Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2018-443-RC2, 2018
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Interactive comment

Interactive comment on "Chlorine-initiated oxidation of n-alkanes under high NOx conditions: Insights into secondary organic aerosol composition and volatility using a FIGAERO-CIMS" by Dongyu S. Wang and Lea Hildebrandt Ruiz

Anonymous Referee #2

Received and published: 17 July 2018

General comments

Wang et al. present results from environmental chamber experiments of C8-C12 alkane oxidation initiated by chlorine under dry/humid and high NOx conditions. They show that yields are higher than for OH-initiated oxidation of the respective alkanes, indicative of the importance of these reactions for SOA production. Identified compounds include organonitrates, organochlorides. FIGAERO-CIMS data are used to look into

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the connection of chemistry and volatility via a new way of representing thermograms.

Overall, this is a very well written paper, and the study and interpretation of results are sound. I therefore recommend this paper to be published after minor revisions. Apart from a few specific comments (see below), I have two general comments regarding the manuscript.

First, the manuscript would profit from a few more lines on its atmospheric relevance. Using alkanes as VOC precursors, and performing experiments under high NOx conditions indicates the authors wanted to simulate an urban/polluted atmosphere. A short discussion on this, including the importance of CI- oxidation in such environments, as well as the choice of RH conditions, would give the study more (atmospheric) importance.

Second, there is somewhat a disconnect in the narrative between section 3.1 and section 3.2, which also represents a disconnect between ACSM and FIGAERO-CIMS data. I suggest the authors try to connect these two parts better. Section 3.1 (SOA and organic chloride formation) is entirely ACSM based. Why? Why were FIGAERO-CIMS data not used? Some statements made in a tentative manner could be confirmed/looked into using FIGAERO-CIMS data (see specific comments below).

Specific comments

P. 1, I. 26/ p. 2 l. 11: Where is chlorine oxidation important? See comment above, the paper would benefit from a few more lines on its atmospheric relevance. P. 2, I. 32-33: You specifically mention here low NOx, as presumably the cited study was done under such. What are then the implications for your study? I suggest reformulating this sentence. P. 4, I. 28: UMR, why not HR? In Figure 5 you present molecular formulae of compounds, indicating HR analysis. Please clarify. P. 5, I. 11: This could be confirmed with FIGAERO-CIMS data. Why were they not added? P. 5, I. 18-19: I- should cluster with Cl2. Why do you use the Cl- signal to track Cl2? Please clarify. P. 5, I. 21-22: Did you see any evidence of that in FIGAERO-CIMS gas-phase measurements? P. 6,

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I. 1-2: Can you confirm that with the organonitrate measurements of the FIGAERO-CIMS? P. 6, I. 16 – 18: Also here the isotope signal should help you. Without that, the chloronitrate peak cannot be identified (based on Figure S8). P. 6, I. 21 – 22: Did you actually observe that as well if you compare your dry and humid experiments, no? You mention this as a finding in your conclusions as well, but I cannot find it as a result in the manuscript. P. 7, I. 3-4: Are those fragmentation reactions in the particle phase, with subsequent evaporation of the resulting compounds? This would be consistent with the observation of loss of SOA mass (mentioned e.g. on p. 5, l. 21 – 22). Please elaborate. Experiments shown here are all under dry conditions. What about humid conditions? P. 7, I. 13 - 14: It becomes clear after discussion of Figure 5, but it would be helpful for the reader to mention here why you use the temperature range of 40 - 140°C. P. 8, I. 8 – 10: What do you base your interpretation of "low-temperature thermal fragmentation products" on? I agree that there must be fragmentation, but I am not sure you have enough evidence for that being thermal fragmentation during desorption. P. 9, section 3.3: How reproducible are your thermograms and corresponding Tmax for one compound and stable conditions? This information should be added e.g. to the supplementary section. P. 11, l. 22 – 23: This sentence is formulated too strongly based on the observations you present in your results section.

Technical corrections

P. 6, I. 8: Should be ACSM P. 8, I. 3: Propose

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