

**EXPERIMENTAL NMR STUDY ON RHODAMINE B BASE*****Bakkialakshmi S. and Menaka. T***Department of Physics, Annamalai University, Annamalai Nagar, India-608002***ABSTRACT**

By using the dyes it is now possible to confirm the structure of the complex formed between the hydroxy propyl β -cyclodextrin and Rhodamine B base. The Proton NMR studies were carried out with pure dye, rhodamine B base and with 1: 1 inclusion complex of rhodamine B base and hydroxy propyl β -cyclodextrin. The change in chemical shift values confirm the formation of inclusion complex of Rhodamine B base with hydroxy propyl β -cyclodextrin.

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Key words: Rhodamine B base, hydroxy propyl β -cyclodextrin, ^1H NMR.**1. INTRODUCTION**

NMR technique consists in exposing the protons in an organic molecule to a powerful field. The protons will process at different frequencies. Now we irradiate these processing protons will steadily changing frequencies and observe the frequency at which absorptions occur. It is generally more convenient to keep the radio frequency constant and the strength of the magnetic field is constantly varied. At some value of the fields strength, the energy required to flip the protons matches the energy of the radiation. Absorption occurs and a signal is observed such a spectrum is called nuclear magnetic resonance spectrum. The most important applications are proton NMR (^1H NMR) and carbon – (^{13}C NMR) NMR spectroscopy. Nuclear magnetic resonance (NMR) spectra of dyes in free and complexed form indicated the probable structure of the complex judging from the proton shifts of the included groups of dyes in the CD cavity. An investigation of the electronic spectral properties of substituted coumarins was given by [Christie. R.M., *et al.*, 1999]. The inclusion complex of 2ABA with β CD is discussed by semi empirical quantum calculations (AM1), absorption, emission, FTIR, ^1H NMR and scanning electron microscope (SEM) [Stalin. *et al.*, 2006]. Effect of β -cyclodextrin, solvents and buffer solutions of different pH on the absorption and fluorescence spectra of 3 amino benzoic acid (3ABA) were investigated [Stalin. T. *et al.*, 2006].

Association constants of dibenzo ($3n + 2$) crown-in ethers using steady-state fluorescence spectroscopy were determined by Tuncer. H. and Erk. C., (2005). The inclusion behaviour of

unsubstituted β -cyclodextrin (β CD) and 2-hydroxy propyl β -cyclodextrin (HP β CD), in solution and solid state was studied [Cannava. C. *et al.*, 2008]. The pH effects on the 1:1 complexation behavior of β -cyclodextrin with the 7-hydroxy-4methyl coumarin and related compounds was investigated by measuring ultraviolet (UV) absorption, circular dichroism (CD), fluorescence and ^1H nuclear magnetic resonance (NMR) spectra and fluorescence lifetimes of the β -CD inclusion complexes formed [Masanori Hoshiyama, *et al.*, 2001]. The effect of cyclodextrin inclusion complex formation on the twisted intramolecular charge transfer (TICT) of the included compound was examined using the TICT – typical dual fluorescence for the p-dimethyl aminobenzoic acid (DMABOA)- β -cyclodextrin (β CD) system in buffered and unbuffered solutions [Yun – Bao Jiang, 1995].

MATERIAL AND METHODS

Rhodamine B base and hydroxy propyl β -Cyclodextrin were purchased from sigma Aldrich company, Bangalore. They were used without further purification. The instrument employed is Bruker 300 MHz (ultrashield) NMR spectrometer, which operates at 33MHz for proton and 75 MHz for BC Nuclei respectively, available at Department of Organic Chemistry, Madurai Kamaraj University, Madurai.

RESULTS AND DISCUSSION

^1H NMR studies were carried out at room temperature and under identical experimental conditions. Proton nuclear magnetic resonance (^1H NMR) spectroscopy has proved to be a useful tool to study β -cyclodextrin inclusion complexes [Lehman, J. and Peter E.K., 1991, Agbara, R.A. *et al.*, 1989, Turro, N.J. *et al.*, 1980]. The resonance assignments of the protons in β -cyclodextrin are well established.

* Corresponding author: +91

E-mail address: befun-chitra@rediff.com

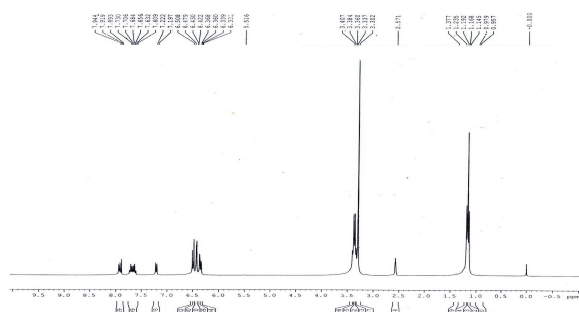


Fig. 1 ¹H NMR spectra of Rh B base

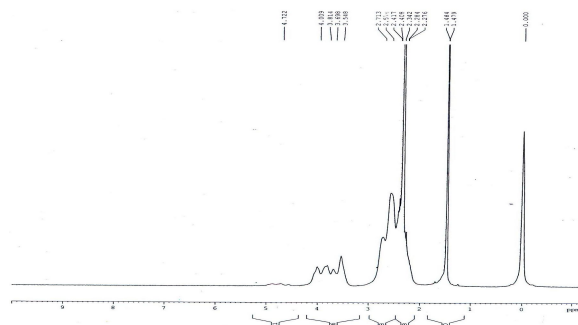


Fig. 2 ¹H NMR spectra of HPβCD

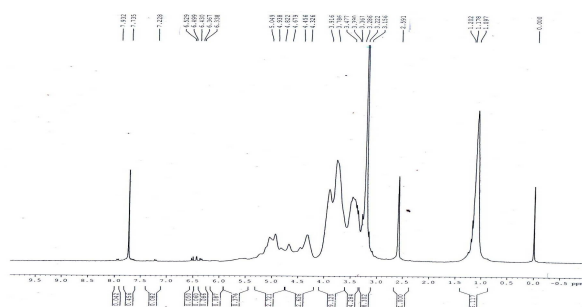


Fig. 3 ¹H NMR spectra of Rh B base + HPβCD complex

¹H NMR spectra of Rhodamine B base, hydroxy propyl β-cyclodextrin and the 1 : 1 inclusion complex of Rhodamine B base and hydroxy propyl β-cyclodextrin are given in Figs. 1, 2 and 3 respectively. The chemical shift values are presented in Table 1.

Table 1 H¹ – NMR chemical shift data of Rh B base and inclusion complex with HPβCD

Proton	Rh B base	HPβCD	Complex	Δδ Rh B base complex
H-1	7.9	3.6	2.5	5.4
H-2	3.3	2.5	4.6	1.3

CONCLUSION

It is assumed that Rhodamine B base molecules not only interact with hydroxy propyl β-cyclodextrin and also form the inclusion complex of Rhodamine B base with hydroxy propyl β-cyclodextrin. The change in chemical shift values conform the complex formation.

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