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CONTENTS

One Pot Synthesis, Spectroscopic Characteriztion, and Computational Studies of Benzo[*d*][1,3]dioxol-5-yl(3-(4-isopropylphenyl)oxiran-2-yl)methanone and Benzo[*d*][1,3]dioxol-5-yl(3-(4-chlorophenyl)oxiran-2-yl)methanone

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ABSTRACT

One pot synthesis of two benzo[d][1,3]dioxol-5-yloxiran-2-yl) methanone derivatives involve two stages first one chalcone synthesis followed by epoxide synthesis.The synthesized product were characterized by ^{1}H NMR,^{13}CMR and HRMS spectroscopic technique. The density functional theory calculations were performed using B3LYP/6-31+G (d, p) basis set for the optimization of molecular geometries. In addition to this The optimized molecular geometry, quantum and structural entities such as bond length, total energy, electron density distribution in highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), charge distribution, electronegativity, absolute hardness, softness, electrophilicity, chemical potential, charge transfer in molecules have been computed.. All the calculations have been computed in the gas phase.

KEYWORDS: One pot synthesis, FMO, benzo[d][1,3]dioxol-5-yloxiran-2-yl) methanone.

INTRODUCTION

Chalcone possess a broad spectrum of biological activity, due to the presence of the alpha beta unsaturated system. Chalcones are act as precursor for synthesis of different intermediates like pyrazoline, isooxazole, pyrimidine, benzodiazepines [1-2] etc. The development of heterocyclic compounds with epoxide groups has piqued researchers' interest. Epoxide, sometimes known as epoxy, is just a three-membered cyclic ether. Two carbon atoms, one oxygen atom. Epoxide is extensively used as a precursor in the production of a variety of chemicals. The Weitz-Scheffer reaction, which uses hydrogen peroxide under alkaline circumstances to oxidise a chalcone to an epoxychalcone, is a good example of green chemistry [3-4]. Epoxychalcone is an intermediary and a precursor to a wide range of chiral chemicals and natural products [5-7] and has outstanding biological and pharmacological active ingredients [8-10]. In addition, life-threatening infections caused by pathogenic bacteria and fungi, which are becoming more common, as well as ubiquitous epidemics around the world, have prompted many research groups from all over the world working on novel antibacterial and antifungal agents in order to avoid the rise of various infectious diseases and the rise of multi drug resistance microbial organisms [11-14].

In defining the structural and electrical properties of atoms and molecules, Density Functional Theory has become increasingly popular. The major goal of this research is to synthesize the title molecule and investigate its molecular structure, vibrational spectra, and electronic properties using experimental and computational methods. We present the one pot synthesis of benzo[d][1,3]dioxol-5-yl(3-(4-isopropylphenyl)oxiran-2-yl)methanone and benzo[d][1,3]dioxol-5-yl(3-(4-chlorophenyl)oxiran-2-yl)methanone, which involves two stages, first one chalcone synthesis followed by epoxide and an analysis of their molecular structure, as well as a DFT investigation at the B3LYP/6-31+G(d,p) level. In addition to FMOs, a 6-31+G (d, p) basis set was used to investigate ionisation potential, electronegativity, global Electrophilicity index, and chemical potential.

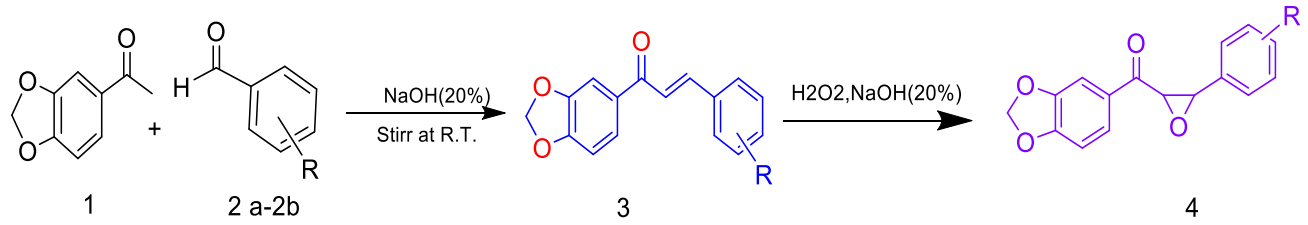
EXPERIMENTAL

Table 1 Abbreviations for Synthesized compounds

Sr.No.	Name of compound	Abbreviations
1	benzo[d][1,3]dioxol-5-yl(3-(4-isopropylphenyl)oxiran-2-yl)methanone	BDIOM
2	benzo[d][1,3]dioxol-5-yl(3-(4-chlorophenyl)oxiran-2-yl)methanone	BDCOM

Material and Methods: The Chemicals used are purchased for synthesis are of analytical grade were used without further purification. The melting point of the compound was determined in an open capillaries and uncorrected. The ^{1}H NMR and ^{13}C NMR spectra were recorded on Brucker Avance NEO 500MHZ NMR spectrometer using TMS as an internal standard, in addition to this high resolution mass spectra were recorded for further confirmation of the synthesized molecules. Progress of the Reaction is monitored by thin layer chromatography using aluminum sheets precoated with UV fluorescent silica gel Merck 60 F254 and were visualized by UV lamp by using n-hexane and ethyl acetate solvent system.

Synthesis: In first step substituted aromatic aldehyde mainly 4-isopropyl benzaldehyde and 4-chlorobenzaldehyde (0.001 mol) was added in a conical flask containing 10 mL of methanol,to this 5ml of 20% NaOH,then methylene dioxyacetophenone were added (2, 0.001 mol) was added and resulting mixture was stirred on magnetic stirred,progress of the reaction monitored by thin layer chromatography ,after completion of the first step ,to the same conical flask 30% H_2O_2 were added,at cold conditions,then stirred for 2 -3 hrs white solid products were formedafter completion of the reaction reaction queched with ice cold water ,product was filtered and recrystallised by suitable solvent, The progress of the reaction was monitored by thin layer chromatography. The structures of these compounds were confirmed on the basis of their Mass, ^{1}H and ^{13}C NMR spectral analysis.



Scheme 1. Synthesis of BDIOM and BDCOM

Spectral analysis of synthesized compounds:

Benzo[d][1,3]dioxol-5-yl(3-(4-isopropylphenyl)oxiran-2-yl)methanone: ^{1}H NMR (500 MHz, DMSO) δ7.62(dd,J=8.2, 1.7Hz, 1H), 7.50(d, J=8.5Hz 2H), 7.48(d, J=1.7Hz, 1H), 7.21(d, J=8.5Hz, 2H), 7.12(d, J=8.2Hz, 1H), 6.07(s, 2H), 4.64(d, J=1.7 Hz, 1H), 4.03(d, J=1.7Hz, 1H 2.95 – 2.79 (m, 1H), 1.26 (d, 6H). ^{13}C NMR (126 MHz, DMSO) δ 190.85, 152.12, 149.11, 147.98, 132.98, 129.89, 126.33, 125.08, 108.22, 107.11, 102.12, 59.22, 58.33, 33.13, 23.68, 23.63.HRMS Observed 310.1278 calculated 310.35.

Benzo[d][1,3]dioxol-5-yl(3-(4-chlorophenyl)oxiran-2-yl)methanone: ^{1}H NMR (500 MHz, $CDCl_3$) δ7.72(dd, J=8.2, 1.7Hz, 1H), 7.62(d, J=8.5Hz 2H), 7.50 (d, J=1.7Hz, 1H), 7.41(d, J=8.5Hz, 2H), 7.08(d, J=8.2Hz, 1H), 6.17(s, 2H), 4.78(d, J=1.9Hz, 1H), 4.13(d, J=1.9Hz, 1H) ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.57, 152.74, 148.55, 134.93, 134.15, 130.26, 129.03, 127.12, 125.08, 108.21, 107.98, 102.10, 60.82, 58.53. HRMS Observed 302.5147 calculated 302.71

Computational study: The DFT calculations were performed on an Intel (R) Core (TM) i7 personal computer using Gaussian-03 program package. The DFT /B3LYF method with 6-31+G (d, p) basis set level. [18-20] were used to study the geometry of the title compound. The molecular electrostatic potential was computed using the same method for the optimised structure in the gas phase in order to investigate the reactive sites of the BDIOM AND BDCOM molecule.

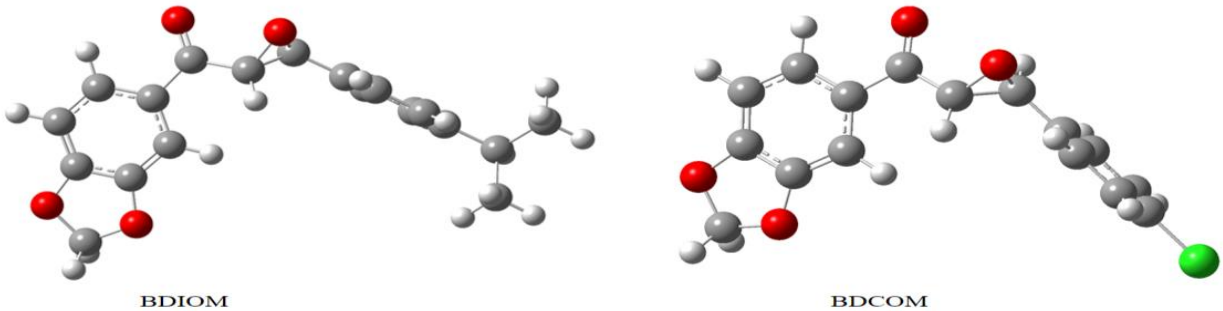


Figure 1: Optimized structure of BDIOM AND BDCOM at DFT/B3LYP method with 6-31 +G (d, p) basis set

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Molecular geometry: The optimized structure of the molecule BDIOM and BDCOM are shown in figure 1 both the molecule containing C1 point group symmetry,dipole moment 5.5226 and 8715 debye indicates polar nature of the compound.the bond length shown in figure 2,data of bond length given in table 2 from that plot the graph of connectivity vs bond legth are shown in fig.3,The carbonyl bond length(C15-O16) are 1.22 A^0 for BDIOM and BDCOM respectively,epoxide skelton bond lengths (C17-C18) are 1.50 A 0,C17-O21 C18-O21 ARE 1.43,1.42 OF BDIOM C17-O21 ,C18-O21 are 1.43 ,1.42 respevtively for BDCOM.

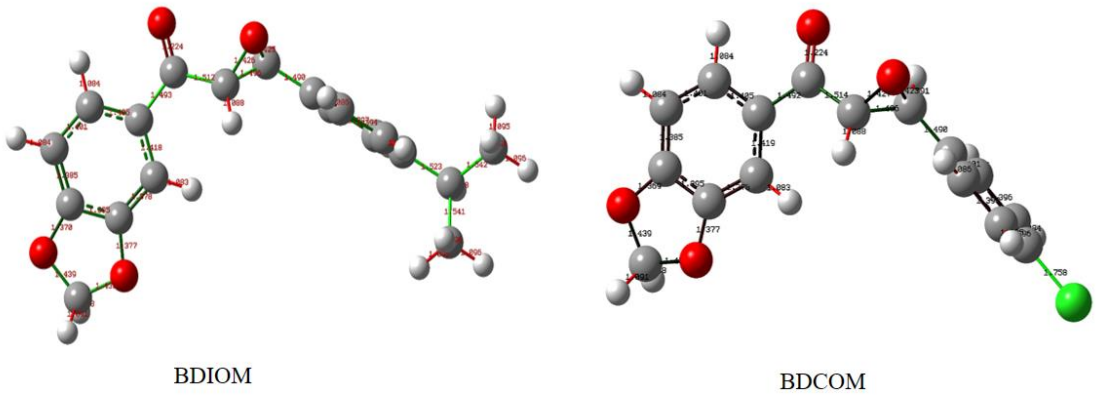

Figure 2: Bond length of BDIOM and BDCOM

Table 2 Optimised geometrical parameters of BDCPP-1at B3LYP/6-311G++ (d,p)

Connectivity	Bond length	Connectivity	Bond length	Connectivity	bond length	Connectivity	bond length
C1-C2	1.39	C17-H19	1.09	C1-C2	1.40	C17-C18	1.50
C1-C6	1.38	C17-O21	1.43	C1-C6	1.38	C17-H19	1.09
C1-O13	1.38	C18-H20	1.09	C1-O13	1.38	C17-O21	1.43
C2-C3	1.38	C18-O21	1.42	C2-C3	1.38	C18-H20	1.09
C2-O14	1.37	C18-C22	1.49	C2-O14	1.37	C18-O21	1.42
C3-C4	1.40	C22-C23	1.40	C3-C4	1.40	C18-C22	1.49
C3-H8	1.08	C22-C24	1.40	C3-H8	1.08	C22-C23	1.40
C4-C5	1.41	C23-C25	1.40	C4-C5	1.41	C22-C24	1.40
C4-H9	1.08	C23-H26	1.09	C4-H9	1.08	C23-C25	1.40
C5-C6	1.42	C24-C27	1.39	C5-C6	1.42	C23-H26	1.09
C5-C15	1.49	C24-H28	1.09	C5-C15	1.49	C24-C27	1.39
C6-H10	1.08	C25-C29	1.40	C6-H10	1.08	C24-H28	1.09
C7-H11	1.09	C25-H30	1.09	C7-H11	1.09	C25-C29	1.40
C7-H12	1.10	C27-C29	1.41	C7-H12	1.10	C25-H30	1.08
C7-O13	1.43	C27-H31	1.09	C7-O13	1.43	C27-C29	1.40
C7-O14	1.44	C29-C32	1.52	C7-O14	1.44	C27-H31	1.08
C15-O16	1.22	C32-C33	1.54	C15-O16	1.22	C29-Cl32	1.76
C15-C17	1.51	C32-C34	1.54	C15-C17	1.51	-	-
C17-C18	1.50	-	-	-	-	-	-

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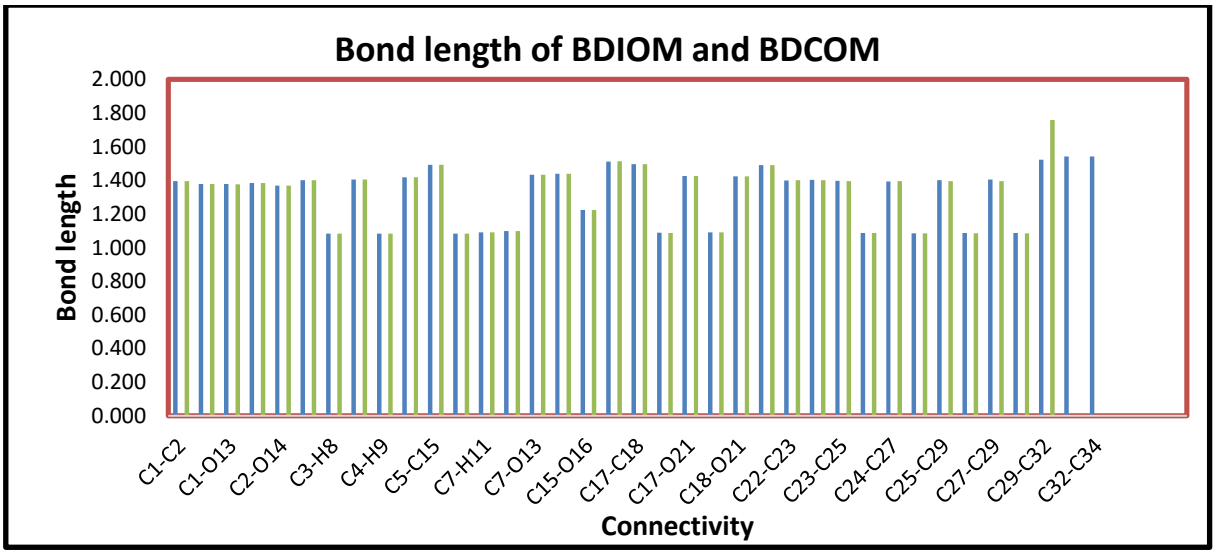

Figure 3 Graphical representation of bond length of synthesized compound

Mulliken atomic charges: Mulliken atomic charges are calculated for BDIOM and BDICOM compounds and are shown in figure, table anad graphical representation ,In BDIOM molecule C6 is carry higher negative charge -0.941,-0.965 and C22 carry higher positive charge 0.556 in nature,C2 carry higher positive charge 0.476,from the MESP plot maximum electron density is situated at epoxide and carbonyl region.

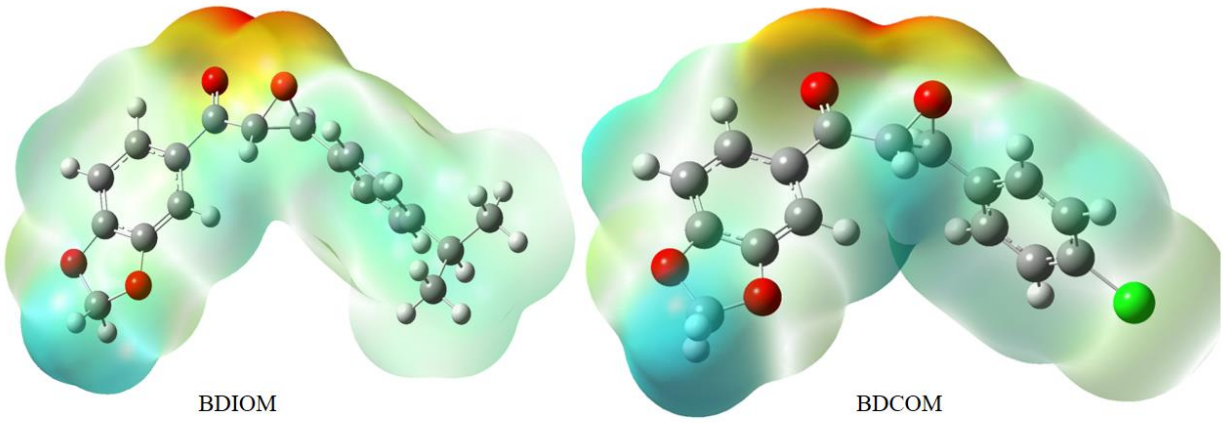

Figure 4: MESP of BDIOM and BDCOM

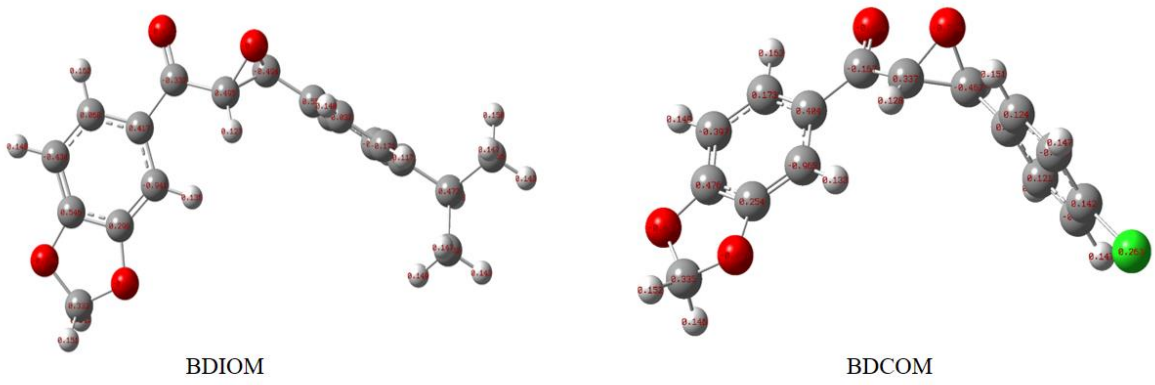

Figure 5: Mulliken atomic charges of BDIOM and BDCOM

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Table 3 Mulliken Atomic charges of BDIOM and BDCOM

BDIOM				BDCOM			
Atom	**Charge**	**Atom**	**Charge**	**Atom**	**charge**	**Atom**	**Charge**
1 C	0.296	22 C	0.556	1 C	0.254	17 C	0.337
2 C	0.546	23 C	-0.375	2 C	0.476	18 C	-0.462
3 C	-0.434	24 C	-0.032	3 C	-0.397	19 H	0.128
4 C	0.068	25 C	-0.056	4C	0.173	20 H	0.150
5 C	0.417	26 H	0.120	5 C	0.404	21 O	-0.256
6 C	-0.941	27 C	-0.171	6 C	-0.965	22 C	0.052
7 C	0.332	28 H	0.140	7 C	0.335	23 C	0.121
8 H	0.148	29 C	-0.225	8 H	0.149	24 C	0.124
9 H	0.162	30 H	0.119	9 H	0.163	25 C	-0.512
10 H	0.135	31 H	0.117	10H	0.133	26 H	0.128
11 H	0.151	32 C	0.472	11H	0.152	27 C	-0.293
12 H	0.145	33 C	-0.562	12 H	0.146	28 H	0.151
13 O	-0.406	34 C	-0.565	13 O	-0.407	29 C	0.142
14 O	-0.409	35 H	0.118	14 O	-0.407	30 H	0.147
15 C	-0.337	36 H	0.149	15 C	-0.167	31 H	0.147
16 O	-0.412	37 H	0.143	16 O	-0.409	32 Cl	0.263
17 C	0.495	38 H	0.147				
18 C	-0.494	39 H	0.150				
19 H	0.127	40 H	0.147				
20 H	0.146	41 H	0.143				
21 O	-0.266						

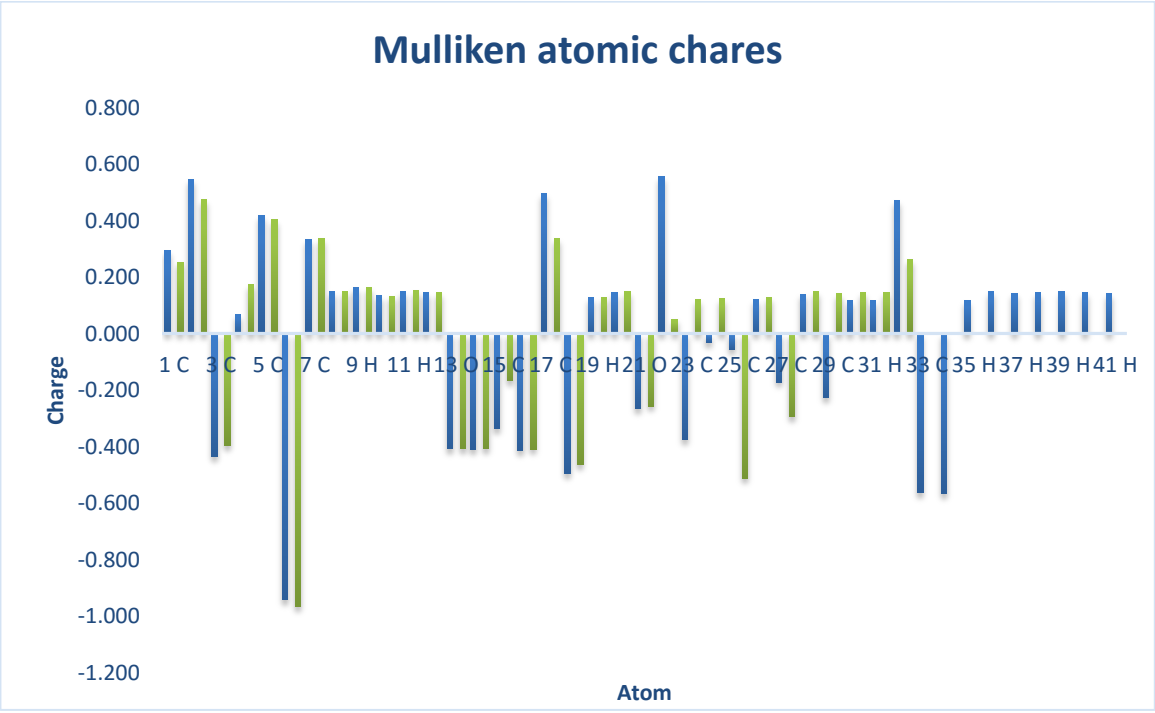

Figure 6: Graphical representation of Mulliken atomic charges of BDIOM and BDCOM

Global Chemical reactivity descriptors: The electron donating and receiving ability of a molecule can be defined using the value of HOMO and LUMO energy. These mo lecular orbitals play vital role in electronic and optical properties, luminescence, photochemical reaction, UV-VIS, quantum chemistry and pharmaceutical studies as well as provide the information of biological mechanism [21-25]. The frontier molecular orbital's (i.e., FMO's) energy gap supports to indicate the stability of structure. Besides, FMO's also informs about the kinetic stability and chemical reactivity of a molecule. Furthermore, the FMO's helps for pre dicting the most reactive position of a studied molecule.

The calculated energy value of HOMO and LUMO orbitals are -6.355,-6.455 and -2.013,-2.168 eVfor BDIOM AND BDICOM respectively. The FMO's energy gap of the BDIOM AND BDICOM were found to be 4.3423 and 4.2874 eV 0.08657 eV. With larger the HOMO and LUMO energy gaps, the less chemical reactivity, biological activity, and polarizability of the examined. The frontier molecular orbital distribution of the compound was depicted in Fig. 7 Compound BDICOM(I= 6.455eV) has higher ionization potential than BDIOM(I=6.355eV).the electron affinity value is higher for BDICOM(2.168eV) and lower for BDIOM(2.013eV). The fact that the specified molecule's electrophilicity index is higher indicates that it has a higher binding capacity with biomolecules and can act as an electrophilic species[15,16,17].here BDCOM has higher electrophilicity index(4.3359) than BDIOM(4.0308).

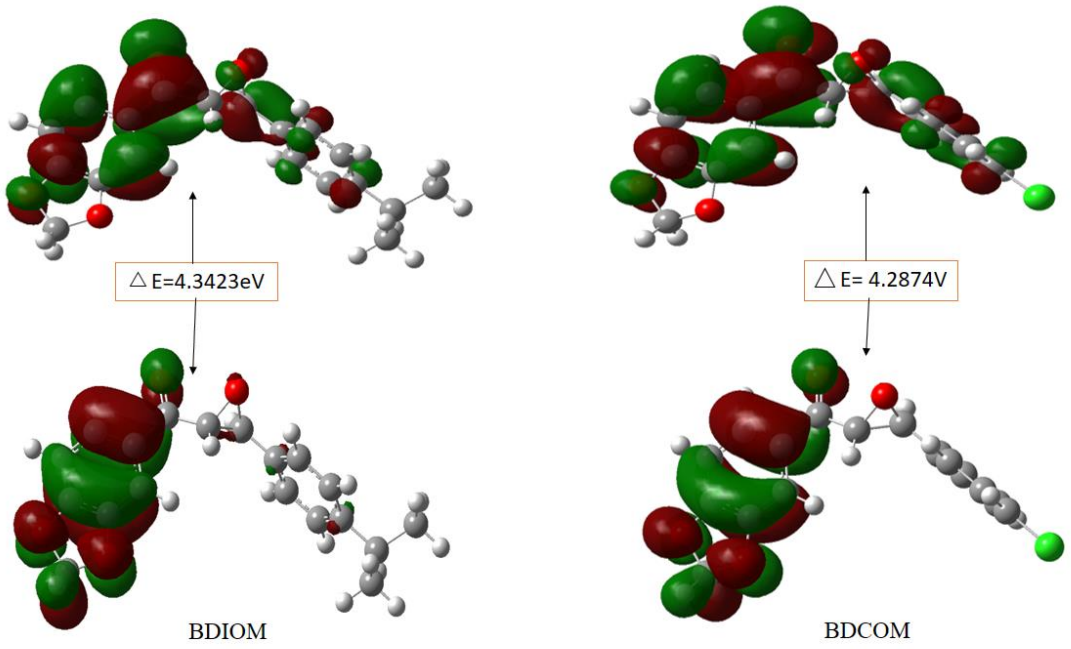

Figure 7: HOMO-LUMO plot of BDIOM and BDCOM

Table 4 Electronic and Global reactivity parameters

ENTRY	E HOMO	E LUMO	Eg	I	A	X	η	S	(μ	ω	NMAx	Dipole moment
BDIOM	-6.355	-2.013	4.3423	6.355	2.013	4.1837	2.1712	0.4606	-4.1837	4.0308	1.9269	5.522608
BDCOM	-6.455	-2.168	4.2874	6.455	2.168	4.3116	2.1437	0.4665	-4.3116	4.3359	2.0113	4.871528

CONCLUSION

The one-pot technique of chalcone synthesis is more convenient, requires less purification, and is faster than the traditional two-step process. The structure of produced compounds was validated using spectroscopic techniques such as proton NMR, CMR, and HRMS.The Density Functional Theory B3LYP/6-311++G (d, p) basis set was utilised to investigate various structural and electrical properties. The same degree of technique was used to investigate features such as the HOMO-LUMO energy gap, molecule electrostatic potential, and global reactivity descriptors. BDIOM has a dipole moment of 5.52 debye, which makes it more polar than BDCOM. Furthermore, the HOMO-LUMO energy gap is 4.34 eV for BDIOM and 4.29 eV for BDCOM, respectively, and thermodynamic parameters such as enthalpy, entropy, and polarizability are determined. The DFT study provides information on the molecule's optimal structure and reactivity

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CONFLICT OF INTEREST

The author declares that they have no conflict of interest.

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