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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 #1

Received and published: 28 September 2018

This is highly technical paper that provides some important insights into the capability of a method based on quantum chemistry and statistical thermodynamics to accurately predict the saturation vapor pressure of small organic substances with a very large number of hydrogen-bond forming functional groups (hydroxy, peroxy). The relevance of the work derives from the importance of such compounds as SOA forming oxidation products of isoprene, and the fact that such substances clearly fall far outside of the applicability domain of group contribution-based prediction methods commonly used in the SOA community. The paper convincingly demonstrates that the prediction method greatly overestimates the impact of intramolecular hydrogen bonding on saturation vapor pressure, which leads to overprediction by as much as three orders of

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magnitude. It also explores several approaches to addressing this issue and makes recommendation on how more realistic estimates could be obtained. Considering the highly technical nature of the material, the paper is well written and also accessible to those not intimately familiar with theoretical chemistry.

I have little to criticize but feel strongly about the fact that the paper uses non-SI units for pressure and energy. The guidelines for authors of manuscript submitted to ACP explicitly states: "The metric system is mandatory and, wherever possible, SI units should be used." Please, no lame excuses, such as "it is customary in the theoretical chemistry community to use calories" or "the measured vapor pressures we use for comparison were reported in mbar". There is absolutely no reason why it is not possible to use Pascal for pressure and Joule for energy. The unit of Pascal for pressure was introduced in 1971, i.e., well before most, if not all, of the authors of this manuscript were born!

Page 3, line 26 and 27: use Pascal

Page 8, line 25: use kJoules

Page 18: All of the data in Table 1 should be reported in units of Pascal

Page 20: The vapor pressures in Table 3 should be reported in units of Pascal

Page 21: All of the data in Table 4 should be reported in units of Pascal (The table caption suggests that Table 4 also report activity coefficients, which does not appear to be the case)

Page 23, 24 and 26: Figures 2, 3 and 5: the y-axis should have values reported in units of Pascal

The name of the software is COSMOtherm and not COSMOTherm. This should be changed throughout the manuscript.

Page 2, line 28: "catechol" instead of "cathecol"

Page 3, line 15: “nor” instead of “or”

Page 3, line 30: “up to four” instead of “up four”

Page 11, line 14: “can be recommended” instead of “can recommended”

Page 13, Line 15: “EVAPORATION” instead of “EVAPO -RATION”

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