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Synthesis of 7-Formyl-8-hydroxyquinoline, Infrared Spectra its HF and DFT Calculations and Assignment of Vibrations Modes

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Abstract

In this work, 7-Formyl-8-hydroxyquinoline (7F8HQ) has been synthesized and its Fourier transform infrared spectra at solid phase were recorded in the region of 4000-400 cm^{-1}. The vibrational infrared intensity bands of 7-Formyl-8-hydroxyquinoline in ground state have been calculated by HF and density functional theory (DFT) with 6-311G(dp) basis set respectively. The calculated frequencies have been scaled which compared with experimental infrared spectra. The normal modes of vibration obtained from HF and density functional theory methods are in good agreement with the experimental data.

Key Words: 7-Formyl-8-hydroxyquinoline, Infrared spectra, HF, Density Functional Theory.

1 Introduction

8-Hydroxyquinoline and its derivatives are well known for their antifungal, antibacterial and antiamoebic activities [1]. These molecules are widely employed as a good fluorogenic ligand binding with many metal cations due to its low quantum yield in aqueous and some organic solutions [2]. Quinoline derivatives have attracted special interest due to their therapeutic properties [3]. Quinoline sulphonamides have been used in the treatment of tuberculosis, malaria, diabetes and cancer [4-7]. The electrical conductivity, corrosion inhibition and spectrophotometric properties of 7-formyl-8-hydroxyquinoline and its transition metal complexes were reported [8]. The tin, cobalt, copper, zinc, cadmium and silver with 7-formyl-8-hydroxyquinoline complexes were prepared [9], their electrical conductivity and 7-formyl-8-hydroxyquinoline ability to act as a corrosion inhibitor for aluminium was determined. Recently, V. Arjunana et al.[10] have investigated ab initio and DFT studies on 7-bromo-5-chloro-8-hydroxyquinoline, and Arici and Yilmaz [11] have carried out Infrared Spectra, Density Functional Theory and Hartree-Fock Theoretical Calculations of 2-Methyl-8-quinolinol. Theoretical calculations based on Time-dependent density functional theory (TD-DFT) were carried out for the quinolin-8-yl benzoate (8-OateQ) compound to understand the effect of O-substituent on the electronic absorption of 8-hydroxyquinaline (8-HQ)[12]. But up to now, to our best knowledge no ab initio and DFT calculation has been reported on 7-formyl-8-hydroxyquinoline. In this study, we report ab initio HF and DFT/B3LYP, BLYP calculation results on 7-formyl-8-hydroxyquinoline. The aim of this study is to give optimal molecular geometry, vibrational wavenumbers and modes of the free 7-formyl-8-hydroxyquinoline.

2 Experimental details

2.1 Preparation of the 7-formyl-8-hydroxyquinoline

The 7-formyl-8-hydroxyquinoline (7F8HQ) was prepared according to a previous study [13]. 1,45 g (0,1 mol) of 8-hydroxyquinoline was added to 8,5 ml (0,01 mol) of chloroform and 90 ml of 15% NaOH. The reaction mixture was heated under reflux for 4h, on a water bath until the solution became brown in color. After cooling, the pH of the solution was adjusted to 5,5-5,8 using 0,01 M HCI. A pale brown product was separated and left to coagulate, then filtered off and recrystallized from 80 % ethanol, mp 225^0 C and yield 15 %. The infrared spectra of the resulting molecule 7-formyl-8-hydroxyquinoline(7F8HQ) were recorded in the region 4000-400 cm^{-1}, using Bruker FTIR IFS 66/S spectrophotometer equipped with ATR module at Kahramanmaraş Sutçu Imam University. The observed infrared of 7-formyl-8-hydroxyquinoline is shown in Fig. 1.

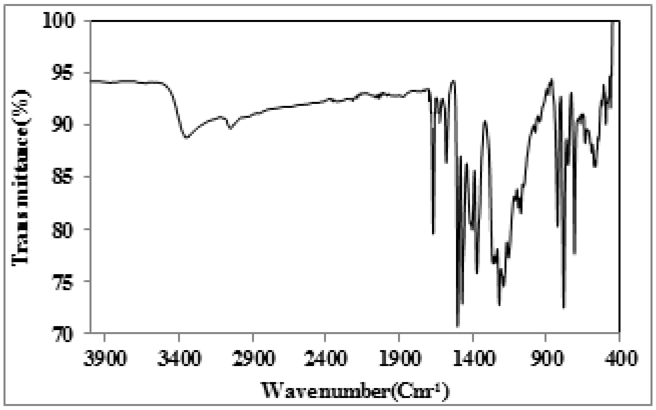


Figure 1: The infrared spectra of 7-formyl-8-hydroxyquinoline

3 Computational details

The HF and DFT calculations of the title compound were carried out with Gaussian 09W program [14] on a personal computer. The Becke-3-Lee-Yang-Parr (B3LYP) functional [15, 16] were used to carry out both the HF and DFT analysis with the standard 6-311G(d,p) basis set. The normal coordinate analysis of the title compound has been computed at the fully optimized geometry by assuming C_s point-group symmetry. All the calculated vibrational frequencies are scaled by 0,9085 for HF/6-31G(dp) and 0,9669 for B3LYP/6-311G(dp) [17]. The scale factors used to minimize the deviation between the computed and the experimental frequencies. Molecular geometry is not restricted and all the calculations are performed by using GaussView molecular visualization program [18].

4 Results and discussion

4.1 Vibrational assignments

The molecular structure of the 7-formyl-8-hydroxyquinoline consists of 20 atoms and belongs to C_s point group of symmetry. The formyl and OH group attached as orto to the planer naphthalene molecule as show in Fig.2. The fifty four fundamental modes of vibrations for the compound are distributed into the irreducible representations under C_s symmetry as 36 A' and 18 A'' species, *i.e.*, Γ_{Cs} = 36 A' + 18 A''. All vibrations are active in both IR and Raman spectra. All the frequencies are assigned in terms of fundamental, overtone and combination bands.

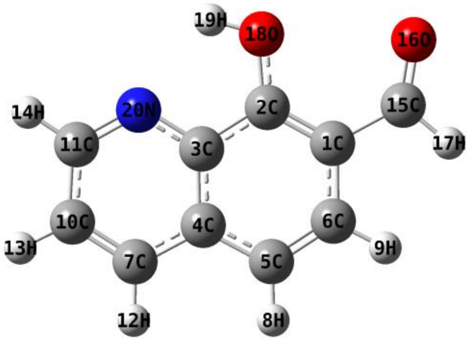


Figure 2: Molecular structure of 7-formyl-8-hydroxyquinoline

The observed and calculated frequencies using HF/6-311G** and DFT/ B3LYP/6-311G** with their relative intensities and probable assignments are given in Table 1.

Table 1 the observed infrared wavenumbers and calculated frequencies using HF/6-311G** and DFT/ B3LYP/6-311G** their intensities and probable assignments of 7-formyl-8-hydroxyquinoline molecule

No.	Spc.	Calculation/ HF/6-311G**			Calculation/DFT/B3LYP/6-311G**				
		Uscl. (cm^{-1})	Scl.^{a} (cm^{-1})	Inf.Int.	Uscl. (cm^{-1})	Scl.^{b} (cm^{-1})	Inf.Int.	Exp.Inf.	Approx. Assignment
1	A"	75,0853	68	1,699	73,5408	71	0,499	-------	Formyl torsion
2	A"	140,1255	127	0,091	138,2976	134	3,128	-------	γ ring
3	A"	171,2636	156	5,501	165,5989	160	7,077	-------	γ ring
4	A'	201,5778	183	2,733	184,2251	178	2,173	-------	δ(C- Formyl)
5	A"	269,2377	245	0,001	251,3847	243	0,048	-------	γ (CCC)+ γ Formyl
6	A"	325,5988	296	5,183	299,0768	289	6,508	-------	γ (CCC)
7	A"	326,5495	297	4,873	302,5947	295	3,444	-------	γ (CCC)
8	A'	397,4741	361	2,983	373,1948	361	2,971	-------	δ(CCC)
9	A"	483,9899	485	0,835	443,3299	428	0,176	-------	γ (CCC)+ γ (CN)
10	A'	537,8559	488	2,343	502,0187	485	1,451	463 w	δ C-(OH)
11	A"	546,2550	496	2,366	505,7230	489	2,126	495 w	γ (CCC)
12	A'	561,1445	511	20,728	524,7901	507	15,031	-------	δ(CCC)
13	A'	604,1607	549	11,981	569,6148	550	9,990	-------	δ(CCC)+ δ(CN)
14	A"	638,6484	581	10,862	601,7957	582	1,545	580 m	γ (CCC)
15	A"	657,7485	597	0,005	622,7617	602	2,819	595 m	γ (CCC)
16	A'	658,9835	599	4,302	691,3966	668	15,072	639 w	δ(CCC)
17	A"	753,6923	685	44,469	705,8761	682	11,203	678 w	γ (OH)
18	A'	755,1744	686	12,073	718,8180	695	95,548	710 s	δ(CCC)
19	A'	827,5084	752	75,412	778,4986	753	58,170	756 m	δ(CCC)
20	A"	862,0609	783	0,368	783,4816	758	0,928	784 vs	γ(C-H)
21	A"	897,0008	815	12,335	817,5282	790	13,656	-------	γ(CCC)
22	A"	928,6109	844	50,292	842,7401	815	42,255	826 s	γ(C-H)
23	A'	969,2623	830	5,090	906,3223	876	4,765	-------	δ(CCC)
24	A'	1050,2786	954	69,287	964,5938	933	0,252	-------	δ(CCC)
25	A"	1082,7182	984	0,396	971,4274	938	0,154	-------	γ(C-H)
26	A'	1086,8088	987	7,763	987,6698	955	64,655	-------	δ(CCC)
27	A"	1087,9009	988	0,084	1005,1539	972	0,280	-------	γ(C-H)
28	A"	1221,4625	1019	0,068	1031,9018	998	0,134	-------	γ(C-H) in Formyl
29	A"	1143,1136	1038	2,158	1061,7002	1026	6,186	1070	γ(C-H)
30	A'	1188,3033	1079	4,820	1131,4051	1094	38,811	1093 m	δ(C-H)
31	A'	1214,7931	1104	46,954	1163,3040	1125	2,366	1126 m	δ(C-H)
32	A'	1270,6846	1154	21,273	1198,6431	1159	42,884	1162 s	ν C-(OH)
33	A'	1309,6075	1189	16,294	1237,2014	1196	9,601	1195 s	δ(C-H)
34	A'	1329,0457	1207	36,034	1244,6148	1203	23,003	1224 vs	δ(C-H)
35	A'	1394,2819	1266	25,589	1308,2441	1265	20,616	1260 s	δ(C-H)
36	A'	1408,5096	1280	30,664	1310,1075	1266	19,024	1270 s	ν(C-C) + ν(C-N)

37	A'	1469,1420	1335	84,431	1348,7176	1339	98,812	------	ν(C-C)
38	A'	1516,8891	1378	28,237	1417,0661	1370	32,319	1373 s	δ(C-H) in Formyl
39	A'	1538,5056	1398	167,189	1434,6005	1299	65,243	------	ν(C-C)
40	A'	1562,3734	1419	24,407	1444,6667	1397	44,284	1409 s	δ(O-H)
41	A'	1585,4598	1440	23,972	1468,8333	1420	56,977	1419 s	ν(C-C)
42	A'	1610,2895	1463	99,115	1492,0606	1443	42,490	1471 vs	ν(C-C)
43	A'	1659,7865	1508	88,123	1539,0323	1488	65,946	1506 vs	ν(C-C)
44	A'	1775,9613	1613	68,723	1609,4333	1556	45,643	-------	ν(C-C)
45	A'	1801,2180	1636	55,877	1641,1571	1587	7,032	1582 m	ν(C-C)
46	A'	1822,6371	1652	79,916	1655,9376	1611	152,097	1628 w	ν(C-C) + ν(C=N)
47	A'	1995,5501	1813	406,255	1789,5117	1730	274,857	1677 m	ν(C=O) in Formyl
48	A'	3081,0490	2799	145,743	2841,7829	2748	175,971	-------	ν(C-H) in Formyl
49	A'	3321,7073	3017	17,659	3155,2026	3050	16,628	-------	ν(C-H)
50	A'	3323,4155	3019	6,387	3159,3377	3055	4,073	-------	ν(C-H)
51	A'	3335,0391	3029	7,544	3171,3512	3066	5,653	-------	ν(C-H)
52	A'	3348,2758	3042	19,102	3183,8803	3078	14,374	3048 w	ν(C-H)
53	A'	3359,8035	3052	17,780	3194,9912	3089	15,183	------	ν(C-H)
54	A'	4064,1310	3692	167,929	3578,1979	3460	133,010	3368 br	ν(O-H)

Scaling factor (s.f^{a}.): 0.9085, s.f^{b}.: 0.9669, Uscl.:Unscaled, Scl.:Scaled, Inf.Int.:Infrared intensity, Spc.:species, br.:broad, m.: medium. s.:strong, w.:weak, v.:very, ν:stretching, δ:in-plane bending, γ:out of plane bending, Exp.Inf.:Experimental infrared .

4.4 Formyl group vibrations

The C–H stretching vibrations of the formyl group [19] usually appear in the region of 2871–2806 cm^{-1}. Hence in the present work, C–H stretching vibration was not observed but wave number was computed at 2799 cm^{-1} (Nos. 48) by HF/6-311G(d,p) and at 2748 cm^{-1} by DFT/B3LYP/6-311G(d,p) methods. This band has been observed as medium strong in infrared spectra at 2869 cm^{-1} [20] and 2854 cm^{-1} [21]. The strong band observed at 1373 cm^{-1} in the infrared spectrum is assigned to the in plane bending C-H stretching vibration of formyl group. The 1373 cm^{-1} band calculated to be at 1378 cm^{-1} (Nos. 38) by HF/6-311G(d,p) and at 1370 cm^{-1} by DFT/B3LYP/6-311G(d,p) methods. Also this band has been observed in infrared spectra at 1420 cm^{-1} [20], 1373 cm^{-1} [21] and 1390 cm^{-1}[22]. The C=O stretching vibration gives rise to a strong band in the range 1815–1680 cm^{-1} [23–25]. The strong band in infrared spectra at 1677 cm^{-1} is attributed to the C=O stretching vibration of the formyl group. This band has been calculated to be at 1813 and 1730 cm^{-1} by HF and DFT respectively. But, the calculated wavenumbers (Nos.47) are moved away from the experimental value. The C=O stretch vibrations observed to be at 1685(vs), 1693 (vs) and 1746(vs) [20-22] respectively. Also the C=O band for 7-Formyl-8-hydroxquinoline molecule has been observed at 1675 cm^{-1} in the infrared spectra [8,26]. The observed formyl group vibrations are in good agreement with the calculated values and literature.

4.2 O-H Vibrations

The O-H stretching vibrations are sensitive to hydrogen bonding. The non-hydrogen bonded or free hydroxyl group absorbed strongly in 3700-3500 cm^{-1}[27]. For solids, liquids and concentrated solutions a broad band of less intensity is normally observed. If present, inter-molecular hydrogen bonding would reduce the O-H stretching band to 3550-3200 cm^{-1} region [28]. The computed wave number for the O–H stretching is at 3692 cm^{-1} (Nos. 54) by HF/6-311G(d,p) and 3460 cm^{-1} by B3LYP/6-311G(d,p) while in the experimental FT-IR spectrum has been observed at 3368 cm^{-1}. The reason for the shift to a low value of the O-H frequency is probably due to the presence of weak intramolecular hydrogen bonding between the O–H and nitrogen atom. The 3368 band for 7-Formyl-8-hydroxquinoline molecule has been observed at 3400 cm^{-1} in the infrared spectra [8]. The O–H in-plane bending vibrations are mixed with C–H stretching vibrations. The O-H in-plane bending vibration is observed in the region

1440- 1260 cm^{-1} [29]. The experimentally observed strong band at 1409 cm^{-1} has been assigned to O–H in-plane bending vibration which shows good agreement with computed wave number at 1409 cm^{-1} (Nos. 40) by HF/6-311G(d,p) and at 1397 cm^{-1} by B3LYP/6-311G(d,p) methods. The O–H out-of-plane bending vibrations appear as broad region around 700–600 cm^{-1}. The weak band observed at 678 cm^{-1} at spectrum is assigned to O–H out-of-plane bending vibration, which shows good correlation with computed wave number at 685 cm^{-1} (Nos.17) by HF/6-311G(d,p) and at 682 cm^{-1} by B3LYP/6-311G(d,p) methods. The very strong band observed at 1162 cm^{-1} which is the C-(OH) stretching band have been calculated at the to be 1154 cm^{-1} by HF/6-311G(d,p) and at 1159 cm^{-1} by B3LYP/6-311G(d,p) methods (Nos.32). Some researchers have assigned the C-(OH) stretching band around 1200 cm^{-1} in substituted benzenes and pyridine molecule [30,31].This C-(OH) stretching band has been observed at 1160 cm^{-1} for 7-Formyl-8-hydroxquinoline molecule in the infrared spectra [8]. The 463 cm^{-1} band can be attributed to the C-(OH) in-plane-bending vibration. The O–H in-plane and out-of-plane, C-(OH) stretching and in-plane-bending vibrations are observed in accordance with a previous report [10].

4.3 C-H Vibrations

Usually, CH stretching vibration at aromatic structures have observed in the 3000-1100 cm^{-1} region [30] as pure vibrations. In the present work, the band observed at 3048 cm^{-1} in the infrared spectrum is assigned to the aromatic CH stretching vibration. The band at 3048 cm^{-1} have been calculated to be at 3042 and 3078 cm^{-1} by HF and DFT(Nos.52), respectively. The C-H in plane bending and out of plane bending vibration generally lies in the 1300-1000 cm^{-1} range and 950-800 cm^{-1} respectively [33-35]. The bands observed at 1260, 1195, 1126 and 1095 cm^{-1} in the spectrum are assigned to the C-H in plane bending mode. The C–H out-of-plane bending vibrations are found at 1070, 826 and 784 cm^{-1}. Theoretically computed frequencies for C–H in-plane and C–H out-of-plane bending vibrations by HF and DFT/B3LYP/6-311G(d, p) methods showed excellent agreement with the recorded spectrum. Except for vibration (Nos.29), all the bending vibrations are in line with the literature.

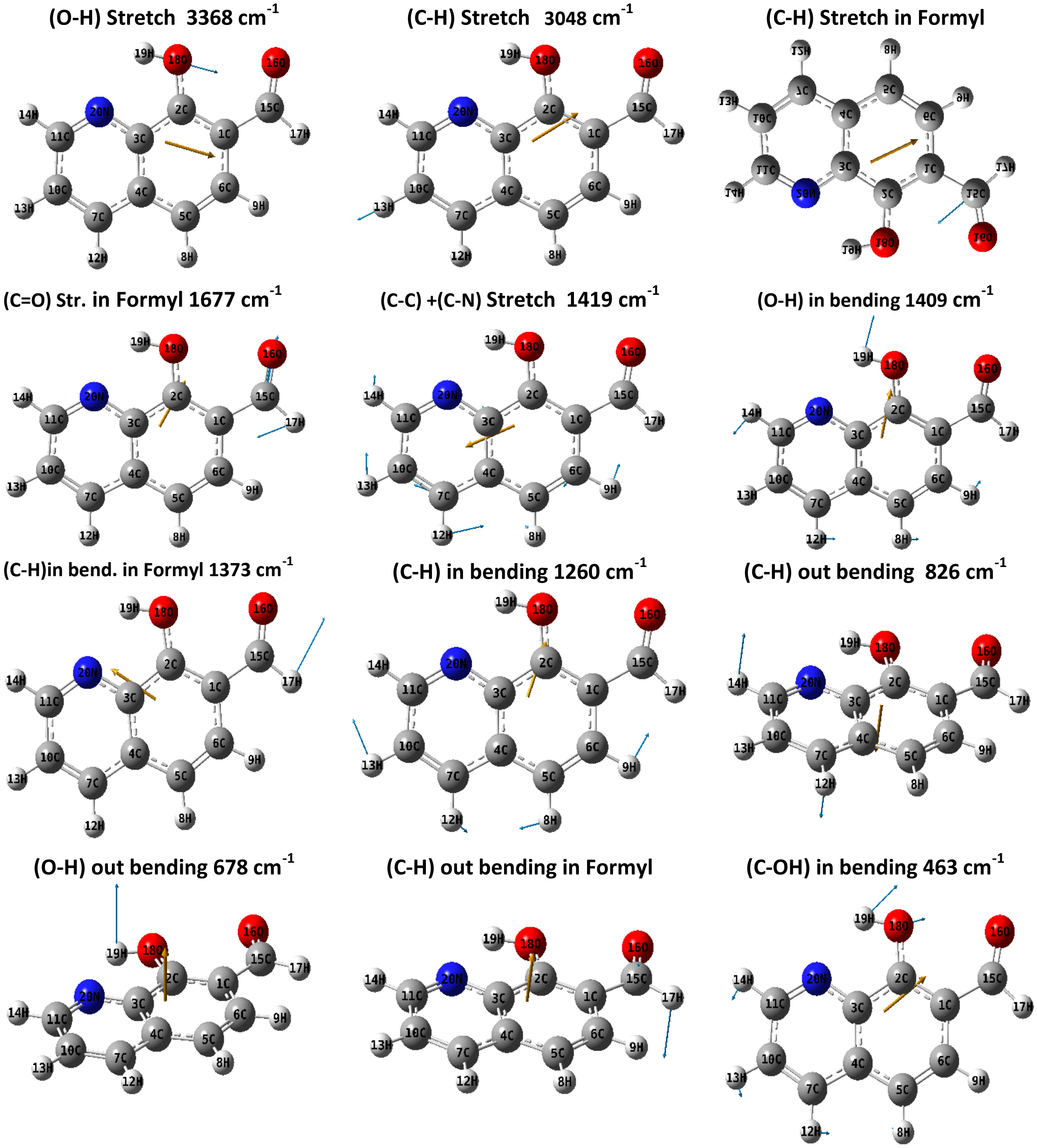
4.4 C-C Vibrations

The carbon–carbon stretching vibrations are very much prominent in the spectrum of pyridine and its derivatives and are highly characteristic of the aromatic ring [36]. In general the bands of C-C stretching vibrations in aromatic compounds appear in the region of 1200 to 1650 cm^{-1} [37]. The bands at 1629 (C=N combination), 1582, 1506, 1471, 1419 and 1270 cm^{-1} in infrared spectra are assigned to C-C stretching vibration. The theoretically computed wave number also present consistent agreement with the experimental observation at 1652, 1636, 1508, 1463, 1440 and 1280 cm^{-1} by HF/6-311G(d,p) and at 1611, 1587, 1488, 1443, 1420 and 1266 cm^{-1} by DFT/B3LYP/6-31G(d,p) methods. As shown in the Table 1, theoretically computed frequencies showed agreement with the recorded experimental spectrum. In the present study, 756, 710 and 639 cm^{-1} in spectrum are assigned to the CCC in plane bending stretching vibrations. The band at 710 cm^{-1} is calculated to be at 686 cm^{-1} (Nos. 18) by HF/6-311G(d,p) and at 695 cm^{-1} by DFT/B3LYP/6-311G(d,p) methods. The 639 cm^{-1} band is calculated to be 599 cm^{-1} (Nos. 18) by HF/6-311G(d,p) and at 668 cm^{-1} by DFT/B3LYP/6-311G(d,p) methods. The medium two bands are assigned to CCC out of plane bending at 595 and 580 cm^{-1}. These bands has been calculated to be at 597(Nos. 15), 581 cm^{-1} (Nos. 14) by HF/6-31G(d,p), 602, 587 cm^{-1} by DFT/B3LYP/6-31G(d,p) methods, respectively. The above results are close agreements with the literature [10,21,38]

4.5 C-N vibrations

The C-N stretching vibrations in side chine are rather difficult task, since there are problems in identifying these frequencies from other vibrations [39]. The C-N stretching vibrations usually lies in the region 1200-1400 cm^{-1} The experimentally observed strong bands at 1629 and 1270 cm^{-1} has been assigned to C=N and C-N stretching vibrations respectively. These bands has been calculated to be at 1652 (Nos. 46), 1280 cm^{-1} (Nos. 36) by HF/6-31G(d,p) and 1611, 1266 cm^{-1} by DFT/B3LYP/6-311G(d,p) methods, respectively. The C=N stretch vibration has been observed at 1625 cm^{-1} for 7-Formyl-8-hydroxquinoline molecule in the infrared spectra [8]. All the vibrations are in line with the literature.

Some significant vibration animasion modes for 7-formyl-8-hydroxyquinoline molecule is shown in Figure 3.


(O-H) Stretch 3368 cm^{-1}

(C-H) Stretch 3048 cm^{-1}

(C-H) Stretch in Formyl

(C=O) Str. in Formyl 1677 cm^{-1}

(C-C) +(C-N) Stretch 1419 cm^{-1}

(O-H) in bending 1409 cm^{-1}

(C-H)in bend. in Formyl 1373 cm^{-1}

(C-H) in bending 1260 cm^{-1}

(C-H) out bending 826 cm^{-1}

(O-H) out bending 678 cm^{-1}

(C-H) out bending in Formyl

(C-OH) in bending 463 cm^{-1}

Figure 3: Some significant vibration modes of the 7-formyl-8-hydroxyquinoline molecule

5 CONCLUSION

Infrared spectra have been obtained for 7-formyl-8-hydroxyquinoline molecule. Also the molecular vibrational frequencies of the fundamental modes of the 7-formyl-8-hydroxyquinoline molecule have been obtained from quantum mechanical calculations. The geometry was optimized at Cs symmetry using the HF and DFT(B3LYP) method with 6-311G(dp) basis set. The theoretical results were compared with the experimental observed vibrational wavenumbers. The infrared absorption and computed intensities provided accurate results, comparable with the experimental data from the literature for similar compounds.

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