

Charge-Tagged *N*-Heterocyclic Carbenes

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Supplementary Material

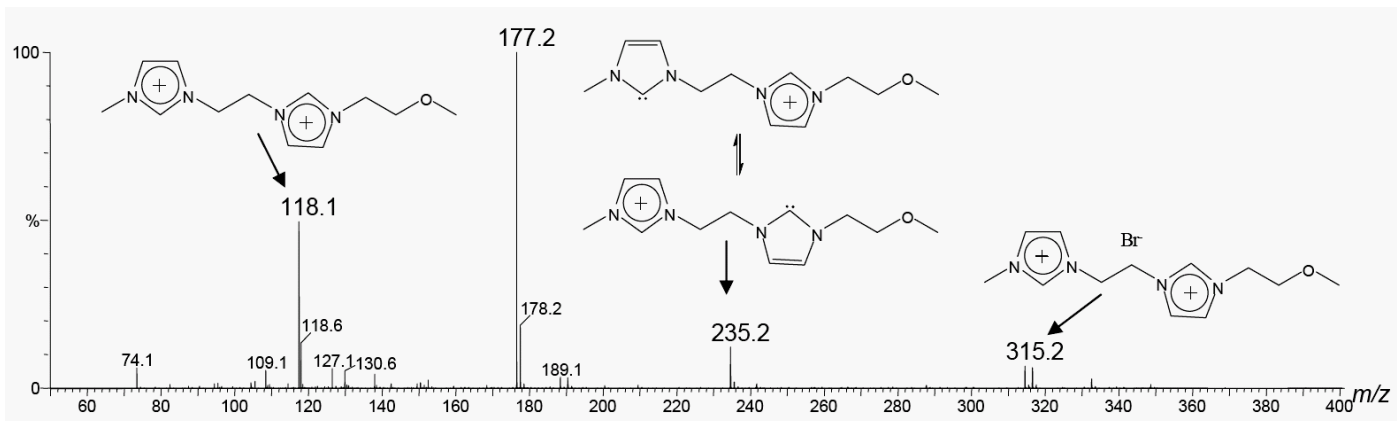


Figure S1 - ESI(+)-MS of a methanolic solution of **3f**.Br₂. Note the detection of the doubly charged imidazolium ion **3f**²⁺ of m/z 118.1 (as well as the isotopologue ion of m/z 118.6) and the singly charged [**3f**.Br]⁺ of m/z 313/315, and the unprecedented charge-tagged carbene **4f**⁺ of m/z 219 directly sampled from solution (or formed via in-source CID of [**3f**.Br]⁺).

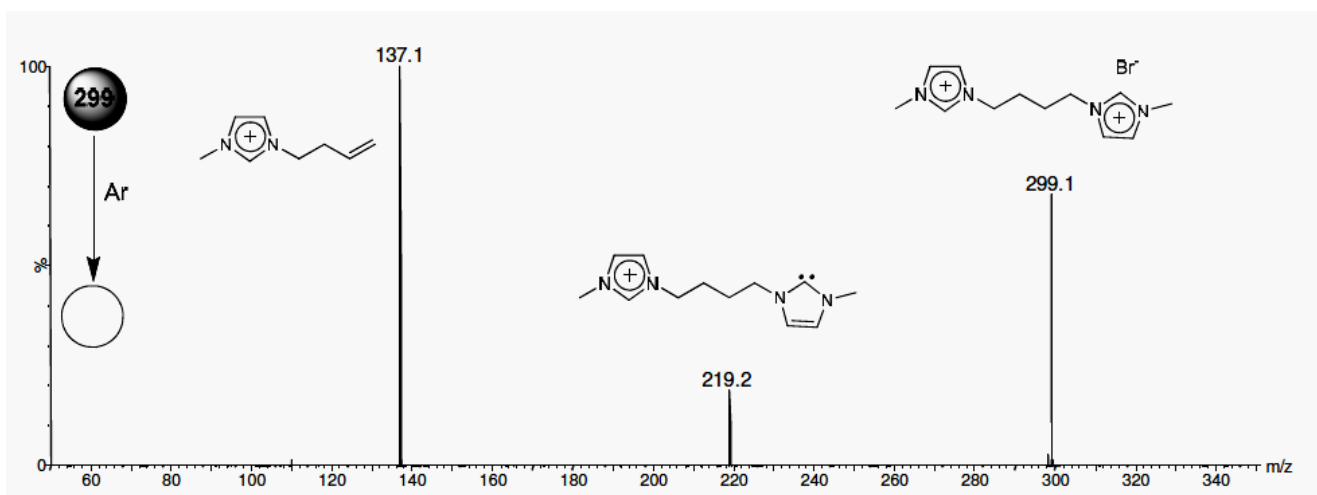


Figure S2 – ESI(+)-MS/MS of [3a.Br]⁺ of *m/z* 299.

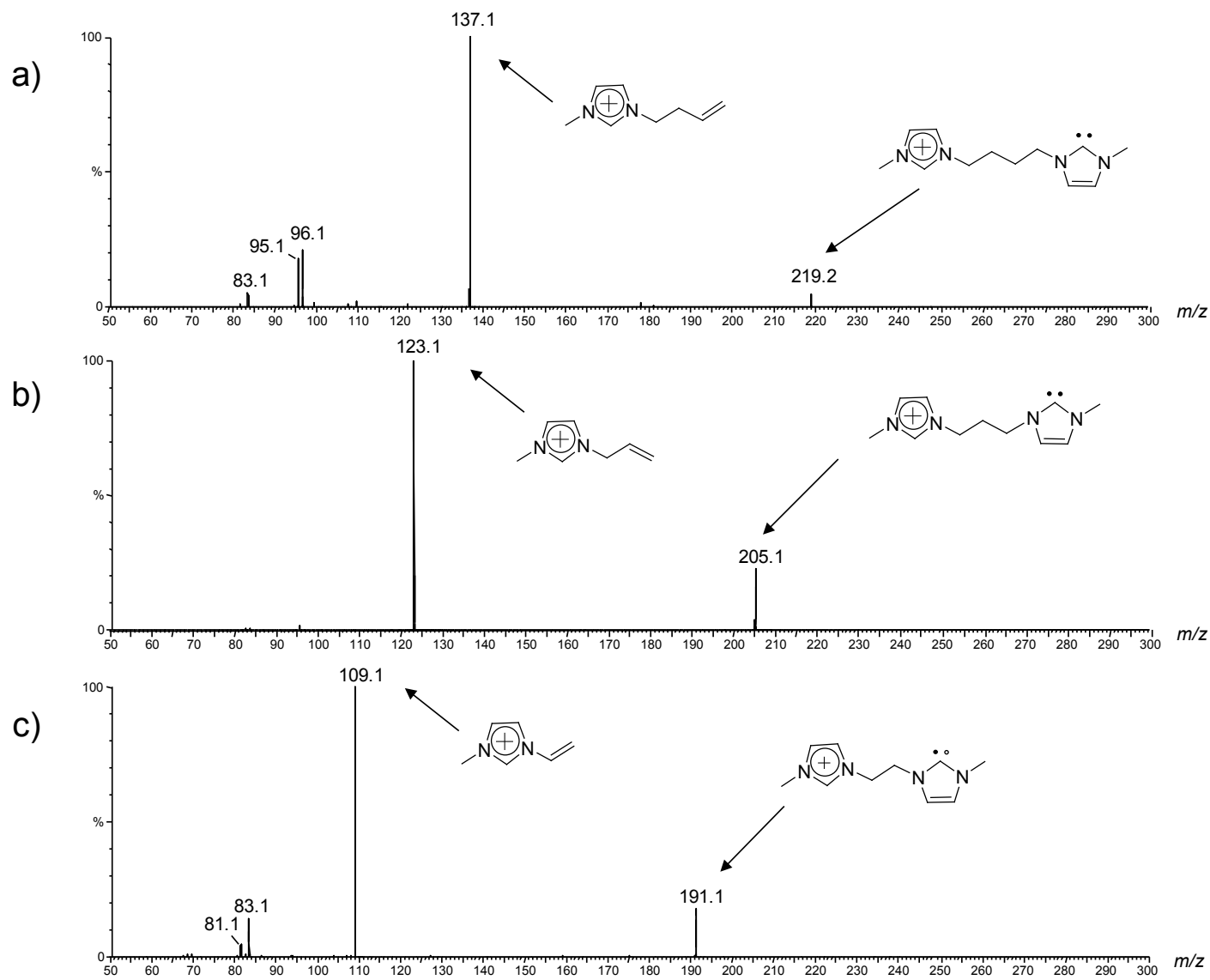


Figure S3 – ESI(+)-MS/MS for the charge-tagged carbenes a) $4a^+$ of m/z 219 b) $4b^+$ of m/z 205 and c) $4c^+$ of m/z 191.

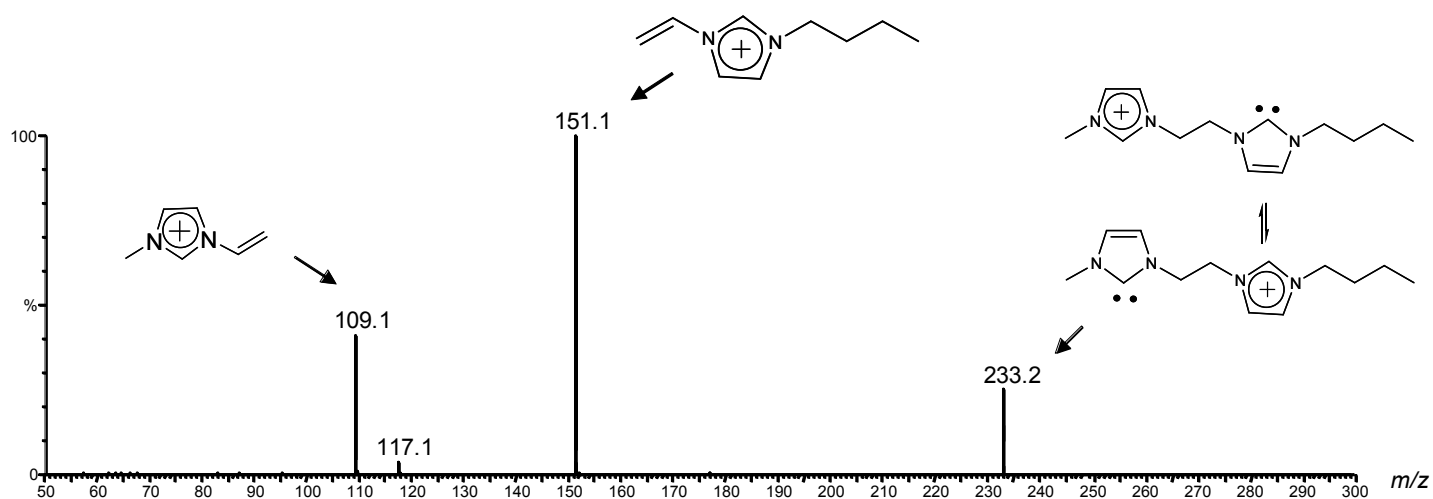


Figure S4 - ESI(+)-MS/MS of the asymmetric charge-tagged carbene **4e⁺** of *m/z* 233.

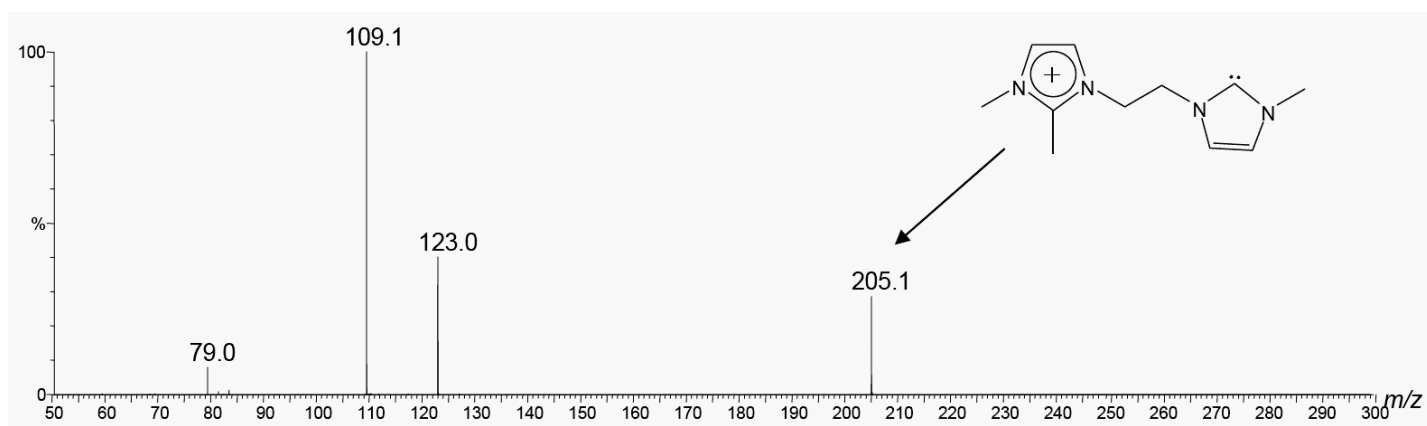


Figure S5 – ESI(+)-MS/MS for the charge-tagged carbene **4d**⁺ of *m/z* 205.

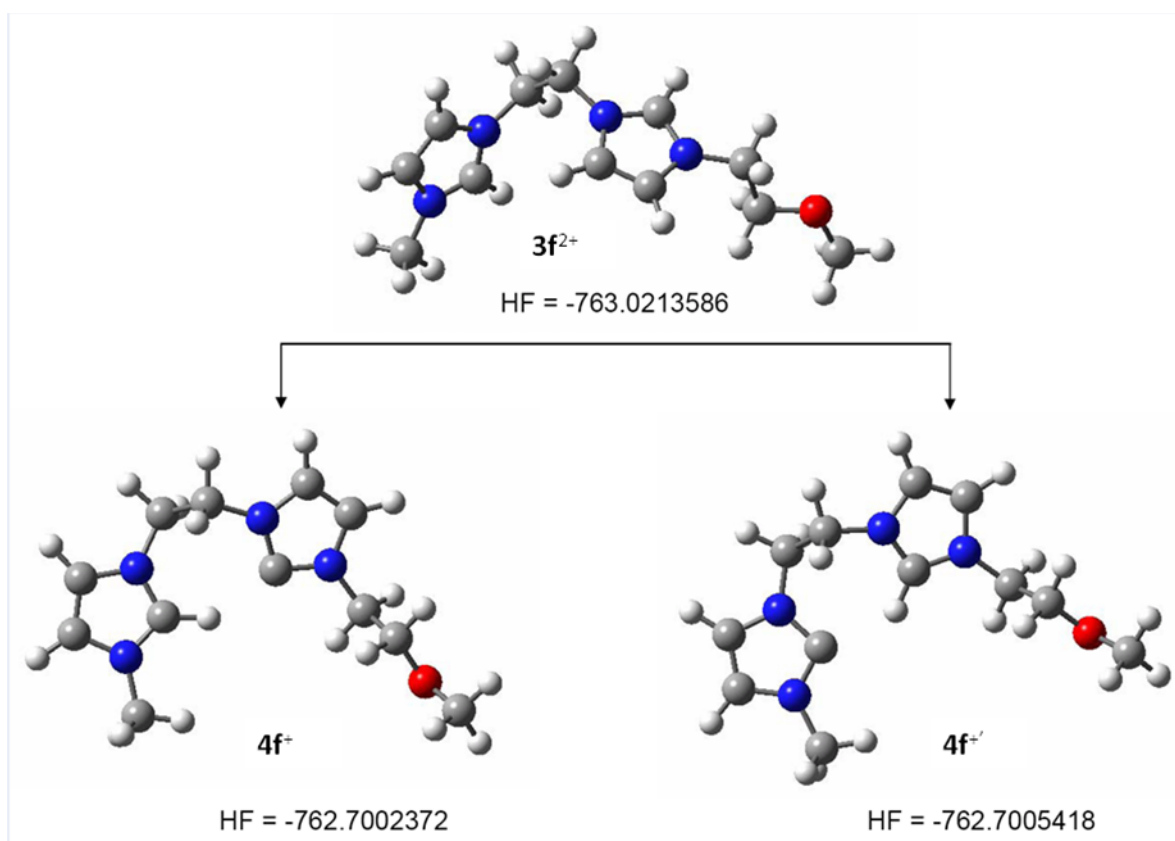


Figure S6. Beck3LYP 6-31G+(d,p) energies (HF energies in hartrees) and optimized structures for the isomeric $4f^+$ and $4f^{+'}$.

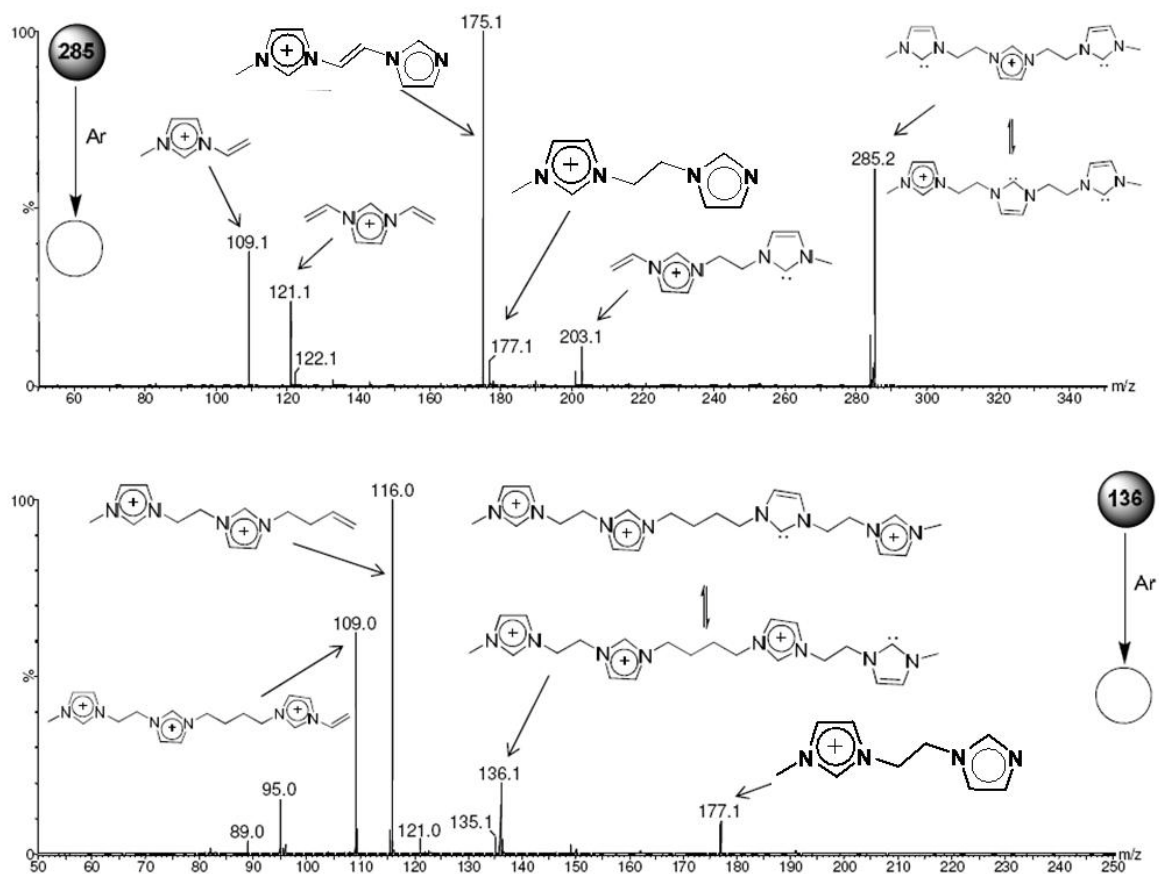
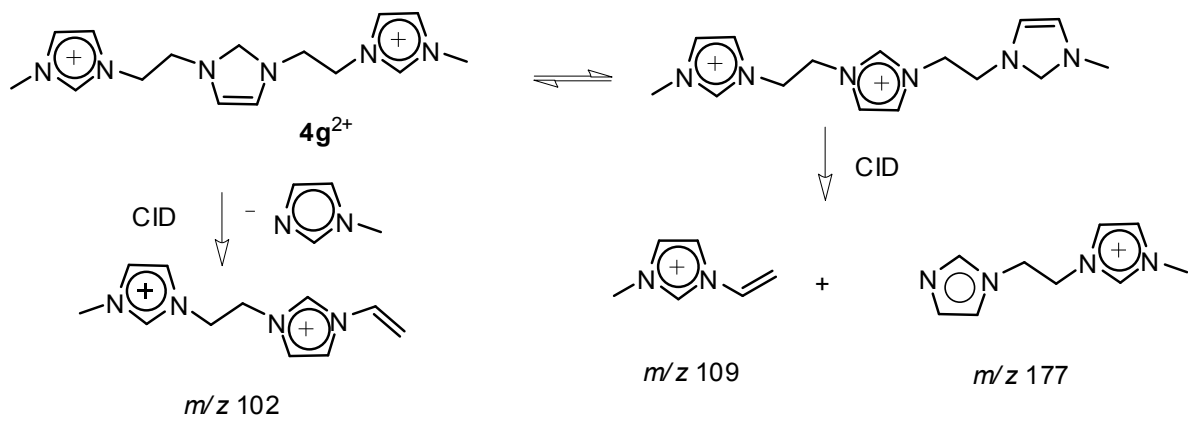


Figure S7 – ESI(+)-MS/MS of a) the singly charged di-carbene **4h**⁺ of *m/z* 285 and b) the triply charged mono-carbene **4j**³⁺ of *m/z* 136.



Scheme S1