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Electronic spectral study of 2,5-Dimethoxy-4-nitroaniline by Density Functional Theory

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Abstract
In the present work, the ultraviolet spectral study of 2,5-Dimethoxy-4-nitroaniline has been carried out experimentally and theoretically in acetone, ethanol and methanol in the range of 200-500 nm in the solution phase. Predicted electronic absorption spectra from time-dependent density functional theory (TD-DFT) calculation have been analysed and compared with the experimental UV visible spectrum. The effects of amino, methoxy and nitro group substitution in benzene ring have been analysed. The electronic properties such as excitation energy, absorption wavelength $\lambda_{max,}$ oscillator strength (f) and energy of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are calculated by Hartree-Fock (HF) and time-dependent density functional theory (TD-DFT).
Keywords: Ultraviolet spectrum, 2,5-Dimethoxy-4-nitroaniline, HOMO, LUMO, Hartree-Fock, Density functional theory

1. INTRODUCTION

The remarkable use of aniline is, in diazotization reaction, to obtain a lot of numbers of organic compounds. That's why it has very important role in daily life. Aniline is a six-membered homoaromatic simplest amine, containing – NH_2 functional group. Aniline has significant industrial commodity chemicals and also use for fine chemical synthesis. Due to having electron rich benzene ring aniline goes to electrophilic aromatic substitution, but after the formation of diazonium salt through diazotization reaction this diazonium salt goes to a huge number of nucleophile substitution and form a lot number of compounds used in daily life. They have been exclusively used for chemical dyes industries [1] pharmaceutical sector [2] electro optical world [3]. Nonlinear optical molecules are much more interesting because of their wide applications of optical signal processing, data storage and telecommunication, optical computing [4-8]. Antibacterial activity of some half-substituted compounds has been discussed by Vidhya et al [9-11] for treatment of cancer is of great importance. Cancer is curse for society so its study is too much important in field of research. Aniline is also responsible for bladder cancer [12], forest dieback reported in WHO report in 1995. The beautiful use of anilines and their derivative is to form indigo dye for blue jeans in the dye industry [13-16]. Polyaniline an important derivative of

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anilines is considered as an emerging conducting polymer in the polymer industries due to its methodical preparation environmental stability and having good electrochemical properties [17-18].For this purpose, details of various studies conducted on aniline and its derivatives are very important. There are molecular geometry changes due to extended interaction of amino group a with an aromatic ring [19-20]. The inclusion of any group for atom by substitution in the parent aniline also leads to charge distribution variation in the molecule widely affects the geometry and its vibrational parameters [21]. Shanker et al [22] studied 2-chloro-6-methylaniline with Raman and infrared spectra. A detailed study of spectral analysis and NLO, NBO, and HOMO-LUMO of 2, 3-diflouroaniline and 2,4-difluoraniline have been done. Vibrational Spectral and first order hyperpolarizability of - N-Phenylbenzene sulfonamide and 2,5-difluoro nitrobenzene calculated have been [23-25]. Spectral investigation 2,5,6-trichloroaniline and 4-chloro-3-ferrocylaniline have been studied [26-27]. Synthesis and antibacterial effect of diaryl methylamine-based imines were studied [28].Ti Lim et. al. reported the effect of the location of anilino (-NHPh) and primary amino ($-NH_2$) groups in azo dye compounds [29]. Yi Ding et al. azo and studied the vibrational assignments HOMO – LUMO overlap of photostable yellow disperse dyes of anthraquinone based [30]. H.T Vo et al studies of the effect of alkyl-amine group on aniline [31].

2. EXPERIMENTAL DETAILS

The investigated compound 2,5-Dimethoxy-4-nitroaniline (2,5DM4NA) was purchased from Tokyo chemical (TCI) India Pvt. Ltd with stated purity of more than 99.9% and was used as such to record UV-Visible spectra without further purification. The absorption spectrum of 2,5DM4NA was recorded by UV/Vis's spectrometer U3900, Hitachi in the range of 400-200nm in three solvent Acetone, Ethanol and methanol at central Instrumentation Facility, Jamia Millia, Islamia, New Delhi. For the purpose Spectro quality grade solvents were distilled.

3. COMPUTATIONAL DETAILS

In the present work after getting the data and spectrum recorded by experimentally by spectrophotometer of the compound 2,5-Dimethoxy-4-nitroaniline (2,5DM4NA) the theoretical calculations are carried out. Two different methods are applied for these calculations, Hartree - Fock (HF) and density functional Theory (DFT). For making structure and visualize the geometry the Gauss view molecular visualization program was sun while for the calculations of vibrational geometrical, electronic and thermodynamic parameters Gaussian- 09 program set was employed [32]. Three parameters that are combined with DFT by Lee, Yang and Parr (LYP) is electron correlation functional. These three-hybrid functional group (B3) [33] parameters by Becke's were used for DFT calculations make one single election density functional method B3LYP [34]. In this work two different theory HF and B3LYP with same basis sets, 6-311++ (d,p) are used for the titled compound. Basis sets are very important in these quantum calculations. Baris sets are groups of wave functions for orbitals of the molecules, be it is the

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possibility to change in size of these orbitals the by the multiple split valence wave function.After optimized the structure title compound at the two different basis set by the two empirical quantum chemical theory, Hartree-Fock and density functional theory, the bond length, dihedral angle and bond angle was calculated.For Electronic absorption spectral analysis, TD-SCF method was carried out by Hartree- Fock (HF) and density functional theory (DFT) methods at 6-311G(d,p) basis sets of the title compound. Electronic properties such maximum absorption wavelength(λmax), excitation energy (E), oscillator strength (f), HOMO-LUMO energies also calculated of the 2,5DM4NA. These electronic properties that is obtained by the optimized structure of the title compound have been studied in various solvent like as, acetone, ethanol, methanol by these two empirical theories. Other parameters such as, chemical potential, ionization potential, electron affinity, electronegativity, HOMO-LUMO energy gap also calculated of the titled compound. These HOMO-LUMO energies are related to ionization potential, electron affinity. Parameters such as Global Hardness, Global softness and electrophilicity index also calculated by these HOMO-LUMO energies.

4. RESULT AND DISCUSSION

4.1 MOLECULAR GEOMETRY

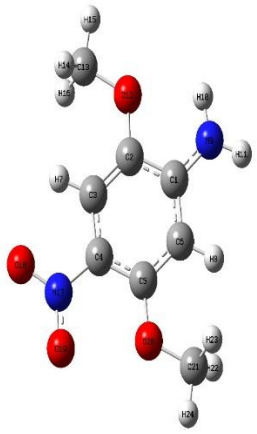

Figure 4.1 Optimized geometric structure of 2,5-Dimethoxy-4-nitroaniline with numbering of atoms.

In the present study the Optimized geometric structure of title compound 2,5DM4NA with numbering of atoms explained. For the geometrical demonstration of the title compound, Cs point group symmetry has been taken account for this. In this research study Cartesian coordinate analysis of theoretical force constant took into consideration.The computation has

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been started with 212 symmetry adapted basis functions ,212 symmetry adapted Cartesian basis functions ,414 primitive gaussians, for 52 alpha and 52 beta electrons with nuclear repulsion energy 815.6262 Hartree, assuming C_s point group symmetry of the optimized structure of title compound. To find out the optimized structure, conformation and orientation of $-NO_2$ and methoxy group in aniline molecule polarised set 6-311++G(d,p) are used in this investigation

4.2 UV-VISIBLE ABSORPTION SPECTRA

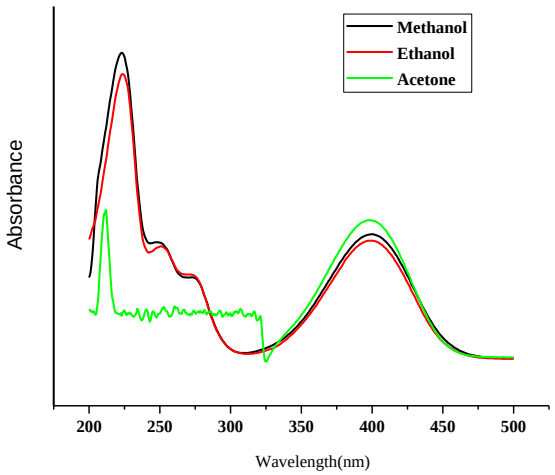

Figure 4.2 (a): Experimental Absorption spectra of 2,5-Dimethoxy-4-nitroaniline in different solvent

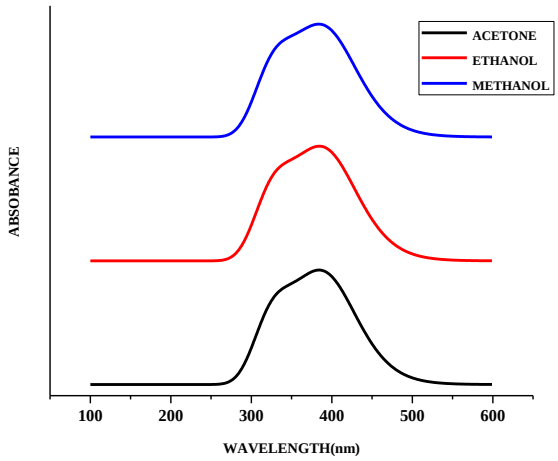

Fig. 4.2(b):TheoreticalAbsorption Spectra of 2,5-Dimethoxy-4-nitroaniline by B3LYP/6-311G(d,p) in different solvent

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In present research, electronic absorption spectra i.e., ultraviolet analysis of 2, 5dimethoxy-4-nitroanaline are discussed. Comparing the value of theoretical λmax and experimental λmax with the help of Density Function Theory (DFT) and Hartree-fock Theory (HFT) these both are computational quantum mechanical modeling theories to determine the electronic structure of a given chemical compound and in finding theoretical λmax value and find how near to Experimental λmax value. When we talk about finding the value of λmax [maximum wavelength of electronic absorption] the first concept which comes in our mind is Woodward-Fieser rule this is classical method of calculating the value of theoretical λmax. This rule gives some base values which helps in calculating the value of theoretical λmax like: - Homo Annular dienes = 253nm,Hetro Annular dienes = 215nm, Butadiene or Conjugated dienes = 217nm ,Alkyl substituted = 5nm ,Exocyclic Double Bond = 5nm ,Double bond with extended conjugation = 30nm .By using all the above given data first calculate the theoretical λmax for aniline according to Woodward-Fieser rule which is equal to 230nm and is more than that of benzene i.e. benzene have 202nm according to Woodward-Fieser rule. This difference is due to alkyl substitution in benzene, that's why aniline have more value than benzene. Due to the substitution of incoming group if the value of λmax increases it is called Bathochromic shift or red shift i.e. shift of absorption to longer wavelength when compare to benzene [35-38]. Sometimes Chromophores and Auxochromes including solvent also is responsible for the change in the value of λmax which increases the value of λmax or decreases the value of λmax (blue shift or Hypsochromic shift). Chromophores are the covalently bonded unsaturated groups responsible for the electronic absorption like C=C, C=O, $-NO_2$ etc. are some of the examples of Chromophores whereas Auxochromes are the saturated group, which when attached to Chromophore changes their intensity as well as wavelength. e.g.: - NH_2, Cl, OH etc.

Similarly, Electron withdrawing group (EWG) and Electron donating group (EDG) also play considerable role when we calculate the value of λmax. Electron withdrawing groups are also capable to acts as chromophore and they shift primary absorption band to longer wavelength but not affect the value of secondary absorption band. Some examples of Electron withdrawing group are $-SO_2$, $-NH_2$, -CN, -COOH, $-COCH_3$, -CHO, $-NO_2$ etc. If we talk about the Electron donating group, they have capability to change the value of λmax of primary absorption band as well as secondary absorption band. Ex: - CH_3, Cl, Br, OH, OCH_3, NH_2, etc [39-41].

The compound for study is disubstituted derivatives of aniline i.e., 2,5 dimethoxy-4-nitroaniline here methoxy group act as Electron donating group. If both the substituents are same either are electron donating group or both are electron withdrawing group then they show same effect on λmax as observed in mono substituted benzene or aniline derivatives. By using HF Theory with the help of all data given in table4.1(b), the theoretical λmax of 2,

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5dimethoxy-4-nitroaniline in the three different solvents namely ethanol, methanol and acetone calculated. The values of λmax calculated from HF Theory are 252.46nm, 232.34nm and 220.69nm, when 2, 5dimethoxy-4-nitroaniline is dissolved in ethanol, methanol and acetone respectively whereas experimental value of λmax that obtained by experimentation is 398.5nm, 252.5nm and 223.5nm by using ethanol as solvent, 398.5nm, 252.5nm and 223.5nm by using methanol as a solvent and 392.5nm and 212nm by using acetone as a solvent. The experimental value of λmax of 2, 5dimethoxy-4-nitroaniline is same when use ethanol and methanol as solvent this due to the polarity difference, ethanol and methanol have same polarity.

When the value of theoretical λmax of 2, 5dimethoxy-4-nitroaniline Table 4.1(a) was calculate by using DFT (Density Function Theory) obtained different values using ethanol, methanol and acetone respectively as a solvent. The values calculate are 395.58nm, 336.75nm and 314nm when ethanol used as solvent, 395.6nm, 336.97nm and 314.35nm when methanol is used as solvent and 395nm, 336nm and 315nm when acetone is used as solvent.

The theoretical values obtained with the help of DFT are more closure to the experimental values as compare with HF theory. This proves that DFTs is more accurate than HF Theory.

Table 4.1(a): Electronic absorption spectra of 2,5-dimethoxy-4-nitroaniline [Absorption wavelength (λ_{max}nm), Excitation Energy (eV) and Oscillator Strength (f)] using B3LYP/6-311g(d,p) basis set.

Solvents	λ_{max}(Experimental)	λ_{max} (Theoretical)	E	f	Assignments
Ethanol	398.5 252.5 223.5	395.58 336.75 314.35	3.1342 3.6818 3.9442	0.2243 0.1449 0.0475	n→π* n→π* π→π*
Methanol	398.5 252.5 223.5	395.63 336.97 314.42	3.1338 3.6794 3.9458	0.211 0.1468 0.0454	n→π* n→π* π→π*
Acetone	398.5 - 212	395 336 315	3.1388 3.6860 3.9435	0.2244 0.1418 0.0498	n→π* n→π* π→π*

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Table 4.1(b): Electronic absorption spectra of 2,5-dimethoxy-4-nitroaniline [Absorption wavelength (λ_{max}nm), Excitation Energy (eV) and Oscillator Strength (f)] using HF /6-311g(d,p) basis set.

Solvents	λ_{max}(Experimental)	λ_{max} (Theoretical)	E	f	Assignments
Ethanol	398.5	252.46	4.911	0.3129	n→π*
	252.5	232.34	5.3363	0.0451	n→π*
	223.5	220.69	5.6181	0.0222	π→π*
Methanol	398.5	252.58	4.9088	0.3149	n→π*
	252.5	232.30	5.3373	0.0439	n→π*
	223.5	220.70	5.6179	0.0226	π→π*
Acetone	398.5	252.48	4.9106	0.3114	n→π*
	-	232.21	5.3393	0.0425	n→π*
	212	220.66	5.6188	0.0229	π→π*

4.4 HOMO LUMO ENERGY

The energy difference between LUMO's and HOMO's is known as energy gap. This energy gap leads the chemical stability of molecule. This energy gap is also responsible for physical properties of the molecules like electrical transport or electron conductivity, kinetic stability, chemical hardness -softness, optical polarizability, kinetic stability of any molecule. More parameter that is calculated by these HOMO LUMO energies and energy gap is electrophilicity index, which is responsible for the energy lowering of a ligand between donor and acceptor. Electron affinity, electron negativity chemical potential was also calculated by the HOMO LUMO energy [42-47]. Ionization potential I of the molecule is equal to energy of E_{HOMO}. For hardness and softness of the molecule this energy gap is responsible. If large energy gap is observed between HOMO and LUMO, then molecule will not easily polarizable and treated hard while with less energy gap molecule treated as soft molecule. In the molecule, having large energy gap, intramolecular charge transfer (ICT) interaction that is responsible for the chemical properties of the molecule is not taking place. In table 4.2 (a)and table 4.2 (b). The energy of HOMO, LUMO, $HOMO_{-1}$(second highest) and $LUMO_{-1}$ (second lowest) in different solvents of **2,5-Dimethoxy-4-nitroaniline** calculated by both theories with 6-311++G (d, p) basis sets also reported.

For the calculation of different physical and chemical parameters such as Ionization potential, chemical potential, electron affinity, global hardness-softness, electronegativity and electrophilic index complete equations is used as follows Ionization potential(I)=-$E_{HOMO;}$ Electron affinity

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(A)=- $E_{LUMO;}$ Electronegativity (σ)=- (μ); Chemical Potential (μ)= (E_{HOMO}+ E_{LUMO})/2; Global softness (S)=1/ η; Global Hardness(η)= (E_{HOMO}- E_{LUMO})/2; Electronegativity (σ)=- μ Fig. 4 .3and fig. 4.4 is reflected the contours of the HOMO and LUMO in different solvents using HF/6-311++G(d, p) and B3LYP/6-311G(d,p) basis set.

Table 4.2 (a): Calculated energy value (eV) of 2,5-Dimethoxy-4-nitroanilineby using B3LYP/6-311G(d,p) basis set

Solvents	E_{HOMO}	E_{LUMO}	E_{HOMO-1}	E_{LUMO+1}	ΔE	∂E	E_{Total}(Hartree)
Acetone	-0.221	0.093	-0.252	0.017	0.128	0.235	-721.35
Ethanol	-0.221	0.093	-0.252	0.017	0.128	0.235	-721.35
Methanol	-0.221	0.093	-0.252	0.017	0.128	0.235	-721.35

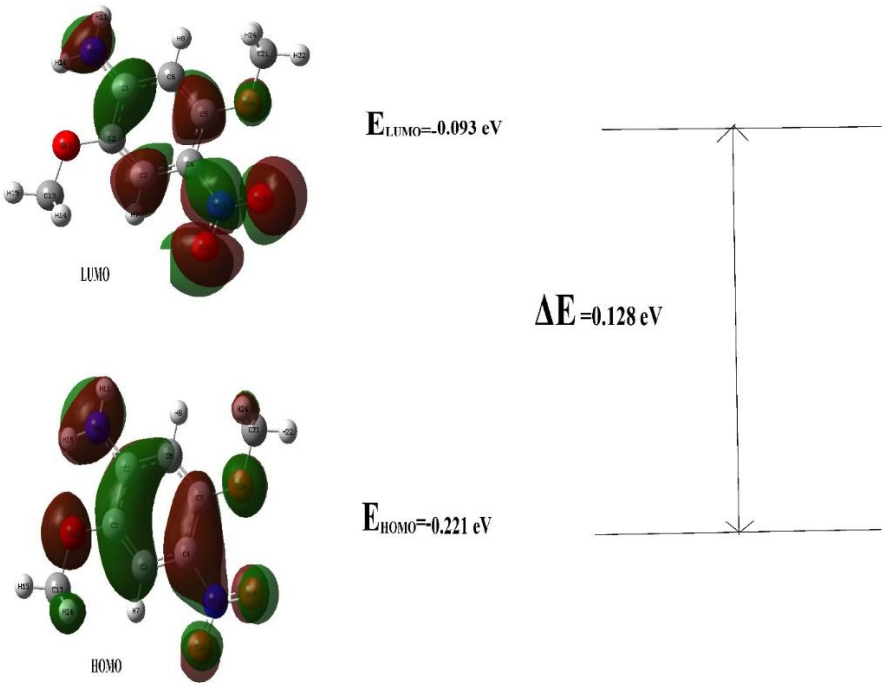

Figure 4.3(a): Computed HOMO-LUMO contours of 2,5-dimethoxy-4-nitroaniline with energy gap at B3LYP/6-311G(d,p) basis set.

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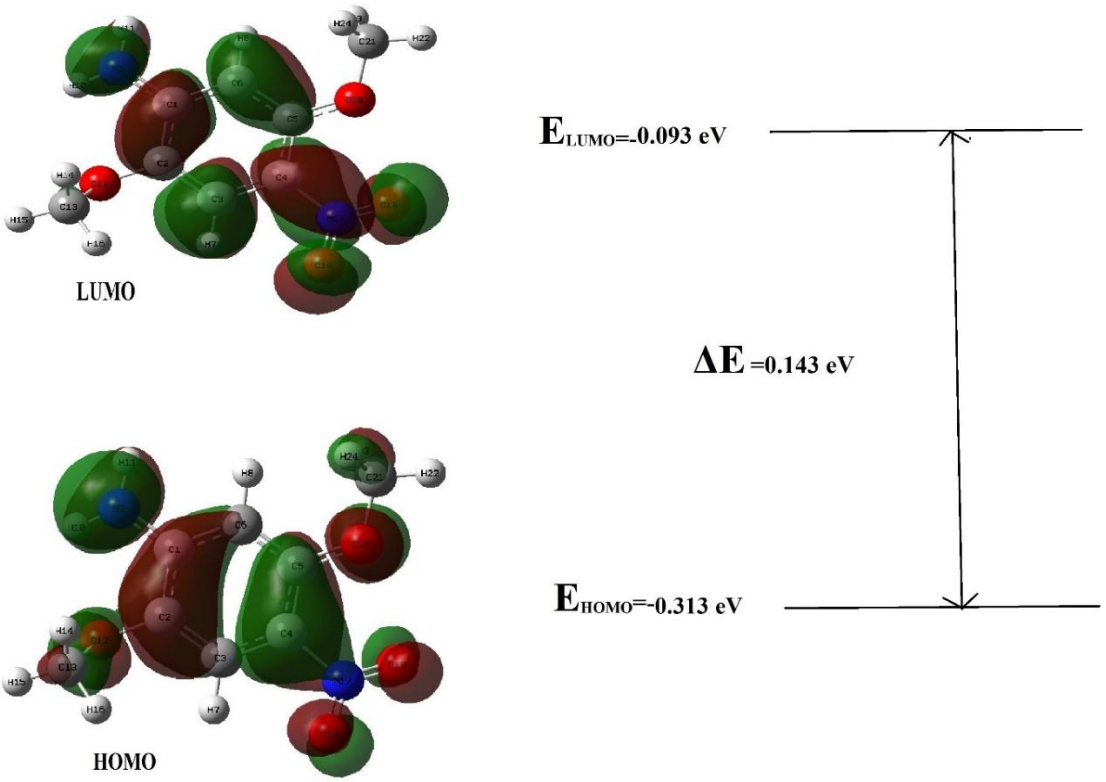

Figure 4.3(b): Computed HOMO-LUMO contours of 2,5-dimethoxy-4-nitroaniline with energy gap at HF/6-311G(d,p) basis set

Table 4.2(b): Calculated energy value (eV) of 2,5-dimethoxy-4-nitroaniline by using HF/6-311G (d, p) basis set

Solvents	E_{HOMO}	E_{LUMO}	E_{HOMO-1}	E_{LUMO+1}	ΔE	∂E	E_{Total}(Hartree
Acetone	-0.313	0.188	-0.346	0.158	0.143	0.184	-716.98
Ethanol	-0.313	0.188	-0.346	0.158	0.143	0.184	716.98
Methanol	-0.313	0.188	-0.346	0.158	0.143	0.184	716.98

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Table 4.2(c): Computed Ionization Potential (I), Electron Affinity (A), Chemical Potential (μ), Global Hardness (η), Global Softness (S, eV^{-1}), Electronegativity(σ) and Electrophilicity Index (ω) of 2,5-dimethoxy-4-nitroaniline using HF/6-311++G(d, p) and B3LYP/6-311G(d,p) basis set [Values are same for all the three solvents]

Parameters	HF/6- 311++G(d,p) values (eV)	B3LYP/6- 311++G(d,p) values (eV)
EHOMO	-0.313	-0.221
ELUMO	-0.188	-0.093
Ionization potential(I)	0.313	0.221
Electron affinity (A)	0.188	0.093
Chemical Potential (μ)	-0.250	-0.157
Global Hardness(η)	-0.063	-0.064
Global softness (S)	-15.873	-15.625
Electronegativity (σ)	0.250	0.157
Electrophilicity index (ω)	-0.5	0.193

5 CONCLUSION

In the present work, the optimized molecular structure, the U.V. absorption analysis, and HOMO-LUMO energies of the compound 2,5-dimethoxy-4-nitroanilinewas calculated at two different theories HF and TD-DFT using two basis sets 6-3114++G (d, p) and 6-31++G (d, p). We compare theoretical and experimental results, and make a conclusion that the TD-DFT calculations give deep insight into the molecular geometries, HOMO-LUMO energy and energy gap also suggest the reactive nature of the tilted compound. The low energy gap also suggests the molecule is soft and easily polarizable. The low value E_{HOMO} indicates that tilted compound gives easily the electrons, means low ionization potential. The data obtained from the above analysis with different basis sets by HF and DFT give good agreement with the experiment one. In the light of this work, it is observed that there is an insignificant difference between the values reported by two theories but DFT has an advantage over HF.

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