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Studies of Substituent and Solvent Effect on Spectroscopic Properties Of 6-OH-4-CH3, 7-OH-4-CH3 and 7-OH-4-CF3 Coumarin

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Abstract : This paper reports the solvent effects on the electronic absorption and fluorescence emission spectra of 6-OH-4-CH3, 7-OH-4-CH3 and 7-OH-4-CF3 coumarin derivatives having -OH, -CH3 and -CF3 substituent at different positions in various solvents (Polar and Non-Polar). The first excited singlet state dipole moment and ground state dipole moment were calculated using Bakhshiev, Kawski-Chamma-Viallet and Reichardt-Dimroth equations and were compared for all the coumarin studied. In all cases the dipole moments were found to be higher in the excited singlet state than in the ground state indicating a substantial redistribution of Π-electron density in the excited state. The angle between the excited singlet state and ground state dipole moment is also calculated. The red shift of the absorption and fluorescence emission bands, observed for all the coumarin studied upon increasing the solvent polarity indicating that the electronic transitions were Π → Π* nature.

Keywords : coumarin, solvent effects, absorption spectra, emission spectra, excited singlet state dipole moment, ground state dipole moment, solvatochromism
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