



## **DFT STUDIES, STRUCTURAL DETERMINATION, CHEMICAL PROPERTIES AND TOPOLOGICAL ANALYSIS OF 1-ACETYL-2-(4-ETHOXY-3-METHOXYPHENYL) CYCLOPROPANE**

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### **Abstract**

In the present study, structural, wave functional, electronic and charge transfer properties of 1 acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane is investigated by making the use of DFT tools Gaussian 09 W, and Gauss View. The optimized geometrical parameters, wave functional properties like reduced density gradient, chemical bonding and electron localization function are reported. The calculated energies of HOMO and LUMO have been found to represent the electron excitation properties. Spectroscopic wave numbers (IR) is investigated computationally and experimentally. The Mulliken and natural atomic charge distribution also were calculated.

### **Keywords**

Mulliken, Gaussian, DFT, NBO, wavefunction.

### **INTRODUCTION:**

Cyclopropane does not occur naturally but derivatives are known in some fatty acids. These cyclopropanes were also used in the medicinal field for general anaesthetics [1]. Cyclopropane itself is mainly of theoretical interest but many of its derivatives are of commercial or biological significance [2]. Acetyl with cystein has been used to cure lung disease [3].

In the past decades, density functional theoretical (DFT) calculation is an effective tool to predict the molecular structure, charge transfer interaction, and inter- and intramolecular hydrogen bonding. Various reports are accessible in the literature concerning the structure and DFT studies [4]. Many reports have commended the success of DFT in comparison to other conventional methods, in computing molecular and chemical properties such as geometries, harmonic frequencies and energies [5]. DFT approach is found to be the best compromise between accuracy and computational cost in comparison to other conventional methods [6].



In the present work 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane was optimized by the DFT method. Vibrational assignments were calculated at B3LYP method. The HOMO LUMO analysis was reported to study molecular reactivity and stability of the molecule. Topology analysis was done to determine the electron density and localization of electron. Geometry optimization such as bond length, bond angle and dihedral angle has been carried out in the gas phase by B3LYP level of DFT. Global reactivity descriptors (ionization potential, electron affinity, electron negativity, global hardness, softness, electrophilicity index and chemical potential) were predicted with the help of HOMO LUMO values. The energy gap value suggests the possibility of charge transfer within the molecule. The intra and intermolecular interactions which exist within the compound is analyzed by different methods namely the topological analysis LOL, ELF and the reduced gradient of the density.

### COMPUTATIONAL DETAILS

In this study, the computational analyses are conducted by the Gaussian09W software. The molecular geometry of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane is initially optimized from B3LYP/6-31 G (d) basis sets. The molecule is viewed by Gauss view 5.0 animation program. The molecular interactions of the compound is studied and analyzed by NBO 3.1 and HOMO-LUMO calculations. The ELF, LOL and NCI are analyzed using Multiwfn software and VMD 1.9.3 is used to visualize the results.

### OPTIMIZED GEOMETRY:

The optimized structure of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane is calculated at B3LYP/6-311++G (d, p) levels. The optimized molecular structure along with numbering of atoms and geometric parameters such as bond length, bond angle and dihedral angle of the title molecule is obtained using Gaussian09 software as shown in Figure 1. The bond length, bond angle and dihedral angle parameter are shown in Table 1.

**Table 1. DFT optimized geometrical parameters (bond length, bond angle and dihedral angle) of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane.**

Bond length	values	Bond angle	Values	Dihedral angle	Values
C <sub>1</sub> -O <sub>2</sub>	1.4307	O <sub>2</sub> -C <sub>1</sub> -H <sub>14</sub>	109.6	H <sub>14</sub> -C <sub>1</sub> -O <sub>2</sub> -C <sub>3</sub>	-61.5
C <sub>1</sub> -H <sub>14</sub>	1.0969	O <sub>2</sub> -C <sub>1</sub> -H <sub>15</sub>	109.4	H <sub>15</sub> -C <sub>1</sub> -O <sub>2</sub> -C <sub>3</sub>	56.9
C <sub>1</sub> -H <sub>15</sub>	1.0966	O <sub>2</sub> -C <sub>1</sub> -H <sub>16</sub>	107.7	C <sub>16</sub> -C <sub>1</sub> -O <sub>2</sub> -C <sub>3</sub>	177.6
C <sub>1</sub> -C <sub>16</sub>	1.5161	C <sub>1</sub> -O <sub>2</sub> -C <sub>3</sub>	118.8	O <sub>2</sub> -C <sub>1</sub> -C <sub>16</sub> -H <sub>17</sub>	60.7
O <sub>2</sub> -C <sub>3</sub>	1.3644	O <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub>	116.5	O <sub>2</sub> -C <sub>1</sub> -C <sub>16</sub> -H <sub>18</sub>	-179.7
C <sub>3</sub> -C <sub>4</sub>	1.412	C <sub>3</sub> -C <sub>4</sub> -C <sub>5</sub>	119.8	O <sub>2</sub> -C <sub>1</sub> -C <sub>16</sub> -H <sub>19</sub>	-59.7
C <sub>4</sub> -C <sub>5</sub>	1.3878	C <sub>3</sub> -C <sub>4</sub> -O <sub>20</sub>	121.6	C <sub>1</sub> -O <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub>	-175.9
C <sub>4</sub> -O <sub>20</sub>	1.3732	C <sub>4</sub> -C <sub>5</sub> -C <sub>6</sub>	121.8	O <sub>2</sub> -C <sub>3</sub> -C <sub>4</sub> -C <sub>5</sub>	178.5



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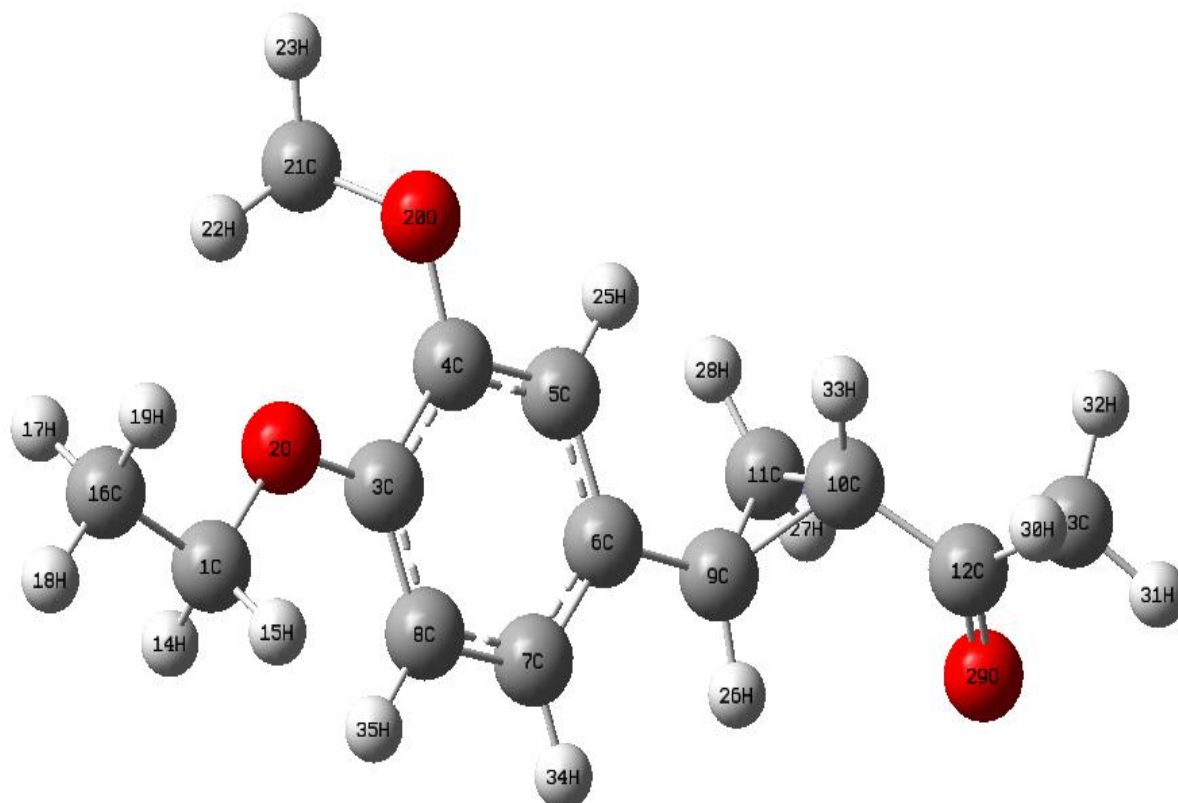
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C <sub>5</sub> -C <sub>6</sub>	1.4022	C <sub>6</sub> -C <sub>5</sub> -H <sub>25</sub>	121.4	C <sub>8</sub> -C <sub>3</sub> -C <sub>4</sub> -O <sub>20</sub>	-177.0
C <sub>5</sub> -H <sub>25</sub>	1.0843	C <sub>5</sub> -C <sub>6</sub> -C <sub>7</sub>	117.6	C <sub>3</sub> -C <sub>4</sub> -C <sub>5</sub> -C <sub>6</sub>	0.2
C <sub>6</sub> -C <sub>7</sub>	1.3947	C <sub>7</sub> -C <sub>6</sub> -C <sub>9</sub>	119.6	C <sub>3</sub> -C <sub>4</sub> -O <sub>20</sub> -C <sub>21</sub>	-69.3
C <sub>6</sub> -C <sub>9</sub>	1.4891	C <sub>6</sub> -C <sub>7</sub> -C <sub>8</sub>	121.3	C <sub>4</sub> -C <sub>5</sub> -C <sub>6</sub> -C <sub>7</sub>	0.5
C <sub>7</sub> -C <sub>8</sub>	1.3962	C <sub>6</sub> -C <sub>7</sub> -H <sub>34</sub>	119.6	H <sub>25</sub> -C <sub>5</sub> -C <sub>6</sub> -C <sub>7</sub>	179.9
C <sub>7</sub> -H <sub>34</sub>	1.0846	C <sub>7</sub> -C <sub>8</sub> -H <sub>35</sub>	119.0	C <sub>5</sub> -C <sub>6</sub> -C <sub>7</sub> -C <sub>8</sub>	-0.5
C <sub>8</sub> -H <sub>35</sub>	1.0817	C <sub>6</sub> -C <sub>9</sub> -C <sub>10</sub>	120.5	C <sub>5</sub> -C <sub>6</sub> -C <sub>7</sub> -H <sub>34</sub>	179.6
C <sub>9</sub> -C <sub>10</sub>	1.5443	C <sub>6</sub> -C <sub>9</sub> -C <sub>26</sub>	114.5	C <sub>5</sub> -C <sub>6</sub> -C <sub>9</sub> -C <sub>10</sub>	47.1
C <sub>9</sub> -H <sub>26</sub>	1.0846	C <sub>9</sub> -C <sub>10</sub> -C <sub>12</sub>	117.3	C <sub>5</sub> -C <sub>6</sub> -C <sub>9</sub> -H <sub>26</sub>	-173.5
C <sub>10</sub> -C <sub>11</sub>	1.5151	C <sub>9</sub> -C <sub>10</sub> -H <sub>33</sub>	115.5	C <sub>6</sub> -C <sub>7</sub> -C <sub>8</sub> -H <sub>35</sub>	-179.5
C <sub>10</sub> -C <sub>12</sub>	1.4909	C <sub>9</sub> -C <sub>11</sub> -H <sub>27</sub>	116.9	C <sub>6</sub> -C <sub>9</sub> -C <sub>10</sub> -C <sub>12</sub>	137.7
C <sub>10</sub> -H <sub>33</sub>	1.084	C <sub>9</sub> -C <sub>11</sub> -H <sub>28</sub>	118.6	C <sub>6</sub> -C <sub>9</sub> -C <sub>10</sub> -C <sub>33</sub>	-6.0
C <sub>11</sub> -H <sub>27</sub>	1.0833	C <sub>10</sub> -C <sub>12</sub> -C <sub>13</sub>	116.3	C <sub>6</sub> -C <sub>9</sub> -C <sub>11</sub> -H <sub>27</sub>	-145.2
C <sub>11</sub> -H <sub>28</sub>	1.0833	C <sub>10</sub> -C <sub>12</sub> -O <sub>29</sub>	121.7	C <sub>6</sub> -C <sub>9</sub> -C <sub>11</sub> -H <sub>28</sub>	1.3
C <sub>12</sub> -C <sub>13</sub>	1.5147	C <sub>12</sub> -C <sub>13</sub> -H <sub>30</sub>	110.0	C <sub>9</sub> -C <sub>10</sub> -C <sub>12</sub> -C <sub>13</sub>	-140.0
C <sub>12</sub> -O <sub>29</sub>	1.2172	C <sub>12</sub> -C <sub>13</sub> -H <sub>31</sub>	110.1	C <sub>9</sub> -C <sub>10</sub> -C <sub>12</sub> -O <sub>29</sub>	39.4
C <sub>13</sub> -H <sub>30</sub>	1.0949	C <sub>12</sub> -C <sub>13</sub> -C <sub>32</sub>	110.0	C <sub>10</sub> -C <sub>12</sub> -C <sub>13</sub> -H <sub>30</sub>	57.6
C <sub>13</sub> -H <sub>31</sub>	1.0891	C <sub>1</sub> -C <sub>16</sub> -H <sub>17</sub>	110.8	C <sub>10</sub> -C <sub>12</sub> -C <sub>13</sub> -H <sub>31</sub>	178.9
C <sub>13</sub> -H <sub>32</sub>	1.095	C <sub>1</sub> -C <sub>16</sub> -H <sub>18</sub>	109.8	C <sub>10</sub> -C <sub>12</sub> -C <sub>13</sub> -H <sub>32</sub>	-59.9
C <sub>16</sub> -H <sub>17</sub>	1.0922	C <sub>1</sub> -C <sub>16</sub> -H <sub>19</sub>	110.7	C <sub>4</sub> -O <sub>20</sub> -C <sub>21</sub> -H <sub>22</sub>	62.9
C <sub>16</sub> -H <sub>18</sub>	1.0932	C <sub>4</sub> -O <sub>20</sub> -C <sub>21</sub>	116.3	C <sub>4</sub> -O <sub>20</sub> -C <sub>21</sub> -H <sub>23</sub>	-177.8
C <sub>16</sub> -H <sub>19</sub>	1.092	O <sub>20</sub> -C <sub>21</sub> -H <sub>22</sub>	111.3	C <sub>4</sub> -O <sub>20</sub> -C <sub>21</sub> -H <sub>24</sub>	-59.4
O <sub>20</sub> -C <sub>21</sub>	1.4326	O <sub>20</sub> -C <sub>21</sub> -H <sub>23</sub>	105.9		
C <sub>21</sub> -H <sub>22</sub>	1.0915	O <sub>20</sub> -C <sub>21</sub> -H <sub>24</sub>	110.4		
C <sub>21</sub> -H <sub>23</sub>	1.0896				
C <sub>21</sub> -H <sub>24</sub>	1.0958				



**Figure 1: 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane optimized molecular structure with numbering system**

The bond lengths ( $C_1-C_{16}$ ), ( $C_{10}-C_{11}$ ) and ( $C_{12}-C_{13}$ ) are larger than the C-C bond and this is due to the electron transfer from lone pair oxygen to the carbon atom. Bond lengths ( $C_7-C_8$ ) and ( $C_4-C_5$ ) is lesser than actual bond length this is due to the presence of hydrogen atom attached to the carbon atom. ( $C_5-C_6$ ) and ( $C_3-C_4$ ) are approximately in the same bond length. ( $C_1-H_{14}$ ), ( $C_1-H_{15}$ ) and ( $C_{13}-H_{35}$ ) are found to be larger, which is due to the existence of single bond. The calculated bond length of  $C_{12}-O_{29}$  and  $C_3-O_2$  is  $1.2172\text{\AA}$  and  $1.3644\text{\AA}$  respectively. The bond length differences in the C-O groups are due to different environments of oxygen. ( $C_4-C_5-C_6$ ) and ( $C_6-C_7-C_8$ ) are higher than  $120^\circ$  indicating the presence of hyper conjugate interaction. ( $C_6-C_5-H_{25}$ ) bond angle is larger than  $120^\circ$  indicates the delocalization of charge in methyl group. The decrease in bond angle ( $C_9-C_{10}-C_{12}$ ) ( $117.3805$ ) and increase in ( $C_3-C_4-O_{20}$ ) ( $121.6149$ ) and ( $C_{10}-C_{12}-O_{29}$ ) ( $121.7414$ ) shows the possibility of hydrogen bond. Small changes in bond length can be explained in terms of substitution effect due to the charge distribution on the carbon atom of the benzene ring [7].



## NBO ANALYSIS:

The natural bonding orbital calculations were performed using the NBO 3.1 program level basis set. The natural bond orbital (NBO) analysis has proved to be an effective tool for chemical interpretation of hyper conjugative interaction and electron density transfer from the filled lone pair electron [8].

The energy  $E(2)$  associated with each donor (i) to an acceptor (j) delocalization is determined from the second order perturbation method

$$E(2) = \Delta E_{ij} = \frac{q_i F(i,j)^2}{\epsilon_j - \epsilon_i}$$

Where,  $q_i$  represents the population of donor orbital tenancy. The larger the  $E(2)$  values, the more intensive is the interaction between electron donors and electron acceptors. The result of NBO analysis on the title molecule is summarized in table 2.

**Table 2. Second order perturbation theory analysis of Fock matrix in NBO basis at basic set**

Donor (i)	ED	Acceptance (j)	ED	E(2) (kcal/mol <sup>-1</sup> )	E <sub>j</sub> -E <sub>i</sub> a-u	F(i-j) a-u
$\pi(C_3-C_8)$	1.97638	$\pi^*(C_4-C_5)$	0.3509	17.92	0.29	0.065
	1.97638	$\pi^*(C_6-C_7)$	0.36225	19.24	0.30	0.069
	1.97638	$\pi^*(C_6-C_7)$	0.36225	188.43	0.02	0.080
$\pi(C_4-C_5)$	1.70342	$\pi^*(C_3-C_8)$	0.39224	19.00	0.28	0.067
		$\pi^*(C_6-C_7)$	0.36225	19.01	0.30	0.068
$\pi(C_6-C_7)$	1.67468	$\pi^*(C_3-C_8)$	0.39225	19.60	0.27	0.066
		$\pi^*(C_4-C_5)$	0.3509	20.02	0.28	0.067
$\sigma(C_9-C_{10})$	1.89001	$\sigma^*(C_{10}-C_{11})$	0.03247	6.39	0.84	0.067
LP <sub>1</sub> O <sub>20</sub>	1.95113	$\sigma^*(C_3-C_4)$	0.04025	5.75	1.03	0.069

The intramolecular hyperconjugative interactions are formed by the orbital overlap between  $\pi(C-C)$  and  $\pi^*(C-C)$  bond orbitals which results intramolecular charge transfer (ICT) causing stabilization of the system. The  $E(2)$  values for interactions between bonding and antibonding orbitals is found to be the highest for donors  $\pi(C_3-C_8)$  and  $\pi(C_6-C_7)$  corresponding to acceptors



$\pi^*$  (C<sub>6</sub>-C<sub>7</sub>) and  $\pi^*$  (C<sub>4</sub>-C<sub>5</sub>), having E(2) values of 188.43 kcal/mol and 20.02 kcal/mol respectively. These interactions contribute greatest to the stabilization of the molecule.

The notable interaction from  $\pi$ (C<sub>6</sub>-C<sub>7</sub>) conjugate to the antibonding orbitals of  $\pi^*$ (C<sub>4</sub>-C<sub>5</sub>) with stabilization energy (20.02) respectively. The delocalization of  $\pi$  electron from  $\pi$ (C<sub>6</sub>-C<sub>7</sub>) and  $\pi$ (C<sub>3</sub>-C<sub>8</sub>) to corresponding acceptor of antibonding orbitals as  $\pi^*$ (C<sub>6</sub>-C<sub>7</sub>) and  $\pi^*$ (C<sub>3</sub>-C<sub>8</sub>) with values 19.24, 19.60 KJ/Mol respectively. The electron density of the conjugated  $\pi$ (C<sub>3</sub>-C<sub>8</sub>) bond (1.67468) and  $\pi^*$ (C<sub>3</sub>-C<sub>8</sub>), (C<sub>4</sub>-C<sub>5</sub>) bonds (0.39 and 0.35) of the aromatic ring revealed the strong electron delocalization. The interaction of atoms in the molecule contain lone pair of electron localized on O<sub>20</sub> (LP1) with the adjacent atom  $\sigma^*$  (C<sub>3</sub>-C<sub>4</sub>) with stabilization value of 5.75 kJ/mol.

### MULLIKEN ATOMIC CHARGES:

Total atomic charge on the atoms of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane was obtained by Mulliken population analysis. Mulliken charges which are, of course, the cheapest and fastest way to calculate charges. However, this method tends to give qualitative results and is very much dependent on basis set as well condition of medium. Mulliken population analysis have numerous flaws, such as atomic charges that are extremely sensitive to the type of orbitals used, sometimes unphysical negative values for charges, and show unreasonable charge distribution for molecules with high ionic characteristics [9,10]. The atomic charge values were acquired by the Mulliken population analysis which have been calculated using B3LYP level of theory with 6-311++G(d,p) as basis set. Table 3 lists the calculated Mulliken atomic charge values of the title molecule. Figure 2 shows the graphical representation of the analysis of Mulliken atomic charges.

The oxygen atom has more negative charges where the hydrogen atom H<sub>26</sub> (0.283561) has more positive charge than the other hydrogen atoms. The result suggests that the atoms bonded to the hydrogen atom and all oxygen atoms are electron acceptor and the charge transfer takes place from H to C. The highest electronegative atom O<sub>29</sub> which makes the neighbouring atoms C<sub>10</sub> and C<sub>12</sub> are positive.

**Table 3. Mulliken charge distribution of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane**

Atoms	Mulliken atomic charges	Natural charges
C	-0.015411	-0.02565
O	-0.121031	-0.55795
C	-0.414860	0.28386



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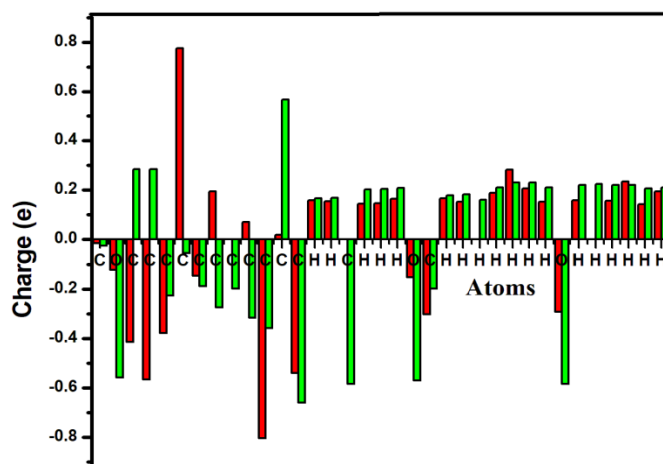
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C	-0.566918	0.28399
C	-0.37739	-0.22638
C	0.775503	-0.05661
C	-0.145200	-0.18748
C	0.193699	-0.27316
C	0.234396	-0.19752
C	0.069472	-0.31542
C	-0.804782	-0.35759
C	0.018781	0.56721
C	-8.541022	-0.66107
H	0.159020	0.16604
H	0.154785	0.16863
C	-0.675064	-0.58469
H	0.144850	0.20350
H	0.146570	0.20487
H	0.164886	0.20805
O	-0.151481	-0.57080
C	-0.301004	-0.19725
H	0.166459	0.17887
H	0.151646	0.18164
H	0.128003	0.16109
H	0.188429	0.21141
H	0.283561	0.23139
H	0.207578	0.23049
H	0.153112	0.21135
O	-0.291371	-0.58508
H	0.159202	0.22152
H	0.178222	0.22390
H	0.156840	0.22023
H	0.234183	0.22076
H	0.142320	0.20643
H	0.194365	0.21143



**Figure 2: Mulliken charge distribution chart of 1 acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane**

### HOMO-LUMOENERGY GAP:

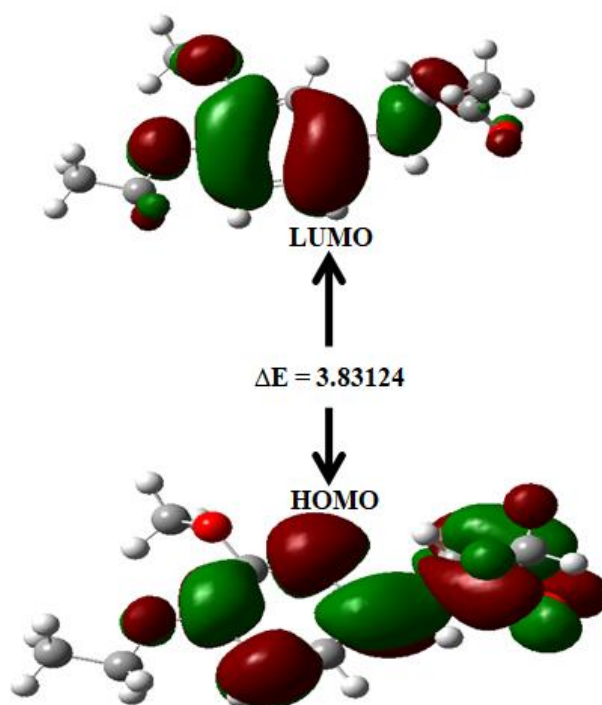
There are several ways to calculate energies. The first and the simplest one involves the difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied orbital (LUMO) of a neutral system [11]. The HOMO and LUMO energy gap can be used to explain the molecular stability and chemical reactivity. This form corresponds to the frozen orbital approximation as the ground state properties are used to calculate excitation values. The HOMO and LUMO energy gap has been calculated by DFT level. The visualization of FMOs (HOMO and LUMO) and HOMO-LUMO gap are shown in figure 3.

$$\text{HOMO energy} = 8.2435$$

$$\text{LUMO energy} = 4.47226$$

$$\text{HOMO-LUMO energy gap} = 3.83124$$





**Figure 3: HOMO-LUMO orbitals of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane.**

**Table 4. Global reactivity descriptors of the title molecule**

Molecular Properties	Mathematical Description	Energy(eV)
$E_{HOMO}$	Energy of HOMO	-8.2435
$E_{LUMO}$	Energy of LUMO	-4.41226
Energy Gap	$\Delta E_g = E_{HOMO} - E_{LUMO}$	3.83124
Ionization Potential (IP)	$IP = -E_{HOMO}$	8.2435
Electron Affinity (EA)	$EA = -E_{LUMO}$	4.41226
Electronegativity ( $\chi$ )	$\chi = -1/2(E_{LUMO} + E_{HOMO})$	6.32188
Chemical potential ( $\mu$ )	$\mu = 1/2(E_{LUMO} + E_{HOMO})$	-6.32788
Global Hardness( $\eta$ )	$\eta = 1/2(E_{LUMO} - E_{HOMO})$	3.83124
Softness (S)	$S = 1/2\eta$	1.9156
Electrophilicity index ( $\omega$ )	$\omega = \mu^2/2\eta$	5.2257



The chemical reactivity descriptors of compounds such Ionization Potential (I) value is 8.2435, electron affinity (EA) value is 4.41226, Electro negativity (X) value is 6.32788, Chemical potential ( $\mu$ ) value is -6.32788, global hardness ( $\eta$ ), softness value is 3.83126, Electrophilicity index ( $\omega$ ) value is 5.2257 were obtained. The calculated chemical reactivity values are set out in Table 4. The energy gap between HOMO and LUMO is obtained as 3.83124. So the stability of the molecule is high.

The smaller energy gap leads the molecule to be less stable and more reactive while large energy gap leads to more stable less reactive systems [12]

#### **VIBRATIONAL ANALYSIS:**

Vibrational spectroscopy has been shown effective in the identification of functional groups of organic compounds as well as in studies on molecular conformations [13]. The molecular structure of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane consists of 35 atoms which undertake 99 fundamental normal mode vibrations. The FT-IR vibrational wave numbers were determined theoretically by the DFT method using the basis set B3LYP/6-31+G(d,p). The normal mode vibrational frequencies are calculated at the B3LYP level was scaled by 0.967 in order to reasonably agree with experimental data. The experimentally observed and computed scaled wavenumbers have presented in Table 5. The computed scaled wave numbers agree well with experimental wave numbers. The experimental and the simulated FT-IR spectra is given in figure 4.

**Table 5. Detailed assignments of experimental and theoretical wave numbers of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane**

Wave number	IR intensity	vibration
3134	—	$\gamma_{asy}C_{11}-H_{28}$ $\gamma_{asy}C_{11}-H_{27}$
3119	—	$\gamma_{sy}C_8-H_{35}$ $\gamma_{sy}C_7-H_{34}$
3093	—	$\gamma_{sy}C_5-H_{25}$ $\gamma_{sy}C_{11}-H_{27}$ $\gamma_{sy}C_{10}-H_{33}$
3083	—	$\gamma_{sy}C_7-H_{34}$ $\gamma_{sy}C_8-H_{35}$ $\gamma_{sy}C_9-H_{26}$
3074	—	$\gamma_{sy}C_{10}-H_{33}$ $\gamma_{sy}C_9-H_{26}$
3068	—	$\gamma_{sy}C_{10}-H_{33}$



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		$\gamma_{sy}C_9-H_{26}$
3061	–	$\gamma_{asy}C_{13}-H_{30}$ $\gamma_{asy}C_{13}-H_{31}$ $\gamma_{asy}C_{21}-H_{22}$ $\gamma_{asy}C_{21}-H_{23}$
3047	–	$\gamma_{sy}C_{11}-H_{27}$ $\gamma_{sy}C_{11}-H_{28}$
3047	–	$\gamma_{asy}C_{16}-H_{19}$ $\gamma_{asy}C_{16}-H_{17}$
3029	–	$\gamma_{asy}C_{16}-H_{18}$ $\gamma_{asy}C_{16}-H_{17}$
3010	–	$\gamma_{asy}C_{21}-H_{22}$ $\gamma_{asy}C_{21}-H_{34}$
3000	2985	$\gamma_{asy}C_{13}-H_{30}$ $\gamma_{asy}C_{13}-H_{32}$
2961	–	$\gamma CH_3$
2953	–	$\gamma_{asy}C_1-H_{15}$ $\gamma_{asy}C_1-H_{14}$
2945	–	$\gamma_{asy}C_{13}-H_{30}$ $\gamma_{asy}C_{13}-H_{31}$
2932	2935	$\gamma_{sy}C_{21}-H_{24}$ $\gamma_{sy}C_{21}-H_{23}$
2916	–	$\gamma_{sy}C_1-H_{15}$ $\gamma_{sy}C_1-H_{14}$
1730	–	$\gamma O_{29}-C_{12}$
1612	1686	$\gamma CC$
1574	1590	$\gamma CC$
1514	1519	$\gamma_{in}C_1-C_{14}$ $\gamma_{in}C_1-C_{15}$
1497	–	$\beta_{in}CH_2$
1490	–	$B_{out}CH_3$
1479	–	$\beta_{in}CH_2$ $\beta_{in}CH_2$
1465	–	$\beta_{in}CH_3$ $\beta_{in}CH_2$



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1464	–	$\beta_{in}CH_2$ $\beta_{in}CH_2$
1454	–	$\beta_{out}CH_3$
1454	–	$\beta_{in}CH_2$
1444	–	$\beta_{in}CH_2$
1414	–	$\beta_{in}CH_2$ $\gamma CC$
1431	–	$\beta_{out}CH_2$
1395	1391	$\beta_{out}CH_2$
1374	–	$\beta_{out}CH_2$
1363	–	$\beta_{in}CH_3$
1334	–	$\gamma C_{10}-H_{33}$
1300	1311	$\gamma CC$
1272	–	$\beta_{out}CH_2$
1272	1272	$\beta_{out}CH_2$
1253	1240	$\gamma C_5-H_{25}$
1220	–	$\gamma C_9-H_{26}$
1203	–	$\beta_{in}CH_2$
1180	–	$\beta_{out}CH_3$
1167	–	$\beta_{in}CH_2$
1156	–	$\beta_{in}CH_2$ $\beta_{out}CH_3$
1145	–	$\gamma CC$ $\gamma CH$
1142	1144	$\beta_{out}CH_3$
1134	–	$\gamma CH$ $\beta_{in}CH_2$
1115	–	$\gamma_{asy}CH$ $\beta_{out}CH_3$
1107	–	$\beta_{in}CH_2$ $\beta_{in}CH_3$
1084	–	$\beta_{out}CH_2$



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1050	–	$\gamma C_8-H_{35}$ $\beta_{out}CH_2$
1043	–	$\gamma C-O$
1029	1032	$\beta_{out}CH_2$
1026	–	$\beta_{out}CH_3$
1013	–	$\beta_{out}CH_2$
949	961	$\beta_{in}CH_2$
924	–	$\beta_{in}CH_2$ $\beta_{in}CH_2$
921	920	$\beta_{in}CH_3$
911	–	$\gamma CC$ $\gamma C_8-H_{35}$
893	–	$\gamma C_7-H_{34}$
876	–	$\gamma C_5-H_{25}$
862	–	$\beta_{out}CH_2$
821	–	$\beta_{in}CH_2$
805	–	$\beta_{in}CH_2$
785	–	$\beta_{in}CH_2$ $\gamma C_8-H_{35}$ $\gamma C_7-H_{34}$
766	769	$\beta_{in}CH_2$ $\beta_{out}CH_2$
763	–	$\beta_{in}CH_2$
712	–	$\beta_{in}CH_2$
693	–	$\beta_{in}CH_2$
635	627	$\beta_{in}CH$
604	–	$\beta_{in}CH_2$
582	–	$\beta_{in}CH_3$ $\beta_{in}CH_2$



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575		$\beta_{in}CH_3$ $\beta_{in}CH_2$
523		$\beta_{in}CH_3$ $\gamma CC$
453		$\beta_{in}CH_3$ $\beta_{in}CH_2$
466		$\gamma CC$ $\beta_{in}CH_2$
422		$\beta_{in}CH_3$
409		$\beta_{in}CH_3$
351		$\beta_{in}CH_3$ $\beta_{in}CH_2$
349		$\beta_{in}CH_3$
312		$\gamma CC$ $\beta_{in}CH_3$
273		$\beta_{in}CH_3$ $\beta_{in}CH_2$
257		$\beta_{in}CH_3$ $\beta_{in}CH_2$
248		$\beta_{in}CH_3$ $\beta_{in}CH_2$
202		$\beta_{in}CH_3$ $\beta_{in}CH_2$



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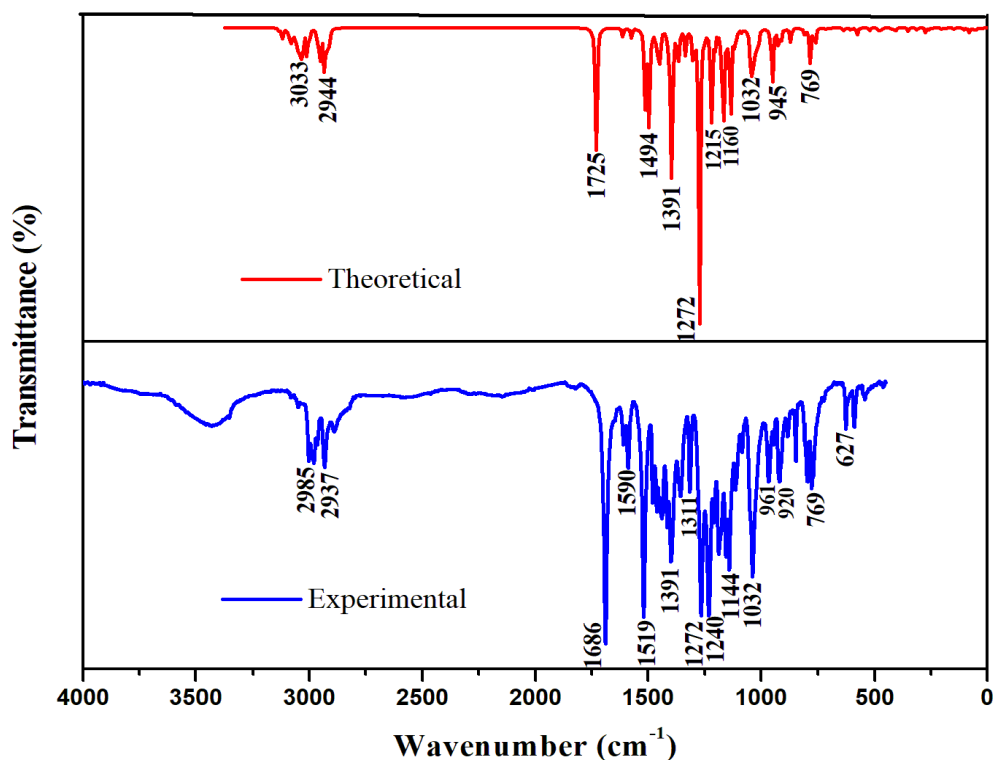
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185		$\beta_{in}CH_3$
151		$\beta_{in}CH_3$
144		$\beta_{in}CH_3$
134		$\beta_{in}CH_3$ $\beta_{in}CH$
125		$\beta_{in}CH_3$
104		$\beta_{in}CH_3$ $\beta_{in}CH_2$
101		$\beta_{in}CH_3$
81		$\beta_{in}CH_3$ $\beta_{in}CH_2$
64		$\beta_{in}CH_3$ $\beta_{in}CH_2$
53		$\beta_{in}CH_3$
35		$\beta_{in}CH_3$ $\beta_{in}CH_2$
21		$\beta_{in}CH_3$



**Figure 4: Experimental and simulated FT-IR spectra of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane**

#### **METHOXY GROUP VIBRATIONS:**

When the electron donating methyl (CH<sub>3</sub>) group is directly attached to an oxygen atom, the C–H stretching and bending bands can shift energetically due to the associated electronic effects. This causes a spread of O–CH<sub>3</sub> stretching vibrational bands over a larger region than that of the C–CH<sub>3</sub> group. There is one methoxy (-OCH<sub>3</sub>) group attached to phenyl ring of the title compound. Basically, nine fundamentals are assigned to the CH<sub>3</sub> group, namely, symmetric stretch; in-plane stretch (*i.e.*, in-plane hydrogen deformation modes), symmetric bending, in-plane rocking, out-of-plane rocking, twisting hydrogen bending modes and out-of-plane hydrogen bending modes inclusive of CH<sub>3</sub> out-of-plane stretch [14]. The deviation in wavenumber was because of the slight difference in the orientation of the methoxy group. The C–H in plane bending of CH<sub>3</sub> group is observed at 920 cm<sup>-1</sup>(weak) and out plane bending is observed at in 1144 cm<sup>-1</sup> (strong) and 1032 cm<sup>-1</sup> (very strong) in FTIR. DFT calculation gives the mode for CH<sub>3</sub> stretching is observed at 2961 cm<sup>-1</sup>. The theoretical in plane bending modes





were seen at 1363  $\text{cm}^{-1}$ , 1107  $\text{cm}^{-1}$ , 924  $\text{cm}^{-1}$ , 582  $\text{cm}^{-1}$ , 575  $\text{cm}^{-1}$ , 523  $\text{cm}^{-1}$ , 453  $\text{cm}^{-1}$ , 351  $\text{cm}^{-1}$ , 349  $\text{cm}^{-1}$ , 312  $\text{cm}^{-1}$ , 273  $\text{cm}^{-1}$ , 257  $\text{cm}^{-1}$ , 202  $\text{cm}^{-1}$ , 185  $\text{cm}^{-1}$ , 151  $\text{cm}^{-1}$ , 144  $\text{cm}^{-1}$ , 134  $\text{cm}^{-1}$ , 125  $\text{cm}^{-1}$ , 104  $\text{cm}^{-1}$  and 101  $\text{cm}^{-1}$ . The dft modes of outplane bending were observed at 1490  $\text{cm}^{-1}$ , 1465  $\text{cm}^{-1}$ , 1454  $\text{cm}^{-1}$ , 1180  $\text{cm}^{-1}$ , 1156  $\text{cm}^{-1}$ , 1142  $\text{cm}^{-1}$ , 1115  $\text{cm}^{-1}$  and 1026  $\text{cm}^{-1}$ .

### **C-H VIBRATIONS:**

The hetero aromatic structure shows the presence of C-H stretching vibration in the region 3100–3000  $\text{cm}^{-1}$  which is the characteristic region for the ready identification of C-H stretching vibration [15]. These vibrations are not found to be affected due to the nature and position of the substituent. In the present study, two medium FT-IR bands are observed at 2985  $\text{cm}^{-1}$  (weak), 2937  $\text{cm}^{-1}$  (weak) and 1519  $\text{cm}^{-1}$  (weak) for symmetrical and asymmetrical stretching, respectively. In our calculations, C-H stretching vibration is predicted at 3000  $\text{cm}^{-1}$ , 2932  $\text{cm}^{-1}$ , 1514  $\text{cm}^{-1}$  and 1253  $\text{cm}^{-1}$  by B3LYP/6-311G (d) level, which are in good agreement with the experimental assignments. The C-H in plane bending of the title compound in FTIR is obtained at 627  $\text{cm}^{-1}$  and the corresponding theoretical value is observed at 635  $\text{cm}^{-1}$ . The other theoretical C-H asymmetric stretching vibrations were found at 3134  $\text{cm}^{-1}$ , 3061  $\text{cm}^{-1}$ , 3047  $\text{cm}^{-1}$ , 3029  $\text{cm}^{-1}$ , 3010  $\text{cm}^{-1}$  and 2953  $\text{cm}^{-1}$ . The symmetrical stretching vibrations are seen at 3119  $\text{cm}^{-1}$ , 3093  $\text{cm}^{-1}$ , 3083  $\text{cm}^{-1}$ , 3074  $\text{cm}^{-1}$ , 3068  $\text{cm}^{-1}$ , 2953  $\text{cm}^{-1}$ , 2945  $\text{cm}^{-1}$  and 2916  $\text{cm}^{-1}$ .

### **C-C VIBRATIONS:**

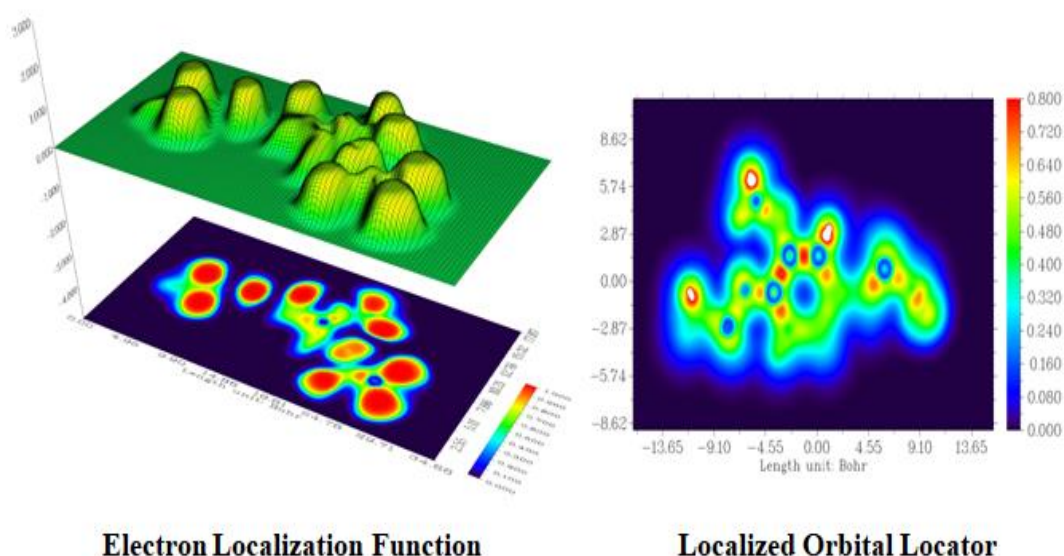
The aromatic compounds of C-C ring stretching vibrations exhibit in the range of 1625-1453  $\text{cm}^{-1}$  [16]. In the aromatic six-membered rings viz., phenyl regions, there are two or three bands due to skeletal vibrations. Here in this study, the observed theoretical frequencies assigned to C-C aromatic phenyl ring vibrations are observed 1612  $\text{cm}^{-1}$ , 1574  $\text{cm}^{-1}$  and 1300  $\text{cm}^{-1}$ . The strong stretching C-C bands of FT-IR peak at 1686  $\text{cm}^{-1}$  (very strong), 1590  $\text{cm}^{-1}$  (medium) and 1311  $\text{cm}^{-1}$  (weak) in the FT-IR spectrum have a close agreement with the theoretical value.

### **CH<sub>2</sub> vibrations:**

For the assignments of CH<sub>2</sub> group frequencies, basically six fundamentals can be associated to each CH<sub>2</sub> group namely, CH<sub>2</sub>sy–symmetric stretch; CH<sub>2</sub>asy – asymmetric stretch; CH<sub>2</sub> sciss–scissoring and CH<sub>2</sub> rock – rocking modes which belong to inplane vibrations. In addition to that, CH<sub>2</sub>wag – wagging and CH<sub>2</sub> twist – twisting modes of CH<sub>2</sub> group would be expected to be for out-of-plane symmetry species [17]. The theoretical in plane bending were seen at 1497  $\text{cm}^{-1}$ , 1479  $\text{cm}^{-1}$ , 1465  $\text{cm}^{-1}$ , 1464  $\text{cm}^{-1}$ , 1454  $\text{cm}^{-1}$ , 1449  $\text{cm}^{-1}$ , 1444  $\text{cm}^{-1}$ , 1414  $\text{cm}^{-1}$ , 1156  $\text{cm}^{-1}$ , 1134  $\text{cm}^{-1}$ , 1107  $\text{cm}^{-1}$ , 821  $\text{cm}^{-1}$ , 763  $\text{cm}^{-1}$ , 604  $\text{cm}^{-1}$ , 422  $\text{cm}^{-1}$ . For the title molecule, the in-plane bending vibrations are assigned at 961  $\text{cm}^{-1}$  (weak) and 769  $\text{cm}^{-1}$  (weak) in FT-IR while the related simulating frequencies are found at 949  $\text{cm}^{-1}$  and 766  $\text{cm}^{-1}$ . The most vital point is that certain CH<sub>2</sub> modes are generally coupled with bending vibrations.

## ELF-LOL

The topological analysis of the electron localization function and localized orbital locator are the tool used for performing covalent bond analysis. The covalent region has high LOL value, the electron depletion regions between valance shell and inner shell are shown in by the blue circle around nuclei [17,18]. Colour shade maps of the ELF and LOL for the compound are displayed in Figure 5.

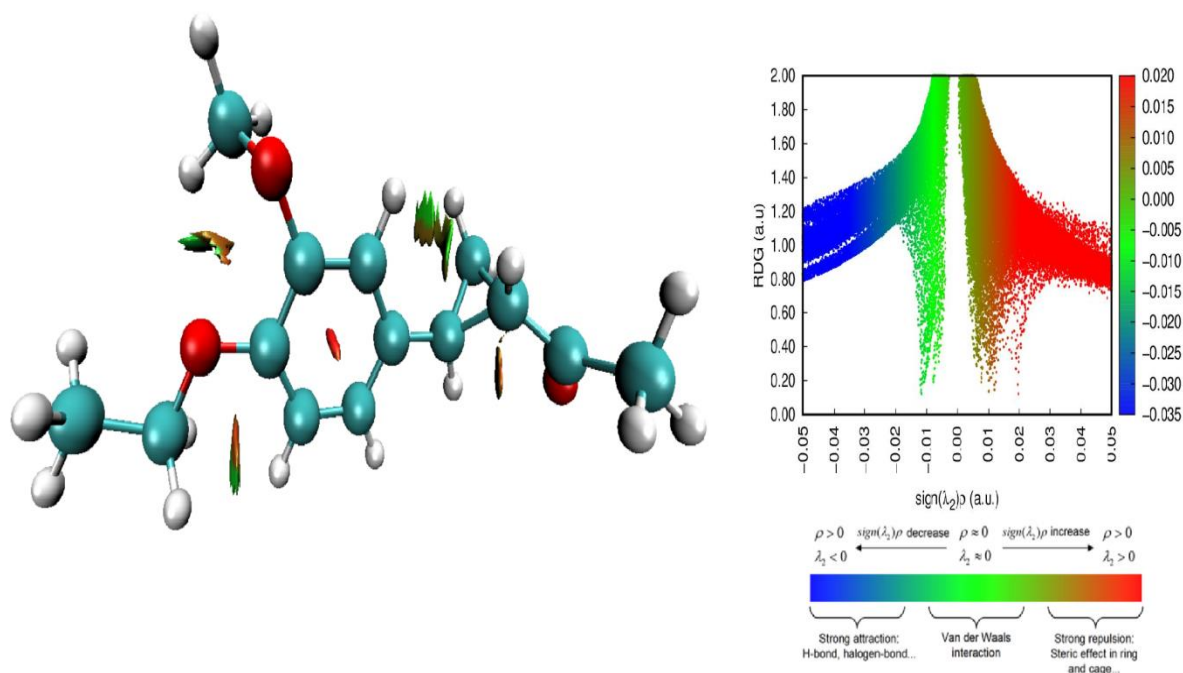


**Figure 4: colour filled map of ELF and LOL of the molecule**

A large ELF or LOL value in the region indicates high localization of electron or a nuclei shell in that region. The red colour indicates intrude into interstitial space between boundary atoms. The value of ELF and LOL ranges from 0.0 to 1.0. Where values greater than 0.5 describes the region of electron localization. Where as values less than 0.5 indicates the presence of highly localized bonding and non bonding electron. Red colour is in < 1 range [19,20]. The red colour around hydrogen atoms with maximum value bespeaks the presence of bonding and nonbonding electrons. High ELF or LOL values indicated by red colour around hydrogen atoms shows high localization of electrons due to the ubiety of covalent bond, a lone pair of electrons or a nuclear shell in that region. The central region of some hydrogen atom in the LOL is white as the electron density exceeds the upper limit of colour scale.

## RDG ANALYSIS:

RDG forms the base of reactivity studies Gradient feature has been implemented. Interaction move from weak to strong reaction and vice versa [21]. Reduced Density Gradient is an electron density of the dimensionless quantity and its first derivative. By mapping  $\rho(r)$  against  $\text{sign}(\lambda_2)$ , nature and strength of interactions present in the molecule can be understood [22]. A Greater enticing ( $\lambda^2 < 0$ ) or repulsive ( $\lambda^2 > 0$ ) non covalent interaction demonstrated by a higher absolute value electron density at the interaction of critical points [23]. 2D scatter plot and the 3D RDG isosurface densities of the title molecule are depicted in figure 6.



**Figure 6: 2D scatter and Isosurface density plots of 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane.**

Red colour indicates repulsive interactions, blue colour indicates hydrogen bonding and green colour indicates vanderwaals interaction. In the RDG isosurface, the red spike shows the steric repulsion observed in the centre of aromatic ring. The RDG scatter graph manifests the red contour between 0.10 and 0.20 au clarifies the repulsive exchange contribution. This plot illustrates the steric repulsive force between the aromatic carbon atoms. While the red-green mixed spike regions of interactions are observed between the ring hydrogen and neighbouring oxygen.

## CONCLUSION



In the present work, molecular structure, vibrational frequency (FTIR) and quantum chemical calculations studies have been formed on 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane in order to identify its structural and spectroscopic features. Experimental FT-IR spectral analysis was performed and recorded wave numbers were compatible with calculated wave numbers. The FMO demonstrates the energy gap of the title molecule 3.8312 eV which indicates 1-acetyl-2-(4-ethoxy-3-methoxyphenyl) cyclopropane is more chemically stable. NBO analysis is used to contemplate the hyper-conjugative interaction of the molecule stability and charge delocalization. With the help of RDG plot surface analysis, the interactions take place (Vanderwaals interaction and steric effect) within the molecule is classified.

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