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Crystallographic report

Coordination polymers containing $Cd(NO_3)_2$ and $Cd(H_2O)_2^{2+}$ units bridged by btp ligands (btp = 2,6-bis(*N*′-1,2,4-triazolyl)pyridine)

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There are two kinds of coordination polymers in the title compound: one contains $Cd(NO_3)_2$ units bridged by 2,6-bis(*N*′-1,2,4-triazolyl)pyridine (btp) ligands and the other contains $Cd(H_2O)_2^{2+}$ bridged by btp ligands. The two coordination polymers are connected through hydrogen bonds. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium(II); coordination polymer

COMMENT

Two 2,6-bis(*N*′-1,2,4-triazolyl)pyridine (btp) ligands bridge $Cd(NO_3)_2$ units to form one coordination polymer (Fig. 1a) and, separately, the other two btp ligands bridge $Cd(H_2O)_2^{2+}$ units to form a second type of coordination polymer (Fig. 1b). There are two uncoordinated NO_3^- anions between the two polymers to balance the charge. The Cd–N distances range from 2.323(5) to 2.363(5) Å. The Cd1–O(NO_3) distances are 2.387(5) and 2.413(7) Å, and the Cd2–O(H_2O) distances are 2.279(4) and 2.331(4) Å. The O–Cd1–O and O–Cd2–O angles are 177.21(19)° and 170.77(17)° respectively. The $Cd(NO_3)_2$- and $Cd(H_2O)_2^{2+}$-containing polymers are stacked alternately through hydrogen bonds (Fig. 1c).

EXPERIMENTAL

Colorless crystals were isolated under the conditions such that an aqueous solution of $Cd(NO_3)_2$ was carefully layered by a methanol solution of btp.[1,2] IR (KBr): $\nu(H_2O)$ 3451, ν(btp) 3102, and $\nu(NO_3^-)$ 1384 cm^{-1}. Anal. Found: C, 31.67; H, 2.30; N, 32.85. Calc. for $C_{36}H_{32}Cd_2N_{32}O_{14}$: C, 31.75; H, 2.37; N, 32.92%. Intensity data were collected at 150 K on a Nonius Kappa-CCD diffractometer using Mo Kα ($\lambda = 0.71073$ Å) radiation for a colorless crystal $0.10 \times 0.16 \times 0.26$ mm^3. $C_{36}H_{32}Cd_2N_{32}O_{14}$, $M = 1361.74$, monoclinic, Pn, $a = 13.3066(2)$ Å, $b = 13.6343(3)$ Å, $c = 13.6510(2)$ Å, $\beta = 97.8044(12)°$, $V = 2453.55(7)$ $Å^3$, $Z = 2$, 10150 unique data ($\theta_{max} = 27.5°$), $R = 0.039$ (9161 reflections with $I \geq 2\sigma(I)$), $wR = 0.097$ (all data). The metric crystal data are consistent (after transformation and a shift of origin) with a higher symmetry space group, and refinement could be achieved employing a disordered model. However, the unambiguous presence of reflections of the type $0k0$ for $k = 2n + 1$ supports the present model. Programs used: DENZO-SMN software package, SHEXTL V5.0, ORTEP-3. CCDC deposition number: 236173.

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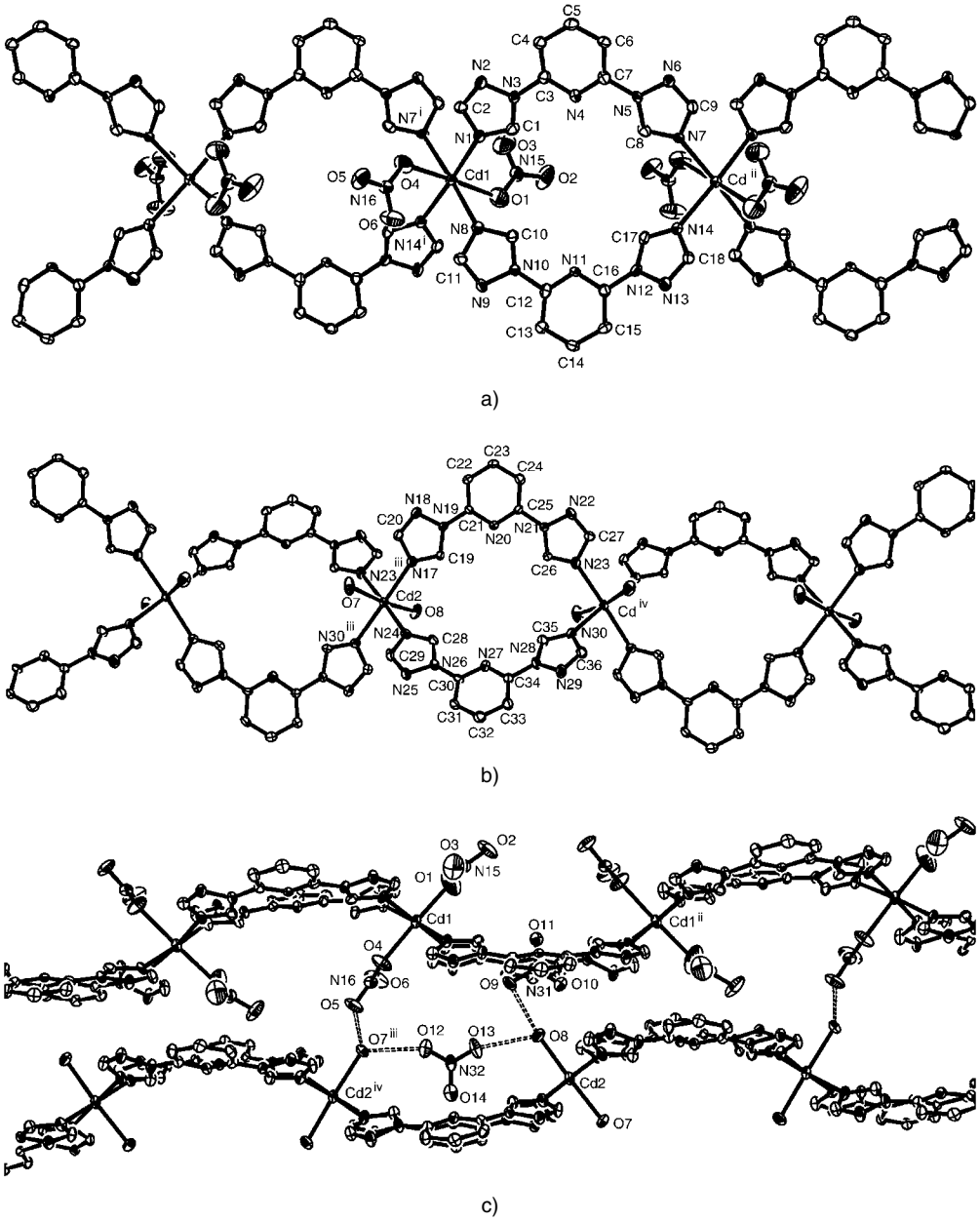

Figure 1. (a) Structure of the coordination polymer containing $Cd(NO_3)_2$ units bridged by btp ligands with hydrogen atoms omitted for clarity. Selected bond distances and angles: Cd1–N1 2.360(5), Cd1–N8 2.341(6), Cd1–$N7^{i}$ 2.354(5), Cd1–$N14^{i}$ 2.349(5), Cd1–O1 2.413(7), Cd1–O4 2.387(5); O1–Cd1–O4 177.21(19)°. (b) Structure of the coordination polymer containing $Cd(H_2O)_{2+}$ units bridged by btp ligands with hydrogen atoms omitted for clarity. Selected bond distances and angles: Cd2–N17 2.363(5), Cd2–N24 2.323(5), Cd2–$N23^{iii}$ 2.327(5), Cd2–$N30^{iii}$ 2.362(6), Cd2–O7 2.331(4), Cd2–O8 2.279(4) Å; O7–Cd2–O8 170.77(17)°. Symmetry operation: (i) $\frac{1}{2}+x$, $-y$, $-\frac{1}{2}+z$, (ii) $-\frac{1}{2}+x$, $-y$, $\frac{1}{2}+z$, (iii) $-\frac{1}{2}+x$, $1-y$, $\frac{1}{2}+z$, (iii) $\frac{1}{2}+x$, $1-y$, $-\frac{1}{2}+z$. (c) Structure of the two kinds of coordination polymers associated via hydrogen bonds. Hydrogen bond distances: $O7^{iii}\cdots O5$ 2.821(6), $O7^{iii}\cdots O12$ 2.747(6), O8···O13 2.771(6), O8···O9 3.040(6) Å.