Crystallographic characterization and elucidation of unconventional interactions of small molecules

Saikat Banerjee¹, Antonio Bauzá², Antonio Frontera², Amrita Saha¹
¹Jadavpur University, Kolkata, India, ²Departament de Química, Universitat de les Illes Balears, Palma (Balears), Spain
E-mail: saikatbanerjee2211@gmail.com

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 \([\text{Zn}_2(L)_2(\text{Na})\text{N}_3]\) 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 \(n-n\), CH-\(n\), n-hole and C-H\(\cdots\)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.


Keywords: Crystal structures, DFT study, Supramolecular interactions

Acta Cryst. (2017), A70, C958