Visualizing Non−Covalent interactions between Propylamine and 2-Chlorobenzyl alcohol in Benzene: Theoretical and Dielectric relaxation studies

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Abstract. The non−covalent interactions of propylamine (pa) with 2-chlorobenzyl alcohol (2cbOH) in benzene have been studied by theoretical and dielectric relaxation studies. In the theoretical method, the optimized structure of pa2cbOH is achieved by the DFT method in B3LYP/6-311++G (d,p) basis set at ground level d,p orbitals. The Vibrational energy distribution analysis is adopted to find the vibrational assignment of pa2cbOH, as well as it compared with the experimental observations. Stability, electronic effects are determined through the chemical reactivity parameters with the help of FMO analysis. The hydrogen bonding and Vander Waals interactions of pa2cbOH are confirmed with reduced density gradient (RDG) isosurface. In Dielectric relaxation analysis, various dielectric parameters like $\varepsilon'$, $\varepsilon''$, $\varepsilon_0$ and $\varepsilon_\infty$ were determined for five different mole ratios of pa2cbOH. Higasi’s single frequency equation and Gopalakrishna’s single frequency concentration variation methods are validated by measuring the multiple relaxation time $\tau_1$ and relaxation time $\tau_2$ for group rotation of pa2cbOH. The strength of hydrogen bonding and other weak interactions were determined using the values $\tau_1$ and $\tau_2$.

1. Introduction

Studying molecular interactions or non−covalent interactions (NCI) are important in the field of protein folding, drug delivery, biology and materials science [1−3]. NCI’s are involved in more dispersed variations of electromagnetic interactions between molecules or within the molecule in the form of inter or intramolecular interactions [4]. It is the governing force determining the conformational determinations of single molecules and the preferred binding sites for molecular clusters [5]. Among many forms of NCI, this study made an attempt of studying molecular association in the form of hydrogen bonding between propyl amine (pa) and 2−chlorobenzyl alcohol (2cbOH) in non−polar solvent benzene. Both propyl amine (pa) and 2−chlorobenzyl alcohol (2cbOH) are profoundly effective chemicals; Propylamine in the mixture has an assortment of applications, particularly it is in treating depressions/anti-depressant, dysthymic disorder, panic attack [6]. Also, it is utilized as an intermediate or finishing mediator in drugs, paints, synthetic rubbers, resin, fibre, and
fabric materials [7]. And 2-chlorobenzyl alcohol is a probable intermediate in metabolic activities [8-11]. The title molecule pa2cbOH has theoretically simulated, and its molecular geometrical factors, non–covalent bond length, and bond angles have been attained using B3LYP/6-311++/G(d,p). VEDA 4 program [12] has been used to determine the vibrational assignments using PED. The Reduced density gradient analysis confirmed the presence of hydrogen bonding and other weak integrations in pa2cbOH.

2. Materials
The AR graded propylamine is purchased from Merck chemicals Pvt. Ltd with assay ≥99.0% (GC) and 2-chlorobenzyl alcohol is obtained from Avra synthesis Pvt. Ltd with assay 99%. The purchased chemicals are in the good assay; hence it is used directly for the studies without any purification.

3. Methods
There are two methods adopted to visualize non–covalent interactions between propylamine and 2-chlorobenzyl alcohol in benzene; they are (i) theoretical studies and (ii) dielectric relaxation studies. The methods are described below in detail.

3.1. Theoretical studies:
Theoretical studies of propylamine with 2-chlorobenzyl alcohol (pa2cbOH) are simulated using Gaussian 09W [13] software. The optimized structure of pa2cbOH is acquired at the basic set B3LYP/6-311++ G (d,p) in the ground state (G) with d, p orbitals. The vibrational assignments of pa2cboH are obtained by utilizing the VEDA-4 program; also the vibrational assignments are correlated along the experimental observations. The experimental FTIR spectrum of pa2cbOH is recorded using a Perkin Elmer system at 4×10⁻² m⁻¹ resolution with a scanning speed of 10×10⁻² m⁻¹. The relative stabilization of the active site of the title molecule is influenced by steric and electronic effects [14], they are predicted theoretically with the help of Global chemical reactivity descriptors (GCRD) obtained from the LUMO and HOMO. Besides, theoretically reduced density gradient (RDG) analysis is adopted to investigate the possibilities of non–covalent interactions in pa2cbOH.

3.2. Dielectric relaxation studies
Various dielectric relaxation parameters such as static dielectric constants (ε₀) are measured using a Dipole meter at room temperature by heterodyne beat method. The Abbe’s refractrometer is used to measure refractive index. The values of dielectric constant (ε′) and dielectric loss (ε″) were obtained at 9.43 GHz in X-band microwave frequency. Using the measured dielectric values, relaxation time (τ₁)-average, dielectric relaxation time (τ₂)-overall, relaxation time (τ₀)-mean and the energy parameters such as molar free energy of activation for viscous flow (Δfₚ) and the molar free energy of dielectric relaxation (Δfᵣ) of propylamine with 2-chlorobenzyl alcohol has been calculated over five different molar ratios (i.e.,1:3, 1:2, 1:1, 2:1 and 3:1) at room temperature. Oswald’s viscometer is used to measure the viscosities of pa2cbOH at room temperature. Propylamine and 2-chlorobenzyl alcohol were separately dissolved in benzene at the molar concentration (0.3mol/L). The dissolved solutions were mixed in five mole ratios at continual measurements. The maximal deviation of dielectric constant occurred at the equimolar ratio of the solutes in all the systems, it is apparent that the disparity is owing to the association of 1:1 complexes.

4. Results and Discussion
4.1. Theoretical studies
In this study, theoretical studies are focused to predict the non–covalent interactions between propylamine and 2-chlorobenzyl alcohol via geometrical parameters, vibrational assignments, FMO, GCRD, and RDG analysis.

4.1.1. Optimized structure.
The molecular structure of propylamine with 2-chlorobenzyl alcohol was combinedly drawn using Chem. Office software (2004) [15] and named as pa2cbOH which is displayed in figure 1 [1]. The molecular structure pa2cbOH is optimized using DFT/B3LYP at 6-311++ basic set in the ground state G with d, p orbitals [16]. In the optimized structure, atoms were named and numbered. The theoretically obtained values of the geometrical parameters (optimized), bond length and bond angles are given in Table 1. The molecule pa2cbOH has sixteen C-H bond lengths, nine C-C bond lengths, one C-O, C-Cl & C-N bond length, and two N-H bond lengths. The maximal value of the bond length found for C₁₈-H₂₂ is 1.6854Å and the bond angle H₁₆-N₁₇-C₁₈ is 140.4395°. Especially bonding between H₁₆ and N₁₇ is referred to as hydrogen bonding, length of hydrogen bond is 1.5 Å [17].

![Optimized molecular geometry of propylamine and 2-chlorobenzyl alcohol (pa2cbOH) with numbered atoms.](image)

Table 1 Bond lengths and bond angles of optimized pa2cbOH in DFT/B3LYP/6-311++/G(d,p)

| Atoms          | Bond length (Å) | Atoms          | Bond angle (degree) |
|----------------|-----------------|----------------|---------------------|
| C₁–C₂          | 1.54            | C₂–Cl₉–O₈      | 109.4718            |
| C₁–O₈          | 1.43            | C₂–Cl₉–H₁₀     | 109.4726            |
| C₁–H₁₀         | 1.07            | C₂–Cl₉–H₁₁     | 109.4697            |
| C₁–H₁₁         | 1.07            | O₈–Cl₉–H₁₀     | 109.4717            |
| C₂–C₃          | 1.3552          | O₈–Cl₉–H₁₁     | 109.4704            |
| C₂–C₇          | 1.54            | H₁₀–Cl₉–H₁₁    | 109.4711            |
| C₃–C₄          | 1.54            | C₁–C₂–C₃       | 120.0034            |
| C₃–Cl₉         | 1.76            | C₁–C₂–C₇       | 119.9967            |
| C₄–C₅          | 1.3552          | C₃–C₂–C₇       | 119.9999            |
| C₄–H₁₂         | 1.07            | C₂–C₃–C₄       | 119.9993            |
| C₅–C₆          | 1.54            | C₂–C₃–Cl₉      | 120.0004            |
4.1.2. FTIR analysis.

The FTIR spectrum of pa2cbO at 1:1 mole ratio has recorded in the range of 4000–400 cm$^{-1}$. The characteristic region of the methyl group; such as $\gamma_s$ (–CH$_3$) and $\gamma_a$ (–CH$_3$) are in 2880-2860 cm$^{-1}$ and 2970–2950 cm$^{-1}$ respectively. For the title molecule, the peaks 2861.26 and 2912.28 are assigned to $\gamma_s$ (–CH$_3$) and $\gamma_a$ (–CH$_3$) respectively. The $\gamma_a$ (–CH$_3$) frequency is theoretically calculated at 2967.86 cm$^{-1}$. The peaks at 1363.75 cm$^{-1}$ and 1472.37 cm$^{-1}$ are designated to CH$_3$ in–plane & out of plane.
bending respectively. The methylene group vibrations such as $\gamma(-CH_2)$ and $\gamma_{as}(-CH_2)$ vibrations of molecules occur in 1470, 1430 cm$^{-1}$, and 2843–2863 cm$^{-1}$ respectively, the peak 2718.18 cm$^{-1}$ is assigned to $\gamma(-CH_2)$. The $(-CH_2)$ out of plane bending is theoretically observed at 963.88 cm$^{-1}$. The values of methyl and methylene vibrations are in agreement with the literature [21–23]. Usually determining $\gamma_{s}C-N$ frequency is a little arduous due to the complicated region [22, 24], for pa2cbOH, the $\gamma_{s}(C-N)$ was observed at 1243.33 cm$^{-1}$. The peaks 1060.02 cm$^{-1}$ and 1033.67 cm$^{-1}$ are assigned to C–C–C bending vibrations its corresponding theoretical peak was observed at 1050.99. The aromatic ring (C=C–C) stretching vibration causally lie in the region 1450–1615 cm$^{-1}$. For the title molecule, it is observed at 1634.47 cm$^{-1}$ and its congruent theoretical frequency is at 1502.33 cm$^{-1}$. The characteristic region of Ar $\gamma_{s}(C-H)$ is 3130–3070 cm$^{-1}$, it is observed experimentally at 3077.02 cm$^{-1}$ and its congruent theoretical peak is identified at 3082.11 cm$^{-1}$, the values are in agreement with the literature [21–22]. The characteristic region of Ar(C–H) in-plane & out of plane bending is in the region 1225–950 cm$^{-1}$ and 900–670 cm$^{-1}$ respectively. For pa2cbOH, peaks at (1125.19, 940.04, and 937.06 cm$^{-1}$) and 859.99 cm$^{-1}$ are assigned at Ar (C–H) in-plane and out of plane bending respectively. The values are in agreement with the literature [25]. The C–O–H stretching & bending frequencies are observed at (2718.18, 2657.76 cm$^{-1}$) and 1440.82 cm$^{-1}$ respectively. The calculated $\gamma_s$ C–O–H frequency is at 3034.35 cm$^{-1}$, it is slightly deviated to the upper region, due to the presence of halogen (heavy) atom [26]. The stretching frequency of C–Cl is observed at 802 cm$^{-1}$, 746.66 cm$^{-1}$ its corresponding calculated peak is at 817.78 cm$^{-1}$. The $\gamma_{s}$(C=O) observed at 1787.96 cm$^{-1}$. The $\gamma_{s}$(–NH$_2$) frequency appeared at 3217.81 cm$^{-1}$. The NH$_2$ scissoring frequency appeared at 1564.70 cm$^{-1}$ and its corresponding theoretical frequency calculated at 1655.81 cm$^{-1}$. The NH$_2$ wagging band was observed at 695.95 cm$^{-1}$ and 647.78 cm$^{-1}$, it corresponding theoretical frequency calculated at 761.97 cm$^{-1}$. The characteristic region of O–H stretching frequency is 3550–3200 cm$^{-1}$, is it observed at 3305.02 cm$^{-1}$, and its theoretically calculated peaks are at 3400.81 cm$^{-1}$ and 3554.7 cm$^{-1}$. The peak of NH$_2$ is slightly deviated and merged with O–H vibrations, which indicates the scissoring and wagging have slightly deviated. This deviation is due to the formation of hydrogen bonding between NH$_2$ of propylamine and O–H of 2–chlorobenzyl alcohol. The length of the hydrogen bond is 1.5Å [17], which is obtained theoretically at B3LYP/ 6.311++/G(d,p).

![Fig.2. Experimental and theoretical FTIR spectrum of pa2cbOH](image)

4.1.3. FMO and GCRD analysis.
The chemical stability of molecules can be recognized with the help of the HOMO and LUMO [11]. Electron donating capability was represented by HOMO whereas electron-accepting capability was represented by LUMO [27]. The energy gap amid HOMO LUMO of organic molecules is appreciably implying the possibility of charge transfer. In general, the lowest energy electronic excitation is achievable in a molecule. If the energy gap is large, electron excitation required high energy [28] though the excitation energies for an electron decrease when the gap decreases. The HOMO and LUMO energies are theoretically calculated by the adopted level and it is displayed in Fig. 3. In the 1950’s Kenichi Fukui developed the frontier molecular orbital (FMO) theory, which focused on HOMO and LUMO [29].

![Energy diagram of pa2cbOH](image)

**Table 2** The FMO and GCRD values and GCRD of pa2cbOH.

| Energy values (eV) | HOMO       | LUMO       | \( \Delta E_{\text{HOMO-LUMO}} \) |
|------------------|------------|------------|-------------------------------|
|                  | \(-6.8543\) | \(-0.8236\) | \(6.0307\)                   |
| Ionization potential (I) | 6.8543     |            |                               |
| Electron affinity (A)          | 0.8236     |            |                               |
| Chemical potential (\(\mu\))   | \(-3.0154\) |            |                               |
| Electron negativity (\(\chi\)) | 3.8389     |            |                               |
| Absolute hardness (\(\eta\))   | 3.0154     |            |                               |
| Softness (S)                 | 0.3316     |            |                               |
| Net electrophilicity (\(\Delta \omega \pm\)) | 5.6413   |            |                               |
| Electrophilicity index (\(\omega\)) | 1.5076     |            |                               |

Electrical properties are used to investigate by utilizing frontier molecular orbitals [FMO]. Chemcraft 1.7 software [30] was utilized to draw HOMO and LUMO energy diagram. The most elevated occupied molecular orbitals of donating the electron and lowest occupied molecular orbital accept the electron. The HOMO energy values are electron \(E_{\text{HOMO}} = -6.8543\) eV and LUMO energy values are \(E_{\text{LUMO}} = -0.8236\) eV. The total energy difference value is \(E = 6.0439\) eV. The blue colour pointed to the positive stage and the red colour pointed to the negative stage [31]. The ionization potential (I), electron affinity (A), electron negativity (\(\chi\)), chemical potential (\(\mu\)), hardness (\(\eta\)), softness (S), electrophilicity index (\(\omega\)), the values are calculated using the literature [32-35] and listed table 2.

4.1.4. Reduced density gradient

Usually, the non-covalent interactions in a system of molecules can be studied through the isosurfaces of Reduced Density Gradient (RDG) [36]. For pa2cbOH, the interactions are found to be weak, which are obtained by frequency calculations. Isosurface of the optimized geometry of 1:1 complexed title molecule has been computed by giving 0.5 isovalue as an input of Multiwfn program [37]. Figure 3 (a) visualizes colour gradient of different interactions; it is obtained using Chemcraft software [38]. Fig.4 (a) clearly illustrated the various types of the interactions and the colour gradient to stand for \(\rho (r)\) and \(\lambda_2\) value and filled in the isosurface (RDG) it clearly described the types of the interactions. The interactions of pa2cbOH are graphically represented in the isosurface through three different colour schemes; red corresponds to steric effects, blue corresponds to hydrogen bonding interactions and green corresponds to van der Waals effects [39]. For pa2cbOH, the contact (propylamine) \(\text{H}_2\text{N} \cdots \text{H-}\)
O (2-chlorobenzyl alcohol) exists and appears in blue colour in Fig. 4(a), it indicates the hydrogen bonding interactions. The region in green colour suggesting the existence of weak (propylamine) \( H_2N \cdots Cl \) (2-chlorobenzyl alcohol) interactions due to Vander Waals effects. The Green and red patches between Cl and C=H of 2-chlorobenzyl alcohol represent the Vander Waals and very week repulsive steric interactions. [40]

![Fig. 4.](image)

**Fig.4.** For pa2cbOH, (a) Colour gradient representation of different interactions (b) graphical representation of RDG vs. the electron density multiplied by the 2nd largest eigenvalue of Hessian matrix

4.2. Dielectric relaxation studies

The present study is an attempt to find non-covalent interactions between propylamine and 2-chlorobenzyl alcohol in benzene. This study is based on the Higasi method [41] to validate the single frequency equation proposed by Debye. The Debye equation defining slopes \( a' \) and \( a'' \) to determine the average relaxation time (\( \tau_1 \)), overall relaxation time (\( \tau_2 \)), and geometric meantime (\( \tau_0 \)). The values of relaxation time (\( \tau \)) for the title molecule has been measured for the five different mole ratio 1:3, 1:2, 1:1, 3:1, 2:1 at room temperature. The value of relaxation time was found maximal at the 1:1 mole ratio. It is because of the H bonding between N atom in the NH\(_2\) group of propylamine and hydroxyl hydrogen of 2-chlorobenzyl alcohol, the formation is like (propylamine) \( H_2N \cdots H-O \) (2-chlorobenzyl alcohol). The hydrogen bond length is 1.5Å [17] (ie., N17…H16), which is theoretically calculated and given in table 1. The increase in relaxation time could be due to raising the effectual size of the molecular rotating unit [41]. The values of relaxation time decreases apparently for other mole ratios. The value of relaxation time at the 1:1 ratio is also determined by the Gopalakrishna method [42], the obtained value is in agreement with Higasi’s method. The value of dipole moment of the title molecule is calculated using Higasi’s and Gopalakrishna’s method for the equal mole ratio and it is given in table 3. The values of \( \Delta f_\eta \) and \( \Delta f_\tau \) are calculated, the value of \( \Delta f_\tau \) was found to be higher than \( \Delta f_\eta \). This is due to the influence of viscous flow. This involves both translational and rotational forms of motion and the values are given in table 4.

| Ratio   | \( W_2 \) | \( \varepsilon_0 \) | \( \varepsilon' \) | \( \varepsilon'' \) | \( \varepsilon_\infty \) | Relaxation Time (in \( 10^{-12} \) s) |
|---------|-----------|-----------------|----------------|----------------|----------------|----------------------------------|
|         |           |                 |                |                |                | Higasi’s Method | Gopalakrishna’s Method |
|         |           |                 |                |                |                | \( \tau_1 \) | \( \tau_2 \) | \( \tau_0 \) | \( \tau \) |
| 1:3     | 0.0240    | 2.8408          | 2.6083         | 0.2632         | 2.1800         | 13.6688           | 14.6828           | 14.1667           |               |
| 1:2     | 0.0261    | 2.8808          | 2.6183         | 0.2816         | 2.1900         | 14.6251           | 15.4938           | 15.0532           |               |
| 1:1     | 0.0303    | 2.9703          | 2.6364         | 0.3020         | 2.2250         | 16.5522           | 18.3767           | 17.4406           | 16.8607         |
| 2:1     | 0.0344    | 2.8719          | 2.6203         | 0.2709         | 2.2290         | 15.9100           | 15.4341           | 15.6702           |               |
| 3:1     | 0.0365    | 2.8363          | 2.6283         | 0.2614         | 2.2180         | 14.3783           | 13.2278           | 13.7911           |               |
Table 4 The values of dipole moment (μ), activation free energies (Δf_θ and Δf_τ) of pa2cbOH in benzene at 1:1 ratio

| Parameter                        | Values  |
|----------------------------------|---------|
| Dipole moment (in D)             |         |
| 1. By Higasi’s Method            | 3.7823  |
| 2. By Gopalakrishna’s Method     | 6.8026  |
| Activation Energy                |         |
| 1. Δf_θ                          | 15.67   |
| 2. Δf_τ                          | 14.17   |

5. Conclusion
In the present work, the non−covalent interactions between propylamine and 2-chlorobenzyl alcohol in benzene have been studied by adopting the DFT method at B3LYP/6-31++G(d,p) basic set as well as dielectric relaxation method. The comprehensive interpretation of the optimized geometrical structure of the title molecule have given the information about the structural parameter such as bond length and bond angle, especially the presence of intermolecular hydrogen bonding between amino and hydroxyl groups was confirmed. The vibrational spectral assignments of pa2cbOH have been carried out using PED analysis. The detailed description of vibrational modes and the presence of intermolecular hydrogen bonding, the experimental and theoretical calculations have been compared. The HOMO-LUMO energy orbitals, global chemical reactivity descriptors, the electrophilic and nucleophilic attack calculated by the reactive site. Through RDG isosurface, the presence of hydrogen bonding and other interactions were determined. The Dielectric relaxation analysis, relaxation time of the pa2cbOH molecule has been calculated using Higasi and Gopalakrishna method, it confirms the complex formation is maximum at 1:1 ratio due to hydrogen bonding between propylamine and 2-chlorobenzyl alcohol.

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