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Vibrational Analysis of Flavone

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Abstract: In this study, the experimental and theoretical study on the structures and vibrations of flavone are presented. FT-IR and FT-Raman spectra of the molecule have been recorded in the 400-4000 cm^{-1} region and the 5-3500 cm^{-1} region, respectively. The molecular geometry and vibrational frequencies of flavone in the ground state have been calculated by using Density Functional method (B3LYP) in conjunction with 6-311++G(d,p) and 6-31++G(d) as basis sets.

Key Words: Infrared spectra, Raman Spectra, Hartree-Fock, Density functional theory, Flavone

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