

Explanation of EI Fragmentation Mechanisms for PCP Related Compounds

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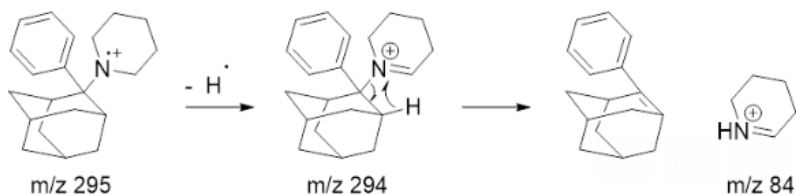
8/20/2022

James,

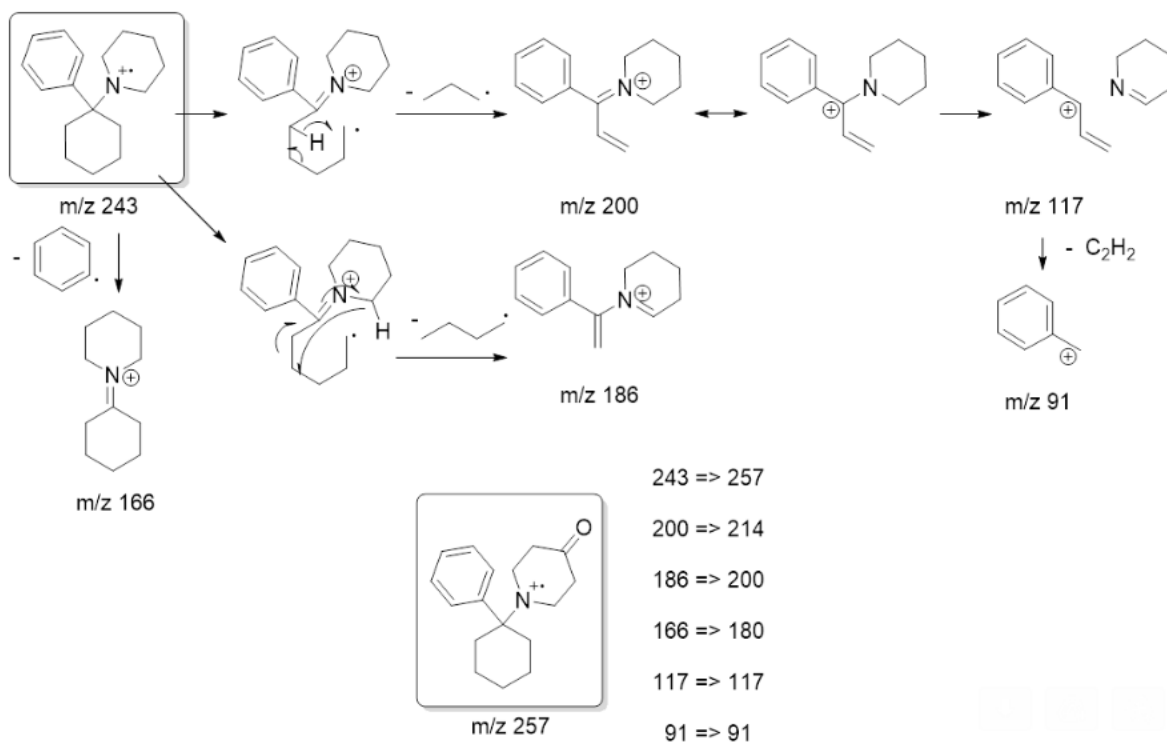
I have some explanation here.

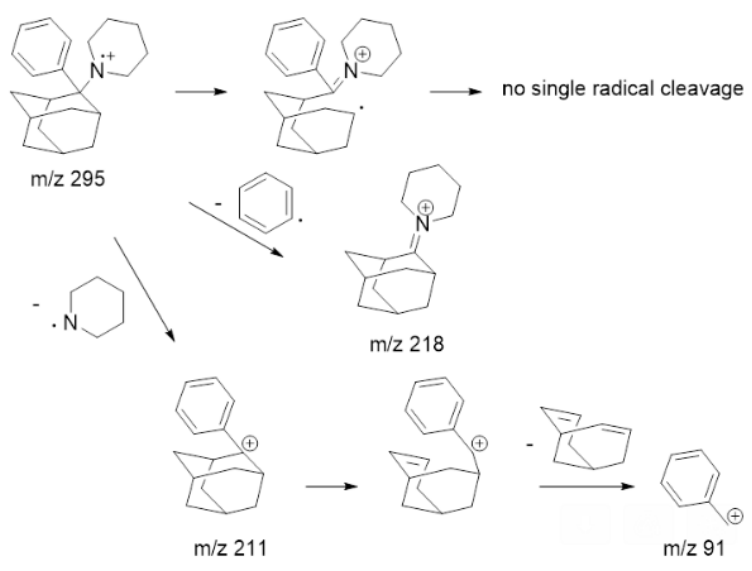
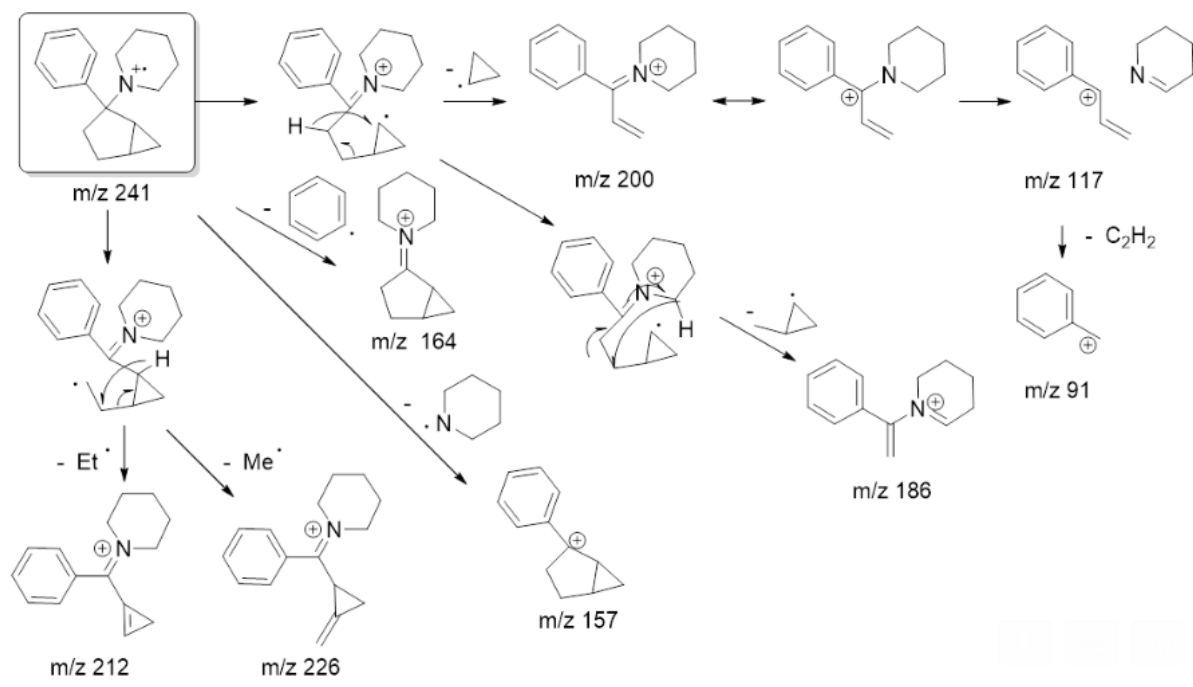
First, all of these compounds have an important M-H, probably losing one H in position alpha to the N.

They all show m/z 84 (with the keto compound it is seen at 98) and this 84 arises from something like this:



Then, the main difference between these PCP derivatives is the possibility of a good radical cleavage (or not) from the cyclohexyl ring. If not, only the peaks at M-77 and M-84 remain and are intense by default. The neutral loss M-77 is the aromatic ring. In PCP, the loss of 43 is intense and dominates the further cleavages. The cyclopentyl-cyclopropyl derivative can cleave a small radical, but that is not very important and the losses of 77 and 84 predominate. In this case, the peaks at 200 and 186 are the same as in PCP.





At least, this is reasonable.
 Regards,
 Martin