Synthesis and properties of new fluorinated isoxazoles

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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, and play an important role in the synthesis of novel liquid-crystalline materials.

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 organic compounds properties.[1] Taking into account the vast amount of exciting research on fluorinated liquid crystals that has been reported, the understanding of how this small atom affects the control of the liquid-crystalline materials characteristics is crucial.

In the present work we have investigated the behaviour between isoxazoles containing hydrocarbons and perfluorocarbons chains starting from basic benzaldehyde and styrene. This comparison of behaviour is very applicable to liquid crystals, which almost always possess hydrocarbon chains in their molecular structure. There are different approaches to prepare disubstituted isoxazoles, here we have prepared a collection of isoxazoles using the reactions shown in the Figure 1. The oxime, previously prepared, reacts with the alkene by [3+2] 1,3-dipolar cycloaddition to give the 3,5-diarylisoxazoline that is oxidized to the correspondent isoxazole.[2]

![Figure 1: Synthesis of isoxazolines by [3+2] 1,3-dipolar cycloaddition followed by MnO2-oxidation reaction.](image)

A wide variety of substituents has been used, then R₁ and R₂ represent perfluorinated or alkyl chains, including mono and trisubstituted, they also represent the fluorine atoms directly bonded to the aromatic ring. The results obtained until now evidence that the inclusion of the fluorine modifies the intermolecular interactions, melting point, transition temperatures, absorption and emission spectra. This work contributes to a better understanding of the structure–property relationship in simple molecules such as 3,5-diarylisoxazoles containing or not fluorine atoms and facilitates the design of new and more complex compounds.

References:

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