Interactive comment on “Formation of Highly Oxygenated Low-Volatility Products from Cresol Oxidation” by Rebecca H. Schwantes et al.

Anonymous Referee #1

Received and published: 7 November 2016

General comment:

The authors present a mechanistic study of toluene photo-oxidation. They focus on the chemistry of first and higher generation products from toluene photooxidation. As analytical tool they apply CF3O- CIMS. The results are compared to MCM3.31; and missing parts according to the new results were added /modified in two steps. These model improvements led to better consistency between the model results and measurements. Quantification was in parts inherently limited by absence of suited calibration compounds. Very positively, the authors put some efforts in characterizing the sensitivity of their CIMS for the expected compounds and compound classes. The authors also show the importance of higher generation product to SOA formation. The results are new and interesting, and as toluene is an abundant aromatic VOC, they are an important contribution for understanding VOC degradation and SOA formation in the atmosphere. The very interesting paper is well structured, and overall well written. However, I had some difficulties to follow some of the parts in the experimental section. I have the impression that this did not depend so much on the level of details that are given, but on notations and "unlucky" formulations. I think with a little effort that could be improved easily. I will list some examples below.

The manuscript should be published in ACP after the authors considered the minor points below.

Minor comments:

The scope of abstract and conclusion are not quite balanced. While the abstract focus more on o-cresol and benzaldehyde, the conclusion focus solely on 3-methyl catechol.

p.1, line 10: this sentence is somehow askew. It requires either reformulation or a reference to the yield 0.7, like "reported yield" or so.

Section 2.1 Experimental Design: here some info about the light source(s) is (are) missing: You refer to H2O2 photolysis as OH source on one hand, but later to jNO2 as a measure of photooxidation and a light source to prevent NO3 formation. I suggest, shortly to describe the main features / spectral dependence of your light source.

p.5, line 1ff: this is difficult to follow. Why do you speak about complex interaction when you obviously address the analyte CF3O complex. Similar the analyte F- adduct is formed by F transfer, but formation process and result are not identical. Also p.5, line 25 ff: "Traditionally, an analyte (A) is detected either at the F- transfer reaction (A+19) or complex formation (A+85)." Probably, better "detected" as "F- adduct" or "CF3O-complex"?!

p.5, line 8: is the 500 ml glass bulb the FTIR cell?

p.5, line 14ff: I don’t understand what are result and consequence from these comparisons. Please, clarify.
I guess the bulb was meanwhile empty of o-cresol?

It would be helpful to mention that “your” purified air is somewhat humid (RH?). Or is it O2 in air vs N2 that makes the difference?

“Likely the presence of water destabilizes the molecular ion formed from CF3O− ionization leading to more fragmentation.” I guess, you mean that the presence of water affects F− transfer adduct most?!! Please clarify.

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I find the use of the word “consistent” difficult to misleading (here and at some instances). Please, check and maybe reformulate to be clearer.

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