

Chemistry Department

## Optimizing Ionic liquids for CCS

Molecular Structure & Interactions NMR group

MSI NMR group



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(Pos-doc researcher)

- Graduated in *Applied Chemistry* (1996, FCT/UNL).
- PhD in *Organic Chemistry* (2003, UNL).
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## Objectives

Ionic liquids (ILs) have been proposed as alternative materials for Carbon Capture and Sequestration (CCS). My goal is to understand the CO<sub>2</sub> solvation process in ILs. To accomplish this I study neat ILs in order to learn more about their liquid structure and also ILs/solvent mixtures to gain an insight into all the interactions taking place.

## Methodology

I use conventional and High Pressure NMR (HP-NMR) to study ILs (Fig. 1). In our group we developed an HP-NMR methodology that allows the study of IL structure and the solvation mechanism. This methodology is focused on NOE and multinuclear diffusion NMR experiments (Fig.2), using the PGSE techniques. HP-NMR combined with molecular simulations (Fig. 3) provides an insight to the nature of cation/anion/CO<sub>2</sub> relationship.

## Expected Results

Through our NMR rationalization approach we aim to achieve a molecular detailed picture of CO<sub>2</sub> solvation in ILs that allows the proposal of new and improved ILs, tailored for CO<sub>2</sub> capture and, in the long run to contribute to the climate change mitigation efforts.

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Fig. 1 – HP-NMR tubes

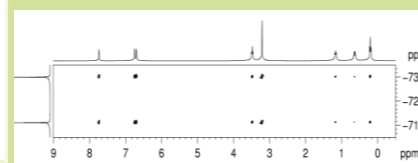


Fig. 2 – <sup>1</sup>H, <sup>19</sup>F-HOESY spectra of BMIMPF<sub>6</sub> at 80 bar CO<sub>2</sub>

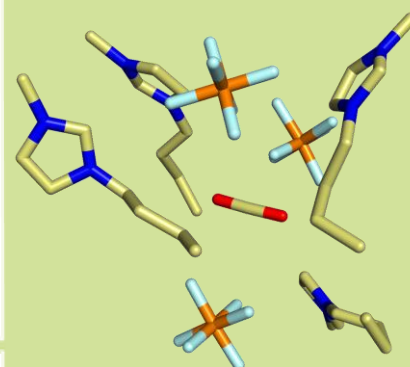


Fig. 3 – IL/CO<sub>2</sub> MD simulation