



## Detection by ESI-MS of Negative Charge-Tagged NHC

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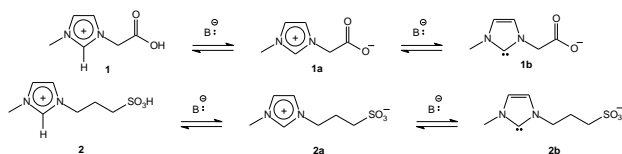
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### INTRODUCTION

Ionic liquids (IL) are a class of compounds that are used in several areas of technology. Imidazolium-based IL can be deprotonated at C2 position, due to the relative acidity of the C2-H hydrogen,<sup>1</sup> leading therefore to the formation of N-Heterocyclic carbenes (NHC). NHC are highly reactive species that possess a very short half-life,<sup>2</sup> being a hard task its experimental detection. We report herein the use of a negative charge tag for imidazolium NHC derivatives detection and characterization by ESI(-)MS/MS).

### RESULTS AND DISCUSSION

**MAI.CI (1)** and **MSI.CI (2)** are functionalized imidazolium IL (Scheme 1) that upon a double deprotonation afford charge-tagged NHC.



Scheme 1. Negative charge-tagged NHC.

Compounds **(1)** and **(2)** were submitted to ESI(-)MS experiments displaying ions of  $m/z$  139 and  $m/z$  203 (Figure 1).

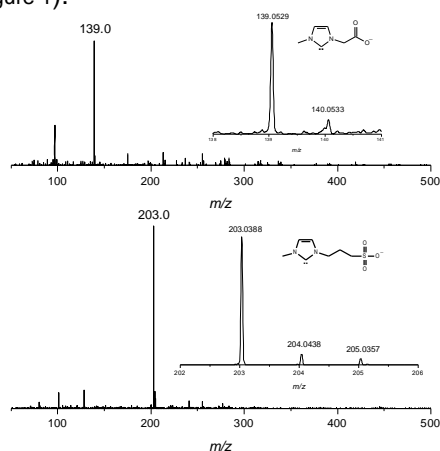


Figure 1. ESI(-)MS of IL **1** and **2** after KOtBu addition.

To confirm the structure of the detected ions, these charge-tagged NHC were submitted to ion-molecule gas phase reactions (Figure 2, Scheme 2).

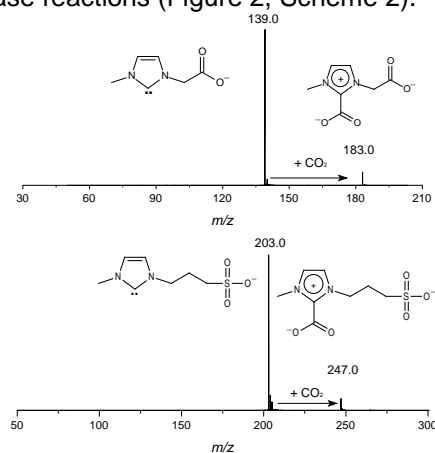
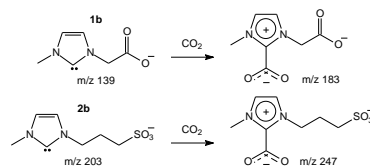


Figure 2. ESI(-)MS for the ion-molecule gas phase reactions.



Scheme 2. Gas-phase carboxylation of **1b** and **2b**.

The incorporation of the CO<sub>2</sub> in the structures are in accordance with the expected reactivity of NHC derivatives

### CONCLUSION

NHC derivatives from functionalized imidazolium IL are detected by ESI-MS negative ion mode due to the presence of a charge tag in the IL structures.<sup>3</sup>

### ACKNOWLEDGEMENTS

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