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μ_2-Diiodotetrakis(2-hydroxymethyl-1-methyl-1-imidazole-N^3)dicadmium(II) bis[triiodo(2-hydroxymethyl-1-methyl-1-imidazole-N^3)cadmate(II)] dihydrate

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There are two types of Cd in the title compound, the six-coordinated Cd atom in the cation is in a distorted octahedral geometry while the four-coordinated Cd in the anion shows a distorted tetrahedral geometry. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; cadmium; 2-hydroxymethyl-1-methyl-1-imidazole; iodine

COMMENT

d^{10} metals, such as zinc(II) and cadmium(II) atoms, coordinated by rigid aromatic ligands often display intriguing photo properties.[1–3] The crystal structure of the title compound comprises a centrosymmetric dinuclear $[Cd_2I_2(2\text{-hydroxymethyl-1-methyl-1-imidazole})_4]^{2+}$ cation, two mononuclear $[CdI_3(2\text{-hydroxymethyl-1-methyl-1-imidazole})]^-$ anions, and two lattice water molecules. As shown in Fig. 1, in the dinuclear cation, the independent Cd1 is chelated by the O and N atoms from a pair of imidazole ligands, and its coordination is completed with two μ_2–I^- bridges, resulting in a distorted octahedral geometry. In the anion, Cd2 is coordinated by N atoms from the imidazole ligand, and three I^- atoms forming a distorted tetrahedral geometry; the Cd2–O3 distance of 2.905(18) Å is considered to be too long for a significant bonding interaction between these atoms.

EXPERIMENTAL AND RESULTS

2-Hydroxymethyl-1-methyl-1-imidazole (0.1 g), was dissolved in distilled water (3 ml), CdI_2 (0.1 g) in ethanol (5 ml) was added and the solution was stirred in 50 °C for 10 min. The pH was adjusted to ~7.5 by dilute NaOH and the solution was kept in the dark at room temperature. The colorless plate-like crystals deposited after 5 weeks, yield ~40%. Data collection was performed at 296(2) K on a Bruker AXS SMART CCD diffractometer (Mo–Kα, $\lambda = 0.71073$ Å) for a crystal of $0.02 \times 0.35 \times 0.46$ mm^3. $C_{30}H_{52}Cd_4I_8N_{12}O_8$, $M = 2173.64$, triclinic, P-1; $a = 7.7374(9)$, $b = 10.378(1)$, $c = 19.907(2)$ Å; $\alpha = 80.838(2)$, $\beta = 82.432(2)$, $\gamma = 68.265(2)°$; $V = 1461.3(3)$ Å^3. $R = 0.040$ for 3688 of the 6663 reflections ($\theta_{max} = 27.5°$) with $I > 2\sigma(I)$. Programs used were teXsan, SHELXL-97 and ORTEP. CCDC deposition number is 242787. The O3 atom was disordered and thus modelled isotropically.

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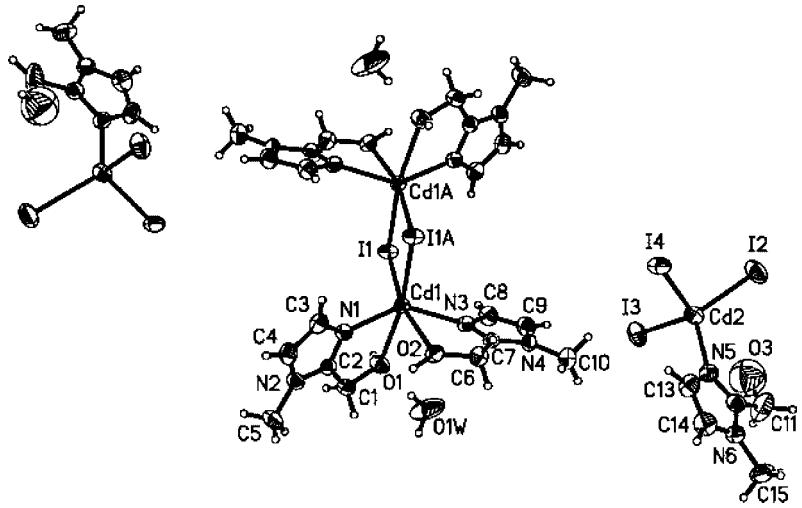

Figure 1. *ORTEP* plot of $C_{30}H_{52}Cd_4I_8N_{12}O_8$. Selected bond distances and angles: Cd1–I1 2.8635(9), Cd1–O1 2.514(5), Cd1–O2 2.619(5), Cd1–N1 2.202(6), Cd1–N3 2.229(6), Cd1–I1A 2.9467(9), Cd2–I2 2.740(1), Cd2–I3 2.761(1), Cd2–I4 2.816(1), Cd2–N5 2.254(7) Å; I1–Cd1–O1 92.7(1), I1–Cd1–O2 166.5(1), I1–Cd1–N1 112.5(2), I1–Cd1–N3 100.1(2), O1–Cd1–O2 92.7(2), O1–Cd1–N1 69.0(2), O2–Cd1–N3 67.78(2), N1–Cd1–N3 139.9(2), I1–Cd1–I1A 92.32(2), O1–Cd1–I1A 167.6(1), O2–Cd1–I1A 84.9(1), N1–Cd1–I1A 98.6(2), N3–Cd1–I1A 102.9(2), I2–Cd2–I3 112.07(3), I2–Cd2–I4 106.68(3), I3–Cd2–I4 111.29(3), I2–Cd2–N5 119.9(2), I3–Cd2–N5 107.2(2), I4–Cd2–N5 98.9(2), Cd1–I1–Cd1A 87.68(2)°. Symmetry transformation: A: $-x$, $2-y$, $-z$.