The revised manuscript submitted by Wang et al is a substantial improvement. However, in a few cases I believe that additional clarification is needed in the author's responses. As both reviewers ask for justification of the applied methods it is a bit disappointing to see this comment being swept under the rug. My main concern is improper literature citations, which leads to a loose and quite regional referencing, which does not give credit to the original findings and developed methodologies. In many cases the this implies that the statement referenced is not actually addressed in the cited papers.

Original comment and response are given in italic below.

Line 32: "Even if the concentration of NH3 exceeds that of DMA by 10-100 orders of magnitude, the cluster formation rate of PA-DMA cluster formation is much higher than that of the PA-NH3 cluster system."

This is a consistent finding with other acid-base clusters. Please elaborate on that this is not a unique finding and refer to the relevant literature.

Response: Thank you for your nice comment. The cluster formation rate of PA-DMA cluster formation is much higher than that of the PA-NH3 cluster system.This is not an isolated finding. For example, Ning et al. also found that the cluster formation rate of HIO3-DMA is higher than that of the HIO3-NH3 cluster system(Ning et al., 2022).

Citing Ning et al here, does not give credit to the original finding that DMA outcompetes ammonia in acid-base nucleation and the general finding that base strength governs nucleation potential in acid-base clustering. This was originally shown by Kurtén et al (https://doi.org/10.5194/acp-8-4095-2008) in 2008. As this is a quite seminal paper that essentially drove the entire community to investigate DMA in nucleation it should be acknowledged for this finding. Subsequently, for SA-base nucleation the fact that base strength dictate nucleation potential has been shown by Olenius (https://doi.org/10.1063/1.4819024), Ortega (https://doi.org/10.5194/acp-12-225-2012), Elm (https://doi.org/10.1021/acs.jpca.7b08962 and https://doi.org/10.1021/acs.jpca.7b05658) and Myllys (https://doi.org/10.1021/acs.jpca.8b02507 and https://doi.org/10.5194/acp-19-9753-2019). All this work outdates Ning et al. substantially. The finding that base strength governs nucleation potential in acid-base clustering has also been further extended to other acid systems in the Clusteromics series of papers.

Computational methods: Funelling approach:
The applied computational workflow follows a standard routine, which is inspired by the funnelling approaches by Temelso et al. (https://doi.org/10.1021/acs.jpca.7b11236) and Kubecka et al. (https://doi.org/10.1021/acs.jpca.9b03853). It would be worth mentioning these works in the paper for justifying the workflow. What parameters were used in the ABCluster calculations.

Choice of DFT functional: Why did you choose the ωB97X-D functional for yourstudy? Please justify your choice by referring to potential benchmarks that demonstrate that this functional performs well for atmospheric molecular clusters.

Choice of basis set: Please justify the choice of the 6-31++G(d,p) basis set for the final geometry optimization and vibrational frequency calculations.

DLPNO-CCSD(T)/aug-cc-pVTZ: Please justify that DLPNO-CCSD(T)/aug-cc-pVTZ yield sufficiently accurate binding energies of the clusters. Which PNO convergence criteria were used in the calculations and were (T) fully iteratively calculated?

Response: Thank you for your nice comment. Many previous studies have adopted these methods and applied them to a wide range of acid-base cluster systems(Ning et al., 2026; Zhang et al., 2021; Liu et al., 2023). normal PNO was used in the calculations.

The authors did not really address this comment. A similar comment was also raised by the other reviewer. I am also not quite satisfied with the response that *"Many previous studies have adopted these methods and applied them to a wide range of acid-base cluster systems"*, as this is not a justification. The applied computational methodology is based on substantial amount of research that has been carried out to identify the best methodology to sample atmospheric molecular clusters.

1) The applied computational workflow follows the funnelling approaches originally proposed by Temelso et al. (https://doi.org/10.1021/acs.jpca.7b11236) and Kubecka et al. (https://doi.org/10.1021/acs.jpca.9b03853). It would be worth mentioning these works in the paper for justifying the workflow. Also please state the ABCluster parameters used.

2) A large effort has been carried out to identify that the ωB97X-D functional is the best choice for modelling atmospheric molecular clusters. This choice has been based on extensive benchmarks carried out for both the binding energies and geometries of atmospheric molecular clusters.

   Binding energy benchmarks:
   https://doi.org/10.1039/c3cp52616j
   https://doi.org/10.1039/c6cp06851k
   https://doi.org/10.1021/acs.jctc.2c00825

   Geometry benchmarks:
   https://doi.org/10.1021/acs.jctc.4c01046
   https://doi.org/10.1021/acsomega.6c00573

   The authors should justify their choice of functional based on such grounds.

3) The fact that the very small and quite old pople style basis set 6-31++G(d,p) is sufficient for modelling atmospheric molecular clusters is also based on extensive benchmarks:
10.1016/j.cplett.2014.09.060
10.1016/j.comptc.2016.10.015
https://doi.org/10.1021/acsomega.6c00573

4) The application of DLPNO in molecular cluster studies was first advocated by Myllys et al (https://doi.org/10.1021/acs.jpca.5b09762) and subsequently benchmarked by Schmitz et al (https://doi.org/10.1021/acsomega.0c00436). Also please state which PNO convergence criteria were used in the calculations and were (T) fully iteratively calculated?

The authors do not need to cite all these papers, but some of them can be used for justification of the methods. If the quantum chemical methods are not properly justified, how can we trust the results derived from them?