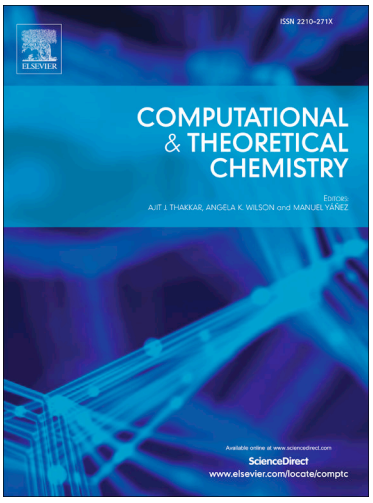

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Computational Study of Effect of Solvents on Vibrational Spectra of Coumarin 500

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Abstract

Optimized structure of coumarin 500 has been obtained in gas phase and in solvents like methanol, ethanol, dimethyl sulfoxide and CCl_4 using density functional theory calculations with B3LYP/6-311+G(d,p) functionals. The calculated frequencies of certain vibrational bands of coumarin 500 are observed to shift in solvents. To understand the origin of these shifts, HOMO-LUMO analysis of ultra-violet visible spectra of coumarin 500 has been carried out in different solvents. The detailed study of charge transfer interactions in coumarin 500 is done using natural bonding orbital and molecular electrostatic potential analysis. Assignments of various vibrational bands have been obtained and effect of charge transfer interactions in solvents on these bands has been studied.

Keywords: Vibrational spectra, HOMO-LUMO, Density Functional Theory, Natural Bond Orbital, Solvation, Coumarin Dyes.

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