ORIGINAL RESEARCH PAPER

Engineering

Volume : 6 | Issue : 12 | December : 2016 | ISSN - 2249-555X | IF : 3.919 | IC Value : 79.96

A study on the effect of substituent's on UV absorption spectroscopy

KEYWORDS: Coumarin-1, UV-absorption, n-butyl amine, tricthyl amine.

S.Bakkialakshmi
Department of Physics, Annamalai University, Annamalainagar, Tamilnadu, India-608 002.

M. Shakthi
Christ Institute of Technology, Pondicherry

K.B.Renuga Devi
Rajiv Gandhi College of Engineering and Technology, Pondicherry

ABSTRACT *In the present work one of the important dyes, coumarin-1 has been subjected to phtophysical analysis. Though the influence of the electron-donating groups such as amino, substituted amino, hydroxyl alkoxy groups, etc. at position-7 of the coumarin ring system has been extensively studied, the luminescent properties of the coumarin moieties with an acetoxy substituent here not been explored. Herein it is attempted to study the variation of absorption behavior of coumarin-1 with two aliphatic amines n-butyl amine and triethyl amine.*

1. Introduction

The photophysical properties of coumarin and its derivatives depend on the nature and position of a substituent group in the parent molecule and also vary with surrounding media. Coumarin are used as non-linear optical chromophores and as an excellent probe to study salvation dynamics in homogenous solutions as well as organized meida [1-7]. In the recent past, humerous coumrin hetro derivatives have been synthesized and the possibility of their applications as lager dyes, organic scientillators and triplet sensitizes have been explored (8-12). Photochronic and redox properties of a series of 2H-Pyrano [3,2-c] Chromen-5-one derivatives were investigated by the UV/Vis absorption spectroscopy (13).

2. Materials and Methods

Coumarin-1, N-butyl amine, triehtylamine, DMF and DMSO were purchased from Sigma Aldrich company, Bangalore and were used without further purification. The concentration used for coumarin-1 is 5 x 10^{-6} M. UV/Vis absorption spectra were taken using 1650 PC SHIMADZU UV-Visible Spectrometer.

3. Results and Discussion

The measurements have been made in three different solvents water, Dimethyl Formamide (DMF) and Dimethyl Suphoxide (DMSO). The absorption maxima (λ_A) and the molar extinction coefficient (ε_A) were presented in Table 1.

Table:1. Absorption, emission, Ionization potential, Electron affinities of charge transfer complexes, Molar extinction co-efficient (log ε), Solvent parameter (Z) and Stoke's shifts (cm^{-1}) of Coumarin1 in different solvents.

Solvents	λ_{abs} (nm)	λ_{emi} (nm)	ID (ev)	EA	log ε (M^{-1} cm^{-1})	Z (nm)	Stoke's shift $\Delta\upsilon$ (cm^{-1})
Water	381	457	9.32	0.86	-2.118	$7.5x10^{10}$	4364.88
DMF	368	430	9.47	0.75	-2.117	$7.76x10^{10}$	3918.09
DMSO	376	440	9.38	0.82	-2.12	$6.88x10^{10}$	3868.47

The absorption spectra of cou-1 in all the solvents consist of absorption bands of longer wavelengths. There is no change in the shape of the spectra while different solvents were used. Only slight changes were observed in the values of molar extinction coefficient in different solvents.

It was observed that absorption intensities increase with increasing concentrations of NBA & TEA. These are shown in figs. 1-6. The plot of $\left\{\left[\frac{1}{A-A_0}\right]\right.$ and $\left.\left[\frac{1}{NBA}\right]\right\}$ & $\left\{\left[\frac{1}{A-A_0}\right]\right.$ and $\left.\left[\frac{1}{TEA}\right]\right\}$ with results in a straight line as in Figs. 7&8. From the slope values of this plot, K_g was evaluated and tabulated. This is the ground state formation constant and these are given in Table 2&3.

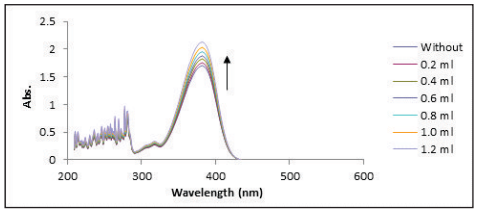

Fig.1. Absorption spectra of Coumarin1 in different concentrations of NBA (mol dm^{-3}) in Water (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012

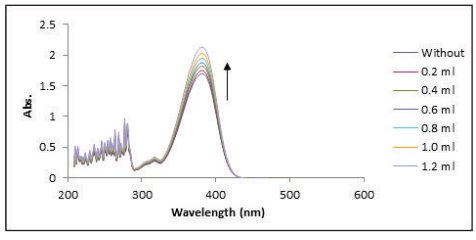

Fig.2. Absorption spectra of Coumarin1 in different concentrations of NBA (mol dm^{-3}) in DMF (1) 0, (2) 0.002, (3) 0.004, 4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012

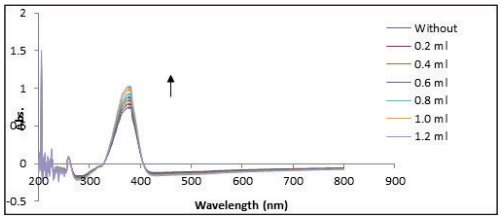

Fig.3. Absorption spectra of Coumarin1 in different concentrations of NBA (mol dm^{-3}) in DMSO (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012

Volume : 6 | Issue : 12 | December : 2016 | ISSN - 2249-555X | IF : 3.919 | IC Value : 79.96

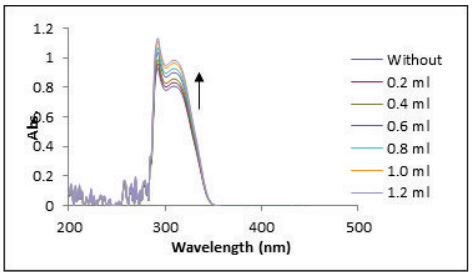

Fig.4. Absorption spectra of Coumarin1 in different concentrations of TEA (mol dm^{-3}) in Water (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012

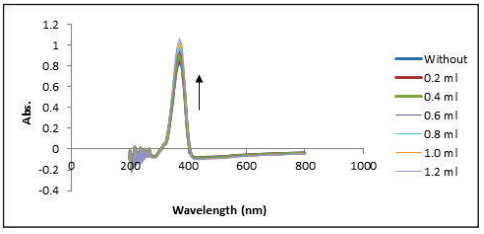

Fig.5. Absorption spectra of Coumarin1 in different concentrations of TEA (mol dm^{-3}) in DMF (1) 0, (2) 0.002, (3) 0.004, 4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012

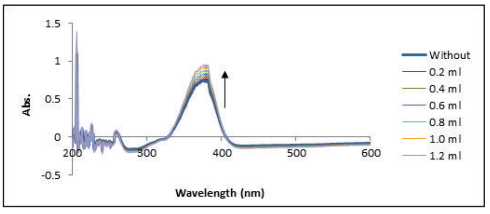

Fig.6 Absorption spectra of Coumarin1 in different concentrations of TEA (mol dm^{-3}) in DMSO (1) 0, (2) 0.002, (3) 0.004, (4) 0.006, (5) 0.008, (6) 0.010, (7) 0.012

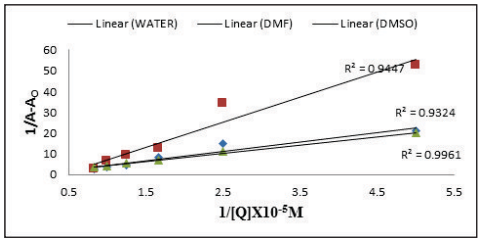

Fig.7. Plot of [1/A-A_0] and 1/[Q] for Coumarin1 with NBA in different solvents (1.Water, 2.DMF, 3.DMSO)

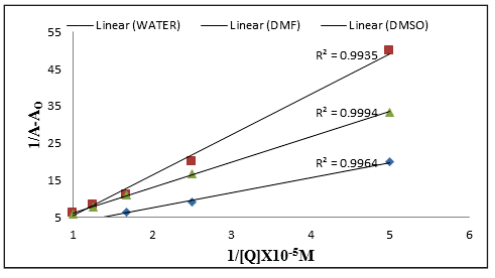

Fig.8. Plot of [1/A-A_0] and 1/[Q] for Coumarin1 with TEA in different solvents (1.Water, 2.DMF, 3.DMSO)

Table: 2. Formation Constant K (M^{-1}) and Free energy ΔG (KJmol^{-1}) of Coumarin1 with NBA in different solvents.

Solvents	K_g (M^{-1})	K_c (M^{-1})	ΔG_g (KJmol^{-1})	ΔG_c (KJmol^{-1})
Water	8.95	0.11	-5376.26	-5437.37
DMF	8.28	0.005	-5325.07	-13051.2
DMSO	3.76	0.004	-3336.39	-13601.51

Table: 3. Formation Constant K (M^{-1}) and Free energy ΔG (KJmol^{-1}) of Coumarin1 with TEA in different solvents.

Solvents	K_g (M^{-1})	K_c (M^{-1})	ΔG_g (KJmol^{-1})	ΔG_c (KJmol^{-1})
Water	4.66	0.023	-3876.99	-9502.86
DMF	6.61	0.009	-4457.61	-11866.49
DMSO	8.14	0.007	-5282.11	-12499.59

4. Conclusion

The absorption properties of coumarin-1 with NBA and TEA in three different solvents water, DMF and DMSO were discussed clearly. The ground state formation constants were calculated and tabulated.

References

1. Kaholek, M., P.Hradlovic, J. Photo.chem. Photobiol. A, 108 (1997) 283-288.
2. Moriya, T., Bull.Chem.Soc. Jpn, 59 (1986), 961-918.
3. Fletcher, A.N., D.E. Bliss, Appl.Phys. 16 (1978), 289-295.
4. Signore, G., R.Nifosi, L.Albertazzi, B.Storti, R. Bizzarri, J.Am.Chem.Soc., 132 (2010), 1276-1288.
5. Wolfbeis, O.S., E.Furlinger H. Kroveis, H.Z. Marsoner, Fresenius, Z., Anal.Chem. 314 (1983), 119-124.
6. Padhye, M.R., T.S. Varadarajan, A.U., Deshpande, Spectrosc. Lett, 15 (1982) 597-608.
7. Bourson, J., J. Mugner, B. Valeur, Chem.Phys. Lett.920 (1982), 430-432.
8. Specht, D.P., P.A. Martic, S., Farid, Tetrahedron, 38 (1982), 1203-1211.
9. Urano, T., H. Nagasaka, M. Tsuchiyama, S.Shimizu, K.Kawazoe, M. Schimizu, T.Yanaoka, Bull. Chem. Soc. Jpn. 68 (1995), 1661-1668.
10. Kumar, S., R.Giri, S.C. Mishra, M.K. Machwe, Spectrochim. Acta., Part A 51 (1995), 1459-1467.
11. S.Kumar, R.Giri, S.C. Mishra, M.K. Machwe, Indian J. Pure Appl. Phys. 33(1995), 615-622.
12. Kumar, S., R.Giri, S.C. Mishra, M.K. Machewe, Indian J. Pure. Appl. Phys. 36 (1998) – 622-630.
13. Huang, C.N., P.Y. Kuo, C.H.Lin, D.Y. Yang, Tetrahedron, 63 (2004), 10625-10033.