

# Imidazole and benzoimidazole derived new ionic liquid crystal compounds: synthesis, characterisation, mesomorphic properties and DFT computations

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## ABSTRACT

Four new series of ionic liquid crystals derived from imidazole bromonium and benzimidazole bromonium salts with spacer alkyl chain ( $C_n$ ,  $n = 2, 4$ ) were synthesised and characterised. The following tests and measurements have been performed: the FT-IR,  $^1H$ -NMR and  $^{13}C$ -NMR spectroscopy in addition to a CHN elemental analysis techniques. Both the differential scanning calorimetry and the polarising optical microscopy measurements are applied for the evaluation of liquid crystals properties. The outcome confirms the existence of a smectic A liquid crystalline phase. A Density Functional Theory computations were performed to obtain the shape of the molecular structure that corresponds to the ground-state energy.