The Zinc Aqua Complex of a Tetrapodal Pentaamine Ligand and its Reactivity towards Carbon Dioxide

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In the context of derivatisation studies of the pentaamine ligand 2,6-$C_5H_3N[CMe(CH_2NH_2)_2]_2$ (2-(6-(1,3-diamino-2-methylpropan-2-yl)pyridin-2-yl)-2-methylpropane-1,3-diamine, **1**), we explored its zinc(II) coordination chemistry. With $ZnBr_2$ in hot aqueous ethanol, in the absence of Lewis acid, the aqua complex $[Zn(\mathbf{1})(H_2O)]Br_2$ (**2**) is obtained, in which the pentaamine ligand acts as a square-pyramidal coordination cap. Single crystal structure data for the dihydrate of **2** are reported. In methanol solution, the complex is reactive towards carbon dioxide, and spectroscopic data (IR, ^{13}C NMR) indicate the reversible formation of the dinuclear methyl carbonate complex $[(Zn(\mathbf{1}))_2(\mu_2\text{-}(\eta^1\text{-}O,\eta^1\text{-}O)O_2COCH_3)]Br_3$.

Key words: Tetrapodal Pentadentate Ligand, Zinc, Aqua Complex, Carbon Dioxide Fixation