FT-IR Study of Iodophenyl-cholesteryl Carbamates

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FT-IR Study of Iodophenyl-cholesteryl Carbamates. *Some new iodophenyl-cholesteryl carbamates were prepared by two methods: by reaction of cholesterylchloroformate with iodophenyl-amines, in the presence of the pyridine to acid acceptor and by direct reaction of sterols with iodophenyl isocyanate. These compounds were characterizes by IR spectroscopy.*

Key words: *Cholesterol, Carbamates, Cholesterylchloroformate, FTIR Spectroscopy, Liquid Crystals*

INTRODUCTION

In this paper we study two cholesteryl carbamates with iodophenyl group at C-3 sterolic. Many cholesteryl esters, expecially carbamates with halogeno substituent on aromatic structures at C-3 sterolic presents liquid crystals properties.

In recent years we synthesized many cholesteric liquid crystals derived from cholesterol with fluoro and chlorophenyl moiety at C-3 sterolic [1, 2] and the influence of the substituent of the side chains in 3 position was investigated [3-5].

The novel fluorine- containing LC are shown to be suitable for super twisted nematic (STN) but also for thin film transistor (TFT) addresed LC displays [6].

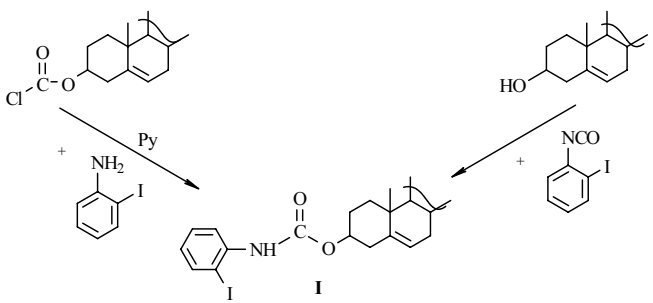
In general, compounds containing a lateral halogeno substituent were synthesized in order to generate a high positive value of the dielectric anisotropy and a low melting point.

RESULTS AND DISCUSSION

The cholesteryl derivative **I** and **II** were prepared by condensation of cholesteryl chloroformate and iodoaniline in the presence of pyridine as proton scravenger [1].

The cholesteryl derivative I was obtain also by direct reaction of cholesterol with o-iodophenyl isocyanate in dry toluene.

The purity of compounds **I** and **II** was checked by TLC.



I **II**

In the IR spectra the most prominent vibrations observed in the iodophenyl cholesteryl carbamates synthesized were the carbonyl group vibration, at 1737 cm^{-1} (strong) for C=O, 1215 cm^{-1} (very strong) for C-Oasym and 1037 cm^{-1} (strong) for C-Osym. NH from urethanic group is a strong vibration at 3451 and 3452 cm^{-1}. For methyl groups from steroid nucleus vibrations were at 2948-2944cm^{-1} and 2867-2864 cm^{-1}.

Table 1 present characteristic vibrations of iodophenyl-cholesterylcarbamates **I** and **II**.

Table 1. IR bands of cholesterylcarbamates **I** and **II**

Compound	IR bands (cm^{-1})				
	C=O	C-O (asim)	C-O (sim)	NH	Another characteristics vibrations
I	1738 (s)	1215 (vs)	1038 (s)	3452 (m)	1529 (s); 1301 (m); 1590 (s); 835 (m)
II	1737 (s)	1215 (vs)	1037 (s)	3451 (m)	1511 (s); 1299 (m); 1590 (s); 834 (m)

EXPERIMENTAL

All solvents were purified by distillation before use. Cholesterol was Merck product; cholesteryl chloroformate, *o*-iodophenyl isocyanate and iodo amines were from Aldrich. The purity of compounds **I** and **II** was checked by TLC silica gel plates 0.25 mm (Merck) and petroleum ether: ethyl ether 9:1 using as eluent mixture.

The FTIR spectra were recorded from pressed KBr pellets using a Jasco 6300 FT-IR spectrometer in the region of 4000 – 400 cm^{-1}, detector TGS, apodization Cosine, software SpectraManager II. The instrument had a spectral resolution of 4 cm^{-1}, which were used in all spectra determinations.

Cholesteryl carbamate **II** from cholesterylchloroformate and cholesteryl carbamate **I** from iodophenyl isocyanate was synthesized by reported methods [5, 7].

CONCLUSIONS AND FUTURE WORK

In the future these iodophenyl cholesterylcarbamates will study to evaluate the effect of iodophenyl group attached at the C-3 position of the sterol nucleus.

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Докладът е рецензиран.