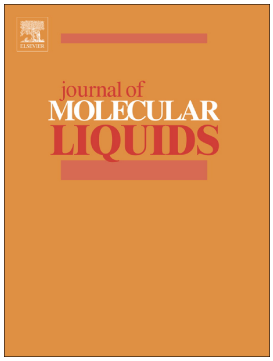

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A Combined Experimental and Computational Investigation ~~on~~of Solvatochromism of Nonpolar Laser Dyes: Evaluation of Ground and Singlet Excited-State Dipole Moments

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Abstract

In the present work, the solvatochromism of two large nonpolar laser dyes Exalite 384 (E384) and Exalite 416 (E416) has been studied by both experimentally and computationally. The steady state absorption and fluorescence spectra have been measured in a series of polar protic, polar aprotic and non-polar/weakly polar solvents to investigate their solvatochromism and determine dipole moments. Various solvent correlation techniques, like Lippert–Mataga, Bilot–Kawski, Kawski–Chamma–Viallet, Bakhshiev and Reichardt methods were used to evaluate the singlet excited and ground state dipole moments. Kamlet– Taft and Catalan solvent parameters were used by means of multiple linear regression (MLR) method to analyze specific and non-specific solute-solvent interactions. Computational studies were carried out to optimize ground and excited state geometries using density functional theory (DFT) and time-dependent density functional theory (TD-DFT), respectively, in vacuum. This study also extends to evaluate the electronic transition energies from ground to first electronic excited state of solvated laser dyes employing semiempirical wave function model. In particular, the semiempirical method ZINDO has been combined with integral equation formalism of polarizable continuum model (IEF-PCM) to calculate solute-solvent interaction potential which is comparatively studied with $E_T(30)$ polarity scale along with experimental. The intramolecular charge transfer and hybridization is demonstrated by natural bond orbital analysis (NBO). The ground (μ_g) and excited state dipole moments (μ_e) of these dyes computed and those determined experimentally are compared and the results are discussed.