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Synthesis, Characterization and Theoretical Insights into Molecular Properties of 2-(4-fluorophenyl)-4*H*-chromen-4-one

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ABSTRACT

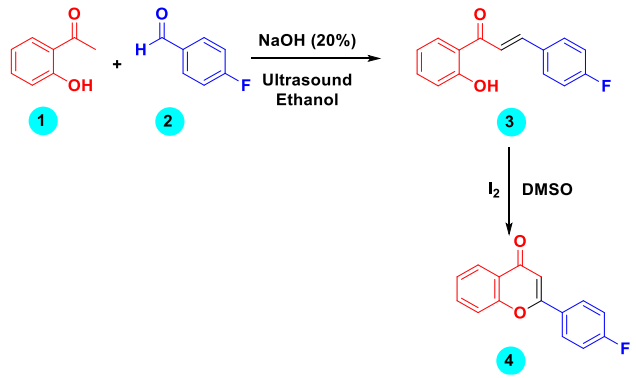
Flavone scaffold is one of the most often perceived parts in biologically active organic compounds. In light of this, a flavone; 2-(4-fluorophenyl)-4*H*-chromen-4-one (FPC) has been synthesized, characterized and studied by using density functional theory (DFT) at B3LYP/6-31G(d,p) basis set. The geometry of the FPC molecules has been optimized by using B3LYP/6-31G(d,p) basis set and in-depth structural analysis on bond lengths and bond angles has been discussed. The HOMO-LUMO analysis and various quantum chemical parameters are computed and discussed for the better understanding of chemical behaviour of the title molecule. Molecular electrostatic potential (MEP) surface investigation is presented to understand the reactivity sites of the title molecule.

1. Introduction

Flavonoids are a diverse group of plant-derived compounds [1]. They are well-known plant secondary metabolites that have been discovered in foods such as bananas, vegetables, olive oil, tea, and red wine. The pharmacological potential of natural products is gaining popularity [2-4]. Researchers have been studying flavonoids as oxidative reaction inhibitors and anti-inflammatory agents in recent years [5, 6]. They have been shown to have anxiolytic, antiviral, antiprotozoal, anti-microbial, and anti-carcinogenic properties [7-12]. Usually chalcones are the precursors used for the synthesis of flavones. Chalcones also possess notable pharmacological properties [13-21]. Green chemistry principles have been utilized for the synthesis of variety of compounds [22-26]. The ultrasound strategy has been previously used for the synthesis of chalcones [27]. Accordingly ultrasound methodology has been employed for the synthesis of precursor, i.e. chalcone. DFT computations provide investigators with a plethora of data about the molecules' spectral and quantum chemical parameters, enabling researchers to examine chemical behaviour [28-37]. The chromones 6,8-dichloro-2-(4-chlorophenyl)-4H-chromen-4-one and 6,8-dichloro-2-(4-Methoxyphenyl)- 4H-chromen-4-One were previously studied using DFT methodology to explore structural and spectroscopic properties [38, 39]. DFT approaches have already been shown to be useful in studies of reaction mechanisms. Assigning the correct UV-Visible and vibrational bands has been an easy task due to the contrast of theoretical and experimental IR vibrations. In view of the above, this present work made on a DFT study of 2-(4-fluorophenyl)-4*H*-structural, chromen-4-one's spectral, and molecular properties.

2. Experimental Methods

The chalcone (**3**) was synthesized from 2-hycroxyacetopheone (**1**) and 4-fluorobenzaldehyde (**2**) as per previously reported method [21]. The chalcone (**3**) (0.01 mol) was taken in round bottom flask containing DMSO solvent. To this catalytic amount of I_2 was mixed and resulting mixture was refluxed until formation of the product. The reaction was monitored by TLC. After completion of the reaction, reaction mixture was transferred in a beaker containing crushed ice. The precipitated product formed was filtered, washed with water and sodium thiosulfate until free from I_2. The crude product was recrystallized to afford pure product (**4**). The synthesis is given in Scheme 1.



Scheme 1 Synthesis of 2-(4-fluorophenyl)-4*H*-chromen-4-one

Table 1 Physicochemical and spectral data of FPC

Properties	Characteristics
Systematic Name of the Product	2-(4-fluorophenyl)-4H-chromen-4-one
Abbreviation used	FPC
Physicochemical data	Yield: 75%, Colour: White solid, m.p. : 155 °C
^{1}H NMR (400 MHz, $CDCl_3$)	400 MHz, d (ppm): 6.73-6.75(s, 1H), 7.41 (m, 1H), 7.69 (m, 1H), 7.51-7.53 (m, 1H), 8.19 (m, 1H), 7.45-7.47 (m, 2H), 7.81-7.83 (m, 2H)
HRMS	Calculated: 240.0586 [M+H], Observed: 240.0588 [M+H].

2.1 Computational Details

DFT calculations were performed on an Intel (R) Core (TM) i5 computer using Gaussian-03 program package without any constraint on the geometry [40]. The geometry of the molecules studied here 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. Absorption energies (λ in nm), oscillator strength (ƒ), and transitions of title molecule have been calculated at TD-B3LYP/6-31G (d, p) level of theory for B3LYP/6-31G(d,p) optimized geometries. To investigate the reactive sites of the title molecules, MEP was computed using the same method. All the calculations were carried out for the optimized structure in the gas phase.

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3. Results and Discussion

3.1 Optimized Molecular Structure

The optimized molecular structure of the title molecule FPC is given in Fig. 1. The molecule FPC is having C1 point group symmetry and the dipole moment is 5.0279 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 FPC, the C=O (C16-O20) bond length is 1.2307 Å. The C-F (C20-F26) bond length is 1.3462 Å. The bond lengths in C-O are 1.3649 Å (C7-O23) and 1.3734 Å (C13-O23). Amongst aromatic C=C bond lengths, C3-C4 bond is the longest (1.406 Å) and the shortest is C14-C16 (1.3868 Å). Other bond lengths are also in good agreement. All the bond angles are also in good agreement.

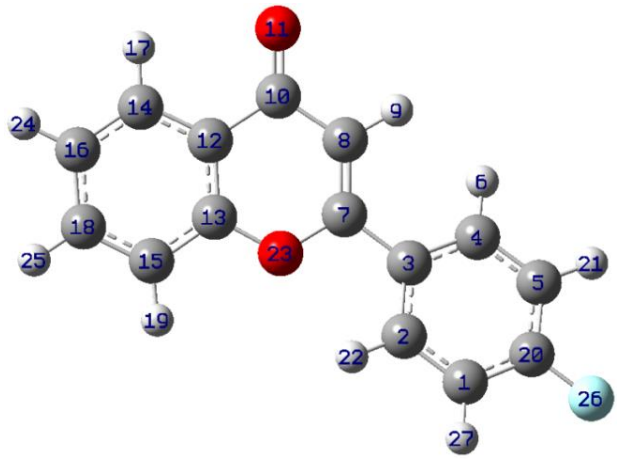

Fig. 1 Optimized molecular structure of FPC

Table 2 Optimized bond lengths of FPC at B3LYP/6-31G(d.p)

Bond Lengths (Å)			
C1-C2	1.3917	C10-O11	1.2307
C1-C20	1.39	C10-C12	1.4817
C1-H27	1.0843	C12-C13	1.4
C2-C3	1.4058	C12-C14	1.4036
C2-H22	1.0832	C13-C15	1.398
C3-C4	1.406	C13-O23	1.3734
C3- C7	1.4742	C14-C16	1.3868
C4- C5	1.3903	C14-H17	1.085
C4-H6	1.0843	C15-C18	1.3889
C5- C20	1.3913	C15-H19	1.0846
C5- H21	1.0842	C16-C18	1.4046
C7- O8	1.3583	C16-H24	1.0854
C7-O23	1.3649	C18-H25	1.0858
C8-H9	1.0823	C20-F26	1.3462
C8-C10	1.4578	-	-

Table 3 Optimized bond angles of FPC at B3LYP/6-31G(d.p)

Bond Angles (°)			
C2-C1-C20	118.7831	C10-C12-C13	119.844
C2-C1-H27	121.5646	C10-C12-C14	121.5517
C20-C1-H27	119.6521	C13-C12-C14	118.6032
C1-C2-C3	120.9161	C12-C13-C15	121.5911
C1-C2-H22	119.6387	C12-C13-O23	121.8179
C3-C2-H22	119.444	C15-C13-O23	116.5899
C2-C3-C4	118.6536	C12-C14-O16	120.507
C2-C3-C7	120.4998	C12-C14-H17	117.3648
C4-C3-C7	120.8465	C16-C14-H17	122.1282
C3-C4-C5	120.9707	C13-C15-C18	118.7177
C3-C4-H6	120.0384	C13-C15-H19	119.3815
C5-C4-H6	118.9789	C18-C15-H19	121.9007
C4-C5-C20	118.756	C14-C16-C18	119.8684
C4-C5-H21	121.5636	C14-C16-H24	120.2573
C20-C5-H21	119.6766	C18-C16-H24	119.8743
C3-C7-C8	126.1016	C15-C18-C16	120.7124
C3-C7-O23	111.9959	C15-C18-H25	119.3558
C8-C7-O23	121.8985	C16-C18-H25	119.9317
C7-C8-H9	120.2747	C1-C20-C5	121.9145
C7-C8-C10	122.509	C1-C20-F26	119.1022
H9-C8-C10	117.2078	C5-C20-F26	118.9823
C8-C10-O11	123.403	C7-O23-C13	120.055
C8-C10-C12	113.8609	O11-C10-C12	122.7342

3.2 Global Descriptors Study

The pictorial representation of HOMO-LUMO orbitals is given in Fig. 2. The electronic parameters such as E_{HOMO}, E_{LUMO}, ionization enthalpy (I), and electron affinity (A) are given in Table 4. The quantum chemical parameters like electronegativity (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 FPC is 4.55 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 0.4396 and 2.275 eV respectively. The ease of removal of an electron is governed by its chemical potential Pi and it is likewise identified with its electronegativity (χ). A good electrophile is described by a higher value of global electrophilicity (ω) and the higher value of ω indicates good nucleophile. Observed results suggest that the molecule FPC has a higher value of global electrophilicity (ω = 3.7394 eV), and 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 1.8132 eV.

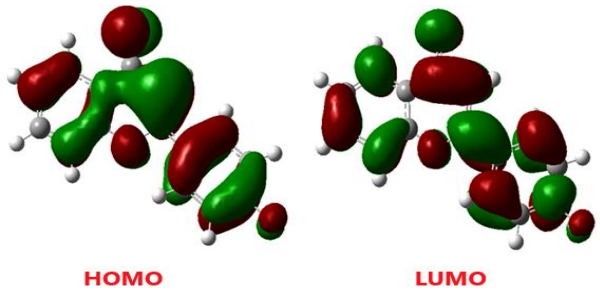

Fig. 2 HOMO-LUMO properties of FPC

Table 4 Electronic parameters of FPC

E_{Total} (a.u.)	E_{HOMO} (eV)	E_{LUMO} (eV)	I (eV)	A (eV)	E_g (eV)
-827.31	−6.40	−1.85	6.40	1.85	4.55

Note: Abbreviations: I, ionization potential; A, electron affinity; Note: $I = -E_{HOMO}$ and $A = -E_{LUMO}$

Table 5 Global reactivity parameters of FPC

χ (eV)	η (eV)	σ (eV^{-1})	ω (eV)	Pi (eV)	ΔNmax (eV)	Dipole moment (Debye)
4.125	2.275	0.4396	3.7394	-4.125	1.8132	3.4640

Note: $\chi = (I + A)/2$; $\eta = (I - A)/2$; $\sigma = 1/\eta$; $\omega = Pi^2/2\eta$; $Pi = -\chi$; $\Delta Nmax = -Pi/\eta$. Abbreviations: χ, electronegativity; η, absolute hardness; σ, global softness; ω, global electrophilicity; Pi, chemical potential; ΔNmax, maximum no. of electron transferred.

3.3 Mulliken Atomic Charges

The Mulliken atomic charges of the FPC molecule are calculated by DFT/B3LYP method with 6-31G(d,p) basis set in the gaseous phase and are given in Table 6. Mulliken atomic charges reveal that all the hydrogen atoms have a net positive charge but H17 and H22 atoms have a more positive charge than other hydrogen atoms and therefore they are more acidic. These two hydrogen atoms are flanked between two C=C groups. Amongst, carbon atoms, the C10 atom have the highest net positive charge (0.410979) as it is attached to an electronegative oxygen atom. On the other hand C8 atom has the highest negative charge (-0.186337).

Table 6 Mulliken atomic charges

Atom	Charge	Atom	Charge
1 C	-0.143342	14 C	-0.112416
2 C	-0.098615	15 C	-0.119032
3 C	0.045639	16 C	-0.088379
4 C	-0.105502	17 H	0.124073
5 C	-0.148913	18 C	-0.085850
6 H	0.109620	19 H	0.104105
7 C	0.315796	20 C	0.364054
8 C	-0.186337	21 H	0.113232
9 H	0.109041	22 H	0.115507
10 C	0.410979	23 O	-0.544596
11 O	-0.519430	24 H	0.096524
12 C	0.036938	25 H	0.098476
13 C	0.285938	26 F	-0.288878
-	-	27 H	0.111367

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3.4 Molecular Electrostatic Potential Surface Analysis

Fig. 3 shows the MEP plot of FPC. The use of MEP plot 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. The studied molecule FPC should high electrophilic reactivity zone from MEP plot.

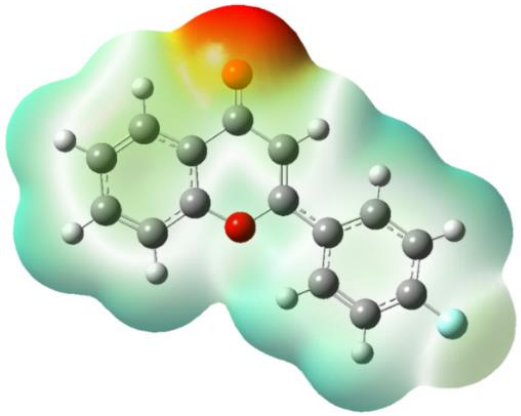

Fig. 3 Molecular electrostatic potential plot of FPC

4. Conclusion

The DFT approach was used to analyse different aspects of FPC using the B3LYP/6-31G (d,p) basis set. The tile molecule 2-(4-fluorophenyl)-4*H*-chromen-4-one geometry is optimised using the B3LYP/6-31G(d,p) basis sequence. It has been addressed how to configure geometrical parameters such as bond lengths and bond angles. Frontier molecular orbital analysis shows that the molecule is undergoing the irrevocable charge transition. Electronegativity, absolute hardness, global softness, global electrophilicity, chemical potential, maximum charge transmitted, and other quantum chemical parameters are measured and addressed. The electrophilic reactivity sites in the title molecule has been observed from the molecular electrostatic potential surface plot. Results of Mulliken atomic charges reveal that H17 and H22 atoms have a more positive charge and hence more acidic.

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