

Interactive comment on “Interaction between Dicarboxylic Acid and Sulfuric Acid-Base Clusters Enhances New Particle Formation” by Yun Lin et al.

Anonymous Referee #3

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This manuscript presents a theoretical study on the interactions between succinic acid (SUA) and sulfuric acid (SA) – ammonia (AM)/dimethylamine (DMA) clusters in presence of water molecules. The application of the results in atmospheric new particle formation (NPF) is discussed. Overall, this study tackles how a multi-component system, which is more realistic in terms of atmospheric NPF, evolves and provides some of the novel insights into the interaction between organic acids and SA-base clusters. On the other hand, the results and their implication could have been presented in a way that is easier to be followed. The authors are advised to address the following concerns before a recommendation can be made.

C1

1. The atmospheric concentrations of NPF precursors are especially important when one wants to discuss the implication of a theoretical calculation. In fact, the authors failed to find a reliable source for the key species that appear in this study. The concentration of SUA is referred from Kawamura and Kaplan, 1987, which actually presents concentrations of particulate SUA and should not be used in a clustering system. The concentration of SA is set at 10^5 molecule cm^{-3} , which is at least one order of magnitude lower than many measurement values.

2. In many cases, the authors compare ΔG and then conclude that SUA (and/or other molecules) either promote or hinder the growth of clusters. This is fine when the difference between two ΔG is large. On the other hand, one probably wants to include the concentrations of gaseous precursors and clusters, do the math, and then obtain something like a branching ratio when the difference is small, instead of simply using “promotion or hindrance”. Following this point, I would like to see a clear definition of “promotion or hindrance” in the manuscript. Is it a comparison between the current step of reaction/clustering or a comparison of the further growth of formed cluster from the current step?

3. Given the comprehensive calculation that has been performed, I suppose the authors could suggest a pathway (or multiple possibilities with relative weight for each) on how the complex clusters are formed? e.g., how is (SA)(DMA)(AM)(SUA)(W)₆ formed? Will water be added to cluster at the beginning? A summary like this would be welcome, even for a smaller cluster if such a pathway is too complex for a big cluster.

Minor comments, 4. The reference list should be carefully checked. Some of the references are not in an alphabetical order. Also, I suppose what in Line 75 should be “Xu and Zhang (2012)”.

Interactive comment on Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2018-975>, 2018.

C2