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Synthesis, spectroscopic and dft based quantum chemical study of (2*E*)-1-(4-chlorophenyl)-3-[4-(propan-2-yl) phenyl] prop-2-en-1-one

Nutan V. Sadgir [1*], Sunil L. Dhonnar [1], Bapu Jagdale[1] and Bhagyashri Waghmare[2]

[1*]Department of Chemistry, L.V.H. Arts, Science, and Commerce College, Panchavati,
Nashik (M.S) India.

[2]Department of Chemistry M.S.G. Arts, Science and Commerce College, Malegaon,
Nashik (M.S.) India

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Abstract: The (2*E*)-1-(4-chlorophenyl)-3-[4-(propan-2-yl) phenyl] prop-2-en-1-one was synthesized by condensation reaction between 4-isopropyl benzaldehyde and 4-chloroacetophenone in ethanol as solvent. The synthesized compound was characterized by FT-IR and Proton NMR techniques. The optimized molecular geometry, bond length, Mulliken atomic charges, bond angles, vibrational frequencies, the dipole moment of title compound have been computed by density functional theory (DFT) using a standard B3LYP method with 6-311++G (d, p) basis set by using Gaussian-03 (W) package. The various thermochemical properties, global chemical reactivity descriptors, FMO analysis and molecular electrostatic potential (MEP) were also investigated at the same level of theory.

Keywords: DFT, B3LYP, HOMO-LUMO, MESP

1. INTRODUCTION

Chalcone is a common name for the, α-β unsaturated ketones that are made by condensing an aromatic aldehyde with substituted acetophenone in the presence of a base [1]. Kestanecki coined the term "chalcones," and Tambor's other chalcone names are benzalacetophenone and phenyl styryl ketone. Chalcones are chemically 1, 3-diaryl-2-propene-1-ones, which have two aromatic rings connected by a three-carbon, -unsaturated carbonyl system (-CHβ=CHα-C=O). [2, 3] On both the phenyl ring and a conjugated double bond, chalcones have a fully delocalized electron mechanism.

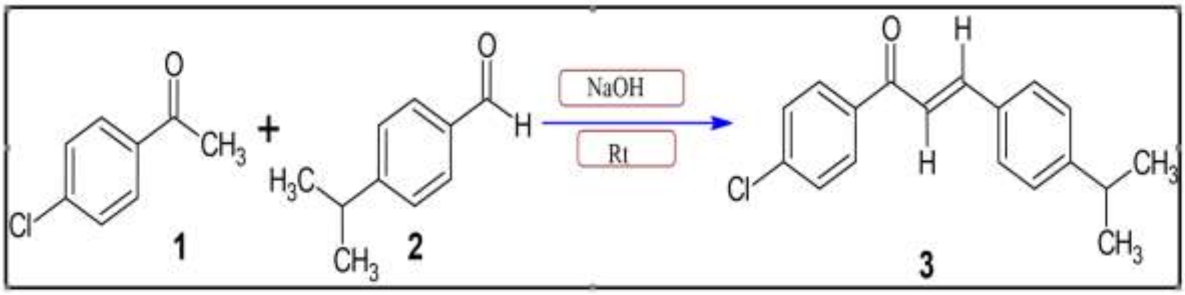
Antimicrobial[4-6]], anti-inflammatory[7], analgesic[8], antiplatelet [9], anti-ulcerative[10], antimalarial[11], anticancer[12], antiviral[13], antileishmanial [14], antioxidant [15], antitubercular [16], antihyperglycemic [17], immunomodulatory[18], antifungal[19], cardiovascular[20], and anti-HIV[21] properties have been recorded for chalcone and its derivatives.

Different molecular and spectroscopic properties of molecules are studied using density functional theory. Most researchers have been working on various computational models to study structural, chemical, spectroscopic, and other properties of Organic compounds nanomaterials, metal complexes for theoretical aspects in recent years [22-28]. Therefore, to study structural, electronic and spectroscopic properties of (2*E*)-1-(4-chlorophenyl)-3-[4-(propan-2-yl) phenyl] prop-2-en-1- one, Here we combined theoretical and experimental study of the title compound of DFT method at B3LYP functional and 6-311++G (d, p) basis sets combination.

2. EXPERIMENTAL

2.1 Material and physical measurement: The Chemicals used for synthesis are of AR grade. Melting point was determined in an open capillary and uncorrected. FT-IR spectrum of title compound was recorded on Shimadzu spectrometer. The sample was prepared using a KBr disc technique. The ^{1}H NMR was recorded on Brucker Avance 500 MHZ spectrometer using TMS as an internal standard. The sample is dissolved in CDCl3. Reaction was monitored by thin layer chromatography by using n-hexane and ethyl acetate solvent system.

2.2 Synthesis of (2*E*)-1-(4-chlorophenyl)-3-[4-(propan-2-yl) phenyl] prop-2-en-1-one: The title compound was synthesized by well-known Claisen-Schmidt condensation of 4-chloroacetophenone (0.01mol) and 4-(propan-2-yl)-benzaldehyde were dissolved in ethyl alcohol and 5 ml of NaOH was added dropwise to the reaction mixture, progress of the reaction was monitored by Thin Layer Chromatography. After completion of the reaction was quenched by pouring into the crushed ice, then neutralized by diluting HCl, the precipitate obtained was filtered the crude product dried and crystallized by using ethyl alcohol. The reaction is shown in scheme 1.



Scheme 1: Synthesis of (2*E*)-1-(4-chlorophenyl)-3-[4-(propan-2-yl) phenyl] prop-2-en-1-one

2.3 Computational details: The DFT calculations were performed on an Intel (R) Core (TM) i7 personal computer using Gaussian-03 program package. The DFT /B3LYF method with 6-311++G (d, p) basis set level. [29-36] were used to study the geometry of the title compound.

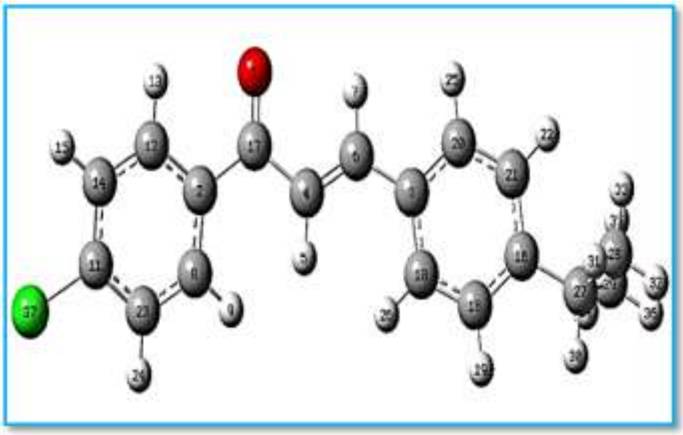


Fig. 1: Optimized structure of title compound at DFT/B3LYP method with 6-311++G (d,p) basis set

3. RESULTS AND DISCUSSION

3.1 Spectral Data of the title compound: FT-IR (KBr,cm^{-1})IR- (C=O) 1625 cm^{-1} , (C=C) 1540-1583 cm^{-1}, aromatic(C-H) 2943 cm^{-1} ,(C-Cl) 550cm^{-1}, ^{1}H NMR (500 MHz,CDCl3, δ/ppm): 1.2 (d, 6H), 2.6(m, 1H), 7.4 (d, 1H J= 15.5 Hz), 7.76 (d, 1H J=15.5 Hz) ,7.4 (d,2H), 7.5(d 2H), 7.34(d 2H), 7.42(d,2H)

3.2 Molecular Geometry: The title compound total 37 atoms are present. The optimize structure of the title compound with the labelling of the atoms shown are **Fig.2** The molecular structure of the title compound contains two six membered rings in which, one is 4-isopropyl substituted ring attach to C=C of enone system (ring B) and another ring is a 4-Chloro substituted ring attach to carbonyl group (ring A).The structural entities; bond length and bond angle are obtained for the optimized structure are shown in **table 1**.The presence of α, β-unsaturated ketone is indicated by the shorter bond length O$_2$-C$_{17}$ and C$_4$-C$_6$ are found to be 1.225 Å, 1.347 Å respectively. The C $_{11}$-Cl$_{37}$, 1.756 Å and found within the expected range. All the bond lengths and bond angles are in good agreement with the structure of the title compound [37-40].The dipole moment of the title compound is 4.49 Debye which indicates polar nature of tile compound. The calculated (C$_{17}$ C$_4$ C$_6$ C$_3$) torsion angle is 179.03^{0} confirms the molecule exhibits E configuration.

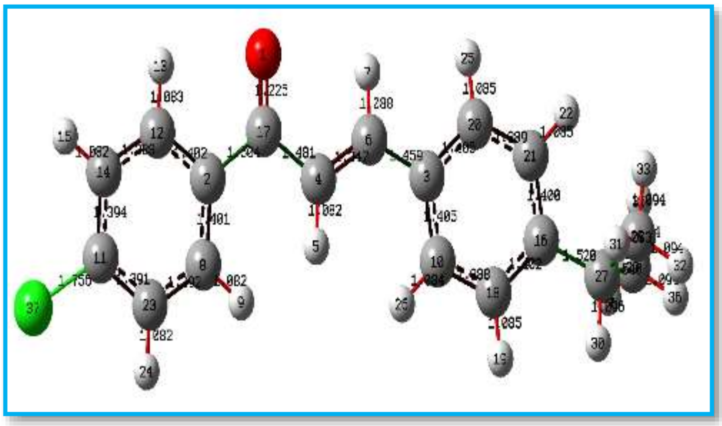


Fig.2: Bond length of the title compound

Table 1: The bond length and dihedral angle of title compound calculated at B3LYP/6-311++G (d, p) level

Connectivity	**Bond Length [Å]**	**Connectivity**	**Bond Angle [°]**	**Connectivity**	**Bond Angle [°]**
O1-C17	1.225	O1-C17-C4	121.69	C12-C14-H15	120.09
C2-C12	1.402	O1-C17-C2	119.55	C12-C2-C17	117.83
C2-C8	1.401	C2-C8-H9	120.75	H13-C12-C14	120.51
C2-C17	1.504	C2-C12-H13	118.35	C14-C11-C23	121.20
C3-C6	1.459	C2-C12-C14	121.14	C14-C11-Cl37	119.42
C3-C10	1.405	C2-C17-C4	118.75	C16-C18-H19	119.16
C3-C20	1.406	C2-C8-C23	120.99	C16-C21-H22	119.99
C4-C6	1.347	C3-C6-H7	115.90	C16-C21-C20	121.02
C4-H5	1.082	C3-C6-C4	127.98	C16-C27-C28	111.84
C4-C17	1.481	C3-C10-H26	120.10	C16-C27-C29	111.82
C6-H7	1.088	C3-C20-H25	119.01	C16-C27-H30	106.82
C8-H9	1.082	C3-C20-C21	121.36	C18-C16-C21	117.67
C8-C23	1.392	C3-C10-C18	120.857	C18-C10-H26	119.04
C10-H26	1.084	C4-C6-H7	116.11	C18-C16-C27	120.67
C10-C18	1.388	H5-C4-C6	120.96	C20-C21-H22	118.99
C11-Cl37	1.756	H5-C4-C17	118.57	C21-C20-H25	119.63
C11-C14	1.394	C6-C4-C17	120.46	C21-C16-C27	121.67
C12-H13	1.083	C6-C3-C10	123.663	C23-C11-Cl37	119.38
C12-C14	1.388	C6-C3-C20	118.80	C27-C28-H31	111.28
C14-H15	1.082	C8-C23-C11	119.08	C27-C28-H33	111.30
C16-C18	1.402	C8-C23-H24	120.77	C27-C28-H32	110.46
C16-C21	1.400	C8-C2-C17	123.60	C27-C29-H36	110.46
C16-C27	1.520	C8-C23-H24	120.77	C27-C29-H34	111.27
C18-H19	1.085	C8-C2-C12	118.56		
C20-H25	1.085	H9-C8-C23	118.25		
C20-C21	1.389	C10-C3-C20	117.53		
C21-H22	1.085	C10-C18-C16	121.56		
C23-H24	1.082	C11-C14-H15	120.07		
C27-C28	1.540	C11-C23-H24	120.15		
C27-C29	1.540	C11-C14-C12	119.02		

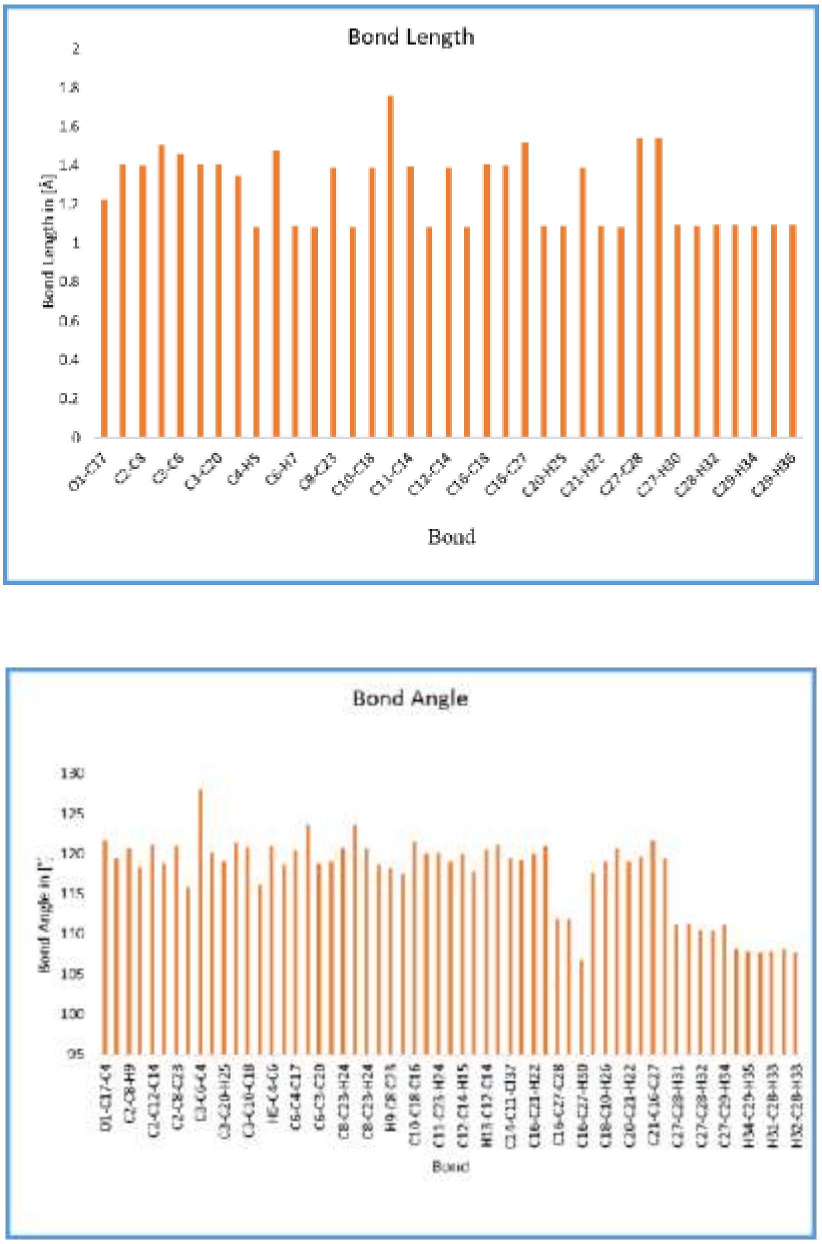


Fig.3: (a) The Graphical representation of bond length and **(b)** Bond Angle

3.3 Vibrational frequency Assignment: Experimental IR spectrum was recorded in the region of 4000-500 cm^{-1} is shown in fig.4a. Comparison of vibrational assignment of title compound by Experimental IR spectrum with theoretical IR spectrum Title compound contains total 37 atoms with 86 fundamental modes of vibration. Theoretical and experimental IR spectrum is shown in **Fig 4a** and **4b.**Carbonyl stretching frequency of alpha beta unsaturated ketone in the range of 1700-1600 cm^{-1}, the experimental carbonyl stretching frequency of title compound 1643 cm^{-1} and theoretically it is 1648 cm^{-1} this confirms presence of carbonyl group, lower value of IR frequency is due to conjugation of enone system with the aromatic rings. Experimental IR at 1554cm^{-1} and theoretical IR at 1560cm^{-1} is due to the Ar-C=C- stretching vibrations. Out of plane bending vibrations experimentally at 972.12 cm^{-1} and theoretically at 972cm^{-1} indicates the trans geometry of alkene. The C-H experimental and theoretical is stretching vibration 3047 cm^{-1} and 3054 cm^{-1} respectively

Table 2: Selected Experimental and theoretical vibrational assignments of title compound

Selected mode no.	Calculated (Scaled) frequencies in cm^{-1}	Calculated IR intensity	Experimental Frequencies cm^{-1}	Assignment
101	3062.586444	7.6235	-	υ C-H of ring a and b
99	3054.040487	19.4394	3047	υ_{asymm} C-H of ring b
95	2975.569568	33.4327	-	υ C-H of isopropyl group
93	2969.446087	86.6014	-	υ asymm of C-H of isopropyl group
88	1648.831373	158.0349	1643	υ C=C,C=O
87	1587.721532	62.4122	1585	υ C=C,C=O
86	1569.120377	653.7728	-	υ C=C and CH (Ring b)
85	1560.641711	84.0718	1554	υ C=C of ring b
83	1533.984862	63.3761	1500	υ C=C of ring a
79	1445.035773	12.8212	-	υ C=C and CH (Ring a and b)
77	1429.914524	0.0256	1423	υ C=C and CH (Ring a)
71	1307.156514	185.7343		υ C=C
67	1269.540845	88.4362	1257	υ C=C and CH (Ring b)
62	1176.765782	142.112	-	υ C=C of ring b
60	1151.550883	91.1439	1153	υ C=C and CH (Ring a)
55	1057.401161	122.1066	1037	υ C=C and CH (Ring b)
53	1001.982216	118.6453	-	υ
51	986.188057	149.2858	972	υ_{γ} CH (C=C)
45	924.8090	0.0004	910	υ CH (Ring a)υ
42	860.767246	1.5088	852	υ CH(C=C)
30	629.36311	1.3765	636	υ CH (Ring b)

υ - stretching; asym-asymmetric; sym-symmetric; def-deformation; β-In-plane bending; γ-out of plane bending, ρ-rocking, Γ-torsion

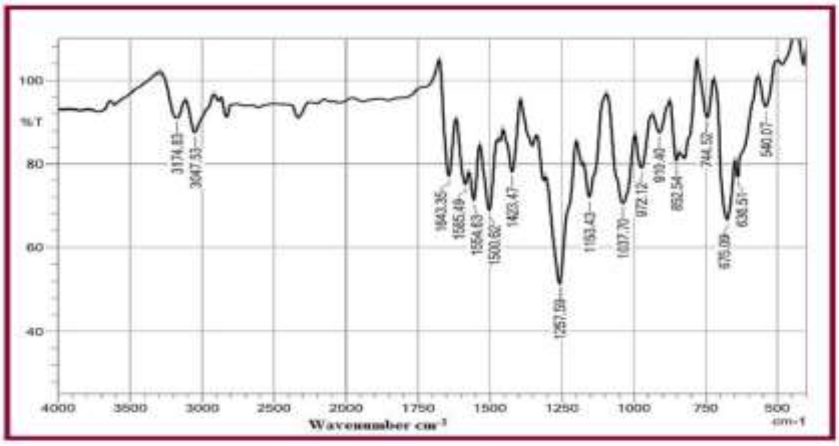


Fig.4a: FT-IR spectrum experimental

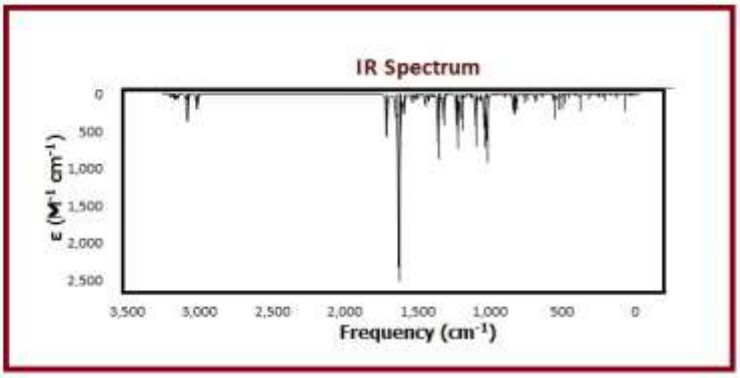


Fig.4b: Simulated FTIR spectrum of the title compound

3.4 Global Chemical reactivity descriptors: Analysis of the Frontier molecular orbitals explained electron excitation from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbitals (LUMO). A molecule with a small frontier orbitals gap is generally associated with a high chemical reactivity, low kinetic stability and is also termed as soft molecules. A hard molecule has a large HOMO-LUMO gap and a soft molecule has a small HOMO-LUMO gap. HOMO-LUMO plot of title compound is shown in **Fig.5** The HOMO-LUMO energy value and energy gap values for title compound were computed by the TD-DFT method at B3LYP/6-311++G (d, p) basis set in gas phase. The computed gas phase HOMO and LUMO energies are -7.2328 eV and -2.7225 eV respectively. Whereas the energy gap of title compound is 3.9891eV. From the HOMO-LUMO energies various chemical reactivity parameters have been derived. The Ionization potential (I), Electron Affinity (A), Chemical hardness (ɳ), Chemical softness (S), Electronic chemical potential (μ), Global Electrophilicity index (ω) parameters were calculated based on Koopman's theorem [41] equation 1-4 [42-43]. The HOMO-LUMO energies and global reactivity parameters are listed in table 5.The global hardness (η) of 1.9945eV, Chemical Softness (S) 0.5014eV, chemical potential (μ) -4.569 eV, electrophilicity Index (ω) 5.233eV suggest the good stability of the compound.

$$\eta = \tfrac{1}{2}\,(I - A)\ldots\ldots \qquad (1)$$

$$S = 1/\eta\ldots.. \qquad (2)$$

$$\mu = -\tfrac{1}{2}\,(I+A)\ldots \qquad (3)$$

$$\omega = \mu^2 / 2\eta\ \ldots.. \qquad (4)$$

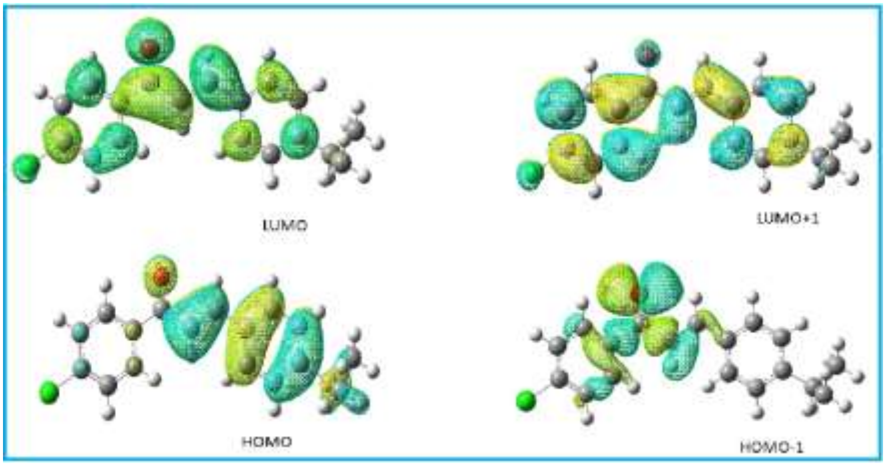


Fig.5: Frontier molecular orbitals of title Molecule

Table 3: Global chemical reactivity indices calculated at B3LYP/6-311G++(d,p) level

Parameters	**B3LYP/6-311++G(d,p)**
E_{LUMO} (eV)	-2.577eV
E_{HOMO} (eV)	-6.561eV
$\Delta E = E_{LUMO}-E_{HOMO}$ (eV)	3.98eV
Electron affinity (A)	2.577eV
Ionization Energy (I)	6.561eV
Global Hardness (η)	1.9945eV
Chemical Softness (S)	0.501eV
Electronic chemical potential (μ)	-4.569eV
Global electrophilicity Index (ω)	5.223Ev

3.5 Mulliken atomic charges: The Mulliken atomic charges play an important role to know the chemical reactivity of compounds. The Mulliken atomic charges calculated and reported on title compound is shown in **Fig.6 ,** As indicated in **table 4** The $C_{2,}$ C3 atom carries the higher positive charge 1.094,1.035 respectively. Among other carbon atoms and therefore expected to be the site for nucleophilic attack on title compound, whereas C_8 carries a higher negative charge -1.163 in all carbon atoms. The Molecular electrostatic potential plot is shown in **Fig.8,** this gives information about the chemical reactivity of sites. As seen from the figure that, the regions exhibiting the negative electrostatic potential are localized to the carbonyl group. The dipole moment of the title compound is 4.49 Debye indicates polar nature.

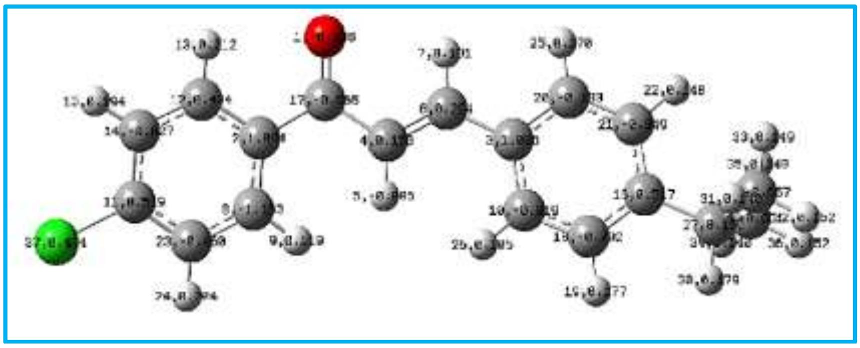


Fig. 6: Mulliken atomic charges representation

Table 4: Mulliken atomic charges of Title compound at B3LYP/6-311++G (d, p) level

Atom	Charge	Atom	Charge
1 O	-0.238	20 C	-0.133
2C	1.094	21 C	-0.349
3C	1.034	22 H	0.148
4C	0.153	23 C	-0.460
5H	-0.086	24 H	0.204
6C	0.294	25 H	0.170
7H	0.191	26 H	0.105
8C	-1.163	27 C	0.150

9H	0.119	28 C	-0.657
10C	-0.919	29 C	-0.661
11C	0.519	30 H	0.179
12C	0.434	31 H	0.140
13H	0.212	32 H	0.152
14C	-0.827	33 H	0.149
15H	0.194	34 H	0.140
16C	0.517	35 H	0.148
17C	-0.965	36 H	0.152
18C	-0.792	37Cl	0.474
19H	0.177		

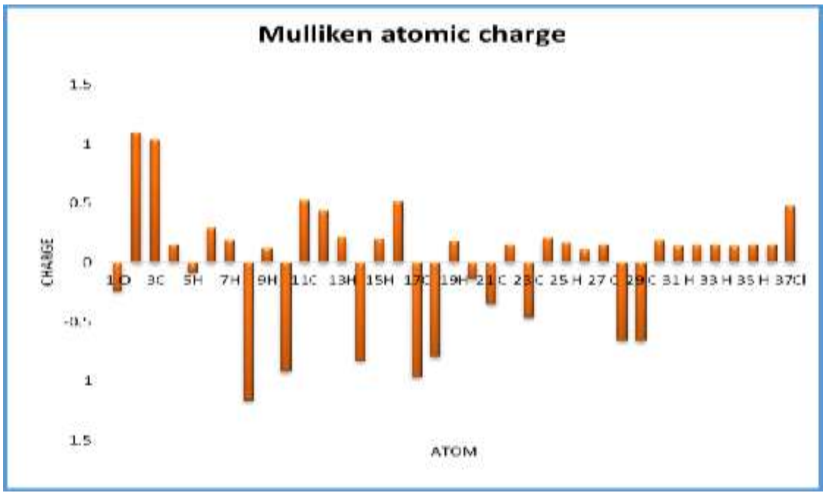


Fig.7: The Mulliken atomic charge plot of title molecule

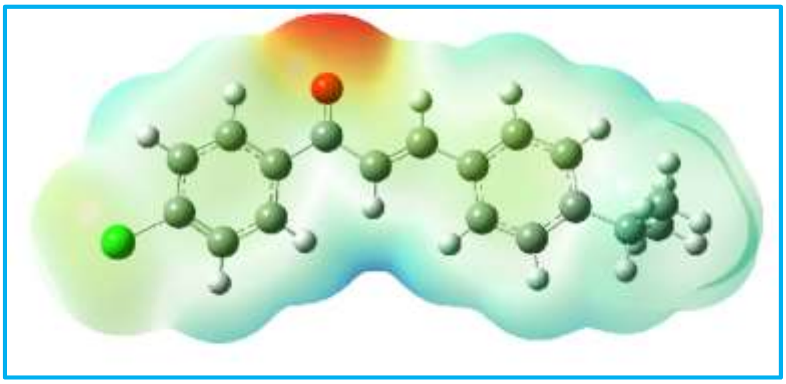


Fig.8: Molecular electrostatic potential surface of title compound

4. CONCLUSION

The (2*E*)-1-(4-chlorophenyl)-3-[4-(propan-2-yl) phenyl] prop-2-en-1-one was synthesized and characterized by using FT-IR and ^{1}H NMR. To study different structural and electronic parameters by using Density Functional Theory B3LYP/6-311++G (d, p) basis set used. The properties like the

HOMO-LUMO energy gap, molecular electrostatic potential, and global reactivity descriptors have been explored using the same level of method. The dipole moment of title compound is 4.49 Debye shows polar nature. C_2 carbon carries higher a higher positive charge among all the other carbon atoms and whereas C_8 carries a higher negative charge in all carbon atoms In addition to this energy of HOMO-LUMO energy gap is 3.98 eV, thermodynamic properties like Enthalpy, Entropy, and Polarizability are calculated. From the DFT study gives information about the optimized structure and reactivity of molecule.

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Conflict of interest

The author declares that they have no conflict of interest.

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Corresponding author: Nutan Sadgir,

Department of Chemistry, L.V.H. Arts, Science, and Commerce College, Panchavati,

Nashik (M.S) India. Contact no. 918485811767