GROWTH AND VIBRATIONAL SPECTROSCOPIC INVESTIGATIONS OF NONLINEAR OPTICAL MATERIALS

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Principal Investigator Dr. I. Hubert Joe Co-Investigator Prof. V. K. Rastogi

SUMMARY OF THE PROJECT WORK

Nonlinear optical (NLO) materials have recently attracted much attention because of their potential applications in emerging optoelectronic technologies. Materials with large second order optical nonlinearities find wide applications in the area of laser technology, laser communication and data storage technology.

Organic materials have been showed in recent years to possess superior second order nonlinear optical properties compared to the more traditional inorganic materials. Amino acids and their complexes belong to a family of organic materials that have applications in NLO. Aminoacids are interesting materials for NLO applications as they contain a proton-donor carboxyl acid (COO^-) group and the proton-acceptor amine (NH_3^+) group with them.

The high efficient NLO materials for photonic application was theoretical predicted using by quantum chemical modeling of the materials using the Gaussian'09W program package. A large number of amino acid based organic- and semi-organic NLO crystals, with special emphasis on the L-Alanine, L-Valine, L-Glutamine, L-Proline, and L-Arginine were grown using slow evaporation technique. The second harmonic generation (SHG) efficiency of the grown crystals was evaluated using Kurtz-Perry technique and it was found to be higher than that of urea. The molecular structural features of the different grown crystals contributing to NLO properties have been investigated. The intramolecular charge transfer (ICT) from the donor to the acceptor component of the NLO chromphore through the π-conjugated bridge for the push-pull molecules. And, the intra- and inter-molecular hydrogen

bonding interactions between the cationic and anionic species of the compounds in the salt forming crystals have been shown to play an important role in making the materials into NLO active. Enhanced nonlinear optical activity of the molecular system, which is a consequence of the large value of second-order polarizability, 'β' is found to be associated with the intramolecular charge transfer, resulting from the electron-acceptor groups. Vibrational (FTIR and NIR-FT-Raman) characterization of all organic, semi-organic NLO crystals have been performed to understand the structural parameters responsible for NLO properties.

The important results of project activity have been published in international peer-reviewed journals *Viz.*, Journal of Physical Chemistry A, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Journal of Molecular Structure and at international/national conferences .