

Área: ORG

Synthesis and photophysical properties of substituted 2-benzylidene-1-indanones as precursors for the evaluation of novel liquid crystals

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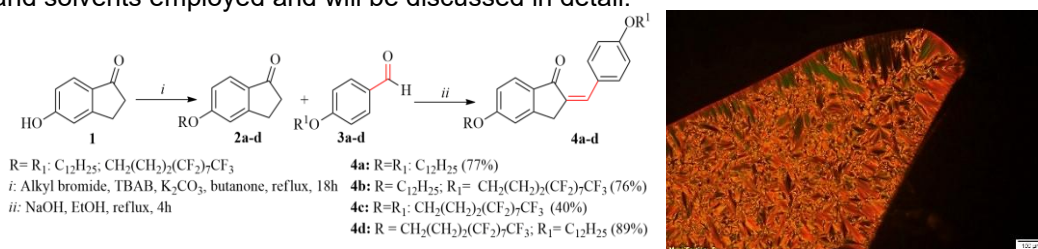
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Highlights

Synthesis of new 2-benzylidene-1-indanone, shows potential for liquid-crystalline mesophases, promising photophysical properties, strongly influenced by substituents and solvents.

Abstract

This work reports the synthesis of four 2-benzylidene-1-indanone derivatives, focusing on their photophysical and thermal properties, as well as the structure–property relationships in mesophase formation, with the objective of broadening the applicability of these compounds. To obtain the **4a-d** derivatives, substituted 4-hydroxy-1-indanones were first synthesized,¹ followed by the preparation of compounds **2a-d** through aldol condensation with aldehydes previously prepared according to literature procedures (Scheme 1).² Compounds **4a-d** were isolated as yellow, white, and beige solids, and characterized by ¹H and ¹³C NMR spectroscopy. In this context, compounds **4a**, **4b**, and **4d** did not exhibit liquid crystalline activity, showing only solid–solid transitions. Furthermore, it is noteworthy that compound **4b** formed needle-shaped crystals upon heating, followed by the isotropic state. In contrast, sample **4c** exhibited a smectic C (SmC) mesophase above 157.9 °C, and transitioned to the isotropic state at 169.35 °C. Upon cooling, the SmC mesophase reappeared above 168.21 °C, followed by a crystal–crystal transition between 149.98 and 116.92 °C. Therefore, it is concluded that the less flexible semiperfluoroalkyl chain promotes the formation of ordered liquid-crystalline phases, due to the high polarity, stability, and low polarizability conferred by substituent.¹ This property is further supported by the DSC analysis obtained for this sample and will be presented subsequently. In addition, the photophysical studies of these compounds are consistent with literature data,³ showing absorption bands at 350 nm and emission around 438 nm. It is also worth noting that the spectral properties depend on the polarity of both substituents and solvents employed and will be discussed in detail.



Scheme 1. Synthesis, texture of mesophase SmC for **4c**

¹Lopes, L. D., & Merlo, A. A. *Molecular Crystals and Liquid Crystals*, v. 1, n. 612, p.149–157, 2015

²Ren, T. B., Xu, W., et. al., *Angewandte Chemie - International Edition*, n. 25, v. 57, p. 7473–7477, 2018

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