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Coordination driven and/or H-bonded M(II)-N,N-dialkylisonicotinamide networks
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The search for strategies enabling assembling of transition metal complexes into multidimensional frameworks is one of the major challenges in crystal engineering. The metal embedded supramolecular networks, having specific dimensions and topologies are associated with many magnetic, electronic, zeolitic, catalytic and optical properties thus leading to the creation of “functional materials” [1], [2], [3]. Coordination polymerization or hydrogen bonding are the two strategies employed in assembling metal complexes into multidimensional networks. Recently, a combination of the two has also been used effectively to increase the dimensionality. The strength of coordinate bond along with the flexibility imparted by hydrogen bonding provide ideal environment for multi-dimensional framework expansion. Among various ligands used for construction of supramolecular networks, the pyridine based ligands such as nicotinic acid, isonicotinic acid and their amide derivatives are ideal as they have the structural adaptability for both: metal-ligand coordination [4], [5] as well as the intermolecular hydrogen bonding [6].

Our work involving the Metal(II)-N,N-dialkylisonicotinamide complexes [7] has shown that these fully substituted amide derivatives of isonicotinic acid provide the necessary rigidity and binding sites that enhance the chances of formation of coordination networks instead of isolated entities and therefore provide a fertile route to metal organic frameworks (MOF’s). Furthermore, intermolecular interactions among 1D coordinated and/or H-bonded chains make feasible the formation of more complex networks (2D and 3D). Each of these levels contains remarkable features making the complexes unique from a structural point of view. This work also reinforces the role played by counter ions present in the lattice such as perchlorates and nitrate to enable assembling of metal complexes into networks. To explore the magnetism among such systems, in depth magnetic measurements (variable temperature magnetic susceptibility, epr etc.) have also been made [7].

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Five new metal-organic frameworks: novel topologies and characteristics.
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Metal-organic frameworks (MOFs) are a subgroup of coordination polymers and coordination networks. We are engaged in the preparation of MOFs using a range of common metal salts and organic ligands, including multitypic aromatic carboxylates. Topological analysis is a useful tool for analysing coordination networks. It allows one to see the arrangement of molecules in a structure in a simple manner and therefore helps in the determination of why that structure was formed. This enables a more systematic design of coordination polymers.

Three MOFs were prepared from gadolinium(III) nitrate and 5-nitroisophthalic acid (NIA) using the same method with only the concentration of starting materials in the solvent system varying. [Gd(NIA)(DMF)]·1.5H2O (1), [Gd(NIA)(DMF)]·3H2O (2) and [Gdd(NIA)(DMF)(H2O)]·4DMF·xH2O (3) have a distinctive paddle-wheel motif with four NIA molecules coordinated to a pair of gadolinium metal centres.

Network analysis revealed the six connected (4^2.8^3)-pcu net for 1. 1 and 2 are related by rotation around one C-C bond which reduces the symmetry of the network. This is easy to see through the topology as the six-connected node reduces to a four-connected node. 2 is found to have the square and tetrahedron four-connected (4^8.8^4)-pts net. 3 has the unprecedented four-, five- and six-connected (4^6.6^4.6^4.6^8)-net (Figure 1). The four-connected node of 3 is the same as that square four- node of the pts net while the six-connected node is the same as that of the pcu net.