

N°1504 / PC

TOPIC(s) : Alternative solvents / Clean reactions

## Effect of the Alkyl Substituent in the Mesomorphic Properties and Conductivity of 2-Picolinium Ionic Liquid Crystals

### AUTHORS

Andreia F. M. SANTOS / FCT-NOVA, LAQV-REQUIMTE, DEPARTMENT OF CHEMISTRY, NOVA SCHOOL OF SCIENCE AND TECHNOLOGY, NOVA UNIVERSITY OF LISBON, CAMPUS DE CAPARICA, CAPARICA

Maria H. GODINHO / FCT-NOVA, I3N/CENIMAT, DEPARTMENT OF MATERIALS SCIENCE, NOVA SCHOOL OF SCIENCE AND TECHNOLOGY, NOVA UNIVERSITY OF LISBON, CAMPUS DE CAPARICA, CAPARICA

J. L. FIGUEIRINHAS / IST-UL, CEFEMA AND DEPARTMENT OF PHYSICS, INSTITUTO SUPERIOR TÉCNICO, UNIVERSITY OF LISBON, AV. ROVISCO PAIS, 1, LISBON

Luis C. BRANCO / FCT-NOVA, LAQV-REQUIMTE, DEPARTMENT OF CHEMISTRY, NOVA SCHOOL OF SCIENCE AND TECHNOLOGY, NOVA UNIVERSITY OF LISBON, CAMPUS DE CAPARICA, CAPARICA

Madalena DIONÍSIO / FCT-NOVA, LAQV-REQUIMTE, DEPARTMENT OF CHEMISTRY, NOVA SCHOOL OF SCIENCE AND TECHNOLOGY, NOVA UNIVERSITY OF LISBON, CAMPUS DE CAPARICA, CAPARICA

Corresponding author : Madalena DIONÍSIO / madalena.dionisio@fct.unl.pt

### PURPOSE OF THE ABSTRACT

Thermotropic ionic liquid crystals are molecular salts, which self-assemble into liquid crystals whose mesophase is thermally induced. These materials have emerged during the last decades due to fact that they combine the characteristics of both liquid crystals and ionic liquids, allowing the design of new molecules with broad variability of polarity, solubility, viscosity, transition temperatures and electrochemical window, as well as defined anisotropic physical properties [1]. It is known that the mesomorphic behaviour is associated to the combination of the rigidity addressed to the cation and the flexibility of the alkyl moiety. In the case of the latter, sizes between C6 and C18 have been reported as suitable to imprint the desired ordering to form a liquid crystal [2]. In this context, ionic liquid crystals (ILCs) based on 2-picolinium bromides possessing different alkyl substituents were prepared, namely [C6-2-Pic][Br], [C12-2-Pic][Br] and [C16-2-Pic][Br]. The syntheses of ILCs were carried out on a microwave apparatus to avoid the use of organic solvents, which revealed to be an effective and greener alternative when compared to the conventional heating methods. Moreover, all materials were characterised by spectroscopic techniques ( $^1\text{H}$  and  $^{13}\text{C}$ -NMR; ATR-FTIR), Thermogravimetric Analysis, Differential Scanning Calorimetry, Polarized Optical Microscopy and X-Ray Powder Diffraction. In general, it was observed that the mesomorphic behaviour changes with the alkyl chain where [C6-2-Pic][Br] is non-thermomesomorphic, as no temperature-driven liquid crystalline transitions are detected. On the other hand, upon heating, [C12-2-Pic][Br] exhibits a smectic phase with ordered layers, while [C16-2-Pic][Br] has a disordered lamellar liquid crystalline phase. Furthermore, conductivity of all materials was measured from 10<sup>-1</sup> to 10<sup>6</sup> Hz and over a large temperature range between -90 and 160 °C. The plot of conductivity at low frequencies against temperature reciprocal is sensitive to the phase transitions/transformations undergone by the respective material. Moreover, it clearly illustrates the different charge transport mechanism associated to each material, going from non-Arrhenius ([C6-2-Pic][Br]) to Arrhenius-type ([C12-2-Pic][Br] and [C16-2-Pic][Br]) with several regimes.

Acknowledgments: This work was supported by the Associate Laboratory for Green Chemistry LAQV (UID/QUI/50006/2019), i3N (UID/CTM/50025/2019) and CeFEMAS (UID/CTM/04540/2019), which are financed by national funds from FCT-MCTES and by FEDER funds through the COMPETE 2020 Program. The authors also thank the National Funds through FCT-MCTES and POR Lisboa 2020, under the projects numbers POCI-01-0145-FEDER-007688, PTDC/CTM-REF/30529/2017 (NanoCell2SEC) and Action European Topology

Interdisciplinary Action (EUTOPIA CA17139). A. F. M. Santos acknowledges FCT-MCTES for the PhD Grant (SFRH/BD/132551/2017).

## FIGURES

FIGURE 1

FIGURE 2

---

### KEYWORDS

Ionic Liquid Crystals | Alkyl 2-Picolinium Salts | Differential Scanning Calorimetry | Dielectric Relaxation Spectroscopy

---

### BIBLIOGRAPHY

- [1] N. Kapernaum, A. Lange, M. Ebert, M. A. Grunwald, C. Haege, S. Marino, A. Zens, A. Taubert, F. Giesselmann and S. Laschat, *ChemPlusChem*. 2022, 87, 1-38.
- [2] A. A. Fernandez and P. H. J. Kouwer, *Int J Mol Sci*. 2016, 17, 731 (1-31).