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Atmospheric Measurement Techniques Discussions

Interactive comment on "MS/MS studies on the selective on-line detection of sesquiterpenes using a flowing afterglow-tandem mass spectrometer" *by* J. Rimetz-Planchon et al.

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Comment: This is a very interesting paper papving a way towards a practial use of tandem mass spectrometry for analyses of SQT present in air. It is good to see that only even electron (nonradical) ions are produced from protonated product ions but that both radical and nonradical ions are produced from the radical cations. Is there any way the observed fragmentation could be rationalised with reference to the structures of the SQT molecules? It woudl be really useful to give a scheme with structures and indicate which are the major neutral fragments lost in CID. It really looks promissing in

the terms of potential for determining the identity of SQT from the in-situ data.

Reply: We thank the reviewer for his positive and encouraging comments. With respect to the question on how to rationalize the observed fragmentation with reference to the structures of the SQT molecules, however, we have no conclusive answer. The only information that is certain concerning the neutrals formed is the mass difference between the precursor ion and the formed fragment ions. As the structures of the precursor and fragment ions are not known and the thermochemical information is not available, it is not obvious to predict the structure of the neutrals lost. Furthermore, concurrent pathways leading to the same mass difference may be accessible at higher ECM values. Thus, using only this mass difference it is very uncertain to associate one or more neutrals to it. Due to these uncertainties, no information on neutrals formed in the CID process will be included in the article and the discussion of energetically allowed fragmentation pathways will only be possible after detailed quantumchemical calculations, which is beyond the scope of this article.

Interactive comment on Atmos. Meas. Tech. Discuss., 3, 4285, 2010.