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Title of Ph.D. Thesis : **Structural, Electronic and Spectroscopic Studies of
Non Linear Optical Conjugated Molecules and
Organic Dyes.**

Abstract

With the rapid technological development in the field of photonics and opto-electronics, optical materials with large and fast third order nonlinearity have acquired great importance. Among various materials, nonlinear optical (NLO) organics have attracted the attention of physicists and chemists due to their ease of processing, chemical flexibility, and easy processing of their good quality thin films and crystals. In the present research work we have set employed Z-scan experimental technique and performed experiments to investigate nonlinear absorption coefficient (β), nonlinear refractive index (n_2) and third order susceptibility (χ^3) for the diamino and dihydroxy anthraquinone derivatives using low power CW lasers.

The major outcomes of the present work are outlined as:

- The solutions of different concentrations for 1, 4-Diamino-9, 10-Anthraquinone (14-DAAQ), 1, 2-Diamino-9, 10-Anthraquinone (12-DAAQ), 1, 5-Diamino-9, 10-Anthraquinone (15-DAAQ) and 2, 6-Diamino-9, 10-Anthraquinone (26-DAAQ) were prepared. The Z-scan results reveal that the DAAQ dyes in solution exhibit reverse saturable absorption and self defocusing effects at 532 nm, which are observed to be concentration dependent. The obtained values β , n_2 and χ^3 for 14-DAAQ, 12-DAAQ and 15-DAAQ in solutions are found to be of the order of 10^{-4} (m/W), 10^{-11} (m/W) and

10^{-5} (esu), respectively. However, for 26-DAAQ dye solution for which the values of β , n_2 and χ^3 are found as $\sim 10^{-5}$ (m/W), 10^{-13} (m/W) and 10^{-8} (esu), respectively. The NLO response of 12-DAAQ in solution has also been examined with other excitation wavelength 405 nm, where the dye has negligible linear absorption (off-resonance). It has been found that the nonlinear optical parameters for 12-DAAQ with 532 nm excitation source are larger than that obtained with 405 nm.

- The obtained values of nonlinear optical parameters for DAAQ dyes-polymer composite films are higher as compared to those in liquid media. The values of nonlinear optical parameters for DAAQ dyes-polymer composite films are comparable to those of DAAQ dyes-polymer films. The nonlinear optical studies carried on AQ dyes reveal that these dyes show high values of third order susceptibility with low power CW laser.
- Quantum chemical methods have also become an important tool to evaluate NLO response in organic molecules and dyes. Theoretically evaluated, molecular hyperpolarizability (β) is a key parameter determining the second order NLO behaviour. In this context, we have examined the molecular hyperpolarizability for all the AQ dyes by employing Density Functional Theory (DFT) using Gaussian 03 software package. We have also, designed seven conjugated organic structures and investigated the effect of different donors and acceptors across a conjugated pyridine molecule on molecular hyperpolarizability by employing ab-initio Hartree Fock calculations and DFT. The dependence of the hyperpolarizability of different molecular structure on the nature of donor and acceptor on the pyridine is discussed on the basis of molecular orbital picture by employing quantum chemical calculations.
- The results obtained for DAAQ and DHAQ dyes are quite encouraging for possible applications in optical limiting and opto-electronic devices.