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Molecular structure, FT-IR, vibrational assignments, HOMO–LUMO analysis and molecular docking study of 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone



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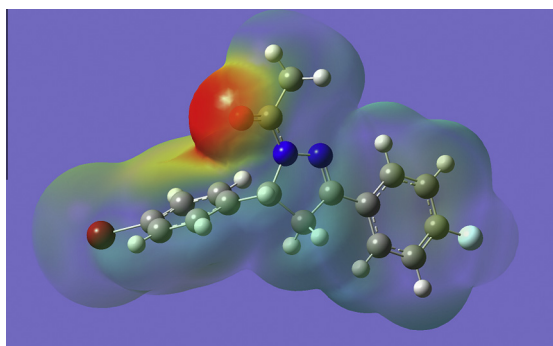
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HIGHLIGHTS

- IR, spectrum and theoretical analysis were reported.
- The wavenumbers are calculated theoretically using Gaussian09 software.
- The wavenumbers are assigned using PED analysis.
- The geometrical parameters are in agreement with XRD data.
- Molecular docking studies are reported.

GRAPHICAL ABSTRACT



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ABSTRACT

The optimized molecular structure, vibrational frequencies, corresponding vibrational assignments of 1-[5-(4-bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone have been investigated experimentally and theoretically using Gaussian09 software package. The title compound was optimized using the HF/6-31G(d) (6D, 7F), B3LYP/6-31G (6D, 7F) and B3LYP/6-311++G(d,p) (5D, 7F) calculations. The B3LYP/6-311++G(d,p) (5D, 7F) results are in agreement with experimental infrared bands. The geometrical parameters are in agreement with XRD data. The stability of the molecule arising from hyper-conjugative interaction and charge delocalization has been analyzed using NBO analysis. The HOMO and LUMO analysis is used to determine the charge transfer within the molecule. Molecular electrostatic potential was also performed. From the MEP it is evident that the negative charge covers the C=O group and the positive region is over the rings. First hyperpolarizability is calculated in order to find its role in nonlinear optics. Molecular docking studies suggest that the compound might exhibit inhibitory activity against TPPII and may act as anti-neoplastic agent.

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Introduction

Pyrazolines are well known amongst five membered azole hetero-cycles. The synthetic routes to pyrazoline derivatives are well cited in literature [1]. Pyrazoline derivatives have attracted considerable interest because of their therapeutic and pharmacological properties. Several of them have been found to exhibit a wide spectrum of biological actions like antimicrobial [2–5], anti-inflammatory, anti-amoebic [6,7], analgesic [8], anticonvulsant [9], antidepressant [10], anticancer [11], neuro-protective [12], antiviral [13], amine oxidase inhibitory [14] and antimyco-bacterial activity [15,16]. Due to these interesting activities of diversely substituted pyrazolines as biological agents, considerable attention has been focussed on this class and in addition pyrazolines have played a crucial part in the development of the theory in heterocyclic chemistry and also used extensively in organic synthesis [17]. Fun et al. [18] reported the single crystal XRD study of the title compound. Binil et al. [19] reported the vibrational spectroscopic study of a pyrazolidinedione derivative experimentally and theoretically. In the present work, the electronic properties and IR spectrum of the title compound is reported with the hope that the results of the present study would be helpful in future synthesis of more potent derivatives. The energies, degrees of hybridization, populations of the lone pairs of oxygen, energies of their interaction with the anti-bonding orbital of the rings and the electron density distributions and $E(2)$ energies have been calculated by NBO analysis using DFT method to predict clear evidence of stabilization originating from the hyper-conjugation of various intramolecular interactions. Since there has been growing interest in using organic materials for nonlinear optical devices, the first hyperpolarizability is also determined theoretically. To evaluate the biological potential of the title compound molecular docking studies of the title compound are reported here.

Experimental

The experimental procedure for the synthesis of the title compound, 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone is described by Fun et al. [18]. In the title molecule, $C_{17}H_{14}BrFN_2O$, the benzene rings form dihedral angles of 6.6° and 85.3° with the mean plane of the 4,5-dihydro-1H-pyrazole ring. The latter ring is planar and the dihedral angle between the benzene rings is 78.9° . In the crystal, weak $C-H \cdots O$ and $C-H \cdots F$ hydrogen bonds link the molecules in corrugated layers [18]. The FT-IR spectrum (Fig. 1) was recorded on Shimadzu-FT-IR infrared spectrometer with KBr pellets.

Computational details

Calculations of the title compound are carried out with Gaussian09 software package [20] using the HF/6-31G(d) (6D, 7F), B3LYP/6-31G (6D, 7F) and B3LYP/6-311++G(d,p) (5D, 7F) basis sets to predict the molecular structure and vibrational wave numbers. Molecular geometry was fully optimized by Berny's optimization algorithm using redundant internal coordinates. Harmonic vibrational wave numbers are calculated using the analytic second derivatives to confirm the convergence to minima on the potential surface. The wave number values computed at the Hartree–Fock level contain known systematic errors due to the negligence of electron correlation [21]. We therefore, have used the scaling factor value of 0.8929 for HF method [21]. The DFT hybrid B3LYP functional tends to overestimate the fundamental modes; therefore scaling factor of 0.9613 has to be used for obtaining a considerably better agreement with experimental data [21]. Parameters corresponding to optimized geometry of the title compound

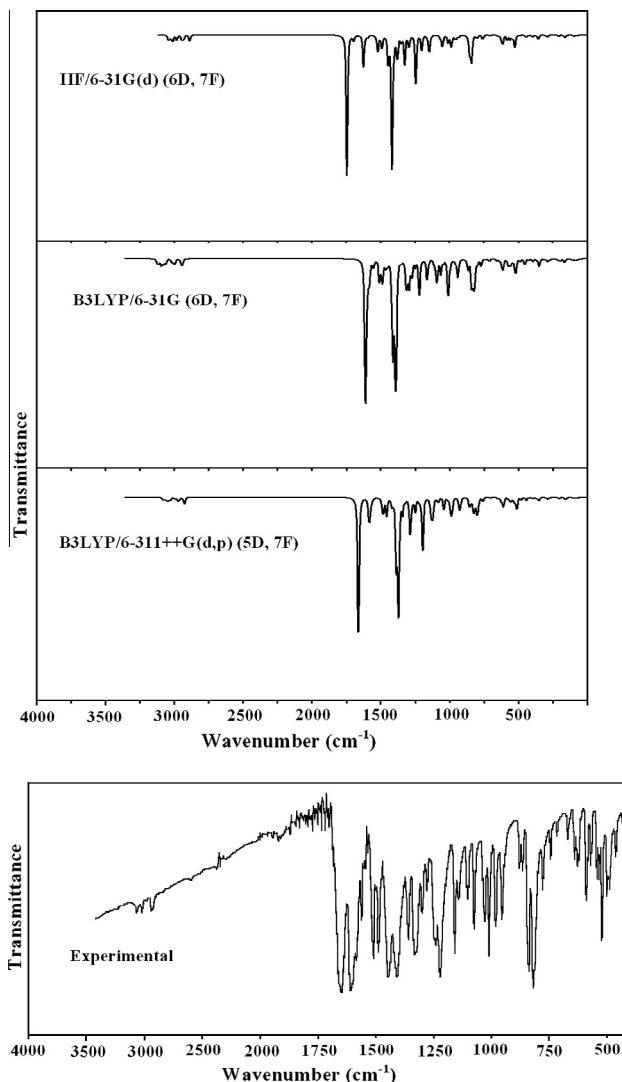


Fig. 1. FT-IR spectrum of 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone.

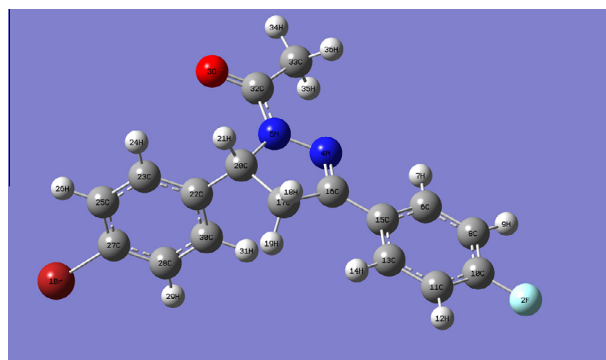


Fig. 2. Optimized geometry (B3LYP/6-311++G(d,p) (5D, 7F)) of 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone.

(Fig. 2) are given in Table S1 (supporting material). The absence of imaginary wave numbers on the calculated vibrational spectrum confirms that the structure deduced corresponds to minimum energy. The assignments of the calculated wave numbers are aided by the animation option of Gaussview program, which gives a visual presentation of the vibrational modes [22]. The potential

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