

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

Anonymous Referee #2

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General This is a very interesting and impressive paper on the oxidation of cresol studied at the Caltech chamber. Generally, it contains a wealth of new findings extending the knowledge on aromatics oxidation considerably.

Apparently, despite the study of aromatics oxidation over some decades now, this appears another field where the now available mass spectrometric techniques allow for the identification of reaction products which have not been identified before, especially for low NO conditions - but see and consider the note below.

On the other hand, the paper confirms a lot of findings as they are implemented into the MCM 3.3.1, many of them for high NO conditions which are expected to be met in regions where aromatic VOC emissions coincide with elevated NO and NO_x levels.

It seems that especially for low NO conditions many new observations are made but

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the authors should include into their paper a discussion where conditions with low NO enabling preference of ROO + HO₂ over ROO + NO can really be met.

The paper has the potential to deliver valuable changes and additions to chemical schemes such as the MCM 3.3.1. as it contains information of the formation of products in oxidation generations beyond one and two.

Overall, I think the paper is a great step forward in the understanding of aromatics oxidation and merits publication in ACP subject to only minor revision.

Details

p3, line 27: While it is understandable to avoid further complications during the present study, it would be extremely interesting to do a similar study at higher RH and then see the coupling to aqueous chemistry

p18, section 4.2.4: Maybe a reference can be given for the classic formation of the endo-peroxide ? I wonder if a intramolecular H-shift could occur in systems like the peroxy / endoperoxides at the different stages of the mechanisms discussed so that a hydroperoxide might form from this and not only by + HO₂ / - O₂ ? Maybe it would be timeöy to discuss such possibility.

Figure 3: The main additions here are on the catechol oxidation.

Figure 4: I do not understand "See Figure 2 " written at the catechol up right in the scheme. Probabyl this should be 'Figure 3 ' ? Please explain / correct.

References: I wonder if the paper

PAN, Shan-Shan, and Li-Ming WANG. "The Atmospheric Oxidation Mechanism of o-Xylene Initiated by Hydroxyl Radicals." Acta Physico-Chimica Sinica 31.12 (2015): 2259-2268.

should be mentioned because it contains remarkable recent considerations on xylene oxidation

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