

Photoinduced FT-IR spectroscopy of conjugated polymer/fullerene composites embedded into conventional host polymer matrices

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Abstract

In this work, we report on the investigation of photoexcited states in conjugated polymer (donor) – fullerene (acceptor) interpenetrating networks (polythiophene derivatives – PC₆₁BM) embedded into conventional polymer hosts like polystyrene, polyvinylcarbazole, polycarbonate or polyvinylbenzenechloride, using photoinduced FT-IR spectroscopy. We discuss the influence of specific host polymer matrices on photoexcited states of the photoactive guests via photoinduced infrared activated (IRAV) modes.

Keywords: Photoinduced absorption spectroscopy, polymer/polymer interfaces, bulk heterojunctions, polythiophene, fullerenes.

1. Introduction

In this work, we studied photophysically active compounds consisting of a conjugated polymer/fullerene composite embedded into a conventional polymeric host material. Our motivation is:

- to achieve a controlled decrease of the polymer inter-chain interactions by diluting the photoactive components in conventional polymers (solid state solution)
- to improve the stability by protection from degradation at ambient conditions [1]
- to enhance the processability of the total composite blend [2]
- to tune the morphology [3]
- to utilise the additional charge transport properties of the host matrices [4]

The spectroscopic study of photoinduced IRAV bands in these compounds has been utilised to understand the influence of the host matrix on the donor-acceptor bulk heterojunction.

2. Experimental

Photoinduced FT-IR spectroscopy has been carried out using a Bruker IFS 66S spectrometer and a chopped argon laser as pump source. Thin film samples have been prepared by coating KBr substrates by spin- or drop casting from solutions of *ortho*-dichlorobenzene containing one weight percent blend dissolved. The blends consisted of 1:1:1 weight ratio of conventional polymer:conjugated polymer:fullerene. Drop cast samples were evacuated for faster drying and improved film quality.

All photoinduced absorption (PLA) measurements are presented as normalised differences in transmission, and are corrected for various optical densities of different samples. Apart from the photoinduced studies, also chemical and electrochemical doping experiments were performed to identify the radical states in the infrared spectra. For chemical doping, a thin film coated on a

ZnSe substrate was exposed to iodine vapour during a short period of time and for the electrochemical doping a three-electrode electrochemical cell was used. Working electrode, counter electrode and reference electrode consisted of a Ge reflection element coated with a Pt layer, a Pt foil, and a Ag/AgCl wire, respectively. The electrolyte solution used was 0,1 M TBABF₄ (TetraButylAmmoniumBF₄) in acetonitrile. The polymeric host materials used in this work were polystyrene (PS), polyvinylcarbazole (PVK), polycarbonate (PC) and polyvinylbenzenechloride (PVBC). The donor materials used in the study were the conjugated polymers (poly)3-octylthiophene (P3OT) and (poly)dihexyloxythiophene (PDHT). Acceptors throughout the work were fullerene derivatives with enhanced solubility such as [6,6]PC₆₁BM (mono-adduct).

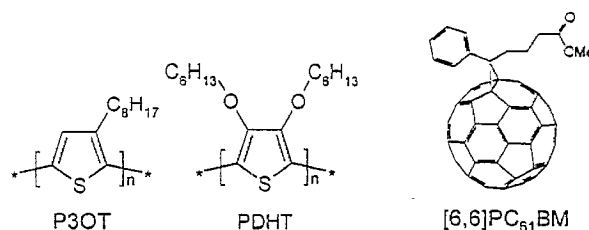


Fig. 1: Molecular structures of donor polymers and acceptor fullerene used in this study.

3. Results and discussion

In Fig. 2a the photoinduced infrared spectra of several composites clearly show electronic photoinduced absorption peaks due to the photoinduced electron transfer [5] as a distinctive feature at around 1700 cm⁻¹. It has a FWHM of approximately 1000 cm⁻¹ and is correlated with the photoinduced IRAV bands below 1500 cm⁻¹, (displayed in larger scale in Fig. 2b).

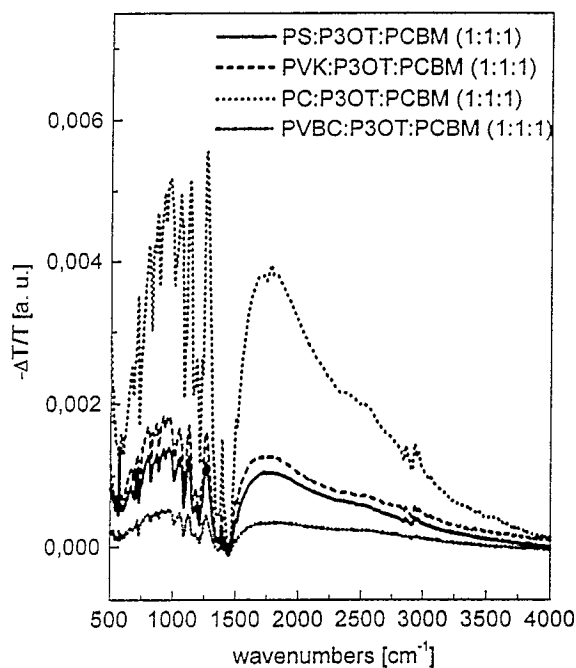


Fig. 2a: Photoinduced IR spectra of several composites.

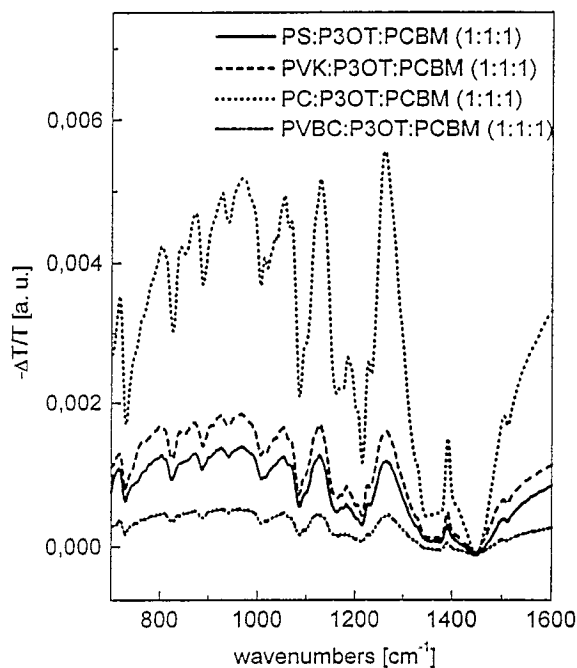


Fig. 2b: Photoinduced IRAV bands.

Compared to the pure systems without host matrices we see no significant shifts of IRAV peak positions. The intensity changes of the IRAV bands are correlated with the dilution as well as with morphology effects in solid state matrices.

In Fig. 3 the photoinduced IR spectra are compared with spectra of chemically and electrochemically doped samples.

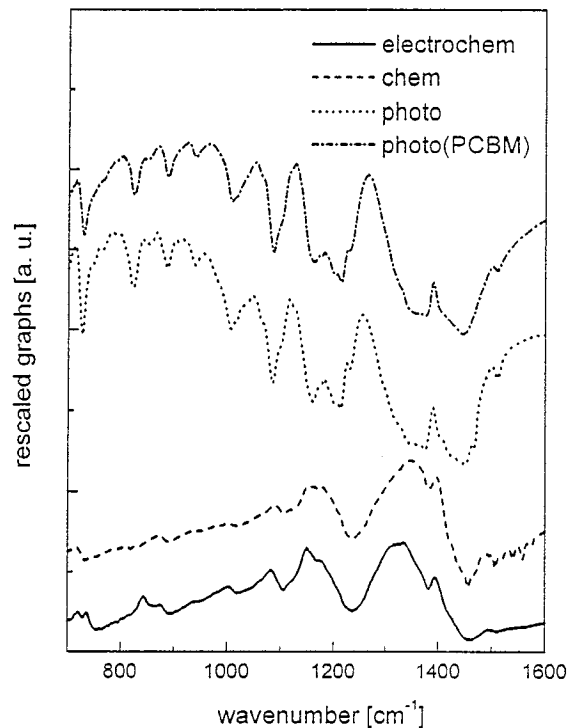


Fig. 3: Comparison of photoinduced and doping induced IRAV bands.

4. Conclusions

Embedding of the conjugated polymer/fullerene charge transfer systems into conventional host polymers up to 50% has been studied. Photoinduced electron transfer has been preserved in these blends, with qualitative scaling due to dilution effects. P3OT shows stronger electron donor activity compared to PDHT. Comparison between chemical, electrochemical and photoinduced doping showed different response for different doping techniques. [6][7] The morphology of blends is a crucial parameter for the photoinduced activity.

5. References

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