Vibrational spectroscopic studies of hydrogen-bonded complexes between 2,5-dihydroxy-P-benzoquinone and amines

Moustafa M. Habib^{a,*}, Hoda A. Al-Wakil^b, Aly El-Dissouky^b and Nesrine M. Refat^b

^a *Chemistry Department, Faculty of Education, Alexandria University, Alexandria, Egypt*

^b *Chemistry Department, Faculty of Science, Alexandria University, Alexandria, Egypt*

Abstract. A series of 1 : 1 hydrogen-bonded complexes between 2,5-dihydroxy-P-benzoquinone (DHBQ) and various nitrogen bases of different strengths were prepared. The FT-IR spectra of the prepared complexes were examined in different regions. It has been found that the protonic and carbonyl vibrations are strongly affected by protonation. The intensity of protonic vibrations was estimated, the base line was corrected by using Perkin-Elmer Paragon 1000 program. A maximum was found at $pK_a = 5.6$ in the correlation between the intensity and pK_a (amines) suggesting a critical behavior. The same value was located as a deep minimum in the correlation between the center of gravity of the protonic vibrations, ν_{cg} cm^{-1} , and the pK_a of the amines confirming the critical behavior in some of the studied complexes. The effect of the contribution of the second OH group to the IR absorption profile was discussed. Finally, the FT-IR spectra of some deuterated complexes were presented and analysed.

1. Introduction

Quinones have been the subject of numerous biological studies [1–3]. They exhibit a variety of redox reactions which are coupled to protonation reaction, this unique behavior is probably the main reason that quinones have been studied for more than 40 years with various techniques [4–6].

Considerable attention has been given to the separation of derivatives for applications in material science, for example, they have been used in the development of artificial photosynthetic systems [7], charge conducting materials [8], electrode coating [9], coating of material surface [10] and opto-electronic device display system [11].

Hydroxybenzoquinones are very important substances especially in pharmacological profiles [12] and as chelating agents [13,14]. However, the data reported on the hydrogen-bonded complexes of hydroxybenzoquinones with various proton acceptors is limited. The spectrophotometric determination and thermodynamic parameters of 1 : 1 proton transfer equilibria between 2,5-dihydroxy-3,6-dichlorobenzoquinone (chloranilic acid) and some amines in 1,4-dioxan were presented [15]. Moreover, the IR, NMR and UV spectra of a series of hydrogen-bonded complexes between chloranilic acid and various amines were reported [16,17]. The X-ray and AMI [18,19] structural studies of 1 : 1 hydrogen-bonded complexes of DHBQ with some pyridines were reported. The packing diagram of the crystal studies was presented. DHBQ is connected on one side through a asymmetric hydrogen bond, 2.72 Å, long to a symmetry-related DHBQ molecule ($\text{OH} \cdots \text{O}$) and on the other side to the nitrogen base ($\text{OH} \cdots \text{N}$).

*Corresponding author.

$$\text{AH} \cdots \text{B} \xrightleftharpoons{K_{\text{PT}}} \text{A}^{-} \cdots \text{HB}^{+} .$$

(AB)
(PT)

More questionable seems to be the interpretation of the IR spectra of hydrogen bonded complexes in the solid state. Therefore it seemed justified to carry out further IR spectra for hydrogen-bonded complexes in the solid state especially on interesting H-bonded molecular complexes between dihydroxy-p-benzoquinone and amines. The integrated intensity for many hydrogen bonded systems were estimated in solution [25] and in polyethylene matrix [26] while its estimation in the solid state is not reported.

The FT-IR spectra are presented in different regions to show the effect of the hydrogen bond formation on the different vibrational modes. Another important aim of this work was the estimation of the integrated intensities (A , $\text{kg mol}^{-1} \text{cm}^{-2}$) and the center of gravity ν_{cg} cm^{-1} of the protonic vibrations. The correlations between ν_{cg} , A and pK_a (amines) will give more informations about the position of the critical point of the studied hydrogen-bonded complexes. An important aim of this work was the discussion of the contribution of the second proton donor group, OH, to the IR absorption profile.

2,5-Dihydroxy-p-benzoquinone, acetonitrile and the amines were of spectroscopic grade. The liquid amines were distilled before using and stored in brown bottles. The crystalline complexes of DHBQ with the different amines were prepared by precipitation from equimolar solution of the components in acetonitrile. The deuterated derivatives were obtained from D₂O solutions at room temperature. The solution of DHBQ in acetonitrile is yellow suggesting the presence of the H₂A form [19]. The composition of the complexes were confirmed by carbon, hydrogen and nitrogen elemental analysis. The analysis provided that 1 : 1 complexes were formed, in Table 1, the elemental analysis and the melting points of the complexes together with the stoichiometry were collected. The FT-IR spectra of the solid complexes were recorded on a Perkin-Elmer Paragon 1000 spectrophotometer with a resolution power 1 cm⁻¹ in KBr pellets. The used KBr was Perkin-Elmer IR spectroscopic grade which was oven dried at 140°C. The KBr pellets thickness was estimated by using a micrometer.

Table 1
Melting points, elemental analysis and stoichiometry of DHBQ complexes with amines

Amine	% Observed			% Calculated			Stoichiometry	m.p.°C
	C	H	N	C	H	N		
2-Cyanopyridine	59.88	3.16	11.74	59.01	3.27	11.47	1:1	164
6-Nitroquinoline	58.1	2.9	9.7	57.32	3.18	8.92	1:1	158
Pyridine	60.01	3.89	5.86	60.27	4.11	6.39	1:1	137
Piperidine	58.77	6.92	6.30	58.66	6.66	6.22	1:1	170
4-Aminopyridine	55.36	4.43	11.95	56.41	4.27	11.96	1:1	147
Morpholine	52.36	6.78	7.14	52.86	5.72	6.16	1:1	168
2,6-Dimethylquinolin	68.11	4.93	4.08	68.69	5.05	4.71	1:1	153
Benzylamine	62.85	4.71	5.11	63.15	5.26	5.67	1:1	160
N-ethylpiperidine	60.98	6.89	4.78	61.66	7.5	5.53	1:1	120
2-Amino-3-methylpyridine	57.27	4.12	10.93	58.06	4.83	11.29	1:1	112
2-Aminopyridine	56.38	3.68	11.33	56.41	4.27	11.96	1:1	82
Ethylenediamine	48.23	4.31	13.21	48.48	5.05	14.14	1:1	210

3. Methods of calculations

The centers of gravity of the protonic vibrations ν_{cg} (cm^{-1}) were computed with a reproducibility of 30 cm^{-1} by using the equation [27]

$$\nu_{cg} = \frac{\sum A\nu}{\sum A} (\text{cm}^{-1})$$

in the range $4000\text{--}400 \text{ cm}^{-1}$, where A is the absorbance and ν is the wave number.

The integrated intensities of the protonic vibrations were computed with a reproducibility of 3% utilizing the equation [25,26]

$$A = \frac{2.3}{dc} \int \log \frac{I_0}{I} d\nu = \frac{2.3}{dc} \times \text{area} (\text{kg mol}^{-1} \text{ cm}^{-2}),$$

where d is the thickness of KBr pellet, c is the molal concentration. The area under the spectral peaks from $4000\text{--}400 \text{ cm}^{-1}$ in the absorbance-wave number scale was computed by using Perkin-Elmer Paragon 1000 program.

4. Results and discussion

The variation of the FT-IR spectra with increasing the pK_a values of the amines is illustrated in Fig. 1. The spectra, to a large extent, resemble those for other systems reported in the literature [28,29]. Figure 1a represents the FT-IR spectrum of DHBQ where a sharp band appears at 3331 cm^{-1} due to OH stretching vibration. Figures 1b, 1c represent the FT-IR spectra of the molecular complexes 2-cyanopyridine-DHBQ and 6-nitroquinoline-DHBQ, the ν_{OH} band broadened and shifted to lower frequencies 2891 and 2459 cm^{-1} , respectively.

Fig. 1. FT-IR spectra of (a) 2,5-dihydroxy-P-benzoquinone and its complexes with (b) 2-cyanopyridine, (c) 6-nitroquinoline, (d) 2,6-dimethylquinoline and (e) piperidine.

Passing through the critical region represented by the complex 2,6-dimethylquinoline-DHBQ, Fig. 1d, quite different spectra can be seen. The most striking feature of these spectra is the broadening of the protonic band, and the hydrogen bonded complexes absorb over almost the entire IR region producing so called “continua” [30].

One can observe in Fig. 1d, the complete disappearance of the IR adsorption above 2000 cm^{-1} , on the other hand, the infrared spectrum reveals strong and broad band between 1800 and 400 cm^{-1} assigned to nearly symmetrical (OHN) hydrogen bond. Spectrum 1e, represents example of the proton transfer complexes, DHBQ-piperidine.

Fig. 2. FT-IR spectra of (a) 2,5-dihydroxy-P-benzoquinone complexes with (a) 2-aminopyridine, (b) 2-amino-3-methylpyridine, (c) 4-aminopyridine, (d) benzylamine and (e) ethylenediamine between 4000 and 400 cm^{-1} .

Where a sharp band appeared at 2998 cm^{-1} due to ν_{NH^+} . One can see a considerable resemblance of ν_{OH} band for DHBQ and ν_{NH^+} band for piperidine complex, they seemed to be mirror images to each other.

It seems interesting to discuss the FT-IR spectra of the hydrogen-bonded complexes between DHBQ and the nitrogen bases including the amino group separately as follows. Theoretical calculations on the electronic structure of aminopyridins [31] showed that protonation is easier at the ring N atom than at the amino N atom. Figure 2 represents the FT-IR spectra of the hydrogen-bonded complexes between

various nitrogen bases including NH_2 group and DHBQ. Figure 2a represents the FT-IR spectrum of 2-aminopyridine–DHBQ complex where the absorption above 2000 cm^{-1} is completely disappeared except from $\nu_{\text{NH}_2}^{\text{as}}$ and $\nu_{\text{NH}_2}^{\text{s}}$ vibrations at 3323 and 3166 cm^{-1} , respectively. One can see in Fig. 2a an excessive broadening of the protonic vibration and Evan's hole at 760 cm^{-1} , consequently the complex between 2-aminopyridine and DHBQ can be considered as a critical one. For 2-amino-3-methylpyridine–DHBQ complex, Fig. 2b, one can observe two absorption peaks at 3470 and 3313 cm^{-1} attributed to $\nu_{\text{NH}_2}^{\text{as}}$ and $\nu_{\text{NH}_2}^{\text{s}}$, the band at 2862 cm^{-1} can be assigned to ν_{NH^+} . Figure 2c represents the spectrum of 4-aminopyridine complex where $\nu_{\text{NH}_2}^{\text{as}}$ and $\nu_{\text{NH}_2}^{\text{s}}$ appeared at 3332 and 3166 cm^{-1} , respectively, the ν_{NH^+} was recorded at 2872 cm^{-1} . In case of benzylamine complex, Fig. 2d, a broad band near 3000 cm^{-1} was recorded which could be assigned to $\nu_{\text{NH}_3^+}^{\text{as}}$ and $\nu_{\text{NH}_3^+}^{\text{s}}$ vibrations overlapping with ν_{CH_2} and ν_{CH} vibrations.

For ethylenediamine complex, Fig. 2e, an absorption peak near 3000 cm^{-1} was recorded attributed to $\nu_{\text{NH}_3^+}^{\text{as}}$ and $\nu_{\text{NH}_3^+}^{\text{s}}$ vibrations through the formation of homoconjugated cation $(\text{NHN})^+$, confirmed by the disappearance of asymmetric and symmetric vibrations of NH_2 group.

It has been found that both the stretching frequencies of the carbonyl and $\text{C}=\text{C}$ groups of DHBQ moiety were affected by the proton transfer process. Hence the FT-IR spectra were examined in the $1700\text{--}1500\text{ cm}^{-1}$ region, the spectra are presented in Fig. 3. Figure 3a represents the FT-IR spectrum of DHBQ, the carbonyl and $\text{C}=\text{C}$ stretching vibration frequencies were found at 1612 and 1647 cm^{-1} , respectively. For the molecular complexes represented by 6-nitroquinoline–DHBQ complex, Fig. 3b, the absorption peaks at 1619 and 1604 cm^{-1} attributed to asymmetric and symmetric stretching vibrations of the carbonyl group while the absorption peak at 1650 cm^{-1} attributed to the stretching vibration frequency of $\text{C}=\text{C}$ group. For the critical region complex 2,6-dimethylquinoline–DHBQ complex, Fig. 3c, the $\nu_{\text{C}=\text{O}}$ was located at 1615 cm^{-1} and $\nu_{\text{C}=\text{C}}$ was located at 1647 cm^{-1} . For the proton transfer complex piperidine–DHBQ complex, Fig. 3d, both $\nu_{\text{C}=\text{O}}$ and $\nu_{\text{C}=\text{C}}$ were shifted to lower frequencies at 1584 and 1633 cm^{-1} , respectively. These results could be interpreted in terms of appreciable conjugation including the hydroxyl, ethylene and carbonyl group of DHBQ. This conjugation was favored by the planarity of the molecule and the lack of a hydrogen atom due to protonation of the ring [18]. Consequently, both $\nu_{\text{C}=\text{C}}$ and $\nu_{\text{C}=\text{O}}$ were shifted to lower frequencies.

It seems important to discuss the contribution of the second OH group ($\text{OH}\cdots\text{O}$) to the infrared absorption profile. This contribution in the stretching vibration region from 3200 to 400 cm^{-1} can be clearly observed in the proton transfer complex of DHBQ with morpholine (Mo). The IR spectra of DHBQ–Mo and DHBQ–Mo-d are shown in Fig. 4. Two proton absorption regions in both spectra are assigned to the $\nu(\text{O}\cdots\text{H}\cdots\text{O})$ [or $\nu(\text{O}\cdots\text{D}\cdots\text{O})$] and $\nu(\text{NH}^+\cdots\text{O}^-)$ [or $\nu(\text{N}^+\cdots\text{O}^-)$] stretching vibrations. The low frequency absorption for DHBQ–Mo is intense with numerous Evan's holes and extends in the range $700\text{--}1500\text{ cm}^{-1}$, for DHBQ–Mo-d this region located between 500 and 1500 cm^{-1} and is characterized by weak intensities. The maximum of this continuum is at 1028 cm^{-1} for DHBQ–Mo while upon deuteration it moves to 860 cm^{-1} . The isotopic ratio $\nu(\text{O}\cdots\text{H}\cdots\text{O})/\nu(\text{O}\cdots\text{D}\cdots\text{O})$ is about 1.2. The high frequency absorption in the $2400\text{--}3150\text{ cm}^{-1}$ shows doublet structure and is centered at 2650 and 2200 cm^{-1} for DHBQ–Mo and DHBQ–Mo-d, respectively. The isotopic ratio $\nu(\text{N}^+\cdots\text{H}\cdots\text{O}^-)/\nu(\text{N}^+\cdots\text{D}\cdots\text{O}^-)$ is equal 1.2. The spectroscopic behavior of these complexes shows ionic character of both adducts and asymmetric proton or deuteron density distribution of hydrogen bonds. The contribution of the second OH group in the protonic deformation region from 1500 to 1000 cm^{-1} was analysed, Fig. 5. The infrared spectrum of DHBQ is shown in Fig. 5a where $\delta_{\text{C}\cdots\text{O}\cdots\text{H}}$ is recorded as a group of bands extending from 1118 to 1327 cm^{-1} [13], the long frequency band at 1379 cm^{-1} is attributed to the ring

Fig. 3. FT-IR spectra of (a) 2,5-dihydroxy-P-benzoquinone and its complexes with (b) 6-nitroquinoline, (c) 2,6-dimethylquinoline and (d) piperidine between 1700 and 1500 cm^{-1} .

vibrational mode. Figure 5b represents the complex of DHBQ with morpholine where δ_{NH}^+ can be recognized at 1100 cm^{-1} . The absorption peak at 1158 cm^{-1} is presumably attributed to δ_{NH} of morpholine. The lower frequency band at 1039 cm^{-1} is attributed to the out-of-plane deformation γ_{OH} . The band at 1240 cm^{-1} can be assigned to $\delta_{\text{C-O}}$ and the two absorption peaks at 1326 and 1399 cm^{-1} can be attributed to δ_{OH} of $(\text{OH} \cdots \text{O})$ hydrogen-bond. This assignment is based on comparison with the deuterated analogue, Fig. 5c. The 1326 and 1399 cm^{-1} bands are shifted to a lower frequency, 1223 cm^{-1} , hence

Fig. 4. FT-IR spectra of (a) DHBQ-Mo and (b) DHBQ-Mo-d between 3200 and 400 cm^{-1} .

they represent δ_{OH} . The 1240 cm^{-1} band is shifted to a higher frequency 1258 cm^{-1} , consequently it represents uncoupled $\delta_{\text{C-O}}$ vibration with δ_{OH} . Below 1250 cm^{-1} one can observe an absorption peak at 1102 cm^{-1} attributed to δ_{ND} mode.

It is clearly observed that, even in the case where a continuous absorption occurs, in most systems a band appears on the high frequency side which could be attributed to asymmetric vibrations and contribution of the second OH to the IR profile. It has almost as a rule, a fine structure and is asymmetric so it is difficult to determine the ν_{OH} or ν_{NH} positions. However, the center of gravity of the broad protonic absorption band ν_{cg} cm^{-1} was computed in the range 4000–400 cm^{-1} , the ν_{cg} values were collected in Table 2. The relationship between ν_{cg} and pK_a is represented in Fig. 6 where two branches are obtained. The left hand one represents ν_{OH} and the right hand side branch represents ν_{NH^+} . A deep minimum was recorded at $\text{pK}_a \cong 5.6$ which could be assigned to the critical behavior. The scattering of some experimental points was probably due to the packing effect, where different packing of the molecules in different complexes could affect the bridge polarization.

The integrated intensity A , $\text{kg mol}^{-1} \text{cm}^{-2}$ for the protonic vibration of the studied crystalline complexes was calculated in the range from 4000–400 cm^{-1} . The amines, their pK_a values, the intensity, the area under the absorption peak, the molality and the pellet thickness were gathered in Table 2. The base line was corrected by a very good sample preparation. It is also corrected utilizing Perkin-Elmer Paragon 1000 program. The correction depends on 4 numerical field parameters represent the possible order of flatting and are called slope, bow, skew and wave. These parameters can be represented by the following three linear equations

$$\begin{aligned} \text{Bow} &= -0.1367 \text{ slope} + 0.0308, & R^2 &= 0.0997, \\ \text{Skew} &= -0.6978 \text{ slope} + 0.0141, & R^2 &= 0.01955, \\ \text{Wave} &= -0.0329 \text{ slope} - 0.0904, & R^2 &= 0.047. \end{aligned}$$

Fig. 5. FT-IR spectra of (a) DHBQ, (b) DHBQ-Mo and (c) DHBQ-Mo-d between 1500 and 1000 cm^{-1} .

The correlation between the integrated intensity and pK_a of the amines is shown in Fig. 7. The correlation consists of two straight lines with intersection at ≈ 5.6 . The line at the left-hand side represents H-bonded complexes and the other right hand side represents proton transfer complexes. The maximum at $\text{pK}_a \approx 5.6$ represents the critical point where the proton is nearly equally shared between O and N

Table 2

Gravity center ν_{cg} cm^{-1} , absolute intensity A , area under the curve, molality and thickness of the KBr pellets of the investigated complexes

Amine	pK _a	ν_{cg} cm^{-1}	$10^6 A$ $\text{kg mol}^{-1} \text{cm}^{-2}$	Area	Molality	Thickness (cm)
2-Cyanopyridine	1.39	1668.88	1.34	1669.93	0.0328	0.087
6-Nitroquinoline	2.72	1629.38	3.1	1404.61	0.011	0.089
Pyridine	5.22	1406.98	4.32	2509.89	0.015	0.089
2,6-Dimethylquinoline	5.46	1358.22	5.49	3448.87	0.0168	0.086
2-Aminopyridine	6.86	1372.81	2.13	2191.36	0.026	0.091
2-Amino-3-methylpyridine	7.43	1424.90	1.83	1829.12	0.0255	0.090
Morpholine	8.49	1469.03	2.76	1160.28	0.0102	0.094
4-Aminopyridine	9.11	1483.95	2.31	1151.8	0.0142	0.092
Benzylamine	9.33	1530.21	2.11	1614.59	0.0189	0.093
N-ethylpiperidine	10.45	1573.28	0.68	1156.49	0.042	0.092
Ethylenediamine	10.71	1847.71	1.2	1610	0.033	0.091
Piperidine	11.2	1615.27	0.36	1261.27	0.088	0.089

Fig. 6. Correlation between ν_{cg} and pK_a.

atoms. Consequently, both correlations between ν_{cg} , A and pK_a are concurring together in locating the critical point at 5.6.

It is worth noting that the present correlations between ν_{cg} , A and pK_a of the amines resemble those reported in the literature for carboxylic acids and phenols-amine systems [16,17,32–34].

5. Conclusions

- (1) The FT-IR spectroscopic studies reveal a strong H-bond between DHBQ and the investigated amines.
- (2) The second OH-group of DHBQ (not involved in H-bond with the amines) contributes in the IR absorption profile.

Fig. 7. Correlation between A and pK_a .

- (3) An interesting finding from this work is the base line correction of the IR profile in the solid state leading to an accurate estimation of the integrated intensity.
- (4) It is worth-noting that the critical point corresponding to the maximum at $\text{pK}_a = 5.6$ in the correlation between the integrated intensity and pK_a is in excellent agreement with the position of a deep minimum in the correlation between ν_{cg} and pK_a confirming the possibility of estimating the integrated intensity in crystalline H-bonded systems.

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