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Crystallographic report

catena-Poly[aqua(phenyl-1,3-bisoxyacetato) tris(pyridine)cadmium(II)], $[(H_2O)(C_5H_5N)_3(O_2CCH_2OC_6H_4OCH_2CO_2)Cd]_n$

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The $[O_2CCH_2OC_6H_4OCH_2CO_2]^{2-}$ group bridges adjacent planar $[(H_2O)(C_5H_5N)_3Cd]^{2+}$ units into a linear chain. The carboxyl groups occupy opposite sites in the octahedral environment of the cadmium atom. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium; phenyl-1,3-bisoxyacetatic acid; polymer structure

COMMENT

In recent years, self-assembly metal complexes with multifunctional carboxylic acids ligand have attracted considerable attention in supramolecular chemistry and crystal engineering.[1–3] The reaction of pyridine, cadmium dinitrate tetrahydrate and phenyl-1,3-bisoxyacetate sodium afforded the cadmium(II) coordination polymer $[(H_2O)(C_5H_5N)_3(O_2CCH_2OC_6H_4OCH_2CO_2)Cd]_n$ (Fig. 1). Crystallography shows that the cadmium atom is coordinated by two oxygen atoms of two phenyl-1,3-bisoxyacetate ligand, three pyridine nitrogen atoms and one water molecule that define an octahedral geometry. The $[O_2CCH_2OC_6H_4OCH_2CO_2]^{2-}$ ligand bridges adjacent planar $[(H_2O)(C_5H_5N)_3Cd]^{2+}$ units into a linear chain that propagates along the *b* axis. The two symmetry-independent chains have similar coordination geometries and topologies.

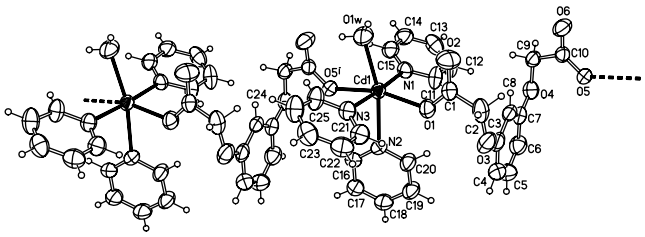

Figure 1. A portion one of the two polymeric $[(H_2O)(C_5H_5N)_3(O_2CCH_2OC_6H_4OCH_2CO_2)Cd]_n$ chains. Selected bond distances and angles for the unprimed molecule: Cd1–O1 2.261(5), Cd1–$O5^i$ 2.342(4), Cd1–O1w 2.354(5), Cd1–N1 2.332(5), Cd1–N2 2.475(5), Cd1–N3 2.333(6) Å; O1–Cd1–$O5^i$ 163.4(2), O1–Cd1–O1w 113.2(2), O1–Cd1–N1 92.3(2), O1–Cd1–N2 81.5(2), O1–Cd1–N3 90.7(2), $O5^i$–Cd1–O1w 83.4(2), $O5^i$–Cd1–N1 88.3(2), $O5^i$–Cd1–N2 81.9(2), $O5^i$–Cd1–N3 89.4(2), O1w–Cd1–N1 89.2(2), O1w–Cd1–N2 165.0(2), O1w–Cd1–N3 88.1(2), N1–Cd1–N2 92.8(2), N1–Cd1–N3 176.6(2), N2–Cd1–N3 89.2(2)°. Translation code: $i = x, y - 1, z$.

EXPERIMENTAL

The compound was synthesized by the addition of pyridine (3 ml) and cadmium dinitrate tetrahydrate (6.16 g, 20 mmol) to an aqueous solution of phenyl-1,3-bisoxyacetatic acid (9.04 g, 40 mmol). Colorless prisms were isolated from the filtered solution at room temperature over several days. Anal. Found: C, 50.89; H, 4.37; N, 7.01. Calc. for $C_{25}H_{25}N_3O_7Cd$: C, 50.73; H, 4.26; N, 7.10%. The

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room-temperature X-ray intensities were measured on a Rigaku Raxis-Rapid diffractometer for a colorless $0.18 \times 0.26 \times 0.38\ mm^3$ crystal. $C_{25}H_{25}CdN_3O_7$, $M = 591.88$, triclinic, $P\bar{1}$, $a = 8.699(2)$, $b = 10.322(2)$, $c = 29.362(6)$ Å, $\alpha = 80.17(3)$, $\beta = 87.28(3)$, $\gamma = 81.95(3)°$, $V = 2571.4(9)$ Å^3, $Z = 4$, 11 460 unique reflections, $R = 0.080$ for 9392 $I > 2\sigma(I)$ reflections. The final difference Fourier map had two large peaks (>4 e$^-$Å^{-3}), one at 1.35 Å from the C8 atom and the other at the same distance from the C8′ atom, but is otherwise featureless. The spurious peaks are related to the non-crystallographic relationship between the two independent molecules (the unprimed atoms being related to the primed atoms by $(\frac{1}{2} + x, \frac{1}{2} - z)$, but the treatment of such pseudosymmetry was not attempted. Programs used: SHELXS-97, SHELXL-97, ORTEP-II. CCDC deposition number: 235936.

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