Ultrasound Assisted Synthesis, Molecular Structure, UV-Visible Assignments, MEP and Mulliken Charges Study of (E)-3-(4-chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one: Experimental and DFT Correlational

ROHIT S. SHINDE

PG Department of Chemistry, Mahatma Gandhi Vidyamandir’s Arts, Science and Commerce College, Manmad, Taluka-Nandgaon, District- Nashik, India-423104. (Affiliated to Savitribai Phule Pune University, Pune, maharashtra, India.

Abstract
Present investigation deals with the synthesis and density functional theory study (DFT) of a chalcone derivative; (E)-3-(4-chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (CPMPP). The synthesis of a CPMPP has been carried out by the reaction of 4-methoxyacetophenone and 4-chlorobenzaldehyde in ethanol at 30°C under ultrasound irradiation. The structure of a synthesized chalcone is affirmed on the basis of FT-IR, 1H NMR and 13C NMR. The geometry of a CPMPP is optimized by using the density functional theory method at the B3LYP/6-31G(d,p) basis set. The optimized geometrical parameters like bond length and bond angles have been computed. The absorption energies, oscillator strength, and electronic transitions have been derived at the TD-DFT method at the B3LYP/6-31G(d,p) level of theory for B3LYP/6-31G(d p) optimized geometries. The effect of polarity on the absorption energies is discussed by computing UV-visible results in dichloromethane (DCM). Since theoretically obtained wavenumbers are typically higher than experimental wavenumbers, computed wavenumbers were scaled with a scaling factor, and vibrational assignments were made by comparing experimental wavenumbers to scaled theoretical wavenumbers. Quantum chemical parameters have been determined and examined. Molecular electrostatic potential (MEP) surface plot analysis has been carried out at the same level of theory. Mulliken atomic charge study is also discussed in the present study.

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CONTACT Rohit S. Shinde chemistry.rss@gmail.com PG Department of Chemistry, Mahatma Gandhi Vidyamandir’s Arts, Science and Commerce College, Manmad, Taluka-Nandgaon, District- Nashik, India-423104. (Affiliated to Savitribai Phule Pune University, Pune, maharashtra, India.

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Introduction
Chalcone is the trivial name given to the α,β-unsaturated ketones, which are synthesized by condensing an aromatic aldehyde with an substituted acetophenone in the presence of a base. Chalcones are not only important precursors in the synthesis of many biologically active molecules, but they also make up a significant part of natural products. Chalcones as well as their synthetic analogues show large number of medicinal properties. They are crucial in the production of a wide variety of remedial compounds. They have shown remarkable curative efficacy in the treatment of a variety of diseases. Chalcone-based derivatives have gotten a lot of attention because of their simple structures and diverse pharmacological effects.

The synthesis of these compounds has been reported using a variety of techniques and schemes. Aldol condensation and Claisen-Schmidt reaction continue to be the most widely used processes for synthesis of chalcones. In the presence of an aqueous alcoholic alkali, Claisen-Schmidt condensation occurs between equimolar amounts of a substituted acetophenone and substituted aldehydes. Chalcones and their heterocyclic analogues have a wide range of pharmacological properties, including anticancer, antioxidant, anti-inflammatory, antifungal, antiviral, antibacterial, antiproliferative, antitumor, antimalarial, antidiabetic, anticonvulsant, and many others, making them a significant scaffold in medicinal chemistry.

Green Chemistry has played vital role for designing many synthetic molecules without causing environmental hazards. In that ultrasound technique is proved to be highly efficient. DFT is a method that can provide a good deal of information regarding the physical and chemical behavior of the molecules. In this unique circumstance, I would like to present current research on ultrasound assisted synthesis, molecular structure, UV-visible assignments, MEP, and Mulliken charges study of (E)-3-(4-chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one: a DFT and experimental study correlational.

Experimental
Chalcones were synthesized by base catalyzed Claisen-Schmidt condensation reaction of appropriately 4-methoxyacetophenone (1) and 4-chlorobenzaldehyde (2) by literature method. Anequimolar mixture of 4-methoxyacetophenone and 4-chlorobenzaldehyde in 10 mL ethanol in a 50 mL conical flask equipped. Then appropriate amount of KOH solution was added drop wise to the reaction mixture. The alkaline mixture was exposed to ultrasound irradiation until formation of the product (checked by TLC). After this, reaction mixture was neutralized by 1:1 HCl whereby the precipitation occurred. On filtering off, the crude chalconewas dried in air and recrystallized by ethanol to give pale yellow crystals of chalcone (3).

![Scheme 1 Synthesis of titled compound](image)

Table 1: Physicochemical and Spectral data of CPMPP molecule

| Systematic Name of the Product                  | (E)-3-(4-Chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one |
|------------------------------------------------|---------------------------------------------------------|
| Abbreviation used                              | CPMPP                                                   |
| Physicochemical data                           | Yield: 88%, Colour: pale yellow crystals,               |
| FT-IR IR (KBr, cm⁻¹)                          | 470, 532.35, 694.37, 771.53, 833, 995, 1087, 1211, 1327, 1489, 1597, 1666, 3047 |
| ¹H NMR (400 MHz, CDCl₃)                        | 3.90 (s, 3H), 6.97-7.01 (m, 2H), 7.37-7.41 (m, 2H), 7.52 (d, J = 15.7 Hz, 1H), 7.55-7.59 (m, 2H), 7.75 (d, J = 15.7 Hz, 1H), 8.02-8.06 (m, 2H) |
| ¹³C NMR (100 MHz, CDCl₃)                       | 55.65, 114.05, 122.44, 129.33, 129.66, 130.98, 131.07, 133.74, 136.30, 142.55, 163.70, 188.48 |
Computational Study
DFT calculations were performed on an Intel (R) Core (TM) i5 computer using Gaussian-03 program package without any constraint on the geometry. The geometry of the molecules studied in this is optimized by DFT/B3LYP method using 6-31G(d,p) basis set. The FMO analysis and quantum chemical study has been performed using same basis set.

Table 2: Optimized Bond Lengths of CPMPP molecule obtained at B3LYP/6-31G(d,p)

| Bond lengths (Å) | C1-C2      | C1-C6      | C1-O27     | C2-C3      | C2-C4      | C3-C4      | C3-H8      | C4-C5      | C4-C11     | C5-C6      | C5-H9      | C6-H10     | C11-C12    | C11-O16    | C12-H13    | C12-C14    | C14-H15    |
|------------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|
|                  | 1.4038     | 1.4033     | 1.359      | 1.3865     | 1.4077     | 1.0843     | 1.4028     | 1.4941     | 1.3902     | 1.3902     | 1.0846     | 1.0833     | 1.4871     | 1.2314     | 1.084     | 1.3472     | 1.0889     |

Table 3: Optimized Bond Angles of CPMPP molecule obtained at B3LYP/6-31G(d,p)

| Bond lengths (°) | C2-C1-C6 | H15-C14-C17 | C2-C1-O27 | C6-C1-O27 | C1-C2-C3 | C1-C2-H7 | C1-C2-C4 | C1-C2-H8 | C4-C3-H5 | C1-C6-H10 | C5-C6-H10 | C4-C11-C12 | C4-C11-O16 | C12-C11-O16 | C11-C12-H13 | C11-C12-C14 | H13-C12-C14 | C12-C14-H15 | C12-C14-C17 |
|------------------|----------|-------------|-----------|------------|----------|----------|----------|----------|----------|-----------|----------|-------------|------------|--------------|--------------|-------------|--------------|-------------|-------------|-----------|
|                  | 119.6544 | 116.1539    | 115.6855  | 124.66     | 120.158  | 118.4593 | 118.0568 | 118.341 | 119.4349 | 120.9931  | 119.572   | 119.3039    | 120.1517   | 120.5244     | 119.0571    | 119.8758    | 121.6015    | 115.8011    | 128.045     | -          |

Results and Discussion
Optimized Molecular Structure
The optimized molecular structure of the title molecule CPMPP is given in Figure 1. The molecule CPMPP is having C1 point group symmetry and the dipole moment is 3.1533 Debye. The optimized geometrical parameters; bond lengths and bond angles of the title molecule have been computed and presented here in Table 2 and Table 3. In the molecule CPMPP, the C=O (C11-O16) bond length is 1.2314 Å. The C-Cl (C24-Cl28) bond length is 1.7559 Å. The bond lengths in C-O are 1.359 Å (C1-O27) and 1.422 Å (O27-C29). Amongst aromatic C=C bond lengths, C17-C19 bond is the longest (1.4086 Å) and the shortest is C2-C3 (1.3865 Å). Other bond lengths are also in good agreement. All the bond angles are also in good agreement.
Global Descriptors Study
The pictorial representation of HOMO-LUMO orbitals is given in Figure 2. The electronic parameters such as EHOMO, ELUMO, ionization enthalpy (I), and electron affinity (A) are given in Table 4. The quantum chemical parameters like electro negativity (χ), absolute hardness (η), softness (σ), electrophilicity (ω), chemical potential (Pi) are presented in Table 5. The frontier molecular orbital (FMO) analysis suggests that the energy gap in the molecule CPMPP is 4.06 eV. The lower HOMO-LUMO energy gap demonstrates the inevitable charge transfer is happening within the molecule. The global softness (σ), and the absolute hardness (η) values are 0.4926 and 2.03 eV respectively. The ease of removal of an electron is governed by its chemical potential Pi and it is likewise identified with its electro negativity (χ). A good electrophile is described by a higher value of global electrophilicity (ω) and the higher value of ω indicates good nucleophile. Our results suggest that the molecule CPMPP has a higher value of global electrophilicity (ω = 4.2625 eV), so it is most likely to accept electrons readily and also would undergo nucleophilic attack easily. As Pi value increases, the ability of a molecule to lose an electron increases. The maximum charge transfer is in the title molecule is 2.0493 eV.

**Fig. 2: HOMO-LUMO pictures of CPMPP molecule**

| Table 4: Electronic parameters of CPMPP molecule |
|-----------------------------------------------|
| Entry | E (a.u.) | E_{HOMO} (eV) | E_{LUMO} (eV) | I (eV) | A (eV) | Eg (eV) |
|-------|---------|---------------|---------------|-------|-------|--------|
| CPMPP | -1228.18| -6.19         | -2.13         | 6.19  | 2.13  | 4.06   |

| Table 5: Global reactivity parameters of CPMPP molecule |
|--------------------------------------------------------|
| Entry | χ (eV) | η (eV) | σ (eV⁻¹) | ω (eV) | Pi (eV) | ΔNmax (eV) | Dipole Moment (Debye) |
|-------|-------|-------|----------|-------|--------|------------|----------------------|
| CPMPP | 4.16  | 2.03  | 0.4926   | 4.2625| -4.16  | 2.0493     | 3.1533               |

UV-Visible Analysis
The absorption energies (λ in nm), oscillator strength (f) and electronic transitions of the CPMPP molecule were computed at the TD-DFT-B3LYP/6-31G (d,p) level of theory for the optimized structure. The absorption energies (λ in nm), oscillator strength (f) and transitions of CPMPP molecule and experimental UV-Vis spectral analysis are given in Table 6. The theoretical UV-Vis absorption results were simulated up to three singlet excited states. The experimental UV-Vis spectra were recorded in the DCM solvent. Likewise, the theoretical UV-Vis spectra were computed in the gas phase, and the DCM solvent. The theoretical and experimental UV-Vis spectral images are depicted in Figure 3 and Figure 4. The first singlet state (S1) is found to be at 382.50 nm in the gas phase and 368.76 nm in DCM. The experimental UV-visible absorption band is centred at 375.02 nm in DCM solvent. This result suggests that the theoretical UV-Vis absorption results are in acceptable concurrence with the UV-Vis absorption experimental results. The HOMO-LUMO electronic transition corresponds to the 71 -> 72 configurations. The solvent effect on the HOMO-LUMO absorption wavelength of the DPPPm molecule is found to be a blue shift (hypsochromic
shift) as per the UV-Vis absorption theoretical data. The second singlet excited state (S2) is present at 338.93 nm (gas phase) and 350.05 nm (DCM) in the theoretical UV-Vis absorption spectrum. The second gas phase singlet excited state and also DCMO is composed of only one configuration, namely 71 -> 72 configurations. The third gas phase singlet excited state (S3) is from 69 -> 72, 70 -> 72, and 71 -> 73 and 69 -> 72, 70 -> 72 in DCM. The third absorption band is located at 307.68 nm (gas phase) and 315.08 nm (DCM).

Fig. 3: Experimental UV-Visible spectra in DCM

Fig. 4: Simulated UV-Visible spectra in gas phase and DCM of CPMPP molecule

Table 6: Absorption wavelength (\(\lambda\) in nm), coefficient, oscillator strength (\(f\)), and electronic transitions of titled compound computed at TD-DFT B3LYP/6-31G(d,p) level of theory (Experimental value of absorption wavelength (\(\lambda\) in nm) given in bracket)

| State | Config | Coefficient | \(f\) | \(\lambda\), nm | Config | Coefficient | \(f\) | \(\lambda\), nm |
|-------|--------|-------------|------|----------------|--------|-------------|------|----------------|
| I     | 69 -> 72 | 0.67881 | 0.0002 | 382.5 | 69 -> 72 | 0.68263 | 0.0019 | 368.76 |
|       | 69 -> 73 | 0.10098 | -0.1239 |      | 70 -> 72 | 0.10238 |      | (375.02) |
| II    | 71 -> 72 | 0.70176 | 0.6207 | 338.93 | 71 -> 72 | 0.70087 | 0.8907 | 350.05 |
| III   | 69 -> 72 | 0.12029 | 0.4056 | 307.68 | 69 -> 72 | -0.10306 | 0.2899 | 315.08 |
|       | 70 -> 72 | 0.67825 |      |      | 70 -> 72 | 0.68537 |      |      |
|       | 71 -> 73 | -0.10087 |      |      |      |      |      |      |

**Vibrational Study**

The experimental and theoretical IR spectrum of the title compound is given in Figure 5. In the given spectra, scaled theoretical IR values and experimental IR values are depicted. The comparison between the experimental and scaled IR values has led to the correct assignment of the vibrational bands. The CPMPP molecule consists of 32 atoms with 90 normal modes of vibration. Because of the anharmonicity of the incomplete treatment of electron correlation and the use of a finite one-particle basis set, computed harmonic vibrational wavenumbers are usually higher than experimental ones. B3LYP method was used to calculate harmonic frequencies using 6-31G(d,p) basis sets, which were then scaled by appropriate scaling factor. The BLYP/6-31G(d,p) method produced better results, with a deviation from the experiment of less than 30 cm\(^{-1}\).

The aromatic C-H vibrational stretching is located at 3047 cm\(^{-1}\) in the in the experimental IR spectrum and at 3020 cm\(^{-1}\) theoretically predicted IR spectrum. This definitely suggests a great deal of agreement between the two compared values. The C=C stretching vibrations is observed at 1601 cm\(^{-1}\) and 1597 cm\(^{-1}\) in the experimental and theoretical IR spectra respectively. The another important C=C
vibration was found at 1489 cm\(^{-1}\) and 1473 cm\(^{-1}\) in the experimental and theoretical IR spectra respectively. The C-H bending vibrations are found at 1327 cm\(^{-1}\) and 1308 cm\(^{-1}\) in the experimental and theoretical IR spectra respectively. The C-O stretching vibration is found at 1211 cm\(^{-1}\) in the experimental IR spectrum and at 1194 cm\(^{-1}\) in the theoretical IR spectrum. The 1087 cm\(^{-1}\) in the experimental and 1108 in the experimental are attributed to C-C stretching vibrations. The experimental 995 cm\(^{-1}\) matches with the theoretical 1002 cm\(^{-1}\) is occurred due to the bending vibrational mode. Throughout this regard, the correlation was used to correctly assign vibrational bands to the title compounds, and the IR spectra of the titled compound have a very strong correlation.

**Mulliken Atomic Charges and Molecular Electrostatic Plot Analysis**

The Mulliken atomic charges of the CPMPP molecule are calculated by DFT/B3LYP method with 6-31G(d,p) basis set in the gaseous phase and are given in Table 7. Mulliken atomic charges reveal that all the hydrogen atoms have a net positive charge but H15 and H31 atoms have a more positive charge than other hydrogen atoms and therefore they are more acidic. Amongst, carbon atoms, the C11 atom have the highest net positive charge (0.372919) as it is attached to an electronegative oxygen atom. On the other hand C12 atom has the highest negative charge (-0.141075).

![Experimental IR and Theoretical IR spectra showing selected vibrational assignments of CPMPP molecule](image)

**Table 7: Mulliken atomic charges of CPMPP**

| Atom | Charge | Atom | Charge |
|------|--------|------|--------|
| 1 C  | 0.362574 | 17 C | 0.127545 |
| 2 C  | -0.128205 | 18 C | -0.123597 |
| 3 C  | -0.112476 | 19 C | -0.105209 |
| 4 C  | 0.038662 | 20 C | -0.073641 |
| 5 C  | -0.107676 | 21 H | 0.104888 |
| 6 C  | -0.137000 | 22 C | -0.074632 |
| 7 H  | 0.098792 | 23 H | 0.094380 |
| 8 H  | 0.087747 | 24 C | -0.093211 |
| 9 H  | 0.120507 | 25 H | 0.115548 |
| 10 H | 0.092396 | 26 H | 0.114129 |
| 11 C | 0.372919 | 27 O | -0.512859 |
| 12 C | -0.141075 | 28 Cl | -0.013042 |
| 13 H | 0.081235 | 29 C | -0.083420 |
| 14 C | -0.090049 | 30 H | 0.118400 |
| 15 H | 0.122194 | 31 H | 0.129564 |
| 16 O | -0.503478 | 32 H | 0.118091 |

Figure 6 shows the molecular electrostatic potential plot. The use of a molecular electrostatic potential can be used to evaluate phenomena such as nucleophilic and electrophilic positions, solvent effects, hydrogen bonding interactions, and so on. MEP is mainly used to establish the reactive sites of molecules, enabling researchers to predict how one particle will interact with another. The various electrostatic potential values at the molecule’s surface are expressed by different colours. Electrophilic reactivity is correlated with the red and yellow zones, which lead to high electron density. The blue sections, on the other hand, reflect low electron density and nucleophilic reactivity, while the green colours represent regions of zero potential.

**Conclusion**

Present investigation deals with the synthesis and DFT study of a chalcone derivative; (E)-3-(4-chlorophenyl)-1-(4-methoxyphenyl)prop-2-en-1-one. The synthesis of a CPMPP has been carried out by the reaction of 4-methoxyacetophenone and 4-chlorobenzaldehyde in ethanol at 30°C under ultrasound irradiation. The structure of a synthesized chalcone is affirmed on the basis of FT-IR, 1H NMR and 13C NMR. The geometry of a CPMPP is optimized by using the density
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functional theory method at the B3LYP/6-31G(d,p) basis set. The molecule CPMPP is having C1 point group symmetry and the dipole moment is 3.1533 Debye. The optimized geometrical parameters like bond length and bond angles have been computed. The quantum chemical parameters like electro negativity, absolute hardness, softness, electrophilicity, chemical potential are presented. The FMO analysis suggests that the energy gap in the molecule CPMPP is 4.06 eV. The lower HOMO-LUMO energy gap demonstrates the inevitable charge transfer is happening within the molecule. The absorption energies, oscillator strength, and electronic transitions have been derived at the TD-DFT method at the B3LYP/6-31G(d,p) level of theory for B3LYP/6-31G(d,p) optimized geometries. The effect of polarity on the absorption energies is discussed by computing UV-visible results in DCM. The solvent effect on the HOMO-LUMO absorption wavelength of the CPMPP molecule is found to be a blue shift as per the UV-Vis absorption theoretical data. Mulliken atomic charges reveal that all the hydrogen atoms have a net positive charge but H15 and H31 atoms have a more positive charge than other hydrogen atoms and therefore they are more acidic. Amongst, carbon atoms, the C11 atom have the highest net positive charge (0.372919) as it is attached to an electronegative oxygen atom. On the other hand C12 atom has the highest negative charge (-0.141075).

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Conflict of Interest
There is no conflict of interest for this work.

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