Abstract

This thesis deals with the study of interference of pyridine moiety in amide-to-amide recognitions and the generation of coordination polymer based functional materials to explore properties such as guest inclusion, luminescence, gas storage and separation. Four classes of molecules considered for this purpose were (1) mono-pyridyl amides, (2) bis-pyridyl amides in which amide groups were separated by alkyl spacers having odd number of carbon atoms, and two ester based ligands, (3) 1,3-phenylenediisonicotinate, and (4) benzene-1,3,5-triyltriisonicotinate. Pyridine interference in amide-to-amide recognition was studied based on mono-pyridyl and bis-pyridyl amides, in which the amide groups are separated by odd number of alkyl chain. Further, coordination complexes of the same molecules were prepared with the aim of understanding the subtleties in transfer of molecular recognition information from organic materials to their coordination complexes and also to study the robustness of the hydrogen bonding patterns in the presence of counter anions. The role of molecular flexibility of the ligand in variation of dimensionality of the coordination polymers was explored with the complexes of phenylenediisonicotinate. An identical 2D coordination polymer based on tri-ester molecule, benzene-1,3,5-triyltriisonicotinate had been synthesized in the presence of different metal atoms, anions, and a series of diverse aromatic guests, without any significant change in the network or packing of the layers. Interestingly, the layers were shown being capable of exchanging the metal ions which were integral part of the network, while the guest molecules remained intact. The coordination polymers produced in the presence of $CHCl_3$ and MeOH were observed to exhibit breathing transition from closed to open form upon sorption of N_2/H_2. Further, a simple solid solution approach based on metal was adopted which offered an easy way to modulate gate opening pressure, and improved uptake capacities of iso-structural coordination polymers. These layered coordination polymers have the potential for the absorption for environmentally hazardous molecules like iodine and polycyclic-aromatic hydrocarbon (PAH) molecules and adsorptive based separation of the PAH molecules.

Key words: amide-to-amide recognition, synthon interference, coordination polymer, metal exchange, gas sorption, gate opening, breathing transition, separation.