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## Preface

Transition metal compounds have received significant attention from chemists in recent years not only due to their fascinating architectures involving various non-covalent interactions but also due to their potential applications in variety of fields. In this context, it can be mentioned that the study of metal organic compounds involving interesting synthons continues to remain as a major research area for the synthetic chemists. This thesis provides an innovative approach to explore non-covalent interactions in supramolecular assemblies of coordination compounds and their biological relevance.

The present thesis focuses on the synthesis, supramolecular assemblies and antiproliferative evaluation of a few transition metal complexes. The thesis also emphasizes the investigation of the energetic features of a few unconventional non-covalent interactions theoretically using various computational tools.

In Chapter 1, introductory concepts on the topics of relevance for the thesis have been discussed. This chapter discusses the basics of supramolecular chemistry, the non-covalent interactions, the recent development in crystal engineering and the various computational methods used for studying non-covalent interactions. The thesis also highlights a detail review on the anticancer activities of transition metal complexes. The aims and objectives of the thesis work have been highlighted at the end of the chapter. In Chapter 2, pyridinedicarboxylate based isostructural Co(II), Mn(II) and Zn(II) coordination compounds have been reported with unconventional antiparallel CO $\cdots$ CO interactions. Chapter 3 deals with the synthesis, structural investigations and theoretical studies of three Mn(II) complexes involving mixed N-and O-donor ligands. Two of the Mn(II) compounds are polymers involving energetically significant anti-parallel nitrile $\cdots$ nitrile interactions, while; enclathration of the guest molecules have been discussed for the remaining unusual cocrystal hydrate of Mn(II). Chapter 4 describes the synthesis, structural investigations and antiproliferative activities of three isostructural Co(II), Mn(II) and Zn(II) compounds involving 2-chlorobenzoate and 3-cyanopyridine ligands. Chapter 5 emphasizes on the crystal structures and anticancer activities of Co(II), Ni(II) and Cu(II) complexes involving 2,6-pyridinedicarboxylate and pyridine ligands. The self-assembled dimers in the supramolecular assemblies have been further investigated theoretically.

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**Albert Schweitzer**

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