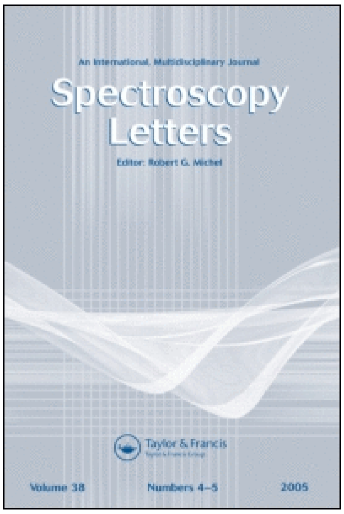

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ELECTRONIC TRANSITIONS OF DI-HYDROXY NAPHTHALENE MOLECULES

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ELECTRONIC TRANSITIONS OF DI-HYDROXY NAPHTHALENE MOLECULES

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ABSTRACT

The electronic transitions of di-hydroxy naphthalene molecules are found to be shifted towards higher wavelength side, when hydroxyl groups are substituted in the naphthalene molecule. The changes in the position and intensity of the electronic bands depend upon the charge transfer property of the substituent. The present paper correlates the electronic transitions observed in the photoacoustic spectra of naphthalene, 1,3-dihydroxy naphthalene (DHN), 1,4-DHN and 1,5-DHN in the region 250–400 nm. The electronic transitions of these molecules have been interpreted using the optimised geometries and CNDO/S-CI methods. Assignments of the observed electronic transitions are made on the basis of radiative and non-radiative transitions. A good agreement is found between the experimental and calculated results.

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Key Words: Photoacoustic spectroscopy; Di-hydroxy naphthalene; Electronic transitions; CNDO calculations; Polycyclic aromatic hydrocarbons

INTRODUCTION

Hydroxyl substituted naphthalene are of wide interest to physicists, chemists, biologists and industrialists equally. In fact, the complex mixtures of substituted polycyclic aromatic hydrocarbons (PAHs), some of which are carcinogenic or mutagenic, from an important class of molecules for experimental and theoretical studies. These are found in treated and untreated water[1], plant tissues[2], coal-derived samples[3] and other fossil fuels. Moreover, they are used as food-grade and antioxidants in foodstuffs[4], oil and oil additives[5], and in plastics[6]. Naphthols, in particular, are used in pharmaceuticals and in the synthesis of some laser dyes[7]. These substituted aromatics and their radical cations are highly fluorescent, a property attributed to π-electron excitation. The spectroscopic study of these compounds is helpful in understanding the intramolecular and intermolecular charge transfer processes, molecular structures, identification of analytes at trace concentration levels, and in the study of interactions of molecules with their environment etc.

Electronic absorption spectra of monohydroxyl-derivatives of naphthalene have been studied both experimentally as well as theoretically by several workers[8–19]. Daglish[20] and Hercules et al.[21] have reported the absorption spectra of hydroxyl-substituted naphthalenes in the region 220–400 nm. Fujii et al.[22] have reported the electronic absorption spectra of four dihydroxyl-naphthalenes, 1,4-, 1,8-, 2,3- and 2,7- with C_{2v} symmetry in isoctane solution from 190 nm to 400 nm region at room temperature. The photoelectron (PE) spectra of hydroxyl-substituted naphthalene are rare; only 1- and 2-naphthols appear to have been studied by Utsunomiya et al.[15] in the region 6 to 20 eV.

The fluorescence spectra of mono and few dihydroxyl-naphthalenes have also been reported by Hercules et al.[21]. Suzuki et al.[23] have studied the temperature dependence of the fluorescence and polarization spectrum of 1-naphthol in a glycerin solution. The room temperature phosphorescence (RTP) and fluorescence (RTF) of hydroxyl-substituted aromatics adsorbed on solid surface have been studied by Dalterio et al.[24–25] and Bello et al.[26].

Recently, we have studied mono-hydroxyl substituted naphthalene molecules by photoacoustic (PA) spectroscopy[27–29]. The PA spectra of naphthalene and naphthols in boric acid glass have been successfully explained and interpreted by CNDO/S-CI molecular orbital method in the region 250–400 nm[30–31]. Additional bands in the PA spectra of naphthalene and naphthols are attributed to non-radiative transitions. Also the radiative as well as non-radiative transitions of naphthols are found to be shifted towards the higher wavelength region when compared with the parent molecule i.e., naphthalene molecule.

In the present paper, we are reporting the photoacoustic and optical absorption spectra of 1,3-DHN, l,4-DHN and 1,5-DHN molecules in boric acid glass in the region 250–400 nm. The PA spectra of obtained experimentally have been interpreted on the basis of CNDO/S-CI molecular orbital calculations [20–21] and compared with the naphthalene molecule.

EXPERIMENTAL

Dihydroxy naphthalene molecules were obtained from M/S Fluka AG (Switzerland) and boric acid crystals of AR grade was obtained from M/S Glaxo Laboratories Ltd. (India). The boric acid glass doped with these naphthols was prepared by the method described elsewhere[32].

The experimental set-up of PA spectrophotometer used for these studies was developed at National Physical Laboratory, New Delhi[33]. The PA spectrophotometer used here has a Jarrell-Ash monochromator having a linear dispersion of 1.65 nm/mm. The radiation from 1000-watt xenon arc lamp is modulated at 40 Hz by a variable frequency mechanical chopper. The modulated radiation after passing through proper optics uniformly irradiates sample and the carbon black (used as reference) placed in two acoustically sealed cylindrical stainless steel cells. Two lock-in amplifiers using the time constant of 10 seconds amplify the signals obtained from the microphones. The ratio of these two signals is a normalised spectrum and is recorded on a X-Y recorder. The schematic representation of the experimental set-up is given elsewhere[34].

The optical absorption spectra were recorded on JASCO UV-VIS-NIR spectrophotometer (Model V-570).

RESULTS AND DISCUSSION

The electronic transitions of 1,3-DHN and 1,4-DHN in the region 250–400 nm are studied by different workers[20,35–38] and found two radiative transitions in this region. Baharvand et al.[37] have studied the electronic absorption spectra of 1,3-DHN and 1,4-DHN. They have studied the effect of temperature dependence on the fluorescence characteristics of these molecules[38]. They have also studied the solvent effect on naphthalene and its derivatives, exhibiting that the change in solvents produces a very small almost negligible Bathochromic change in the absorption and fluorescence wavelength maxima[39].

The electronic absorption spectrum of 1,5-DHN molecules has been studied by some workers[20,35–36] and is known to consist of two electronic transitions in the region 250–400 nm. Similar to other DHNs, both of these transitions are radiative electronic transitions corresponding to the singlet-singlet energy levels. Ashok K. Sharma et al. have studied the electronic transitions of 1,5-DHN and its radical cation. They compared the experimental results with the theoretical calculations using the Longuet-Higgins-Pople (LHP) and Wasilewski type open shell SCF-MO calculations and photoelectron spectral data of molecules[40–43].

However, no one has reported about non-radiative transitions. Here, we are describing the PA spectra of 1,3-DHN, 1,4-DHN and 1,5-DHN molecules in boric acid glass alongwith their conventional absorption spectra. The assignments have been made on the basis of CNDO/S-CI calculations.

1,3-DHN

The conventional absorption spectrum of 1,3-DHN molecules in boric acid glass is shown in Fig. 1. It shows two distinct band systems in the region 250–400 nm. The absorption near 285.2 nm is stronger than the band at 326.9 nm.

The PA spectrum of 1,3-DHN molecules in boric acid glass is shown in Fig. 2. The PA spectrum shows additional bands at 378.0 nm and 354.6 nm of modified intensity and shape. Each band consists of well-developed vibrational modes.

The observed optical spectrum of 1,3-DHN in boric acid glass has two electronic transitions at 326.9 nm and at 285.2 nm respectively. The first electronic transition corresponds with the electronic transition of type $(^1A_{1g}\ 6\ ^1B_{3u})$ of naphthalene molecule and may be assigned as of type $(A_1 6 B_1)$ with the transition moment along the long axis of the molecule. The second electronic transition may be due to the allowed $(A_1 6 B_2)$ transition with the transition moment along the short axis of the molecule. This corresponds with the electronic transition of type $(^1A_{1g}\ 6\ ^1B_{2u})$ of naphthalene molecule. These are assigned as radiative transitions corresponding to the singlet-singlet energy levels. However, in PA spectrum, the origins of these transitions are observed at 323.0 nm and at 281.0 nm respectively.

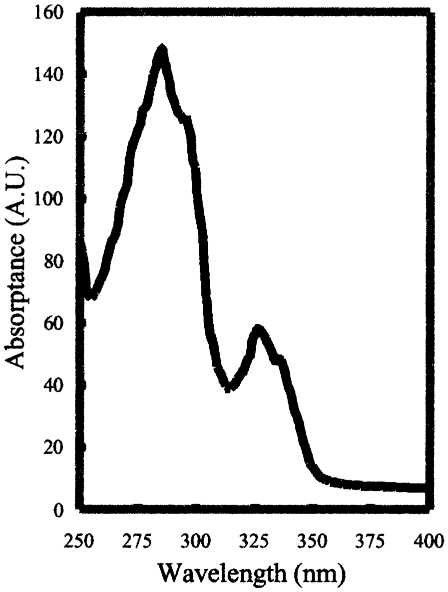

Figure 1. Optical absorption spectrum of 1,3-dihydroxynaphthalene molecule in boric acid glass.

The first radiative transition which is observed with its origin at 323.0 nm in PA spectrum of 1,3 DHN in boric acid glass, has three vibrational bands. The first band at 313.8 nm shows a difference of 910 cm^{-1} from its origin may be assigned to $v_7(b_{1g})$ (C-H in-plane bending). The second band at 310.4 nm, which is at a distance of 1256 cm^{-1} from the origin, is attributed to the OH in-plane deformation[44]. The other band at 306.7 nm showing a difference of 1640 cm^{-1} from its origin, may be due to the combination of $v_8(a_g)$ (C-H out of plane bending) and $v_7(b_{1g})$.

The second radiative transition observed at 281.0 nm in the PA spectrum has two vibrational modes. The band at 274.0 nm, which is at a distance of 907 cm^{-1} from the origin, can be due to $v_7(b_{1g})$ vibrational mode. The next band observed at 268.6 nm, showing a difference of 1640 cm^{-1} is attributed to the combination of $v_8(a_g)$ and $v_7(b_{1g})$.

In PA spectrum of 1,3-DHN, two additional transitions towards the longer wavelength side are observed at 378.0 nm and at 354.6 nm. These may be attributed to non-radiative transitions. The CNDO/S-CI calculations also justify these two additional bands as due to the singlet-triplet (S-T) absorption (lowest energy triplet level). In Table 1, these transitions are denoted as non-radiative transitions.

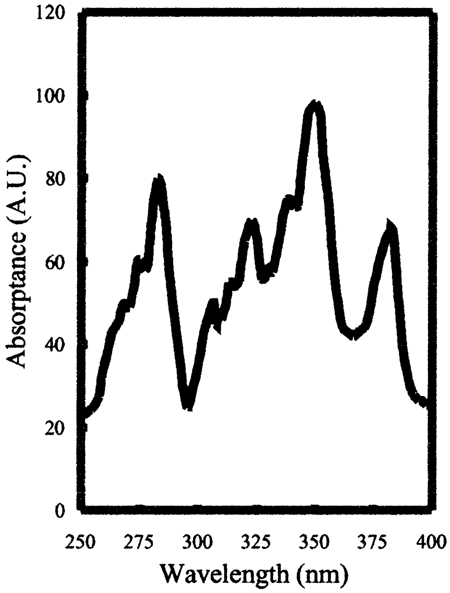

Figure 2. Photoacoustic spectrum of 1,3-dihydroxynaphthalene molecule in boric acid glass.

The first non-radiative transition, which has its origin at 381.0 nm, has no vibrational band attached to it. The origin of second non-radiative transition observed at 354.6 nm, shows two vibrational bands. The first band at 339.5 nm, having a difference of 1256 cm^{-1} may be assigned to OH in-plane deformation. The second band at 329.5 nm showing a difference of 2166 cm^{-1} from its origin is attributed to the combination of $v_7(b_{1g})$ and OH in-plane deformation.

The results obtained by experimental and by CNDO/S-CI molecular orbital calculations are given in Table 1. A good agreement is observed between the experimental and calculated results.

1,4-DHN

The conventional absorption spectrum of 1,4-DHN molecules in boric acid glass is shown in Fig. 3. It shows two distinct band systems in the region 250–400 nm. The absorption at 288.0 nm is stronger than the band at 328.8 nm.

Table 1. Assignments of the Observed Bands in PA and Optical Spectra of 1, 3-DHN in Boric Acid Glass

Transition No.	Calculated Transition Energy (nm)	Observed Maxima Optical (nm)	Observed Maxima PAS (nm)	Observed Maxima PAS (cm^{-1})	Shift from Electronic Origin (cm^{-1})	Assignments
I	**381.0** (S–T)	—	**378.0**	**26,455**	**0**	**Non-radiative**
II	**359.2**	—	**354.6**	**28,200**	**0**	**Non-radiative**
			339.5	29,456	1256	0+1256
			329.5	30,366	2166	0+910+1256
III	**321.2** (0.0479)*	**326.9**	**323.0**	**30,959**	**0**	**Radiative**
			313.8	31,869	910	0+910
			310.4	32,215	1256	0+1256
			306.7	32,599	1640	0+733+907
IV	**281.7** (0.1934)*	**285.2**	**281.0**	**35,587**	**0**	**Radiative**
			274.0	36,494	907	0+907
			268.6	37,227	1640	0+733+907

*The number in parenthesis indicate oscillator strength.

The PA spectrum of 1,4-DHN molecules in boric acid glass is shown in Fig. 4. The PA spectrum shows one additional band at 393.2 nm with modified intensity and shape. Each band consists of a well-developed vibrational mode.

The observed optical absorption spectrum of 1,4 DHN in boric acid glass shows two radiative transitions having their origins at 328.8 nm and at 288.0 nm respectively. The first electronic transition may be due to the allowed ($A_1 6 B_1$) transition with the transition moment along the long axis of the molecule. This corresponds with the electronic transition of type ($^1A_{1g}$ 6 $^1B_{3u}$) of naphthalene molecule. The second electronic transition of 1,4-DHN corresponds with the electronic transition of type ($^1A_{1g}$ 6 $^1B_{2u}$) of naphthalene molecule. This may be assigned as of type ($A_1 6 B_2$) with the transition moment along the short axis of the molecule. Both these transitions are also observed in the PA spectrum with their origins at 324.6 nm and at 288.4 nm respectively. The variation in the positions of above transitions between optical and PA spectrum are due to the time constants used in the lock-in amplifiers.

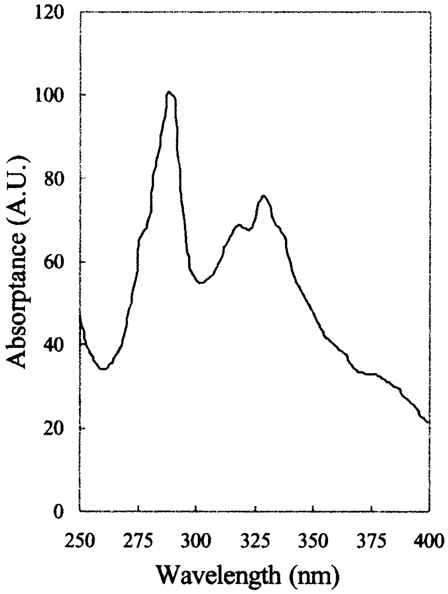

Figure 3. Optical absorption spectrum of 1,4-dihydroxynaphthalene molecule in boric acid glass.

In the PA spectrum, the band at a distance of 1256 cm^{-1} attached with the origin of the first transition at 324.6 nm, is due to OH in-plane deformation. The other band at 308.2 nm, at a difference of 1640 cm^{-1} from the origin, may be due to the combination of $v_8(a_g)$ (C-H out of plane bending) and $v_7(b_{1g})$ (C-H in-plane bending). The third band at 300.1 nm, having a frequency difference of 2510 cm^{-1} from the origin is attributed to the second overtone of OH in-plane deformation[44].

The second radiative transition with its origin at 288.4 nm shows three vibrational modes. The first band observed at 281.0 nm and having a difference of 907 cm^{-1} from the origin is assigned as $v_7(b_{1g})$. The second band at 278.3 nm shows a distance of 1256 cm^{-1} from the origin, may be due to the OH in-plane deformation. The third band at 271.4 nm, at a difference of 2166 cm^{-1} can be assigned as the combination of $v_7(b_{1g})$ and OH in-plane deformation.

The CNDO/S-CI calculations and the structure of observed bands suggest that an additional band observed at 393.2 nm may be due to the nonradiative electronic transition. This is attributed to singlet-triplet absorption (lowest energy triplet level).

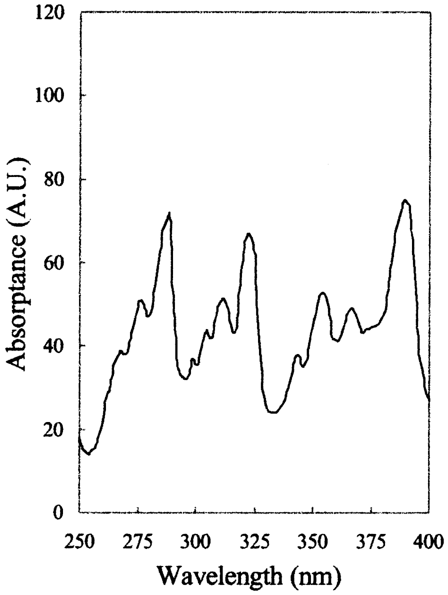

Figure 4. Photoacoustic spectrum of 1,4-dihydroxynaphthalene molecule in boric acid glass.

The first band at 369.4 nm attached to this non-radiative electronic transition, shows a difference of 1640 cm^{-1} from the origin. It may be attributed to the combination of $v_8(a_g)$ and $v_7(b_{1g})$. The second band at 357.3 nm, at a difference of 2556 cm^{-1} from the origin, may be due to the combination of $v_8(a_g)$ and second overtone of $v_7(b_{1g})$. The third band at 346.1 nm, which is at a distance of 3460 cm^{-1} from the origin, may be assigned as the combination of second overtone of $v_8(b_{1g})$, $v_8(a_g)$ and second overtone of $v_7(b_{1g})$.

Table 2 provides assignments of the observed bands in the PA spectrum of 1,4-DHN. A close agreement between the results obtained by experiment and CNDO/S-CI molecular orbital calculations, has been observed.

1,5-DHN

The conventional absorption spectrum of 1,5-DHN molecules in boric acid glass is shown in Fig. 5. It shows two distinct band systems in the region 250–400 nm. The absorption at 289.0 nm is stronger than the band at 332.5 nm.

Table 2. Assignments of the Observed Bands in PA and Optical Spectra of 1, 4-DHN in Boric Acid Glass

		Observed Maxima				
			PAS			
Transition No.	Calculated Transition Energy (nm)	Optical (nm)	(nm)	(cm^{-1})	Shift from Electronic Origin (cm^{-1})	Assignments
I	**400.5** (S–T)	—	**393.2**	**25,432**	**0**	**Non-radiative**
			369.4	27,072	1640	0+733+907
			357.3	27,988	2556	0+736+2 × 910
			346.1	28,892	3460	0+2 × 450+740 +2 × 910
II	**326.1** (0.1048)*	**328.8**	**324.6**	**30,807**	**0**	**Radiative**
			311.9	32,063	1256	0+1256
			308.2	32,447	1640	0+730+910
			300.1	33,317	2510	0+2 × 1256
III	**290.8** (0.2237)*	**288.0**	**288.4**	**34,674**	**0**	**Radiative**
			281.0	35,581	907	0+907
			278.3	35,930	1256	0+1256
			271.4	36,840	2166	0+910+1256

*The number in parenthesis indicate oscillator strength.

The PA spectrum of 1,5-DHN molecules in boric acid glass is shown in Fig. 6. The PA spectrum shows one additional band at 396.6 nm with modified intensity and shape. Each band consists of well-developed vibrational modes.

In the conventional optical absorption spectrum, the two electronic transitions are observed at 332.5 nm and at 289.0 nm respectively. The first electronic transition may be due to the allowed ($A_g 6 B_u$) transition with the transition moment along the longer molecular axis. This corresponds with the electronic transition of type ($^1A_{1g}$ 6 $^1B_{3u}$) of naphthalene molecule. The second electronic transition of 1,5-DHN corresponds with the electronic transition of type ($^1A_{1g}$ 6 $^1B_{2u}$) of naphthalene molecule. This may be assigned as of type ($A_1 6 B_2$) with the transition moment along the shorter molecular axis. These transitions are also observed in the PA spectrum of 1,5-DHN at 329.2 nm and at 291.0 nm respectively. The variation in the positions in these

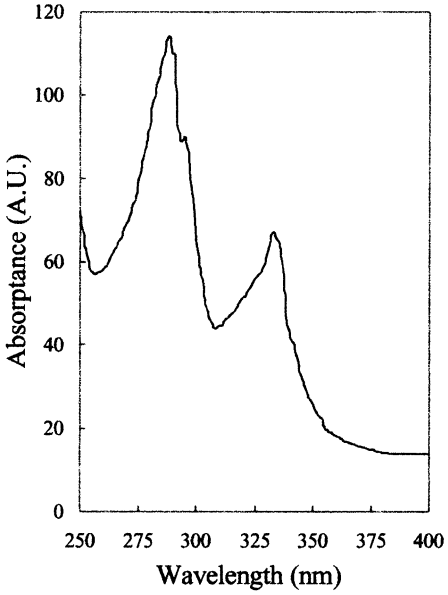

Figure 5. Optical absorption spectrum of 1,5-dihydroxynaphthalene molecule in boric acid glass.

transitions may be due to the time constants used in the lock-in amplifiers.

The electronic transition observed at 329.2 nm shows three vibration bands. The first band observed at 319.6 nm, showing a shift of 907 cm^{-1} from the origin, may be attributed to $v_7(b_{1g})$ (C-H in-plane bending). The other band at 316.1 nm having a difference of 1256 cm^{-1} from the origin, may be due to OH in-plane deformation. The third band at 308.3 nm which is at a distance of 2063 cm^{-1} from the origin, may be assigned as the combination of $v_8(b_{1g})$ (sketal motion of molecule, out of plane bending), $v_8(a_g)$ (C-H out of plane bending) and $v_7(b_{1g})$.

The second radiative transition with its origin at 291.0 nm has three vibrational modes. The first band at 287.3 nm, at a distance of 445 cm^{-1} from the origin is attributed to $v_8(b_{1g})$. The second band at 277.7 nm having a difference of 1640 cm^{-1} from the origin may be due to the combination of $v_8(a_g)$ and $v_7(b_{1g})$. The third band at 271.2 nm showing a shift of 2510 cm^{-1} from the origin may be assigned as the second overtone of OH in plane deformation.

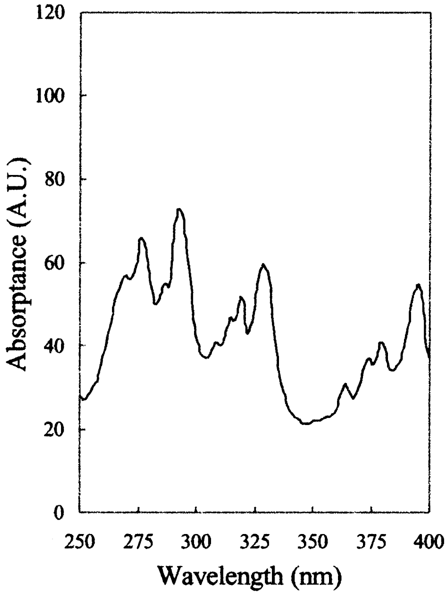

Figure 6. Photoacoustic spectrum of 1,5-dihydroxynaphthalene molecule in boric acid glass.

In the PA spectrum, an additional band at 396.6 nm towards the longer wavelength side is observed. On the basis of CNDO/S-CI calculations, it could be explained as due to the singlet-triplet (S-T) absorption (lowest energy triplet level). This is assigned as non-radiative transition as shown in Table 3.

The origin of this non-radiative transition is observed at 396.6 nm and this transition shows three vibrational modes. The band observed at 379.3 nm, shows a shift of 1153 cm^{-1} from its origin. It may be attributed to the combination of $v_8(b_{1g})$ and $v_8(a_g)$. The other band at 372.4 nm which is at a distance of 1640 cm^{-1} from the origin, may be due to the combination of $v_8(a_g)$ and $v_7(b_{1g})$. The third band at 365.3 nm having a difference of 2163 cm^{-1} from the origin may be assigned as the combination of $v_7(b_{1g})$ and OH in plane deformation.

All the assignments alongwith their values are given in Table 3. A good agreement is observed between the experimental results and the results obtained by CNDO/S-CI molecular orbital calculations.

Table 3. Assignments of the Observed Bands in PA and Optical Spectra of 1, 5-DHN in Boric Acid Glass

Transition No.	Calculated Transition Energy (nm)	Observed Maxima			Shift from Electronic Origin (cm^{-1})	Assignments
		Optical (nm)	PAS (nm)	PAS (cm^{-1})		
I	**401.5** (S–T)	—	**396.6**	**25,214**	**0**	**Non-radiative**
			379.3	26,367	1153	0+445+708
			372.4	26,854	1640	0+733+907
			365.3	27,377	2163	0+907+1256
II	**327.6** (0.1181)*	**332.5**	**329.2**	**30,376**	**0**	**Radiative**
			319.6	31,283	907	0+907
			316.1	31,632	1256	0+1256
			308.3	32,439	2063	0+445+708+910
III	**288.2** (0.2561)*	**289.0**	**291.0**	**34,364**	**0**	**Radiative**
			287.3	34,809	445	0+445
			277.7	36,004	1640	0+733+907
			271.2	36,874	2510	0+2 × 1255

*The number in parenthesis indicate oscillator strength.

Effect of Di-hydroxyl Groups on the PA Spectrum of Naphthalene Molecule

The assignments of observed electronic transitions in the PA spectra of 1,3-DHN, 1,4-DHN and 1,5-DHN molecules in boric acid glass recorded at room temperature are diagramatically shown in Fig. 7.

The PA spectra of 1,3-DHN, 1,4-DHN and 1,5-DHN molecules are shifted towards the higher wavelength region, as compared with naphthalene molecule as well as with 1-naphthol and 2-naphthol. This is because of the fact that the introduction of second OH increases charge density at the substituted ring of naphthalene nucleus. Due to increase in charge density, the dipole moments of these DHNs are more as compared to 1-naphthol and 2-naphthol. The increases in the dipole moment of these DHNs are due to the presence of intra-molecular hydrogen bonding in these molecules, which increase their polarization[45–46]. These arguments are supported by our calculated value of transition energies for these molecules. However, we

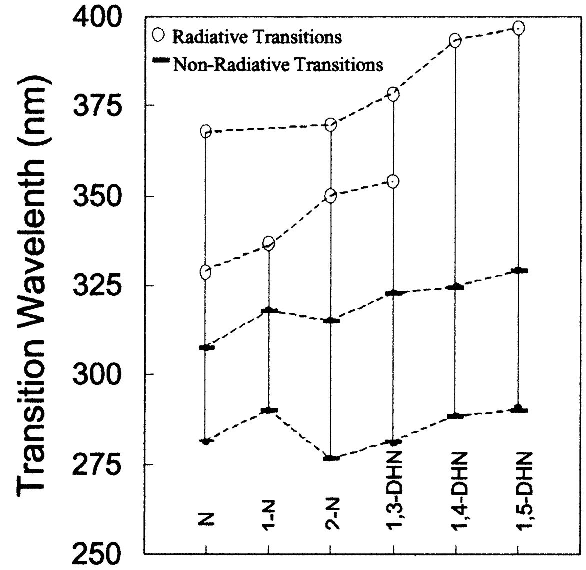

Figure 7. Correlation diagram for electronic transition observed in PA spectra of Naphthalene (N), 1-Naphthol (1-N), 2-Naphthol (2-N), 1,3-DHN, 1,4-DHN, and 1,5-DHN.

could observe only one non-radiative transition in 1,4-DHN and 1,5-DHN molecules.

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