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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Estimating the saturation vapor pressures of isoprene oxidation products $C_5H_{12}O_6$ and $C_5H_{10}O_6$ using COSMO-RS" *by* Theo Kurtén et al.

Anonymous Referee #2

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Atmospheric oxidation products are usually multifunctional. Prediction of their vapor pressures has large uncertainties due to the complicated intramolecular interactions of these molecules. In this paper, the authors compared predicted vapor pressures with experimentally measured values. Thorough comparison using different methods to derive conformers for the calculation of vapor pressure based on COSMO-RS was conducted. These comparisons suggest the possibility of overestimation of saturation vapor pressures due to the overestimation of intramolecular interactions, specifically H-bond, by COSMO-RS. Although in this study, the authors have only selected two isoprene oxidation products which might be due to high computation cost, this method may be applicable to other atmospherically relevant molecules. The results of this study

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suggest the importance of proper treatment of intramolecular interaction and selection of conformers in predicting vapor pressures for multifunctional atmospheric oxidation products. Overall, the description of the method used for the calculation in the paper is clear and well written. The results and discussion are a useful contribution to the literature on the estimation of vapor pressures for multifunctional organic compounds. I have a few minor comments.

Page 7 line 29: The high activity coefficients in WIOM phase (and higher than in pure water) suggests that WIOM phase used in this study may be not a good representative organic phase for isoprene SOA as measured by D'Ambro et al. (2007). Isoprene SOA is much more polar than WIOM phase. This probably won't change the conclusion that "Differences between the measured values and true pure-compound saturation vapor pressures can thus not explain the discrepancy between COSMOTherm results and measurements."

Page 9 line 2: It is not clear why the authors varied c1 between 0.6 and 1.8. Are 0.6 and 1.8 threshold values for c1?

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