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DFT Study of (Rs) - (3-Bromophenyl) (Pyridine-2yl) Methanol

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Abstract: The theoretical study of (RS)-(3-bromophenyl) (pyridine-2yl) methanol has been carried out using DFT at B3LYP/6-311+G (d, p) level. Theoretical IR and normal mode analysis of title compound has also been calculated. The structure activity relationship based on the study of frontier orbital gap and molecular electrostatic potential map of the (RS)-(3-bromophenyl) (pyridine-2yl) methanol has been used to understand the active sites of the molecule under study.

Keywords: Density functional theory, Vibrational analysis, HOMO-LUMO, MESP.

I. INTRODUCTION

The diphenyl methanols, RPh₂COH, exhibit a very rich diversity of supramolecular arrangements, including isolated molecules, hydrogen-bonded dimers, trimers, tetramers and hexamers as well as continuous hydrogen-bonded chains [1]. It is therefore of considerable interest to investigate the influence of an addition potential acceptor of hydrogen bonds as achieved. The vibrational spectroscopic analysis is known to provide immensely invaluable molecular structure elucidation in synergy with quantum chemical calculations. In order to obtain a complete description of molecular dynamics, vibrational wavenumber calculations along with the normal mode analysis have been carried out at the DFT level employing the basis set 6-311++G(d, p). The optimized geometry of molecule under investigation and its molecular properties such as equilibrium energy, frontier orbital energy gap and molecular electrostatic potential energy map, have also been used to understand the properties and active sites of the molecule.

II. COMPUTATIONAL DETAILS

Quantum chemical study of the (RS)-(3-bromophenyl) (pyridine-2yl) methanol has been performed within the framework of the density functional theory [2] with Becke's three-parameter hybrid exchange functional [3] with Lee-Yang-Parr correlation functionals (B3LYP) [4,5] and employing 6-311 ++ G(d, p) basis set using the Gaussian 09 program package [6]. As the DFT hybrid B3LYP functional tends to overestimate the fundamental normal modes of vibration, a scaling factor of 0.9679 has been applied [7, 8]. The vibrational wavenumber assignments have been carried out by combining the results of the Gaussview 5 program [9], symmetry considerations and the VEDA 4 program [10]. The calculated IR spectra has been shown in Fig. 2.

III. RESULT AND DISCUSSION

A. Molecular Geometry Optimization and Energies

The geometry of the title compound has been optimized for the calculation of its molecular properties using DFT at the B3LYP level, with the 631++G(d,p) basis set. The optimized geometry of molecule (Fig. 1) under study is confirmed to be located at the local true minima on potential energy surface, as the calculated vibrational spectra contains no imaginary wavenumber. The optimized structural parameters (bond lengths, bond angles, dihedral angles) of title compound have been shown in Table 1. The (C - O) bond lengths 1.427 Å is found to be close to the standard ester C - O bond lengths [11,12].

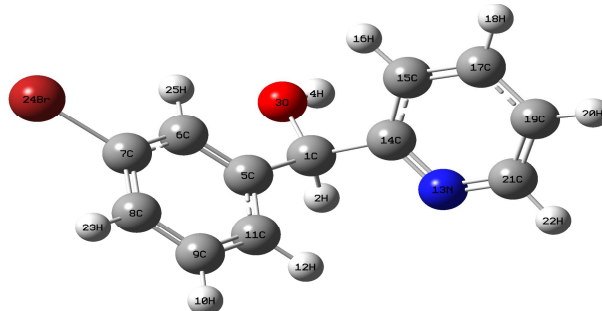


Figure 1. Optimized geometry of (RS)-(3-bromophenyl) (pyridine-2yl) methanol,

B. Vibrational Assignments

The optimized molecular structure belongs to the C_1 point group as it does not display any special symmetry. The overestimation of the vibrational wavenumbers in ab-initio and DFT methods are corrected either by computing anharmonic correlations explicitly or by introducing a scaled field, even directly scaling the calculated wavenumbers with proper factor. The vibrational wavenumbers are calibrated accordingly with the scaling factor of 0.9679 for DFT at B3LYP/6-311++G(d,p) level. The vibrational assignments have been done on the basis of relative intensities, line shape, the VEDA 4 program and the animation option of Gaussview 5.

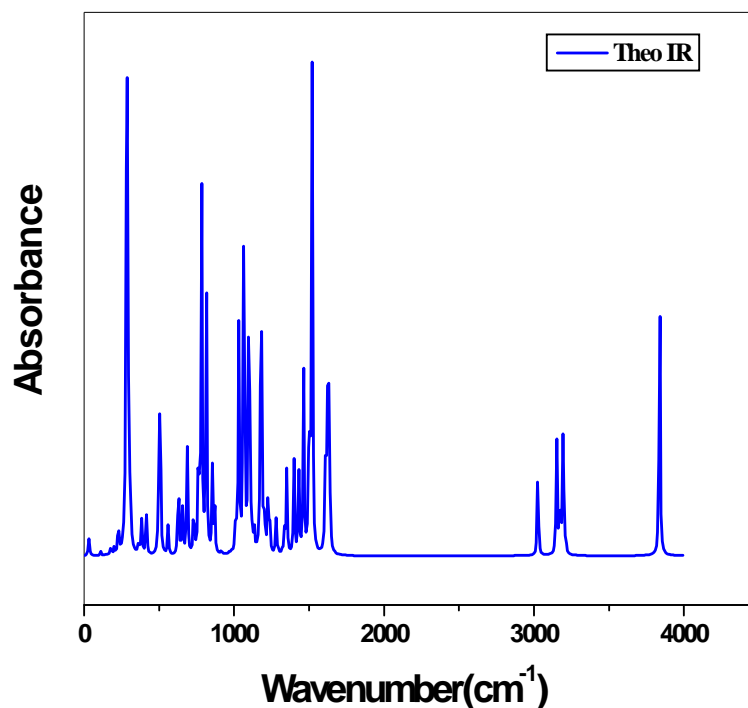


Figure 2. Theoretical IR spectrum of (RS)-(3-bromophenyl) (pyridine-2yl) methanol,

- 1) *O-H vibrations*: The O-H stretching vibration is very sensitive to hydrogen bonding. A free hydroxyl group or a non-hydrogen bonded hydroxyl group absorbs in the range $3700-3500\text{ cm}^{-1}$. The intra-molecular hydrogen bonding present in the system reduces the hydroxyl stretching band to $3559-3200\text{ cm}^{-1}$ region [13]. The scaled wavenumber calculated at 3741 cm^{-1} is identified as O-H stretching with 100% contribution to P.E.D.
- 2) *C-C and C-H vibrations*: C-C stretching wavenumbers are observed as mixed modes in the range 1100 cm^{-1} to 800 cm^{-1} and agree well with the general appearance of C-H and C-C stretching modes. The C-C pure stretching are calculated to be 1583 , 1575 and 1559 cm^{-1} which are also in good agreement with previous studies. The C-H stretching vibration of (RS)-(3-bromophenyl) (pyridine-2yl) methanol has been observed in the range $3110-2929\text{ cm}^{-1}$.
- 3) *Ring vibrations*: The thiophene ring spectral region predominantly involves the C-H, C-C, C-Cl, C-S and C=C stretching, and C-C-C as well as H-C-C-bending vibrations. The bands due to the ring C-H-stretching vibrations were observed as a group of partially overlapping absorptions in the region $3110-3069\text{ cm}^{-1}$ with more than 90% potential energy contribution. Vibrations involving C-H in-plane bending are found in the region $1600-825\text{ cm}^{-1}$.

C. Electronic properties:

The highest occupied molecular orbital (HOMO) is the orbital that primarily acts as an electron donor and the lowest unoccupied molecular orbital (LUMO) is the orbital that largely acts as the electron acceptor. The frontier orbital energy gap helps characterize the chemical reactivity and kinetic stability of the molecule. The frontier orbital energy gap is found to be 5.302 eV .

IV. CONCLUSION

We have performed a detailed quantum chemical studies on (RS)-(3-bromophenyl) (pyridine-2yl) methanol using density functional theory at B3LYP/6311+G(d,p) level. Vibrational spectroscopic analysis has been performed and prominent modes of vibration are assigned and discussed. The HOMO-LUMO gap provides a measure of charge transfer interaction. These findings may stimulate further observations on the biological activity of (RS)-(3-bromophenyl) (pyridine-2yl) methanol and related natural products.

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