Author responses and changes to Manuscript: egusphere-2025-165

Dear editor and reviewers:

We are very grateful for the constructive comments from the editor and reviewers on our manuscript (ID: **egusphere-2025-165**, original title: **Chloric Acid-Driven Nucleation Enhanced by Dimethylamine and Sulfuric acid in the Arctic: Mechanistic Study**. We have studied these comments carefully and have made corresponding revisions which marked in red in the revised manuscript. The all comments and our replies are listed as follows:

<<Comments from Reviewer #Report 1>>

The authors did an excellent job in answering the comments from all reviewers. There are two minor points that I would suggest the authors correct before publication.

Line 100-102: "Engsvang et al.(Engsvang et al., 2024) has investigated the formation mechanism of CA clusters, concluding that CA did not contribute. The formation rate and mechanism of CA-DMA clusters deserve further investigation."

It should be specified that CA-DMA clusters are also included in the study by Engsvang et al. This also means that the second sentence contradict the first one. However, the study by Engsvang was on fairly small clusters (up to 2 acid-base pairs). I suggests the authors perhaps motivate by saying "The formation rate and mechanism

of larger CA-DMA clusters deserve further investigation."

>>**Response:** Thank you for your nice comment. Engsvang et al.(Engsvang et al., 2024) has investigated the formation mechanism of CA clusters, concluding that CA did not contribute. The study by Engsvang was on fairly small clusters (up to 2 acid-base pairs). The formation rate and mechanism of larger CA-DMA clusters deserve further investigation.

Line 117-128 (Configurational sampling): I still do not believe that the references here are doing full justice for the people putting in the hard work of developing the funneling approach and benchmarking the computational methods. Without rigorous testing and benchmarking of the quantum chemical methods, we do not know whether the end results are meaningful. There is a reason why the DLPNO-CCSD(T)/aug-cc-pVTZ//wB97X-D/6-31++G(d,p) level is extensively used. Hence, I am not entirely satisfied with the fact that the authors only cite a few papers that applied the approach.

For instance, the funneling approach based on genetic algorithms has been spearheaded by the Shields' group and Jakub Kubecka:

Funneling approach with OGOLEM:

https://pubs.acs.org/doi/full/10.1021/acs.jpca.7b11236

https://app.jove.com/t/60964/computation-atmospheric-concentrations-molecular-clusters-from-ab

To the best of my knowledge the first group to apply ABCluster in a funneling

workflow was the group of Xiuhui Zhang:

https://doi.org/10.1016/j.chemosphere.2018.03.154

The funneling approach based ABCluster that is basically used by every group now, was developed by Jakub Kubecka:

https://pubs.acs.org/doi/full/10.1021/acs.jpca.9b03853

The DLPNO-CCSD(T) method has been introduced to the field by Nanna Myllys and benchmarked by Schmitz and Elm:

https://pubs.acs.org/doi/full/10.1021/acs.jpca.5b09762

https://pubs.acs.org/doi/full/10.1021/acsomega.0c00436

The choice of the wB97X-D functional and the 6-31++G(d,p) basis set for geometries has mainly been benchmarked by Elm and co-workers:

https://www.sciencedirect.com/science/article/pii/S0009261414008379

https://www.sciencedirect.com/science/article/pii/S2210271X16304297

The overall DLPNO-CCSD(T)/aug-cc-pVTZ//wB97X-D/6-31++G(d,p) methodology is recommended by Smith et al and Elm et al in comprehensive reviews:

https://doi.org/10.1016/j.jaerosci.2020.105621

https://doi.org/10.1016/j.jaerosci.2020.105733

>>**Response:** Thank you for your nice comment. We have cited these references.

Sincerely

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