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Comment on acp-2021-831

Anonymous Referee #1

Referee comment on "The role of organic acids in new particle formation from methanesulfonic acid and methylamine" by Rongjie Zhang et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-831-RC1, 2021

The manuscript by Zhang et al. presents a theoretical evaluation on the role of organic acids in MSA-MA NPF. Among all considered organic acids, they found that formic acid (ForA) has the highest potential to stabilize the MA-MSA cluster and can enhance MSA-MA nucleation at atmospheric conditions via catalyzing the formation of clusters in the initial stage of NPF. The structural factors that affect the enhancing potential of organic acids on MSA-MA NPF were also revealed. The selected topic should be interesting across a range of atmospheric chemistry community. The work is technically well performed and calculated data can well support the conclusion. The manuscript is well written and easy to follow. Therefore, I recommend publication of this manuscript after consideration of the following comments:

- The accuracy of DLPNO-CCSD(T)/aug-cc-pVTZ calculation depends on selected keywords for the convergence. Please clearly present the selected keywords for the DLPNO-CCSD(T)/aug-cc-pVTZ calculation in the Computational Details section.
- Lines 82-83, in my opinion, the range for the number of initial configurations (1000-10000) for each cluster is large and it would be better to explain the reason.
- It is better to test how the selection of coagulation sink affects the core conclusion.
- Line 98, please cite the references for the equation (1).
- Lines 174-175, in order to explain why SucA and AdiA are outliers, the authors should clearly present the even/odd pattern of dicarboxylic acids.
- Please provide the equation for calculating the binding free energy of $(SA)_1(amine)_1(OAs)_1$ in Table S3 and point out whether the calculated $[(SA)_1(amine)_1(OAs)_1]$ is the mean values based on concentration of precursors.
- Please check the guidelines of Atmos. Chem. Phys. for references, and all the references should be cited in the same style.
- Some minor mistakes are shown in the manuscript, e.g., Line 79, “global minimum structures” instead of “global minima structures”; Line 135, “ones” should be

"clusters"; Lines 223-224, it should be written as " The evaporation rate of the $(ForA)_2$ cluster is found to be comparable to that of $(MSA)_2$".