International Research Journal on Advanced Engineering and Management
https://goldncloudpublications.com
https://doi.org/10.47392/IRJAEM.2025.043
e ISSN: 2584-2854
Volume: 03
Issue:02 February 2025
Page No: 270-273

UV-Visible Spectra, HOMO-LUMO Studies on Indole Derivative CBTC Using Gaussian Software

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Abstract
In the present work, spectral and structural properties of indole derivative, 3-chloro-N1-(diethylamino) benzylidene) benzo[-b] thiophene-2-carbohydrazide -(CBTC) is carried out. Semiempirical method and PM6 basis set have been used to study optimized geometry. The UV-Visible spectra in Methanol was obtained using TD-DFT method at 6-31+G (d, p) basis set. The parameters such as wavelength, oscillator strength, and excited state energies have been obtained from UV-Visible spectra. The ground state dipole moment was found to be 5.095 Debye. The HOMO-LUMO energy gap is found to be -0.031 eV and chemical hardness is found to be 0.016 eV.

Keywords: *Indole Derivative, UV-Visible Spectra, TD-DFT, HOMO, LUMO*

1. Introduction
Indole is also known as benzo pyrrole which contains the benzenoid nucleus and has 10 π- electrons (two from Ione pair on nitrogen and double bonds provide eight electrons) which makes them aromatic in nature. Like the benzene ring, electrophilic substitution occurs readily on indole due to excessive π-electrons delocalization. Indole is an important heterocyclic system that provides the indole skeleton occurs in a variety of natural products, predominantly in alkaloids, and is seldom used for the plan of many synthetic compounds with powerful pharmacological activities [1]. In addition, indole is a privileged scaffold in drug discovery programs and their associated biological activities are very much cited in the literature [2]. Gaussian 16 offers new methods and capabilities which allow one to study ever larger molecular systems. Gauss View 6 offers a rich set of building and visualization capabilities. The Gaussian program can also be used to calculate the ground-state dipole moments. Gaussian predicts numerous molecular properties derived from basic computation methods [3]. In this present work, UV-Vis spectra have been obtained using TD-DFT with 6-31+G (d, p) basis set in Methanol. The UV-Vis spectra has also been studied in Butanol, DMSO, and DMF solvents. The HOMO (highly occupied molecular orbital) and LUMO (lower unoccupied molecular orbital) structure has been studied in the gas and liquid phase.

2. Computational Methods
Gaussian 16 program has been used for geometry optimization from the Semiempirical method at PM6 (Parameterization Method 6) basis set. UV-Vis Spectra analyzed using TD-DFT (Time- Dependent Density Functional Theory). Effect of solvent in TD-DFT analyzed using IEFPCM (Integral Equation Formalism Polarizable Continuum Model). Theoretical calculations of HOMO and LUMO structures were drawn from optimized geometry. The HOMO and LUMO surfaces also have been drawn for molecule in the water [4].

Table 1 The Wavelengths Obtained from UV-VIS Spectra

Solvents	Wavelengths (nm)		
	1	*2*	*3*
Ethanol	415.12	316.27	310.02
Methanol	415.89	316.63	310.23
Acetone	414.44	315.96	309.83
Water	417.35	317.31	310.62

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Table 2 Oscillator Strengths Obtained from UV-VIS Spectra

Solvents	Oscillator Strength		
	1	*2*	*3*
Ethanol	0.0815	0.5101	0.1203
Methanol	0.0818	0.5098	0.1232
Acetone	0.0813	0.5103	0.1178
Water	0.0822	0.5091	0.1290

Table 3 Excited State Energies Obtained from UV-VIS Spectra

Solvents	Excited state energies (eV)		
	1	*2*	*3*
Ethanol	2.9867	3.9202	3.9931
Methanol	2.9812	3.9158	3.9966
Acetone	2.9916	3.9241	4.0016
Water	3.0387	3.2782	3.9242

Table 4 HOMO-LUMO Energies and Chemical Hardness

Parameters	Energy (eV) and chemical hardness	
	Gas phase	Water
HOMO	-0.11625	-0.18931
LUMO	-0.08518	-0.06458
Gap	-0.03107	-0.12472
Chemical Hardness	-0.015535	-0.06236

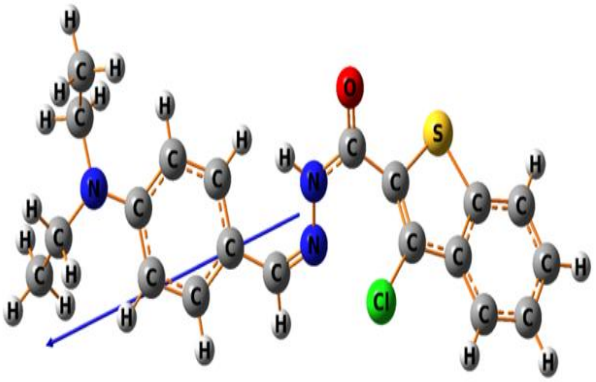

Figure 1 Molecular structure of CBTC

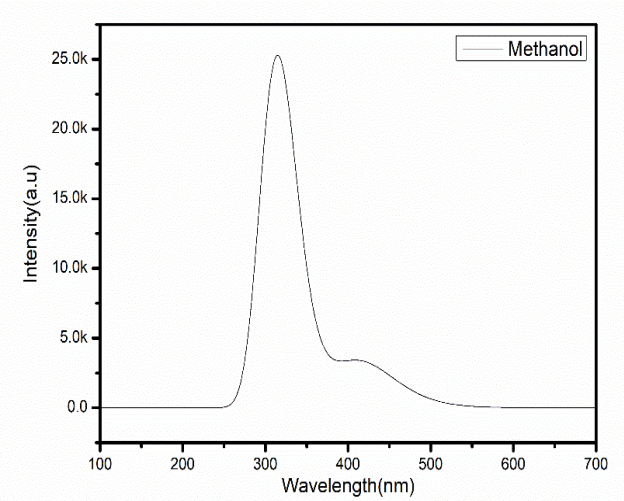

Figure 2 UV-Visible spectra of CBTC in Methanol

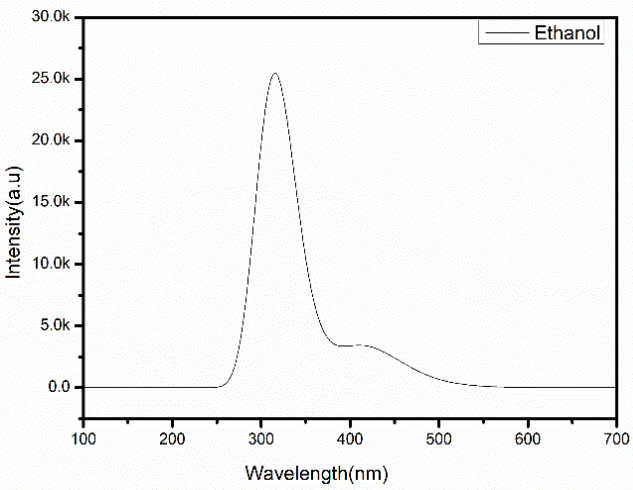

Figure 3 UV-Visible spectra of CBTC in Ethanol

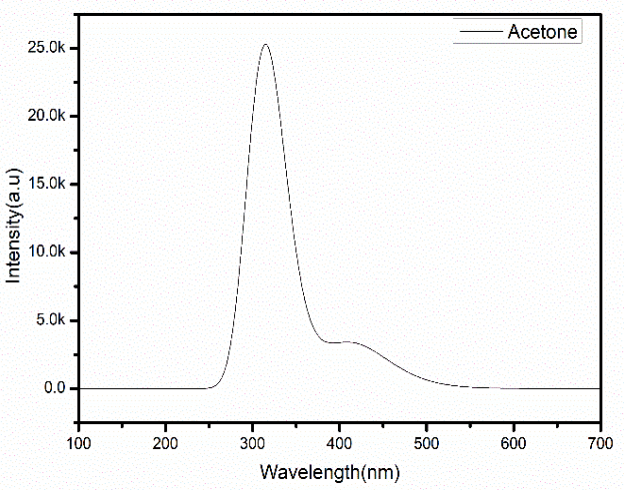

Figure 4 UV-Visible spectra of CBTC in Acetone

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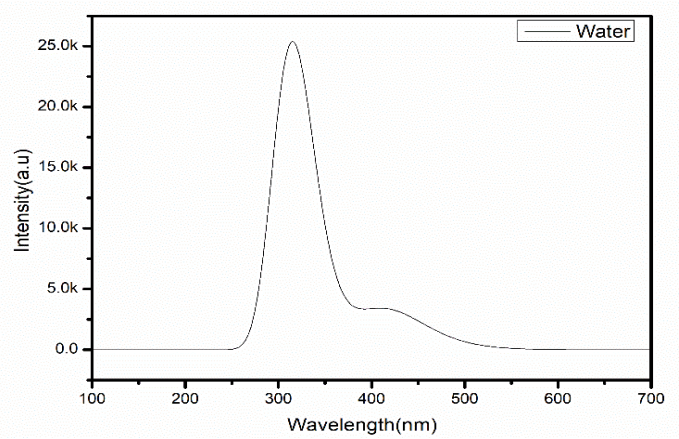

Figure 5 UV-Visible Spectra of CBTC in Water

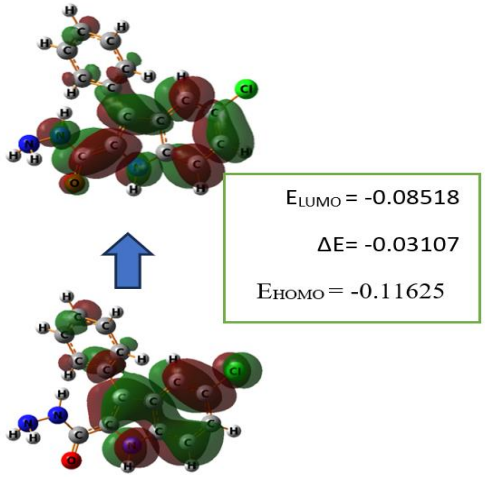

Figure 6 3D Plots of HOMO-LUMO Maps in the Gas Phase.

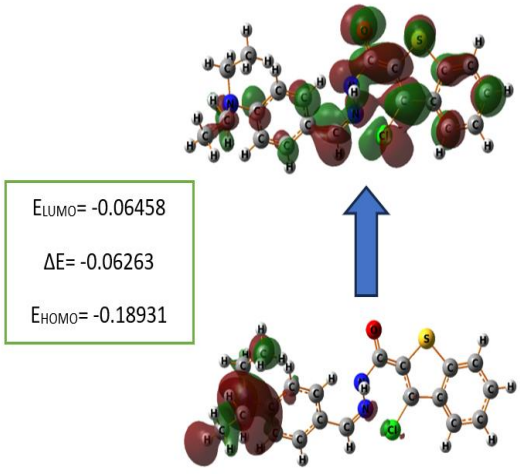

Figure 7 3D Plots of HOMO-LUMO Maps in Water

3. Results and Discussion

3.1. Results

The newly synthesized indole derivative CBTC has been optimized using Semiempirical method at PM6 basis set. The ground state dipole moment of CBTC is 5.095 D for optimized geometry. The optimized geometry has been used to study UV-Visible spectra and HOMO-LUMO surfaces, Shown in Figure 1, Figure 2, Figure 3, Figure 4, Figure 5, Figure 6 & Figure 7.

3.2. Discussion

3.2.1. UV-Visible Spectra

The UV-Vis spectra of CBTC obtained using TD-DFT method in Methanol at 6-31+G (d, p) basis set is as shown in Fig 2. The wavelength, oscillator strength, and excited state energies is as shown in Table 1, 2, and 3 for Methanol, Ethanol, Acetone, and Water. The TD-DFT method was carried out at B3LYP/6-31+G (d, p) basis set. The numbers 1, 2, and 3 corresponds to three excited states of molecule in the respective solvents. The IEFPCM model was used to study the effect of solvents. The absorption maxima occurs for Methanol, Ethanol, Acetone and Water solvents respectively at 415.12 nm, 415.89 nm, 414.44 nm and 417.35 nm. The corresponding oscillator strength and excited-state energies are given in Table 1, 2, and 3 & 4. The wavelength, oscillator strengths, and excited state energies for the second and third states are small compared to the first excited state. The variation of wavelength with respect to intensity in Methanol, Ethanol, Acetone, and Water shows that the interaction between solute and solvent is almost the same. This means that there is no significant variation in absorption due to the solvent effect [5-10].

3.2.2. HUMO-LUMO Surfaces

Molecular orbital gives the information of molecular arrangement. The HOMO surface denotes electron donor and LUMO acceptor. The chemical reactivity of the molecule is denoted by the energy gap. In basic molecular orbital theory, the HOMO energy was associated with ionization potential Z=EHOMO, and LUMO energy associated with electron affinity E=ELUMO. The chemical hardness of the compound is given by (η)=(Z-E)/2. By using HOMO and LUMO

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energy values, we determined chemical quantities of the compound [11-13].

Conclusion

The Indole compound CBTC has been optimized using the semiempirical method using the PM6 basis set. The UV-Visible spectra were analyzed using the TD-DFT method at the B3LYP/6- 31+G (d, p) basis set in Methanol. A comparative study has been made to analyze UV-Vis spectra in Ethanol, Acetone, and Water solvent. The absorption maxima, oscillator strengths for three excited state energies, have been measured form UV-Vis spectra of the selected molecule in Methanol, Ethanol, Acetone, and Water. The HOMO-LUMO energy gap and chemical hardness have been calculated in the gas phase and Water.

Acknowledgment

Vijayalaxmi mallayya, wish to thank to Director and technical staff of USIC, Gulbarga University, Kalaburagi for facilitating the UV-Visible absorption spec trophotometer.

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