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Computational Insights on Molecular Structure, Electronic Properties, and Chemical Reactivity of (*E*)-3-(4-Chlorophenyl)-1-(2-Hydroxyphenyl)Prop-2-en-1-One

VISHNU A. ADOLE[1], PRASHANT B. KOLI[2]*,
RAHUL A. SHINDE and ROHIT S. SHINDE[1]

[1]Department of Chemistry, Mahatma Gandhi Vidyamandir's Arts, Science and Commerce College, Manmad, (Affiliated to SP Pune University, Pune) Nashik-423 104, India.

[2]Department of Chemistry, Arts, Commerce and Science College, Nandgaon, (Affiliated to SP Pune University, Pune) Nashik-423 106, India.

Abstract

In the current examination, (*E*)-3-(4-chlorophenyl)-1-(2-hydroxyphenyl) prop-2-en-1-one has been studied to investigate geometrical entities, electronic properties, and chemical reactivity viewpoints. To inspect structural, spectroscopic, and chemical reactivity aspects, density functional theory method (DFT) at B3LYP/6-311G(d,p) basis set has been employed. The (*E*)-3-(4-chlorophenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one has been synthesized and characterized by FT-IR, ^{1}HNMR, and ^{13}C NMR spectral techniques. The detailed investigation of bond lengths and bond angles is discussed to comprehend the geometrical framework. To explore its chemical behaviour, Mulliken atomic charges, molecular electrostatic potential surface, and electronic parameters are introduced. The imperative exploration of the electronic properties, such as HOMO and LUMO energies, was studied by the time-dependent DFT (TD-DFT) method. The dipole moment of the title molecule is 2.57 Debye with C1 point group symmetry. The most electropositive carbon and hydrogen atoms in the title molecule are C14 and H27 respectively. Amongst aromatic C=C, the C16-C18 is the longest, and C17-C19 is the shortest bond. The molecular electrostatic potential plot predicts the positive electrostatic potential is around hydrogen atoms. The vibrational assignments were made by comparing the experimental FT-IR absorption peaks with the scaled frequencies obtained using computational work. Besides, some significant thermochemical information is obtained using the same basis set using frequencies.

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CONTACT Prashant B. Koli ✉ prashantkoli005@gmail.com 📍 Department of Chemistry, Arts, Commerce and Science college, Nandgaon, District-Nashik.Affiliated to SPPU, Pune, India.

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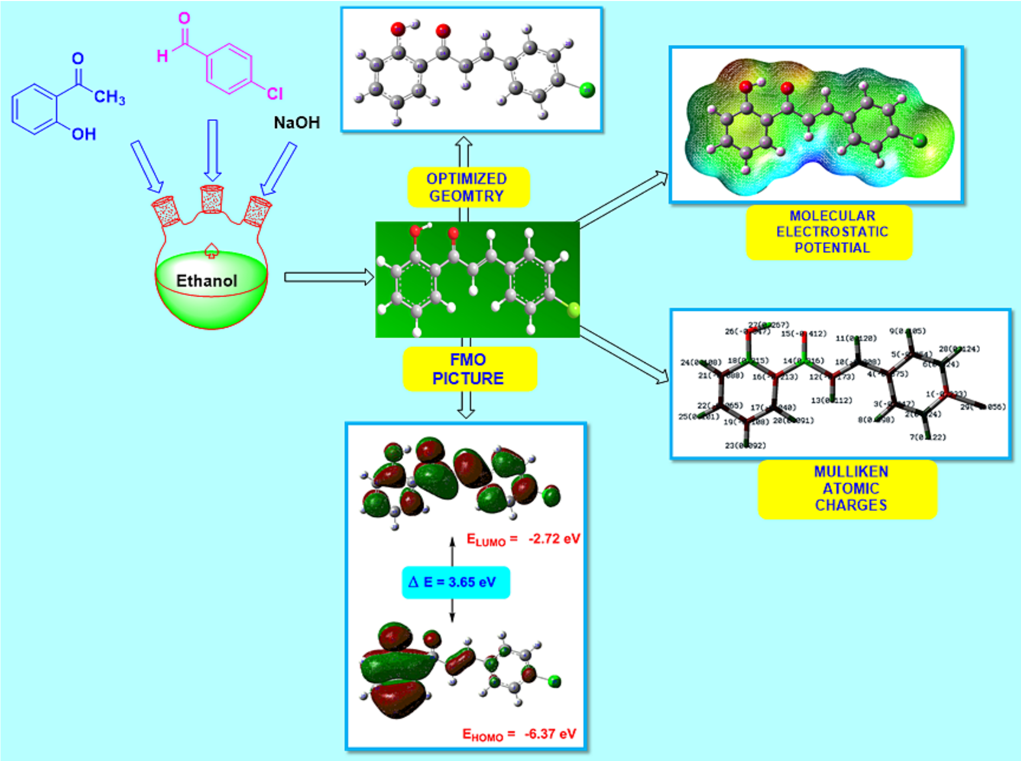


Graphical abstract

Introduction

The rising attention towards chalcone derivatives is the direct consequence of their broad pharmacological applications.[1] Chalcones are naturally occurring biologically potent compounds belonging to the flavonoid family (Figure 1). Apigenin (1), luteolin (2), chrysoeriol (3), and velutin (4) are some important examples of flavones (Figure 2). Synthetically, chalcones are synthesized by Claisen-Schmidt reaction of aromatic ketones and aromatic aldehydes having 1,3- diphenylprop-2-en-1-one as a basic framework. The fantastic medicinal and pharmacological pattern of chalcones includes properties like anticancer,[2] antitumor,[3] anti-diabetics,[4] anti-HIV,[5] antioxidants,[6] antiulcer,[7] antimalarial,[8] cardiovascular,[9] anti-tubercular,[10] antibacterial,[10] antifungal,[12] antiviral,[13] anti-inflammatory,[14] anticonvulsant,[15] antidiuretic,[5] etc. The 2-arylidene indanone derivatives are having a structural framework similar to the chalcones.[16] These compounds have also been explored as biological agents. Besides, chalcones have also been used as versatile intermediates for the synthesis of a variety of heterocyclic compounds having promising therapeutic applications.[17-20] The biologically active aza, thia, and oxa synthetic heterocyclic compounds were synthesized from chalcones.[21-23] Importantly, the chalcone framework can be synthetically manipulated to get a diverse pattern of biological properties.

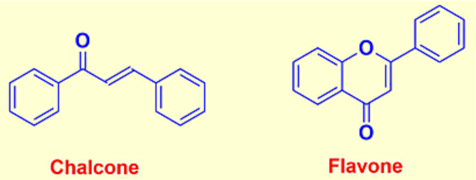


Fig. 1: Structure of chalcone and flavone

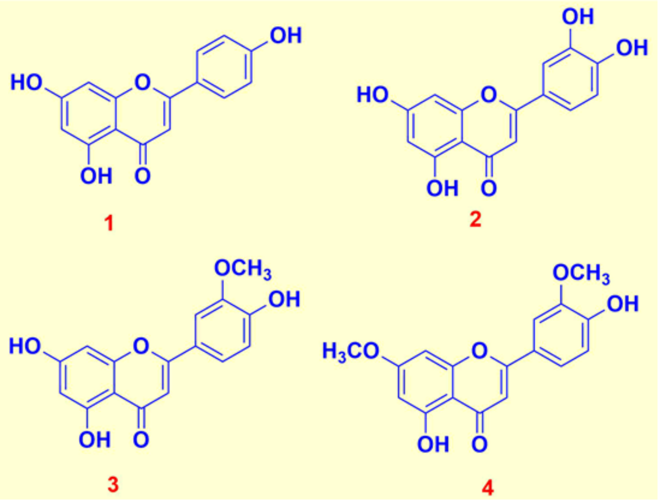


Fig. 2: Some examples of flavones

The DFT computations have been used to study various molecular and spectroscopic properties of the molecules. The compounds like nicotinic acid N-oxide,24 sesquiterpene lactone,[25] mesitylene,[26] 5-nitro-2-(4-nitrobenzyl) benzoxazole,[27] 2-arylidene indanone,[28] 3,5-difluorophenylboronic acid,[29] cyclohexanone oxime,[30] 2-methylpyridine 1-oxide,[31] pycolinaldehydeoxime,[32] o-methoxybenzoates,[33] (E)-1-(4-bromobenzylidene)semicarbazide,[34] 1,5-diphenylpenta-1,4-dien-3-one,[35] 3-(2-Chloro 6-fluorophenyl)-1-(2-thienyl) prop-2-en-1-one,[36] dihydropyrimidinone,[37] 6,8-dichloro-2-(4-chlorophenyl)-4H-chromen-4-one,[38] of 2-[5-(4-chlorophenyl)-4, 5-dihydro-1H-pyrazol-3-yl] phenol,[39] etc. have been studied to explore their structural, electronic, chemical, and spectroscopic facets. In the last decade majority of researchers are working on computational models utilizing some potential nanomaterials for theoretical aspects.[40-43] Utilization of green chemistry principles has been advanced in recent years to reduce the environmental hazard.[44] Considering all these crucial a successful attempt has been made to study structural, electronic, chemical, and spectroscopic properties of the (E)-3-(4-chlorophenyl)-1-(2-hydroxyphenyl) prop-2-en-1-one (4CPHPP). To the best of understanding, this is a primary report on the combined theoretical and experimental study of the title compound 4CPHPP by DFT method at B3LYP/6-311G(d,p) basis set.

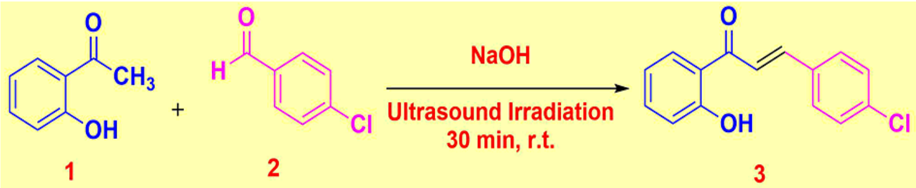
Experimental Details

General Remarks

The chemicals (Make- SD fine chemicals and Avra synthesis) were purchased from Sigma laboratory, Nashik with a high purity of 99 %, and they were used as such without any purification. The FT-IR spectrum of the title compound was recorded on Shimadzu spectrometer. The sample was prepared using a KBr disc technique. The NMR experiment was performed on sophisticated multinuclear FT NMR Spectrometer model Avance-II (Bruker). The compound was dissolved in DMSO-d6. Chemical shifts were reported in ppm relative to tetramethylsilane (TMS) for ^{1}H NMR spectra. The reaction was monitored by thin-layer chromatography using Merck Aluminum TLC plate, silica gel coated with fluorescent indicator F254. All the glass apparatus were cleaned and dried in an oven before use.

Experimental Procedure for the Synthesis of the Title Compound 4CPHPP

The title compound 4CPHPP was Synthesized as per previously reported method.45 In a typical synthesis method 2-hydroxy acetophenone (0.01 mol) and 4-chloro benzaldehyde (0.01 mol) were mixed in ethanol solvent. To this appropriate amount of aqueous NaOH solution was added. Then the alkaline mixture was exposed to ultrasound irradiation. After completion of the reaction (monitored by TLC), the reaction was quenched by pouring onto the crushed ice. It was then acidified, filtered, dried, and recrystallized to give pure crystals of the title compound. The reaction is presented in Scheme 1.



Scheme 1: Synthesis of the title compound 4CPHPP

Computational Method

The molecular structure of 4CPHPP in the ground state (in the gas phase) was optimized by DFT/B3LYP method with a 6-311G(d,p) basis set level, and the optimized structure was used in the vibrational frequency calculations. The molecular geometry optimization has been performed by using Gauss View 4.1 software package. The calculated harmonic vibrational frequencies were scaled by 0.96. The entire calculations were implemented by using Gauss View 4.1 program and Gaussian 03W program package on a computing system.[46] To explore the electronic properties, the theoretical UV-Visible spectra have been investigated by the TD-DFT method with a 6-311G(d,p) basis in the gas phase.

Results and Discussion

Spectral Data of the title Compound 4CPHPP

FT-IR (cm^{-1}) – 3441.01, 3086.11, 2931.80, 1627.92, 1504.48, 1404.18, 1342.46, 1226.73, 1056.99, 786.96; ^{1}H NMR (400 MHz, DMSO-d6); δ (ppm) – 6.98 (m, 2H), 7.19 (m, 2H), 7.43 (m, 2H), 7.52 (m, 1H), 7.83 (m, 2H), 7.89 (m, 2H), 8.13 (m, 1H), 12.69 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d6); δ (ppm) – 117.68, 118.76, 120.06, 121.61, 128.70, 130.37, 130.52, 133.11, 135.68, 136.14, 143.28, 162.45, 193.32.

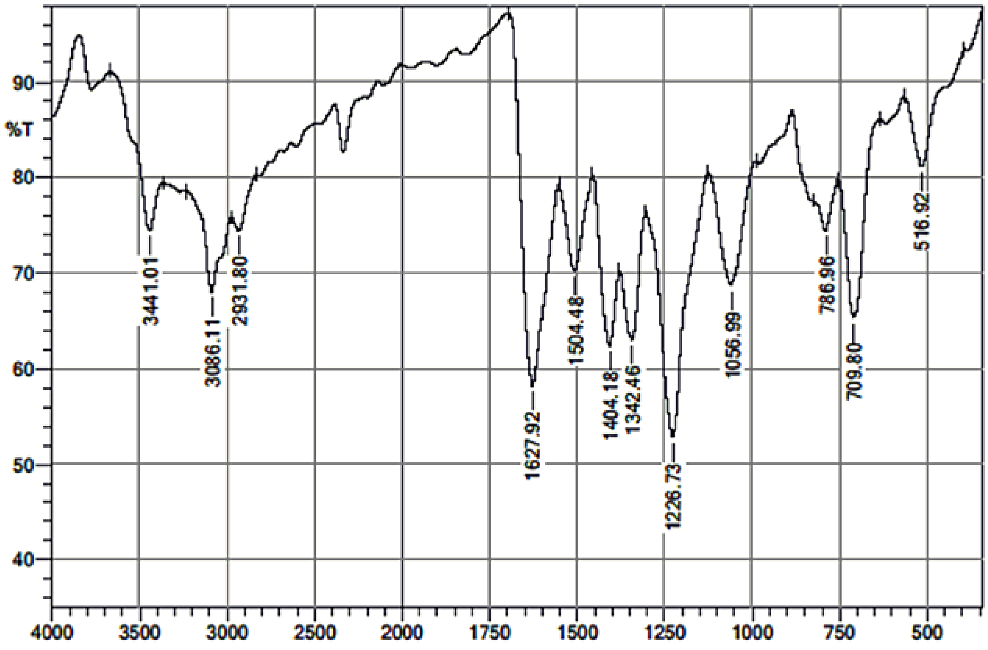


Fig. 3: FT-IR spectrum of the title compound

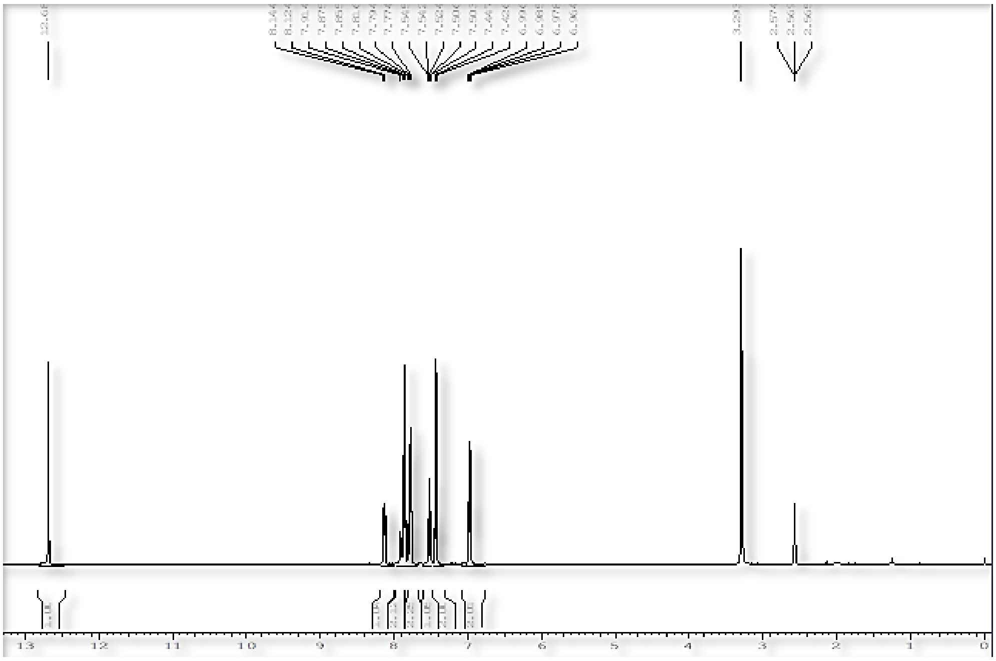


Fig. 4: ^{1}H NMR spectrum of the title compound

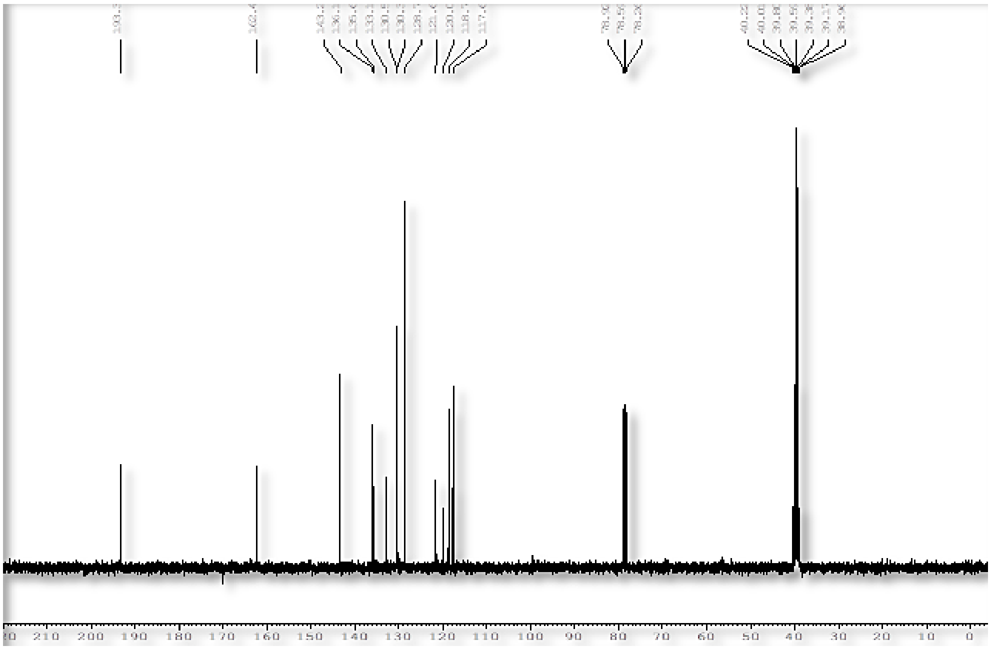


Fig. 5: ^{13}C NMR spectrum of the title compound

The title compound 4CPHPP has been successfully characterized by FT-IR (Figure 3), ^{1}H NMR (Figure 4), and ^{13}C NMR (Figure 5), spectroscopic methods. The important FT-IR absorption signals are 3441.01 cm^{-1} (due to OH stretching vibrations), 3086.11 cm^{-1}(due to Ar-CH stretching vibrations), 1627.92 cm^{-1} (due to C=O and C=C stretching vibrations), and 1504.18 cm^{-1}(Ar C=C stretching vibrations). The important chemical shift value in 1H NMR spectrum is singlet at 12.69 δ which is assigned to O-H proton. The high deshielding is due to the intra-molecular hydrogen bonding between O-H proton and the carbonyl oxygen atom. This is also confirmed in the computational results. Other signals and the total number of protons are exactly matching with the structure of the title compound. The total carbons in the title compound 4CPHPP are 15; however in the ^{13}C NMR spectrum thirteen signals have appeared. This is due to the symmetric nature of the 4-chlorphenyl ring.

Table 1: Optimized geometrical parameters of the title compound at DFT/B3LYP method with a 6-311G(d,p) basis set

Bond lengths (Å)					
C1-C2	1.3944	C6-H28	1.0821	C17-H20	1.0817
C1-C6	1.3901	C10-H11	1.0869	C18-C21	1.4038
C1-Cl29	1.7549	C10-C12	1.3453	C18-O26	1.3353
C2-C3	1.3862	C12-H13	1.0806	C19-C22	1.4019
C2-H7	1.0823	C12-C14	1.4784	C19-C23	1.083
C3-C4	1.4065	C14-O15	1.2441	C21-C22	1.3818
C3-H8	1.0832	C14-C16	1.4754	C21-H24	1.083
C4-C5	1.4047	C15-C27	1.6372	C22-H25	1.0845
C4-C10	1.4593	C16-C17	1.4109	C26-H27	0.9915
C5-C6	1.3896	C16-C18	1.4259	-	-
C5-H9	1.0844	C17-C19	1.3816	-	-

Bond angles (°)					
C2-C1-C6	121.0327	C1-C6-H28	120.1921	C19-C17-H20	118.4684
C2-C1- Cl29	119.3779	C5-C6-H28	120.8569	C16-C18-C21	119.7607
C6-C1-Cl29	119.5894	C4-C10-H11	115.9548	C16-C18-C26	122.5821
C1-C2-C3	119.3428	C4-C10-C12	127.9173	C21-C18-O26	117.6572
C1-C2-H7	119.9106	H11-C10-C12	116.128	C17-C19-C22	119.3288
C3-C2-H7	120.7466	C10-C12-H13	120.9588	C17-C19-H23	120.2778
C2-C3-C4	121.2263	C10-C12-C14	120.091	C22-C19-H23	120.3934
C2-C3-H8	118.5822	H13-C12-C14	118.9503	C18-C21-C22	120.4437
C4-C3-H8	120.1915	C12-C14-O15	119.2758	C18-C21-H24	117.7904
C3-C4-C5	117.8397	C12-C14-C16	120.5044	C22-C21-H24	121.7658
C3-C4-C10	123.5496	O15-C14-C16	120.2199	C19-C22-C21	120.7024
C5-C4-C10	118.6107	C14-C16-C17	123.26	C19-C22-H25	119.8481
C4-C5-C6	121.6076	C14-C16-C18	118.7881	C21-C22-C25	119.4495
C4-C5-H9	119.1691	C17-C16-C18	117.9519	C18-O26-H27	106.3184
C6-C5-H9	119.2233	C16-C17-C19	121.8125	-	-
C1-C6-C5	118.951	C16-C17-H20	119.7192	-	-

Computational Results

The optimized geometry extracted by using Gauss View 4.1 program and Gaussian 03W program package is depicted in the Figure 6. In the title compound 4CPHPP, there are a total of 29 atoms are present. The structural entities; bond lengths and bond angles are obtained for the optimized structure are presented in Table 1. The important bond length values are C14=O15 (1.2441 Å), C12=C18 (1.3453 Å), and O26-H27 (1.0845 Å). The increase in the bond length of the carbonyl group is due to the presence of intramolecular hydrogen bonding. The

C1-Cl29 bond length is 1.7549 Å. The hydrogen bond between the oxygen of carbonyl and hydrogen of hydroxyl has bond length 1.6372 Å. The presence of this bond in the computational result is also proof of the existence of the hydrogen bond. All bond lengths and bond angles are in good agreement with the structure of the title compound. The dipole moment of the title compound is 2.57 Debye which indicates its polar nature.

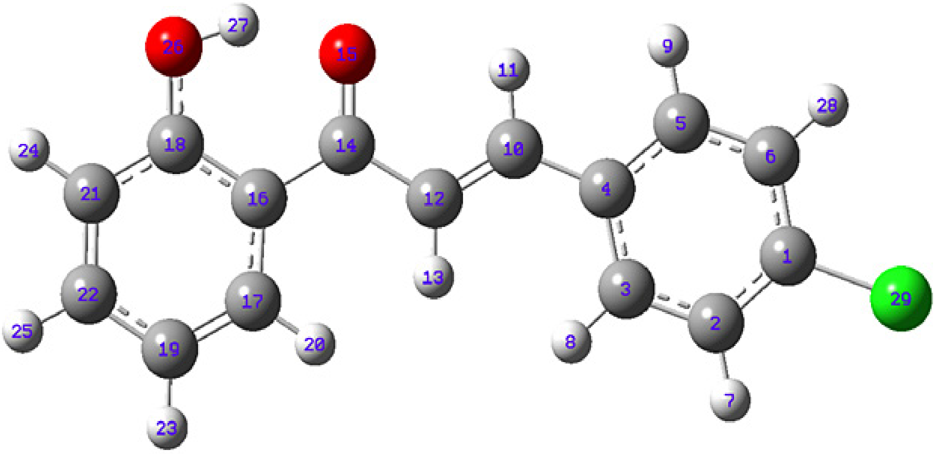


Fig. 6: Optimized molecular structure of the title compound at DFT/B3LYP method with a 6-311G(d,p) basis set

Figure 7 indicates the Mulliken charges in the title compound 4CPHPP. The Mulliken charges are also presented in Table 2. From the Mulliken charges, it can be said that all the hydrogen atoms in the title compound are having a positive charge. This is also confirmed by the molecular electrostatic potential plot. The hydrogen atom which is the most electropositive in nature is H27 as it is attached to the electronegative oxygen atom. Then H7 is the second most electropositive due to the vicinity of the chlorine atom. Amongst all carbon atoms, C14 is the most electropositive in nature. This data is very important to decide the chemical reactivity of the title compound. The molecular electrostatic potential plot (MEP) is depicted in Figure 8. The MEP plot provides information regarding the chemical reactivity sites. The different colours in the MEP plots indicate zones of the positive, negative and neutral potentials. The MEP plot of the title compound indicates that the benzene ring bearing OH group would react more powerfully than the benzene ring bearing chlorine atom. Therefore, the electrophilic aromatic substitution reaction in the title compound is more favourable and selective in the former benzene ring. As predicted by the Mulliken atomic charges and MEP plot, the hydrogen atoms are present in the zones of positive electrostatic potential.

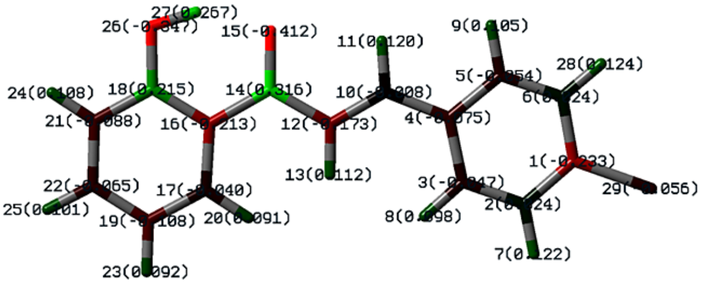


Fig. 7: Mulliken atomic charges in the title compound 4CPHPP

Table 2: Mulliken atomic charges

Atom	Charge	Atom	Charge	Atom	Charge
1 C	-0.232848	11 H	0.120470	21 C	-0.088319
2 C	0.023941	12 C	-0.173175	22 C	-0.065451
3 C	-0.047129	13 H	0.112102	23 H	0.092261
4 C	-0.075108	14 C	0.315522	24 H	0.108219
5 C	-0.054460	15 O	-0.412054	25 H	0.101488
6 C	0.024372	16 C	-0.212886	26 O	-0.346990
7 H	0.122250	17 C	-0.039604	27 H	0.267205
8 H	0.097682	18 C	0.214894	28 H	0.124204
9 H	0.104927	19 C	-0.108467	29 Cl	-0.055737
10 C	-0.007885	20 H	0.090576	-	-

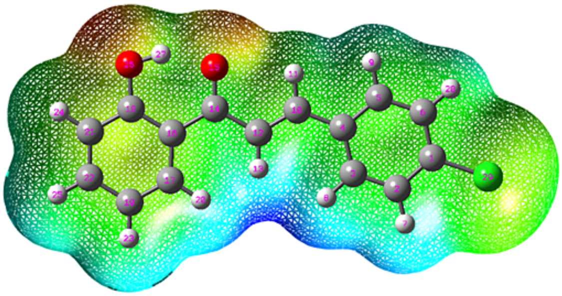


Fig. 8: Molecular electrostatic potential plot of the title compound

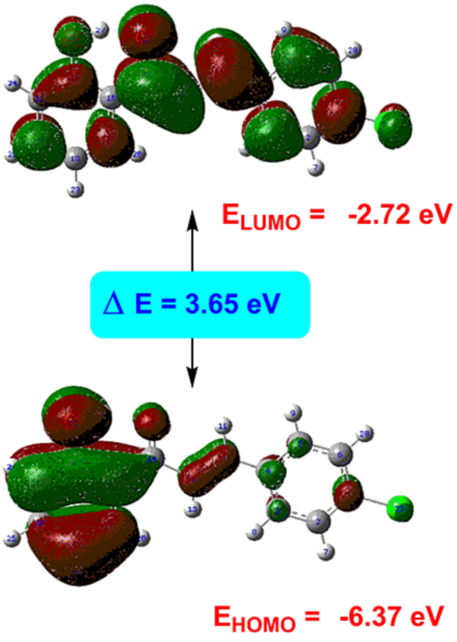


Fig. 9: HOMO-LUMO of the tittle compound 4CPHPP

The HOMO-LUMO presentation of the title compound 4CPHPP is given in Figure 9. The imperative exploration on the electronic properties, such as HOMO and LUMO energies, was studied by the time-dependent DFT (TD-DFT) method at B3LYP/6-311G(d,p) basis set in the gas phase. The HOMO-LUMO energy gap in the title compound is 3.65 eV. The bandgap in the title compound suggests the inevitable charge transfer phenomenon is taking place within the title compound. From the HOMO-LUMO energies, various chemical reactivity parameters have been derived. The chemical potential (μ) and the charge transferred (ΔNmax) values are -4.545 eV and 2.49 eV respectively. The first singlet excitation energy in the title compound is 3.1579 eV and the absorption wavelength 392.62 nm with oscillator strength value (f) = 0.1798. The high value of absorption wavelength is due to presence of the extended conjugation which is known as the bathochromic shift. This excitation energy corresponds to the amount of energy required for the promotion of an electron from HOMO to LUMO.

The theoretical and experimental IR spectra are presented in the Figure 10 and 3 respectively. The vibrational assignments were made by comparing the experimental FT-IR frequencies with the theoretical frequencies obtained by using B3LYP/6-311G(d,p) basis set. The very strong IR absorption peak at 1627.92 cm^{-1} is matching with the theoretical value 1625.28 cm^{-1} is assigned to C=O and C=C stretching vibrations. Another important experimental IR absorption peak is at 3441.01 cm^{-1} which is assigned to OH stretching vibrations is ideally matches the theoretical value which is 3450.35 cm^{-1}. The decrease in both IR absorption frequencies is the consequence of the strong conjugation of the enone system with the aromatic rings. The theoretical IR signal at 1535.83 1504.18 cm^{-1} is due to the Ar C=C stretching vibrations and it is correlated with the experimental value 1504.18 cm^{-1}. Other vibrational data is also in good agreement with the experimental FT-IR frequencies. Thermochemical data obtained from the harmonic frequencies are tabulated in Table 3. The important thermochemical parameters like total Energy (thermal), total heat capacity (Cv), and entropy (S) are evaluated. The entropy value indicates the degree of freedom whereas the total energy suggests the thermal stability of the title compound. The thermodynamic data could be used to predict the other thermochemical parameters also.

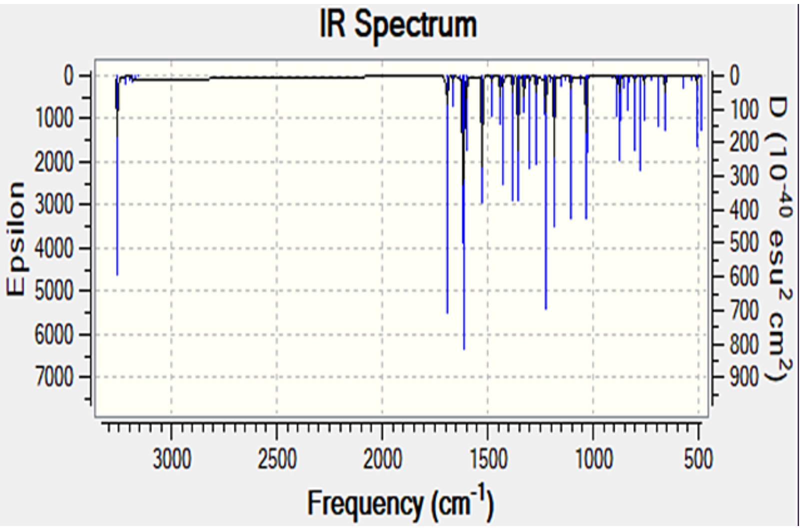


Fig. 10: Theoretical IR spectrum of the title compound

Table 3: Thermochemical data of the title compound

Parameters	Translational	Rotational	Vibrational	Total
Total Energy (Thermal) KCal/Mol	0.889	0.889	145.279	147.056
Total heat capacity (Cv) Cal/Mol/Kelvin	2.981	2.981	52.009	57.971
Entropy (S) Cal/Mol/Kelvin	42.544	34.242	51.6031	128.389

Conclusion

In conclusion, (*E*)-3-(4-chlorophenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one has been explored to study its structural, electronic, and chemical viewpoints. The conclusion of the present research is summarized as-

- The (*E*)-3-(4-chlorophenyl)-1-(2-hydroxyphenyl) prop-2-en-1-one has been synthesized and characterized by FT-IR, ^{1}HNMR, and ^{13}C NMR spectral techniques. DFT method at B3LYP/6-311G(d,p) basis set has been employed.
- The detailed investigation of bond lengths and bond angles is discussed to comprehend the geometrical framework.
- To explore its chemical behaviour, Mulliken atomic charges, molecular electrostatic potential surface, and electronic parameters are introduced.
- The imperative exploration on the electronic properties, such as HOMO and LUMO energies, was studied by the time-dependent DFT (TD-DFT) method.
- The dipole moment of the title molecule is 2.57 Debye with C1 point group symmetry.
- The most electropositive carbon and hydrogen atoms in the title molecule are C14 and H27 respectively. Amongst aromatic C=C, the C16-C18 is the longest, and C17-C19 is the shortest bond.
- The molecular electrostatic potential surface analysis suggested the positive electrostatic potential is around hydrogen atoms.
- The vibrational assignments in the title compound were done by comparing the experimental IR frequencies with the scaled frequencies obtained using computational work. Additionally, some noteworthy thermochemical data is acquired utilizing a similar basis set using frequencies.

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Conflict of Interest

The authors declare that they do not have any conflict of interest.

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