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Poly[[bis(*p*-toluenesulfonato-κO)cadmium(II)]-bis(μ_2-1,3-di-4-pyridylpropane-$\kappa^2 N:N'$)]

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Key indicators

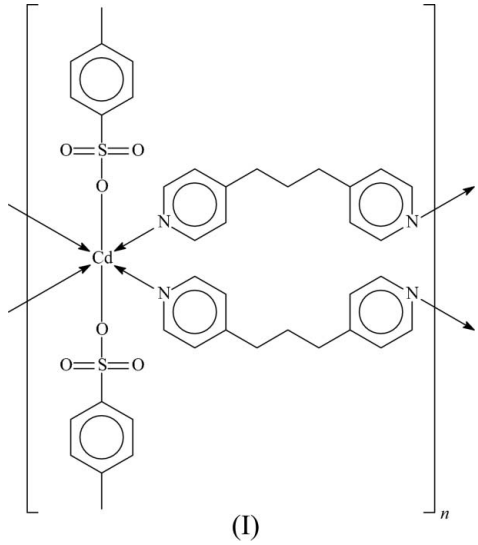
Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.097
Data-to-parameter ratio = 18.4

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

The Cd atom in the title polymeric structure, $[Cd(C_7H_7O_3S)_2(C_{13}H_{14}N_2)_2]_n$, exists in a slightly distorted *trans*-N_2O_4Cd octahedral geometry; the Cd atom lies on a special position of 2 site symmetry. The *p*-toluenesulfonate ligand coordinates in a monodentate mode to the Cd atom, and the 1,3-di-4-pyridylpropane ligand links adjacent Cd atoms into a layer structure.

Comment

The product of the reaction of cadmium bis(*p*-toluenesulfonate) and 4,4′-bipyridine is a 1:1 adduct, which exists as a polymeric structure in which the Cd atom is bridged by two sulfonate groups, as well as by the 4,4′-bipyridine spacer ligand, in a slightly distorted *cis*-N_2O_4 octahedral geometry (Ping *et al.*, 2006). A similar synthesis using the more flexible 1,3-di-4-pyridylpropane ligand has yielded the title 1:2 metal–ligand adduct, (I), in which the metal shows slightly disorted *trans*-N_4O_2 octahedral Cd coordination. The sulfonate group coordinates in a monodentate mode to the Cd atom and the two spacer ligands bridge adjacent metal atoms into a layer structure. Part of the polymeric structure of (I) is shown in Fig. 1 and selected bond lengths and angles are given in Table 1.



(I)

Experimental

Cadmium sulfate (0.21 g, 1 mmol) was dissolved with sodium *p*-tolunesulfonate (0.20 g, 1 mmol) in a small volume of methanol (10 ml). 1,3-Di-4-pyridylpropane (0.20 g,1 mmol) was added. Colourless crystals of (I) separated from the solution after a few days.

Crystal data

$[Cd(C_7H_7O_3S)_2(C_{13}H_{14}N_2)_2]$
M_r = 851.30
Orthorhombic, *Pnna*
a = 24.101 (2) Å
b = 17.286 (1) Å
c = 9.2556 (6) Å
V = 3856.0 (5) Å^3
Z = 4
D_x = 1.466 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.73 mm^{-1}
T = 291 (2) K
Block, colourless
0.31 × 0.22 × 0.16 mm

Data collection

Bruker APEXII area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.790, T_{max} = 0.892
28015 measured reflections
4435 independent reflections
3453 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.05
4435 reflections
241 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 3.6136P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.321 (2)	Cd1—N1^{i}	2.347 (2)
Cd1—O1^{i}	2.321 (2)	Cd1—N2^{ii}	2.337 (2)
Cd1—N1	2.347 (2)	Cd1—N2^{iii}	2.337 (2)
O1—Cd1—O1^{i}	179.7 (1)	O1^{i}—Cd1—N2^{iii}	89.0 (1)
O1—Cd1—N1	87.9 (1)	N1—Cd1—N1^{i}	84.7 (1)
O1—Cd1—N1^{i}	92.3 (1)	N1—Cd1—N2^{ii}	94.6 (1)
O1—Cd1—N2^{ii}	89.0 (1)	N1—Cd1—N2^{iii}	178.5 (1)
O1—Cd1—N2^{iii}	90.9 (1)	N1^{i}—Cd1—N2^{ii}	178.5 (1)
O1^{i}—Cd1—N1	92.3 (1)	N1^{i}—Cd1—N2^{iii}	94.6 (1)
O1^{i}—Cd1—N1^{i}	87.9 (1)	N2^{ii}—Cd1—N2^{iii}	86.3 (1)
O1^{i}—Cd1—N2^{ii}	90.9 (1)		

Symmetry codes: (i) $x, -y+\frac{3}{2}, -z+\frac{3}{2}$; (ii) $x+\frac{1}{2}, y, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

H atoms were positioned geometrically, with C—H distances in the range 0.93–0.97 Å, and were included in the refinement in the riding-model approximation, with U_{iso}(H) = 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 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*.

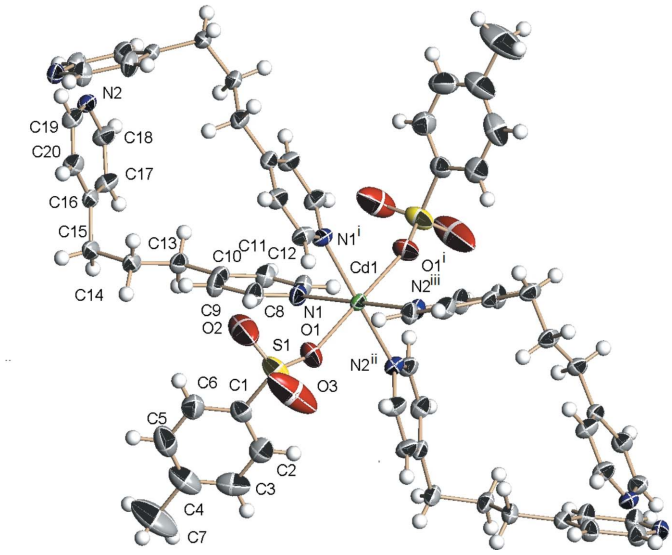


Figure 1
Part of the polymeric structure of $[Cd(C_{13}H_{14}N_2)(C_7H_7SO_3)_2]_n$. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Symmetry codes are given in Table 1.

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