

QUANTUM CHEMICAL CALCULATIONS AND FT-IR, UV LIGHT INTERACTIONS ON BENZOFURAN-2-CARBONYL CHLORIDE

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Abstract: Molecular vibrational frequency analyses of benzofuran-2-carbonyl chloride (BCC) were carried out by infrared (IR) and ultraviolet (Uv-Vis) spectrums from Quantum chemical calculations simulated with experimental data. BCC structure is optimized by HF and DFT methods with standard and higher basis sets of 6-311++G**. Scaled quantum mechanical (SQM) force field frequencies and potential energy distributions (PED) were studied with the help of MOLVIB. The first order hyperpolarizability, polarizability and dipole moment were calculated for non-linear optical (NLO) properties. Frontier molecular orbital, natural bond orbital (NBO) and TD-SCF calculated major contributions are presented. Chemical reactivity, ionization potential, global hardness and softness values of the titled compound were reported. Present investigated organic chemical compound having good optical properties and biological importance were found and results are discussed in detailed.

Keywords: SQM, HF, DFT, FT-IR, UV-Visible spectra.

I. INTRODUCTION

Benzofuran is a popular compound as a natural product and its derivatives have extensive applications. Most of the derivatives have been reported with spectral data of Infrared, Uv-vis and fluorescence simulated with theoretical DFT calculations [1-5]. Benzofuran derivative are easily prepared by simple reactive methods and those are available in nature. Present investigations were obtained carbonyl group and halogen substituted compound. The carbonyl group is a combination of the organic functional group of carbon double band oxygen [R-C=O]. It consists of resonance structure and is based on different resonances around the atomic molecule [6]. Many of research and development organizations are looking for new heterocyclic compound. These organic compounds are plays a virtual role in medical, industrial and many more [7-9]. In this article presents one of the benzofuran derivatives organic compounds "benzofuran-2-carbonyl chloride". It is studied by using density functional theory and experimental Infrared, Uv-vis, Raman spectroscopy methods. Most of the literatures are available on either theoretical optimized or experimental synthesized compounds are reported. For the first time we provide complete structural geometric, vibrational, optical and Raman active studies on titled compound.

II. COMPUTATIONAL METHOD

Day-to-day research is updating with quantum computing methods. In computational chemical simulations can provide accurate results regarding vibrational, molecular structural, chemical and electronic properties of suspects without any experimental wastage and it saves time and expenditure of work. A present study of titled compound "benzofuran-2-carbonyl chloride" (BCC) is optimized at Hartree-Fock (HF) and Density Functional Theory (DFT) respective higher basis set 6-311++G(d,p) at Gaussian09W and visualization program Gauss-View 5.0 [10-11]. Molecular electrostatic potential surface distributions were plotted with the help of Argus Lab [12]. Scaled quantum mechanical force field frequencies and potential energy distributions (PED) of BCC were carried out by Prof. T. Sudius developed MolVib program [13-14]. Infrared spectral data were extracted from MolVib output file by using simirra theoretical program. Uv-Vis spectral analysis for absorption spectra were obtained from the method of time dependent self-consistent field (TD-SCF) simulated with experimental data. Ground and first state exited energy distribution counter surface were extracted from Gaussian molecular orbital check point file. NBO and NLO calculations, atomic mulliken charge distributions and potential electrostatic map were performed by using both HF and DFT calculations.

III. EXPERIMENTAL DETAILS

Benzofuran-2-carbonyl chloride is purchased from Sigma-Aldrich Company with the purity of 97% and it is used for experimental spectral analysis without any father purification.

3.1 UV-Vis Spectral Analysis

The UV-Vis spectrum of BCC was recorded by using 450 MeV synchrotron radiation source at Indus 1, RRCAT, India. The absorbance spectra were recorded at frequency 50 kHz and 1msec exposure time by using ANDOR spectral instrument in the spectral region of 174 - 1020 nm [15]. From the observed spectra, it was strong absorption at 321 nm. From the theoretical TD-SCF method of UV-Vis spectrum also shown approximately same absorbance peak. Therefore both observed and theoretical spectrums were shown in figure 1. One more observation was carried out to the titled compound along with absorption spectra, which is optical energy band gap found at 3.85 eV. It was presented in figure 2.

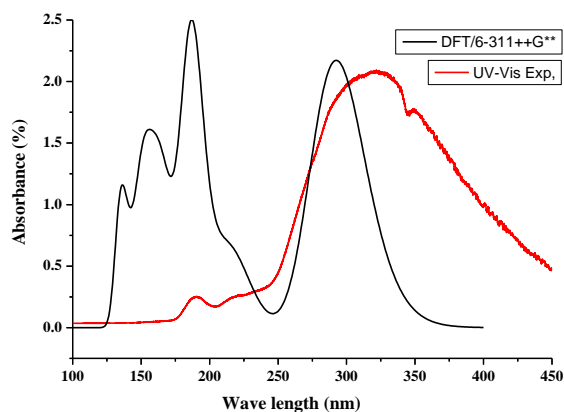


Fig. 1: Experimental and TD-SCF observed UV-Vis Spectrum.

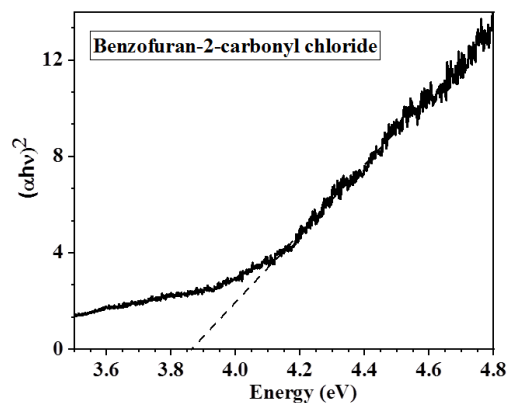


Fig. 2: Optical energy band gap of BCC

3.2 Infrared Spectral Analysis

The FT-Raman spectrum of BCC was recorded at a 4 cm^{-1} resolution with a thermofisher scientific equipped model Nicolet 6700 FT-IR with DTGS KBr detector in the $4000\text{--}400 \text{ cm}^{-1}$. The sample was prepared KBr pellet method and XT-KBr beam splitter was used for this arrangement [16]. Along with experimental spectra of BCC, we obtained theoretical spectrum by using DFT and HF method. That is shown in Figure 3 and more details of vibrational spectra are presented in results and discussion part.

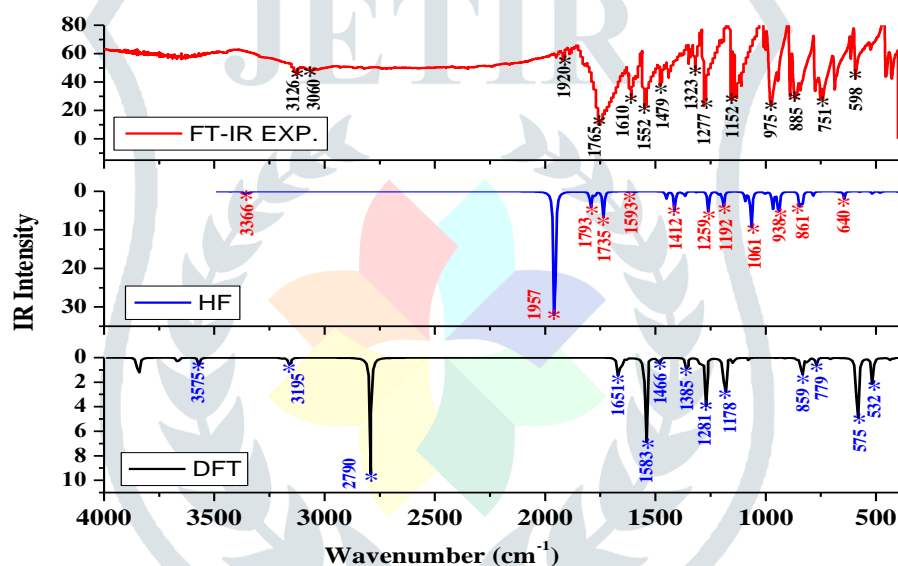


Fig. 3: FT-IR experimental, HF/6-311++G** and DFT/6-311++G** Spectrum.

IV. RESULTS AND DISCUSSIONS

4.1 Molecular Geometry

Molecular structure of BCC is belongs to C_1 point group symmetry and it was optimized by Gaussian09W and visualized by gauss-view 5.0. BCC molecule is contains Chlorine (Cl) and furan connected with benzene ring. Optimized structure of BCC where presented with chemical symbol along with label in Figure 4. Definitions of the internal coordinates of geometry were reported in supplementary table 1. Bond lengths, bond angles and dihedral angles were compared with both HF and DFT data and all comparative values are mostly closed to each other [17-18]. All optimized and experimental bond angles and bond lengths are reported in Table 1.

Potential energy surface scan were carried out to the present compound by both HF and DFT methods with respect to changing dihedral angle of O12-C10-C17-C116. We obtained approximately same shaped curves and energy remains constant. Observed PES curves of DFT and HF are shown in Figure 5 (a) and Figure 5 (b) respectively.

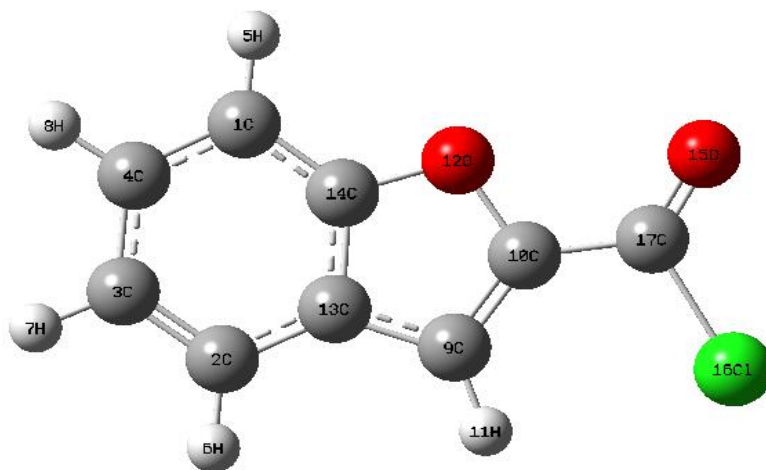


Fig. 4: Optimized Molecular structure of Benzofuran-2-carbonyl chloride along with numbering of atom.

Supplementary material 1: definition of internal coordinates of Benzofuran-2-carbonyl chloride

No.(i)	Symbol	Type	Definition ^a
Stretching			
1-5	R _i	C-H	C1-H5, C4-H8, C3-H7, C2-H6, C9-H11
6-11	R _i	C-C (Ring1)	C1-C4, C4-C3, C3-C2, C2-C13, C13-C14, C14-C1
12-13	R _i	C-C (Ring2)	C13-C9, C9-C10,
14-15	R _i	C-O (Ring2)	C10-O12, O12-C14
16	R _i	C-C (R2sub)	C10-C17
17	R _i	C-O sub	C17-O15
18	R _i	C-Cl sub	C17-Cl16
In-Plane bending			
19-26	γ _i	C-C-H (Ring1)	C14-C1-H5, C4-C1-H5, C1-C4-H8, C3-C4-H8, C4-C3-H7, C2-C3-H7, C3-C2-H6, C13-C2-H6
27-28	γ _i	C-C-H (Ring2)	C13-C9-H11, C10-C9-H11
29-34	γ _i	RING 1	C1-C4-C3, C4-C3-C2, C3-C2-C13, C2-C13-C14, C13-C14-C1, C14-C1-C4
35-39	γ _i	RING 2	C14-C13-C9, C13-C9-C10, C9-C10-O12, C10-O12-C14, O12-C14-C13
40	γ _i	C-C-C (R2sub)	C9-C10-C17
41-42	γ _i	C-C-O R2	O12-C10-C17, C10-C17-O15
43	γ _i	C-C-Cl	C10-C17-Cl16
44	γ _i	O-C-Cl	O15-C17-Cl16
Out-of-plane bending			
45-49	ρ _i	C-H	H5-C1-C14-C4, H8-C4-C1-C3, H7-C3-C4-C2, H6-C2-C3-C13, H11-C9-C13-C10
50	ρ _i	C-O	C17-C10-C9-O12
Torsion			
51-56	τ _i	RING 1	C1-C4-C3-C2, C4-C3-C2-C13, C3-C2-C13-C14, C2-C13-C14-C1, C13-C14-C1-C4, C14-C1-C4-C3
57-61	τ _i	RING 2	C14-C13-C9-C10, C13-C9-C10-O12, C9-C10-O12-C14, C10-O12-C14-C13, O12-C14-C13-C9
62-63		BUTTER	C2-C13-C14-O12, C1-C14-C13-C9
64	τ _i	C-C-O-Cl	C10-C17-O15-Cl16

^aFor numbering of atom refer Fig.4

Table 1: Optimized geometrical parameters of Benzofuran-2-carbonyl chloride obtained by HF and DFT calculations

Bond length ^a	Value(Å)		Bond Angle ^a	Value(°)		Dihedral Angle ^a	Value(°)	
	DFT	HF		DFT	HF		DFT	HF
C1-C4	1.389	1.377	C1-C4-C3	121.74	121.86	C1-C4-C3-C2	-0.011	-0.006
C4-C3	1.410	1.406	C4-C3-C2	121.29	121.01	C4-C3-C2-C13	0.015	0.012
C3-C2	1.385	1.374	C3-C2-C13	118.10	117.93	C3-C2-C13-C14	-0.006	-0.010
C2-C13	1.405	1.398	C2-C13-C14	119.20	119.80	C2-C13-C14-C1	-0.005	0.001
C13-C14	1.408	1.386	C13-C14-C1	123.45	123.22	C13-C14-C1-C4	0.010	0.004
C14-C1	1.389	1.386	C14-C1-C4	116.20	116.14	C14-C1-C4-C3	-0.001	-0.002
O12-C14	1.360	1.342	O12-C14-C13	110.55	110.62	O12-C14-C13-C9	-0.004	0.000
C13-C9	1.430	1.440	C14-C13-C9	105.44	105.18	C14-C13-C9-C10	0.006	0.001
C9-C10	1.366	1.341	C13-C9-C10	106.23	105.46	C13-C9-C10-O12	-0.006	-0.002
C10-O12	1.376	1.356	C9-C10-O12	111.62	112.28	C9-C10-O12-C14	0.003	0.002
C10-C17	1.455	1.461	C10-O12-C14	106.15	106.42	C10-O12-C14-C13	0.001	-0.001
C17-O15	1.186	1.169	O12-C10-C17	115.34	115.33	C17-C10-O12-C9	179.995	179.995
C17-C16	1.825	1.768	C9-C10-C17	133.03	132.37	O12-C10-C17-O15	0.003	0.020
C1-H5	1.082	1.073	C10-C17-O15	127.27	125.87	O12-C10-C17-C116	-179.994	-179.980
C4-H8	1.083	1.075	C10-C17-C116	112.40	114.17	C9-C10-C17-O15	179.998	-179.98
C3-H7	1.083	1.074	O15-C17-C116	120.31	119.95	C9-C10-C17-C116	0.000	0.014
C2-H6	1.083	1.074	C14-C1-H5	121.45	121.64	H5-C1-C4-C14	179.997	179.995
C9-H11	1.077	1.068	C4-C1-H5	122.34	122.20	H8-C4-C3-C1	179.985	179.987
			C1-C4-H8	119.15	119.16	H7-C3-C2-C4	179.995	179.997
			C3-C4-H8	119.09	118.96	H6-C2-C3-C13	179.982	179.988
			C4-C3-H7	119.02	119.09	H11-C9-C13-C10	179.996	179.998
			C2-C3-H7	119.68	119.89			
			C3-C2-H6	121.04	121.16			
			C13-C2-H6	120.85	120.90			
			C13-C9-H11	128.11	127.80			
			C10-C9-H11	125.65	126.72			

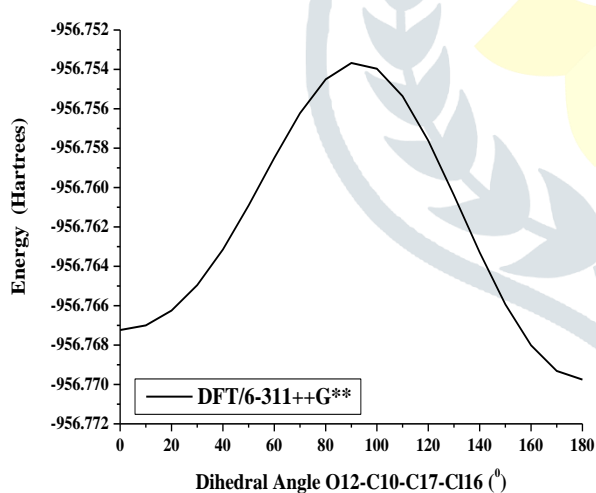


Fig. 5 (a): Potential energy surface scan for dihedral angle O12-C10-C17-C116 of BCC by DFT Method.

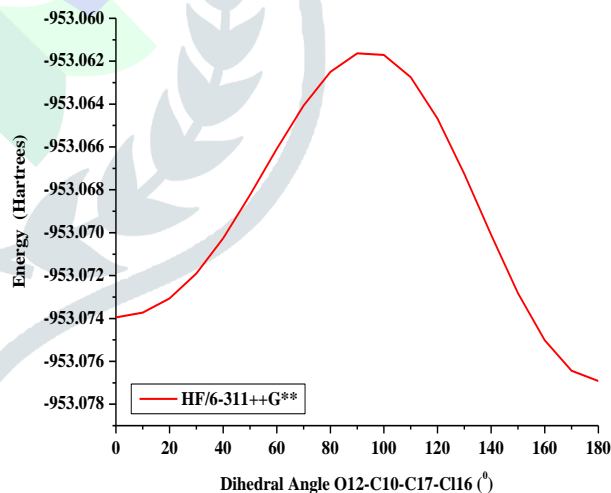


Fig. 5 (b): Potential energy surface scan for dihedral angle O12-C10-C17-C116 of BCC by HF Method.

4.2 Vibrational Analysis

The organic compound of BCC belongs to C₁ point group symmetry with 17 atoms (N=17). Local symmetry and asymmetry coordinates of BCC were defined along with scaled factors and quantum force field calculations in table 3. Non-linear molecule has 45 fundamental modes of vibrations with the reference of three dimensional degrees of freedom 3N-6 (where N is number of atoms in molecule) [19-20]. From the structural geometry of molecule BCC, it has 31 in-plane (2N-3) and 14 Out-of-Plane vibrations (N-3). Total number of fundamental modes of vibration, 45 (Γ_{vib}) = 31 A' (in-plane) + 14 A'' (out-of-plane).

Table 2: Definition of local-symmetry coordinates and the values of corresponding scale factors used to correct The 6-31G++ (d, p) force field calculations of Benzofuran-2-carbonyl chloride

No.(i)	Symbol ^a	Definition ^b	Scale factors
Stretching			
1-5	v(C-H)	R1, R2, R3, R4, R5	
6-11	v(C-C)(Ring1)	R6, R7, R8, R9, R10, R11	
12-13	v(C-C)(Ring2)	R12, R13	
14-15	v(C-O)(Ring2)	R14, R15	
16	v(C-C)(R2sub)	R16	
17	v(C-O)sub	R17	
18	v(C-Cl) sub	R18	
In-Plane bending			
19-22	β (C-C-H) R1	$(\gamma_{19}-\gamma_{20})/\sqrt{2}, (\gamma_{21}-\gamma_{22})/\sqrt{2}, (\gamma_{23}-\gamma_{24})/\sqrt{2}, (\gamma_{25}-\gamma_{26})/\sqrt{2}$	
23	β (C-C-H) R2	$(\gamma_{27}-\gamma_{28})/\sqrt{2}$	
24	β R1 tri	$(\gamma_{29}-\gamma_{30} + \gamma_{31}-\gamma_{32} + \gamma_{33}-\gamma_{34})/\sqrt{6},$	
25	β R1 asy	$(2\gamma_{29}-\gamma_{30} - \gamma_{31}+2\gamma_{32} - \gamma_{33}-\gamma_{34})/\sqrt{12},$	
26	β R1 sym	$(\gamma_{30} - \gamma_{31} + \gamma_{33}-\gamma_{34})/2,$	
27	β R2 asy	$(a-b)(\gamma_{36} - \gamma_{39}) + (a+b)(\gamma_{37} - \gamma_{38})$	
28	β R2 sym	$\gamma_{35}+a(\gamma_{36} + \gamma_{39})-b(\gamma_{37} + \gamma_{38})$	
29	β CCOsub	$(\gamma_{40} - \gamma_{41})\sqrt{2}$	
30	β COCl sc	$(2\gamma_{44} - \gamma_{42} - \gamma_{43})/\sqrt{6}$	
31	β COCl wa	τ_{64}	
32	β COCl ro	$(\gamma_{42} - \gamma_{43})\sqrt{2}$	
Out of plane bending			
33-37	ω (C-H)	$\rho_{45}, \rho_{46}, \rho_{47}, \rho_{48}, \rho_{49}$	
38	ω (C-O)	ρ_{50}	
Torsion			
39	τ R1tri	$(\tau_{51}-\tau_{52}+\tau_{53}-\tau_{54}+\tau_{55}-\tau_{56})/\sqrt{6}$	
40	τ R1asy	$(\tau_{51}-\tau_{53}+\tau_{54}-\tau_{56})/2$	
41	τ R1sym	$(-\tau_{51}-2\tau_{52}-\tau_{53}+\tau_{54}+2\tau_{55}-\tau_{56})/\sqrt{12}$	
42	τ R2asy	$-b(\tau_{57}+\tau_{61})+a(\tau_{58}+\tau_{60})+\tau_{59}$	
43	τ R2sym	$(a-b)(\tau_{60} - \tau_{58})+(1-a)(\tau_{61} - \tau_{57})$	
44	τ Butter	$(\tau_{62} - \tau_{63})/2$	
45	τ COCl	$(\tau_{65} - \tau_{66})$	

C-C Ring Vibrations:

Aromatic C-C ring stretching vibrations occurs at about the range of frequencies 1450-1600 cm⁻¹ and out of plane bending were found at 675-900 cm⁻¹ [21-22]. The computed C-C ring vibrational frequencies were found at 766 - 880 cm⁻¹ corresponding observed frequencies at 751 - 889 cm⁻¹. C-C stretching vibrations are observed at 1441 cm⁻¹ corresponding computing HF and DFT scaled assignments were found 1480 cm⁻¹ and 1466 cm⁻¹ respectively.

C-H Vibrations:

According to vibrational frequencies theory, C-H vibrations were found in-plane stretching at 2700-3600 cm⁻¹ and C-H bending may also observed at about 1375 and 1450 cm⁻¹. In aromatic compounds C-H out of plane bending vibrations were found at about 1000-650 cm⁻¹ [23]. Hartree-Fock (HF) and Density Functional Theory (DFT) computational methods were given accurate C-H assignments at about 3100-3400 cm⁻¹. We found banding C-H frequencies at about 3060 cm⁻¹ and 3126 cm⁻¹.

Carbonyl group:

The vibrational frequency range of C=O carbonyl derivatives were found at 1630-1820 cm⁻¹. The present investigated compound having C=O carbonyl group vibrations with acid chloride, it was found at 1760-1820 cm⁻¹ [24]. From observed FT-IR spectrum specific group of C=O stretching vibrations were found at 1765 cm⁻¹ and theoretical HF spectra shown at 1793 cm⁻¹.

According to theoretical chemist Prof. Peter Pulay recommendations the normal modes of vibrations of BCC were well defined and detailed assignments of fundamental vibrations were presented in table 3 [25-26].

Table 3: Detailed assignments of fundamental vibrations of BCC by normal mode analysis based on SQM force field calculations using HF and DFT method

Mode no.	FT-IR Experimental frequencies (cm ⁻¹)	Theoretical IR frequencies (cm ⁻¹)		IR Activity		Assignments (PED) ^{a, b}
		HF	DFT	HF	DFT	
7	-	3426	3266	3.249	1.700	ω CH (45)
8	-	3366	3207	8.620	2.622	β CHR1 (99)
9	3126	3358	3195	24.283	12.184	β CHR1 (90)
10	-	3345	3184	12.835	5.537	β CHR2 (88)
11	3060	3333	3174	2.558	0.860	β CHR1 (94)
12	1752	1957	1843	1411.823	541.467	β CHR1 (97)
13	1610	1793	1651	137.99	33.796	ω CH (77), τ R1asy (16)
14	-	1735	1621	45.082	4.533	ω CH (90)
15	1548	1623	1583	201.717	135.759	ω CH (87)
16	-	1593	1509	4.795	4.795	ν CHR1 (91)
17	1441	1480	1466	9.485	8.810	ν CHR1 (95)
18	1348	1412	1385	61.596	5.920	ν CHR2 (97)
19	1321	1356	1344	164.206	8.315	ν CHR1 (98)
20	1278	1306	1291	11.439	102.206	ν CHR1 (99)
21	-	1298	1281	38.995	1.496	ω CH (99)
22	-	1288	1213	7.494	2.319	ω CH (55), τ R1tri (26), τ R1asy (11)
23	-	1259	1178	151.844	16.757	B CCOsub (37), B COCLR (34)
24	1133	1213	1151	27.177	144.977	β COCLwa (57), ω CO (31)
25	1112	1192	1132	141.177	7.848	β R1tri (33), β R1asy (22), ν CCR2 (14)
26	-	1110	1026	0.009	6.989	β R1tri (41), β R1asy (35), ν CCR1 (13)
27	-	1092	989	69.607	0.002	β COCLsub (41), ν R2sub (29)
28	975	1081	984	4.937	126.328	β R1sym (49), ν CCR1 (25)
29	943	968	958	303.803	2.650	τ R1asy (51), ω CH (31)
30	889	910	901	22.882	28.850	τ COCL (37), ω CO (34), β COCL wa (14)
31	-	895	880	140.156	13.164	β R2sym (31), ν CCR2 (19)
32	-	875	869	5.766	178.925	ν CCR1 (57), ν CCR2 (19)
33	843	861	859	240.694	9.538	ν CCR1 (46), ν CCR2 (18)
34	775	785	779	102.583	98.761	ν CCR2 (46), ν CCR1 (37)
35	-	769	766	93.168	24.128	ν CCR1 (35), ν CCR2 (22)
36	751	760	759	38.916	46.066	τ butt (44), τ COCL (20)
37	686	723	707	33.776	8.430	ν CCR2 (48), ν CCR1 (39)
38	-	628	624	7.673	2.361	ν CCR1 (79), β R1sym (13)
39	592	610	601	58.591	41.812	τ butt (41), τ COCL (24)
40	-	578	575	0.098	0.049	ν CCR1 (86)
41	-	570	569	0.001	0.001	ν CCR1 (42), ν CCR2 (24)
42	455	534	532	5.974	2.644	ν CCR1 (31), ν COsub (25)
43	428	458	443	21.883	32.019	ν CCR2 (33), ν CCR1 (23), β R2asy (22)
44	-	439	438	16.784	7.906	ν CCLsub(24), ν CCR1 (19), ν R2sub (18)
45	-	378	369	5.503	0.075	ν CCLsub(44), ν CCR2 (18), ν CCR (10)
46	-	294	270	4.665	1.669	τ R2sym (73)
47	-	269	267	5.167	4.883	β COCLR (28), ν CCR1 (17)
48	-	259	256	7.231	3.528	β R2asy (24), ν R2sub (22), β COCLR (14)
49	-	138	128	3.161	1.672	τ R1sym (67), τ R2asy (16)
50	-	96	90	0.190	0.131	ν CCR2 (54), β CCOsub (17)
51	-	61	58	0.136	0.228	τ R2asy (69), τ R1sym (14)

^a Only PED contributions $\geq 15\%$ are listed by DFT method.

^b Abbreviations : ν, stretching; β, in plane bending; ω, out of plane bending; τ, torsion, ss, symmetrical stretching, as, asymmetrical stretching, sc, scissoring, wa, wagging, twi, twisting, ro, rocking, ipb, in-plane bending, opb, out-of-plane bending; tri, trigonal deformation, sym, symmetrical deformation, asy, asymmetric deformation, butter, butterfly, ar, aromatic, sub, substitution, vs, very strong; s, strong; ms, medium strong; w, weak; vw, very weak.

4.3 Molecular Orbital Analysis:

BCC aromatic organic compound were optimized and studied molecular orbital electronic charge distributions. According to Fukui recommendations electronic distributions were justified by frontier orbitals (HOMO-LUMO). We capture different orbital structures along with charged surfaces [27-29]. Highest occupied and lowest unoccupied molecular orbitals of the investigated

compound were found 46 and 47 respectively. From TD-SCF of DFT and HF methods were used. Some of charged orbital surfaces of BCC were presented in figure 6 (a) and 6 (b).

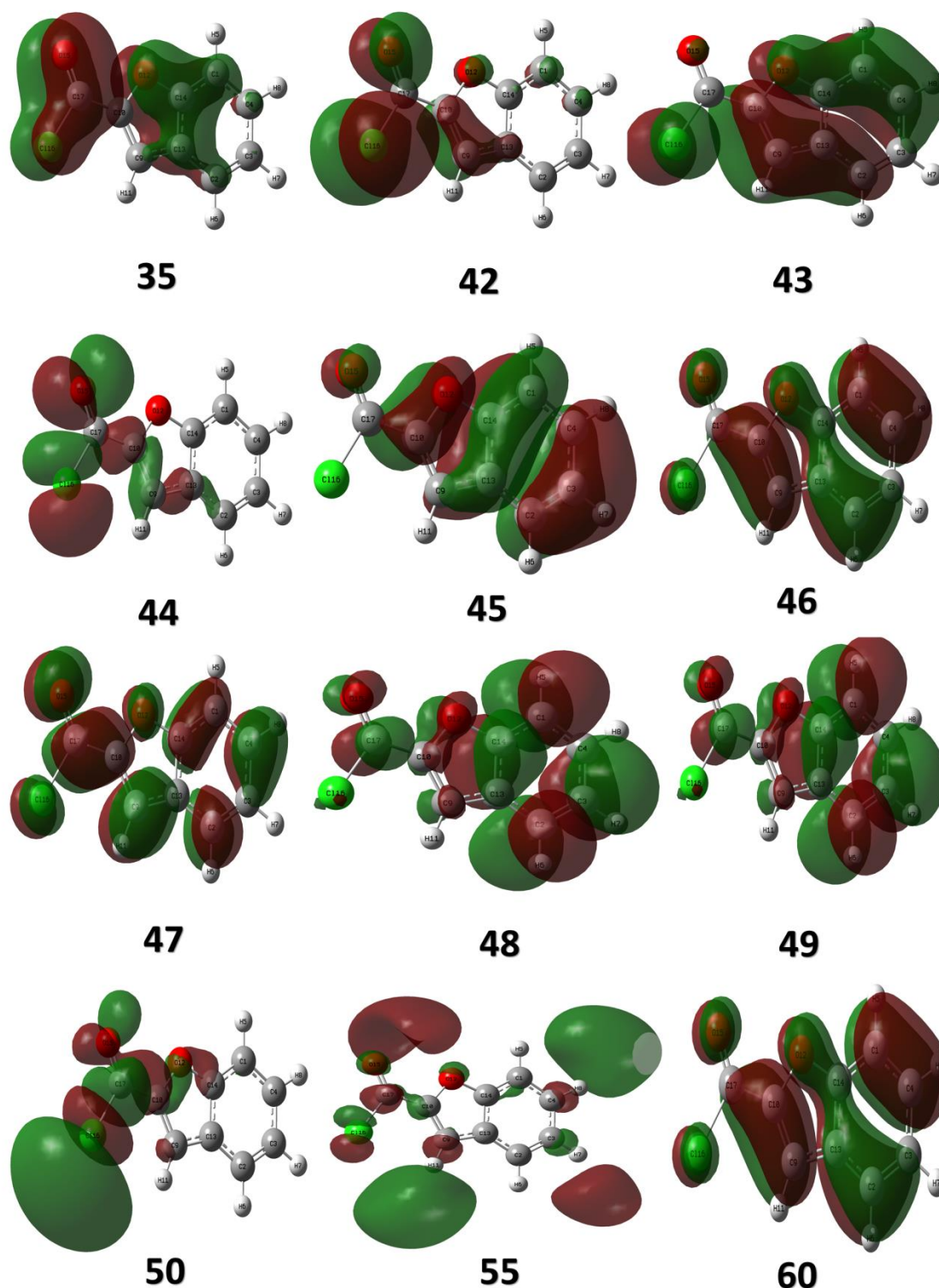


Fig. 6(a): Visualization of molecular orbitals (HOMO: 46 – LUMO: 47) by DFT/TD-SCF method.

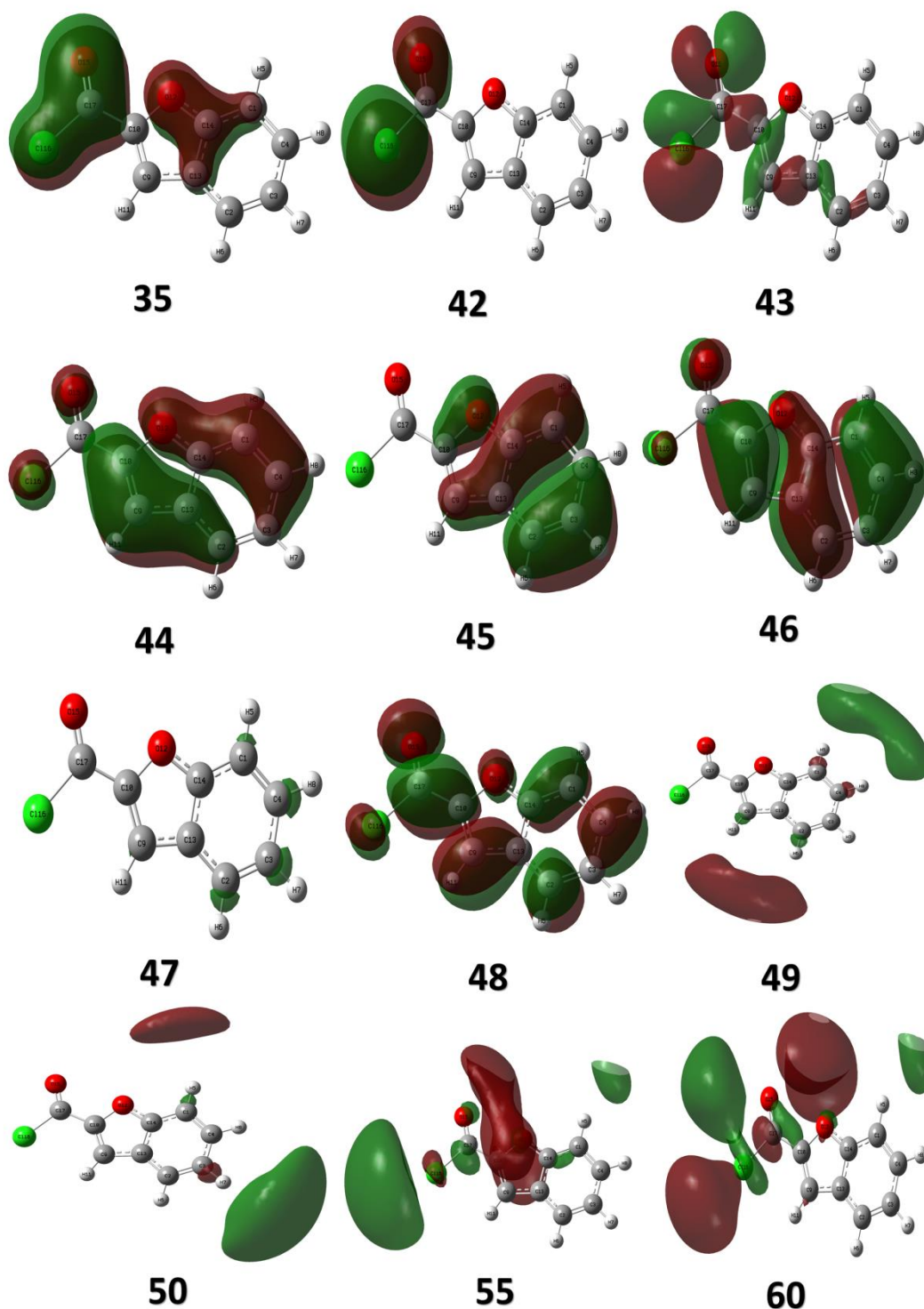


Fig. 6(b): Visualization of molecular orbitals (HOMO: 46 – LUMO: 47) by HF/TD-SCF method.

Different molecular orbitals were shown positive and negative charge distributions. In addition to that, we calculated energy gap and chemical properties of BCC. It was useful to determine the chemical stability of organic compounds and electronic charge distributions [30]. Some of equations were used for these calculations and results were presented in Table 4.

$$\text{Ionization potential (I)} = -E_{\text{HOMO}}$$

$$\text{Electron Affinity (A)} = -E_{\text{LUMO}}$$

$$\text{Chemical potential } (\mu) \text{ (eV)} = -\frac{1}{2}(E_{\text{HOMO}} + E_{\text{LUMO}})$$

$$\text{Electronegativity } \chi = I + \frac{A}{2}$$

$$\text{Chemical hardness } \eta = I - \frac{A}{2}$$

$$\text{Electrophilicity index } \omega = \frac{\mu^2}{2\eta}$$

$$\text{Global Softness } \sigma = \frac{1}{\eta}$$

Table 4: The calculated quantum chemical parameters on Benzofuran-2-carbonyl chloride

Property	DFT/6-311++G**	HF/6-311++G**
Total energy (eV)	-26035.0291	-25934.5562
E _{HOMO} (eV)	-7.1299	-8.9895
E _{LUMO} (eV)	-2.7456	1.0982
Energy gap (ΔE) (eV)	-4.3843	-10.0878
Ionization potential (I) eV	7.1299	8.9895
Electron Affinity (A) eV	2.7456	-1.0982
Electro-negativity (χ)eV	8.5027	8.4404
Chemical Potential (μ)	4.9377	3.9456
Chemical hardness(η)eV	5.7571	9.5386
Electrofilicity index (ω)eV	2.1175	0.8160
Global Softness (σ)eV	0.1736	0.1048
Dipole moment(D)	5.0025	6.0763

4.4 Non Linear Optical Properties:

Non-linear optical materials have wide range of applications in material science. We obtained electric dipole moment μ (D), second order polarizability ($\Delta\alpha$) and first hyperpolarizability (β) from quantum computing methods HF and DFT with the help of finite field approach [31]. Coming to present work of BCC organic material, we extract dipole, polar and hyper Polar values from Gaussian output file. Compared both HF and DFT calculated values and reported in Table 5.

$$\mu = \mu_x^2 + \mu_y^2 + \mu_z^2$$

$$\alpha_o = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}$$

$$\Delta\alpha = 2^{-1/2}[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{xx})^2 + 6\alpha_{xx}^2]^{1/2}$$

$$\beta = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2}$$

$$\beta_x = \beta_{xxx} + \beta_{yyx} + \beta_{zzx}$$

$$\beta_y = \beta_{yyy} + \beta_{xxy} + \beta_{yyz}$$

$$\beta_z = \beta_{zzz} + \beta_{xxz} + \beta_{yyz}$$

Table 5: The electric dipole moment (D), average polarizability, first hyperpolarizability, etc., of BCC by B3LYP/6-311++G**

Components	HF/6-311++G**	DFT/6-311++G**
μ (D)	3.87361011	5.71508058
α_o (esu)	19.4426×10^{-24}	23.0763×10^{-24}
$\Delta\alpha$ (esu)	53.6181×10^{-24}	57.5952×10^{-24}
β total (esu)	9.5857×10^{-30}	15.2862×10^{-30}

4.5 Molecular electrostatic potential surface map (MESP):

Three dimensional electrostatic potential surface were recorded by using Argus lab and presented in Figure 7 (a) & 7 (b). MESP shows clear picture of electrophilic and nucleophilic attacks of BCC [32]. Charge distributions were observed in carbonyl group. From MESP, oxygen atoms (O15 and O12) were get negative charge shows red colour and chlorine atom (Cl16) positive charge shows blue colour.

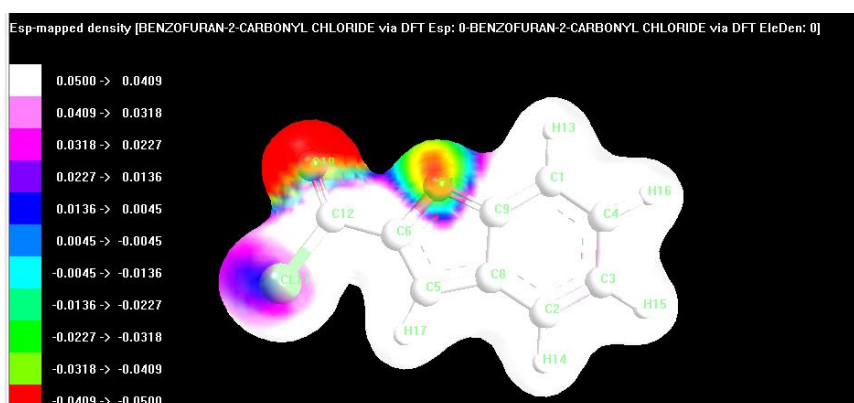


Fig. 7 (a): DFT/6-311++G (d,p) calculated 3D molecular electrostatic potential maps of BCC.

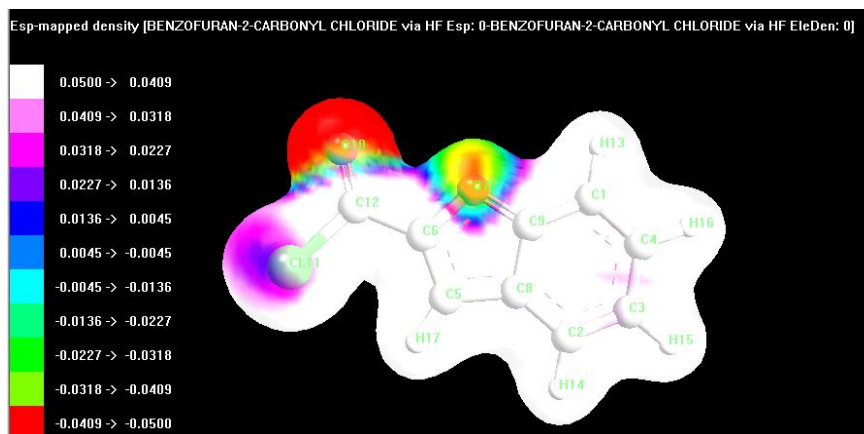


Fig. 7 (b): HF/6-311++G (d,p) calculated 3D molecular electrostatic potential maps of BCC.

4.6 Atomic mulliken charges:

Mulliken population analyses were used to understand partial atomic charge and linear combinations of atomic orbitals from quantum computational methods. It was developed by Robert. S. Mulliken in 1955 [33]. Atomic charges of optimized BCC were computed via DFT and HF method and presented in Table 6.

Table 6: Atomic charges for optimized geometry Benzofuran-2-carbonyl chloride by HF and DFT

S.No.	Atom	Mulliken	
		DFT	HF
1	C1	-0.357908	-0.211708
2	C2	-0.062717	0.038663
3	C3	-0.168932	-0.311217
4	C4	-0.244782	-0.323662
5	H5	0.196817	0.256354
6	H6	0.160322	0.232454
7	H7	0.171519	0.232398
8	H8	0.177270	0.244955
9	C9	-0.198185	-0.386970
10	C10	1.086517	1.009972
11	H11	0.176266	0.262180
12	O12	-0.043177	-0.182382
13	C13	0.943242	0.971227
14	C14	-0.719252	-0.611540
15	O15	-0.098571	-0.229414
16	C16	0.331362	0.297316
17	C17	-1.349793	-1.288625

V. CONCLUSION

The investigated BCC compound structure were optimized and analyzed theoretical vibrational frequency data via DFT and HF method with standard basis set 6-311++G (d,p). FT-IR experimental vibrational frequencies were compared with theoretical scaled frequencies and reported in detailed. Assignments of fundamental vibrations of BCC normal modes analysis based on SQM force field calculations using DFT and HF method. UV-Vis absorbance at 321 nm and optical band gap at 3.85 eV were observed. According to FMO analysis, we found energy gap between molecular orbital from both theoretical methods and reported. From quantum chemical calculations carried out for ionization potential, chemical potential, global chemical softness and dipole moment. Different molecular orbitals were presented for clear picture of electric charge distributions. 3-D MESP were presented for visualization of electrophilic and nucleophilic attack.

ACKNOWLEDGMENT:

The corresponding author, A.Veeraiah is highly grateful to UGC-DAE, IUC-Indore, Government of India (Project code-CSR-IC-BL-56/CRS-173/2016-17/837) and Management of D.N.R.College Association for their financial support and cooperation respectively. Further, the authors are highly grateful to Prof. T. Sundius for Molvib program.

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