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Synthesis and molecular characterization with DFT study of 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)-ethanone

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In this study, we have presented the synthesis and structure analysis of 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)–ethanone. The molecular elucidation is conducted by Fourier transform infrared (FT-IR) and Nuclear magnetic spectroscopy NMR (^{1}H and ^{13}C-NMR). The FT-IR recording in 4000-500 cm^{-1} are done in KBr solid phase, while the NMR spectrum for both ^{1}H and ^{13}C-NMR are done in the DMSO-6. Density functional theory (DFT) was used to stimulate and confirm the structure and molecular characteristics, using the DFT/B3LYP/cc-pVDZ method to study various conformers of the compound and their minimum energies by the scanning potential energy surface. In addition, the molecular electrostatic potential (MEP) map and charge spreading have been plotted for the molecule to account for the chemical reactivity and site selectivity. Furthermore, the thermodynamic properties for the molecule have been studied. A good correlation is found between experimental and simulation studies for FT-IR and NMR results. In the simulation data, the differences of energy between the conformers are found to be very small.

Keywords: Cyclobutane, DFT, MEP, Molecular reactivity, Thermodynamic properties

Cyclobutane $(C_2H_4)_2$ (CYLB) is an alicyclic compound that has van der Waals interaction, and a polar molecule. CYLB is colorless, flammable, water-insoluble, the boiling point is 12 °C and the melting point is -80 °C. CYLB has no commercial and biological importance, but its complex derivatives are very good in biology and biotechnology. For example, 3-substituted cyclobutane carboxylic acid derivatives exhibit anti-inflammatory and antidepressant activity.[1,2] CYLB may be formed by the effect of light on Diel-Alder reaction[3]. In 1887 William Perkin was succeeded in synthesis CYLB-carboxylic acid, it is the first generalized CYLB derivatives[4]. Akhmedov et al. were synthesized 1,1,3-trisubstituted cyclobutane rings from unsaturated derivatives with lewis acids[5]. Recently many researchers have synthesised and characterized CYLB derivatives[6-8]. DFT calculation has a reasonable cost-accuracy ratio for structure analysis in large systems, however, the calculations are always prohibitive and work best for charged systems[9-12]. The combination of DFT calculation and experimental studies leads to understand the characterization of the molecule[13-16]. DFT has higher accuracy of molecular analysis including vibrational frequencies, thermodynamic, electronic properties for a polyatomic molecule[17]. The main objective of this study is to the synthesis and molecular characterization of 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)–ethanone. As a stimulation model of the molecule properties, DFT on the cc-pVDZ basis set has been used.

Experimental Details

Chemicals

All chemicals including Ether $(C_2H_5)_2O$, $CaCl_2$ (anhydrous), $AlCl_3$ (anhydrous), KOH, $Na_2Cr_2O_7$, H_2SO_4 and DMSO-d6 were purchased from Merck, and later used without extra purifications. 6-Chloro-4,5-epoxy-2-methyl-1-hexene was received from the organic Lab at Chemistry Department, Firat University, and it was distilled before use. FT-IR spectra were recorded with the Perkin-Elmer spectrum. The melting point was measured using Electrothermal 9100. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on Bruker ascend 400 NMR spectrometer operating at 400 MHz for ^{1}H and 100 MHz for ^{13}C NMR, using DMSO-d6 as solvent.

Synthesis of 2-chloro-1-(3-mesityl-3-methylcyclobutyl)ethan-1-ol

The experimental setup was four necks round bottom flask were attached with dropping funnel, thermometer, and calcium chloride tube placed in a mechanical mixer. After that, 1500 mL of mesitylene, 167 g of anhydrous $AlC1_3$ were added and followed by addition of 183 g of epoxide compound dropwise at (11-12) °C. The mixture was stirred for 2 h, and then decomposed with 15% HCI. The solution was neutralized with 5% NaOH aliquot. After that was dried with $MgSO_4$ and the solvent was removed on the rotary evaporator. Finally, 247 g of compound 2-chloro-1-(3-mesityl-3-methylcyclobutyl)ethan-1-ol (3) was obtained.

Synthesis of 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)–ethanone

Four-neck conical flask 1000 mL fitted with thermometer, funnel, stirrer and condenser, then sodium dichromate (0.29 mol), 2-chloro-1-(3-methyl-3-(2,4,6-trimethyl cyclohexyl) cyclobutyl) ethan-1-ol (0.52 mol) were added, followed by 50 ml water. H_2SO_4 (75 ml) (68% v/v) was added after 7-8 h of running the experiment at room temperature, from the neck of the funnel. The mixture was stirred for 18 h at room temperature. The solid product was formed and filtered, and then the filtrate was extracted with several portions of diethyl ether. The extracts were combined and dried over anhydrous $CaCl_2$, then recrystallized with ethyl alcohol as compound 4.

Characterization of 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)–ethanone

The reaction illustrated in Fig. 1 yielded, 55% of synthesis of 2-chloro-1-(3-mesityl-3-methylcyclobutyl) ethan-1-one. Molecular characteristics were; melting point: 97-98 °C; FT-IR (KBr, cm^{-1}, υ): 1812 (C=O), 1658 and 1612 (C=C in ring), 3155 (Ar-H); ^{1}H-NMR (400 MHz, DMSO-d_6, δ, ppm): 1.49 (s,3H, -CH_3-(cyclobutane), 2.14 (s, 9H, -CH_3 (mesitylene), 2.35-2.51 (m, 4H, -CH_2)- (cyclobutane), 3.46 (p, 1H, -CH-(cyclobutane), J = 8.80 Hz), 4.55 (s, 2H, CH_2-Cl), 6.71 (s, 2H, Ar-H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ, ppm): In the spectrum drawn by ATP method, (5 peaks for CH_3 and CH_2 s), (20.45, 20.75, 25.24, 37.68, 130.29); (7 pieces of CH and aprotic carbons), 39.77, 40.21, 48.42, 130.29, 134.06, 143.94, 203.90 Elemental analysis (theoretical): C, 72.57; H, 7.99; 0, 6.04; experimental, C, 72.56; H, 8.01; O, 6.07.

Computational study

All theoretical calculations were carried out with Gaussian 09, using combined approach of B3LYP and cc-pVDZ. First, the optimization and the vibrational frequency are confirmed for synthesis of 2-chloro-1-(3-mesityl-3-methylcyclobutyl)ethan-1-one. Second, NMR chemical shift was measured by using the Gauge Independent Atomic Orbital (GIAO) process. Finally, Frontier molecular orbital which is produced by HOMO-LUMO energy level, molecular electrostatic potential (ESP), atomic charge density, and thermodynamic properties were calculated[18, 19].

Results and Discussion

Molecular geometry

The basis set of B3LYP/cc-pVDZ calculated bond lengths, bond angles, and dihedral angles of 2-chloro-1-(3-mesityl-3-methylcyclobutyl)ethan-1-one. Atomic numbering configuration of the theoretical geometric structure using ChemBioDraw and Gaussian View, presented in Fig. 2. The aromatic ring was skewed from the natural hexagon, the bond length for C-C and C=C was equal to 1.39 Å and 1.42 Å, respectively, but the actual bond length between C-C

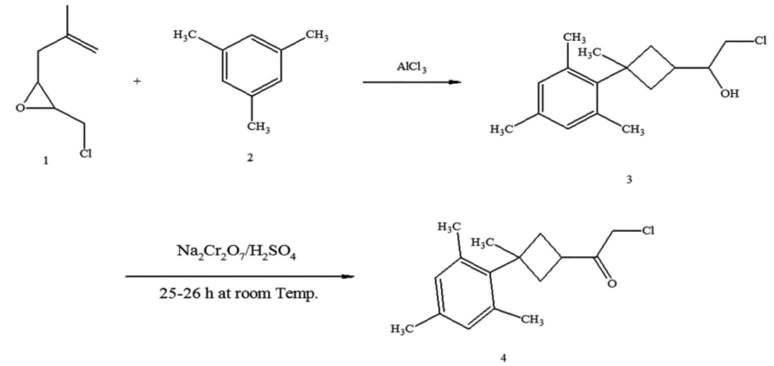

Fig. 1 — The mecahnism of synthesising compounds (4)

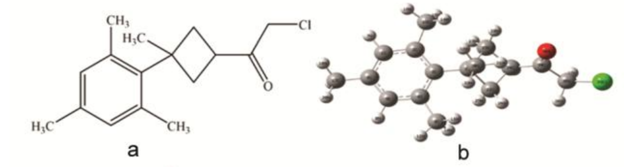

Fig. 2 — The geometrical structure of compound 4 A) Draw by ChemBioView Ultra B) Optimization by Gaussian

and C=C in the benzene ring was equal to 1.34 Å and 1.54 Å, respectively. This variation of bond length is due to the steric effect of the -CH_3 groups in a present compound 4. The real bond length between C-C in cyclobutane was identical to 1.55 Å[20, 21], but in the current study assigned to 1.57 Å, the cyclobutane ring was attached by three different groups. Based on the result of the bond length for C=O and C-Cl, can conclude that our data is well comparable with previous data. The DFT calculations provide narrowing angle of C3-C2-C1, C4-C3-C2, C5-C4-C3, and C6-C1-C2 by 119.85, 117.89, 119.88, and 122.55, respectively. The normal angle for benzene ring is 120°. This shows that this distortion is caused by the replacement of the CH_3 group at positions C2, C4, and C6 with the long-chain in position C3. The variation in bond lengths, bond angles, and dihedral angles are summarized in Table 1.

Table 1 — The geometrical optimization parameters of compound 4 in the ground state

Symbol	Bond Length	Symbol	Dihedral angle
C2-C1	1.40	C4-C3-C2-C1	-5.28
C3-C2	1.42	C5-C4-C3-C2	5.30
C4-C3	1.42	C6-C1-C2-C3	1.38
C5-C4	1.40	C9-C4-C3-C2	-172.76
C6-C1	1.39	C13-C2-C1-C6	-176.94
C9-C4	1.51	C17-C6-C1-C2	-178.07
C13-C2	1.51	C21-C3-C2-C1	178.71
C17-C6	1.50	C22-C21-C3-C2	-142.98
C21-C3	1.53	C23-C21-C3-C2	-41.28
C22-C21	1.57	C24-C21-C3-C2	-129.82
C23-C21	1.57	C34-C24-C23-C21	-105.53
C24-C23	1.54	C35-C34-C24-C23	-167.50
C34-C24	1.51	O38-C34-C24-C23	13.16
C35-C34	1.53	Cl39-C35-C34-C24	-171.27
O38-C34	1.21		
Cl39-C35	1.79		
Symbol	Bond Angle		
C3-C2-C1	119.85		
C4-C3-C2	117.89		
C5-C4-C3	119.88		
C6-C1-C2	122.55		
C9-C4-C3	123.83		
C13-C2-C1	116.27		
C17-C6-C1	121.53		
C21-C3-C2	120.87		
C22-C21-C3	116.96		
C23-C21-C3	117.28		
C24-C21-C3	91.34		
C34-C24-C23	116.32		
C35-C34-C24	113.27		
O38-C34-C24	123.93		
Cl39-C35C34	114.10		

NMR spectroscopy

The basis set of B3LYP/ccpVDZ was used to stimulate ^{1}H- and ^{13}C-NMR spectra of the compound 4, as the experimental approach DMSO was used as a solvent. There were several identical peaks in the ^{1}H- and ^{13}C -NMR spectra of compound 4, as shown in Figs 3 and 4, respectively. The protons in the benzene ring are the first and the most characteristic peaks appeared at 6.75 ppm for both H7 and H8. The second characteristic peak is due to two methyl group on the benzene ring, they are doublet peaks at 2.36 ppm, with a higher intensity including six carbon. Finally, two hydrogen peaks (H36, and H37) were shifted to lower filed meaning higher ppm (4.55 ppm), which is also confirmed to be at 5.6ppm by computational analysis. All of the ^{1}H-NMR shifts and characteristics were shown in Table 2, for both experimental and theoretical calculation.

In the ^{13}C-NMR spectra, carbons of the three methyl group (-CH_3) attached to the benzene ring were recorded experimentally at 20.75, 20.75, 20.45 ppm, and the basis set computed the same range of shifts at 30.47, 30.28, 28.91 ppm, respectively. The carbonyl group (C=O) was recorded at 203.90 ppm and 211.06 ppm experimentally and theoretically, respectively. The aromatic carbon in the benzene ring experimentally appeared around 143.94 ppm and theoretically appeared at 143.41 ppm, as the electronegativity of the chlorine atom and carbonyl group of C35 were shifted to lower filed higher ppm (48.42 ppm) and (64.38 ppm) for experimentally and theoretically, respectively. All of the experimental and theoretical ^{13}C-NMR shifts and characteristics were summarized in Table 3., In general, there was a good agreement between experimental and theoretical data for compound 2-chloro-1-(3-mesityl-3-methylcyclobutyl)ethan-1-one, evidencing the applicability of the basis set to stimulate the molecular characteristics.

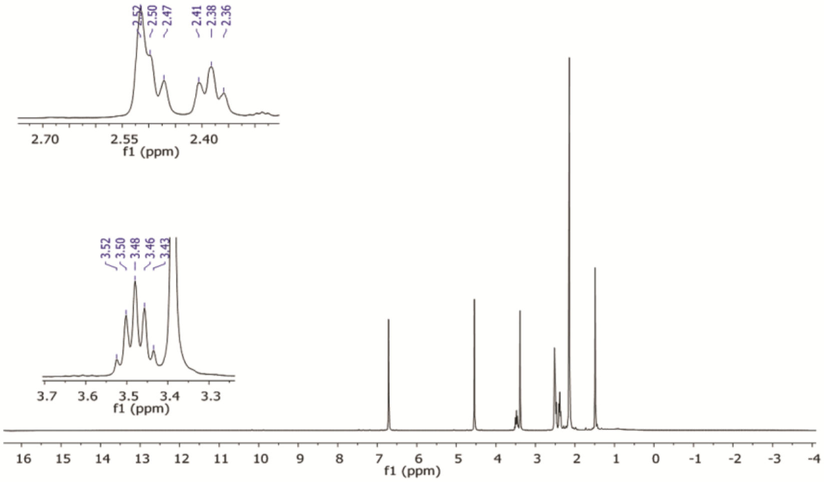

Fig. 3 — ^{1}H-NMR spectra of the compound 3

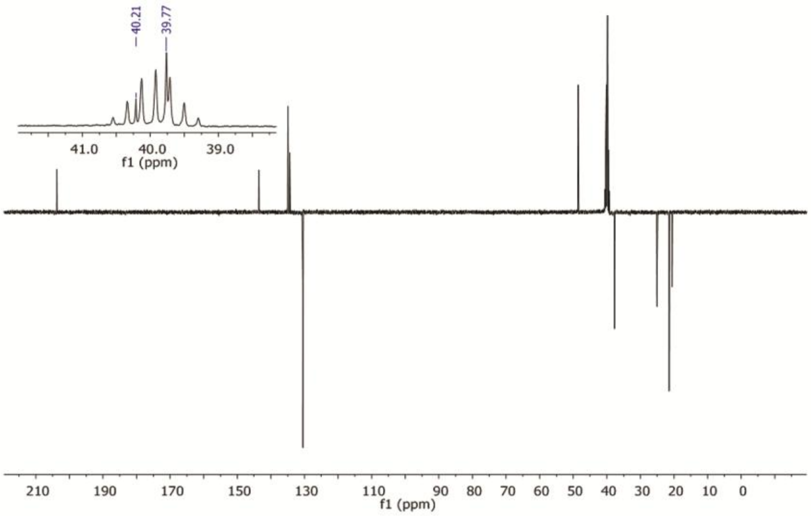

Fig. 4 — ^{13}C-NMR spectra of compound 4

FT-IR Spectroscopy

In the FT-IR measurements for synthesis compounds 2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)-ethanone, an identical peak appeared at 1745 cm^{-1} for C=O. In addition, the peaks for the aromatic benzene ring were recorded at 1658,1612 cm^{-1}. The basis set stimulated the molecular vibration for CO, CH, and CH$_3$ in a very close range to the experimental result, experimental and theoretical FT-IR spectra presented in Fig. 5. The two strong vibrations were observed in IR for CO groups, one is C-O stretching vibrations in a region 1250-850 cm^{-1}[22], and the second vibration is C=O at 1650- 1850 cm^{-1} [23, 24]. The basis set of B3LYP/ccpVDZ recorded very high infrared absorption band at 1812cm^{-1}. The aromatic structures usually display multiple bands between 3000 and 3100 cm^{-1}, which is a characteristic region for vibration stretching C-H [24-26]. The experimental C-H stretching vibration was observed at 3022-3155 cm^{-1}, the same vibration was calculated theoretically at 3156-3012 cm^{-1} using the B3LYP/ccpVDZ method, thus showed a strong correlation between the experimental and theoretical data, Table 4.

The CH group normally generates four fundamental bending vibrations, which are scissoring and rocking, wagging and twisting (in-plane bending) (out-of-plane bend), respectively. Out-of-plane bending vibrations of C-H appeared in the 1000-675 cm^{-1} region, and in-plane bending vibrations of C-H appeared in the 1400-1050 cm^{-1} region [27]. The C-H ring vibrations in-plane bending appeared at 1396-1036cm^{-1} experimentally, while theoretically

Table 2 — Experimental and theoretical chemical shifts (ppm) of 1H-NMR of compound 4

H number	Experimental Results (E)	Theoretical Results (T)
H7	6.75	7.9454
H8	6.75	7.9344
H36	4.55	5.6299
H37	4.55	5.4293
H25	3.52	4.1904
H29	3.50	4.1215
H28	3.48	3.7701
H27	3.46	3.7569
H15	2.52	3.7267
H10	2.52	3.6703
H19	2.52	3.6196
H14	2.36	3.3122
H20	2.41	3.2968
H18	2.50	3.2499
H11	2.47	3.1944
H26	3.43	3.1628
H31	2.41	3.1372
H16	2.38	3.1165
H12	2.37	3.0702
H32	1.5	2.4748
H33	1.5	2.4182

Table 3 — Experimental and theoretical chemical shifts (ppm) of ^{13}C-NMR of compound 4

C number	Experimental Results (E)	Theoretical results (T)
C34	203.90	211.06
C3	143.94	152.64
C2	143.94	143.41
C4	143.94	143.31
C6	134.06	142.40
C1	130.29	135.81
C5	130.29	135.68
C35	48.42	64.38
C21	40.21	54.66
C22	39.77	49.08
C24	39.77	47.19
C23	37.68	44.68
C30	25.24	33.55
C13	20.75	30.47
C9	20.75	30.28
C17	20.45	28.91

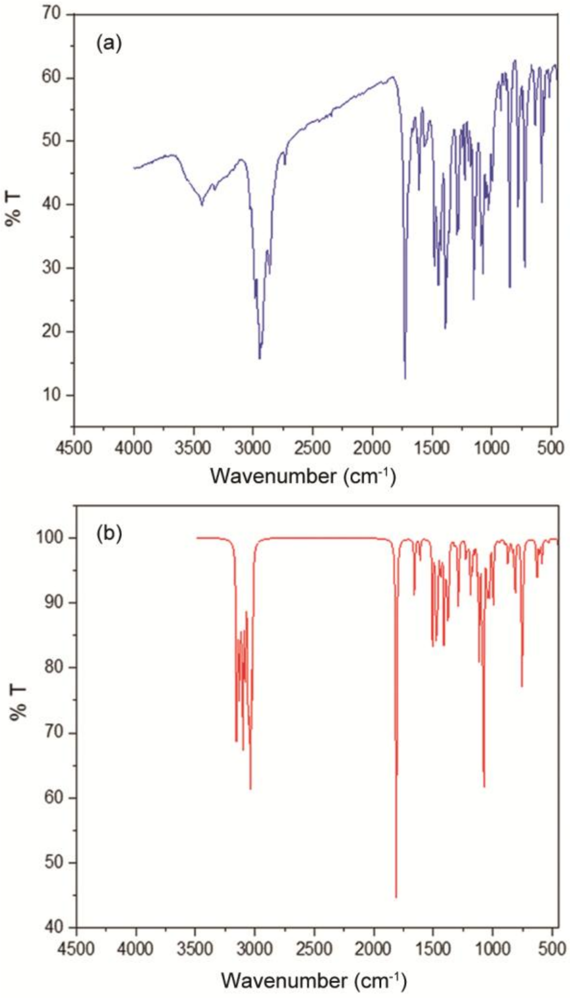

Fig. 5 — FT-IR spectra of compound 4 A) Practical B) Theoretical

appeared at 1398-1033cm^{-1}. The C-H out-of-plane ring bending vibrations appeared experimentally at 1276-1268 cm^{-1} and theoretically at 1265-1225 cm^{-1}. The CH_3 group typically generates nine fundamental vibrations, such as three modes of bending, three modes of stretching, two modes of rocking, and a single mode of torsion. The methyl group's symmetric and asymmetric stretching vibrations usually occur at 2850-3000 cm^{-1}[28]. In the area of 1650, 1156, and 1132 cm^{-1}, the aromatic ring carbon-carbon (C=C) stretching modes appeared, however in theoretical they were appeared at 1658, 1612, 1154, and 1132 cm^{-1}. The difference between measured and observed frequencies were due to; the phase of the compound being measured as the experimental results belong to the solid phase and the theoretical calculations belong to the gaseous phase, and the experimental values reported in the presence of intermolecular interactions, while the calculations were performed on a single molecule.

Molecular reactivity report

Based on the HOMO and LUMO energy bandgap level multiple factors were founded. The ionization potential (I=-E_{HOMO}) is defined as the least quantity of energy available in a gaseous state to remove an

Table 4 — Comparison of the experimental and theoretical vibrational spectra of compound 4

Assignments With TED	Unscaled Frequencies (6-311(d, p)) B3LYP	FT-IR (cm^{-1}) With KBr	Assignments With TED	Unscaled Frequencies (6-311(d,p)) B3LYP	FT-IR (cm^{-1}) With KBr
υsC1H7,C5H8	3155	3156	υsC-Hring	1507	1508
υasC23H27,H28	3147	3148	υCH3	1481-1463	1484-1460
υasC22H25, H26	3134	3140	ScC17,H18,H20	1459,1049	1452
υasC13H14,H16	3133	3132	υC35,H37	1409	1412
υasC9H11,H12	3130	3124	υsCH3	1404	1404
υasC30H31H32	3126	3116	υs-inCH3-ring	1398,1046,1033	1396,1036
υasC35H36,H37	3114	3108	ro-inC24H29	1376	1372
υasC17H18,H20	3112	3100	υasC-ring	1321,1316	1324
υasC30H32,H33	3102	3092	roC35H36,H37	1289	1284
υasC13H15,H16	3099	3084	υs-ouC23H27,H28	1274	1276
υsC9H10,H12	3098	3076	υsouC1H7,C5H8	1265	1268
υsC17H18,H20	3083	3068	roC23H27,C24H29	1261,1225	1260
υsC23H27,H28	3078	3060	υC21C23	1154	1156
υsC35H36,H37	3061	3052	υsC21C22,C23C24	1132	1132
υsC22H25,H26	3055	3044	υasC22C2324	999,996	996,988
υsC13H14,H15,H16	3039	3036	υasC1C5C6	974	972
υsC9H10,H11,H12	3037	3028	υasC21C23C30	943	940
υsC30H31,H32,H33	3034	3020	υasC21C22C23	909,883	908
υsC17H18,H19,H20	3022	3012	roC22H25H26	815	884
υC=O	1812	1745	υsC35Cl39	753	756
υsC=C-ring	1658,1612	1650			

υ, stretching; s, symmetric; as, asymmetric; ro, rocking; ou, out of the plan; in, in a plan sc, scissorin

electron from the atom or molecule. The quantity of discharge energy is referred to as electronic affinity ($A=-E_{LUMO}$) when one electron is attached to the gaseous molecule. Electronegativity $\chi= (I + A)/2$ is the tendency of an atom for attracting electrons. Weight transfer in a molecule is denoted by chemical hardness = $(I - A)/2$. The HOMO and LUMO energy values also used to evaluate other reactivity descriptors, such as chemical potential $\mu= -\chi$, softness $s= 1/2\eta$, and global electrophilicity index = $\mu2/2\eta$ [29, 30]. Usually, the chemical activity of the compound is shown by the energy values of HOMO and LUMO, and the energy difference. The molecule that have lower energy bandgaps are more polarizable, and exhibit high reactivity[31]. Arrangement and energy levels of the orbitals, including HOMO and LUMO, determined by B3LYP/cc-pVDZ for the current compound, are presented in Fig. 6. The findings show that the greater level of energy between HOMO and LUMO is equal to 5.378 eV. All of the parameters on the reactivity of the compound are summarized in Table 5. Only HOMO and LUMO cannot be considered to provide a fair definition of frontier orbitals, as neighboring orbitals may display quasi-degenerate energy levels in the boundary region. For this reason, both the gas phase and the density of states (DOS) were measured using the Gauss Sum 3.0 program, as shown in Fig. 7.

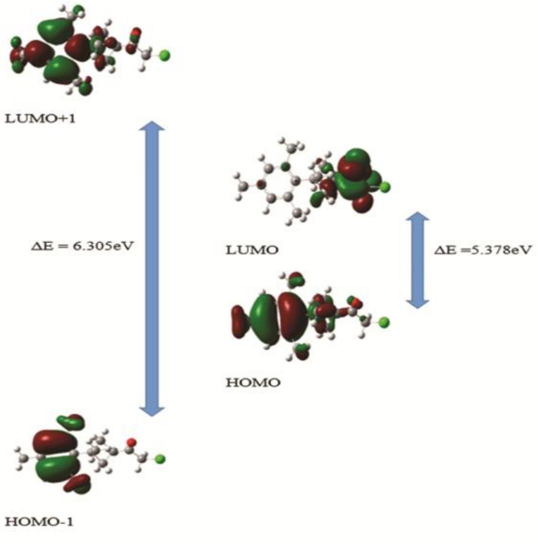

Fig. 6 —Molecular orbital and energy levels of compound 4 calculated by B3LYP/cc-pVDZ

Molecular electrostatic potential (MEP) maps

The molecular electrostatic potential (MEP) for the molecule was calculated to predict the reactive

Table 5 — Electronic parameters of compounds 4

B3LYP/ cc-pVDZ	Equations	Results
E $_{LUMO+1}$ (eV)	E $_{LUMO+1}$ (eV)	-0.115
E $_{LUMO}$ (eV)	E $_{LUMO}$ (eV)	-0.856
E $_{HOMO}$ (eV)	E $_{HOMO}$ (eV)	-6.235
E $_{HOMO-1}$ (eV)	E $_{HOMO-1}$ (eV)	-6.420
ΔE	HOMO - LOMO	5.378
I (eV)	I= - E$_{HOMO}$	6.235
A (eV)	A= - E$_{LUMO}$	0.856
X (eV)	X= I+A/2	3.546
η (eV)	η = I-A/2	2.689
μ (eV)	μ = -(I+A/2)	-3.546
S (eV)	S = 1/2η	0.185
ω (eV)	ω = μ2/2η	2.338

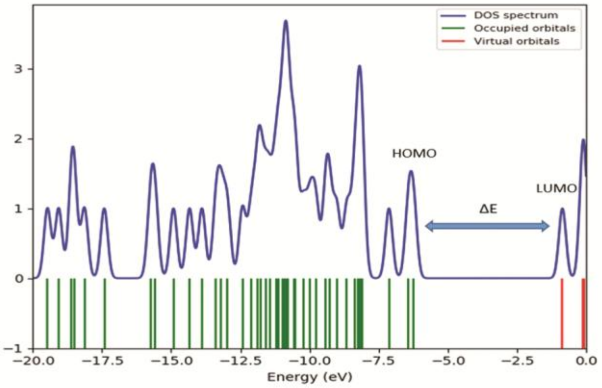

Fig. 7 — The density diagrams of compound 4

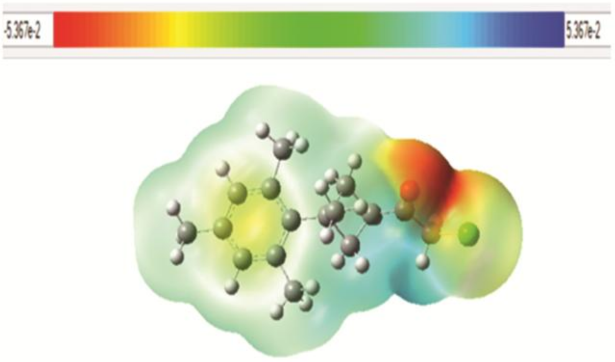

Fig. 8 — Molecular electrostatic potential (MEP) maps of compound 4

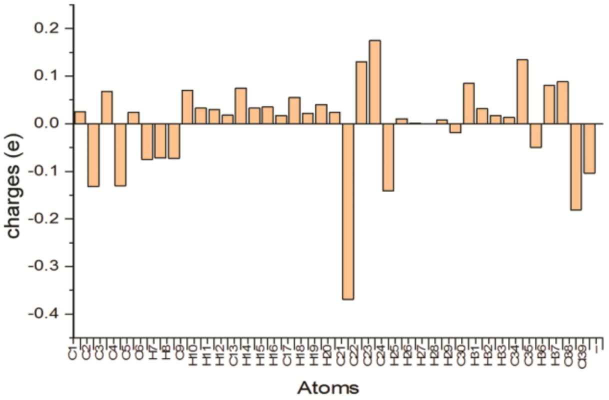

Fig. 9— Mulliken charge distribution of compound 4

electrophilic and nucleophilic attack sites. At the surface of the molecule, different colours represented dissimilarity of the electrostatic potential. The potential increases from red to blue (red < orange < yellow < green < blue), the range map color started from -0.05367 a.u extreme red color to 0.05367 deepest blue color. The positive (blue) regions of MEP are associated with electrophilic reactivity, and nucleophilic reactivity is related to the negative (red) areas. The MEP for the compound a negative area based on the oxygen, and a little bit on chlorine atoms presented in Fig. 8. The maximum positive regions were located on the methyl and cyclobutane groups. The MEP has designated the negative sites are higher electronegative atoms, and the positive sit was lower electronegativity atoms. The MEP surface shows that the C=O was strong repulsion to chlorins atom and reacted with electrophilic compounds.

Mulliken charge distribution

The charge distribution on the molecule greatly influences the vibrational spectrum. The molecular structure of the compound is composed of thirty-nine atoms: twenty-one hydrogens, sixteen-carbon, one oxygen, and one chlorine atom. The plot of the atomic charge distribution for the compound is presented in Fig. 9. Generally, the hydrogen atoms of the compound 4 were positive, while a little number of the carbon atoms with oxygen and chlorine atoms has a negative value. The carbon number 22 it is carbon for cyclobutane ring has a maximum negative value which is indicated to react with the more electrophilic compound. Also, oxygen 38 and chlorine 39 was a negative peak value and reacted with electrophilic compounds.

Thermodynamic parameters

The different thermodynamic properties of the molecule, including thermal energy, rotational temperatures, rotational constants, zero-point vibration energy, basic heat power, and entropy were calculated based on B3LYP/cc-pVDZ at a pressure of 1.00 atom and 298 K, as summarized in Table 6.

Table 6 — Thermodynamic parameters of compound 4

Parameters	B3LYP/cc-pVDZ
Zero-point vibrational energy(kcal/mol^{-1})	206.805
Total energy (a.u.)	-1157.799
Rotational constants (GHz)	
	1.020
	0.155
	0.144
Rotational temperatures (K)	
	0.048
	0.007
	0.0069
Entropy (Kcal mol^{-1} K^{-1})	
Rotational	0.889
Translational	0.889
Vibrational	217.045
Total	218.823

Conclusion

2-chloro-1-(3-methyl-3-mesityl-cyclobutyl)-ethanone is synthesized and characterized by FT-IR and NMR. B3LYP/cc-pVDZ was used to analyze the theoretical calculations including geometrical structure, electronic energy, vibrational motion, and NMR. Comparison between theoretical with experimental results for both FT-IR NMR is noble. The study of the molecular reactivity was determined to form HMOM and LUMO energy level. Molecular electrostatic potential (MEP) maps and Mulliken charge distribution show that the molecule has set for weak electronic interaction. Determination of the thermodynamic properties were calculated to understand the structure reactivity of the molecule.

References

1 Koca M, Kirilmiş C & Arici C, *Acta Crystallogr Sect E Struct Rep Online*, 66 (2010) o523.

2 Brown K, Cater D P, Cavalla J F, Green D, Newberry R A & Wilson A B, *J Med Chem*, 17 (1974) 1177.

3 Heathcock C H, *Science*, 267 (1995) 117.

4 Rosen T, *Comprehensive Organic Synthesis*, (Pergamon Press, Oxford) 1991, pp.395.

5 Akhmedov M A, Sardarov I K, Akhmedov I M, Kostikov R R, Kisin A V & Babaev N M, *Zhurnal Organicheskoi Khimii*, 27 (1991) 1434.

6 Koca M, Kirilmiş C, & Arici C, *Acta Crystallogr E*, 66 (2010) o523.

7 Çukurovalı A, Özdemir N, Yılmaz İ & Dinçer M, *Acta Crystallogr E*, 61 (2005) o1754.

8 Dinçer M, Özdemir N, Çukurovalı A, Yılmaz İ & Büyükgüngör O, *Acta Crystallogr E*, 60 (2004) o1523.

9 Lee D R, Galant N J, Wang H, Mucsi Z, Setiadi D H, Viskolcz B & Csizmadia I G, *J Phys Chem A*, 113 (2009) 2507.

10 Sure R & Grimme S, *J Comput Chem*, 34 (2013) 1672.

11 Omer R A, Ahmed L O, Koparir M & Koparir P, *Indian J Chem*, 59A (2020) 1828.

12 Ahmed L & Omer R, *J Phys Chem Funct Mater*, 3 (2020) 48.

13 Oelichmann H-J, Bougeard D & Schrader B, *J Mol Struct*, 77 (1981) 179.

14 Jayaprakash A, Arjunanet V, Jose S P & Mohan S, *Spectrochim Acta A Mol Biomol Spectrosc*, 83 (2011) 411.

15 Ahmed L & Omer R, *J Phys Chem Funct Mater*, 3 (2020) 9.

16 Omar R A, Koparir P, Ahmed L O & Koparir M, *Turkish Comput Theor Chem*, 4 (2020) 67.

17 Tao X T, Yuan D R, Zhang N, Jiang M H & Shao Z S, *Appl Phys Lett*, 60 (1992) 1415.

18 Ahmed L & Omer R, *Cumhur Sci J*, 41 (2020) 916.

19 Ahmed L & Omer R, *J Phys Chem Funct Mater*, 2 (2019) 66.

20 Raj R K, Gunasekaran S, Gnanasambandan T & Seshadri S, *Spectrochim Acta A Mol Biomol Spectrosc*, 139 (2015) 505.

21 Koparir M, Orek C, Koparir P & Sarac K, *Spectrochim Acta A Mol Biomol Spectrosc*, 105 (2013) 522.

22 Lin-Vien D, Colthup N, Fateley W & Grasselli J, *The handbook of infrared and Raman characteristic frequencies of organic molecules*, (Academic Press-Elsevier, Cambridge) 1991.

23 Sarıkaya E K & Dereli Ö, *J Mol Struct*, 1052 (2013) 214.

24 Koparir P, Karaarslan M, Orek C & Koparir M, *Phosphorus Sulfur Silicon Relat Elem*, 186 (2011) 2368.

25 Moghanian H, Mobinikhaledi A & Monjezi R, *J Mol Struct*, 1052 (2013) 135.

26 Koparir P, *Phosphorus Sulfur Silicon Relat Elem*, 194 (2019) 1028.

27 Tammer, M, *G Sokrates: Infrared and Raman characteristic group frequencies: tables and charts,* (Wiley, Chichester) 2004.

28 Sarıkaya E K, Dereli Ö, Erdoğdu Y & Güllüoğlu M T, *J Mol Struct*, 1049 (2013) 220.

29 Calais J L, *Int J Quantum Chem*, 47 (1993) 101

30 Gázquez J L, *J Mex Chem Soc*, 52 (2008) 3.

31 Srivastava K, Shimpi M R, Srivastava A, Tandon P, Sinhaa K & Velaga S P, *RSC advances*, 6 (2016) 10024.