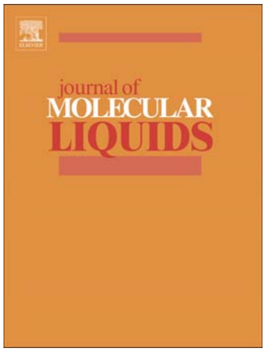

Steady state absorption and fluorescence study: Estimation of ground and excited state dipole moments of newly synthesized pyridazin-3(*2H*)-one derivatives

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Steady state absorption and fluorescence study: Estimation of ground and excited state dipole moments of newly synthesized pyridazin-3(*2H*)-one derivatives

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Abstract

Steady state absorption and emission spectra of newly synthesised pyridazin-3(*2H*)-one derivatives 5-(2-hydoxy-4-methyl-phenyl)-2-phenyl-*2H*-pyridazin-3-one [HMP], 5-(5-bromo-2-hydroxy-phenyl)-2-phenyl-*2H*-pyridazin-3-one [BHP] and 5-(4-chloro-2-hydoxy-phenyl)-2-phenyl-*2H*-pyridazin-3-one [CHP] were studied in different solvents in order to estimate the ground and excited state dipole moments. Ground state dipole moments (μ_g) were estimated using the theoretical method provided by Gaussian-09 program and experimental method suggested by Guggenheim. Ground state dipole moments measured from theoretical and experimental methods for the molecule CHP only are quite close to each other. Thus, molecular geometry taken for this molecule CHP under theoretical and experimental methods may correlate well. Excited state dipole moments (μ_e) of all the three molecules were estimated using solvatochromic shift method. From the results of the effect of solvents on emission spectra it may be inferred that in HMP and BHP molecules there exists $\pi \rightarrow \pi^*$ transition and in CHP molecule there exists $n \rightarrow \pi^*$ transition. Under solvatochromic shift method, three equations proposed by Lippert's, Bakshiev's and Kawski-Chamma-Viallet's were used to find excited state dipole moments and it is found that excited state dipole moments are larger than ground state dipole moments in all the three molecules. This may be due to the fact that, the excited states for all the three molecules are more polar than the ground states. Furthermore, we have analysed the microscopic solvent polarity parameter and effect from empirical measurements of acidity (SA), basicity (SB), polarizability (SP) and dipolarity (SdP).

Keywords: Pyridazin-3(*2H*)-one, Absorption, Fluorescence, Stokes shift, Dipole moment, Microscopic solvent polarity parameter $\left(E_T^N\right)$.

1. Introduction

Absorption and emission spectra of organic molecules are usually modified in solvation process. The effect of solvents on absorption and emission spectra can be used to determine the magnitude and the direction of electric dipole moment of solute molecules in its first electronically excited state. The dipole moment of the electronically excited state is an important property that provides information about the electronic and geometrical structures of the molecule in its short-lived excited state and is often useful in various applications [1]. Several authors have made extensive studies on the estimation of ground and excited state dipole moments for a variety of fluorescence compounds [2-7].