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Comment on acp-2021-831

Anonymous Referee #2

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-RC2>, 2021

The manuscript by Zhang et al. is devoted to the role that organic acids (OA) may play in new particle formation from methanesulfonic acid (MAS) and methylamine (MA) molecules. It is based on high-level quantum chemical calculations of the formation free energies of selected MA-MSA-OA ternary clusters and on results obtained from ACDC (Atmospheric Cluster Dynamics Code) simulations. The main conclusion of the paper is that the formic acid (ForA) molecule is of particular interest because ForA might have an important role in MSA-driven new particle formation (NPF) in relevant atmospheric conditions. The various factors that affect the enhancing potential of the organic acids, especially ForA, on MSA-MA NPF were also thoroughly analysed.

The work is technically well performed and the results of the calculations well support the conclusions. The manuscript is almost clearly written and should be interesting for the community of atmospheric chemists.

I recommend publication of this manuscript after the following (minor) points have been taken into account :

- When comparing the various dicarboxylic acid molecules considered in the calculations, it is found that only maleic and glutaric acid can interact via their two carboxylic groups. It is however surprising that such configuration has not been found for Succinic acid. This has to be discussed.
- Although the ACDC code has been presented elsewhere, it is quite disappointing not having here a brief presentation of its main inputs and outputs. In particular, this would greatly improve understanding of section 3.4 and Figure 6.
- Finally, when comparing the DeltaG values, it should be clearly stated that the discussion in the paper is based on the absolute values, whereas relative values are given in Tables and Figures. Then, « higher values » in the text correspond in fact to « lower values » in the Tables/Figures.

