



On the Ugi mechanism probed by ESI-MS(/MS)

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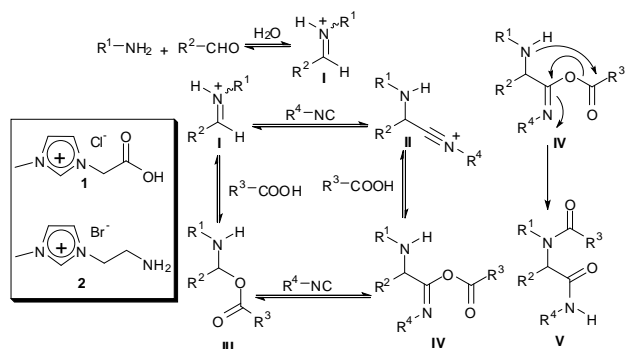
Keywords: Ugi MCR, Charge tags, ESI-MS(/MS).

INTRODUCTION

The interest over multicomponent reactions (MCR) has increased substantially.¹ Among MCR of four components, the Ugi Reaction (U4CR) has attracted special interest owing to its versatility and facility to generate new libraries of bioactive compounds.²

RESULTS AND DISCUSSION

Scheme 1 shows the two charge-tagged reagents used to probe the mechanism and the two accepted reaction pathways for the U4CR.



Scheme 1. Charge-tagged reagents and the two accepted reaction pathways for the Ugi four-component reaction.

Figures 1 and 2 show the ESI(+)-MS/MS (from Water Synapt) spectra of the ions of m/z 343 and of m/z 221, respectively.

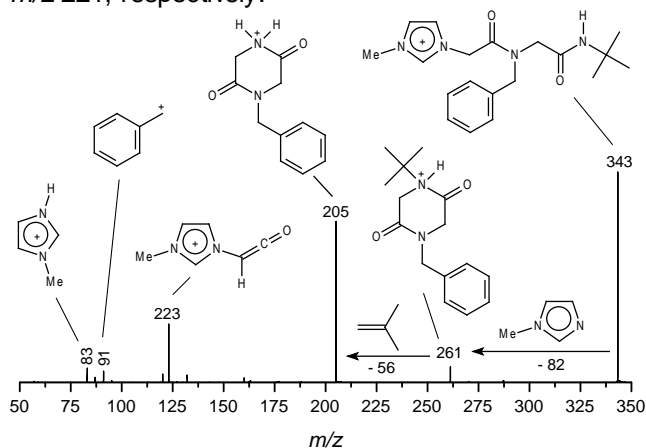


Figure 1. ESI(+)-MS/MS of the ion of m/z 343 (intermediate V).

It is noted that these two ions could only be detected due to the presence of the charge tags.

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The final rearrangement was also evaluated by means of DFT calculations (Figure 3).

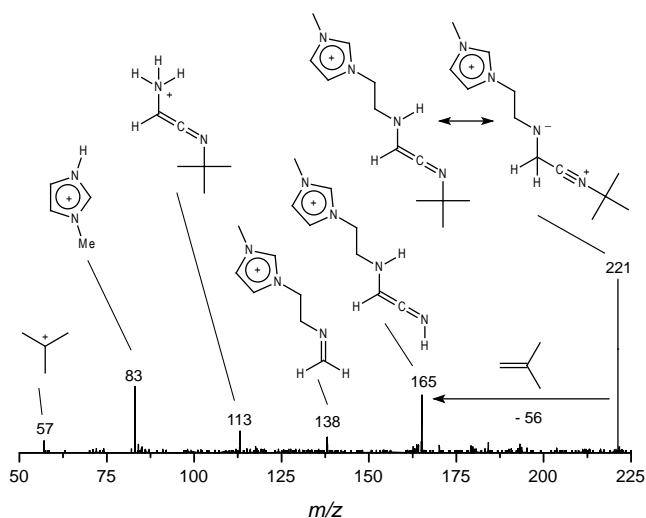


Figure 2. ESI(+)-MS/MS of the ion of m/z 221 (intermediate II).

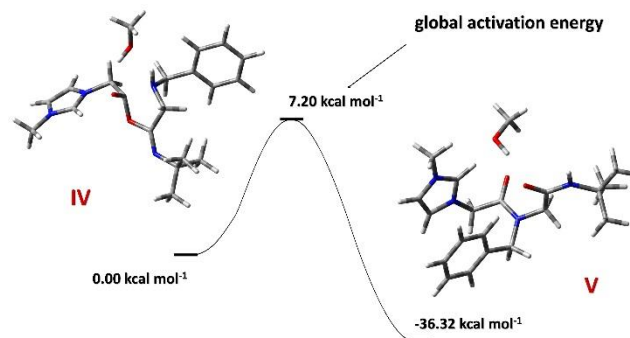


Figure 3. Rearrangement from IV to V. M062X/6-311+G(2d, 2p)//M062X/6-31+G(d,p) level of theory. Methanol has been considered with explicit treatment for the calculated structures.

CONCLUSION

The iminium mechanism seems to be the most probable once its intermediates are the most stable.

ACKNOWLEDGEMENTS

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