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Comment

## ***Interactive comment on “EVAPORATION: a new vapor pressure estimation method for organic molecules including non-additivity and intramolecular interactions” by S. Compernelle et al.***

### **Anonymous Referee #3**

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The authors report about their new vapor pressure estimation model EVAPORATION which needs only molecular structure as input. It is based on a group contribution method and takes non-additivity of functional groups for polyfunctional molecules into account as they occur in secondary organic aerosol. The model uses a large dataset for fitting the necessary parameters, the selection of the dataset is discussed in some detail, which is of use for the community to identify the most important gaps in the experimental data available at present. The authors compare the model results to other pressure estimation methods and experimental data. The model is a significant im-

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provement on present vapor estimation methods and should find immediate application when modeling gas to particle partitioning of secondary organic aerosol.

The manuscript is well written and appropriate figures are provided to support the text. I recommend publication in ACP, however the authors should consider the points below which were already recommended by the previous reviewers:

The distinction between the "simple" additive group contribution method and the "full" model is not completely clear at several locations in the text as well as in the figures. In particular it is not clear to me whether in Fig. 3 and 4 the agreement between modeled and experimental data would improve if the full model of Table 4 would be used instead of the additive model of Table 2.

It would help the reader to understand the different descriptors better if for a few example compounds their assignment would be illustrated (perhaps in an appendix)

Minor comments:

page 13234, line 23: Booth et al., 2011 should be added to the references.

page 13250, first paragraph: While I agree that the differences between a "simple" group contribution method and the measurements of Booth et al. (2010) can not be explained by uncertainties between different types of measurements, there is the possibility that there are problems associated with the measurements of the vapor pressures of the solids as discussed in Soonsin et al. (2010). If you compare the sub-cooled vapor pressures derived from measured vapor pressures of the solids for the dicarboxylic acids of Booth et al. (2010) with direct measurements of the sub-cooled liquids (e.g. Soonsin et al., 2010, Riipinen et al., 2007) they agree within error for succinic and glutaric acid while they disagree for malonic acid. It would be interesting to see measurements of tartaric and citric acid in their liquid state. This discussion is given in the section conclusion, but it would be helpful for the reader if it is mentioned also at this point.

page 13254, line 14: write instead of MG: Marrero and Gani (2001)

Figures: I find Fig.6 very difficult to read, I suggest to print left and right in either separate figures or over two columns so that the assignment to each compound class is easier to see.

#### References:

Booth, A. M., Barley, M. H., Topping, D. O., McFiggans, G., Garforth, A., and Percival, C. J.: Solid state and sub-cooled liquid vapour pressures of substituted dicarboxylic acids using Knudsen Effusion Mass Spectrometry (KEMS) and Differential Scanning Calorimetry, *Atmos. Chem. Phys.*, **10**, 4879–4892, 2010.

Riipinen, I., Koponen, I. K., Frank, G. P., Hyv<sup>o</sup>arinen, A.-P., Vanhanen, J., Lihavainen, H., Lehtinen, K. E. J., Bilde, M., and Kulmala, M.: Adipic and malonic acid aqueous solutions: surface tensions and saturation vapor pressures, *J. Phys. Chem. A*, **11**, 12995–13002, 2007.

Soonsin, V., Zardini, A. A., Marcolli, C., Zuend, A., and Krieger, U. K.: The vapor pressures and activities of dicarboxylic acids reconsidered: the impact of the physical state of the aerosol, *Atmos. Chem. Phys.*, **10**, 11753–11767, 2010.

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