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Interactive comment

Interactive comment on "HOM cluster decomposition in APi-TOF mass spectrometers" *by* Tommaso Zanca et al.

Anonymous Referee #1

Received and published: 13 March 2020

Zanca et al. present numerical simulations of the decomposition of molecular clusters in Atmospheric Pressure interface Time of Flight (APi-ToF) mass spectrometers. APi-ToF has recently evolved into one of the most commonly used techniques to measure the concentration and molecular composition of both neutral and naturally charged atmospheric clusters. In the present manuscript, the potential decomposition of clusters that include highly-oxygenated organic molecules (HOMs) representative of a mass peak commonly observed in ozonolysis of alpha-pinene is studied using a numerical decomposition model that has been developed and previously tested on simple clusters by the same group. Thus, the manuscript contributes essential information for prudent interpretation of mass spectra of molecular clusters in a large number of new particle formation studies, and it is clearly within the scope of AMT. I cannot comment on all the

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technical details of the manuscript but the presented work appears to be well-founded and rigorous. I recommend the following minor revisions for the authors to consider:

p. 5, line 87: The term "RRKM theory" is not explained. Please add a brief explanation.

p. 5, Figure 4: In my opinion, Figure 4 is not necessary. Please consider removing Figure 4.

p. 7/8: Lines 148-156 might be more clearly arranged in a table.

p. 10, Figure 8: Please explain in slightly more detail what you mean by '10 different sets of "noisy" input frequencies'.

p. 10/11, Figure 9a: I don't fully understand the dark bars presented in Figure 9a. While the figure caption suggests that these indicate the average number of fatal collisions, the main text (line 212) suggests that these are the "normalized number of fatal collisions". Please clarify.

p. 12, Figure 10: In the figure legend, change "Fragmentation probability" to "Decomposition probability".

p. 13, Figure 11a: What is represented by the different curves shown in Figure 11a? The colors 'blue' and 'orange' indicate the presence or absence of the quadrupole electric field but what is represented by the set of curves?

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