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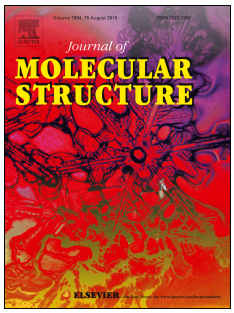

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Vibrational and UV spectroscopic studies of 2-coumaranone by experimental and Density functional theory calculations

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Key words: 2-coumaranone, FT-IR, FT-RAMAN, UV Spectra, Fluorescence imaging, NBO

Abstract:

The vibrational and electronic properties of 2-coumaranone have been reported in the ground state using experimental techniques (FT-IR, FT-Raman, UV spectra and fluorescence microscopic imaging) and density functional theory (DFT) employing B3LYP correlation with the 6-31G(d, p) basis set. The theoretically reported optimized parameters, vibrational frequencies etc., were compared with the experimental values, which yielded good concurrence between the experimental and calculated values. The assignments of the vibrational spectra were done with the help of normal co-ordinate analysis (NCA) following the Scaled Quantum Mechanical Force Field(SQMFF) methodology. The whole assignments of fundamental modes were based on the potential energy distribution (PED) matrix. The electric dipole moment and the first order hyperpolarizability of the 2-coumaranone have been computed using quantum mechanical calculations. NBO and HOMO, LUMO analyses have been carried out. UV