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Rotational diffusion dynamics of fluorescein derivatives in binary mixtures of solvents:

an Experimental and Computational study

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Abstract: With a view to understand the nature of solute solvent interactions, rotational reorientation times of three medium sized dipolar laser dyes viz., dichlorofluorescein (DCF), sodium fluorescein (SF) and keton red (KR) in two binary mixtures namely, aqueous-DMSO and aqueous-1-propanol have been determined employing steady state fluorescence depolarization technique. The experimental results are analyzed in the light of SED hydrodynamic theory. A hook shaped profile for rotational reorientation time versus viscosity is observed in both the binary mixtures of solvents that is likely to shed light on solute-solvent interactions. Further, theoretical study has been carried out using Gaussian 09 software. The optimized geometry, HOMO-LUMO, energy gap, molecular electron potential map (MEPM) were extracted from DFT/B3LYP 6-311g(d) basis set. The hyper conjugation or intra molecular delocalization was estimated from NBO analysis. Strong interactions were observed between $nO_{33} \rightarrow \sigma^*C_{31}$, $\pi N_{38} \rightarrow \sigma^*C_{12}$ and $\pi O_{32} \rightarrow \pi^*(C_{31}-O_{33})$ with E(2) energies of 203.58, 121.89 and 39.92 kJ/mol for SF, KR and DCF.

PRINCIPAL

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