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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Molecular composition and volatility of multi-generation products formed from isoprene oxidation by nitrate radical" *by* Rongrong Wu et al.

Anonymous Referee #2

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The authors describe experimental results of the nitrate radical initiated oxidation of isoprene carried out in a batch-reactor for close to atmospheric conditions. Nitrate radical were generated via the O3 + NO2 pathway. The reaction was conducted in such a way that multiple nitrate radical attacks were possible leading to product formation of the 2nd and 3rd generation. Product formation was followed by a bromide-CIMS. The results are interesting and worth to be published in ACP. Some points should be considered before acceptance of the manuscript can be recommended.

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1. Line 71. “isoprene nitrates”? better: “organic nitrates derived from isoprene oxidation”

2. Line 150, Fig.1a-c: It is stated that approx.90% of consumed isoprene reacted with NO3 based on modeling results. The reaction scheme with the used rate coefficients is not given yet. Please provide this information in the SI. The modeling results should be compared with the measurements of the chemical species depicted in Fig.1 (as done in a couple of other papers of the Jülich group). That gives the readership an impression how good the processes in the experiment have been understood and how accurate the model is.

3. Line 200-212: The authors determined a bulk sensitivity for the organic nitrates. It should be described more in detail what has been done. It is not clear to me why this calibration was not used to set all the measurements on an absolute scale. The authors argue “that the normalized signals are sufficient”. More precise information is better in each case! On the other hand, they did it for C10 products. Why is the calibration only used for higher molecular products? Please comment. It would be fine if the authors could provide the plots of the C5 org.nitrate concentrations (or the yields because the amount of reacted isoprene is known). And please add a discussion regarding the uncertainty of these absolute values.

4. Line 417, Fig.2: In Fig.2 an average spectrum from the complete experiment is given. It would be fine having also a product spectrum from the first injection showing mainly 1st generation products. A couple of possible reaction pathways were mentioned/discussed in the paragraph before, incl. possible RO2 isomerization step leading possibly to HOMs. Nothing is said here regarding the relevance of RO2 isomerization in this reaction system based on the measurements. It would be also very helpful for the readership to have a reaction scheme in the main body that explains the formation of the observed main products, i.e. C5H9NO5, C4H7NO5, C5H9NO4, C5H9NO6, ... What about the formation of the carbonyls HCHO, MVK, MACR? The Vocus PTR-MS is very sensitive at least for the C4-carbonyls.

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