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ATR spectroscopy applied to photochromic polymer analysis

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Abstract

This work reports the use of infrared spectroscopy in the Attenuated Total Reflection (ATR) mode to analyze the interactions between polymeric bases and the spiropyran. Infrared spectroscopy helps to understand the interactions between the different molecules, spiropyran polymeric base and the solvent. Polymethyl methacrylate and cellulose acetate as polymeric base and the spiropyran 1, 3, 3 trimethyl indoline-5-nitro benzopyrane were used. Thin films of different concentrations (0.25%, 0.5%, 1%, 2% and 5%) of spiropyran were deposited in each type of polymeric base. The infrared spectra show the frequencies associated with the chemical bonds of each molecule. A decrease in intensity of absorbance was observed for the C=O stretching mode of the acetate group located at 1720 cm^{-1} and for the C=C and C=N stretching modes at 1642 cm^{-1} associated with spiropyran. A shift in the intensity of the peaks was also observed due to solvent and polymeric base effects on the final film.

Keywords: Spiropyrans; Photochromic materials; Infrared spectroscopy; Structural analysis

1. Introduction

Photochromism is a phenomenon wherein, the absorption spectrum of a single chemical species changes reversibly when it is irradiated by light of a certain wavelength, inducing transformations between molecular states, whose absorption spectra are different. One of the most studied photochromic materials is spiropyran (SP) which absorbs ultra violet (UV) light. On UV illumination the SP's colorless isomer undergoes an heterolytic cleavage of the NO bond to form a colored isomer (merocyanine), which absorbs light in the visible region. The change in coloration (colorless to blue) of the sample is a physical observation of the molecular transformation. This process can be reversed by visible illumination.

Reversible photocoloration is attributed to an equilibrium between the SP (closed, colorless) form and the merocyanine (open, colored) form, as shown in Fig. 1. The *cis*-cisoid isomer is an intermediate product in this molecular transformation and it is associated to the sample degradation [1]. Spiropyran-doped polymers have a great potential for applications in optoelectronic devices, such as data storage films and waveguides [2,3], and in bioelectronic devices, like biosensors for medical purposes [4–6]. When the molecule is in the open merocyanine state, a dipole is generated. By laser illumination or application of an external field, its physical and chemical properties can be controlled. The radical group NO could be changed to generate shifts in the absorption peaks for the merocyanine state. One of the most notable features of these materials, is that

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