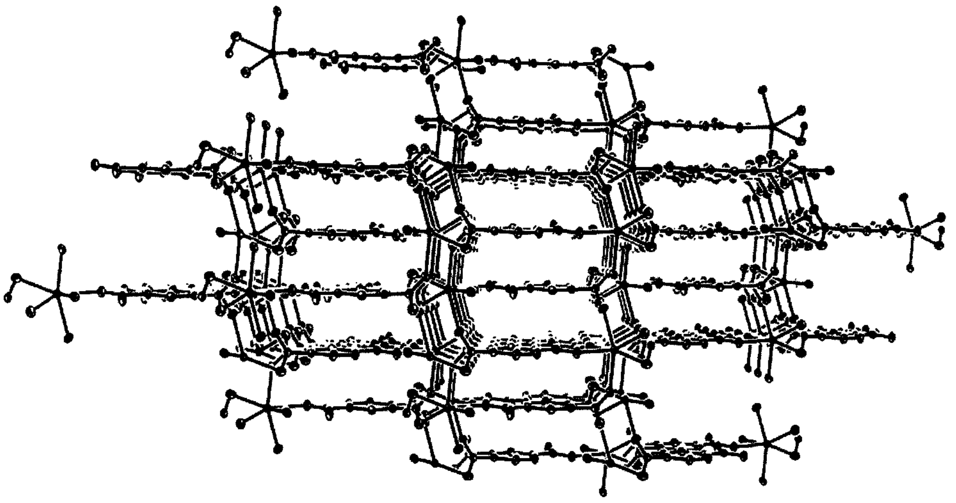

Figure 3. ORTEP plot showing three-dimensional structure of **1** viewed along the *b* axis at the 50% probability level.

COMMENT

Rigid ligands are known as good candidates for assembling coordination polymers, not only because they permit a reasonable predication of the constructed structure, but also because they form structures of higher dimension.[1,2] In particular, the coordination polymers formed by d^{10} metals, such as zinc(II) and cadmium(II) atoms, and the rigid aromatic carboxylate groups often exhibit intriguing photoluminescent properties.[2–5] Here, we report the synthesis and crystal structure of a three-dimensional coordination polymer $[Cd(Hbtc)(H_2O)]_n$ (**1**) (btc = 1, 2, 4-benzenetricarboxylate). Crystallography shows that the cadmium(II) center lies in a distorted octahedral environment defined by one oxygen atom from coordination water and five oxygen atoms belonging to five monodentate carboxylate groups, as shown in Fig. 1. The assembly of **1** can be best viewed as the following two steps: first, the Hbtc ligand acts as a bridging ligand by connecting two adjacent cadmium(II) atoms to form an infinite one—dimensional cadmium chain, as shown in Fig. 2; second, the neighboring chains are further connected together through oxygen atoms of the carboxylate group of the Htbc ligands to generate a three-dimensional architecture, as shown in Fig. 3 viewed along the *b* axis.

EXPERIMENTAL

Synthesis

A mixture of $CdCl_2 \cdot 2.5H_2O$, 1,2,4-benzenetricarboxylic acid anhydride and water in the molar ratio 1.5 : 1 : 926 was adjusted to around pH 6 with 1 mol l^{-1} NaOH, then transferred and sealed in a 25 ml Teflon-lined stainless-steel container. The container was heated to 180 °C and held at that temperature for 1 day, then cooled to 100 °C at a rate of 5 °C h^{-1}, and held for 10 h, followed by further cooling to 30 °C at a rate of 5 °C h^{-1}. The primrose-yellow block crystals of **1** were collected.

CRYSTALLOGRAPHY

Intensity data were collected at 298 K on Smart Apex 2000 diffractometer for a pale-yellow crystal 0.07 × 0.23 × 0.27 mm^3 $C_9H_6CdO_7$, $M = 338.54$, triclinic, P-1, $a = 6.9975(2)$, $b = 7.0573(2)$, $c = 10.0967(3)$ Å, $\alpha = 83.326(2)°$, $\beta = 86.2540(10)°$, $\gamma = 69.2320(10)°$, $V = 462.90(2)$ Å^3, $Z = 2$; 1870 unique data ($\theta = 28.0°$), 1838 data with $I > 2\sigma(I)$. $R_1 = 0.029$, $wR_2 = 0.067$; $\rho_{max} = 0.78$ e Å^{-3} based on 163 parameter. Program used: SHELXL and ORTEP. CCDC deposition number: 198396.

Acknowledgements

We thank the National Science Foundation of China (grant nos, 20271044 and 20273052) and NSF of Fujian Province, P.R. China (E0110001).

REFERENCES

1. Ford PC, Cariati E, Bourassa J. *Chem. Rev.* 1999; **99**: 3625.
2. Tao J, Tong ML, Shi JX Chen XM, Ng SW. *Chem. Commun.* 2001; 2043.
3. Yang SY, Long LS, Huang RB, Zheng LS. *Chem. Commun.* 2002; 472.
4. Yang SY, Long LS, Jiang YB, Huang RB, Zheng LS. *Chem. Mater.* 2002; **14**: 3229.
5. Yuan W, Long LS. *Appl. Organometal. Chem.* 2003; **17**: 257.