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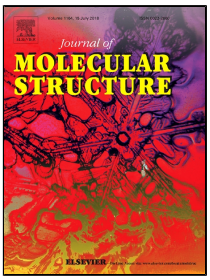

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Spectroscopic (FT-IR, Laser-Raman and NMR) and Conformational Analysis on Novel Pyrazole β-keto ester Compound

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Abstract: Our goal in this study is to submit a comprehensive theoretical study of novel compound. Therefore, we perused and analyzed the experimental (real form) and theoretical (gas form) vibrational frequencies for the most stable conformer of title compound. The crystallographic geometry was used for full geometry optimization, followed by a conformational analysis. The experimental FT-IR and Laser-Raman spectra of the studied molecule were taken in the region (4000-400 cm^{-1}) and (4000-100 cm^{-1}) in gas phase, respectively. For the most stable conformer, the vibrational modes and their assignments and optimized structure parameters (bond lengths, bond angles) were computed by using DFT/B3LYP functional and 6-311++G(d,p) basis set. Gaussian 09W software and GaussView5 interface programs were utilized for all computations. Theoretical mode assignments of the most stable conformer were obtained by using potential energy distribution (PED) with free VEDA 4 software program. The observed FT-IR and Laser-Raman spectra were compared with the calculated theoretical data. The computed vibrational frequencies of C1 conformer were also found in good agreement with the experimental results. The Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) analysis divulge the possibility of charge transfer within the molecule. The proton (^{1}H) and carbon-13 (^{13}C) nuclear magnetic resonance (NMR) chemical shifts were researched for the most stable conformer C1, both experimentally in DMSO-d_6 and theoretically in DMSO with integral equation formalism polarizable continuum model (IEFPCM) method.

Keywords: Pyrazole, β-ketoester, DFT/B3LYP; NMR shifts; IEFPCM

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