

# ELECTRONIC SPECTRA AND SOLVENT EFFECT OF 5-BROMO-2-3-DIHYDROXY PYRIDINE

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## ABSTRACT

*The ultraviolet spectra of 5-bromo-2-3-dihydroxy pyridine have been reported. The ultraviolet absorption spectra of this molecule have been recorded in various solvents in the region 1900-4000 Å<sup>0</sup>. The electronic transition viz  $n-\pi^*$ ,  $\pi-\pi^*$  and  $n-\sigma^*$  have also been discussed along with red and blue shift.*

## I INTRODUCTION

The aromatic compounds like benzene like benzaldehyde, pyridine, pyrimidine, uracil, cytosine and their derivatives are of great biological importance as they play an important role in the structure and properties of nucleic acid [1-2]. However due to their great complexity and low symmetry only a little spectral studied by some workers [3-4]. The vibrational spectra of di-substituted pyridines have also been studied [5], but very little work appears on the IR spectra of tri-substituted pyridines [6]. Further when the N-heterocyclic molecules have some substituent like -OH, -SH and -NH<sub>2</sub>, They may cause tautomerism. Tripathi et al [7] have studied the vibrational and electronic spectra of some substituted pyridine. Some workers [8-10] have also studied the electronic spectra of pyridines and substituted pyridines. In view of these the present paper the ultraviolet absorption spectra of 5-bromo-2-3-dihydroxy pyridine.

## II EXPERIMENTAL

Specpure grade chemical 5-bromo-2,3-dihydroxy pyridine was obtained from M/S Aldrich Chemise, West Germany and used as such. This chemical here-after referred as 5,2,3-BDHP. The purity of the said compound was also confirmed by elemental analysis and melting point determination. The ultraviolet absorption spectra were recorded in various solvents used were of spectroscopic grade. All the solvents used were of spectroscopes grade. The ultraviolet

spectra of the said compound in vapour phase could not be recorded even under the best experimental conditions because of very high melting point of the compound.

### III RESULT AND DISCUSSION

The structural formula of the compound 5,2,3-BDHP is given in Figure 1. The analysis of observed UV bands in different solvents is given in Table 1. The UV spectra of 5,2,3-BDHP in different solvents are given in Figure 2.

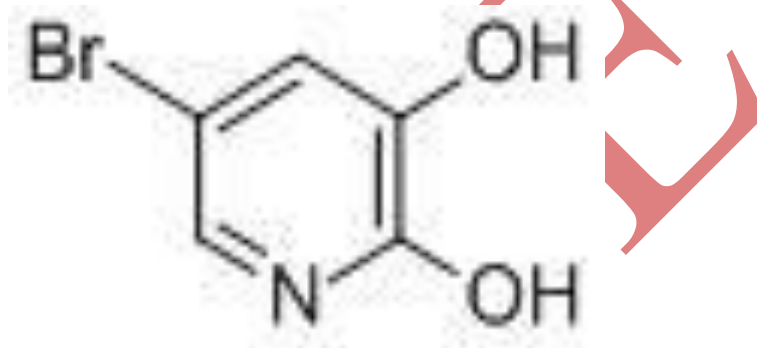


Figure: 1 Molecular Structure Of 5,2,3-BDHP

### IV ELECTRONIC SPECTRA

In case of N-heterocyclic compounds the bands observed at 238 nm corresponds to  $A_1 \rightarrow B_1$  transition which is derived from  $A_{1g} \rightarrow B_{1u}$  transition. According to Yadav et al [11], the bands observed at 2100 and 2000 Å corresponds to  $A_{1g} \rightarrow B_{1u}$  and  $A_{1g} \rightarrow A_{1u}$  transitions respectively. According to Sanyal et al [12], in pyridines  $n-\pi^*$  transition corresponds to out-of-plane transitions while  $\pi-\pi^*$  and  $\pi-\sigma^*$  transitions to in-plane transitions. In view these assignments, the  $n-\pi^*$  transitions at 2030 Å (water)/2090 Å (methanol)/2100 Å (ethanol) and  $\pi-\pi^*$  transitions at 2430 Å (water)/2480 Å (methanol)/2470 Å (ethanol) in 5,2,3-BDHP have been taken to represent in-plane bending while the  $n-\pi^*$  transition bands around at 3050 Å (water)/3070 Å (methanol)/3060 Å (ethanol) in 5,2,3-BDHP have been taken to represent in-plane transitions.

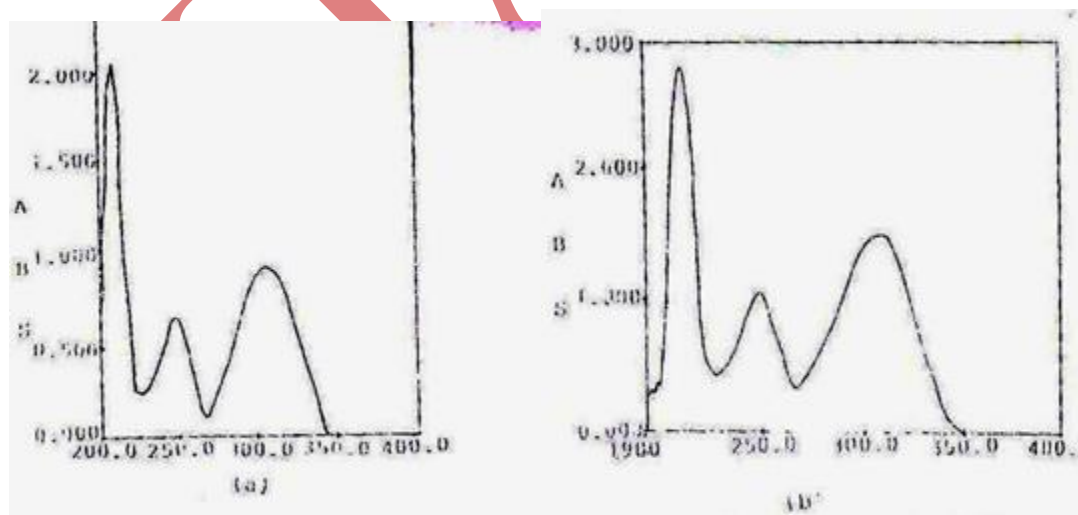
## V SOLVENT EFFECT

Becker et al [13], has suggested the  $\pi-\pi^*$  transitional undergoes a red shift as the polarity of the solvent increases. This is due to the momentary polarization of the solvents by transitions dipole of the solutes [14]. In the present study, in case of  $\pi-\pi^*$  transitions, as the polarity of the solvents increases (ethanol  $\rightarrow$  methanol  $\rightarrow$  water), the red shift has been observed in the said compound (Table 1).

A red shift has also been observed in  $n-\sigma^*$  transitions with the increasing order of polarity of the solvents for the compound which is also clear from Figure 2 and Table. 1 [16].

According to Ram et al [14], the blue shift with increasing polarity of a solvent is the useful means of the recognizing  $n-\pi^*$  transitions. This shift has been observed on changing the solvent in increasing order of polarity. This shift is due to the stabilization of the ground state by hydrogen bonding in ethanol, methanol and water and increase in transition energy which is essential to break or weaken the hydrogen bonding [15-16]. During the present investigation, the  $n-\pi^*$  transition is blue shifted with increasing polarity of the solvents (i.e. ethanol  $\rightarrow$  methanol  $\rightarrow$  water), for 5, 2, 3-BDHP as shown in Table 1 and in Figure 2 respectively.

Furthermore, greater the dielectric constant of the solute, greater will be the degree of solvation [17-18]. Also, as the solvents polarity increases, the attraction between solute and solvent molecules will also increases and hence the system will be more stable. This explains the red shift observed in  $\pi-\pi^*$  and  $\pi-\sigma^*$  transitions in the said molecule (Table 1) on going from methanol  $\rightarrow$  ethanol  $\rightarrow$  water solvent.



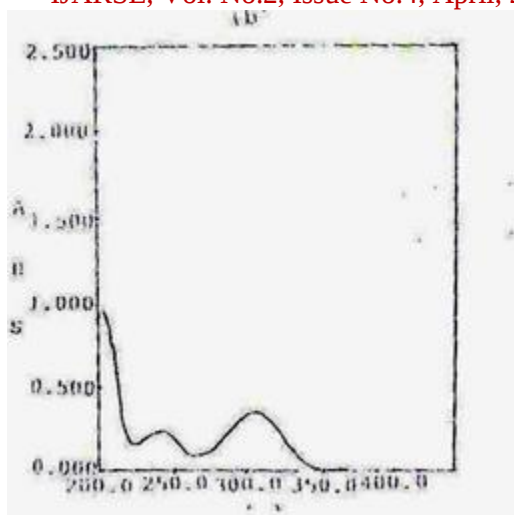


TABLE 1

Solvent Effect on Electronic Transition of 5,2,3-BDHP

(All values are in Å)

| SOLVENT  | DC*  | RI**   | 5,2,3-BDHP |             |              |
|----------|------|--------|------------|-------------|--------------|
|          |      |        | $n-\pi^*$  | $\pi-\pi^*$ | $n-\sigma^*$ |
| Ethanol  | 25.0 | 1.3773 | 3060       | 2470        | 2100         |
| Methanol | 32.0 | 1.3362 | 3070       | 2480        | 2090         |
| Water    | 80.5 | 1.3380 | 3050       | 2430        | 2030         |

Where, \*DC= Dielectric Constant

\*\*R.I.= Refractive Index

**REFERENCES**

- (1) B. S. Yadav, Vipin Kumar and M.K. Yadav, Indian J Pure & Appl Phys, **36** (1998) 557.
- (2) B. S. Yadav, Israt Ali, Padeep Kumar and Preeti Yadav, Indian J Pure & Appl Phys, **45** (2007) 982.
- (3) Rajat M.Issa, Abdalla M. Khedr and Helen Rizk, Journal of Chinese Chemical Society, **55** (2008) 875-884.
- (4) J H. S. Green, W. Kyneston and H.M. Paiseley, Spectrochimica Acta, **19** (1963) 549.
- (5) Vir Singh, Vipin Kumar, M.K. Yadav, B.S. Yadav and Seema, Asian J of Chem., **9(3)** (1997) 411.
- (6) R S Tripathi and B R Pandey, Indian J Pure & Appl Phys, **13** (1975) 416.
- (7) R S Tripathi, Indian J Pure & Appl Phys, **11** (1973) 277.
- (8) N Sundaraganesan, S.Iiakiamani, H. Saleem and S. Mohan, Indian J Pure & Appl Phys, **42** (2004) 588.
- (9) N. Mataga and T. Kuboto, "Molecular and Electronic Spectra", (Marcel Dekker Inc, New York) (1970).
- (10) B S Yadav, M K Singh, Seema and Vir Singh, Oriental J Chem, **14**(1998) 397.
- (11) B.S. Yadav, Vir Singh, Vipin Kumar and M.K. Yadav, Asian. J. Chem., **9 (3)** (1997) 372.
- (12) N.K. Sanyal S.L. Srivastava and R. K. Goel, Indian J Pure & Appl Phys, **16** (1978) 719.
- (13) R.S. Becker, A.B.F., Duncan, F.A. Matsen, D.R. Scott and W. West, "Chemical Applications of Spectroscopy", (John Willey and Sons, New York) (1968).
- (14) K. Ram, B. R. Pandey, and R. S. Tripathi, J. Chem., Phys, **74** (1977) 1250.
- (15) J.N. Murrell, "The Theory of the Electronic Spectra of Organic Molecules", (Chamman and Hall, London) (1971).
- (16) H. Suzuki, "Electronic Absorption Spectra and Geometry of Organic Molecules", (Academic press, New York) (1967).
- (17) I. L. Finer, "Organic Chemistry", (English language Book Soc, UK **I** (1975).
- (18) G. Herzberg, "Molecular spectra and Molecular structure" (Van Nostrand Reinhold Co New York) (1966).