SYNTHESIS AND CHARACTERIZATION OF ORGANIC NONLINEAR OPTICAL CRYSTALS

Final Report of the Minor Research Project

Submitted to the

University Grants Commission

(UGC Ref. No.: MRP(S)-0290/12-13/KLMG002/UGC-SWRO, Dated 29.03.2013)

By

Dr. RAVIKUMAR C

DEPARTMENT OF PHYSICS
CMS COLLEGE, KOTTAYAM
KERALA– 686 001, INDIA

MARCH 2016

EXECUTIVE SUMMARY OF THE WORK

Conjugated organic structures have been studied as prospective building blocks for second-order nonlinear optical materials in view of their potential application in the area of photonics. Some of the advantages of organic materials include ease of synthesis, scope for altering the properties by functional substitutions, inherently high nonlinearity, high damage resistance, etc. Most of the amino acids contain a deprotanated carboxylic acid group (COO^-) and protanated (NH_3^+) amino group. This dipolar nature exhibits peculiar physical and chemical properties in amino acids, thus making them ideal candidate for NLO applications. An understanding of the electronic origin of molecular NLO response is of fundamental scientific interest as well as a crucial component in the development of state-of-the-art NLO materials. The interest of studying the vibrational experimental and theoretical spectra of conjugated chromophores is a great importance in modern nonlinear optical processes. A brief account of the investigated work is summarized below.

FTIR and Raman spectral analysis of crystallized potential NLO chromophore benzaldehyde thiosemicarbazone ($C_8H_9N_3S$) has been performed with the support of theoretical investigation of equilibrium geometry, various bonding features, and harmonic vibrational wavenumbers using B3LYP method. The role of optical nonlinearity of the crystal is analyzed as a consequence of enhanced intensity of 8a mode leading to higher degree of conjugation.

Structure and nonlinear optical properties donor – acceptor structure L-asparaginium tartrate (LAT) have been studied by FT-IR and Raman spectra. The geometry, charge transfer interaction, and harmonic vibrational wavenumbers have been calculated with the help of B3LYP density functional theory method. The SHG efficiency was evaluated by Kurtz and Perry powder reflection technique.

Technologically, nonlinear optical processes are the basic tools of optoelectronic and photonic applications. Current work is focused on design of NLO chromophores in view of the potential applications in various photonic technologies. Necessarily too many of the applications and the probable uses of the vibrational spectra of NLO materials are to be widely recognized.