

Área: ORG

Exploring the Hantzsch reaction for the synthesis of pyridine-based luminescent discotic liquid crystals

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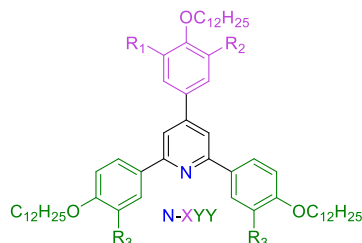
¹ Universidade Federal de Santa Catarina, Florianópolis, Santa Catarina, Brasil.Palavras Chave: Liquid Crystals, Pyridine, *Hantzsch Synthesis*, Organic Electronics, Luminescence, Discotic Materials.

Highlights

Synthesis of Pyridine-Derived Discotic Liquid Crystals via the Hantzsch Methodology for Application in Organic Electronics.

Resumo/Abstract

Although Organic Light-Emitting Diodes (OLEDs) are widely known and used devices in everyday life. Their efficiency remains limited, mainly due to the low light extraction within the device. A promising strategy to overcome this limitation is the alignment of the light-emitting material [1]. In this context, liquid crystals (LCs) stand out as ideal candidates, as they exhibit self-organization as an intrinsic characteristic [2] and can be designed to display luminescence. Therefore, five structures derived from the 2,4,6-triphenylpyridine core were designed and its synthesis planned to occur by the multicomponent Hantzsch methodology [3]. The structures were designed to feature a varied number of aliphatic chains at different positions, aiming to stabilize mesomorphism, reduce symmetry in order to lower transition temperatures, and assess how these structural modifications will affect the thermal, liquid-crystalline, and photophysical properties. Moreover, by comparison with similar molecules containing benzene or 1,3,5-triazine as the central unit, the synthesis of these compounds will allow the evaluation of the effect of the pyridine ring on the material's properties, given that the nitrogen atoms in the central ring promote greater structural planarity due to the absence of hydrogen atoms in these positions. So far, two molecules have been successfully synthesized, N-211 and N-122. Furthermore, the synthetic route reported in the literature was optimized using microwave, reaching greater efficiency and yield in the synthesis. Although both compounds did not exhibit liquid-crystalline behavior, both showed melting points close to room temperature, which is a promising indication that the remaining planned structures may stabilize mesophases within this temperature range.



N-122 R₁, R₂: -H; R₃: -OC₁₂H₂₅
N-211 R₁, R₃: -H; R₂: -OC₁₂H₂₅
N-222 R₁: -H; R₂, R₃: -OC₁₂H₂₅
N-311 R₃: -H; R₁, R₂: -OC₁₂H₂₅
N-322 R₁, R₂, R₃: -OC₁₂H₂₅

Figure 1: Structure of the target molecules

References:

- [1] FIELDS, S. Simulation and Modeling: Surface-plasmon modeling drives OLED design, cutting efficiency loss. *Laser Focus World* (2017).
- [2] WÖHRLE, T. et al. Discotic Liquid Crystals. *Chemical Reviews* vol. 116 1139–1241 (2016).
- [3] Medeiros, J. V. S. et al. Experimental and theoretical study of the photochemical properties and acidochromism of nonconventional 2,4,6-triarylpyridine-based materials. *Dyes and Pigments* 230, 112361 (2024).

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