

# CH-LINES IN IR-SPECTRA OF CARBYNOIDS

*E.M. Baitinger, I.G. Margamov*

*Chelyabinsk State Pedagogical University, Lenin av., 69, Chelyabinsk, 454080, Russia*

## Introduction

During the last 40 years the physical properties of carbyne have been intensively studied. However not all of its features are investigated yet. In particular it concerns the electronic structure and optical characteristics. This field is important for electronics and engineering, where the application of film technologies has developed a lot lately.

The complexity of this research is due to the fact that most electrical and optical properties are sensitive to inessential details of synthesis of carbyne and carbynoids. The latter are substances that, contrary to carbyne, contain a considerable number of impurities and imperfections, which are part of the structure of the chains or interchain space. Co-orientation of the chains, their cross-linking, folds etc. also considerably modify the properties of this one-dimensional carbon phase.

This abstract is devoted to experimental study of the influence of the synthesis conditions of amorphous carbyne on some of its optical parameters.

## Results and discussion

Properties of two series of carbynoid samples different in the way of their chemical processing have been studied with the help of IR-spectroscopy. Both the series were synthesized on the surface of a poly(vinylidene fluoride) film through chemical dehydrofluorynation by treating the film during various periods of time at room temperature with a mixture of saturated (20%) alcoholic KOH solution with organic solvent, which serves as a catalyst of chemical dehydrofluorynation. In the first series acetone was used in the volumetric ratio 1:9, and in the second series — tetrahydrofuran (TGF) in the ratio 2:3. The time of synthesis for the first series varied from 2 to 60 minutes, and in the second — from 10 to 120 minutes. After dehydrofluorynation all the samples were washed sequentially in ethanol, acetone and water. Any additional treatment of films was not carried out.

The studies of IR-absorption were carried out with the spectrometer Specord-75-IR by a two-beam method in a transmission mode in an interval of wave numbers 400-4000  $\text{cm}^{-1}$  (0,05-0,5 eV) at room temperature. The instrumental error makes  $\pm 1$  and  $\pm 2$   $\text{cm}^{-1}$  in the range of 400-2000 and 2000-4000  $\text{cm}^{-1}$ , accordingly. The

shape of spectra and position of features are well reproduced. However in the interval of small photon energies (wave numbers 400-1200  $\text{cm}^{-1}$ ) the IR-spectra give little information and thus are not considered here.

Some most typical spectra of PVDF and carbynoid films obtained under the influence of two different catalysts (I, II — the first series, III-V — the second series) and several times of synthesis are shown in Fig. 1. The basic description of IR-spectra for these carbon materials is known [1]. If photon energy is less than 0,25 eV (wave numbers less than 2000  $\text{cm}^{-1}$ ) a number of absorption lines are formed, which can be caused by double carbon-carbon bonds (1500-1800  $\text{cm}^{-1}$ ) [2], carbonyl groups (1700  $\text{cm}^{-1}$ ) [2] and/or water (1700  $\text{cm}^{-1}$ , 3400  $\text{cm}^{-1}$ ) [3].

We are interested in spectral range of about 3000  $\text{cm}^{-1}$  (0,37 eV), where the intensive absorption by carbon-hydrogen bonds is revealed. In our spectra these are exhibited as a doublet (in a spectrum V in Fig. 1 one can see even the third peak). The position of the doublet peaks differs approximately by 50  $\text{cm}^{-1}$  (6,2 meV). Both their intensity and the half-height-width depend on time of dehydrohalogenation, (which reached 120 min) and on the catalyst characteristics. The common tendency is the decrease of CH-lines intensity the more the time of synthesis is. However this tendency is not monotonous.

Besides for the second series of carbynoids (spectra III-V) the appearance of a non-resonant background and also wide absorption band 1800-3700  $\text{cm}^{-1}$  (at photon energy 0,22-0,46 eV) is characteristic.

This phenomenon, which is revealed for the first time, evidences a considerable heterogeneity of the chain. This heterogeneity becomes more essential as the dehydrohalogenation stage increases.

Besides the common interpretation of this phenomenon connected with the existence of the carbon-hydrogen bonds and cross-linked fragments of the chain, the occurrence of absorption in this interval is possible due to polar conductivity of the chain.

## Conclusions

The presented data show the dependence of spectral features of carbon-hydrogen bonds on time of synthesis and influence of a catalyst of the reaction of creation of carbyne. It is revealed, that with the increase of dehydrohalogenation period a non-resonant background and a wide absorption band appear and significantly increase at the range of 1800-3700  $\text{cm}^{-1}$ .

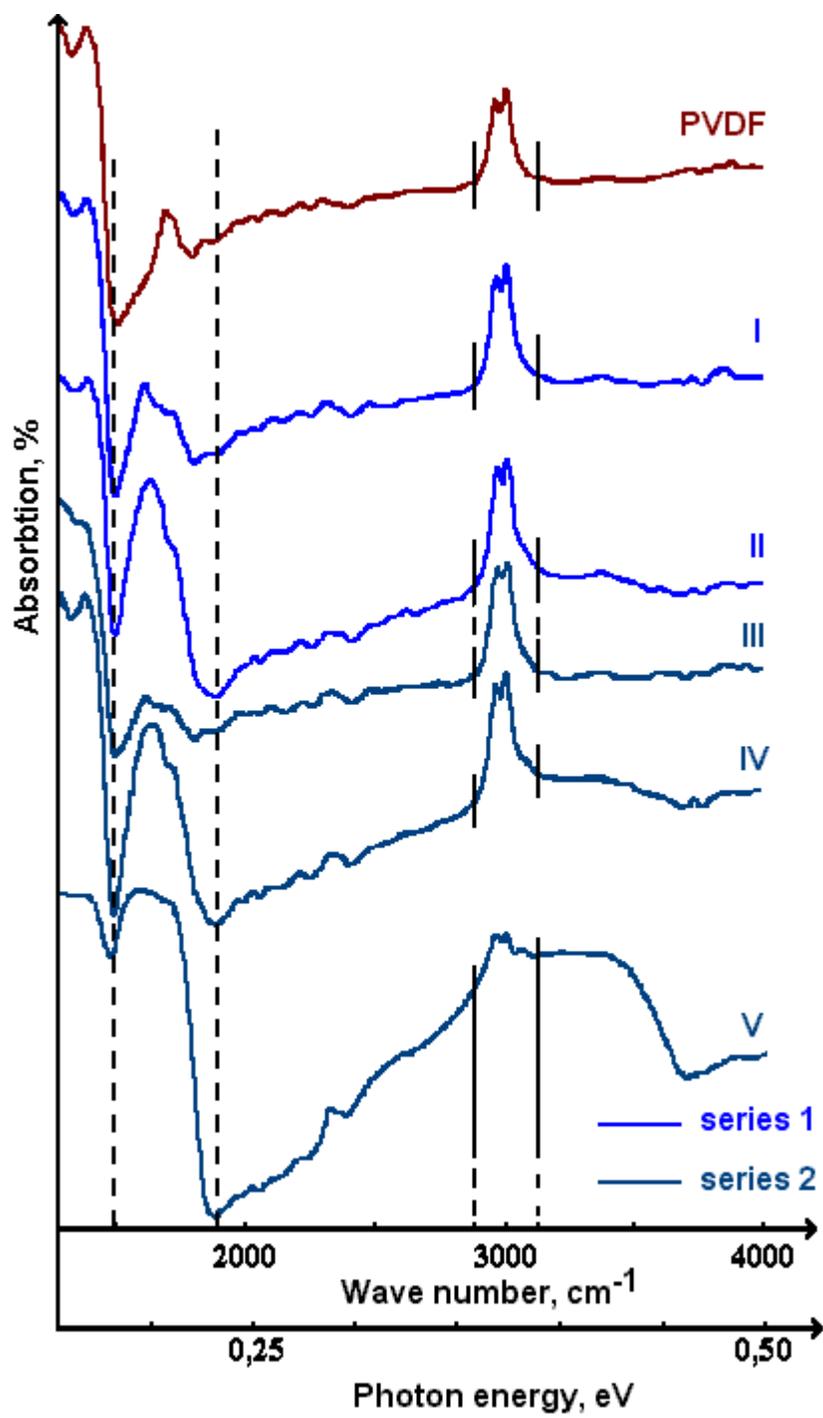
The latter can be a consequence of polar conductivity of carbene chains.

### References

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**Figure 1.** IR-spectra of PVDF and carbinoid samples. The number of the spectra according the following synthesis time: I — 40, II — 120, III — 2, IV — 10, V — 60 min.