EFFECT OF DOPING RATIO ON OPTICAL PROPERTIES OF 5(6) CARBOXYFLUORESCEIN DOPED POLYSTYRENE FILMS

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Abstract: The effect of 5(6) Carboxyfluorescein dye on microstructural and optical properties of the polystyrene is studied. The FTIR study shows the shift in peaks indicates the interaction of 5(6) Carboxyfluorescein with PS. The UV-Vis study shows two absorption regions with the red shift and hence correspondingly two optical energy band gaps. Due to the variation of optical band gap and activation energies with different dopant concentrations, the existence of additional levels in the doped samples which reflects the modification in the microstructure of the dye doped polystyrene.

Keywords: Dye, polystyrene, optical studies, microstructure.

Introduction: The chromofore dye molecules incorporated in matrices like polymer, silica gel and polynucleotides etc. which shows many marked differences because of the environment and molecular orientation of the dye in polymer matrix. This dye doped films have wider applications in optics and electronics have made rapid progress in recent years. Due to their different optical properties it is possible to observe both molecular aggregates and single isolated molecules in the films which identify by different luminescent behavior [1, 2]. In view of this in the present work the effect of 5(6) Carboxyfluorescein (5(6) CF) dye on optical and microstructural properties of the polymer polystyrene (PS) are studied.

Experimental: The polymer Polystyrene used in this work is obtained in powder form from M/s. s.d. fine-Chem. Ltd, Mumbai and the 5(6) Carboxyfluorescein dye is obtained from Aldrich chemical co, USA. The 5(6) Carboxyfluorescein doped PS films were prepared by solution casting method using

THF organic solvent [3]. The FTIR spectra of the prepared films were obtained using NICOLET FTIR-6700. UV-Vis study was performed using SHIMADZU (UV-1601) spectrometer in the wavelength range 195-700nm.

Results and Discussion:

FTIR and UV-Visible Studies: FTIR offers quantitative and qualitative analysis for organic and inorganic samples. Fourier Transform Infrared Spectroscopy (FTIR) identifies chemical bonds in a molecule by producing an infrared absorption spectrum. The spectra produce a profile of the sample, a distinctive molecular fingerprint that can be used to screen and scan samples for many different components. FTIR is an effective analytical instrument for detecting functional groups and characterizing covalent bonding information of the polymers with organic chromofore dyes [4]. FTIR spectral assignments of 5(6) Carboxyfluorescein doped polystyrene is show in the below Table1.

Table 1: FTIR peak assignments of Pure and 5(6) CF doped PS.

Wave numbers (cm^{-1})		Peak Assignments
Pure Polystyrene	PS/5(6)CF composite	
-----	3434-3633	O-H stretching vibration
3064	3064-3125	C-H stretching vibration
2998	2998-3054	C-H asymmetric stretching
2923	2923-2926	C-H symmetry stretching
2866	2860-2866	CH_2 stretching vibrations
-----	1705-1731	C=O stretching vibration
1583	1521-1571	C=C stretching vibration
1444	1444-1450	C-H bond stretching
-----	1370-1359	O-H stretching vibration
1260	1253-1260	C-H stretching vibration
-----	1109	C-O stretching vibration
1072	1069-1072	C-H skeletal vibration
790	757	C-H deform

The above findings in the case of 5(6) CF doped PS, the FTIR spectra shows shift in the corresponding bands and appearance of new peaks with a change in intensities. This indicates the considerable interaction between PS and 5(6) CF. As the dopant concentration increases, these interactions results in the formation of dopant aggregates or agglomerates leading to a certain phase separation into a polymer-rich phase and a dopant-rich phase. Also modifies the microstructural properties of PS [5].

UV-visible light spectrum, causing a transition to a high-energy electronic state and subsequently emits photons as it returns to its initial state. Some energy within the molecule is lost through heat or vibrations, so that the emitted energy is less than the exciting energy; i.e., the emission wavelength is always longer than the excitation wavelength [6]. The UV–visible absorption spectra of pure polystyrene as shown in fig.1. as well as 5(6) CF doped PS spectra is shown in the Fig. 2. The Figure shows that there are two absorption peaks in the region 342nm and 461nm.

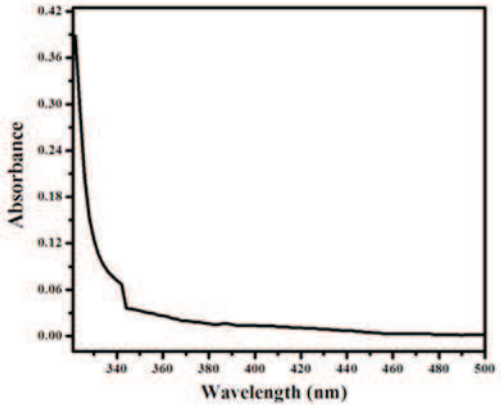

Figure 1. UV-Vis absorption spectra of pure PS.

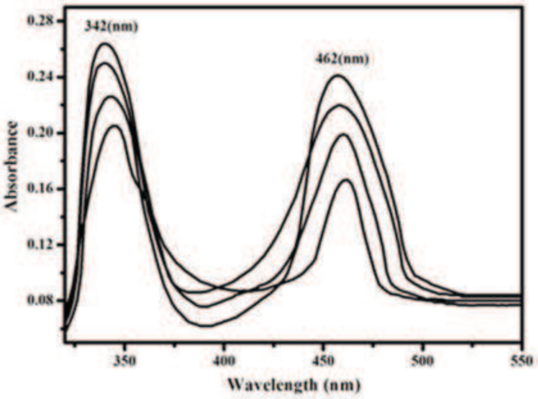

Figure 2. UV-Vis absorption spectra of 5(6) CF doped PS.

These peaks get red shift with increasing dopant concentration in polystyrene matrix. We notice from the figure that the increase in molar concentration lead to increase in the intensity of absorption spectra contain contributions from monomers and aggregates which make the spectrum broader according to Beer – lambert law [7,8].

The corresponding optical energy band gap and optical activation energy is calculated using Mott and Davis relation [9]. It is observed that increasing dopant concentration decrease in energy band gap and activation energy. The variation of the calculated values of energy band gap (Eg) and activation energy (Ea) may reflect the role of dye content and modifying the electronic structure of the PS matrix due to appearance of various polaronic and defect levels. These implications can be explained in the following sense.

The decrease of Eg and Ea may be attributed to the induced energy states due to chromofore dye doping [10, 11].The calculated values of optical energy band gap (Eg) and activation energy (Ea) are given in Table. 2.

Doping level (wt %)	E_{g1}	E_{g2}	E_{a1}	E_{a2}
pure PS	**3.87**	---	**0.32**	----
1	**2.96**	**2.53**	**0.38**	**0.48**
5	**2.91**	**2. 41**	**0.35**	**0.46**
7	**2.88**	**2.38**	**0.31**	**0.41**
10	**2.31**	**2.02**	**0.26**	**0.37**

Table 2: calculated optical energy band gaps and activation energy bands of pure PS and 5(6) CF doped PS.

Conclusions: In this study the effect of doping concentration on the optical and microstructural properties of PS/5(6) CF composite films are carried out. The FTIR spectra indicates possible interaction between dye and PS. Using UV-Visible absorption spectra the optical parameters like optical energy band gap and activation energy were determined and the variation of these parameters suggests the existence of defects and molecular orderings within the 5(6) CF doped PS films. This property can be utilized for optical devices and optical storage applications etc.

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