

## ***Interactive comment on “Effect of Inorganic-to-Organic Mass Ratio on the Heterogeneous OH Reaction Rates of Erythritol: Implications for Atmospheric Chemical Stability of 2-Methyltetrols” by Rongshuang Xu et al.***

**Anonymous Referee #1**

Received and published: 30 December 2019

This is the review of the manuscript entitled “Effect of Inorganic-to-Organic Mass Ratio on the Heterogeneous OH Reaction Rates of Erythritol: Implications for Atmospheric Chemical Stability of 2-Methyltetrols” by Xu et al.

This study examines the photochemical stability of pure erythritol particles and particles containing erythritol and ammonium sulfate (AS) against oxidation by OH radicals. Erythritol serves as a surrogate of 2-methyltetrols, a common compound of isoprene-derived secondary organic aerosols. Reactive uptake of OH and subsequent degradation of erythritol in the particulate phase were determined as a function of inorganic-

C1

to-organic mass ratio (IOR). This was achieved using an aerosol flow reactor coupled to a soft atmospheric pressure ionization source (Direct Analysis in Real Time, DART) attached to a high-resolution mass spectrometer. It is found that the reactive uptake coefficient of OH decreases as the amount of AS increases. Furthermore, the results suggest that the reaction products due to OH oxidation are not significantly affected by the presence of AS. Since in the ambient methyltetrols are associated with AS, this study concludes that the chemical lifetime of methyltetrols is prolonged and may render methyltetrols stable against OH oxidation under humid conditions.

The topic of this study fits well within the scope of ACP. I do not have major comments on this work, mostly minor ones and technical in nature. However, I suggest to carefully proofread the manuscript to improve the English language.

P. 9, top paragraph: Just a comment to better understand the origin of HSO<sub>4</sub><sup>-</sup>. As the particles are heated and vaporize (ammonia is gone), the SO<sub>4</sub><sup>2-</sup> can abstract a hydrogen from the organic molecule? This leads to the detection of HSO<sub>4</sub><sup>-</sup>? Since HSO<sub>4</sub><sup>-</sup> signal does not change significantly between non-oxidized and the oxidized case, reactivity of OH with SO<sub>4</sub><sup>2-</sup> or HSO<sub>4</sub><sup>-</sup> (and maybe NH<sub>4</sub><sup>+</sup>) is not significant? A bit of rewording and better integration of previous studies would make this section easier to understand.

Derivation of the OH uptake coefficient necessitates the particle diameter. It appears that a polydisperse aerosol was applied. It would be helpful to plot the aerosol size distribution or give the corresponding distribution parameters. Did the authors measure the aerosol distribution before and after oxidation to assess potential volatilization of the particles upon oxidation?

How is the uncertainty of presented uptake values derived? Likely the width of the aerosol size distribution and the uncertainty in AIOMFC derived mfs values contribute to the overall uncertainty?

Addition of the MD simulation is a neat feature. However, its validity depends strongly

C2

on established parameters, applied fields, etc. It would have been nice to show that the simulated system or another test case behaves as expected. Here, things may get more complicated since  $\text{NH}_4^+$  and  $\text{SO}_4^{2-}$  ions will be differently distributed within the particles? This could not be addressed as stated in text but could be discussed looking at previous studies (e.g., Tobias and Jungwirth groups).

P. 12., l. 10-13: Please be more specific. Do you expect salting in or salting out for the particle systems you investigated? Will it change for the different IOR?

Figure 2b: The legends using color bars are a bit confusing and maybe, I misunderstand those. Does the color coding of the experimental data has a relationship with the color coding of the ambient sulfate to 2-methyltetrol ratio? No ambient data is plotted and thus one wonders the meaning of that legend. The text already stated that the ambient ratio is much higher than the one probed in experiments. Same with the sulfate to erythritol ratio. There is no change in the color bar and the data are not plotted as a function of this ratio. This could be done by using a 3D plot. Also, the legends are not described in figure caption.

Suggested technical corrections:

p. 1, l. 26: ...inorganic salts often coexist in atmospheric. ...

p. 9, l. 1: The  $\text{HSO}_4^-$  likely originated. ...

p. 9, l. 5: ...before and after oxidation (...) showed no significant change. ...

---

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2019-981>, 2019.