

Charge-tagged ligands derived of 1,3-imidazolium ion as catalyst precursor of copper, nickel and palladium

Felipe F. D. Oliveira,* Priscila M. Lalli, Eduardo M. Schmidt, Peter Bakuzis, Alexandre A. M. Lapis, Marcos N. Eberlin, Brenno A. D. Neto

Laboratory of Medicinal and Technological Chemistry, Chemistry Institute, University of Brasília (IQ-UnB).

*felipefeitosa.oliveira@gmail.com

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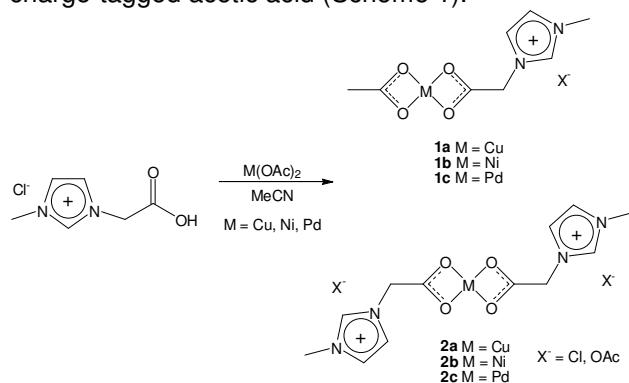
INTRODUCTION

ESI-MS is a soft ionizing technique,¹ which may allow an online monitoring of a plethora of reactions. Valuable information such as coordination, oxidation states of metal center and others may be obtained by ESI-MS.

Based on that, we synthesized a charge-tagged ligand as a precursor to an *in situ* formation of a charge-tagged catalyst palladium, copper and nickel. Herein, we describe the gas phase chemistry of the palladium-derivatives.

RESULTS AND DISCUSSION

All metal derivatives were synthesized *in situ* using a charge-tagged acetic acid (Scheme 1).



Scheme 1. Mono and doubly charge-tagged complexes expected to be generated *in situ*.

The monitoring of the reaction with palladium by ESI(+)-MS(MS) allowed the detection and characterization of two sets of abundant: *m/z* 304, corresponding to the mono-charged **1c**, and that of *m/z* 445 corresponding to the doubly charged **2c** associated to an OAc⁻ anion, that is, [**2c.OAc**]⁺.

In the mono-charged species **1c**, it is observed the loss of the acetate radical. The doubly charged species **2c** (Figure 1) shows the loss of an acetate radical, indicating that the acetate radical is directly linked to the metal center, as shown Scheme 2.

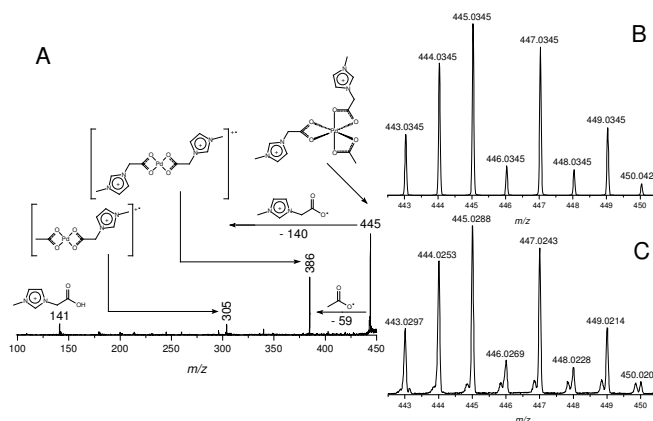
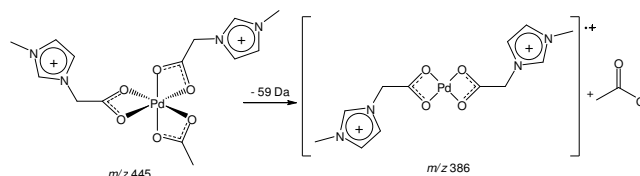


Figure 1. (A) ESI(+)-MS/MS of [**2c.OAc**]⁺ *m/z* 445 and its (B) calculated and (C) experimental isotopologue patterns.



Scheme 2. Possible route for dissociation of [**2c.OAc**]⁺.

Moreover, some coordinating solvent (acetonitrile) species could be detected and characterized by ESI-MS.

CONCLUSION

The use of a charge-tagged ligand allowed an interesting chemistry for its palladium complex in the gas phase and helped towards a better understanding of some catalytic active species generated using palladium derivatives.

ACKNOWLEDGEMENTS

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