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Structural Study of RH6G Dye Doped PVA+NH_4SCN Gel Electrolyte

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Abstract : In this work XRD of RH6G dye doped PVA gel electrolytes were studied. RH6G dye doped PVA gel electrolytes were synthesized by freezing-thawing method using PVA, NH_4SCN as an electrolyte, DMSO as a solvent and RH6G used as a dopent. The synthesized samples were characterized by XRD. XRD of 1and 2 drops RH6G dye doped PVA+NH_4SCN gel electrolyte shows amorphous in nature. The broad peak observed at $2\theta = 18^0$ for 1 drop RH6G dye doped 0.5,1 and 1.5 gm PVA gel electrolyte and at $2\theta = 19^0$ for 1 drop RH6G dye doped 2 and 2.5 gm PVA gel electrolyte. For 2drop RH6G dye doped PVA+NH_4SCN gel electrolyte a wide peak around 20.50^0 is observed.

Keyword : PVA, NH_4SCN, RH6G, Freezing-Thawing method, XRD.

Introduction

The preparation and study of polymer electrolytes remain an area of frontier research and are influencing the modern and future technologies of solid state and electrochemical devices such as rechargeable batteries, fuel cells, supercapacitors, smart windows and transparent conductors etc. [i–iii]. This is mainly due to the low cost, ease of device fabrication, interesting electrical, optical and electrochemical properties. Many potential applications of the electrolytes may be realized via modification of their conductivity and investigation of their electrochemical properties [iv–vii]. Extensive studies have been carried out of the effects of doping on the conductivity of polymer electrolytes [i, iv, v, viii]. These polymer electrolytes exhibit maximum conductivity for a certain wt. % ratio of the dopant and polymer [iv]. In order to enhance the conductivity of the polymer electrolytes, Mohammad A et.al and Reddy Ch et al [iv, ix] mixed inorganic salt and alkali into the host polymer electrolyte.

Rhodamine 6G (RH6G) is a cationic laser dye from the xanthene family have been used extensively as a sensor [x], nonlinear optical material [xi] and photosensitizer [xii]. The present study deals with synthesis and study of XRD of RH6G dye doped PVA+NH_4SCN gel electrolyte.

Experimental

Chemicals

In the present study polyvinyl alcohol (PVA), ammonium thiocyanate (NH_4SCN), aprotic solvent dimethyl sulfoxide (DMSO) and Rhodhamin 6G are of AR grade use for synthesis of dye doped polymer gel.

Synthesis

Initially, 30 ml ionic liquid (liquid electrolyte) of 0.2 M solution of NH_4SCN+DMSO was prepared. The concentration of ionic liquid was kept constant. Then PVA of required amount was added in the ionic liquid at 70 ^{0}C with constant stirring and continued for one hour maintaining the temperature. Then the prepared sol was allowed to cool to room temperature so as to form the gel electrolyte. Five different gel samples were prepared by varying the quantity of PVA in NH_4SCN electrolyte and it was 0.5, 1, 1.5, 2 and 2.5 gm in each 30 ml ionic liquid electrolyte. 1 M concentration of RH6G in DMSO was prepared and added to the prepared sol by drop method. The concentration of RH6G was varied by adding 1, 2, 3 drops in each sample of the first series. Thus in all 15 gel samples of RH6G dye doped PVA+NH_4SCN were prepared.

Result and Discussion

In order to investigate the effects of RH6G dye on the structure of PVA+NH_4SCN gel electrolyte, XRD studies have been carried out. The XRD patterns were recorded at room temperature using X'pert –pro Diffractometer with CuKα radiation (λ=1.5056 Å) in 2θ (Bragg's angle) range at a scan speed of 3^0/ min. ($10^0 \leq 2\theta \leq 40^0$).

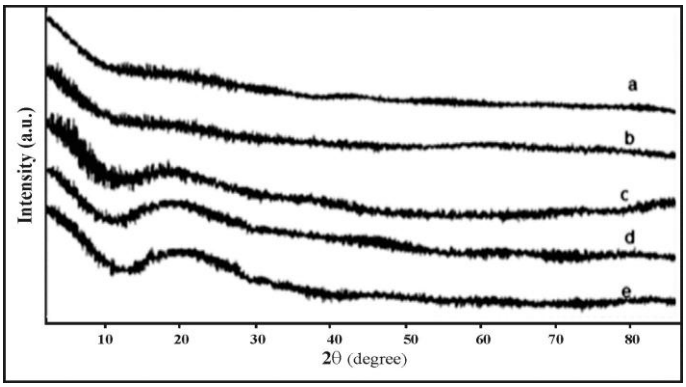

Figure 1:- XRD pattern for 1 drop RH6G dye doped (a) 0.5,(b)1,(c)1.5,(d) 2,(e) 2.5 gm PVA+NH_4SCN gel electrolytes.

Table 1:- Data obtained from XRD of 1 drop RH6G dye doped 0.5, 1, 1.5, 2, 2.5 gm PVA+NH_4SCN gel electrolytes.

PVA in gm	2θ= scattering angle (in degree)	θ (in degree)	d= inter - planar spacing Å	R= inter – chain length Å
0.5	18	9	4.9248	5.4891
1	18	9	4.9248	5.4891
1.5	18	9	4.9248	5.4891
2	19	9.5	4.6818	5.2183
2.5	19	9.5	4.6818	5.2183

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Figure 1 shows X-ray diffraction patterns for 1drop RH6G dye doped 0.5, 1, 1.5, 2 and 2.5 gm PVA gel electrolytes. A hump is observed in each diffractogram, indicating that all the samples are amorphous in nature. However size of the hump changes with concentration of PVA**.** The broad peak observed at $2\theta = 18^0$ for 1 drop RH6G dye doped 0.5,1 and 1.5 gm PVA gel electrolyte and at $2\theta = 19^0$ for 1 drop RH6G dye doped 2 and 2.5 gm PVA gel electrolyte it is related to PVA polymer host [xiii]. Careful observations revealed that 1 drop RH6G dye doped 0.5 and 1 gm PVA gel electrolyte are found to be more amorphous than 1 drop RH6G dye doped 1.5,2,2.5 gm PVA gel electrolytes. Hump is found to be broader for higher loading of PVA. As the concentration of PVA increases peak height increases and found to be shifted to slightly higher value of 2θ. It also indicates that all ingredients (PVA, NH_4SCN, DMSO and RH6G) were mixed properly to form a gel electrolyte [xiv].

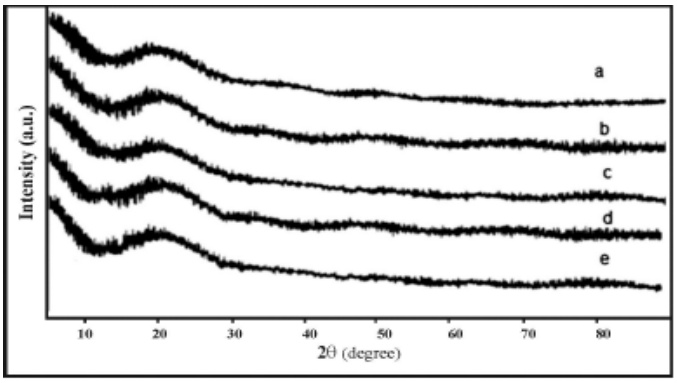

Figure 2:- XRD pattern for 2 drop RH6G dye doped (a) 0.5, (b) 1,(c) 1.5, (d) 2,(e) 2.5 gm PVA+NH_4SCN gel electrolytes.

Table 2:- Data containing scattering angle, inter - planar spacing and inter – chain length for 2 drops RH6G dye doped various concentration of PVA gel electrolytes.

PVA in gm	2θ= scattering angle (in degree)	θ (in degree)	d= inter - planar spacing Å	R= inter – chain lengthÅ
0.5	20.50	10.25	4.3296	4.8257
1	20.50	10.25	4.3296	4.8257
1.5	20.50	10.25	4.3296	4.8257
2	20.50	10.25	4.3296	4.8257
2.5	20.50	10.25	4.3296	4.8257

Figure 2 (a), (b), (c), (d), (e) shows X-ray diffraction patterns for 2 drops RH6G dye doped 0.5, 1, 1.5, 2, 2.5 gm PVA gel electrolytes respectively. It shows the amorphous structure with a wide peak around 20.50^0. An absence of typical crystalline peaks in the diffraction spectra of gel electrolyte is an indication of the removal of the PVA shape during the heating process [xv].

The inter - planar spacing d is obtained from Bragg's Law [xvi] i.e.

$$n\lambda = 2d\sin\theta$$

Where,

n- order of diffraction
λ - Wavelength of X – ray (1.5405 Å)
θ - Angle of diffraction

The inter – chain separation is obtained by using the formula [xvi].

$$R = \frac{7}{2\pi} \times \frac{\lambda}{2\sin\theta}$$

Where,

R - The inter chain length
λ - Wavelength of X-ray
θ - The scattering angle

Peak position, inter planer spacing d and inter chain length R for all the 1 drop RH6G dye doped PVA gel electrolytes are enclosed in Table 7.1.1. Thus only slight change in 2θ values as well as interplaner distance d and inter chain length R is observed at higher concentration of PVA.

Peak position, inter planer spacing d and inter chain length R for all the 2 drops RH6G dye doped PVA gel electrolytes are enclosed in Table 7.1.2. It is observed that the value of 2θ as well as inter planer distance and inter chain length is found to be constant for all 2 drops RH6G dye doped PVA gel electrolytes this might be due to the increased concentration of dye.

The undoped and RH6G dye doped PVA gel electrolyte shows amorphous nature. As observed the 2θ value of RH6G dye doped PVA gel electrolyte shifted toward lower value but as concentration of dye increases for 2 drops, 2θ values shifted slightly to a higher value. Also the inter planer distance and inter chain length decreases as concentration of RH6G dye in PVA gel electrolyte increases, confirming the chemical interaction between PVA, NH_4SCN and RH6G [xvii].

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