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Vibrational assignments of α-acetyl - γ- butyrolactone by ab initio Hartree-Fock and Density Functional methods

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Abstract: The Fourier transform infrared and FT-Raman spectra of α-acetyl-γ-butyrolactone have been recorded in region 4,000–400 and 4,000–100 cm^{-1} respectively. A complete assignment and analysis of fundamental vibration modes of the molecule have been carried out. The observed fundamental modes have been compared with harmonic vibration frequencies computed using density functional theory calculations by employing B3LYP functional at 6-311+G(d,p) level. UV–Visible spectrum of the compound has been recorded and electronic properties, such as highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies have been calculated with B3LYP/6-311++G(d,p) level. These calculated energies show that charge transfer occurs within molecule. Mulliken population analysis and thermodynamic properties of title compound have also been calculated.

Keywords:α-acetyl-γ-butyrolactone, DFT, HF, FT-IR, FT-RAMAN, UV, HOMO-LUMO.

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