# THEORETICAL INVESTIGATION OF MOLECULAR STRUCTURE, HOMO-LUMO, HYPERPOLARIZABILITY, NBO ANALYSIS AND DENSITY OF STATES CALCULATION OF BUTENAFINE

R.K.SANGEETHA[a], S. AYYAPPAN[b,*]
*[a]Department of Physics, Sri Eshwar College of Engineering, Coimbatore, India*
*[b,]Department of Physics, Government College of Technology, Coimbatore, India*

Molecular geometry vibrational wave number of butenafine was investigated using HartreeFock and DFT method with HF and B3LYP/6-31+G(d,p) basis set. The potential energy distribution of the vibrational wave number is found to be in good agreement with experimental values. A detailed NBO analysis of butenafine was done with B3LYP method. U-V visible absorption spectra of the titled molecule is calculated by PCM model using water as solvent. The U-V visible spectra of the titled molecule dissolved in water were recorded in the range of 200-900 nm. The calculated values of U-V spectra are the most reproduced experimental data. The density of states, Homo-lumo and electrostatic potentials were calculated and analyzed. The dipole moment and hyperpolarizability result shows the butenafine has non linear optical properties. The natural bonding analysis was calculated by HF and B3LYP method.

## 1. Introduction

The recent advances in medicine principally in antifungal therapy have introduced new fungicides, in order to reduce the antagonistic, invasive and therauptic treatments. Ostensible fungal infections are common throughout the globe. There are three main anamorphic genera of dermatophyte, responsible for the group of infections generally known as tinea (namely Trichophyton, Microsporumand Epidermophyton). These infections are transmissible and transmitted via physical contact with arthroconidia, which are generated from dermatophyte filaments. Tinea infections affect the keratinised cells of the skin, hair and nails and are named according to the anatomical site infected. Trichophyton rubrum and Trichophyton mentagrophytesare the leading cause of tinea pedis, and tinea rubrum. Epidermophytonfloccosumand tinea mentagrophytesare due to tinea cruris [1]. Butenafine [(4-*tert*-butylphenyl) methyl] (methyl) (naphthalen-1-ylmethyl) amine, a sole approved representative which belongs to the class of a phenol-substituted benzylamine derivatives was synthesized by Maeda etal. (T. Maeda, T. Arika, K. Amemiya, and K. Sasaki, Chem. Pharm. Bull., in press) has the molecular weight of 353.93 and an empirical formula $C_{23}H_{27}N.HCl.$ is a outstanding antifungal which possess a chemical structural arrangement indistinguishable to allylamine [2]. It works by killing sensitive fungi by interfering with the formation of the fungal cell membrane and weakening it. It has greater robustness when compared to azole derivatives and naftifine. Butenafine is slightly soluble in water, freely soluble in ethanol, methanol and chloroform, an effective antibiotic character of antifungal activity is visible; and is particularly active against dermatophytes, aspergilli, dimorphic fungi,and dematiaceous fungi (Maeda et al., in press). The desired result of butenafine was notably superior to those of tolnaftate, clotrimazole and bifonazole[3].Several studies made explicit antimyotic and anti inflammatory properties with butenafine. The current work deals with the theoretical calculation of hyperpolarizability, Homo-lumo and density of states of butenafine using the fundamental tools of computational technique so called density functional theory.

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* Corresponding author: ayyappan@gct.ac.in

## 2. Computational details

The optimization of molecular structure of the titled molecule and the corresponding vibrational frequencies was calculated using HF and DFT with B3LYP/6-31+G(d,p) basis set using Gaussian software [4] .The geometrical structures of the title of the compound have been first optimized with full relaxation of potential energy and without any constraints and the geometry. The natural bonding analysis (NBO), hyperpolarizability, Homo-lumo and molecular electrostatic potential (MESP) were calculated by B3LYP/6-31+G(d,p)basis set [5]. The potential energy scanning (PES) of the titled molecule was calculated by using the same basis set. The density of state (DOS) is also estimated by B3LYP/6-31+G(d,p)method.

## 3. Results and discussion

### 3.1 Molecular geometrical structure analysis

The optimized bond length and bond angle in butenafine were determined using HF and DFT with B3LYP/6-31+G (d,p) basis set as listed in table (1) in accordance with atomic numbering scheme diagram as shown in figure (1). The total energy of the butenafine is obtained by RHF and RB3LYP as -941.3475 and -947.71068 Hartree respectively. The most of the optimized structure of the parameter such as bond length, bond angle and tetrahedral angles were also investigated by HF and B3LYP/6-31+G (d,p) basis set as presented. The benzene ring, naphthalene and $CH_3$ groups were noticeable in the titled molecule. The $C_5$–$C_7$, $C_8$-$C_{13}$ and $C_3$- $C_6$ bonds are occupied by larger bond length values when compared to the other C-C bond. This may be due to affect of substitution of nitrogen and methyl groups [6-9].
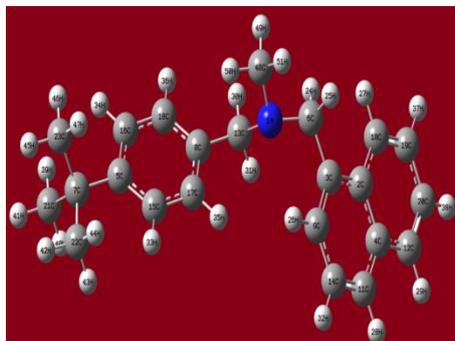


*Fig. 1. Geometrical molecular structure of Butenafine.*

The optimized bond angle of C-C in butenafine is in the range of 1.515Å – 1.378Å for aromatic ring and 1.539Å – 1.547Å for outside ring, while the initiation of substituent of methyl group causes a slight differences between the C-C bond length. The nitrogen present in between the two carbon atoms of the titled molecule and its N-C bond length value is 1.46 Å. The increase of the C-C bond length in the substituent is accompanied by slightly changes in bond angles $C_5$-$C_{16}$-$C_{18}$ , C $_8$-$C_{17}$- $C_{15}$ and $C_8$-$C_{18}$- $C_{16}$ are 20.6°,21.1°and 19.5° respectively.

*Table. 1  Calculated bond length (A°), bond angle (°) and Dihedral angle (°) of butenafine usingB3LYP/6-31+G(d,p) basis set.*

| Bond length(A°) | | Bond angle(°) | | Dihedral angle(°) | |
|---|---|---|---|---|---|
| Parameter | Value | Parameter | Value | Parameter | Value |
| N1-C6 | 1.464 | C4-C12-H29 | 118.4 | C2-C4-C11-C14 | -0.4 |
| N1-C13 | 1.468 | C20-C12-H29 | 120.4 | C2-C4-C11-H28 | 180.0 |
| N1-C48 | 1.460 | N1-C13-C8 | 113.8 | C12-C4-C11-C14 | 179.2 |
| C2-C3 | 1.434 | N1-C13-H30 | 110.9 | C12-C4-C11-H28 | -0.4 |
| C2-C4 | 1.435 | N1-C13-H31 | 107.3 | C2-C4-C12-C20 | 0.5 |
| C2-C10 | 1.423 | C8-C13-H30 | 109.0 | C2-C4-C12-H29 | -179.8 |
| C3-C6 | 1.522 | C8-C13-H31 | 109.1 | C11-C4-C12-C20 | -179.1 |
| C3-C9 | 1.378 | H30-C13-H31 | 106.5 | C11-C4-C12-H29 | 0.6 |
| C4-C11 | 1.418 | C9-C14-C11 | 120.3 | C15-C5-C7-C21 | -121.1 |
| C4-C12 | 1.419 | C9-C14-H32 | 119.4 | C15-C5-C7-C22 | -0.9 |
| C5-C7 | 1.539 | C11-C14-H32 | 120.3 | C15-C5-C7-C23 | 119.2 |
| C5-C15 | 1.400 | C5-C15-C17 | 121.6 | C16-C5-C7-C21 | 59.3 |
| C5-C16 | 1.402 | C5-C15-H33 | 120.2 | C16-C5-C7-C22 | 179.5 |
| C6-H24 | 1.103 | C17-C15-H33 | 118.2 | C16-C5-C7-C23 | -60.5 |
| C6-H25 | 1.096 | C5-C16-C18 | 120.6 | C7-C5-C15-C17 | -179.7 |
| C7-C21 | 1.546 | C5-C16-H34 | 119.9 | C7-C5-C15-H33 | 0.3 |
| C7-C22 | 1.540 | C18-C16-H34 | 118.5 | C16-C5-C15-C17 | -0.1 |
| C7-C23 | 1.547 | C8-C17-C15 | 121.1 | C16-C5-C15-H33 | 180.0 |
| C8-C13 | 1.515 | C8-C17-H35 | 119.3 | C7-C5-C16-C18 | 179.6 |
| C8-C17 | 1.396 | C15-C17-H35 | 119.5 | C7-C5-C16-H34 | 0.0 |
| C8-C18 | 1.397 | C8-C18-C16 | 121.2 | C15-C5-C16-C18 | -0.1 |
| C9-C14 | 1.412 | C8-C18-H36 | 119.5 | C15-C5-C16-H34 | -179.6 |
| C9-H26 | 1.083 | C16-C18-H36 | 119.4 | C5-C7-C21-H39 | -60.0 |
| C10-C19 | 1.375 | C10-C19-C20 | 119.5 | C5-C7-C21-H40 | 60.3 |
| C10-H27 | 1.082 | C10-C19-H37 | 119.8 | C5-C7-C21-H41 | -179.9 |
| C11-C14 | 1.371 | C20-C19-H37 | 119.7 | C22-C7-C21-H39 | 177.3 |
| C11-H28 | 1.085 | C12-C20-C19 | 119.8 | C22-C7-C21-H40 | -62.5 |
| C12-C20 | 1.373 | C12-C20-H38 | 120.3 | C22-C7-C21-H41 | 57.3 |
| C12- H29 | 1.085 | C19-C20-H38 | 119.9 | C23-C7-C21-H39 | 59.8 |
| C13-H30 | 1.106 | C7-C21-H39 | 111.8 | C23-C7-C21-H40 | -179.9 |
| C13-H31 | 1.094 | C7-C21-H40 | 110.9 | C23-C7-C21-H41 | -60.1 |
| C14-H32 | 1.084 | C7-C21-H41 | 110.3 | C5-C7-C22-H42 | 180.0 |
| C15-C17 | 1.393 | H39-C21-H40 | 107.8 | C5-C7-C22-H43 | -60.8 |
| C15-H33 | 1.082 | H39-C21-H41 | 107.8 | C5-C7-C22-H44 | 60.8 |
| C16-C18 | 1.391 | H40-C21-H41 | 108.2 | C21-C7-C22-H42 | -59.0 |
| C16-H34 | 1.084 | C7-C22-H42 | 109.6 | C21-C7-C22-H43 | 60.1 |
| C17-H35 | 1.084 | C7-C22-H43 | 111.8 | C21-C7-C22-H44 | -178.2 |
| C18-H36 | 1.086 | C7-C22-H44 | 111.8 | C23-C7-C22-H42 | 59.2 |
| C19-C20 | 1.412 | H42-C22-H43 | 107.6 | C23-C7-C22-H43 | 178.4 |
| C19-H37 | 1.084 | H42-C22-H44 | 107.5 | C23-C7-C22-H44 | -60.0 |
| C20-H38 | 1.084 | H43-C22-H44 | 108.3 | C5-C7-C23-H45 | 179.7 |
| C21-H39 | 1.092 | C7-C23-H45 | 110.4 | C5-C7-C23-H46 | 59.8 |
| C21-H40 | 1.093 | C7-C23-H46 | 111.7 | C5-C7-C23-H47 | -60.5 |
| C21-H41 | 1.095 | C7-C23-H47 | 110.9 | C21-C7-C23-H45 | 59.8 |
| C22-H42 | 1.093 | H45-C23-H46 | 107.8 | C21-C7-C23-H46 | -60.1 |
| C22-H43 | 1.093 | H45-C23-H47 | 108.1 | C21-C7-C23-H47 | 179.6 |
| C22-H44 | 1.093 | H46-C23-H47 | 107.8 | C22-C7-C23-H45 | -57.6 |
| C23-H45 | 1.095 | N1-C48-H49 | 112.9 | C22-C7-C23-H46 | -177.6 |

| Bond length(A°) | | Bond angle(°) | | Dihedral angle(°) | |
|---|---|---|---|---|---|
| Parameter | Value | Parameter | Value | Parameter | Value |
| C23-H46 | 1.092 | N1-C48-H50 | 109.7 | C22-C7-C23-H47 | 62.2 |
| C23-H47 | 1.093 | N1-C48-H51 | 109.7 | C17-C8-C13-N1 | -51.8 |
| C48-H49 | 1.106 | H49-C48-H50 | 108.0 | C17-C8-C13-H30 | -176.1 |
| C48-H50 | 1.091 | H49-C48-H51 | 108.3 | C17-C8-C13-H31 | 68.0 |
| C48-H51 | 1.092 | H50-C48-H51 | 108.2 | C18-C8-C13-N1 | 129.8 |
| Bond angle(°) | | Dihedral angle(°) | | C18-C8-C13-H30 | 5.5 |
| C6-N1-C13 | 111.0 | C13-N1-C6-C3 | -76.8 | C18-C8-C13-H31 | -110.4 |
| C6-N1-C48 | 111.2 | C13-N1-C6-H24 | 48.0 | C13-C8-C17-C15 | -178.3 |
| C13-N1-C48 | 111.7 | C13-N1-C6-H25 | 163.0 | C13-C8-C17-H35 | 2.2 |
| C3-C2-C4 | 118.9 | C48-N1-C6-C3 | 158.2 | C18-C8-C17-C15 | 0.2 |
| C3-C2-C10 | 123.4 | C48-N1-C6-H24 | -77.0 | C18-C8-C17-H35 | -179.4 |
| C4-C2-C10 | 117.7 | C48-N1-C6-H25 | 38.0 | C13-C8-C18-C16 | 178.2 |
| C2-C3-C6 | 121.0 | C6-N1-C13-C8 | 170.0 | C13-C8-C18-H36 | -1.9 |
| C2-C3-C9 | 119.1 | C6-N1-C13-H30 | -66.7 | C17-C8-C18-C16 | -0.3 |
| C6-C3-C9 | 119.8 | C6-N1-C13-H31 | 49.2 | C17-C8-C18-H36 | 179.6 |
| C2-C4-C11 | 119.5 | C48-N1-C13-C8 | -65.3 | C3-C9-C14-C11 | 0.3 |
| C2-C4-C12 | 119.3 | C48-N1-C13-H30 | 58.0 | C3-C9-C14-H32 | -179.7 |
| C11-C4-C12 | 121.1 | C48-N1-C13-H31 | 173.9 | H26-C9-C14-C11 | -179.7 |
| C7-C5-C15 | 123.1 | C6-N1-C48-H49 | 60.8 | H26-C9-C14-H32 | 0.3 |
| C7-C5-C16 | 120.0 | C6-N1-C48-H50 | -178.7 | C2-C10-C19-C20 | 0.0 |
| C15-C5-C16 | 116.9 | C6-N1-C48-H51 | -60.0 | C2-C10-C19-H37 | -180.0 |
| N1-C6-C3 | 114.3 | C13-N1-C48-H49 | -63.8 | H27-C10-C19-C20 | 179.5 |
| N1-C6-H24 | 110.3 | C13-N1-C48-H50 | 56.7 | H27-C10-C19-H37 | -0.4 |
| N1-C6-H25 | 107.6 | C13-N1-C48-H51 | 175.4 | C4-C11-C14-C9 | 0.5 |
| C3-C6-H24 | 110.2 | C4-C2-C3-C6 | 178.4 | C4-C11-C14-H32 | -179.5 |
| C3-C6-H25 | 108.2 | C4-C2-C3-C9 | 1.3 | H28-C11-C14-C9 | -179.8 |
| H24-C6-H25 | 105.9 | C10-C2-C3-C6 | -0.9 | H28-C11-C14-H32 | 0.1 |
| C5-C7-C21 | 109.5 | C10-C2-C3-C9 | -178.0 | C4-C12-C20-C19 | 0.1 |
| C5-C7-C22 | 112.4 | C3-C2-C4-C11 | -0.5 | C4-C12-C20-H38 | 179.9 |
| C5-C7-C23 | 109.4 | C3-C2-C4-C12 | 179.9 | H29-C12-C20-C19 | -179.7 |
| C21-C7-C22 | 108.1 | C10-C2-C4-C11 | 178.8 | H29-C12-C20-H38 | 0.1 |
| C22-C7-C23 | 108.1 | C3-C2-C10-C19 | 179.9 | C5-C15-C17-H35 | 179.5 |
| C13-C8-C17 | 121.4 | C3-C2-C10-H27 | 0.3 | H33-C15-C17-C8 | 180.0 |
| C13-C8-C18 | 121.0 | C4-C2-C10-C19 | 0.6 | H33-C15-C17-H35 | -0.5 |

The bond angle C-N-C value is 111° were estimated by B3LYP/6-31+G(d,p) basis set method. The nitrogen atoms are doped in between naphthalene and benzene groups so that the bond angles varying from 109.7°– 112.19° are affected by the exchange of electron density in between the two groups.

### 3.2 Dipole moment  andHyperpolarizability

The dipole moment and the first order hyperpolarizability were calculated by HF and B3LYP/6-31+G(d,p) basis set method[10,11]. The dipole moment and the first order hyperpolarizability of the titled molecules were calculated as shown in table(2). It can be seen that there is a additive contributions of diagonal polarizability [13]. The total dipole moment of butenafine for HF and B3LYP/6-31+G(d,p) method is 0.7768 Debye and 0.7194 Debye respectively. The mean first order hyperpolarizability of the title of molecule is predicted by HF and B3LYP method and the values are $0.83202 \times 10^{-30}$e.s.u and $0.72435 \times 10^{-30}$e.s.u   respectively [14].It is observed that the  dipole moment and the hyperpolarizabilty values are more appropriate for HF than the DFT method[15]. The mean hyperpolarizability of the butenafine is approximately

two times greater than hyperpolarizability of urea[16-18] .This values shows that there is a significant presence of the non linear optical properties of the butenafine.

*Table 2. Calculated Dipole moment (μ) in Debye and hyperpolarizability (β) of butenafine by HF / 6-31+G (d,p) and  B3LYP/6-31+G(d,p) method.*

| μ value | HF/6-31+G(d,p) | B3LYP/6-31+G(d,p) |
|---|---|---|
| $\mu_x$ | -0.3376 | -0.1677 |
| $\mu_y$ | -0.6783 | 0.1139 |
| $\mu_z$ | 0.1226 | 0.19636 |
| $\mu$ | -0.8933 | 0.14256 |
| β value | HF/6-31+G(d,p) | B3LYP/6-31G+(d,p) |
| $\beta_{xxx}$ | 3.3064 | 12.0604 |
| $\beta_{yyy}$ | 3.3371 | 82.4864 |
| $\beta_{zzz}$ | -8871 | 9.6420 |
| $\beta_{xyy}$ | 25.0318 | 134.2059 |
| $\beta_{xxy}$ | 8.8601 | -2.9464 |
| $\beta_{xxz}$ | 49.8579 | 29.7797 |
| $\beta_{xzz}$ | -13.7675 | 49.1429 |
| $\beta_{yzz}$ | -10.1864 | 13.8516 |
| $\beta_{yyz}$ | -14480 | 50.3614 |
| $\beta_{xyz}$ | 9.2433 | 156.2073 |
| Total | -23275.3173 | 534.7912 |
| In e.s.u. | $194.798 \times 10^{-30}$ | $4.476 \times 10^{-30}$ |

### 3.3. U-V Visible and Homo-lumo studies

The U-V visible spectra of the titled molecule is also been resolved. The absorption wavelength, excitation energy and oscillation strength were determined by time dependent density functional theory. The result coincides with the experimental findings values as shown in table(3).The absorption wavelength of the titled molecule calculated by TD-DFT/B3LYP/6-31+G(d,p) is 283n that compliments to the experimental wavelength  ($\lambda$=287nm) [19].The U-V visible analysis carries the major contribution energy among the Homo-Lumo and frontier orbital [20-21].
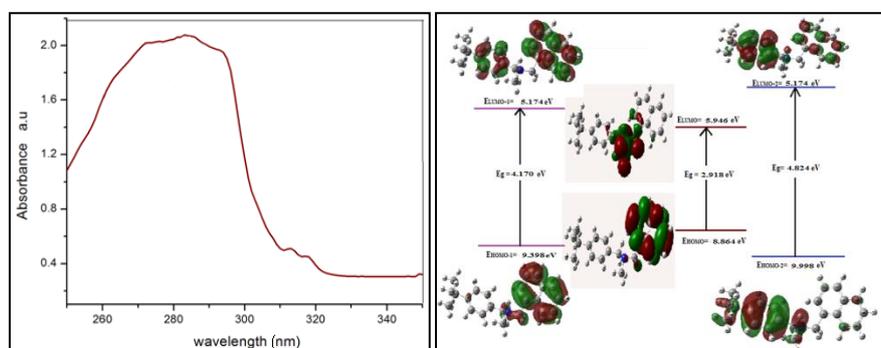


*Fig.2. (a and b).Experimental UV-Vis absorbance spectra and Frontier Molecular diagram of Butenafine.*

The energy gap between Homo- lumo depends on interaction between π and π* interaction of the titled molecule. The electron absorption energy corresponding to the transition from the ground level to first excited state, that is one electron excitation exists from the highest occupying molecular orbital to lowest unoccupied molecular orbital. Generally, lowest unoccupied molecular orbital is π- bond nature[22].

*Table 3. Experimental and computed absorption wavelength (λ), excitation energies (E) and oscillation strength (f) butenafine by B3LYP/6-31+G(d, p) method.*

| Exp wavelength (nm) | Theoretical wavelength (nm) | Excitation level | Transition state | Excitation energy(E) (eV) | Oscillation strength (f) |
|---|---|---|---|---|---|
| 311 | 310 | I | 85→87 86→87 | 4.007 | 0.0186 |
| | 299 | II | 85→87 86→87 | 4.147 | 0.1892 |
| 287 | 283 | III | 83→87 85→88 86→88 | 4.3846 | 0.0040 |

The naphthalene group is delocalised over the whole C-C bonding interactions, so that Homo is located over the naphthalene groups of the titled molecule. Homo to Lumo transition implies an electron density transfer from aromatic ring part of π- conjugate system to the lone pair nitrogen atom [23].The energy gap between the Homo- lumo is 2.918 eV. The Homo, lumo and frontier orbital energy transition level as shown in table(3). The lumo represents an electron acceptor and Homo represents the ability to donate electron as shown in energy level diagram in Figure(2.b).

### 3.4 Density of states

Total density of states and partial density of states were enumerated by using B3 LYP/6-31+ G(d,p) basis set. The total density of state (TDOS) and partial density of states (PDOS) of nitrogen, naphthalene group, methyl groups, benzene group and $CH_2$ group as shown in figure(3).DOS plot shows the population analysis in each orbital and demonstrates a simple view of the constitute molecular orbital in energy range from – 1.5 a.u. to +2.5 au. The partial density of states of $CH_3$ groups of the titled molecule is predominated to the naphthalene and benzene. At all the partial density of state , the energy distribution is through the energy line[24]. The density state value of nitrogen atom in this molecule is lower but the energy distribution is up to 2 a.u. as shown in figure (3). The positive value of OPDOS represents the bonding orbitals and the negative value represents the anti bonding orbitals. The negative value of OPDOS appears only in Lumo regions which is critical as observed. The density of states of the titled molecule is the energy distribution through carbon atom, than the other atoms such that the density of states of carbon is predominant in this molecule[25].
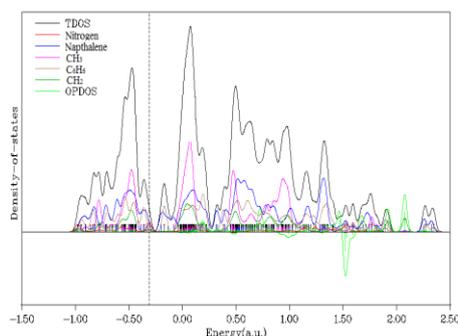


*Fig.3. Total and partial density of states diagram of Butenafine.*

### 3.5. Natural Bonding Orbitals Analysis

Natural Bonding Orbital analysis provides the most accurate and possible Maxwell Lewis structure and highest percentage of density of orbital .It enhance the analysis of inter and intra molecular interactions based on interaction between filled and virtual orbital of the titled molecule[29].The second order Perturbation theory analysis of Fock matrix evaluates the donor and acceptor from the NBO analysis of the titled molecule.The result of interaction is loose occupants from the concentration of electrons in the Lewis structure into the empty non Lewis structure[30].The NBO analysis also describes the bonding intense of the natural hybrid orbital system. The bonding $N_1$-$C_6$, $N_1$-$C_{13}$ and $N_1$-$C_{48}$ is 1.980 interacts with anti bonding $C_3$ and $C_8$ stabilization energy values are 13579, 12890 and 15384 kcal/mol. The bonding $C_{22}$ –$H_{44}$ (1.9889) interacts with $C_{48}$ (0.0002) with stabilization energy 90391 kcal/mol, where as high stabilization energy predicts as relatively high charge transfer from one methyl group to another methyl group of carbon[31]. From the NBO analysis table(4), the C-C interaction is very stronger than the C-N interaction. The molecular stabilization depends on the C-C interactions and the stabilization energy calculated based on NBO analysis is shown in table(4).

*Table 4. Second Order perturbation theory analysis of Fock matrix in NBO basis for butenafine by B3LYP/6-31+G (d, p) method.*

| Donor (i) | ED/e | Acceptor (j) | ED/e | E(2) kcal/ mol | E(j)-E(i) a.u. | F(i,j) a.u. |
|---|---|---|---|---|---|---|
| N1 - C 6 | 1.9881 | C3 | 0.0001 | 13579 | 0.02 | 0.495 |
| N1 - C13 | 1.9802 | C 3 | 0.0001 | 12890 | 0.01 | 0.332 |
| N1 - C48 | 1.9860 | C8 | 0.0067 | 15384 | 0.02 | 0.521 |
| C4 - C12 | 1.9698 | C22 - H44 | 0.0066 | 3067 | 0.06 | 0.394 |
| C 5 - C16 | 1.9709 | C22 - H 44 | 0.0066 | 5418 | 0.04 | 0.42 |
| C6 - H25 | 1.9673 | C 16 - H34 | 0.0323 | 1580 | 0.06 | 0.281 |
| C10 - C19 | 1.9793 | H26 | 0.0008 | 1365 | 0.63 | 0.882 |
| C10 - C19 | 1.9793 | C 7 - C 23 | 0.2354 | 17533 | 0.03 | 0.676 |
| C11 - H28 | 1.9795 | N1 | 0.0004 | 216 | 3.1 | 0.733 |
| C11 - H28 | 1.9795 | C6 | 0.0001 | 12260 | 0.21 | 1.453 |
| C11 - H28 | 1.9795 | C21 - H40 | 0.0060 | 2552 | 0.36 | 0.858 |
| C12 - C20 | 1.9774 | C48 | 0.0000 | 1196 | 0.1 | 0.309 |
| C12 - C20 | 1.9774 | C22 - H44 | 0.0066 | 1264 | 0.05 | 0.225 |
| C13 - H30 | 1.9859 | C 8 | 0.0067 | 32547 | 0.01 | 0.591 |
| C13 - H 31 | 1.9705 | C15 - C17 | 0.0149 | 1175 | 0.03 | 0.163 |
| C18 - H36 | 1.9798 | C3 | 0.0001 | 19336 | 0.03 | 0.738 |
| C18 - H36 | 1.9798 | C 8 - C 18 | 0.0233 | 5807 | 0.06 | 0.526 |
| C19 - C20 | 1.9781 | C2 | 0.0001 | 67017 | 0.32 | 4.125 |
| C19 - C20 | 1.9781 | H25 | 0.0005 | 29704 | 0.38 | 2.997 |
| C19 - C20 | 1.9781 | C15 - C17 | 0.0149 | 1378 | 2.97 | 1.809 |
| C19 - H37 | 1.9806 | C8 | 0.0067 | 8986 | 0.04 | 0.541 |
| C21 - H40 | 1.989 | C48 | 0.0022 | 10971 | 0.26 | 1.514 |
| C22 - H44 | 1.9889 | C10 | 0.0007 | 31274 | 2.21 | 7.439 |
| C 22 - H44 | 1.9889 | C11 - H28 | 0.0147 | 10953 | 3.49 | 5.528 |
| N1 | 1.9994 | C48 | 0.0001 | 3409 | 2.5 | 2.604 |
| N1 | 1.9994 | H51 | 0.0001 | 2800 | 3.13 | 2.642 |
| N1 | 1.9994 | C9 - C14 | 0.0167 | 929 | 6.13 | 2.139 |
| C11 | 1.9988 | H51 | 0.0002 | 13257 | 0.21 | 1.484 |
| C11 | 1.9988 | C9 - C14 | 0.0167 | 935 | 2.23 | 1.294 |

### 3.6. The potential energy surface scanning

The potential energy surface scanning is performed by Gaussian software using DFT/B3LYP/ 6-31+G(d,p) level of approximations. The $C_8$ -$C_{13}$- $N_1$-$C_{48}$ and $C_3$- $C_6$- $N_1$- $C_{48}$ dihedral angles varies in steps of 10º to 360º. Two minimum energy curve has been obtained for $C_8$- $C_{13}$- $N_1$-$C_{48}$ at angle of 130º and 270º in the potential energy curve as shown in figure(5).The

maximum potential of the titled molecule obtained is at 70º and 210º respectively[32]. The two minimum potential energy values of the titled molecule is -1408.53887 Hartree and the two maximum potential value is -1408.52705 Hartree.
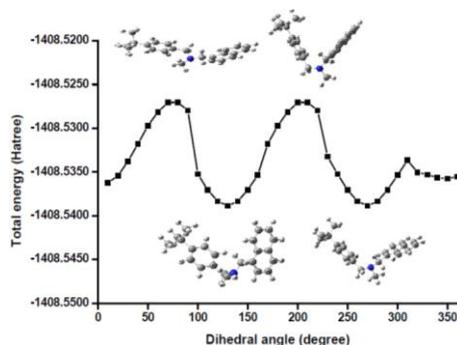


*Fig. 5. Potential energy surface scanning diagram of Butenafine.*

### 3.7. Thermal properties

The steady state thermodynamic function such as heat capacity, entropy, change in enthalpy for the butenafine molecule were obtained from B3LYP/6-31+G(d,p). The thermal parameters values are calculated with respect to change in temperature. The steady state thermodynamic function of the titled molecule increases with increasing temperature ranging from 100K to 1000 K as shown in Fig. 6.
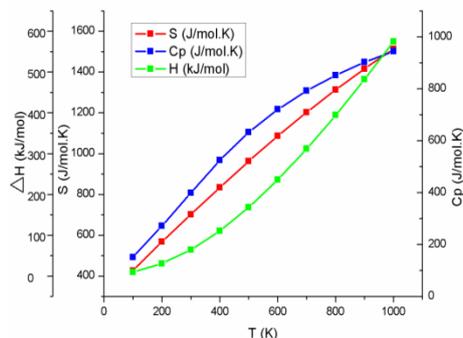


*Fig.6. The graph drawn between Temperature vs entropy(S), change in Enthalpy($\Delta$H) and heat capacity (Cp) diagram of Butenafine.*

The steady state thermodynamic function [33-34]are fitting in equations are given below

$$S = 335.43 + 15.111T + 2.435 \times 10^{-2}T^2$$
$$C_P = 128.5 + 35.9123T + 5.788 \times 10^{-2}T^2$$
$$\Delta H = -114 + 25.1268T + 4.05 \times 10^{-2}T^2$$

The correlation equation between the heat capacity, entropy and change in enthalpy with temperature were fitted by quadratic equations and their corresponding $R^2$ values are 0.96333, 0.99638 and 0.96513 respectively.The steady state thermodynamic data of the title molecule is helpful for the further studies of the molecules.

## 4. Conclusions

We have carried out HF and B3LYP/6-31+G (d, p) method along with the structure and geometrical parameters of butenafine using B3LYP/6-31+G (d, p) basis set method.The electronic transitions have been calculated in the water environment using PCM model, TD-DFT/B3LYP/6-31+G(d,p) shows the charge transfer within the molecule.

The Homo-lumo of the butenafineillustrates more clearly about the involvement of density of charge transfer between the acceptor and donor groups. The density of states of the butenafine is also studied. The change in thermodynamic parameters relates heat capacity, entropy and enthalpy with changing temperature. The correlations between the thermodynamic parameters and temperatures are obtained.

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