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Diiodobis(2-hydroxymethyl-1-methyl-1-imidazole-N^3)cadmium(II)

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The Cd atom in $Cd(Hmmi)_2I_2$ is five-coordinate with a trigonal bipyramidal geometry in which the apical sites are occupied by I and O atoms. Copyright © 2005 John Wiley & Sons, Ltd.

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

COMMENT

In the course of metalloenzyme model studies, we have isolated a mononuclear complex $Zn(Hmmi)_2Cl_2$ (Hmmi = 2-hydroxymethyl-1-methyl-imidazole),[1] in which only the N atom is coordinating to the central metal ion, while the O atom is free. Recent reports have shown that d^{10} metals, such as Zn(II) and Cd(II) ions chelated by rigid aromatic groups, promise intriguing photoelectronic properties.[2,3] In the CdI_2 adduct, Fig. 1, Cd is chelated by O and N atoms from one imidazole ligand, one N from a second imidazole ligand and two I atoms, resulting in a trigonal bipyramidal geometry. Extensive hydrogen bonding interactions between hydroxymethyl groups give rise to a chain structure.

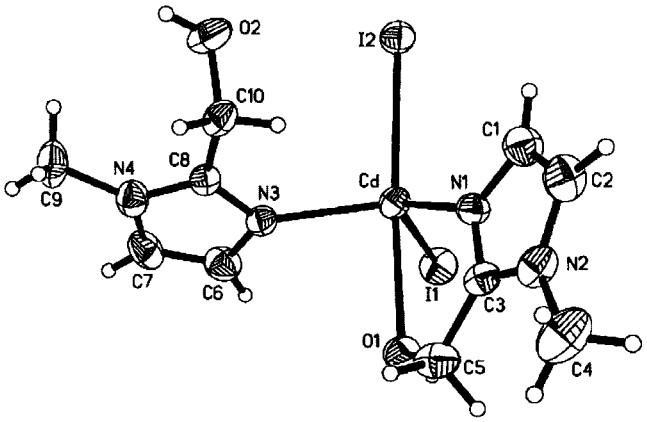

Figure 1. Molecular structure of $Cd(Hmmi)_2I_2$. Selected bond distances and angles: Cd–I1 2.744(1), Cd–I2 2.840(1), Cd–O1 2.658(7), Cd–N1 2.234(8), Cd–N3 2.259(8) Å; N1–Cd–N3 118.3(3), I1–Cd–I2 109.2(1), I1–Cd–N1 122.2(2), I1–Cd–N3 107.7(2), I2–Cd–O1 163.8(2), O1–Cd–N3 84.2(2)°.

EXPERIMENTAL

CdI_2 (0.1 g) in ethanol (5 ml) was added to an aqueous solution (3 ml) of Hmmi (0.1 g). The solution was stirred at 50 °C for 10 min, and dilute NaOH was added until a white precipitate appeared. The pH of the solution was then adjusted to ~6.5 with HNO_3 and a clear solution resulted. After filtration, the filtrate was kept in the dark at room temperature. Some colorless rhombic block crystals suitable for X-ray analysis were deposited after one month, yield ~30%. Data collection was performed at 293(2) K on a Bruker AXS SMART CCD diffractometer (Mo–Kα, $\lambda = 0.71073$ Å) on a crystal of $0.10 \times 0.11 \times 0.16$ mm^3. $C_{10}H_{16}CdI_2N_4O_2$, $M = 590.47$, monoclinic, $P2_1/n$, $a = 8.612(1)$, $b = 14.243(2)$, $c = 14.302(2)$ Å, $\beta = 99.800(3)°$, $V = 1728.7(4)$ Å^3, $Z = 4$. $R = 0.047$ for 1609 of the 2838 reflections ($\theta_{max} = 25.0°$) with $I > 2\sigma(I)$. Programs used were teXsan, SHELXL-97 and ORTEP. CCDC deposition number is 235496.

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