ABSTRACT

Title of the thesis: Exploring diverse solid-state structural assemblies of some organic compounds and metal complexes in the context of crystal engineering

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X-ray diffraction and crystallography is undoubtedly one of the most powerful analytical technique to elucidate the structure of crystalline materials at the molecular level. The crystallographic study of the solid-state structures of organic compounds and metal complexes has attracted intense attention due to their fascinating structures and properties. The subject, namely crystal engineering, evolved from an intersection of crystallography and chemistry, but nowadays it employs crystallography, spectroscopy, and computation. The study and understanding of weak forces are necessary to develop new applications in supramolecular chemistry across a diversity of fields. The interplay of the cooperative weak noncovalent interactions is certainly of great importance in building multidimensional structures.

In this proposed dissertation, various compounds will be synthesized and structurally characterized by X-ray diffraction. The investigations proposed herein are aimed at systematically studying different noncovalent interactions in building extended solid-state networks to gain knowledge in this nascent field. Therefore, it is aimed to explore the robust feature of non-covalent interactions in building multi-dimensional supramolecular frameworks. Attempts have been made to explore several supramolecular structural diversities for the first time in solid-state. Hirshfeld surface analysis has been performed to quantify non-covalent interactions. The non-covalent interactions have also been successfully characterized by using several theoretical studies, such as DFT calculations, QTAIM analysis, NCI Plot Index, PIXEL calculations, etc.

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