ABSTRACT

Crystals are the unacknowledged pillars of the world of modern technology. Crystal growth is basically a process of arranging atoms, ions, molecules or molecular assemblies into regular three-dimensional periodic arrays. The growth of single crystals and their characterization towards device fabrication have assumed great impetus due to their significance in both academic and applied research. The first chapter presents an outline to various crystal growth and characterization techniques and a brief description of nonlinear optics.

Growth of single crystals can be regarded as a phase transformation into the solid state from the solid, liquid or vapour state. Crystals were grown by solution growth technique. The grown crystals were subjected to various characterization tools to study their properties. The present work is aimed at the growth and characterization of picrates, acid-adduct, 2-methylimidazolium hydrogen succinate, 2,6-diaminopyridinium 4-nitrophenolate 4-nitrophenol and a comparative study on conventional solution and unidirectional method grown potassium sodium tartrate tetrahydrate single crystals.

The second chapter deals with the growth of orthonitroaniline -picric acid and imidazolium picrate single crystals by low temperature solution growth method. The solubility was measured in different solvents and the material was purified by repeated recrystallization processes. The grown single crystals have been subjected to various characterization studies.
The structural, thermal, optical and mechanical properties were studied for the grown picrates. HRXRD study shows the crystalline perfection. FT-IR and Laser Raman studies confirm the functional groups present in the picrate compounds. Dielectric behaviour was studied for different axes and temperatures. The computational calculation based on the density functional theory at the basic sets level has been used to compute the first order hyperpolarizability of the title material.

The third chapter deals with the growth of 2-methylimidazolium hydrogen succinate (2MISA) single crystals. The cell parameters were determined using the single crystal X-ray diffraction studies and the crystalline perfection was tested by HRXRD. Dielectric tensorial behaviour of the grown single crystal was studied with varying frequency. The frequency dependence of conductivity supports hopping mechanism. The thermal stability of 2MISA was analyzed using TG/DTA measurements, which infer the material is thermally stable up to 176°C. Mechanical stability and hardness of the grown crystal were studied by Vickers hardness tester. The second harmonic output was measured using Kurtz-Perry powder method.

The fourth chapter deals with the growth of an adduct 4-aminobenzoic acid-nicotinic acid. Single crystal was grown by slow evaporation solution growth method using ethanol and water mixture as the solvent. It belongs to monoclinic crystal system and its lattice parameters were determined using single crystal XRD analysis. Thermal analysis carried out reveals the melting point and thermal stability of the grown crystal. The dielectric permittivity, loss and a c conductivity data establish the normal
behavior of organic compounds. Using DFT theory, the calculated tensorial components were $\varepsilon_{xx} = 347.16$, $\varepsilon_{yy} = 192.18$, $\varepsilon_{zz} = 130.32$ and $\varepsilon_{xz} = 6.37$. Hardness study indicates that the hardness increases with increasing load. From the mechanical studies yield strength and elastic stiffness constant were calculated. The chemical etching study shows the elongated rectangular etch patterns. On increasing the etch period the shape of etch pits also increases.

The growth and characterization of 2,6-diaminopyridinium 4-nitrophenolate 4-nitrophenol has been discussed. It is a promising NLO crystal with orthorhombic crystal system. The various properties were analyzed by different characterization techniques. Its hardness behaviour is dealt in detail. The structural perfection and growth features of the grown crystals were studied by High Resolution X-ray diffraction (HRXRD). Fourier transform infrared spectral analyses were used to confirm the functional group of the synthesized material. Factor group analysis predicts IR and Raman active modes of vibrations theoretically. The UV-Visible studies were carried out for the grown crystal. The second harmonic generation tested using Kurtz-Perry powder test shows 1.3 times of KDP. The dielectric behaviour was analyzed. The computational calculation based on the density functional theory has been used to compute the first order hyperpolarizability of the title material.

The sixth chapter deals with the comparative study on growth and characterization of Potassium sodium tartrate tetrahydrate by conventional solution growth and unidirectional Sankaranarayanan-Ramasamy method. The grown crystals by both methods were cut and polished, subjected to
various characterization methods such as HRXRD, UV-Vis, hardness, dielectric, Laser damage threshold and the properties were compared. The structural perfection of the grown crystals were analyzed by High Resolution X-ray diffraction (HRXRD) studies and compared. The UV-Visible study implies the optical quality of the SR grown PST crystals is better than that of conventional solution grown crystals. The value of dielectric permittivity is high in the case of SR grown crystal when compared to the conventional solution grown crystal. The hardness value of PST crystal is greater for SR grown crystal and withstands load up to 60 g, above which cracks were observed. From the mechanical measurements stiffness constant and yield strength have been evaluated. The measured laser damage threshold (higher value) for the SR grown PST single crystal indicates that the crystal has a lesser defects. It was found that SR method grown crystal possesses good optical, mechanical, structural and dielectric properties when compared to conventional solution grown crystal.

The details of synthesis, growth, characterization, summary of the present investigation and suggestions for future research work are presented in chapter seven.