Most of the active pharmaceutical ingredients (API) exist as crystals. Development of new drugs or modifications of drugs can be effected by complexation of the drug substance with metals or other elements. Thus organometallic complexes have an important role in modern pharmaceutical industry. More over metal organic frameworks (MOF) can be used as drug carriers in drug delivery systems since these materials possess plenty of nano pores. In this context, knowledge of crystal structure of (API) is essential in many aspects. First of all the changes in crystal structure can modify the physico-chemical properties of a drug which in turn affects the bioavailability and the biopharmaceutical properties of a drug. Polymorphism has an important role in pharmaceutical industry since it affects the shelf life and activity of a drug. It causes patent problems and sometimes serious health hazards.

This thesis report describes the growth and characterization of complexes of some vitamin B complex members –nicotinic acid, thiamine and folic acid - and the sodium complex of the antimalarial drug quinine salicylate, an alkaloid. Till date, almost all such complexes are synthesized by hydrothermal methods at elevated temperatures. So a trial has been made to grow such crystals at ambient temperature. The self assembly of molecules during the formation of a crystal is affected by pH values and concentration of reactants. Hence inorder to evaluate such parameters, the crystals except thiamine iodide were grown in sodium metasilicate gel medium. The grown crystals were characterized and the crystal structure was also determined. The thermal and dielectric properties of the crystals which have wide applications in modern pharmaceutical industry and drug delivery systems were also studied.

This thesis consists of eleven chapters. The first introductory chapter contains a brief description of the role of crystals in the pharmaceutical industry and the importance of vitamins and the alkaloid used in this work. A brief literature survey is also included in this chapter.
The second chapter summarises different crystal growth techniques with emphasis on gel technique. This chapter also includes the different characterization techniques used in this work and their relevance in pharmaceutical industry.

The third chapter describes the growth and characterization of nicotinic acid crystals. The crystal structure has been determined using single crystal XRD data and is characterized by FT-IR, elemental, scanning electron microscopy and UV-Vis-NIR spectroscopy. The thermal analysis of the sample was conducted from TGA/DTA/DTG studies which provide thermal and kinetic parameters. Dielectric studies were also done to calculate the plasma energy and polarisability.

The fourth chapter discusses the growth of manganese nicotinate crystal in sodium metasilicate gel medium and its characterization by FT-IR, elemental studies, UV-Vis-NIR spectroscopy and scanning electron microscopy. SXRD data was used to determine the crystal structure. The kinetic and thermal parameters calculated from TGA/DTA/DTG studies are also provided. The Penn value and electronic polarisability calculations using dielectric studies and lattice parameters form part of the study. The optical band gap determined from electronic spectrum has been used to calculate the electronic polarisability. These values of polarisability were compared with that calculated using Clausius-Mossotti relation.

Chapter 5 deals with the growth and characterization of gel grown calcium nicotinate crystals. The optical microscopy reveals the morphology of the crystal. The crystal structure has been determined from SXRD data. The characterization was done using techniques such as FT-IR, elemental, electronic spectroscopy and SEM. The data obtained from TGA/DTA/DTG were used to calculate the kinetic and thermal parameters. The variation of dielectric parameters with frequency was also analysed.

Details of the growth and characterization of cadmium nicotinate crystals are presented in chapter 6. SXRD has been used to determine the crystal structure. FT-IR, elemental, and electronic spectroscopy were used to characterize the grown crystals. The thermal studies were carried out to analyse the thermal stability of the crystal and kinetic and thermal parameters were calculated from the obtained data. The dielectric data has been used to calculate the Penn value and electronic polarisability.
Chapter 7 consists of the growth and characterization of thiamine iodide crystals grown by slow evaporation technique. The crystal structure was determined from SXRD data. The functional groups were identified using FT-IR spectrum. Elemental analysis was carried out to determine stoichiometry of the crystal. The crystals were subjected to TGA/DTA/DTG to determine the thermal stability. The data obtained from these studies have been used to calculate kinetic and thermal parameters. The variation of dielectric parameters with frequency was recorded. The UV-Visible spectrum of the crystal was also determined. The electronic polarisability of the crystal was calculated from dielectric constant and optical band gap.

The growth and characterization of gel grown folic acid crystals are described in chapter 8. The SEM analysis shows that the grown spherulitic crystals consist of a collection of nano single crystals. The size of these nano crystals were determined from PXRD data. The functional groups were identified using FT-IR spectrum and the chemical composition of the crystal was determined by elemental analysis. Optical band gap was determined from UV-Vis-NIR spectroscopy and the result obtained was used to calculate electronic polarisability. The thermal stability was analyzed from TGA/DTA/DTG data and the kinetic and thermal parameters were calculated from these data. The dielectric spectrum shows a decrease in dielectric constant with increase in frequency.

Chapter 9 consists of the growth and characterization of calcium complex of folic acid crystals. PXRD confirms its crystalline nature and the SEM pictures show its surface roughness. The FT-IR spectrum confirms the functional groups as well as the considerable amount of coordinated water and water of crystallisation present in the crystal. The elemental analysis was used to deduce the molecular formula. The details of the dielectric property and the electronic absorption spectrum of the crystal have also been discussed.

Chapter 10 contains the details of the growth and characterization of gel grown sodium salicylate complex of quinine crystals which is used in the treatment of malaria. The crystal and molecular structures were determined from single crystal XRD. The PXRD data has also been presented because it can act as a fingerprint of the complex.
The functional groups have been identified using FT-IR data and the chemical composition from elemental analysis. The dielectric property of the crystal with change in frequency has also been studied. The thermal stability of the crystal was determined using TGA/DTA. These data were used to calculate thermal and kinetic parameters. The electronic polarisability of the crystal has been calculated from UV-Vis-NIR spectrum.

Chapter 11 summarises the results included in the thesis. There are reports that metal complexes of active pharmaceutical ingredients may alter the biological activity of ligands. A knowledge of intermolecular interactions involved in the crystal packing can be of use in designing metal organic frameworks with desired properties. Further studies are required in this direction.

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