Abstract

The thesis deals with exploration of crystal engineering strategies for the design of novel materials with predictable functional properties. In particular, the exploration of hydrogen bonds or coordination bonds as templates for alkenes or bis-alkenes to promote their solid state [2+2] dimerization/polymerization is discussed elaborately. For this purpose, two classes of molecules have been chosen: 1) unsymmetrical bis-pyridyl olefins containing amides (UBOs) and 2) phenyl and pyridyl substituted bis-(acrylamido)alkanes in which amide groups were separated by alkyl/aryl-alkyl spacers. The intended work can be classified as three parts based on the nature of the materials: 1) organic molecules, 2) Ag(I)-CPs and 3) CPs of Cu(II), Cd(II) and Zn(II). The study deals with elucidation of importance of molecular geometries, coordination environments, crystallization conditions, hydrogen bonding or other non-covalent interactions, role of solvents and anions in determining the supramolecular self-assembly, solid state reactivity and their properties. The key outcome of the studies is the synthesis of crystalline organic polymers and Coordination polymers of organic polymers (CPOPs) via single-crystal-to-single-crystal (SCSC) [2+2] reactions which are otherwise impossible to synthesis by conventional methodologies. The synthesized materials are shown to explore functional properties such as plasticity, transparency, dye sorption and gas permeability.

Key words: amide-to-amide recognition, solid state [2+2] photochemical reaction, SCSC, coordination polymer, organic polymer, plastic film, transparency, gas permeability.