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Data Article

Synthesis and characterization data of monocationic and dicationic ionic liquids or molten salts

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ABSTRACT

Data presented in this article are related with the research paper entitled "Ecotoxicity assessment of dicationic versus monocationic ionic liquids as a more environmentally friendly alternative" [1]. The present article describes the synthesis steps and characterization data of a set of twenty-six imidazolium, pyrrolidinium and pyridinium-based ionic liquids (ILs) or molten salts: nine monocationic and seventeen dicationic. Specifically, the chemical structure of the compounds was confirmed by ¹H NMR, ¹³C NMR and ¹⁹F NMR spectroscopy and mass spectrometry (MS). Other data such as physical state at room temperature, melting point temperature (for solids at room temperature) and thermal decomposition temperature (when melting was not reached before decomposition) of the ILs or molten salts are also reported here.

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Specifications Table

Subject area	Chemistry
More specific subject area	Synthesis and characterization of ionic liquids or molten salts
Type of data	Tables, figures

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How data was acquired	¹ H, ¹³ C and ¹⁹ F NMR spectra were recorded on a Jeol model EX270 instrument. MS was recorded on a Bruker MicroTOF 61 spectrometer. Melting point temperature was recorded on a Büchi Melting Point B-540 instrument. Thermal decomposition temperature was acquired by Differential Scanning Calorimetry on a DSC 2920 (TA instruments) instrument.
Data format	<i>Raw and analyzed data</i>
Experimental factors	<i>Samples were dried under vacuum overnight before their characterization.</i>
Experimental features	<i>Relevant data on the characterization of the ILs or molten salts were determined.</i>
Data source location	<i>University of Murcia, Murcia, Spain, Europe</i>
Data accessibility	<i>The data are provided with this article.</i>
Related research article	<i>M.G. Montalbán, G. Villora, P. Licence, Ecotoxicity assessment of dicationic versus monocationic ionic liquids as a more environmentally friendly alternative, Ecotox. Environ. Safe. 150 (2018) 129–135.</i>

Value of the Data

- All the steps for the synthesis of the ILs or molten salts here described and the methods can be followed by other researchers.
 - The chemical synthesis of some of these ILs or molten salts had not been reported before.
 - NMR spectra and MS data of the ILs or molten salts synthesized are useful for structural characterization of these and other similar ILs or molten salts.
 - Data on melting point and decomposition temperature of these ILs or molten salts can be valuable for the design of their applications.
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1. Data

The abbreviations, molecular weights and structures of the ILs or molten salts are presented in [Table 1](#). The synthesis steps necessary for the preparation of the ILs or molten salts are described then in detail. After the report of the chemical synthesis of the ILs or molten salts, their characterization (NMR spectra and MS) is included. [Figs. 1–20](#) show the ¹H NMR and ¹³C NMR spectra of the novel compounds. Finally, [Table 2](#) collects the physical state of the ILs or molten salts at room temperature, their colour, melting point (for solids at room temperature) and decomposition temperature (when melting is not reached before thermal decomposition).

2. Experimental design, materials, and methods

See [Table 1](#)

3. Synthesis and characterization of ILs

C₈(MIm)Br was synthesized following procedures described in the literature with modifications [\[2,3\]](#). 100 mmol of 1-methylimidazole was placed in a round bottom flask fitted with a reflux condenser and an additional funnel under a static atmosphere of Ar. 110 mmol of 1-bromooctane was added dropwise *via* a pressure equalising addition funnel while the mixture was stirred at 60 °C under inert atmosphere. The additional funnel was removed and the reaction mixture was stirred at

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