

Interactive comment on “Oxygenated products formed from OH-initiated reactions of trimethylbenzene: Autoxidation and accretion” by Yuwei Wang et al.

Anonymous Referee #1

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GENERAL COMMENTS

In this manuscript the authors present results of an experimental study of the products of the reaction of trimethylbenzene isomers with OH radicals in the absence and presence of NO_x. Reactions are conducted in a flow tube reactor and gas-phase products are analyzed using three types of online mass spectrometry that in combination allow detection of products ranging from very low to very high oxidation state. The authors detect a variety of monomer and dimer products that are not currently incorporated into the Master Chemical Mechanism, which is widely used to model the atmospheric chemistry of organic compounds. The authors propose structures for the compounds

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(they are preliminary since only elemental formulas and deuterium labeling data are available) and mechanisms by which they could be formed. Fortunately, the authors have kept the paper concise, and not attempted to overinterpret the results or overwhelm readers with data. Although it is difficult to judge the importance of the results because of the lack of quantitative analysis, aromatics are an important class of compounds whose chemistry is not well understood, the work is technically sound, and it should be useful for others to build on. I think the paper should be published in ACP after the following minor comments and have been addressed.

SPECIFIC COMMENTS

1. Line 227-228: How can an oxidation product have an oxidation state lower than TMB?
2. Lines 260-262 (and elsewhere): Because of the high sensitivity of the nitrate-CIMS to oxidized products I do not think you can assume that products formed in these experiments did not involve multiple OH reactions. For example, in the work by Krechmer et al., EST (2016) they formed multigeneration products in chamber experiments in which the lights were only on for 10 s.
3. Line 325-326: The proposed isomerization of the bicyclic alkoxy radical would never compete with ring-opening pathways. See Vereecken and Peeters, PCCP (2009, 2010) estimation methods for these pathways.
4. Line 362: Please provide support (such as references) for the assumption of identical charging efficiencies. Given the high sensitivity of the nitrate-CIMS to oxidation state and chemical structure this sounds like a very poor assumption. I suspect this makes the fractions quoted in sections 3.3 and 3.4 misleading and possibly results in wrong conclusions. The only way I think one can deal with this is to always refer to these as a comparison of fractional signals or some such thing.
5. Line 407-409: Can you distinguish peroxy nitrates by time profiles, since they should

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decay by reversible decomposition on short timescales (though they may be reformed)?

TECHNICAL COMMENTS

1. Line 289: Should be “summarizes”.
2. Line 345: Should be “more O atoms”.
3. Line 362: Should replace “charge” with “charging” or “ionization”.
4. Line 457: Delete “a”.
5. Line 459: Should be “linearly dependent”.

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2020-165>, 2020.