Response to Reviews

We highly appreciate the comments from the reviewers and all the points have been addressed in the revised paper. We hope that the following responses are satisfying and that the paper can be accepted for publication. The reviewers' comments have been reproduced in blue text below, followed by our point-by-point replies. The page numbering refers to the marked manuscript.

Reviewer #1 - Theo Kurtén

Astrid Norskov Pedersen, Yosef Knattrup and Jonas Elm have used computational methods to study the effect of three atmospherically relevant tricarboxylic acids on sulfuric acid - base clustering. I collaborate extensively with professor Elm, and in the interest of full transparency I am therefore writing this review openly (i.e. without the typical anonymity of peer review in our field). Readers (and editors) may themselves then judge how they wish to weight my review compared to that of other, presumably less closely affiliated, reviewers. (For example, it is probably not a surprise to anyone that I approve of the general methodology used here, having been involved in numerous similar studies myself. . .)
With this caveat out of the way, my overall impression of the manuscript is very positive: this is a well-conducted study on a relevant topic, carried out with appropriate methods. Nevertheless, there are a few issues I'd like to discuss with the authors. Please bear with me for a relatively lengthy review, which however contains only relatively few and simple suggested "action items" for the authors. (To aid their work, I've spelled out these suggested action items at the end of each longer issue.)

1)Page 3, lines 66-68. This slightly misrepresents the chemistry, and the "ester issue". First, gas-phase dimers are believed to (predominantly, though not necessarily solely) be formed by cross-reactions of PEROXY radicals. (The reaction does indeed go through a alkoxy-alkoxy intermediate, but that mechanistic detail is less relevant to this big-picture overview, and probably doesn't even need to be mentioned here). Second, the Peräkylä 2023 paper suggests specifically that part of these gas-phase dimers are actually esters rather than peroxides. Third, the Kenseth paper then shows that esters actually measured (by cromatography-based methods) from the particle phase are almost certainly formed by condensed-phase reactions, i.e. the condensed-phase esters are not the same (= do not have the same structure or formation mechanism) as the (speculated) gas-phase esters. This does not prove that the gas-phase esters don't exist - it is indeed quite difficult to explain the mass spectra e.g. in Peräkylä (and many other studies) without them. However, it does suggest that if formed, these gas-phase esters very rapidly rearrange (react/isomerize) once in the condensed phase. (Based on discussions with Christopher Kenseth himself, there are plenty of potential mechanisms for this). While the authors are of course correct that molecules formed exclusively in the condensed phase will not participate in NPF, the existence (or more accurately, the likely concentration range) of gas-phase esters should still be considered an open question. (Suggested action item: please reformulate accordinlgy).

Author reply:

We agree with Theo that the discussion about accretion product formation in the introduction was slightly misleading. We have rewritten the paragraph, such that the discussion is more clear.

Page 3 from:
These are believed to be formed by gas-phase cross reaction of two alkoxyradicals to form an accretion product[Peräkylä et al., 2023]. However, Kenseth et al. [2023] argue that they can only be produced in the particle phase, leaving them unable to participate in NPF.

To:
These are believed to be formed by gas-phase cross reaction of two peroxy radicals to form an accretion product [Peräkylä et al., 2023]. However, Kenseth et al. [2023] studied the structures, and formation mechanism, of four different dimeric accretion products found in atmospheric particles, and concluded that accretion products, specifically those containing *cis*-pinic acid subunits, are formed through particle-phase nucleophilic addition reactions.

2)On the subject of likely concentration ranges, I'm interested in hearing the rationale for the 1-10 ppt range used for tricarboxylics in the modelling.
I also did some back-of-the-envelope calculations, in the spirit of asking, in a manner hopefully familiar to the authors, "what would it take for tricarboxylics to reach a certain concentration?". Let's first assume the precursor is something like alpha-pinene, with typical (non-winter, forest) mixing ratios (based on a quick literature browsing) between 1 ppt and 1 ppb (i.e. about 2.5E7…2.5E10 molecules per cm3). The main (daytime) oxidant for alpha-pinene is usually OH, with a concentration of about 1E6 molecules per cm3, and a reaction rate with a-pinene of around 5-6 x 1E-11 cm3 per molecule and second at the relevant temperatures (using the rate expression from the MCM website). Let's say the molar (not mass) yield of tricarboxylics is somewhere between 1 and 10% of the oxidation (noting that the latter is certainly an overestimate). So then the production rate of tricarboxylics is between 15 and 150 000 molecules per cm3 and s. Let's round up to 20…200 000 to account for O3 oxidation also (and get rid of a significant figure). To get a steady-state concentration, we now need a loss term. For a highly soluble and condensable, but chemically relatively stable, molecule like a tricarboxylic, the condensation sink (CS) should be a good estimate of the loss in the absence of substantial nucleation by tricarboxylics (I'll come back to this soon!). Typical CS values are between 0.01 and 0.0001 per s, with the former corresponding to very polluted and the latter to very clean areas. So we get (setting P = CS x [tricarb], where P is the production rate derived above, and solving for the tricarboxylic acid concentration [tricarb]) a steady-state concentration of 1500 per cm3 (low-end source, high-end CS) to 1.5E9 per cm3 (high-end source, low-end CS). OK, 10 ppt = 2.5E8 is within that range. However to actually get to 10 ppt, we need to simultaneously assume (i.e. the answer to the "what would it take" question is):
-a high-end precursor concentration (close to 1 ppb)
-a very high yield of tricarboxylics from oxidation (closer to 10% than 1%)
-a very low condensation sink (at least not above 0.001 per second).
So while we cannot rule out 10 ppt based on a back-of-the-envelope analysis, it's worth noting that it is certainly a "maximum possible upper limit" type of estimate. (It's worth noting that we probably CAN rule out e.g. 100 ppt!)
I would also note that if the tricarboxylics are driving substantial nucleation, then that is an

additional loss term that quickly limits the steady-state concentration. (E.g. a J - rate of 1 per cm3 and s, with on average N tricarboxylics in the nucleating cluster, would correspond to a loss rate of N per cm3 and s…) So we can't really have tricarboxylic-enhanced J - rates above, or even close to, 0.01 per cm3 and s, and tricarboxylic steady-state concentrations above 1 ppt. On the other hand, nucleation is not inherently a steady-state phenomenon, so I guess we could speculate that tricarboxylics first build up to some > ppt threshold, and are then quickly depleted in a short nucleation burst).

Similar reasoning of course applies to all potentially nucleating complex organics (e.g. "HOM dimers"), not just tricarboxylics - it's hard to build up substantial steady-state reservoirs of compounds that form with relatively low yields from oxidation of precursors that are not super-abundant to begin with.

Note: while I'd like to hear a bit about the reasoning behind the 10 ppt upper limit in the authors' response, the only actual action item I'm suggesting for the actual manuscript is that the authors acknowledge that 10 ppt is, while not completely impossible, a very high number indeed for something like a tricarboxylic.

Author reply:

We agree that the concentrations of the tricarboxylic acids is difficult to estimate, and that 10 ppt is an upper-bound estimate for the concentration of each of the tricarboxylic acids. The concentration range of OOM from 0-10 ppt was chosen as it is what is usually expected for organic oxidation products, and it allows for easy comparison with our previous papers. We do not think it is an issue that the upper limit of the concentration is at a high estimate, given that the largest enhancement for the majority of the systems happens at the lower end of the concentration range, when we go from 0 to 0.5 ppt, and capping the concentration range at 8 ppt or 4 ppt would not change the main conclusions in the paper. To enhance clarity and avoid confusion, we have added a sentence to the manuscript, stressing that the 10 ppt is an upper limit to the OOM concentrations.

Page 12 from:

The sulfuric acid concentration was fixed at 10^6 molecules cm^{-3}, the OOM concentration varied from 0–10 ppt, and the concentration of the bases were studied for two extremes with a "lower limit" and an "upper limit". These were set as follows: AM (10 ppt, 10 ppb), MA (1 ppt, 100 ppt), and DMA/TMA (1 ppt, 10 ppt), with the low concentration limit likely best representing the actual concentrations observed in the ambient atmosphere.

To:

The sulfuric acid concentration was fixed at 10^6 molecules cm^{-3}, and the concentration of the bases were studied for two extremes with a "lower limit" and an "upper limit". These were set as follows: AM (10 ppt, 10 ppb), MA (1 ppt, 100 ppt), and DMA/TMA (1 ppt, 10 ppt), with the low concentration limit likely best representing the actual concentrations observed in the ambient atmosphere. The OOM concentration was varied from 0–10 ppt, where 10 ppt should be considered an upper-bound estimate, only possible with close to 1 ppb concentration of the precursor, about 10% yield of the tricarboxylic acid, and a condensation sink below 0.001 s^{-1}.

3)What is the rationale for using 278.15 K in the ACDC simulations rather than 298.15 K? Is the cluster formation negligible at 298.15 K? Or have some relevant experiments been reported specifically at this temperature? Also, given that monoterpene emissions are strongly temperature-dependent, is it not even less probable to encounter 10 ppt mixing ratios of tricarboxylics at 278 K?

Author reply:
Similarly to the concentrations, the temperature in the ACDC simulations are chosen to be consistent with the Clusteromics series of papers, allowing for easy comparison between molecules. These conditions also correspond to spring-time boreal forest areas, where nucleation is seen to occur frequently. However, we agree with Theo that this rationale should be explicitly stated.

Page 12 from:
The simulations were performed at 278.15 K and 1 atm, using the settings described in Section 2.3.

To:
The simulations were performed at 278.15 K and 1 atm, reflecting the conditions of spring-time boreal forest areas, using the settings described in Section 2.3.

4)The authors rationalize the stability of the PDPE-containing clusters by the flexibility of the molecule. This may well be true in the context studied here (tricarboxylic acids stabilising sulfuric acid -base clusters), but it contrasts in an interesting way with our recent study (https://pubs.rsc.org/en/content/articlelanding/2025/cp/d5cp01931a) where we found that flexibility, in the sense of efficient H-bonding inside a monomer, is a strong predictor for INefficient pure organic cluster formation among a series of "HOM dimer" candidates. The two statements do not necessarily contradict each other. In addition to focusing on pure organics rather than mixed organic-inorganic clusters, our study did not, for example, contain any di- or tricarboxylics. It could be that the stronger H-bonds formed by the carboxylic acids, especially between them and the inorganic cluster constituents, negates the "efficient internal H-bonding leads to reduced cluster formation potential" effect we reported. However, in an older study involving both me and Jonas Elm, we did find some evidence for intramolecular bonding affecting cluster stabilities also for linear dicarboxylic acids (https://pubs.acs.org/doi/10.1021/acs.jpca.9b08020), albeit only for the largest studied case (suberic acid), and with substantial associated entropy-enthalpy compensation. In any case, it would be interesting to see the lowest-energy (and/or lowest free energy) monomers for the three acids studied here - are there any internal H-bonds in any of them (apart from the presumably relatively weak bond between the C=O and O-H in the SAME carboxylic acid group, which tends to be always present)? The suggested action item here is that at minimum, the authors show and briefly discuss the monomers in terms of potential internal H-bonding, and possibly comment on the different role that "flexibility" seems to be playing in their study and ours.

Author reply:
While the results from Kähärä et. al. certainly are interesting, they do not completely contradict the results presented in this paper. In our case the flexibility is needed to allow all three acid groups to efficiently interact with the cluster, but at the same time the tricarboxylic acid monomer does not have an excessive amount of intramolecular interactions, which would

be ineffective for clustering. However, we agree that this apparent discrepancy between the two studies should be addressed in the manuscript. A short discussion has been added to the manuscript, and the monomer structures have been added to the Supporting Information.

Added page 8:
This is in contrast to Kähärä et al. who studied a total of 143 dimers consisting of different OOMs, including accretion products. They found that inflexible molecules formed more stable molecules, than flexible molecules, even if they had a low bulk saturation vapor pressure, due to their decreased likeliness to form internal hydrogen bonds as monomers. Out of the three OOMs studied here, only PDPE shows a single internal hydrogen bond. The monomer structures are included figure S1. This is not the definitive parameter that determines the stability of the clusters, and the flexibility of PDPE is thus favorable.

5)Please add units to the x-axes in Figures 7-9 (I assume ppt).

Author reply:
We appreciate the comment and acknowledge that this is an oversight at our end. Figure 7-9 have been altered to increase legibility. The x-axis title and units have been added, the y-axis is now shared across panels for direct comparison, and the markers have been made consistent across all three figures.

6)I am a bit worried about the boundary conditions used for the ACDC simulations, and their effect on the results. If I interpret the discussion around line 125-128 correctly, the "pure SA-base" clusters are required to have at least 4 sulfuric acids and 3 bases to be counted as "nucleated", while the organic clusters need less of each (such that one OOM can replace up to one base, and/or up to two sulfuric acids). I understand the reasoning here - if the OOMs are enhancing the nucleation, then it makes sense that they can be counted as "replacing one or two inorganic molecules". (For simpler notation, I here refer also to the amines as "inorganic", despite them having C-H bonds, and thus technically also being organic molecules.) And if we knew for sure that the OOMs are enhancing the nucleation, then probably something like these boundary conditions are, in the absence of data on the larger clusters, possibly the best guess we have for the "cluster formation potential", as the authors define it. However, as I see it, the main research question of the study is IF the tricarboxylic OOMs have a substantial enhancing effect on the cluster formation potential (and thus nucleation), or not. This being the case, the boundary conditions used here risk assuming the answer to this question before it has even been stated. (Or to put it another way, there is a risk of circular reasoning if the boundary conditions are set based on an assumption that the OOMs enhance nucleation, which in turn is based on simulations using these boundary conditions.) To illustrate what I mean, let's take a hypothetical "inert" organic compound, which behaves in the following way: 1)1 or 2 inert molecules stick to the inorganic clusters, with low enough evaporation rates that they are essentially always present in them, 2)further inert molecules do not stick to the clusters, and 3)the inert molecules do not affect (in either way) the addition of acids and bases. Using the outgrowing cluster definitions of the authors, they would find a huge "enhancement effect" from such inert organics (as you now only need to form clusters with 3 or even just 2 SA rather than the full 4 SA)- despite them (by definition) not actually affecting the SA-base clustering process at all. This is of course quite hypothetical - no real molecule will behave in this fashion - but it illustrates the problem. I strongly urge the authors to redo the simulations reported in Figures 7-9 so that the boundary conditions (outgrowing cluster definitions) in terms of SA and base molecules required for “nucleation” are exactly the same for both the “organic” and “inorganic” case. If the enhancement effect from these simulations is substantially smaller than that observed in the current simulations, then at least part of the effect originates in the assumed boundary conditions rather than the actual clustering chemistry or physics. The “real” cluster formation potential is then likely to lie somewhere between the two alternatives (outgrowing cluster definitions), and there is probably no accurate way of knowing better without actually studying the full set of (as yet too large to be computed) clusters. This is, I think, an inherent limitation of the otherwise elegant “cluster formation potential” approach. It might be that the best way to present results in these types of cases would be as some sort of shaded areas rather than single lines, with the limits of the shading given by different boundary condition definitions. So my suggested action item is to show these types of shaded areas in Figures 7-9.

Author reply:
To check this, we have have tested the effect of the organics by choosing two outgrowing clusters: 3sa2dma2pdpe and 3sa2dma0pdpe, and tested at 0 ppt pdpe and 10 ppt pdpe (1ppt dma, low concentration regime). The enhancement is about 3 times less than the box used in our article as we go from $J_{\text{out}} = 0.41$ cm^{-3}scm^{-1}, at 0 ppt to $J_{\text{out}} = 55.85$ cm^{-3}scm^{-1} at 10 ppt. Hence, the “order of magnitude” for the enhancement is still the same. We therefore still have confidence in our results, that the organics presented enhance the particle formation, while still acknowledging that the clusters studied are too small to be considered particles. We have chosen to not include the range in the graphs since we do not believe these two box sizes are comparable, and we do not have the data for the $(SA)_3(OOM)_2(BASE)_3$ structures. Furthermore, the inclusion of the 3sa3dma1pdpe cluster is maybe more questionable, however, removing this cluster from the outgrowing does not make a noticeable difference (10 ppt pdpe, 1 ppt dma, changed from $J_{\text{out}} = 96.290136$ cm^{-3}scm^{-1} to $J_{\text{out}} = 96.290135$ cm^{-3}scm^{-1}. We have adressed this in the manuscript.

Page 5 from:
In this study, we explicitly calculated thermodynamic data for the SA–OOM–Base clusters up to size 2 × 2 × 2, while the data for the SA–Base clusters up to size 3 × 3 was obtained from Kubečka et al. [2023]. The outgrowing clusters are therefore chosen to be $(SA)_4(\text{base})_3$, $(SA)_3(OOM)_2(\text{base})_2$, $(SA)_2(OOM)_3(\text{base})_2$ and $(SA)_3(OOM)_1(\text{base})_3$. Given that these outgrowing clusters are fairly small, the systems are artificially stable, and the critical cluster size may not yet have been reached, meaning the calculated formation rates are overestimated.

To:
In this study, we explicitly calculated thermodynamic data for the SA–OOM–Base clusters up to size 2 × 2 × 2, while the data for the SA–Base clusters up to size 3 × 3 was obtained from Kubečka et al. [2023]. The outgrowing clusters are therefore chosen to be one monomer larger than we have data for: $(SA)_4(\text{base})_3$, $(SA)_3(OOM)_2(\text{base})_2$, $(SA)_2(OOM)_3(\text{base})_2$ and $(SA)_3(OOM)_1(\text{base})_3$. Given that these outgrowing clusters are fairly small, the systems are artificially stable, and the critical cluster size may not yet have been reached, meaning the calculated formation rates are overestimated. Furthermore, given that these clusters do not have an equal number of SA and base monomers, it might artificially overestimate the enhancement factor of the OOM. To test this, we performed a simulation for smaller clusters

with $(SA)_2(PDPE)_3(DMA)_2$ and $(SA)_3(PDPE)_0(DMA)_2$ at 278.15 K, 1 ppt DMA, SA concentration of 10^6 molecules cm^{-3}, and PDPE at 0 and 10 ppt. We find an enhancement factor of 137 compared to 396 with the other box sizes. The enhancement is still in the same order of magnitude, illustrating that the enhancement from the OOM is not driven by the boundary conditions.

7)It might be interesting for readers to see estimates of the radii (radiuses) of the clusters in Figures 4 and 6. (This can be done for example by computing the volume in a quantum chemistry programme, using some reasonable default electron density value, assuming a spherical cluster, and solving for r).

Author reply:
We agree with Theo that this would be interesting for readers, and add more context to the cluster structures presented in the study. A short comment has been made in the manuscript, and the radii have been added to the Supporting Information.

Added page 11:
The diameter of the $(SA)_2(DMA)_2(PDPE)_2$ cluster is above 1 nm, and both the $(SA)_2(DMA)_2(CHA)_2$ and $(SA)_1(DMA)_1(PDPE)_2$ is close to 1 nm in diameter, making them near the lower limit of experimental measurement techniques (Vanhanen et al., 2011). The cluster radii of the clusters in figure 4 and figure 6 are given in table S1.

Reviewer #2

Decision: Minor revision. The authors have the methodology, the data, and the conceptual framework to produce an outstanding paper, but avoid some essential work in the discussion and presentation, leaving the paper in parts underdeveloped. I suggest to accept the paper after revisions, that do not necessitate further calculations. The authors should consider addressing the following two points: (A) the tables, figures and plots should be revised. I attached some specific suggestions in the PDF. This can be considered as minor revision. (B) The comparison of the tricarboxylic acid results presented in this work with the "cluster-of-functional-groups" approach from their previous work should be addressed in more detail. One worked-out comparison in the discussion section would probably suffice as minor revision.

Author reply:
We will answer these individually in the next points

(1) Scientific significance: Excellent. The chosen systems follow a consequent strategy building on previous work, and the results enable a meaningful discussion of the "cluster-of-functional-groups" approach introduced by the authors earlier. However, this discussion remains very superficial in the present work and is left as an open question in the conclusion. Notably, the authors themselves propose comparing the current results with their previous ones as a future task. It is unclear why this comparison is not carried out in the present work. Should the "cluster-of-functional-groups" concept be properly and thoroughly discussed in light of the new results, this would elevate the manuscript's scientific significance.

Author reply:
We agree that the cluster-of-functional-groups was not discussed in-depth. They were meant as an outlook for a much more extensive study. We have removed the places mentioning the benchmarking of the approach in the manuscript.

Page 14 removed:
This is in agreement with the calculated cluster formation potentials in our previous work using the “cluster-of-functional-groups” approach

Page 14 removed:
thus validating the suitability of the “cluster-of-functional-groups” approach.

Page 15 removed:
This is also very similar to the results from the “cluster-of-functional-groups” approach. This illustrates that the “cluster-of-functional-groups” approach can be used in the future to identify more complex multifunctional HOMs that could potentially contribute to NPF

Page 15-16 removed:
The data from this work can be used to gauge the accuracy of the “cluster-of-functional-groups” approach, for example, by directly comparing the binding Gibbs free energies of the clusters studied in this paper with the $(SA)_{1-2}(Base)_{1-2}(Carboxylic\ Acid)_3$ clusters from “cluster-of-functional-groups”. Assessing the accuracy of the approach will allow us to apply it for more complex multi-functional highly oxygenated molecules (HOMs) in the future.

(2) Scientific quality: Outstanding The employed methodology is appropriate for the given task, is grounded in extensive prior benchmarking, and the approximations are communicated transparently. The results are discussed with care, and the written text contains correct statements and useful discussion. The scientific approach and methodology represent the state of the art, established by the authors over the last decade, and are of outstanding quality in the field. This aspect does not hold the paper back.

Author reply:
We appreciate the positive comments.

(3) Presentation quality: Good. The presentation of results in the written text is handled with care. However, the presentation in the figures is flawed in several places, bringing the overall assessment down. These issues are straightforward to address, and specific suggestions are provided in the attached PDF. The presentation quality can be easily elevated.

Author reply:
As requested by the reviewer, we have combined Table 1 with Figure 2. For the cluster potential plots, we have fixed the markers and made them share the same y-axis. For the binding free energies, we have split up the $(SA)_1$ and $(SA)_2$ clusters, to better see the differences in binding Gibbs free energies. For the remaining structure plots, we have added the binding Gibbs free energies below the names.

The comments in PDF annotations are quite scattered, making it quite difficult to answer in that format. We have therefore taken the liberty of paraphrasing some of the major questions here. The language changes will not be explicitly discussed here but are shown in the "track-changes" document.

Regarding the level of theory being too technical for an abstract.

Author reply:
We believe that including these technical details are important, as these define how "trustworthy" the results are. Likewise specifying ACDC was necessary, as this defines the way the cluster formation potentials are simulated/calculated similar to a level of theory.

Regarding the "density" error for the lower concentration regime

Author reply:
We tested the lowest nucleation rate case of the SA-AM-MBTCA system and found a similar maximum difference of 24 %. If we assume that the error in the cluster formation potential is directly given by the error in the evaporation rate, the factor that the rate changes is given as $f = \exp(\Delta G_{\text{error}}/RT)$, i.e., at room temperature, where $RT \approx 0.59$ kcal/mol, a $\ln(1.25) * 0.59$ kcal/mol $= 0.13$ kcal/mol error would yield the same change. The exponential growing error in binding free energies is therefore expected to be more severe than the error in the assumed density. We have added this to the manuscript.

Page 12 from:

Given that, for the OOMs, only the density of MBTCA was available in the literature, the effect of changing density was tested on the system yielding the highest nucleation rates (10 ppt PDPE, [SA] = 10^6 molecules cm^{-3} and 10 ppt DMA). When the density was set to that of agaric acid, a tricarboxylic acid with a relatively low density of 1.115 g cm^{-3}, the cluster formation potential was 260.71 cm^{-3} s^{-1}. When the density was set to that of citric acid, another tricarboxylic acid, but with a relatively high density of 1.665 g cm^{-3}, the cluster formation potential was 206.54 cm^{-3} s^{-1}. Thus, the change in density is insignificant relative to other error sources, and the density for all three molecules was set to that of MBTCA, 1.430 g cm^{-3}

To:
Given that, for the OOMs, only the density of MBTCA was available in the literature, the effect of changing density was tested on the system yielding the highest nucleation rates (10 ppt PDPE, [SA] = 10^6 molecules cm^{-3} and 10 ppt DMA) and the lowest nucleation rates (10 ppt MBTCHA, [SA] = 10^6 molecules cm^{-3} and 10 ppt AM). When the density was set to that of agaric acid, a tricarboxylic acid with a relatively low density of 1.115 g cm^{-3}, the cluster formation potential was 260.71 cm^{-3} s^{-1} and 3.99×10^{-7} cm^{-3} s^{-1}, respectively. When the density was set to that of citric acid, another tricarboxylic acid, but with a relatively high density of 1.665 g cm^{-3}, the cluster formation potential was 206.54 cm^{-3} s^{-1} and 3.22×10^{-7} cm^{-3} s^{-1}, respectively. This is a factor of 1.26 and 1.24, respectively. If we assume the error in the cluster formation potential is directly given by the error in the evaporation rate, the factor the rate changes is given as $f = \exp(\Delta G_{\mathrm{error}}/RT)$. This mean that at room temperature, where $RT \approx 0.59$ kcal/mol, a $\ln(1.26) * 0.59$ kcal/mol ≈ 0.14 kcal/mol error would yield the same change. The exponential growing error in the binding free energies is therefore expected to be more severe than the error in the assumed density and we therefore set the density for all three molecules to that of MBTCA, 1.430 g cm^{-3}

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