

Crystallographic characterization and elucidation of unconventional interactions of small molecules

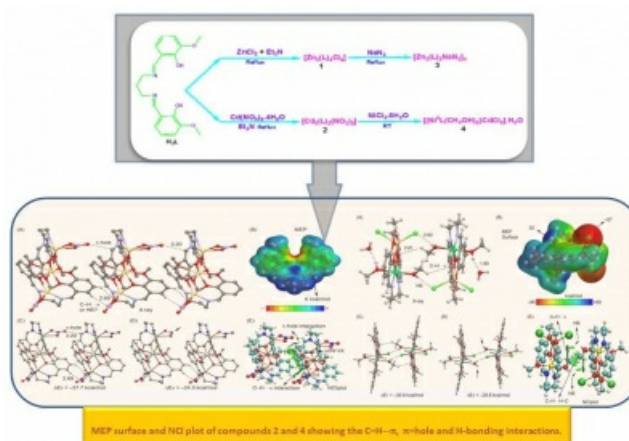
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We have synthesized and X-ray characterized one Zn(II) and one Cd(II) trinuclear complexes (1-2) from a bicompartamental Schiff base ligand. From complex 1, an 1D $[Zn_2(L)2(Na)N_3]_n$ (3) polymer has been derived with a rare $\mu_1,1$ azido bridging. From complex 2, a dinuclear Cd(II)-Ni(II) (4) complex has been derived which gives evidence in favour of preferential site selection of the inner core of the ligand towards 3d and 4d metal ions. Complexes 1-4 show interesting supramolecular architectures in solid state involving different unconventional weak forces like π - π , CH- π , π -hole and C-H...H-C interactions along with conventional H-bonding interactions. Several theoretical tools like DFT, NCI, MEP etc. were used to have insight view of these interactions.

[1] Banerjee, S. et al. (2016). RSC Advances, 6, 39376-39386.

[2] Banerjee, S. et al. (2016). Journal of Coordination Chemistry, 69(20), 3092-3106.



Keywords: [Crystal structures](#), [DFT study](#), [Supramolecular interactions](#)