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Synthesis of Liquid Crystals Precursors Containing the Isoxazole Core

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INTRODUCTION

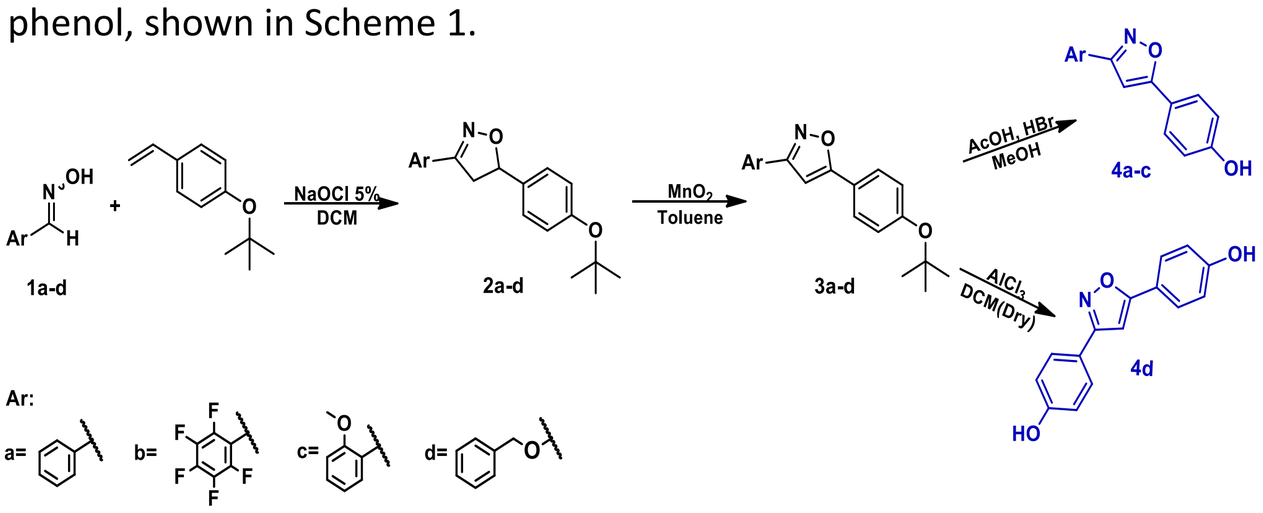
In the world of 5-membered heterocycles, the isoxazole gets some attention due to its wide employability in biological, pharmaceutical and technological products. Beyond their well-known medicinal properties, isoxazoles are interesting intermediates in organic synthesis[1], and play an important role in the achievement of novel liquid-crystalline materials[2].

The combination of different characteristics as small size, high polarity, great stability (due to the high strength of the C-F bond) and low polarizability has stimulated the study of fluorine influence on the control of the liquid-crystalline materials characteristics[3].

In the present work we have synthesized and characterized new bromine-terminated isoxazoles which will be connected to glycerol framework to produce polymerizable liquid crystals allyl monomers.

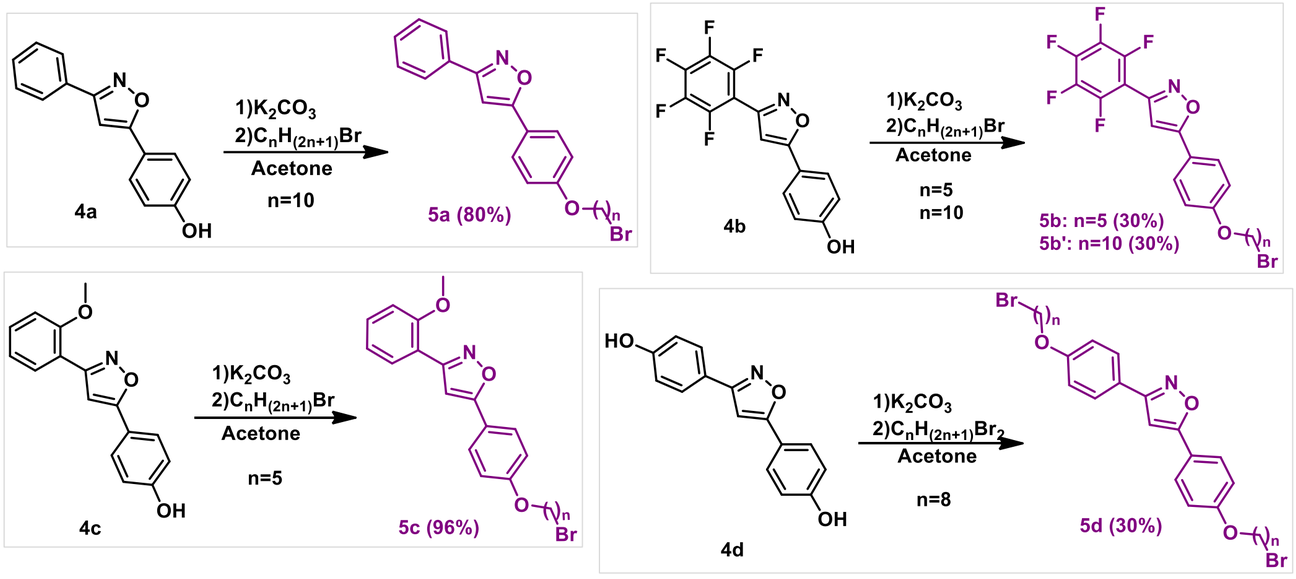
RESULTS AND DISCUSSION

We used the oximes, previously prepared, to obtain the isoxazolines by [3+2] 1,3-dipolar cycloaddition of nitrile oxide with 4-*tert*-butoxystyrene. Followed by MnO_2-oxidation reaction to yield the corresponding isoxazole. To achieve the compounds illustrated below, were necessary remove the protective group in acidic medium or $AlCl_3$ to provide the phenol, shown in Scheme 1.



Scheme 1. Synthetic route to obtain 3,5-disubstituted isoxazoles with phenol group.

After this sequence of reactions, the compounds were alkylated using alkyl dibromide[4] of 5, 8 and/or 10 carbon atoms (Scheme 2).



Scheme 2. Synthetic route for obtaining alkylated **5a-d** compounds with sequences of 5, 8 and 10 carbons.

The products obtained were characterized by ^1H and ^{13}C NMR, Polarized Optical Microscopy (POM) and by Differential Scanning Calorimetry (DSC).

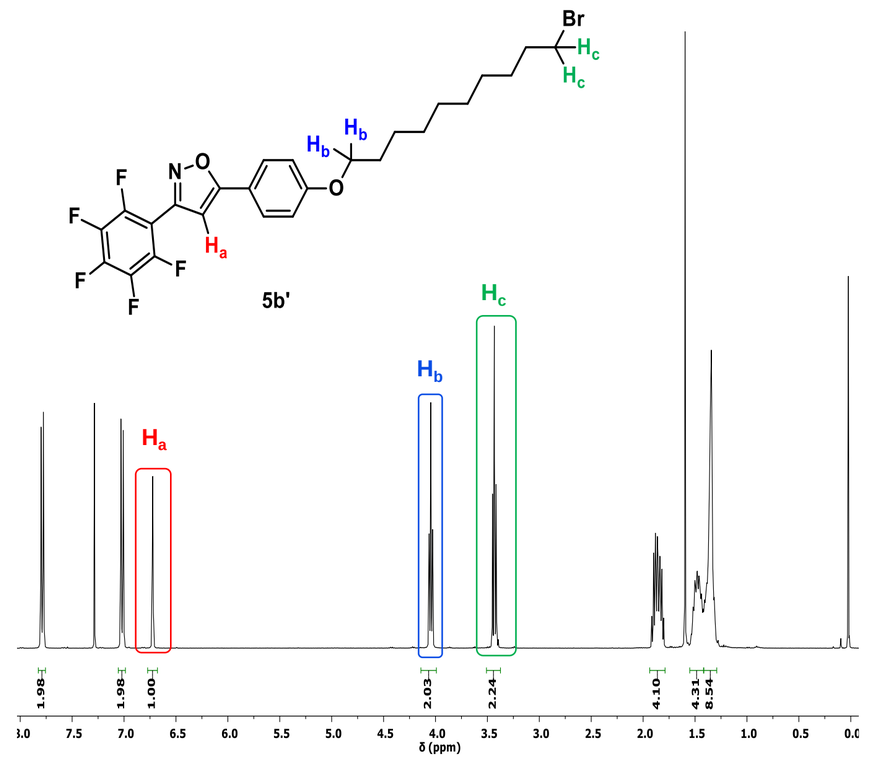


Figure 1. ^1H NMR (300 MHz, $CDCl_3$) of product **5b'.**

In the NMR spectrum we can see the signal of hydrogen atom that characterizes the isoxazole ring (Ha), and two signals Hb and Hc relatated to the methylene group of flexible chain.

CONCLUSION

All the products were obtained with medium yields. Bromine-terminated isoxazoles are excellent advanced precursors to be bonded to the glycerol portion, and then become liquid crystalline materials.

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