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Vibrational assignment, NBO analysis and molecular docking studies ofButyrophenone by Density functional theory

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Abstract: The Fourier-transform infrared spectrum and Fourier-transform Raman Spectrum of Butyrophenonewere recorded in the region 4000-400 $cm^{-1}$and 4000-100 cm^{-1}respectively. A complete vibrational assignment and analysis of the fundamental vibrational modes of the molecule have been compared with the harmonic vibrational frequencies computed using HF and DFT (B3LYP) method by employing 6-311 +G(d, P) basis sets. UV-Visible spectrum of the compound was recorded and the electronic properties, such as HOMO and LUMO energies, The calculated HOMO and LUMO energies show that, the charge transfer occurs within the molecule Stability of the molecule arising from hyper conjugative interations, chare delocalization have been analyzed using natural bond orbital analysis (NBO). Molecular electrostatic otential studies were performed at DFT/B3LYP method using 6-311 +G (d, p) basis sets. Inclusion complex of Butyrophenone with β-cyclodextrin (β-CD) has been investigated by molecular docking method. The other molecular properties like Mulliken population analysis and themodynamic properties of the title compound have been calculated.**Keywords:**Butyrophenone, DFT; FT-IR; FT-Raman, HOMO-LUMO; NBO.

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