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Full Length Research Paper

Solvent effect on absorption and fluorescence of 1-1` binaphtalene aromatic molecule

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The absorption and fluorescence spectra of 1-1` Binaphthalene (1-1` BN) molecule have been studied at different solution states in polar and non polar solvents at room temperature. It is noticed that the absorption spectrum of this molecule is similar to that of Naphthalene molecule at this temperature. The fluorescence spectrum of 1-1`BN molecule differs from that of the Naphthalene molecule. It is also found that a peak shifted towards shorter wavelength in the fluorescence spectrum when the solvent is changed. This is due to the polarity of the polar solvent.

Key words: Absorption spectra, fluorescence spectra, aromatic molecule, Solvent effect.

INTRODUCTION

The aromatic molecule 1-1` Binaphthalene (1-1`BN) has two different distributions (Cis and Trans) as shown in Figure 1. Because of the Cis and Trans distributions in this molecule, its potential curve of the ground state has one minimum value while it has two minima in the excited state (Figure 2). This is because of the two states of the two halves of the molecule when they differ in the energy in the excited state. It had been studied by many researchers in different features (Hochstrasser, 1961; Pauptit and Trotter, 1983; Post et al., 1975). Nakamura et al. (1995) prepared this molecule because of its importance ant its derivatives.

Also, its derivatives are very important. Martinborough et al. (2004) investigated the chiral 1,1-Binaphthyl molecular clefts for the complexation of excitatory amino-acid derivatives. The importance of this molecule by coupling the features of binaphthalene and anthracene, new binaphthalenes with two anthracene switches. A strong CD signal with negative sign due to the interchromophoric exciton coupling was observed. Photodimerization of two anthracene moieties in these binaphthalene molecules can occur. Therefore, chiral molecular switches based on new binaphthalenes with two anthracene moieties were achieved (Martinborough et al., 2004). Tuning the CD spectrum and optical rotation value of a new binaphthalene molecule with two spiropyran units: mimicking the function of a molecular “AND” logic gate and a new chiral molecular switch had been achieved by Zhou et al. (2005).

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EXPERIMENTAL DETAILS

1-1'BN material purified to less than 10^{-7} mole/mole and spectra grade solvents were used. The solvents were cyclohexane, ethanol with concentrations indicated in the figures of absorption and fluorescence spectra of these molecules.

Quartz cells of 1 × 1 × 5 cm in dimensions were used for solution. The used solutions were diluted in order to avoid the self-absorption. The crystal of this molecule was grown on a quartz disc by evaporation technique.

A Pye Unicam Sp800-UV photo spectrometer was used for absorption measurements. Fluorescence spectra measurements involves two parts, the excitation and fluorescence measurements. A xenon lamp (150 watt) and excitation spectrometer (Jarrel Ash 82-410, 0.05) with two gratings 1180 line/mm blazed at 300 nm and the second grating is with 2360 line/mm blazed at 500 nm. For fluorescence spectral measurement G. Zerny-Turner spectroscopy/ spectrograph and EMI 9635 QB photomultiplier (PM) were used

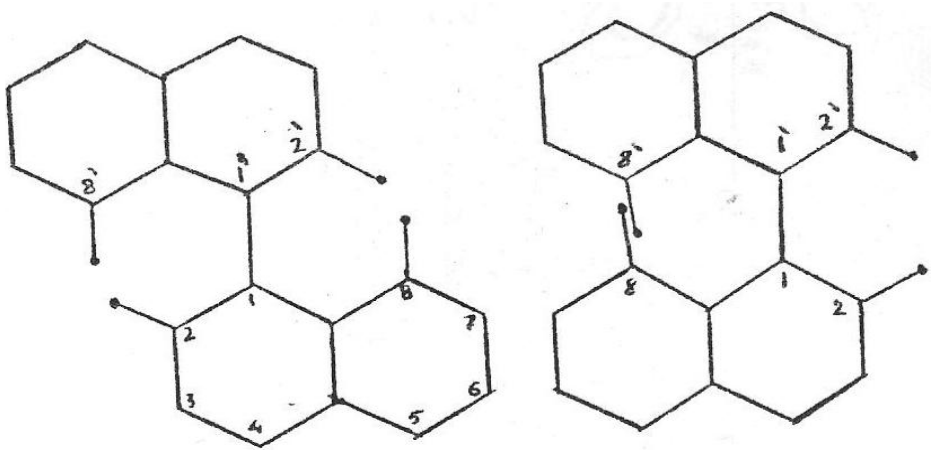

Figure 1. Arrangement of the two rings in 1-1' Binaphthalene (a) Trans distribution, (b) Cis distribution.

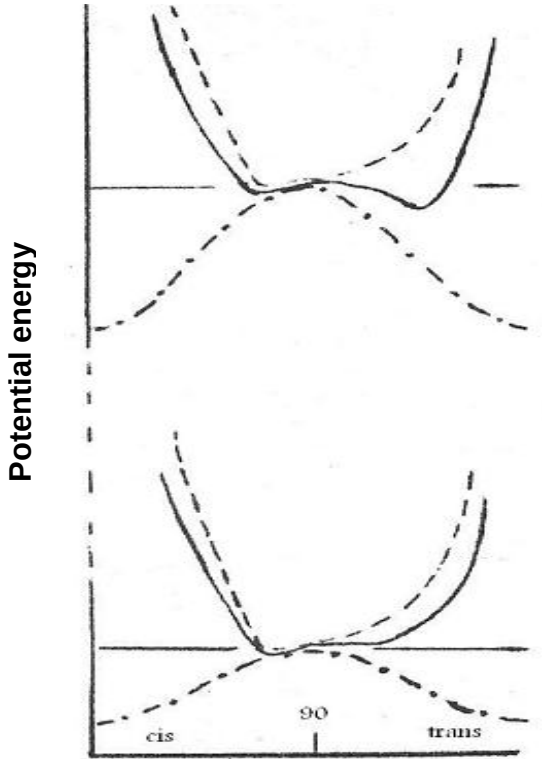

Figure 2. Potential curve of BN molecule.

to measure the fluorescence spectra.

RESULTS

The absorption spectra of 1-1`BN molecule dissolved in ethanol as a polar solvent and in cyclohexane as a non polar solvent at a concentration of 2.9×10^{-5} - 10^{-5} M were measured at room temperature. There was a resemblance in the shape of absorption spectra of this molecule in ethanol (Figure 3), and in cyclohexane (Figure 4). These absorption spectra were compared with the absorption spectra of naphthalene molecule dissolved in ethanol (Hochstrasser, 1961) and cyclohexane (Berlman, 1971). It is seen that there is a remarkable similarity between these absorption spectra with a little blue shift in the absorption spectra of the 1-1`BN molecule dissolved in the above solvents. The wavelength for the 0-0 band of naphthalene dissolved in ethanol and cyclohexane is 315.5 nm while the wavelength of the 0-0 band in 1-1BN molecule in the same solvents is 292 nm.

Fluorescence spectra of 1-1`BN molecule dissolved in different solvents at the temperature were measured (Figures 5 and 6). It is seen that they are different from that of naphthalene molecule in cyclohexane (Berlman, 1971). For 1-1'BN dissolved in ethanol at temperatures 298°K. The fluorescence spectrum starts at wavelength 320 nm and the peak is at 370 nm. In the case of dissolving the molecule in cyclohexane, the spectrum starts at the same wavelength mentioned above and the peak starts to shift toward the shorter wavelength (Blue shift) where the peak at 298°K is at the wave length 354 nm. The values of 0-0 band wave number in the absorption spectrum of 1-1`BNmolecule in cyclohexane and ethanol are identical but different from the results

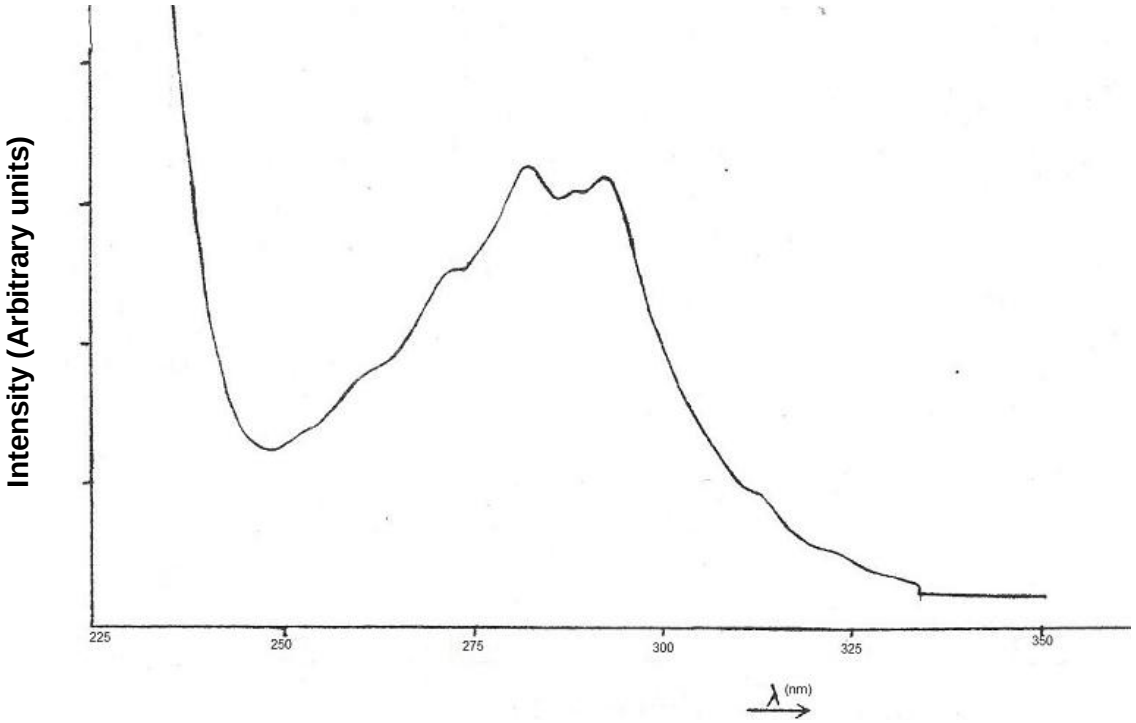

Figure 3. The absorption spectrum of BN solution in Ethanol.

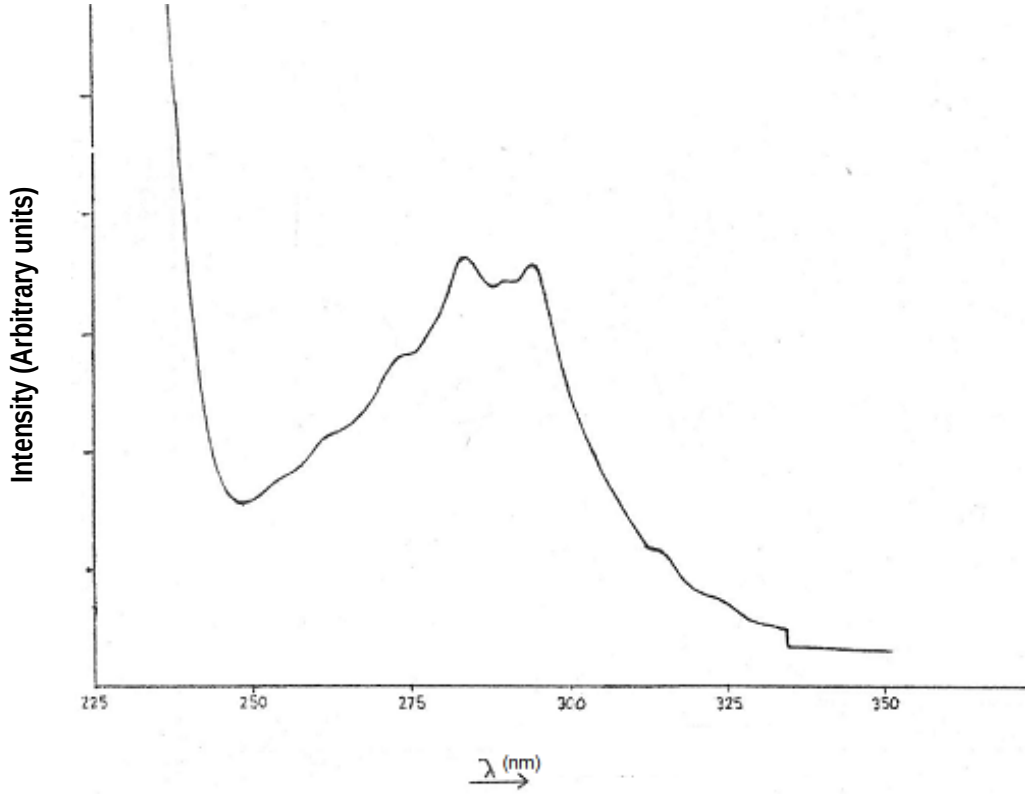

Figure 4. The absorption spectrum of BN solution in Cyclohexane.

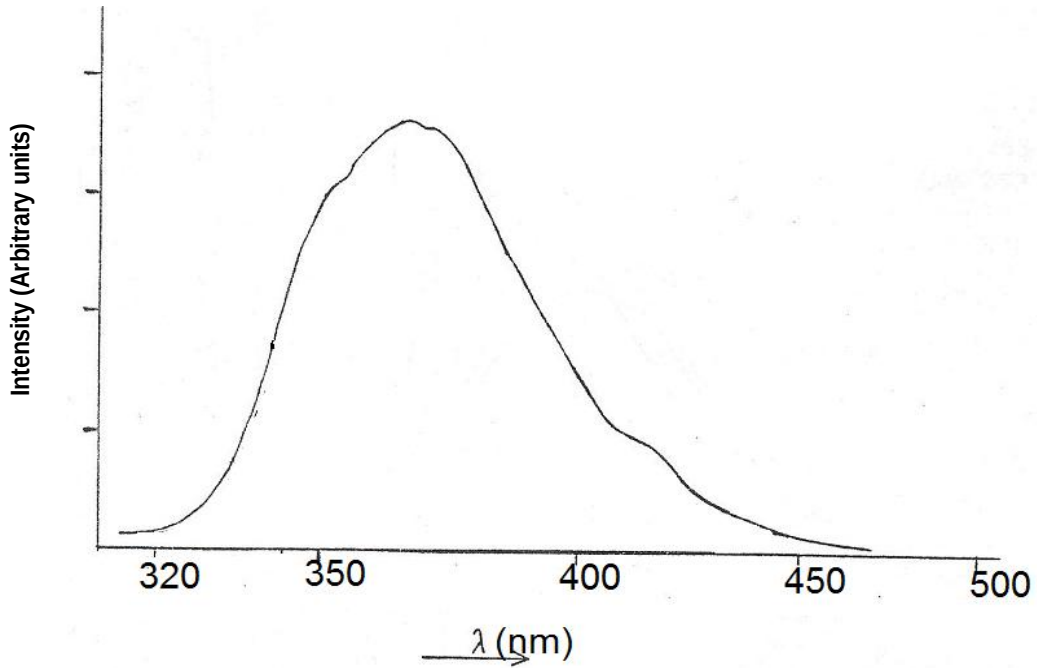

Figure 5. The fluorescence spectrum of BN solution in ethanol at room temperature.

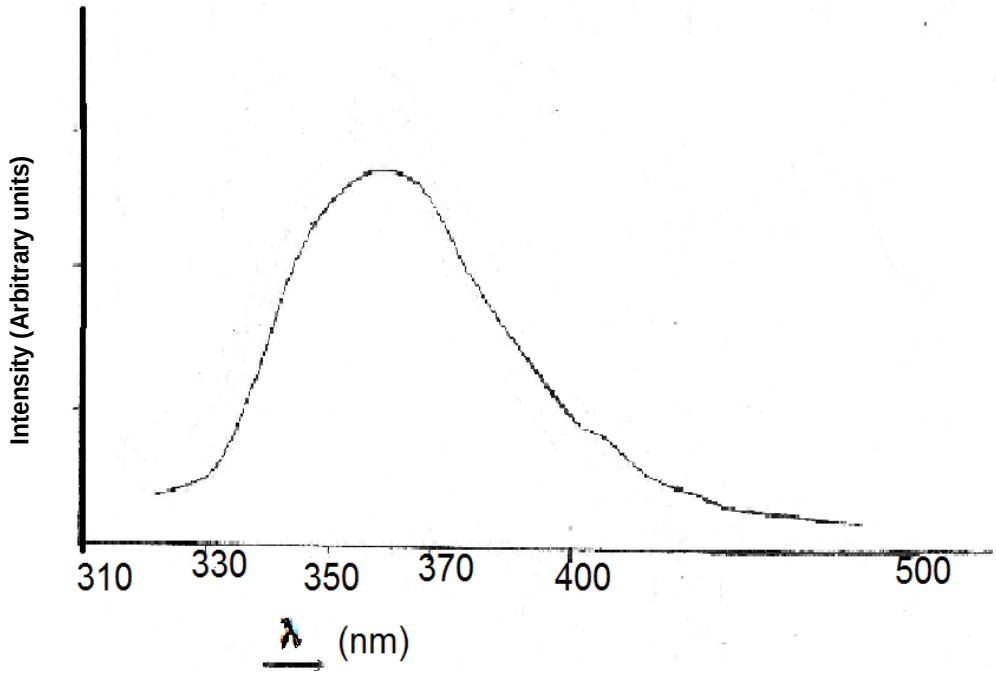

Figure 6. The fluorescence spectrum of BN solution in Cyclohexane at room temperature.

given by Hochstrasser (1961) where he found that 0-0 band is at 319.8 nm and this means that the 0- 0- absorption band is identical to that of the naphthalene.

DISCUSSION

The results obtained can be explained by the position of

the planes of 1-1`BN molecule which are orthogonal or almost orthogonal. The two molecules of the 1-1`BN are non-interacted and also there is no resonance interaction. The molecular spectra of this molecule lie in the UV region of electromagnetic spectrum.

The broad structure band in the absorption spectrum of 1-1`BN molecule which differs from that of naphthalene molecule is due to the swinging (twisting) around the equilibrium angle which is in turn due to the strong hindrance resulted from the spatial distribution of the molecule.

The displacement of 0-0 absorption band of the 1-1`BN molecule in solution from that of the naphthalene molecule is because of the type of distribution in the 1-1`BN molecule which is either cis or trans, that is towards the lower and higher energy respectively where it takes a certain geometrical position with a certain twisting angle in the ground state.

In the excited state, the two halves of the molecule are no longer orthogonal where they are turned apart which leads to the appearance of a fluorescence spectrum different from that of the naphthalene molecule.

The red shift in naphthalene fluorescence spectrum is because the emission spectrum resulted from the short twist grading. The solvent effect had been noticed for the polar one (ethanol) and other one which is non polar (cyclohexane).

REFERENCES

Berlman IB (1971). Handbook of Fluorescence Spectra of Aromatic Molecules, Academic Press, New York.

Hochstrasser RM (1961). The effect of intermolecular twisting on the emission spectra of hindered aromatic molecules: part I. 1,1′ binaphthyl. Can. J. Chem. 39(3):459-470.

Martinborough E, Denti TM, Castro PP, Wyman TB, Knobler CB, Diederich F (2004). Chiral 1,1′-Binaphthyl Molecular Clefts for the Complexation of Excitatory Amino-Acid Derivatives. Helvetica Chimica Acta, 78(5):1037-1066.

Nakamura M, Sawasaki K, Okamoto Y, Takamuku S (1995). Photolyses of derivatives of naphthyl and anthryl phosphates and methylphosphonates. Bull. Chem. Soc. Jpn. 68(11):3189-3197.

Pauptit RA, Trotter J (1983). Crystal structures of optically active naphthidine (4,4′-diamino-1,1′-binaphthyl) and 1,1′-binaphthyl,. Can. J. Chem., 61(1):69-71.

Post MFM, Langelear J, Van Voorst DW (1975). SCF-CI calculations and the assignment of the absorption spectrum of the excimer of 1-methyl naphthalene; relation to 1,1′-binaphthyl Chem. Phys. 4:59-62.

Wang C, Zhu L, Xiang J, Shuai Z, Zhu D (2007). Chiral Molecular Switches Based on Binaphthalene Molecules with Anthracene Moieties: CD Signal Due to Interchromophoric Exciton Coupling and Modulation of the CD Spectrum. J. Org. Chem. 72(12):4306-4312.

Zhou Y, Zhang D, Zhang Y, Tang Y, Zhu D (2005). Tuning the CD Spectrum and Optical Rotation Value of a New Binaphthalene Molecule with Two Spiropyran Units: Mimicking the Function of a Molecular “AND” Logic Gate and a New Chiral Molecular Switch. J. Org. Chem. 70(16):6164-6170.