Self-assembly of chelating, bridging N, N, N donor ligands and Cu(I), Cu(II), Cd(II), Hg(II): Molecular box versus coordination polymer

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Abstract

Three flexible chelating and bridging ligands, (E)-N-(pyridin-2-ylmethylene)-1-(pyridin-3-yl)methanamine(L1), 1-(pyridine-2-yl)-N-(pyridin-3-ylmethyl)methanamine (L01), (E)-N-(pyridin-2-ylmethylene)-1-(pyridin-4-yl)methanamine (L2), have been synthesized. The reaction of these ligands with various metal salts yielded a series of compounds, namely [Cu₂(L1)(PPh₃)₂I₂]₂ (1), [Cu₂(L2)(PPh₃)₂I₂]_n (2), [CuL1(-NO₃)₂]₂ (3), [ZnL1(NO₃)₂]₂ (4), [CdL1(NO₃)₂]₂ [(5), [CdL01 (NO₃)₂]₂ (6) and [HgL1Cl₂]_n (7). The compounds were characterized by elemental analysis, spectroscopic methods (IR, UV–Vis) and X-ray crystallography. X-ray structural analysis of compound 1 reveals the formation of a centrosymmetric tetranuclear compound. The repeat unit of coordination polymer 2 comprises a Cu₂I₂ unit with a triphenyl phosphane substituent on Cu1 linked to an adjacent Cu₂I₂ unit by the ligand L2 that acts as a bridge. Compounds 3, 4, 5 and 6 exhibit a common metallo-cyclophane [M₂(L)₂(NO₃)₄] skeleton. Two M²⁺ cations are linked by two L1 ligands and these ligands chelate to each metal atom through the imine nitrogen (or amine nitrogen) atoms and the nitrogen atom of the 2-pyridyl ring, and bind to the other metal atom of the pair via the nitrogen atoms of the 3-pyridyl rings. Structural studies of 7 revealed the formation of a coordination polymer in which the polymer chain propagates in helical spirals along a twofold screw axis parallel to b. The metal coordination geometries and coordination of the nitrato anions to the metals are noted and discussed.

Keywords: Diimine ligands, Flexible chelating and bridging ligands, Molecular box, Coordination polymer, X-ray structure analyses

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