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## NBO, conformational, NLO, HOMO–LUMO, NMR and electronic spectral study on 1-phenyl-1-propanol by quantum computational methods

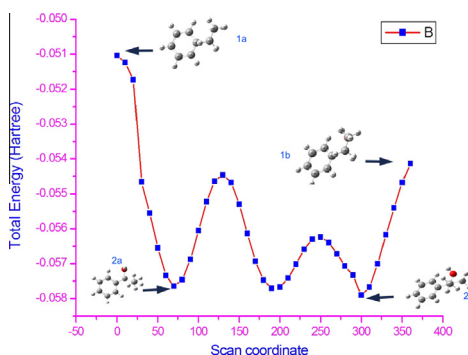
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### HIGHLIGHTS

- The compound 1-phenyl-1-propanol investigated by FT-IR, FT-Raman and NMR and UV–Vis spectroscopic tool.
- The chemical shift is found in favor of its change of chemical property.
- The charge transfer in the molecule by HOMO–LUMO studied in relation with NBO analysis.
- The study of NLO property in relation with polarizability and hyperpolarizability is done.
- Chemical reactivity region have been found along with the Fukui function.

### GRAPHICAL ABSTRACT

1-Phneyl-1-propanol is used as intermediate for composition of fluoxetine anti-depressant drug. It is a major depression drug for pediatric depression. Though the molecule has symmetry, it has different trans–cis structure with tiny different energies. The theoretical vibrational frequencies have been found in good agreement with the corresponding experimental data. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded and chemical shifts of the molecule were compared to TMS by using the Gauge-Independent Atomic Orbital (GIAO) method. A study on the electronic and optical properties, absorption wavelengths, excitation energy, dipole moment and frontier molecular orbital energies are performed using HF and DFT methods.



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### ABSTRACT

In this study, FT-IR, FT-Raman, NMR and UV spectra of 1-phenyl-1-propanol, an intermediate of anti-depressant drug fluoxetine, has been investigated. The theoretical vibrational frequencies and optimized geometric parameters have been calculated by using HF and density functional theory with the hybrid methods B3LYP, B3PW91 and 6-311+G(d,p)/6-311++G(d,p) basis sets. The theoretical vibrational frequencies have been found in good agreement with the corresponding experimental data. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded and chemical shifts of the molecule were compared to TMS by using the Gauge-Independent Atomic Orbital (GIAO) method. A study on the electronic and optical properties, absorption wavelengths, excitation energy, dipole moment and frontier molecular orbital energies are performed using HF and DFT methods. The thermodynamic properties (heat capacity, entropy and enthalpy) at different temperatures are also calculated. NBO analysis is carried out to picture the charge transfer between the localized bonds and lone pairs. The local reactivity of the molecule has been studied using the Fukui function. NLO properties related to polarizability and hyperpolarizability are also discussed.

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## Introduction

1-Phenyl 1-propanol is an organic compound containing an aromatic hydrocarbon with an aliphatic substitution. It is a colorless liquid, soluble in water. It is used as intermediate for composition of fluoxetine anti-depressant drug. Fluoxetine is a major depression drug for pediatric depression. It is also used for obsessive disorder both for adult and pediatric as drug for diseases like bulimia nervosa, panic disorder and premenstrual dysphonic disorder. It is the third most prescribed anti-depressant after sertraline. Other synonyms of alpha-Ethylbenzyl alcohol; Benzyl alcohol, alpha-ethyl-; Benzenemethanol, alpha-ethylalpha-Ethylbenzyl alcohol; Benzyl alcohol, alpha-ethyl. Zhu et al. [1] made DFT study on the candidate molecule, and it was found that while inclusion of 1-phenyl 1-propanol in two modified cyclic decapeptides, it functions as driving force for inclusion of complex formation. This facilitates enhancement of binding affinity of 1-phenyl 1-propanol enantiomer with cyclic decapeptides. Zhoo et al. also made DFT study using B3LYP basis set of the molecule their results reveal that 1-phenyl 1-propanol could form more stable inclusion complex in cyclic decapeptide [2]. And Choi et al. [3] found in their study that 1-phenyl 1-propanol is used as chiral intermediate in the synthesis of the anti-depressant drugs. In the present study, the stable geometry of the molecule is analyzed and discussed with its bond length, bond angle and dihedral angle. The vibrational modes of the molecule is calculated and compared with the experimental values. Spectra of the  $^{13}\text{C}$  NMR and  $^1\text{H}$  NMR is analyzed and chemical shift is calculated comparing with TMS. Electronic transition of the molecule is analyzed to know the site of chromospheres with UV-vis spectra and reactivity center is identified with Fukui function.

## Experimental details

The spectra of the compound 1-phenyl 1-propanol are obtained from spectral library purchased from Sigma-Aldrich Chemicals, USA. The FT-IR spectrum of the compound is recorded using a Bruker IFS 66V spectrometer in the range of  $4000\text{--}400\text{ cm}^{-1}$ . The spectral resolution is  $\pm 2\text{ cm}^{-1}$ . The FT-Raman spectrum of the same compound is also recorded using the same instrument with an FRA 106 Raman module equipped with a Nd:YAG laser source operating at  $1.064\text{ }\mu\text{m}$  line widths with 200 mW power. They are recorded in the range of  $4000\text{--}100\text{ cm}^{-1}$  with a scanning speed of  $30\text{ cm}^{-1}\text{ min}^{-1}$  of spectral width  $2\text{ cm}^{-1}$ . The frequencies of all sharp bands are accurate to  $\pm 1\text{ cm}^{-1}$ . The high resolution  $^1\text{H}$

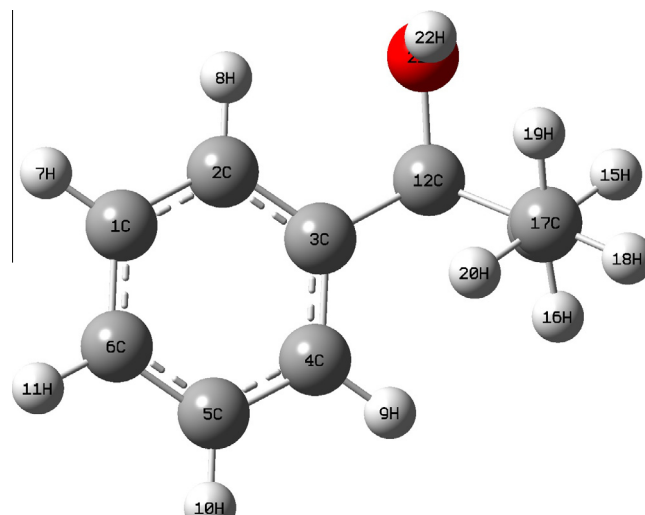


Fig. 2. Optimised structure of 1-phenyl-1-propanol.

NMR and  $^{13}\text{C}$  NMR spectra are recorded using 300 MHz and 75 MHz NMR spectrometer respectively.

## Computational methods

The quantum computational works of the compound are performed using HF and hybrid B3LYP and B3PW91 using the basis sets 6-31+G(d,p) and 6-311+G(d,p). All these calculations are performed using the GAUSSIAN 09W [4] program package on i7 processor in a personal computer. Becke's three-parameter hybrid function (B3) combined with the Lee–Yang–Parr correlation function constitute B3LYP [5,6]. In the same way Becke's three parameter hybrid function (B3) [7] combined with the gradient-corrected correlation functional Perdew and Wang (PW91) [8,9] constitute B3PW91 method. The optimized molecular structure of the molecule is shown in Fig. 2.

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR isotropic shielding are calculated using the GIAO method [10] supported by the TMS B3LYP 6-311+G (2d,p).  $^{13}\text{C}$  isotropic magnetic shielding (IMS) of any X carbon atoms is computed by relation  $\text{CS}_X = \text{IMS}_{\text{TMS}} - \text{IMS}_X$ , where  $\text{IMS}_{\text{TMS}}$  is the isotropic shielding of tetra methyl silene. The  $^1\text{H}$  and  $^{13}\text{C}$  isotropic chemical shifts of the compound with reference to TMS in solvent phase are calculated supported by IEFPCM methods. The electronic properties, HOMO–LUMO energies, absorption wavelengths and oscillator strengths are calculated using the time-dependent self-consistent field theory [11,12] with B3LYP functional for solvent and gas phase. Moreover, dipole moment, nonlinear optical (NLO) properties, linear polarizabilities and first hyperpolarizabilities have also been studied. Fukui function is used to predict both the reactive centers and the possible sites of nucleophilic and electrophilic attack.

## Results and discussion

### Conformational analysis

Conformational analysis was carried out for 1-phenyl-1-propanol by potential energy surface scan to find all possible conformers with B3LYP method using 6-311G(d,p) basis set. The scans were obtained by minimizing the potential energy in all geometrical parameters by varying the torsion angles by steps of  $10^\circ$  in the range of  $0\text{--}360^\circ$  rotation around the bond [13]. The rotation about C14–C12 single bond produces different conformers of the title

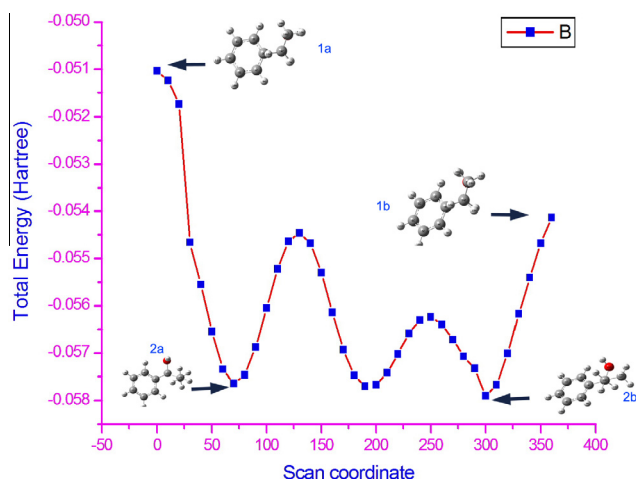


Fig. 1. Conformational analysis.

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