INFLUENCE OF SOLVENT AND THE ELECTRONIC PROPERTIES OF A DYE

S. Bakkialakshmi* and M.Shakthi[a]

Department of Physics, Annamalai University, Annamalai nagar,
Tamilnadu, India-608 002
[a]Department of Physics, Dr.S.J.S.PM CET, Puducherry,
India-605502

Abstract

Influence of solvent, water, and the electronic properties of a dye Coumarin (Cu) with two amines,[(1). n-Butyl amine (NBA) and (2) .Triethyl amine (TEA)] have been calculated. The calculated values have been reported in tables.

Keywords: Coumarin, . n-Butyl amine, Triethyl amine, electronic properties.

1. Introduction

Coumarin, a source for coumaric acid, was identified in 1820 and 1868, was synthesized in a laboratory for the first [1]. It is a pleasant smelling compound which gives a characteristic odor to hay. Other simple coumarins also possess characteristic smells sometimes exploited in per- fumery [2].

Coumarin derivatives also have diverse biological properties, such as enzyme inhibition, hypotoxicity, as well as, carcinogenic, anticoagulant or antibiotic action [3]. Also, some are used as dyes given their efficient light emission properties, high stability, and ease of synthesis [4].

The bicyclic ring system of chromenes, like coumarin, has inspired a number of different synthetic approaches [5,6].

2. Materials and Methods

Coumarin was purchased from Sigma Aldrich Company, Bangalore and was used without further purification. n-Butyl amine and triethyl amine were purchased from S.d fine chemicals (India). UV/Vis absorption spectra were taken using **1650 PC SHIMADZU UV-VISIBLE SPECTROMETER.**

3. Results and Discussion

The main absorption band of Coumarin in visible region corresponds to a transition moment largely parallel to the long axis of the molecule due to π→π* transition. Corresponding absorption maximum at 290 nm is observed in water.

Table 1 presents the absorption spectral data of Coumarin in water. It has been observed that absorption intensities increase with increasing concentrations of the two quenchers, n-butyl amine and triethylamine. These are shown in figs. 1 and 2 respectively. From the figures it can be noted that the absorption intensities increase when the concentration of n-Butyl amine and triethyl amine increase. The absorption maxima occur at 290 nm.

The formation constants for the Coumarin: nBA and Coumarin : TEA complex formation have been determined by analyzing changes in the intensity of absorption with quencher concentration.

The plot of $(1/A-A_0)$ versus [Q] will result in a straight line as shown in Figs.3&4. From the slope values of this plot, K has been evaluated and tabulated (Table 2). This is the ground state formation constant Kg. From this Kg value the free energy change, ΔGg, has been calculated and tabulated (Table 2).

4. Conclusion:

Electronic properties and the influence of solvent have been studied. The ground state formation constant and the free energy change have been calculated and tabulated.

References:

1. R. E. Kirk and D. F. Othmer, "Encyclopedia of Chemical Technology," 5th Edition; John Wiley & Sons Ltd., Chi- chester, 2007.

2. J. R. S. Hoult and M. Paydt, "Pharmacological and Bio- chemical Actions of Simple Coumarins: Natural Products with Therapeutic Potential," *General Pharmacology*, Vol. 27, No. 4, 1996, pp. 713-722. doi:10.1016/0306-3623(95)02112-4

3. E. M. Agostinha, R. Matos, C. C. S. Sousa, *et al*., "Ener- getics of Coumarin and Chromone" *The Journal of Phy- sical Chemistry B*, Vol. 113, No. 32, 2009, pp. 11216- 11221. doi:10.1021/jp9026942

4. J. Preat, D. Jacquemin, *et al*., "Theoretical Investigation of Substituted Anthraquinone Dyes," *Journal of Chemical Physics*, Vol. 415, No. 20, 2005, pp. 1736-1743. doi:10.1063/1.1764497

5. B. A. Chauder, C. C. Lopes, R. S. C. Lopes, A. J. M. da Silva and V. Snieckus, "Phenylboronic Acid- Mediated Synthesis of 2H-Chromenes," *Synthesis*, Vol. 1998, No. 3, 1998, pp. 279-282. doi:10.1055/s-1998-2042

6. K. A. Parker and T. L. Mindt, "Electrocyclic Ring Clo- sure of the Enols of Vinyl Quinones. A 2H- Chromene Synthesis," *Organic Letters*, Vol. 3 No. 24, 2001, pp. 3875-3878. doi:10.1021/ol0167199

Table 1: Absorption spectral data for Coumarin with different quenchers

Samples	Intensity	Wavelength (nm)
Coumarin	0.90	290
Coumarin + NBA	0.96	289
Coumarin + TEA	0.94	288

Table 2: Absorption, Molar restriction co-efficient (log ε), and solvent parameter, Formation constant (K_g) and free energy (ΔG_g) of Coumarin with NBA, TEA

Quenchers	λ_{abs} (nm)	log ε ($M^{-1} cm^{-1}$)	Z (nm)	K_g (M^{-1})	ΔG_g (kJ mol^{-1})
NBA	289	6.764	97.910	0.011	11.601
TEA	288	6.765	98.071	0.0067	11.141

A Monthly Double-Blind Peer Reviewed Refereed Open Access International e-Journal - Included in the International Serial Directories

International Journal in Physical & Applied Sciences

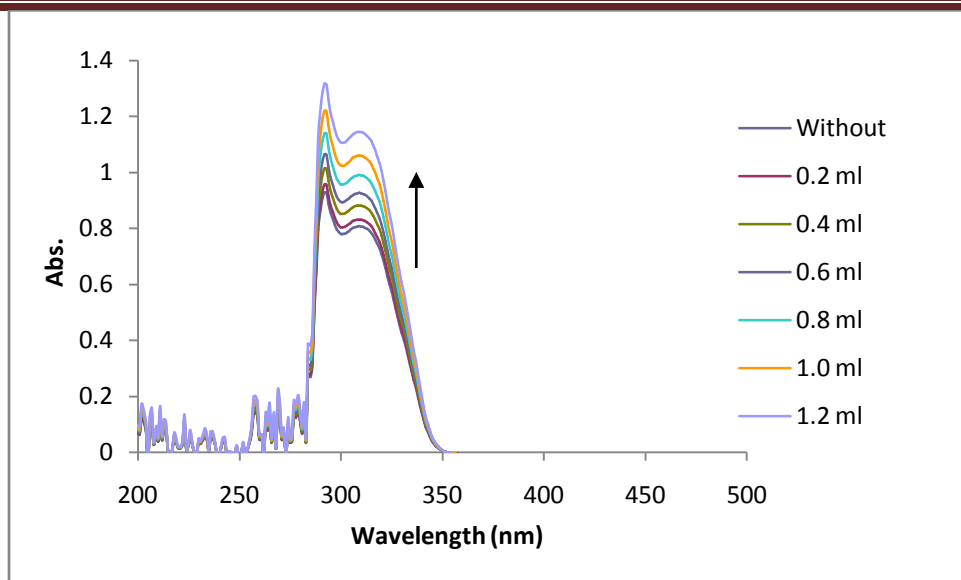http://www.ijmr.net.in email id- irjmss@gmail.com   Page 16

Fig.1 Absorption spectra of Coumarin in different concentration of NBA (mol dm-1)
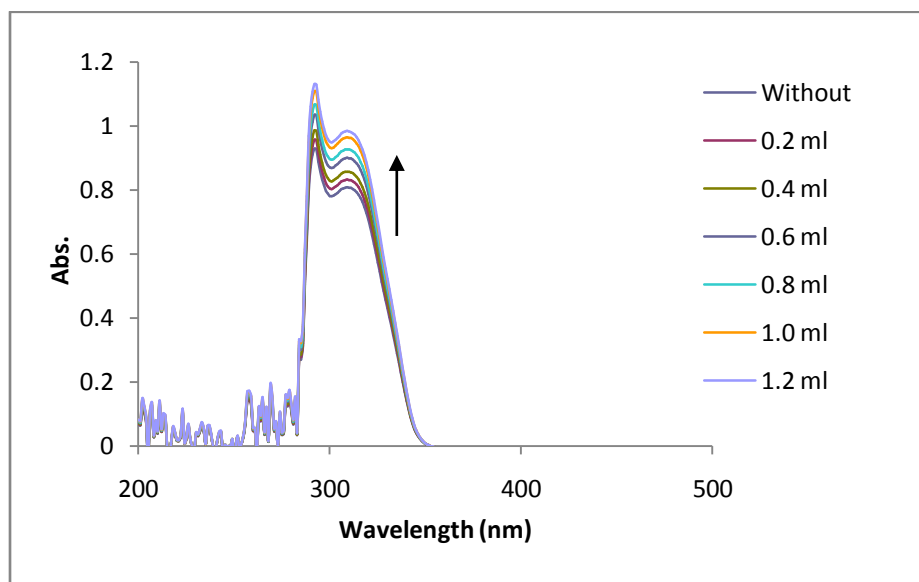**(1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012**

Fig2 Absorption spectra of Coumarin in different concentration of TEA (mol dm-1)
(1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012
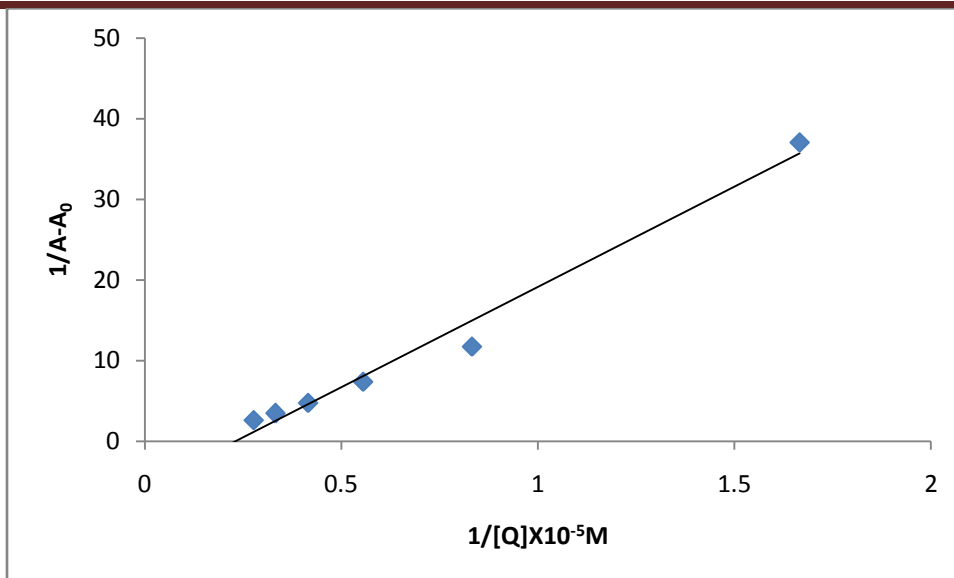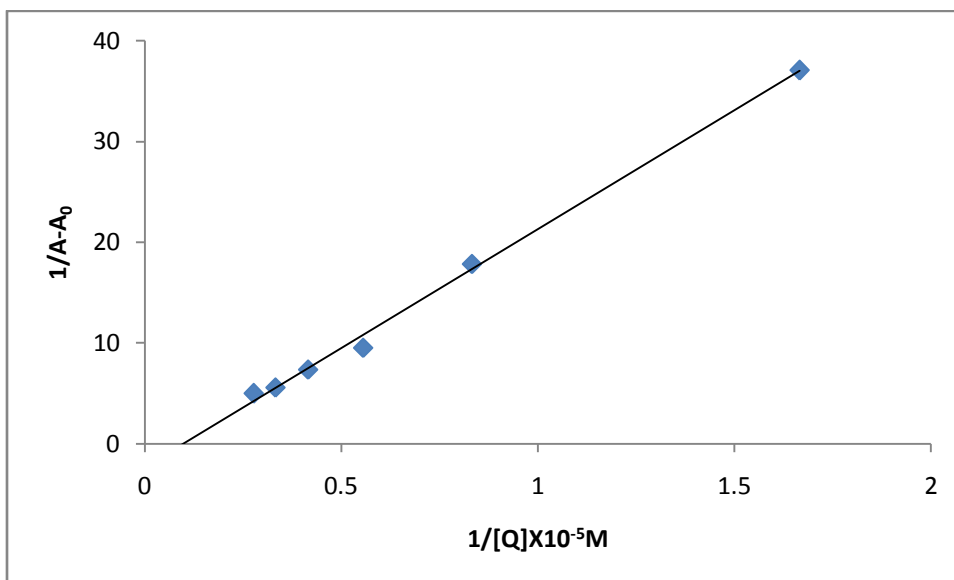
Fig. 3: Plot of 1/A-A0 and 1/[Q] for Coumarin for NBA

Fig. 4: Plot of 1/A-A0 and 1/[Q] for Coumarin for TEA