Abstract of Thesis

Metal organic framework compounds have emerged as an important part of inorganic coordination chemistry during the last two decades. In this thesis, the metal-organic frameworks (MOFs) compounds of 5-substituted isophthalic acids have been investigated. As part of the investigations, preparation of MOF compounds of different 5-substituted isophthalic acids such as 5-aminoisophthalic acid, 5-nitroisophthalic acid and 5-sulphoisophthalic acid have been accomplished. Structures of the newly synthesized compounds were established by single crystal X-ray diffraction technique. Magnetic properties of the transition metal based compounds have been studied by SQUID/PPMS magnetometer. The ligand-sensitized metal-center emission has been studied on the Eu$^{3+}$ and Tb$^{3+}$ doped MOF compounds of Y and La. Up-conversion luminescence properties of Nd based compound have also been studied. The labile nature of the coordinated and lattice water molecules was established by employing dynamic in-situ single crystal to single crystal structural transformation studies. In addition, the site selective substitution in homometallic MOF compounds and their subsequent thermal decomposition to mixed-metal spinel oxides have also been investigated.

In Chapter 1 of the thesis an overview of the metal-organic framework compounds is presented. In Chapter 2, the synthesis, structure and properties of 5-aminoisophthalate compounds of 3d metals and the rare earth metals are presented. In some of these compounds the coordinate and the lattice water molecules can be removed and reinserted with the retention of single crystallinity. Also some of the isostructural compounds exhibits interesting magnetic behaviors. Partial substitution of the Y$^{3+}$/La$^{3+}$ compounds of 5-aminoisophthalate with Eu$^{3+}$/Tb$^{3+}$ exhibits characteristics metal centered emission (red = Eu$^{3+}$ and green = Tb$^{3+}$).

In Chapter 3, the three dimensional compounds of 5-nitroisophthalate and 4, 4’-oxybisbenzoate with cobalt and the high – throughput screening in the synthesis of metal-organic frameworks (MOFs) for the Cu(CH$_3$COO)$_2$.H$_2$O – NIPA – heterocyclic ligand systems are presented.

In chapter 4, the single crystal to single crystal transformation with temperature dependent dimensionality cross-over and structural reorganizations in two copper based compounds of 5-sulfoisophthalate and 5-nitroisophthalate are presented. In chapter 5, the site selective substitution in a homometallic MOF compound and its subsequent decomposition to mixed-metal spinel oxides are presented.