Comparison of theoretical and experimental electronic and optoelectronic properties of HPS compound

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Abstract
We investigated electronic and optoelectronic properties of 1,1,2,3,4,5-Hexaphenyl-1H-silole (HPS) compound for different concentrations and for theoretical (B3LYP and CAM) and experimental methods. Optical parameters such as absorbance band edge, optical band gap and refractive index of the HPS were controlled by concentration. Optical band gap of the HPS decreases from 2.870 to 2.766 eV with increasing concentration. The refractive indices of the HPS were obtained for different concentrations, relations and methods. According to the results obtained, the two theoretical (B3LYP and CAM) results are in harmony with each other, and the experimental and theoretical-B3LYP results are closer to each other. This study contains important and interesting results, especially in terms of comparing the theoretical and experimental electronic and optoelectronic properties of the HPS compound.

1. Introduction

Organic conjugated molecules are becoming increasingly important in applications such as OLED, biosensors, organic field-effect transistors and molecular conductive wires [1–6]. These molecules continue to be of interest to the developing technology due to their optical and electronic properties. For conjugated molecules developed for OLED, good efficiency can be obtained in dilute solutions, but they exhibit poor emission behavior in solid thin films [7, 8]. In 2001, Tang et al. this phenomenon, called aggregation-related emission (AIE), led to a way to achieve high-performance OLEDs [9].

Silole and some of its derivatives have been studied extensively due to their unique electronic properties, high electron attraction, and rapid electron mobility [10, 11]. It also has the lowest empty molecular orbital (LUMO) energy level to the silo which is considered to be the conjugate molecule [12–14]. Silole molecules such as hexapenylsilole (HPS), which exhibit a weak gloss in the solvent but become highly dispersible in their aggregates, have been found to exhibit AIE [15–21]. AIE materials, which are promising for electroluminescence (EL) applications, are used as thin films. The silole molecules studied in this field are 1-methyl-1,2,3,4,5 pentaphenylsilole (MPPS) and 1,1,2,3,4,5-hexapenylsilole (HPS) [18]. By using these materials as fluorescence nuclei a wide variety of functional materials have been developed in fields such as OLEDs, chemosensors, luminescence matrices [22–28].

Considering the different behavior of the 1,1,2,3,4,5-Hexaphenyl-1H-silole (HPS) molecule in the solvent and considering that this molecule can be used as a chemical sensor or optoelectronic material, the optical properties of the molecule should be examined. In this context, the optical and electronic properties of the molecule were analyzed both theoretical and experimental to analyze the behavior of HPS molecule in solvent. First, the most stable structure of the molecule was investigated and it was found to have C2 symmetry without any symmetry challenge. After determining the stable structure of the molecule, the optical parameters were
experimentally found and the optical band gaps were compared with the HOMO–LUMO band intervals calculated theoretically by two different methods. The distance between the HOMO–LUMO energy levels, the total density of state (TDOS or DOS), partial density of state (PDOS) and overlap population density of state (OPDOS or COOP) spectra were calculated to demonstrate the interaction of orbitals between the orbitals, anti-bond and non-bonded orbitals [29–31]. In addition, the non-linear optical properties (NLO) of the HPS molecule were examined and compared with urea as a polar molecule.

2. Experimental details

2.1. Materials
1,1,2,3,4,5-Hexaphenyl-1H-silole (HPS) compound and Dimethylformamide (DMF) solvent were purchased from Sigma-Aldrich. Figures 1(a)–(c) shows the 2D, 3D and crystal structures of the HPS compound.

2.2. The HPS solutions for different concentrations
We regulated the concentrations of the HPS compound as 3.918, 1.385, 0.887, 0.385 and 0.253 mM with an analytical balance (AND-GR-200 Series). These HPS compounds were dissolved in DMF solvent using a digital vortex mixer (Four E’s Scientific CO., Ltd).

2.3. The optical measurements for different concentrations
The optical measurements of the HPS solutions for 3.918, 1.385, 0.887, 0.385 and 0.253 mM were taken using a UV-1800 Spectrophotometer (Shimadzu model) at room temperature.

3. Computational details
HPS molecule have been investigated in terms of optical and electronic properties by DFT/B3LYP method and CAM and 6-311G(d,p) basis set [31–33]. The molecule have been optimized with the same method without any symmetry enforcement. UV–vis and HOMO-LUMO analysis calculations have been also calculated with B3LYP as well as CAM-B3LYP in order to understand the evoked condition analysis. [34, 35]. We have been used GAUSSIAN 09 program package in the calculations [36]. In order to draw DOS diagrams, GaussSum 2.2 program [37] have been used by running log files calculated in GAUSSIAN09 program package. The non-linear optical properties (NLO) of the HPS molecule have been also calculated using DFT/B3LYP method and 6-311G (d,p) basis set.

4. Results and discussion

4.1. Experimental results
Absorbance spectra of the HPS compound for 3.918, 1.385, 0.887, 0.385 and 0.253 mM were recorded and depicted in figure 2. Absorbance spectra of the HPS are not exactly observed at higher concentration (>0.887 mM) and decrease with decreasing concentration. We can say this by looking at the observed curve of the whole peak. Looking at the fully observed spectra of curves, we can say that the maximum peak at 250 nm and another peak at 366 nm are observed. This result indicates that the absorbance spectra of the HPS compound are dominant in the near ultraviolet region and remain at the lowest level in the spectral regions at higher wavelengths.

Transmittance (T) spectrum of a material is also a characteristic feature and it is very important in the investigation of optical properties [38, 39]. The transmittance spectra of the HPS for 3.918, 1.385, 0.887, 0.385 and 0.253 mM is shown in figure 3(a). The transmittance of the HPS for 1.385, 0.887, 0.385 and 0.253 mM increases very sharply in the range of about 370–430 nm with increasing wavelength, while the transmittance of the HPS for 3.918 mM increases very sharply in the range of 400–450 nm. As seen in figure 3(a), a similar sharp increase behavior is observed at wavelengths less than 320 nm.

Important properties of the absorption behavior of a material are investigated by the absorbance band edge (E_{Abs-be}). We obtained the E_{Abs-be} values of the HPS for 3.918, 1.385, 0.887, 0.385 and 0.253 mM from dT/dλ curves versus wavelength (λ) as seen in figure 3(b). Obtained E_{Abs-be} values of the HPS for various concentrations are given in table 1. Absorbance band edge of the HPS varies from 2.725 to 2.825 eV with decreasing concentration. This result shows that the HPS material has a much lower optical band gaps (E_g) than insulators and can be used in semiconductor technology. For this, we investigated the optical band gaps of the HPS for 3.918, 1.385, 0.887, 0.385 and 0.253 mM using the Tauc relation [38, 40].
where $h\nu$ is the photon energy, $A$ is a constant and $m$ is the parameter measuring type of band gaps. The $E_g$ parameters of the HPS were obtained from the $(\alpha h\nu)^2$ curves versus photon energy ($E$) as seen in figure 4(a). Obtained $E_g$ values of the HPS for various concentrations are given in table 1. Optical band gap of the HPS decreases from 2.870 to 2.766 eV with increasing concentration. As seen in figure 4(b), these optical band gaps are close to the absorbance band edge values and are compatible with each other. The obtained $E_g$ values show that the HPS material exhibits semiconductor properties. All these results indicate that the HPS material can be used in electronic and optoelectronic applications.

One of the most important parameters in optical and optoelectronic technology applications is the refractive index ($n$) [39, 41]. To obtain the refractive indices, here are various relations such as Moss, Ravindra, Herve-Vandamme, Reddy and Kumar-Singh. Equations of related approaches are as follows, respectively [42, 43]:

$$(\alpha h\nu) = A(h\nu - E_g)^m$$  \hspace{1cm} (1)
Moss relation is given by

\[ n^4 = \frac{95 \text{ eV}}{E_g} \]  

(2)

Ravindra relation is given by

\[ n = 4.084 - 0.62E_g \]  

(3)

Herve-Vandamme relation is given by

\[ n^2 = 1 + \left( \frac{A}{E_g + B} \right)^2 \]  

(4)

where A is the hydrogen ionization energy 13.6 eV and B = 3.47 eV is a constant assumed to be the difference between the band gap energy and UV resonance energy.

Reddy relation is given by

\[ n = \left( \frac{154}{E_g - 0.365} \right)^{1/4} \]  

(5)

Kumar-Singh relation is given by

\[ n = \frac{3.3668}{(E_g)^{0.32234}} \]  

(6)

For these relations, we calculated refractive indices of the HPS for 3.918, 1.385, 0.887, 0.385 and 0.253 mM. These obtained refractive index values were reflected in figure 5. The refractive index of the HPS varies from 2.305 to 2.830 with various relations and the average n value varies from 2.453 to 2.489 with increasing concentration. These refractive indices are in the range of semiconductor materials.

4.2. Comparison of theoretical and experimental optical results

In this section, we compared optical parameters with theoretical (B3LYP and CAM) and experimental methods. Using the obtained theoretical and experimental optical results, we found the \( E_g \) optical band gaps of the HPS for theoretical and experimental methods from the \((\alpha h \delta)^2\) curves versus \( E \) as seen in figure 6. Obtained \( E_g \) values of the HPS for experimental, theoretical-B3LYP and theoretical-CAM were found to be 2.829, 3.020 and 3.044 eV, respectively. As can be seen, the theoretical optical band gaps are greater than the value of the experimental optical band gap. While the theoretical optical band gaps are closer to each other, the theoretical-B3LYP optical
band gap is close to the experimental optical band gap. The theoretical results also show that the HPS material has an optical band gap of a semiconductor material.

Similarly, we calculated the refractive indexes of the HPS material from different relations [42, 43] using the above experimental and theoretical (B3LYP and CAM) optical band gaps obtained. Figure 7 shows the curves of the refractive indices. The refractive index of the HPS varies from 2.197 to 2.812 with various relations and methods. The theoretical refractive indices are lower than the experimental refractive indices. The average refractive index varies from 2.396 to 2.467 for various relations and methods.

Figure 3. The (a) transmittance spectra and (b) dT/dλ curves versus wavelength (λ) of the HPS for 3.918, 1.385, 0.887, 0.385 and 0.253 mM.
Table 1. The absorption band edge (Ε_{Abs-be}) and optical band gap (Ε_g) parameters of the HPS for various concentrations.

| Concentration (mM) | Ε_{Abs-be (eV)} | Ε_g (eV) |
|--------------------|----------------|----------|
| 3.918              | 2.725          | 2.766    |
| 1.385              | 2.762          | 2.810    |
| 0.887              | 2.774          | 2.829    |
| 0.385              | 2.799          | 2.847    |
| 0.253              | 2.825          | 2.870    |

Figure 4. The (a) (αhν)^2 curves versus photon energy (E) and (b) comparison optical band gaps - absorbance band edges of the HPS for 3.918, 1.385, 0.887, 0.385 and 0.253 mM.
4.3. Frontier molecular orbitals and density of states (DOS) analysis

Frontier molecular orbitals consist of the lowest empty molecular orbital LUMO (conductivity band) and the highest filled orbital HOMO (valence band). The transition between these two orbital provides important information about charge transfer within the molecule [44, 45]. In order to observe the charge transfer in the
HPS molecule, we give the most important transition HOMO-LUMO transition in figure 8. As shown in figure 8, the HOMO orbitals are localized in the central ring, in the phenyl rings named Ring 1 and Ring 4, and the LUMO orbitals are localized in the entire molecule except the rings designated Rings 5. In this figure, the red colors indicate the positive phase and the green colors indicate the negative phase. The transition between HOMO-LUMO energy levels was calculated as 3.65 eV by TD-DFT/B3LYP method and as 6.14 eV in TD-DFT/CAM-B3LYP method for DMF solvent. In gas phase, these values were calculated as 3.64 eV are given in figure 8. The Eg value measured experimentally was found as 2.83 eV in DMF solvent. These results show that the B3LYP method gives more consistent results than the CAM method.

Investigation of the interaction of HOMO-LUMO orbitals in neighboring orbitals can be a true definition [46]. Therefore, Total Density of State (TDOS), Partial Density of State (PDOS), Overlap Population Density of States (OPDOS) functions and orbital information were plotted using the GaussSum 2.2 program [37]. In the B3LYP and CAM method, the HOMO-LUMO energy band gap calculated in DMF solvents was combined with the Eg values and TDOS diagram to form figure 9. According to this diagram, the B3LYP method are better suited to the experiment and the symmetrical appearance of HOMO and LUMO orbitals is noteworthy. In the figure 10 (PDOS) Ring 1-5 and silole, the so-called ring density and orbital data of the rings (HOMO-LUMO) contributions are seen. According to this graph, the contribution of silole ring is the highest in all orbitals. It is seen from figure 8 that 2 phenyl rings bound to the silicon atom named Rings 5 do not contribute to the HOMO orbital and this confirms the HOMO-LUMO energy diagram. Positive, negative, and zero values in the OPDOS diagram indicate interactions with bonding, anti-bonding, and non-bonding, respectively [47] figure 11 denote some of orbitals energy values of the interactions among the selected groups. According to figure 11, Ring1 → silole (pink line), Ring5 ↔ silole (turquoise line) system is negative, that is anti-bonding character.

4.4. NLO (non-linear optical) properties and dipole moment analysis
The nonlinear optical properties of molecules show that they can be used in areas such as optical switching, data discovery, signal processing [48, 49]. The values such as polarizability and hyperpolarizability found in the theoretical study of molecules have an important place in terms of providing information about nonlinear linear optical properties. We obtained the polarizability (α), anisotropy of polarizability (Δα) and first hyperpolarizability (β) values for the HPS molecule from the output file calculated by the B3LYP method by the following equations.

\[
\alpha = 1/3(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})
\]

\[
\Delta \alpha = 1/2((\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{xx} - \alpha_{zz})^2 + (\alpha_{yy} - \alpha_{zz})^2)
\]

\[
\beta = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]
\]

While obtaining these values, atomic units were converted to electronic units and listed in table 2. The data obtained were compared with urea, a polarized molecule and found to be 100 times more polarized than urea (β\text{tot} = 194.7 \times 10^{-33} \text{esu} and Δ\alpha = 3.8312 \times 10^{-24} \text{esu}). According to these results, the HPS molecule can be...
used as a good NLO material. However, the molecule has a homogeneous charge distribution and does not have a large dipole moment. The calculated total dipole moment is 0.0184 Debye and the additive is only due to the $\mu_z$ component. The value of $\mu_x$ and $\mu_y$ components is zero. The dipole moment of the HPS molecule is very small compared to urea. This is due to the high symmetry ($C_2$) of this molecule.

4.5. Mulliken atomic charges analysis
Mulliken populations yield is one of the simplest pictures of charge distribution. In this work, charge distributions of HPS material were computed with B3LYP/6-311G(d,p) method and shown in figure 12. The Si5 atom of the silole ring has the highest positive charge (1.335e), C1 and C4 atoms (−0.365e) have the highest negative charge when compared to other carbon atoms of silole ring. When the whole molecule is examined, it is
seen that H atoms have positive and 0.10e charge and carbon atoms (61 C and 50 C) in phenyl rings (Rings 5) connected to 5Si atom have the most negative charge in the molecule (−0.376e). This may be due to Si-C intermolecular interactions.

Figure 10. The partial electronic density of states (PDOS) diagram of the HPS material.

Figure 11. The overlap population electronic density of states (OPDOS) diagram of the HPS material.
5. Conclusion

Effects on electronic and optoelectronic properties of the HPS compound of different concentrations and theoretical (B3LYP and CAM) and experimental methods were investigated in detail. Absorbance band edge of the HPS varies from 2.725 to 2.825 eV with decreasing concentration, while optical band gap of the HPS decreases from 2.870 to 2.766 eV with increasing concentration. The theoretical optical band gaps are greater than the experimental ones.

Table 2. The dipole moments $\mu$ (D), the polarizability $\alpha$ (a.u.), the average polarizability $\alpha_o (\times 10^{-24}$ esu), the anisotropy of the polarizability $\Delta\alpha (\times 10^{-24}$ esu), and the first hyperpolarizability $\beta (\times 10^{-33}$ esu) of HPS.

| Concentration (mM) | $\mu_{\text{Abs-be}}$ (eV) | $E_g$ (eV) |
|-------------------|------------------|----------|
| $\mu_x$           | 0                | $\beta_{xxx}$ 0.0000 |
| $\mu_y$           | 0                | $\beta_{xyy}$ 0.0000 |
| $\mu_z$           | 0.0184           | $\beta_{yy}$ 0.0000 |
| $\mu_0$           | 0.0184           | $\beta_{yy}$ 0.0000 |
| $\alpha_{xx}$     | 58.7763          | $\beta_{xx}$ $-541.0963$ |
| $\alpha_{xy}$     | $-0.2891$        | $\beta_{xy}$ $631.2229$ |
| $\alpha_{yy}$     | $-0.2891$        | $\beta_{yy}$ $631.2229$ |
| $\alpha_{yz}$     | 73.2181          | $\beta_{yz}$ $-1638.7428$ |
| $\alpha_{xz}$     | 0                | $\beta_{xz}$ 0.0000 |
| $\alpha_{yz}$     | 0                | $\beta_{yz}$ 0.0000 |
| $\alpha_{xx}$     | 76.4401          | $\beta_{xx}$ $3858.8838$ |
| $\alpha_{total}$  | 69.4782          | $\beta_{zz}$ $2460.0517$ |
| $\Delta\alpha$    | 103.0992         | $\beta_1$ 0.0000 |
|                   |                  | $\beta_2$ 0.0000 |
|                   |                  | $\beta$ $1679.0447$ |

Figure 12. The Mulliken charge distribution for HPS material.
than the value of the experimental optical band gap. The theoretical refractive indices are lower than the experimental refractive indices. The HPS material exhibits semiconductor properties and can be used in electronic and optoelectronic applications.

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