Atmospheric Chemistry and Physics Discussions

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Comment on acp-2021-784

Anonymous Referee #2

Referee comment on "Pyruvic acid, an efficient catalyst in SO_3 hydrolysis and effective clustering agent in sulfuric-acid-based new particle formation" by Narcisse Tsona Tchinda et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-784-RC2, 2021

The manuscript titled "Pyruvic acid, an efficient catalyst in SO3 hydrolysis and effective clustering agent in sulfuric acid-based new particle formation" by Tsona et al. discusses the role of pyruvic acid as a catalyst in SO3 hydrolysis. The investigation of whether pyruvic acid can take part in cluster formation brings an interesting addition to the article. The paper is well written and it fits to the scope of the journal.

Specific comments:

1. I would like to see a section in the Methodology on how the cluster conformers were found for the ACDC calculations. Presumably the clusters containing only sulfuric acid and ammonia can be found somewhere in the literature, but how about the clusters containing pyruvic acid? I can see that for the hydrolysis calculations, different conformers of the pyruvic acid were used, but the clusters should have a lot of conformers due to the higher number of molecules as well as the 4 different pyruvic acid conformers, which should be considered in finding the lowest energy cluster.

2. In Fig. 5 (bottom panel), can you discuss why are the enhancement factors of 238 K at 3 and 4*10^9 PA molecules/cm-3 the same, when all other points seem to have the same linear trend with the same slope?

3. Did you run any simulation wher you would have an initial concentration of PASA, formed during the SA formation? Would this have any effect on the cluster formation results or would the PA just evaporate from the cluster, once more SA and NH3 is added through collisions?

Technical corrections:

line 21: "The enhancing effect of PA of examined by evaluating the ratio of the ternary..." There is some typo here.
line 55, 222, 245: giving -> given
line 58: acid in the troposphere -> acids in the troposphere
line 85: You mention only zero-point energies, though later you use also Gibbs free energies. Did you get them also from this calculation?
line 88: "internal reaction coordinate" should be "intrinsic reaction coordinate" for IRC.
line 134: Is there a typo in the birth-death equation, the concentration term is missing from end (the cluster evaporation sink term).
line 156: "second molecule" -> "second H2O molecule"
line 167, 213: "decomposition" is an odd choice of word to describe the formation of a larger molecule from smaller species.
line 172: "previous results studies" a typo?
line 184: "their energies" specify here and in the supplement, what energies they are. Electronic or something else?
line 184: "relati"->"relative"
line 185: "that in during"->"that during"
line 251: Should this be Table S2? That's where the formation energies are. Also, the table caption has one extra superscript in "mol"
line 252: "The binding of PA to SA exhibits similar strength within 1 kcal mol-1 to the binding between two SA molecules" If this means that the energies of PASA and SA2 are within 1 kcal/mol, it should say "within 1.5 kcal/mol".
line 294: "(1 tam)"->"(1 atm)"
line 343: Is there some author missing from "NTT and analysed"?