

Palladium catalyzed Heck-lactonization from *ortho*-iodophenols and enoates: Synthesis of coumarins and the study of the mechanism by electrospray ionization mass spectrometry

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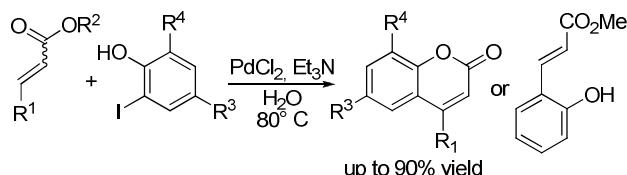
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INTRODUCTION

The arylation of olefins, discovered by Heck and Mizoroki, is one of the most important palladium-catalyzed carbon-carbon coupling reactions.¹ Coumarins display many biological activities² and more recently, could be obtained by Heck-lactonization reaction.³

RESULTS AND DISCUSSION

In earlier studies by our research group, the tandem Heck-lactonization reaction between enoates and *ortho*-iodophenols leading to the corresponding coumarins was investigated under several conditions and three procedures were selected.^{3c} More recently, we extend the scope of this reaction (Scheme 1) and studied this reaction by electrospray ionization mass spectrometry.⁴



Scheme 1. Heck and Heck-lactonization reaction in aqueous medium.

A lot of coumarins, with withdrawing and releasing groups, was synthesized and some examples are showed in the Figure 1.

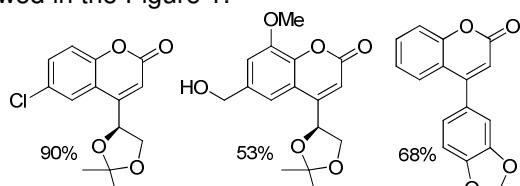


Figure 1. Some coumarins synthesized by Heck reaction.

Intercepted cations by ESI-MS experiment are showed in Figure 2.

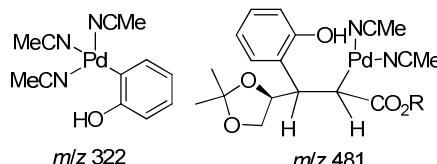


Figure 2. Intercepted cations by MS(+)-MS, after dilution in MeCN.

CONCLUSION

Heck-lactonization reaction gives coumarins in a simple way, in aqueous medium and absence of ligands and the ESI-MS experiment suggest that this reaction goes to the cationic mechanism.

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