ABSTRACT

Title of the thesis: EXPLORING SUPRAMOLECULAR FEATURES OF SOME INORGANIC AND ORGANIC COMPOUNDS IN THE CONTEXT OF CRYSTAL ENGINEERING

Submitted by: Suparna Tripathi **[Index No: 104/16/Phys./24]**

Department: Physics

This thesis includes synthesis and X-ray structural characterization of some inorganic and organic compounds by exploring supramolecular self-assemblies in the solid state. Supramolecular chemistry is the study of noncovalent interactions between molecules. Many new functional materials have been synthesized and structurally characterized by mimicking nature and utilizing the synthesis approaches toward supramolecular chemistry. Although crystal engineering deals with the individual potentiality of weak forces, an exciting aspect is still in a state of infancy, that is, the associative interactions of noncovalent forces to form extended networks and their supramolecular consequences in the solid state.

In this dissertation, X-ray crystallographic and theoretical studies have been critically analyzed various supramolecular architectures of the metal complex and organic compounds. Attempts have been made to understand the grown solids' precise structure and explore intermolecular interactions involved within the structures. Attempts have been made to explore the robust feature of the cooperativity of noncovalent interactions in the context of crystal engineering. Several supramolecular structural diversities have been explored for the first time in the solid-state, where weak interactions play a decisive role in building self-assembled structures. The noncovalent interactions have been quantified by Hirshfeld surface analysis.

The supramolecular interactions have also been successfully rationalized by density functional theory (DFT), Molecular electrostatic potential (MEP), Bader's theory of Atoms in Molecules (AIM), and noncovalent interaction plot index (NCI) to characterize the noncovalent interactions.

Subrata Mukhopadhyay 20/1/2023

Signature of the supervisor

Suparna Tripathi

Signature of the candidate

Dr. Subrata Mukhopadhyay
Professor of Chemistry
Jadavpur University
Kolkata - 700032