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Density Functional Theory Calculations and Crystal Structures of Some Bis-Chalcone Derivatives

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Abstract: The three bis-chalcone compounds, (*2E,6E*)-2,6-bis(3-chlorobenzylidene)cyclohexanone **(1),** (*2E,6E*)-2,6-bis(2,3-dichlorobenzylidene)cyclohexanone **(2)** and (*2E,5E*)-2,5-bis(2,6-dichloro benzylidene) cyclopentanone **(3),** were studied with theoretical and single-crystal X-ray diffraction (XRD) methods. The molecular geometric parameters, frontier molecular orbitals, MEP, normal mode frequencies and the corresponding vibrational assignments, gauge-including atomic orbital (GIAO) ^{1}H-NMR, ^{13}C-NMR chemical shift values of the bis-chalcone compounds in the ground state have been calculated using the density functional (B3LYP) methods with 6-311G (d,p) basis set. These molecules demonstrate apparently a long and flat shape. The each molecule adopt an *(E)* configuration about the central olefinic bonds. The most important feature is stacking mode in the molecules. The calculated results reveal that the optimized geometries can well reproduce the crystal structure. The theoretical vibrational frequencies and ^{1}H-NMR and ^{13}C-NMR chemical shift values show good agreement with the experimental data.

Keywords: *XRD, bis-chalcone, stacking interactions, DFT,* ^{1}*H NMR,* ^{13}*CNMR, FT-IR*

1. Introduction

Chalcones, also known as α,β-unsaturated ketones, are not only important precursors for synthetic manipulations, but also form a major component of the natural products. Chalcones as well as their synthetic analogues display enormous number of biological activities [1-8]. Apart from the biological activities, the photophysical properties of chalcone derivatives also attracted considerable attention from both chemists and physicists. For example, chalcone derivatives have been reported in relation to nonlinear optics (NLO), photorefractive polymers, holographic recording materials, and fluorescent probes for the sensing of metal ions [9–14]. Also, bis-chalcones are an interesting class of compounds because of their use as precursors to potentially bioactive and functional compounds [15-19]. The estimation of relative energies of molecules is very important both in theoretical studies and in the investigation of their chemical reactivity as well as to understand the possible interactions of reactants. Theoretical calculation can give an insight into some of these issues since it can determine the structure of the molecules, the active sites, and atomic level description of interaction mechanisms on the intermediate formation involved in a given reaction [20-23]. Recently, because of their high accuracy

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theoretical calculations have also signicantly contributed to drug discovery and design [24-25]. In connection with these findings, we report herein on the synthesis of some novel bis-chalcones and their theoretical studies.

2. Method

Bis-chalcones (**1-3**) were synthesized following literature procedures by the condensation of cyclohexanone and cyclopentanone with aromatic aldehydes, respectively. [26-27]. Synthesis and spectroscopic details of the compounds are given in these literatures [26-27].

Table 1. Crystal data and structure refinement parameters for the compounds (**1**), (**2**) and (**3**).

	Compound 1	**Compound 2**	**Compound 3**
Empirical formula	$C_{20}H_{16}Cl_2O$	$C_{20}H_{14}Cl_4O$	$C_{19}H_{10}Cl_4O$
Formula weight	343.23	412.11	396.07
Temperature (K)	292(2)	292(2)	292(2)
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/n$	Pnma	$P2_1/c$
Unit cell dimensions			
a (Å)	9.3911(7)	12.8201(8)	4.3340(5)
b (Å)	16.9716(12)	33.116(2)	26.782(3)
c (Å)	10.5793(7)	4.2722(4)	14.8942(19)
α (°)	90	90	90
β (°)	96.71(2)	90	94.57(2)
γ (°)	90	90	90
Volume (Å^3)	1674.6(2)	1813.8(2)	1723.3(3)
Z	4	4	4
D_{calc} (mg m^{-3})	1.361	1.509	1.527
Absorption coefficient (mm^{-1})	0.389	0.658	0.689
F (000)	712	820	715
Crystal description / colour	block/orange	prism/yellow	prism/yellow
Crystal size (mm)	0.47×0.37×0.33	0.40×0.23×0.14	0.20×0.11×0.10
Index ranges	$-11 \leq h \leq 11$, $-20 \leq k \leq 16$, $-12 \leq l \leq 12$	$-15 \leq h \leq 7$, $-21 \leq k \leq 40$, $-5 \leq l \leq 4$	$-5 \leq h \leq 4$, $-30 \leq k \leq 32$, $-18 \leq l \leq 10$
Reflections collected/unique	5303/3167	3493/1740	5534/3250
Completeness	99.50	99.00	99.00
Data / restrains / parameters	3167/0/207	1740/0/118	3250/0/216
Goodness of fit on F^2	1.054	1.026	1.074
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0483$, $wR_2 = 0.0936$	$R_1 = 0.0419$, $wR_2 = 0.0887$	$R_1 = 0.0648$, $wR_2 = 0.1042$
R indices (all data)	$R_1 = 0.0872$, $wR_2 = 0.1122$	$R_1 = 0.0647$, $wR_2 = 0.1021$	$R_1 = 0.1498$, $wR_2 = 0.1369$
Largest difference peak and hole (e Å^{-3})	0.30/-0.47	0.20/-0.18	0.69/-0.71

2.1. X-ray Crystallographic Studies

A suitable single orange block-shaped crystal **(1)** (0.47×0.37×0.33) mm^3, yellow prism-shaped crystal **(2)** (0.40×0.23×0.14) mm^3 and yellow prism-shaped crystal **(3)** **(**0.20×0.11×0.10) mm^3 were selected and mounted on a Rigaku-Oxford Xcalibur diffractometer with an Eos CCD dedector with a fine-focus sealed tube graphite-monochromated MoK$_\alpha$ radiation (k = 0.71073 Å) at 297 K. Data reductions were performed using the CrysAlisPro software which corrects for Lorentz polarisation [28]. The final completeness is 99.50 for **(1),** 99.00 for **(2)** and 99.1 for **(3).** Using Olex2 [29], the each structure was solved with the ShelXT [30] structure solution program, using the Intrinsic Phasing solution method. The model was refined with version of ShelXL [31] using Least Squares minimisation. All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. The details of the crystal data, data collection and structure refinement of the compounds are summarized in Table 1.

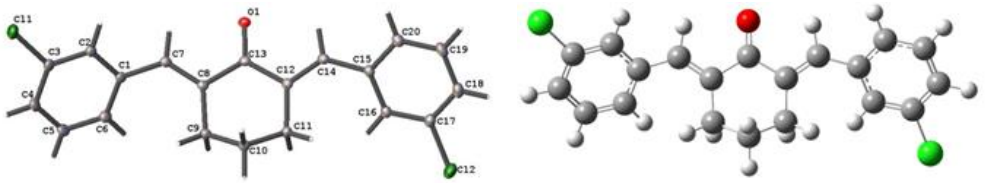
2.2. Computational Methods

Computational calculation of the title compounds were performed by using GaussView molecular visualized program and Gaussian 09W package [32]. The molecular structure of the compounds in the ground state was optimized by Density Functional Theory (DFT) using a hybrid functional B3LYP (Becke's three parameter hybrid functional using the Lee–Young–Parr (LYP) correlation functional) at 6-311G (d, p) double-zeta basis set [33-34]. The geometrical parameters, frontier molecular orbital energies, Molecular Electrostatic Potential (MEP) analysis, frequency (FT-IR) and NMR calculations were obtained from the optimized structures. The true energy minimum at the optimized geometry of the studied compound was confirmed by absence of any imaginary frequency modes. The ^{1}H and ^{13}C isotropic shielding tensors referenced to the TMS calculations were carried out at the same level of the theory. These results were compared with experimental results which was published by Mahdavinia et al and Rahman et al. [26-27].

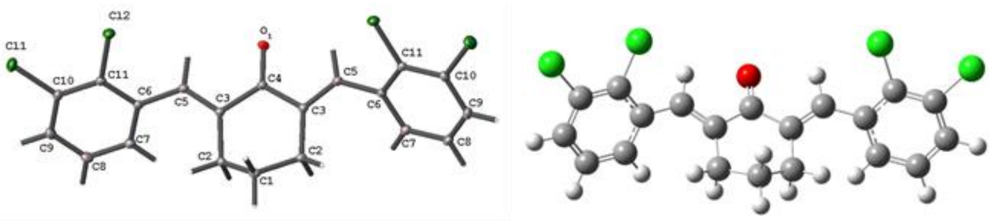
3. Results and discussion

3.1. Experimental Results

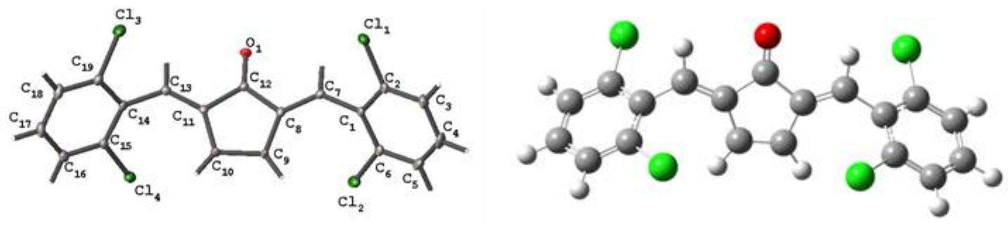
The atomic numbering scheme of the crystal structures and the optimized geometries which have the most favourable conformation of the compound (*2E,6E*)-2,6-bis (3-chloro benzylidene) cyclo hexanone**(1)**, (*2E,6E*)-2,6-bis(2,3-dichloro benzylidene)cyclohexanone **(2)** and (*2E,5E*)-2,5-bis(2,6-dichloro benzylidene)cyclopentanone **(3)** are indicated in Fig.1 (a), (b) and (c). Molecules **(1)** and **(3)** crystallize in monoclinic system with $P2_1/n$ and $P2_1/c$ space group, respectively. Molecule **(2)** crystallizes in triclinic system with Pnma space group. Selected bond distances, bond angles and torsion angles together with corresponding values obtained by means of X-ray crystallographic analysis and DFT calculations are compared and listed in Table 2.



Compound 1



Compound 2



Compound 3

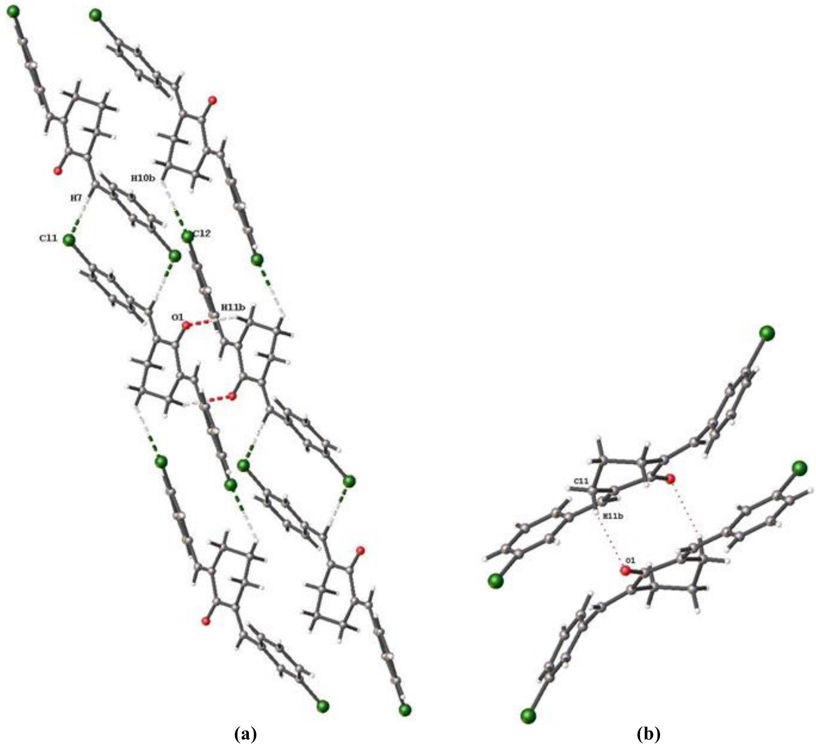
Figure 1. The molecular structure of the compounds (**1**), **(2)** and **(3)** with atom numbering scheme and 30% probability displacement ellipsoids and optimized structures for DFT/ B3LYP/6-311G(d,p) level.

Table 2. Experimental and optimized geometrical parameters of the compounds

	Compound 1			**Compound 2**			**Compound 3**	
	Exp.	**DFT**		**Exp.**	**DFT**		**Exp.**	**DFT**
Bond Length (Å)			**Bond Length**			**Bond Length**		
Cl(1)-C3	1.738(3)	1.760(2)	*Cl(1)*-C10	1.730(3)	1.749(2)	*Cl(1)*-C2	1.735(6)	1.75(2)
Cl(2)-C17	1.737(3)	1.761(2)	*Cl(2)*-C11	1.724(2)	1.747(2)	O1-C12	1.220(6)	1.209(2)
O1-C13	1.225(3)	1.223(2)	O1-C4	1.220(5)	1.220(2)	*Cl(2)*-C6	1.728(5)	1.758(2)
C1-C7	1.465(3)	1.464(2)	C3-C5	1.327(3)	1.347(2)	*Cl(3)*-C19	1.734(6)	1.757(2)
C7-C8	1.338(3)	1.35(2)	C5-C6	1.464(3)	1.468(2)	*Cl(4)*-C15	1.737(5)	1.758(2)
C12-C14	1.344(3)	1.35(2)				C1-C7	1.472(7)	1.472(2)
C14-C15	1.460(3)	1.464(2)				C7-C8	1.345(7)	1.343(2)
						C11-C13	1.318(7)	1.343(2)
						C13-C14	1.472(6)	1.472(2)
Bond Angles(°)			**Bond Angles**			**Bond Angles**		
O1-C13-C8	120.0(2)	120.61(2)	O1-C4-C3	120.26(2)	120.72(2)	C8-C12-O1	126.9(4)	127.11(2)
O1-C13-C12	120.7(2)	120.66(2)	C3-C5-C6	128.6(2)	127.92(2)	C11-C12-O1	125.6(5)	127.12(2)
C1-C7-C8	128.8(2)	130.06(2)	C4-C3-C5	116.0(2)	115.61(2)	C1-C7-C8	129.0(2)	127.44(2)
C12-C14-C15	130.1(2)	130.54(2)	C5-C6-C11	120.7(2)	120.56(2)	C11-C13-C14	128.6(5)	127.43(2)
C2-C3-*Cl(1)*	119.7(2)	119.26(2)	C6-C11-*Cl(2)*	119.38(2)	119.40(2)	C7-C1-C6	123.9(4)	124.35(2)
C18-C17-*Cl(2)*	119.4(2)	119.18(2)				C13-C11-C10	131.4(4)	132.26(2)
C7-C1-C2	118.8(2)	117.47(2)				C1-C6-*Cl(2)*	121.0(4)	120.63(2)
C14-C15-C20	118.7(2)	117.89(2)				C14-C15-*Cl(4)*	120.1(3)	120.63(2)
C7-C8-C13	117.4(2)	115.53(2)				C7-C8-C12	118.3(4)	121.70(2)
C13-C12-C14	116.6(2)	115.39(2)				C12-C11-C13	119.7(4)	121.70(2)
						C2-C1-C7	119.5(5)	119.92(2)
						C13-C14-C19	119.3(4)	119.93(2)
						C2-C1-*Cl(1)*	119.3(4)	119.13(2)
						C14-C19-*Cl(3)*	118.7(4)	119.13(2)
Torsion Angles (°)			**Torsion Angles**			**Torsion Angles**		
C6-C1-C7-C8	-38.3(4)	-31.10(2)	O1-C4-C3-C5	7.5(4)	10.48(2)	C7-C8-C12-O1	168.5(4)	0.91(2)
C12-C14-C15-C16	-30.8(3)	28.67(2)	C3-C5-C6-C7	44.5(4)	43.48(2)	C13-C11-C12-O1	10.9(8)	-0.914(2)
O1-C13-C12-C14	7.9(3)	1.54(2)	C2-C3-C5-C6	4.1(4)	4.69(2)	C1-C7-C8-C9	-0.9(8)	2.41(2)
C7-C8-C13-O1	11.4(3)	-3.28(2)				C14-C13-C11-C10	-0.6(9)	-57.21(2)
						C7-C1-C2-*Cl(1)*	-3.1(6)	1.98(2)
						C13-C14-C19-*Cl(3)*	0.2(6)	-1.98(2)

The compound **(1)** consists of chlorobenzylidene rings which are connected by a cyclohexanone ring and exists in (*E*) configuration with respect to C13=O1 double bond [1.342 Å]. The dihedral angles of between the least-square plane of chlorobenzylidene rings (C1/C6 and C15/C20) and cyclohexanone ring (C8/C13) system is 52.70(2)° and 41.68(2) respectively. The dihedral angles of between the all rings and the molecule plane are 24.20(2)° for (C1/C6) ring, 30.90(2) ° for (C8/C13) ring and 15.86(9) ° for (C15/C20) ring. The molecule is not coplanar. In the molecule **(1),** the central cyclohexanone rings adopts an chair conformation with puckering parameters are Q=0.496(3) Å, $\theta = 131.8(3)$ and ∅=293.8(4) °.

In the crystal (**1**), two adjacent molecules are interconnected by a pair of intermolecular C11-H11B…O1 hydrogen bonds (C11-H11B:0.97(3) Å, H11B…O1: 2.484(3) Å, C11…O1: 3.335 (3) Å, C11- H11B…O1 :146.4 (2) °) which form an inversion dimer (Fig. 2b) resulting in a R_2^2 (10) ring motif [35]. The dimers are further linked into other ring motifs formed via short Cl1…H7 (2.985(2) Å) and Cl2 H10b (3.002(2) Å) along the *(010)* plane as shown in figure 2 (a) and this structure formed 1D supramolecular network. In addition the compound comprise of two weak C-H…O hydrogen bonds. The bond lengths and bond angles are in the normal ranges. They are good aggreement with the reported earlier [36-37-38].



(a) **(b)**

Figure 2. (a) The formation of the sheets and 1D supramolecular network lying parallel to (100) plane in the crystal structure of the compound 1 and **(b)** centrosymetric hydrogen-bonded dimer structure formed *via* intermolecular C-H…O hydrogen bonds around the inversion centre.

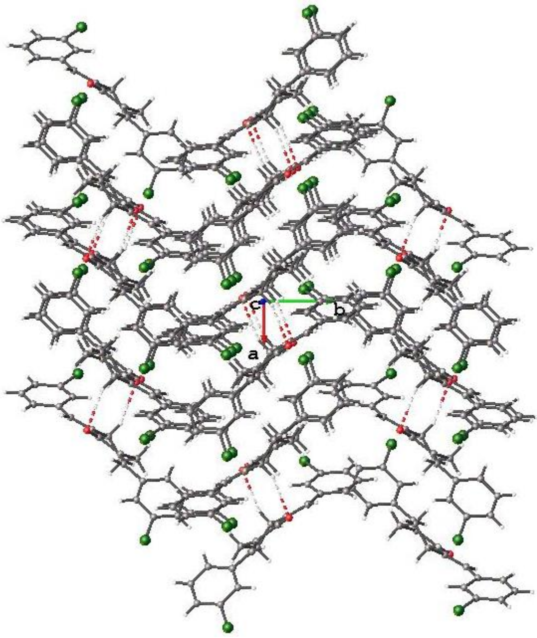


Figure 3. The packing diagram of the compound (1) by C-H…O hydrogen bonds along the *(001)* plane.

The compound **(2)** contains one-half of a molecule in the asymetric unit. The other half of the molecule is generated with x, 1/2-y, z symmetry operator. The molecule has crystallographic mirror symmetry with the C=O bond on the mirror plane. The dihedral angle of between the two phenyl rings (C6/C11 and cyclohexanone ring) is 55.99(2)°. In the molecule **(2),** the central cyclohexanone rings adopts an chair conformation with puckering parameters are Q=0.488(3) Å, $\theta = 130.5(3)$ and $\emptyset$=180.0(4)°. The dihedral angles of between the dichlorobenzylidene rings and cyclohexanone ring with molecule plane are 15.61 (9)° and 44.88(2)° respectively.

The **(2)** includes only weak intramolecular C-H…O hydrogen bond. Packing structure of the molecule **(2)** generate via stacking interactions along the *(101)* plane. In addition to this , there is only C10-Cl1…π [dichlorobenzylidene ring with 3.9186(2) Å (symetry code: x, y,-1+ z)] interactions in the crystal structure.

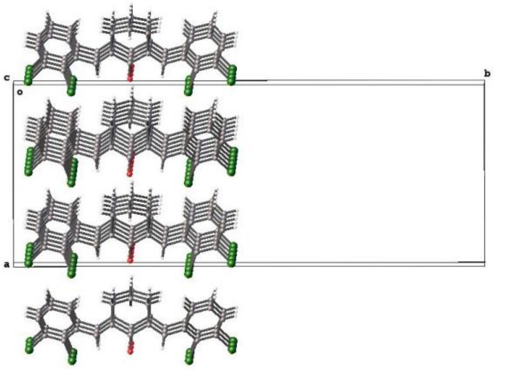


Figure 4. The packing diagram of the compound **(2)** with stacking along the *(101)* plane.

In the compound **(3),** the angles between the planes of the cyclopentanone ring and the two phenyl rings are 60.5(3)° and 62.3(3)°, respectively, and the dihedral angle between the aromatic ring planes is 52.1(3)°. The molecule is not coplanar. In the molecule **(3),** the central cyclopentanone ring adopts an envelope conformation.

The **(3)** consists of only strong C-H…O intermolecular and two weak C-H…O intramolecular hydrogen bonds. The packing diagram of (**3**) is occurred with strong hydrogen bond and intramolecular H7…Cl1 [2.857(5)] short stacking interactions. In the molecule **(3)**, 1D chain occurs along the *(100)* plane via strong C6-Cl2···Cg2, C15-Cl4...Cg3 and C12-O1…Cg1 interactions [Cg2: C1/C6, Cl2···Cg2: 3.681(3) Å; Cg3: C14/C19, Cl4…Cg3:3.744(3) Å and Cg1:C8/C12, O1…Cg1:3.330(4) Å ssymetry code (ii): -1+x, y, z] [figure 6].

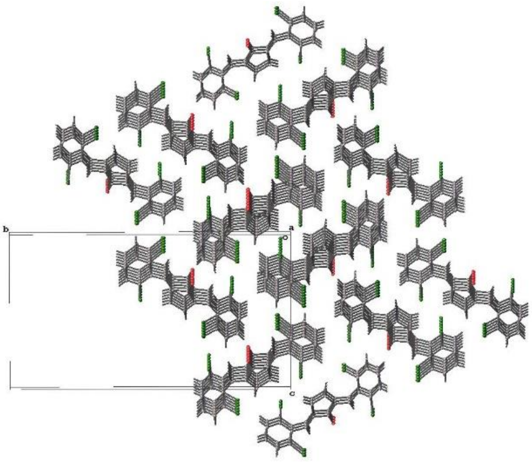


Figure 5. The packing diagram of the compound *(2)* with stacking along the *(101)* plane.

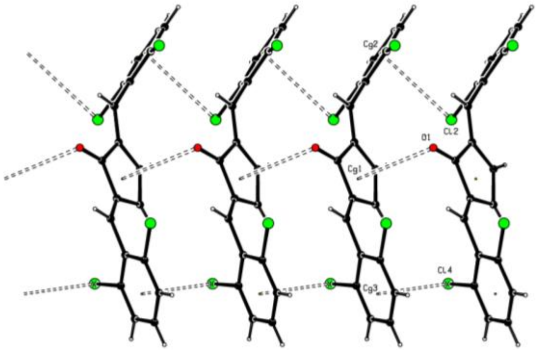


Figure 6. Formation of 1D chain structure of the compound (2).

All molecules demonstrate apparently a long and flat shape. The each molecule adopt an *E* configuration about the central olefinic bonds. The most important feature is stacking mode in the molecules. Some of the experimental and optimized geometrical parameters are listed in Table 2. In general, all the computed parameters are in good agreement with the reported X-ray experimental data. In the Table 2 theoretical studies indicated that , the shorting of the C=C double bonds showing the partial double bond character of the C=C bands which are influenced by adjacent conjugated double bonds. Also, the conformation of these molecules are the result of interaction between the electronic pair of the oxygen in the carbonyl group. According to the theoretical studies, the largest difference between the experimental and calculated bond lengths and bond angles are 0.022 Å and 1.20°. But the torsion angles are slightly differ experimental values. These discrepancies can be explained by the fact that the calculations assume an isolated molecule.

Table 3. Hydrogen bonds (Å, °).

Molecule	D-H···A	D–H	H···A	D···A	D–H···A
1	C7-H7…O1	0.93(3)	2.349(3)	2.736(3)	104.6(2)
	C11-H11B…O1[i]	0.97(3)	2.484(3)	3.335(3)	146.4(2)
	C14-H14…O1	0.93(3)	2.334(3)	2.737(3)	105.8(2)
2	C5-H5…O1	0.93	2.30	2.708(3)	106
3	C4-H4…O1[ii]	0.929(2)	2.556(2)	3.384(2)	148.7(2)
	C7-H7…O1	0.929(2)	2.511(2)	2.870(2)	103.2(5)
	C13-H13…O1	0.930(2)	2.514(2)	2.868(2)	102.9(5)

Symetry code: (i): 2-x,1-y,1-z; (ii): -1+x,1/2-y,1/2+z

3.2. Frontier Molecular Orbitals

The frontier molecular orbitals (HOMO and LUMO) determine the molecule interacts with other species which has great importance in modern biochemistry and molecular biology. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) orbitals could act as electron-donor and electron-acceptor character, respectively [39]. It can be observed from Fig. 7 that the HOMO of the compounds are delocalized on all the atoms except for chlor and hydrogen atoms and mainly on the double bonds, the LUMO of the compounds are delocalized over the entire compound, except for chlor atoms. The HOMO– LUMO gaps are 4.00 eV **(1)**, 4.13eV **(2)**, 3.99 eV **(3)**, respectively. The calculated band gap values indicate that the molecules have stable structure.

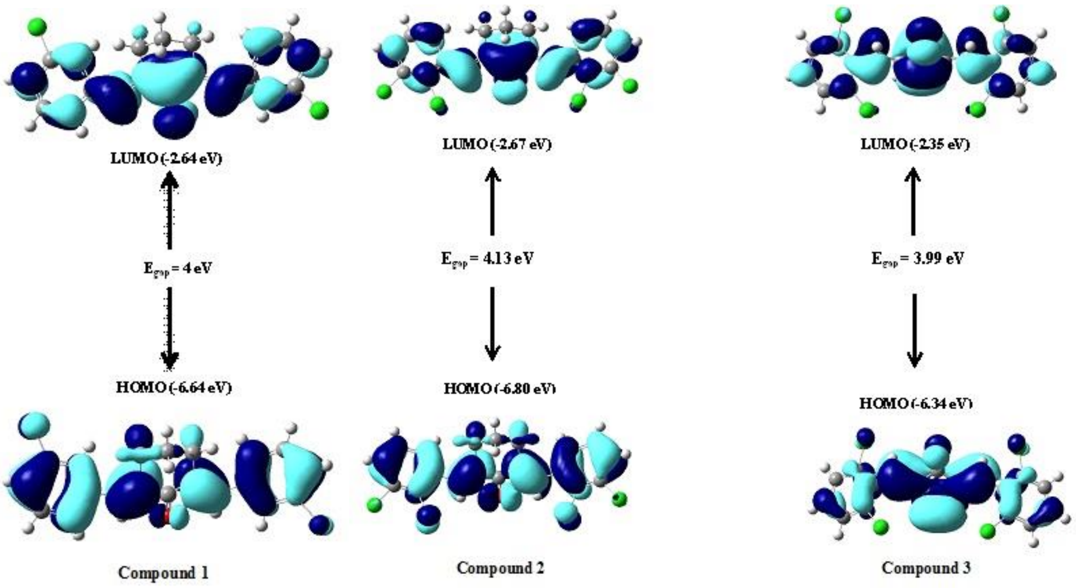
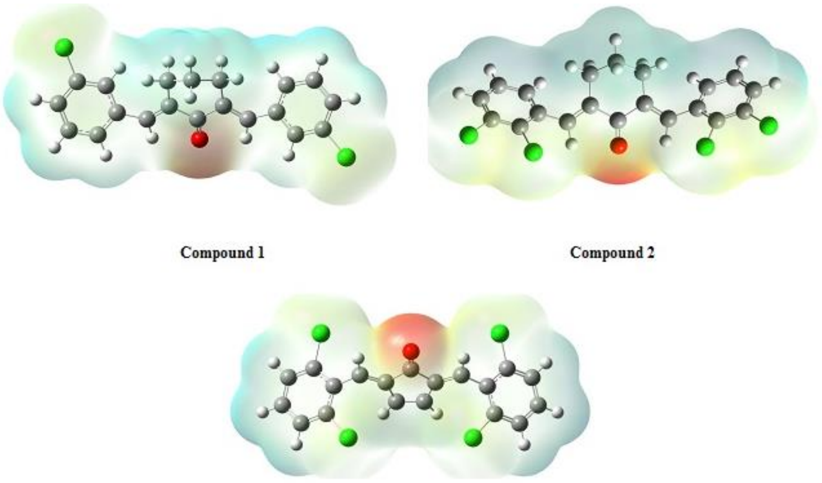


Figure 7. Frontier molecular orbitals of the compounds.



Compound 1

Compound 2

Compound 3

Figure 8. Molecular Electrostatic Potential Surface of the compounds.

3.3. Molecular Electrostatic Potential

In order to identify the reactive sites sensitive to electrophilic and nucleophilic attack, the MEP map (Fig. 8) was calculated for the optimized structure of all compounds. The regions with the strongest negative electrostatic potential are coloured in red and the strongest positive electrostatic potential in blue. The regions with zero potential are represented in green. The MEP of the all molecules indicate that the negative electrostatic potential regions are mainly found over the oxygen atoms these being the most probable sites for electrophilic attack. The positive regions are localized around all the hydrogen atoms, these being the most probable sites for nucleophilic attack. The zero potential regions are localized around the chlor atoms.

3.4. Theoretical NMR Spectroscopy Studies

The carbon and hydrogen chemical shift values of the compounds were calculated based on Gauge-independent atomic orbital (GIAO) method at B3LYP/6-311G(d,p) level of theory [38]. The theoretical values are showed in Table 5. For the B3LYP/6-311G(d,p) method, the chemical shift value of tetramethylsilane (TMS) $\sigma_0(^{13}C)$ = 179.7024 ppm and $\sigma_0(^{1}H)$ = 31.3919 ppm was obtained [31]. For the compounds, NMR spectral data shows that the C13 (compound 1-183.83 ppm), C4 (compound 2-174.22 ppm) and C12 (compound 3-169.25 ppm) atoms have the most chemical shift value that are due to the intramolecular hydrogen bond formed with the carbonyl group. In addition this result indicate *(E)* configuration of the molecules conformations. These ^{13}C NMR values are good aggrement with reported values [36].C10 value for the compound **(1)** and C1 value compound (**2)** have the least one as 23.14 ppm and 23.9 ppm, respectively. This result show that these compounds have chair conformation. ^{1}H-NMR chemical shift values are calculated at 0.84-7.67, 0.8-6.79 and 6.22-6.75 ppm for (**1)**, (**2)** and (**3)** respectively. There is a good agreement between the calculated and previously observed chemical shift values of the compounds [26-27].

3.5. Theoretical Infrared Spectroscopy Studies

The calculated vibrational frequencies are presented with their assignments in the Table 6. The C-H stretching vibrations of aromatic compounds calculated of 3100-3300 cm$^{-1.}$ The scissoring, wagging and rocking of C-H group are 1400-1600 cm^{-1}, 700-800 cm^{-1} and 1100-1200 cm^{-1}, respectively. The methylene groups give rise to C-H stretching band in the region. The wagging, twisting and rocking of the methylene group are calculated 1300-1400 cm^{-1}, 1200-1300 cm^{-1} and 700-800 cm^{-1}, respectively. The C=O stretching give rise to absorption bands in the region of 1700-1800 cm^{-1}. The carbonyl (C=O) carbon-oxygen double bond is formed by overlap of p-orbitals of carbon and oxygen atoms and is highly polar due to the highly electrophilic and the electronegatively of oxygen [40]. The aromatic ring C=C stretching vibration modes were computed at 1600-1700 cm^{-1}. These results are considerably compatible with the experimental data [26-27].

Table 5. Calculated ^{1}C NMR values of the compounds in chloroform

Atom	**Compounds**				**Compounds**		
	(1)	**(2)**	**(3)**	**Atom**	**(1)**	**(2)**	**(3)**
C1	140.58	23.9	137.53	H1a	-	0.8	-
C2	134.21	28.89	146.82	H1b	-	1.11	-
C3	145.09	139.84	128.85	H2a	-	2.22	-
C4	129.83	174.22	128.94	H2b	-	1.90	-
C5	129.34	139.3	129.47	H2	6.9	-	-
C6	127.74	140.22	144.19	H3	-	-	6.71
C7	140.46	129.66	128.22	H4	6.73	-	6.60
C8	138.66	125.91	140.47	H5	6.8	7.68	6.74
C9	28.76	131.43	137.99	H6	6.73	-	-
C10	23.14	143.82	137.99	H7	7.63	6.52	6.73
C11	28.83	143.79	140.47	H8	-	6.56	-
C12	138.45	-	169.25	H9	-	6.79	6.22
C13	183.83	-	126.22	H9a	2.43	-	-
C14	140.49	-	137.53	H9b	2.05	-	-
C15	140.28	-	144.19	H10	-	-	6.22
C16	130.23	-	129.47	H10a	0.84	-	-
C17	144.42	-	128.94	H10b	1.27	-	-
C18	129.87	-	128.85	H11a	2.4	-	-
C19	130.15	-	146.83	H11b	2.07	-	-
C20	132.25	-	-	H13	-	-	6.73
C21				H14	7.67	-	-
				H16	6.85	-	6.75
				H17	-	-	6.60
				H18	6.74	-	6.71
				H19	6.85	-	-
				H20	6.83	-	-

Table 6. Calculated frequencies for the compound.

Bond assignment^{a}	**Scaled frequency, cm^{-1} (Calculated)**		
	1	**2**	**3**
ν_{sym}(C-H)$_{\text{aromatic}}$	3215.08	3209.34	3211.88
ν_{asym}(C-H)$_{\text{aromatic}}$	3176.97	3182.77	3211.86
ν_{sym}(C-H)$_{\text{cyclopentanone}}$	…………..	………..	3230.89
ν_{asym}(C-H)$_{\text{cyclopentanone}}$	…………	…………	3212.93
ν_{sym}(C-H)$_{\text{C7 and C14}}$	3150.19	……….	…………
ν_{sym}(C-H)$_{\text{C7 and C113}}$	……….	…………	3145.91
ν_{asym}(C-H)$_{\text{C7 and C14}}$	3149.30	…………….	………..
ν_{sym}(C-H)$_{\text{C5}}$	……….	3168.04	…………
ν_{asym}(C-H)$_{\text{C5}}$	……….	3167.04	………….
ν_{asym}(C-H$_2$)	3025.49	3035.40	………….
ν_{sym}(C-H$_2$)	3068.82	3075.40	………….
ν(C=O)	1732.86	1739.00	1803.40
ν(C7=C8; C12=C14)	1651.99	…………….	………….
ν(C7=C8; C11=C13)	…………...	……………..	1693.39
ν(C3=C5)	………	1656.71	………..
α(C-H)$_{\text{aromatic}}$	1622.27	1616.84	1619.97
α(C-H$_2$)	1491.78	1492.38	………….
α(C-H)$_{\text{cyclopentanone}}$	……………	…………	1569.67
ω(C-H$_2$)	1362.85	1358.79	……….
τ(C-H$_2$)	1297.22	1298.16	
ω(C-H)$_{\text{aromatic}}$	796.84	761.75	761.75
γ (C-H)$_{\text{aromatic}}$	1156.27	1155.15	1172.19
γ (C-H$_2$)	759.96	753.01	………..
γ (C-H)$_{\text{cyclopentanone}}$	…………	…………….	1178.73

^{a}Abbreviations: *ν*-stretching; α-scissoring; *γ*-rocking;*;* τ-twisting, *ω*-wagging.
Subscripts: *asym*, asymmetric; *sym*, symmetri

4. Conclusion

The three new chalcone compounds namely (*2E*,*6E*)-2,6-bis(3-chlorobenzylidene)cyclo hexanone **(1),** (*2E,6E*)-2,6-bis(2,3-dichloro benzylidene)cyclohexanone **(2)** and (*2E,5E*)-2,5-bis(2,6-dichloro benzylidene) cyclo pentanone **(3)** were studied with theoretical and single-crystal X-ray diffraction (XRD) methods. The molecular geometric parameters, frontier molecular orbitals, MEP, normal mode frequencies and the corresponding vibrational assignments, gauge-including atomic orbital (GIAO) ^{1}H-NMR, ^{13}C-NMR chemical shift values of the bis chalcone compounds in the ground state have been calculated using the density functional theory (B3LYP) methods with 6-311G (d,p) basis set. The bond lengths and bond angles are in the normal ranges and are comparable with the reported earlier. Calculated NMR and FT-IR results are considerably compatible with the experimental data. The each molecule adopt an *E* configuration about the central olefinic bonds. The most important feature of the molecules is stacking mode. In general, all the computed parameters are in good agreement with the reported X-ray experimental data.

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