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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Impact of structure on the estimation of atmospherically relevant physicochemical parameters" *by* Gabriel Isaacman-VanWertz and Bernard Aumont

Anonymous Referee #2

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Isaacman-VanWertz and Aumont conducted comprehensive analysis on important physicochemical properties of organic aerosols (OA), i.e., their vapor pressures, Henry's Law Constants, and gas-phase rate constants, estimated by both structure-based and formula-based methods. They found the predicted property differences between isomers are larger than those caused by different methods. The evaluation of formula-based methods showed reasonable estimations when applied to a mixture of isomers. As molecular structures are often unknown in ambient organic aerosols, formula-based methods are recently developed and adopted to estimate OA properties. This study conducted detailed analysis evaluating formula-based methods and the results, e.g., average of the Daumit method and the modified Li method present-

ing best estimations of vapor pressure, and the development of the PEACh package, provided important information and tools to the aerosol community applying formula-based methods. I am happy to recommend publication of this manuscript in ACP and have only a few minor comments as below:

- While the manuscript is generally written very well, I have several editing comments: (a) define kOH in the abstract. (b) Page 1 Line 29: I suggest modifying "partition between phase and fates". "partition between fates" is not proper. "phase" should be in its plural form. (c) Page 4 Line 97: Change "that" to "than". (d) Page 5 Line 152: Change "condensed phases" to "condensed phase". (e) Page 8 Line 232: Define EPI as Estimation Programs Interface. (f) Page 10 Line 295: What is SB/BK?

- For citations, I suggest adding a few review papers in the Introduction. There was no citation in Lines 22-28 in the Introduction. Ziemann & Atkinson (2012) and Krieger et al. (2012) may be suitable there. Krieger et al. (2018) presenting a data set for validating vapor pressure measurement techniques is suggested to be added around Lines 35-38. Lines 54-72, I understand SIMPOL and EVAPORATION are widely used by the atmospheric community, other estimation methods of the vapor pressure., e.g., Moller et al. (2008), could also be cited and briefly discussed. O'Meara et al. (2014) is also recommended to be added as they also assessed the vapor pressure estimation methods. Page 12 Line 341, you may add Shiraiwa et al. (2014) for "molecular corridors".

- I noticed the authors used fraction of formulas in Fig. 6 as the y-axis. Why in other figures the number of formulas is used instead as the y-axis?

References: Krieger, U. K.; Marcolli, C.; Reid, J. P., Exploring the complexity of aerosol particle properties and processes using single particle techniques. Chemical Society Reviews 2012, 41 (19), 6631-6662.

Krieger, U. K.; Siegrist, F.; Marcolli, C.; Emanuelsson, E. U.; Gøbel, F. M.; Bilde, M.; Marsh, A.; Reid, J. P.; Huisman, A. J.; Riipinen, I.; Hyttinen, N.; Myllys, N.; Kurtén, T.;

Bannan, T.; Percival, C. J.; Topping, D., A reference data set for validating vapor pressure measurement techniques: homologous series of polyethylene glycols. Atmos. Meas. Tech. 2018, 11 (1), 49-63.

Moller, B.; Rarey, J.; Ramjugernath, D., Estimation of the vapour pressure of non-electrolyte organic compounds via group contributions and group interactions. Journal of Molecular Liquids 2008, 143 (1), 52-63. O'Meara, S.; Booth, A. M.; Barley, M. H.; Topping, D.; McFiggans, G., An assessment of vapour pressure estimation methods. Physical Chemistry Chemical Physics 2014, 16 (36), 19453-19469.

Shiraiwa, M.; Berkemeier, T.; Schilling-Fahnestock, K. A.; Seinfeld, J. H.; Pöschl, U., Molecular corridors and kinetic regimes in the multiphase chemical evolution of secondary organic aerosol. Atmos. Chem. Phys. 2014, 14 (16), 8323-8341.

Ziemann, P. J.; Atkinson, R., Kinetics, products, and mechanisms of secondary organic aerosol formation. Chemical Society Reviews 2012, 41 (19), 6582-6605.

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