

Poly[(μ_2 -4,4'-bipyridine- κ^2 N:N')bis(μ_2 -*p*-toluenesulfonato- κ^2 O:O')cadmium(II)]

Lin Ping,^a Zhi-Cheng Wang^a and Seik Weng Ng^{b*}

^aSchool of Materials and Chemical Engineering, Zhongyuan Institute of Technology, Zhengzhou, Henan 450007, People's Republic of China, and

^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study

T = 291 K

Mean σ (C–C) = 0.006 Å

R factor = 0.034

wR factor = 0.087

Data-to-parameter ratio = 18.1

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

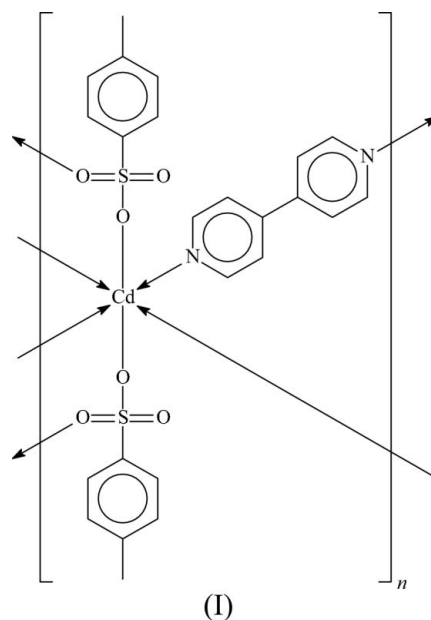
The Cd atom in the polymeric title structure, [Cd(C₇H₇O₃S)₂(C₁₀H₈N₂)]_{*n*}, exists in a slightly distorted *cis*-N₂O₄Cd octahedral geometry. In the crystal structure, two *p*-toluenesulfonate ligands bridge two Cd atoms forming a linear chain, and adjacent chains are linked through 4,4'-bipyridine ligands into a three-dimensional network.

Received 12 July 2006

Accepted 13 July 2006

Comment

Arenesulfonate salts, particularly those of cadmium, tend to exist as well formed crystals and the crystal structures of a large number of cadmium sulfonates have been reported (Cai, 2004). On the other hand, only a few examples of structures of the *N*-heterocycle spacer, 4,4'-bipyridine, which has frequently been used to link metal atoms, have been reported which include a cadmium sulfonate component, *e.g.* cadmium trifluoromethylsulfonate (Xiong *et al.*, 1999), cadmium 2-sulfobenzoate (Su *et al.*, 2005) and cadmium 5-sulfoisophthalate (Li *et al.*, 2004) adducts. In the title structure (Fig. 1), two *p*-toluenesulfonate units bridge adjacent Cd atoms to form a chain along the *a* axis of the monoclinic unit cell; the chain features eight-membered Cd–O–S–O–Cd–O–S–O rings. Adjacent chains are linked through 4,4'-bipyridine ligands. Owing to the *cis* coordination of the N atoms of the 4,4'-bipyridine ligands in the octahedron around the Cd atom (Table 1), the structure adopts a three-dimensional network architecture.



Experimental

Cadmium sulfate (0.21 g, 1 mmol) and sodium *p*-toluenesulfonate (0.20 g, 1 mmol) were dissolved in methanol (10 ml) and to this solution was added 4,4'-bipyridine (0.15 g, 1 mmol). The solution was set aside for several days for the formation of crystals.

Crystal data

[Cd(C₇H₇O₃S)₂(C₁₀H₈N₂)]
M_r = 610.96
 Monoclinic, *P*2₁/*n*
a = 9.7585 (7) Å
b = 18.290 (1) Å
c = 14.246 (1) Å
 β = 96.917 (1)°
V = 2524.1 (3) Å³

Z = 4
D_x = 1.608 Mg m⁻³
 Mo *K*α radiation
 μ = 1.07 mm⁻¹
T = 291 (2) K
 Prism, colorless
 0.39 × 0.29 × 0.22 mm

Data collection

Bruker APEX-II area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.615, *T_{max}* = 0.795

21285 measured reflections
 5757 independent reflections
 4496 reflections with *I* > 2σ(*I*)
R_{int} = 0.041
 θ_{\max} = 27.5°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.034
wR(*F*²) = 0.087
S = 1.03
 5757 reflections
 318 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.7515P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.51 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.68 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cd1—O1	2.310 (2)	Cd1—O4	2.329 (2)
Cd1—O2 ⁱ	2.320 (2)	Cd1—N1	2.324 (2)
Cd1—O5 ⁱⁱ	2.289 (2)	Cd1—N2 ⁱⁱⁱ	2.326 (2)
O1—Cd1—O2 ⁱ	99.65 (8)	O2 ⁱ —Cd1—N2 ⁱⁱⁱ	90.91 (9)
O1—Cd1—O4	84.63 (8)	O4—Cd1—O5 ⁱⁱ	97.11 (9)
O1—Cd1—O5 ⁱⁱ	80.96 (8)	O4—Cd1—N1	168.17 (8)
O1—Cd1—N1	89.88 (9)	O4—Cd1—N2 ⁱⁱⁱ	91.00 (9)
O1—Cd1—N2 ⁱⁱⁱ	167.66 (8)	O5 ⁱⁱ —Cd1—N1	92.35 (9)
O2 ⁱ —Cd1—O4	80.02 (8)	O5 ⁱⁱ —Cd1—N2 ⁱⁱⁱ	88.17 (9)
O2 ⁱ —Cd1—O5 ⁱⁱ	176.98 (8)	N1—Cd1—N2 ⁱⁱⁱ	96.41 (9)
O2 ⁱ —Cd1—N1	90.61 (9)		

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

H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and were included in the refinement in the riding-model approximation. Their displacement parameters were set to 1.2 or 1.5 times *U_{eq}*(C).

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve

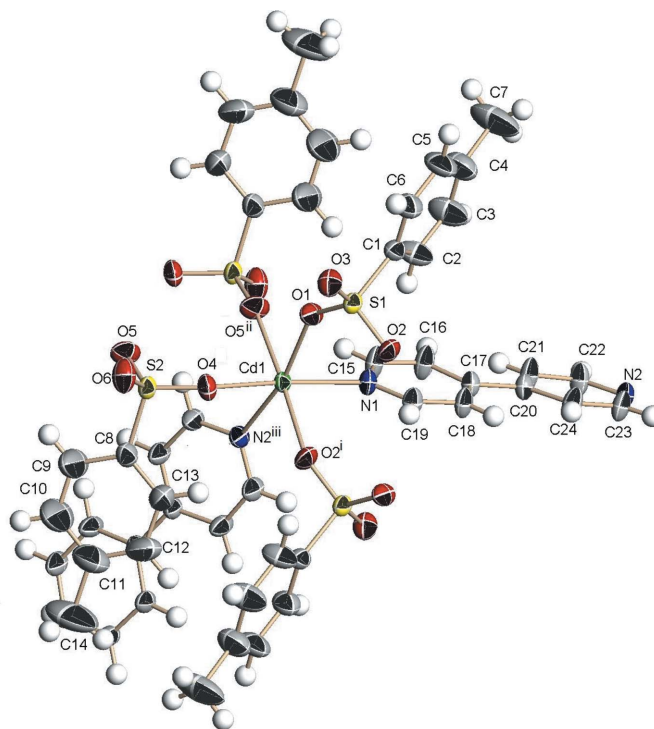


Figure 1

The coordination of Cd in polymeric [Cd(C₁₀H₈N₂)(C₇H₇SO₃)₂]. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. The symmetry codes are given in Table 1.

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

We thank Luoyang Normal College for the diffraction measurements. We also thank Zhongyuan Institute of Technology and the University of Malaya for supporting this study.

References

- Bruker (2004). SAINT (Version 7.12A) and SMART (Version 7.12A). Bruker AXS Inc., Madison, Wisconsin, USA.
 Cai, J.-W. (2004). *Coord. Chem. Rev.* **248**, 1061–1083.
 Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
 Li, X., Cao, R., Sun, D.-F., Bi, W.-H. & Yuan, D.-Q. (2004). *Eur. J. Inorg. Chem.* pp. 2228–2231.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Su, W., Bi, W.-H., Li, X. & Cao, R. (2005). *Acta Cryst.* **C61**, m16–m18.
 Xiong, R.-G., Liu, C.-M., Zuo, J.-L. & You, X.-Z. (1999). *Inorg. Chem. Commun.* **2**, 292–297.