

Vibrational Spectroscopic and Computational Analysis of 5-chloro-2-hydroxy Acetophenone

Palani Murugan, S. Jeyavijayan, Naidu Dhanpal Jayram, K. Viswanathan

Abstract: Fourier Transfer infrared and Raman spectra in the range of 4000-400 cm^{-1} and 3500-50 cm^{-1} were recorded to study the vibrational spectra of 5-chloro-2-hydroxyacetophenone (CHAP). Using density functional theory (DFT/B3LYP) with 6-31+G(d,p) and 6-311++G(d,p) basis sets the various geometrical parameters such as Raman activities, infrared intensities and optimum frequencies were calculated. The HOMO-LUMO energy gap has been computed which confirms the charge transfer of the molecular system. Mulliken's atomic charges associated with each atom and thermodynamic parameters have also been reported with the same level of DFT.

Keywords: 5-chloro-2-hydroxy acetophenone; FTIR; FT-Raman; DFT.

I. INTRODUCTION

The biological and physicochemical properties of acetophenone compounds have shown interesting behaviour in nature through diverse synthesis procedures [1,2]. Recent studies in antibacterial activity of 20 acetophenones using electronic and topological indices have shown interesting structural characteristics [3]. Among them, hydroxy acetophenone is employed as building block for the synthesis of rubbers, plastics, agrochemicals flavor, fragrances and pharmaceuticals. Due to the versatile behaviors of acetophenone, Seth et al. investigated the crystallographic and spectroscopic studies of ortho-hydroxy acetophenones [4]. Recently, many researchers have studied the computational and vibrational spectra of hydroxyacetophenone derivatives [5,6]. Consideration of these factors leads to study the detailed spectral investigation of 5-chloro-2-hydroxyacetophenone (CHAP).

II. EXPERIMENTAL

The fine polycrystalline sample of CHAP was purchased from commercial sources with a stated purity of 99% and they were used as such without further purification. The Fourier transform infrared spectra was recorded in the region

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4000-400 cm^{-1} , using Perkin Elmer FTIR spectrometer equipped with an MCT detector, a KBr beam splitter and globar source. The FT-Raman spectrum of CHAP was recorded on a computer interfaced BRUKER RFS-66V model interferometer in the Stokes region 4000-50 cm^{-1} using Nd: YAG laser operating at 200 mW power continuously with 1064nm excitation.

III. COMPUTATION AND SIMULATION

In the quantum chemical calculations, DFT has proved to be very useful in treating electronic structure of molecules. The DFT calculations were carried out for CHAP with GAUSSIAN 09W program package [7] using the Becke's three parameter hybrids functional combined with the Lee-Yang-Parr correlation (B3LYP) functional [8,9] with standard 6-31+G(d,p) and 6-311++G(d,p) basis sets. The total energy distribution (TED) associated with each vibration is calculated by the MOLVIB program (version V7.0-G77) written by Sundius [10]. The HOMO-LUMO and Mulliken charge analyses have been computed with same level of calculations to elucidate information regarding charge transfer within the molecule.

IV. RESULT AND DISCUSSION

A. Molecular Geometry

Fig. 1 shows the optimized molecular structure of CHAP. DFT structure optimization with standard 6-31+G(d,p) and 6-311++G(d,p) basis sets gives global minimum energy value as -919.577287 and -919.709992 Hartrees, respectively. The optimized geometrical parameters of CHAP calculated by using the above methods in comparison with the experimental data [11] are presented in the Table I. The thermodynamic characteristics like zero point vibrational energy (ZPVE), dipole moment, heat capacity and entropy were computed at same level of calculations for CHAP as presented in Table II. In this study, the dipole moment molecule of CHAP is found to be 3.8702 and 3.8537 Debye, for lower and higher basis sets, respectively. All the thermodynamic data provide helpful information for the further study on the CHAP.

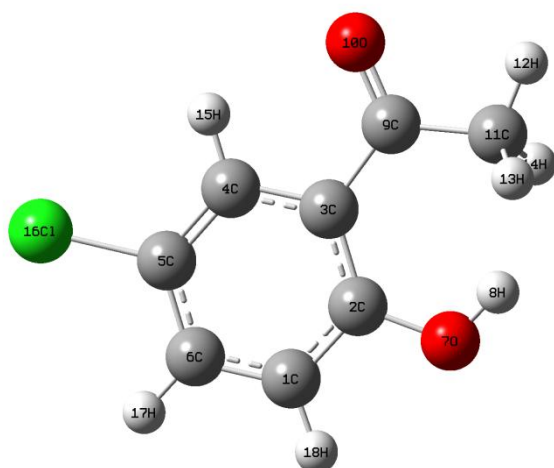


Figure 1. Molecular structure of 5-chloro-2-hydroxy acetophenone

B. Vibrational Spectral Analysis

The molecule under investigation contains 18 atoms and hence it has 48 modes ($3N-6$) of vibrations. The geometry of the molecule CHAP is considered to possess C_1 point group symmetry. The IR and Raman peaks are active for all the vibrations of molecule. The observed FTIR and FT-Raman spectra of CHAP are presented in Fig. 2. The detailed vibrational assignment of fundamental modes of CHAP along with the calculated IR intensities, Raman activities, and normal mode descriptions (characterised by TED) are reported in Table III.

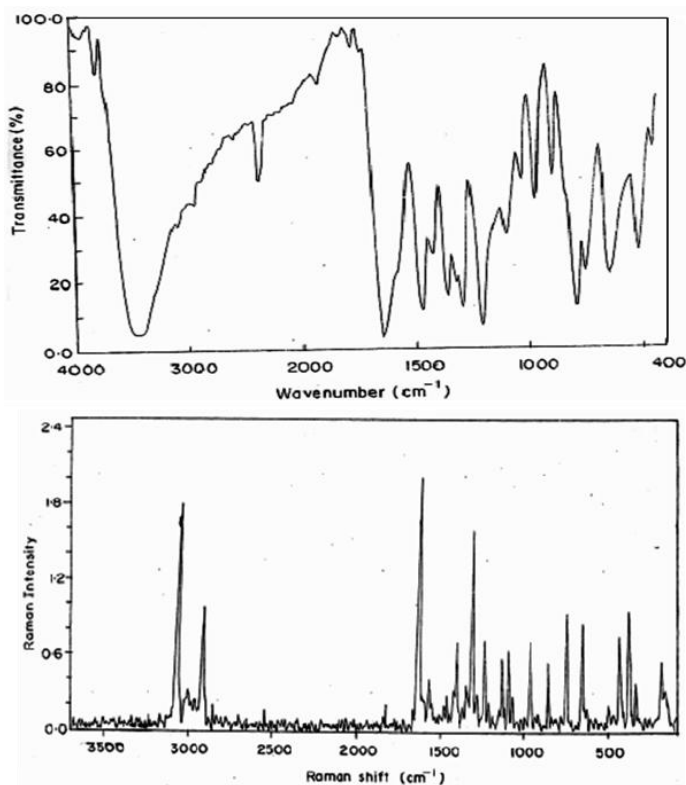


Figure 2. FTIR and FT-Raman spectra of 5-chloro-2-hydroxy acetophenone

Anharmonicity and the general tendency of the quantum mechanical methods show variation in the corresponding experimental quantities and calculated wavenumbers. This

results into overestimate the force constants at the equilibrium geometry. Therefore, in order to improve the calculated values in agreement with the experimental ones, calculated harmonic frequencies are scale down. Using scale factor [12] of 0.96 for B3LYP method, an improved agreement between the computed and experimental frequencies is obtained and listed in Table III.

Table I. Experimental (XRD) and optimized geometrical parameters of 5-chloro-2-hydroxy acetophenone

Bond length (Å)	B3LYP/ 6-31+G(d,p)	B3LYP/ 6-311++G(d,p)	Expt ¹¹
	C1-C2	1.405	
C1-C6	1.391	1.387	1.377
C2-C3	1.417	1.414	1.419
C2-O7	1.391	1.391	1.352
C3-C4	1.418	1.416	1.405
C3-C9	1.495	1.494	1.477
C4-C5	1.381	1.377	1.376
C5-C6	1.4	1.397	1.392
C5-Cl16	1.825	1.827	1.75
C9-O10	1.25	1.247	1.237
C9-C11	1.518	1.516	1.5
Bond angle (°)			
C2-C1-C6	120.84	120.86	120.6
C1-C2-C3	120.6	120.57	120
C1-C2-O7	113.24	113.31	117.9
C3-C2-O7	126.16	126.12	122.1
C2-C3-C4	117.56	117.58	118.7
C2-C3-C9	126.92	126.87	119.8
C4-C3-C9	115.52	115.55	121.5
C3-C4-C5	120.88	120.79	119.8
C4-C5-C6	121.42	121.53	121.5
C4-C5-Cl16	119.64	119.58	118.9
C6-C5-Cl16	118.95	118.89	119.6
C1-C6-C5	118.71	118.67	119.4
C3-C9-O10	119.84	119.71	120.3
C3-C9-C11	122.18	122.2	120
O10-C9-C11	117.98	118.08	119.7

Table II. Theoretically computed thermodynamic parameters of 5-chloro-2-hydroxy acetophenone

Parameter	B3LYP/6-3 1+G(d,p)	B3LYP/6-31 1++G(d,p)
	Zeropoint vibrational energy(kcal mol ⁻¹)	89.4635
Thermal energy (kcal mol ⁻¹)	89.805	88.544
Heat capacity, C_v (calmol ⁻¹ K ⁻¹)	37.579	36.121
Entropy (cal mol ⁻¹ K ⁻¹)		
<i>Total</i>	102.153	97.020

Translational	41.300	41.300	μ_y	2.7931	2.7667
Rotational	30.957	30.949	μ_z	0.0014	0.0011
Vibrational	29.896	24.771	μ_{total}	3.8702	3.8537
Dipole moment (Debye)					
μ_x	-2.6790	-2.6826			

Table III. FTIR, Raman and calculated (unscaled and scaled) vibrational frequencies (cm⁻¹), IR intensity (km mol⁻¹), Raman activity (Å⁴amu⁻¹), and vibrational assignments of 5-chloro-2-hydroxy acetophenone

Sl.No	Experimental frequencies(cm ⁻¹)		Calculated frequencies(cm ⁻¹)								Assignment with TED (%)
	FTIR	FT-Raman	B3LYP/6-31+G(d,p)				B3LYP/6-311++G(d,p)				
			Un Scaled	Scaled	IR intensity	Raman activity	Un Scaled	Scaled	IR intensity	Raman activity	
1	3544(s)	-	3731	3582	142.15	60.08	3748	3598	171.85	99.39	v OH (98)
2	3080(vw)	-	3248	3118	4.28	39.48	3218	3089	8.33	46.74	vCH (96)
3	-	3075(vs)	3246	3117	2.48	140.22	3216	3088	1.13	161.55	vCH (97)
4	-	3011(w)	3231	3102	1.47	52.92	3200	3072	1.19	64.13	vCH (95)
5	2927(w)	2927(vw)	3160	3034	8.95	79.90	3133	3008	5.00	110.34	CH ₃ ips (92)
6	-	2862(s)	3090	2966	10.09	54.61	3064	2941	5.14	40.00	CH ₃ ss (94)
7	2913(s)	-	3021	2900	9.89	125.91	2997	2877	5.85	151.00	CH ₃ ops (90)
8	-	1831(vs)	1665	1599	301.27	40.34	1651	1585	212.01	63.50	CH ₃ ipr (89)
9	1762(w)	-	1633	1568	53.07	47.06	1619	1554	54.98	60.09	vCC (88)
10	1642(vs)	-	1608	1544	33.53	10.51	1594	1530	22.89	15.20	vCC (89)
11	-	1577(ms)	1540	1478	219.91	2.37	1535	1474	189.76	4.83	vCC (85)
12	1470(s)	-	1522	1461	10.98	8.29	1517	1456	12.55	9.11	vCC (86)
13	-	1468(ms)	1512	1451	7.47	5.48	1503	1443	34.12	4.13	v CC (85)
14	1418(ms)	-	1447	1389	81.58	0.42	1436	1379	72.96	0.35	vCC (87)
15	-	1410(s)	1427	1370	27.96	1.76	1424	1367	51.77	1.74	vCC (84)
16	1356(ms)	-	1379	1324	13.56	1.26	1356	1301	3.96	13.26	vCC (82)
17	-	1349(s)	1334	1281	76.70	33.93	1327	1274	10.09	13.15	vCO (80)
18	1318(s)	-	1284	1233	267.53	14.58	1277	1225	254.65	5.89	v CO (81)
19	-	1307(ms)	1252	1202	18.93	1.56	1242	1193	83.82	28.07	b OH (78)
20	1289(ms)	-	1180	1133	33.07	6.14	1170	1123	131.90	7.81	CH ₃ ipb (79)
21	-	1286(s)	1140	1094	66.95	3.42	1133	1088	2.64	7.97	CH ₃ sb (76)
22	-	1239(ms)	1115	1071	22.04	9.05	1105	1061	8.28	21.14	b CH (75)
23	-	1213(s)	1097	1053	13.22	4.74	1091	1047	2.55	4.25	b CH (74)
24	1208(s)	-	1081	1037	7.33	1.22	1074	1031	0.82	0.20	b CH (72)
25	-	1140(s)	1015	974	1.73	0.33	1003	963	2.08	0.07	CH ₃ opb (68)
26	-	1097(ms)	993	953	10.93	10.90	987	948	18.19	15.86	CH ₃ opr (67)
27	-	1070(s)	982	943	12.65	0.12	958	919	11.75	0.13	R asymd (70)
28	1024(w)	-	870	835	40.06	0.56	867	832	5.14	11.87	R asymd (71)
29	-	966(w)	870	835	7.41	13.56	866	831	29.39	0.25	ω CC (65)
30	963(w)	-	751	721	4.62	1.48	733	703	22.37	13.22	ω CC (64)
31	938(s)	-	734	705	17.86	10.56	730	701	0.03	0.33	R trigd (69)
32	881(s)	-	662	636	50.12	4.17	659	633	34.00	4.15	ω OH (63)
33	-	859(w)	644	618	7.59	1.21	628	603	0.06	0.69	b CC (70)
34	791(s)	-	598	574	35.21	3.19	596	572	38.34	2.48	b CC (68)
35	-	748(s)	562	539	24.60	0.89	559	537	9.72	2.53	v CCl (69)
36	746(w)	-	548	526	14.82	1.28	542	521	13.16	0.17	b CO (70)
37	-	654(w)	443	425	0.14	0.19	439	421	0.29	0.03	b CO (67)
38	-	650(w)	390	375	2.95	8.85	389	373	2.40	7.83	t R symd (63)
39	-	648(vw)	378	363	1.72	2.34	376	361	0.74	3.95	t R trigd (60)
40	644(ms)	-	357	343	0.95	2.94	346	332	3.21	4.38	t R symd (62)
41	640(ms)	-	340	326	1.85	1.68	337	324	5.13	0.43	ω CH (61)
42	512(w)	-	325	312	17.95	0.77	294	282	25.43	0.53	ω CH (60)
43	-	498(ms)	297	285	18.81	0.68	281	270	2.66	0.82	ω CH (58)
44	436(vw)	436(s)	248	238	68.30	0.70	172	165	48.08	0.83	b CCl (65)
45	-	378(w)	172	165	8.36	1.37	167	161	0.80	2.08	ω CO (56)
46	-	337(vw)	148	142	10.95	0.83	126	121	5.74	0.35	ω CO (55)
47	-	185(w)	102	97	8.79	1.42	54	52	6.49	1.53	ω CC (54)
48	-	170(ms)	11	10	3.92	0.33	11	11	1.17	0.17	t CH ₃ (51)

O-H Vibrations

The easiest way to confirm bonding strength of any molecule is too precise for the O-H band position. Peaks

stretched in the region of 3500-3600 cm⁻¹ are strong enough to confirm intermolecular hydrogen



bonding system [13]. The vibration peak at 3544 cm⁻¹ confirms CHAP strong absorption due to stretching of O-H bond. The unity confirmation and overall results of molecule was well supported by TED. Table III illustrates vibrations of hydroxyl groups present in plane and out-of plane.

C-H Vibrations

CHAP molecule also consists of C-H vibration due to presence of aromatic compounds. In the present work, stretching band at 3080 cm⁻¹ present in infrared and bands at 3075, 3011 cm⁻¹ from the Fourier Raman confirms C-H stretching vibration and agreed well with the literature [14]. Table III illustrates the in-plane and out-of-plane bending vibrations of C-H group and they are found to be in good agreement with the calculated results.

CH₃Vibrations

A CH₃ group frequencies assignment consists of nine fundamental vibrations. The first three vibrations responsible for stretching, while the bending vibration of molecule decided by another three frequencies. The methyl group movement was decided by two rocking modes and single torsional mode. In case of title compound, at 2862 cm⁻¹, CH₃ symmetric stretch frequency is observed in Raman and in-plane CH₃ stretch frequencies observed at 2927 cm⁻¹ in both IR and Raman spectra. The mentioned frequency numbers well matched with literature report [15] and TED results. Raman studies are enough to find out the complete vibrational in-plane and out of plane modes. In case of CHAP, the FT-Raman bands obtained at 1831 and 1097 cm⁻¹ are assigned to CH₃ in-plane and out-of-plane rocking modes, similarly the bands at 2913 cm⁻¹ in IR and 1140 cm⁻¹ in Raman credited to CH₃ out-of-plane stretching and out-of-plane bending modes, respectively. Also, the band at 170 cm⁻¹ attributed to methyl twisting mode.

C=O Vibrations

In the FTIR spectrum, the vibration due to carbon and oxygen results into carbonyl bonds. They are most characteristic bands [16] occur in the region 1800–1700 cm⁻¹. The wave numbers at 1318 and 1349 cm⁻¹ in the FTIR and FT-Raman spectra, respectively, are assigned as C=O stretching vibrations of CHAP.

C-Cl Vibrations

The vibrations of the halogen atoms are worth to discuss here, since mixing of vibrations are possible due to the lowering of the molecular symmetry [17]. The Raman band at 748 cm⁻¹ has been assigned to C-Cl stretching mode. The C-Cl in-plane bending and out-of-plane bending vibrations are also summarized in the Table III.

C-C Vibrations

The bands between 1400-1650 cm⁻¹ in the aromatic and hetero aromatic compounds are assigned to C-C stretching vibrations [18]. The benzene ring modes predominantly involve C-C bonds. The vibrational frequencies at 1762, 1642, 1470, 1418, 1356 cm⁻¹ in IR and 1577, 1468, 1410 cm⁻¹ in Raman are associated with C-C stretching modes of carbon skeleton. The ring out-of-plane and in-plane bending modes have also been identified in the Table III. All these vibrations are in excellent concurrence with the computed values.

Mulliken Charges Analysis

Charge distributions plays significant role in the calculation of quantum mechanical molecular systems [19].

The electron distributions in CHAP were carried out for the comparison of different choice of the basis sets using Mulliken population analysis. Table IV shows the calculation of Mulliken charge distribution at different basis sets. Electron density rearrangements occur at carbon atom C2 (attached to OH group) due to high negative charge. Similarly, the redistribution occurs at atoms C3 and C5 having positive charges due to the attachment of CO-CH₃ and Cl groups, respectively. A net positive charge is surrounded to hydrogen atom because they are electron acceptors.

HOMO-LUMO Analysis

The electrical and optical properties are responsible for chemical reaction in the molecule. The molecular orbital arrangements such as highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) directly involves in chemical reaction [20] due to overlapping in CHAP. The HOMO-LUMO orbital for CHAP is shown in Fig. 3. In this study, the HOMO is located over ring system, chlorine and oxygen atoms and LUMO: of π nature, (i.e. benzene ring) is delocalized over the whole C-C bond; as a result the HOMO→LUMO transition implies an electron density transfer to the C-C bond of the benzene ring and CO-CH₃ group from chlorine atom. The HOMO-LUMO energy gap is found to be 4.501 eV by B3LYP/6-311++G(d,p) method. This explains the ultimate charge transfer interaction within the molecule, which influences the biological activity of the molecule.

Table IV. Mulliken charges analysis for 5-chloro-2-hydroxy acetophenone

Atoms	Atomic charges (Mulliken)	
	B3LYP/6-31+G(d,p)	B3LYP/6-311++G(d,p)
C1	-0.3403	-0.5451
C2	-1.1625	-1.4285
C3	1.4382	1.3485
C4	-1.5897	-1.0586
C5	0.9714	0.9027
C6	-0.6300	-0.3865
O7	-0.6046	-0.4873
H8	0.4427	0.4248
C9	0.4770	0.0506
O10	-0.4178	-0.3351
C11	-0.9938	-1.1044
H12	0.2529	0.3420
H13	0.2209	0.2650
H14	0.2209	0.2649
H15	0.2535	0.3680
C16	0.3640	0.7515
H17	0.2117	0.3039
H18	0.2047	0.3234

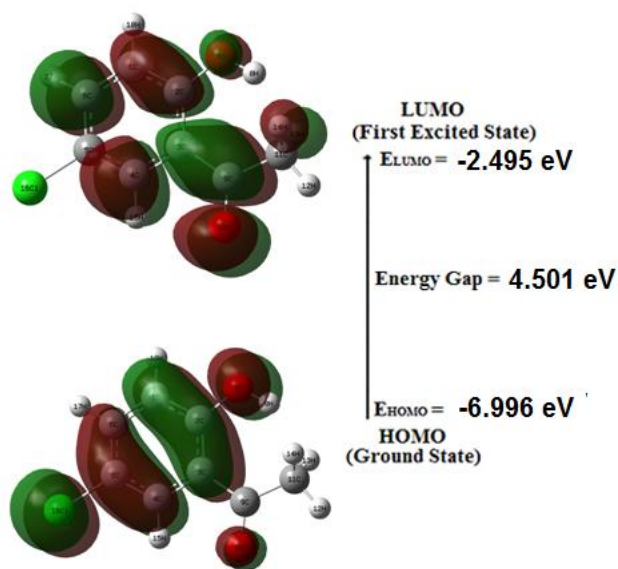


Figure 3. HOMO-LUMO of 5-chloro-2-hydroxy acetophenone

V. CONCLUSION

The vibrational fundamental frequencies of 5-chloro-2-hydroxy acetophenone have been investigated with DFT-B3LYP through 6-31+G(d,p) and 6-311++G(d,p) level calculations. Various parameters such as stabled geometries and frequencies of CHAP were confirmed by FTIR and FT-Raman spectroscopies on the basis of C₁ point group symmetry. The frequency assignment for normal modes is supported by the TED calculation. The perceptiveness of CHAP chemical activity and properties might be confirmed through smaller HOMO-LUMO band gap. In addition, the thermodynamic properties and results of Mulliken's charge of CHAP have been designed and discussed. These outcomes will be of support in the quest of the experimental and theoretical evidence for 5-chloro-2-hydroxy acetophenone in reaction intermediaries, pharmaceuticals and agrochemicals industries.

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