Public Abstract
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Crystal engineering primarily deals with the understanding of intermolecular interactions in the context of crystal packing and thus utilizes this information for the designing and development of novel crystalline solid for targeted application. Supramolecular chemistry helps understanding these intermolecular interactions in the various medium and thus remains an integral part of crystal engineering. These intermolecular interactions are usually weak and non-covalent in nature. Thus, shape and functionality the components of crystalline material have importance in the understanding crystal engineering.
Resorcin[4]arenes and pyrogallol[4]arenes have a unique bowl shape and the upper rim of this bowl is decorated with multiple hydroxyl groups. These structural features led to construction of supramolecular organic frameworks with various architecture and topology. These structures were primarily utilized to understand molecular recognitions and host guest interactions. Thus, in this thesis, we focused on synthesis of novel supramolecular organic frameworks from resorcin[4]arenes and pyrogallol[4]arenes by co-crystallizing these macroccyles with various organic linker molecules such as 4,4’-bypyridine. The major part of this thesis project involved screening and characterization of single crystal structure of these co-crystalline frameworks and analyzing the stability of selected framework in solution as well as in solid form. Application of these novel framework materials in gas sorption and separation is evaluated by exposing the stable framework materials to various gases at specific temperature and pressure. The gas sorption capacity of a specific framework material is attributed to its porosity and thermal stability after desolvation. Various gases such as CO2, Xe, and Kr are absorbed selectively on these porous crystalline materials obtained by manipulating intermolecular interactions.