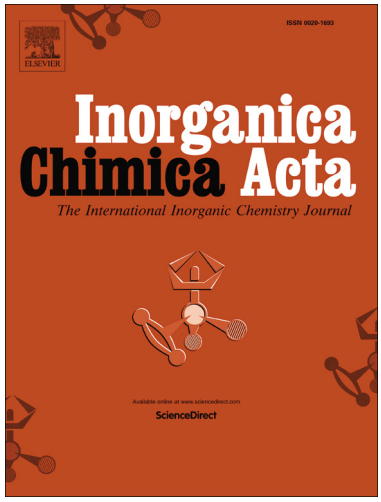

Research paper

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Syntheses of Four New Asymmetric Schiff Bases and Their Cu(II) Complexes: Theoretical Calculations to Rationalize the Packing of Molecules in the Crystals

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Abstract

Four new asymmetric Schiff bases, *N*-α-methylsalicylidene-*N*′-2-hydroxynapthylidene-1,3-propanediamine (H_2L_1), *N*-α-methylsalicylidene-*N*′-5-bromosalicylidene-1,3-propanediamine (H_2L_2), *N*-α-methylsalicylidene-*N*′-3-methoxysalicylidene-1,3-propanediamine (H_2L_3) and *N*-(3-methoxysalicylidene)-*N*′-(2-hydroxynapthylidene)-1,3-propanediamine (H_2L_4) and their Cu(II) complexes [CuL_1] (**1**), [CuL_2] (**2**), [CuL_3] (**3**) and [CuL_4] (**4**) have been synthesized. All the complexes (**1**–**4**) have been structurally characterized by single crystal XRD. The Cu-atom is four coordinated square planar in complexes **1–3** but in **4** a water molecule coordinates to one of its axial positions making it penta-coordinated with square pyramidal geometry. The mononuclear complex molecules of **1** and **2** form infinite 1D columns that are arranged parallel forming 2D sheets where as in **3** they form self-assembled dimers that are inter-connected by weak van der Waals interactions and in **4** the molecules are packed in the form of infinite 1D ladders. The structure of a recently reported complex with a similar asymmetric ligand (H_2L_5) *N*-α-methylsalicylidene-*N*′-salicylidene-1,3-propanediamine where the phenoxido oxygen coordinates mutually to the axial position of another molecule to form a dimer is compared to the present complexes. The packing of the molecules in all the crystals are rationalized by theoretical molecular electrostatic potential surface (MEPS) calculations. DFT calculations show the significant role of CH···π (chelate ring) and π···π (chelate ring) interactions governing the crystal