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Comment to "Detecting supramolecular organic nanoparticles during heat wave by Zhang et al."

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Abstract. Atmospheric new-particle formation is a major source of aerosol particles that influence air quality, cloud properties, and climate. Understanding the molecular mechanisms governing the initial steps of particle formation is therefore essential for accurately representing aerosol formation and its climatic effects in atmospheric models. Zhang et al. (2026c) recently proposed that hydrogen-bond–driven self-assembly of neutral carboxylic acids is a spontaneous and ubiquitous atmospheric new-particle formation mechanism. If correct, this would represent a fundamental shift in the current understanding of atmospheric nucleation.

In this comment, we show that the proposed nucleation mechanism is not adequately supported by the observations or theoretical analysis presented in Zhang et al. The reported particle-composition measurements lack sufficient validation to establish the proposed molecular composition of the smallest particles and do not directly constrain the molecular processes responsible for the earliest stages of particle formation. Furthermore, using the thermodynamic data reported by Zhang et al., we demonstrate that cluster evaporation overwhelmingly exceeds growth by molecular collisions, resulting in negligible particle-formation rates under the reported atmospheric conditions. These kinetic and thermodynamic analyses demonstrate that hydrogen-bond–driven clustering of neutral carboxylic acids cannot explain the reported observations and is unlikely to represent an atmospherically relevant new-particle formation mechanism.

1 Introduction

Recent work by Zhang et al. (2026c) proposes self-assembly of carboxylic acids through hydrogen-bond interactions as an explanation for their observations of atmospheric new-particle formation (NPF) at high temperatures, and further suggest that this represents a common mechanism for NPF under diverse tropospheric conditions. However, the presented evidence does not support this hypothesis. While atmospheric NPF can certainly occur through different mechanisms depending on the environmental conditions, the mechanism proposed by Zhang et al. — hydrogen-bond–driven NPF of pure carboxylic acids —

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is not feasible under the atmospheric conditions investigated. Both the experimental observations and the theoretical analysis contain fundamental limitations that undermine the proposed nucleation mechanism.

The issues leading to incorrect conclusions in the original paper can be divided into two categories: 1) fundamental problems in the interpretation of molecular cluster stability and nanoparticle formation kinetics, which lead to an erroneous theory on nucleation mechanism and 2) limitations in the experimental methodology and interpretation of the measurements. While the experimental uncertainties alone already weaken the conclusions, the theoretical analysis further demonstrates that the proposed hydrogen-bond–driven nucleation mechanism cannot explain the reported atmospheric observations.

2 Results and Discussion

2.1 Cluster thermochemistry

Zhang et al. (2026c) propose that cluster formation begins with the dimerization of glutaric acid (GlA) and toluic acid (ToA). This GlA–ToA complex is referred to as aggregate A_2, and the reported Gibbs free energy of formation at 298 K is -7.7 and -7.6 kcal/mol at the ωB97X-D/6-31++G** (referred to as DFT) and DLPNO–CCSD(T)/aug-cc-pVTZ//DFT (referred to as DLPNO//DFT) levels of theory, respectively. These ΔG values appear unrealistically favorable, as previous quantum-chemical studies have shown that the binding free energy of a doubly hydrogen-bonded carboxylic acid dimer is typically approximately -5 kcal/mol at 298 K using similar DLPNO//DFT levels of theory (Pedersen et al., 2024).

2.1.1 Re-calculation of dimer thermochemistry

As the dimer formation is known to be a key step in further cluster formation, we re-calculated the Gibbs free energy of formation for the GlA–ToA complex. Systematic configurational sampling was performed for the complex and its monomers using Conformer-Rotamer Ensemble Sampling Tool (CREST) (Pracht et al., 2024). We employed CREST using the semiempirical extended tight-binding GFN2-xTB method (Bannwarth et al., 2019), and all conformers within 6 kcal/mol of the lowest energy conformer were selected for further optimization. The structures were re-optimized and frequencies calculated at the DFT level of ωB97X-D/6-31++G** (Chai and Head-Gordon, 2008) using Gaussian 16 RevC.02 (Frisch et al., 2016). We selected conformers within 1 kcal/mol of the lowest DFT Gibbs free energy and calculated the single point energy corrections using DLPNO–CCSD(T)/aug-cc-pVTZ level of theory (Riplinger et al., 2016; Myllys et al., 2016) as implemented in Orca 6.0.1 (Neese, 2025).

The Gibbs free energy of dimerization is calculated using global minimum free energies as $\Delta G = G_{\text{GlA-ToA}} - G_{\text{GlA}} - G_{\text{ToA}}$. The Gibbs free energy is a sum of the single point energy and the thermal contribution to the Gibbs free energy as $G = E_{\text{SPE(DLPNO)}} + G_{\text{thermal(DFT)}}$. For GlA–ToA complex, the Gibbs free energy of GlA–ToA complex formation at 298 K to be -6.6 (DFT) and -5.1 kcal/mol (DLPNO//DFT). Figure 1 presents the minimum free energy structures.

The difference is partly explained by the fact that Zhang et al. (2026a) appear to have manually selected their monomer structures rather than performing systematic configurational sampling. Instead of using the global-minimum structure of the

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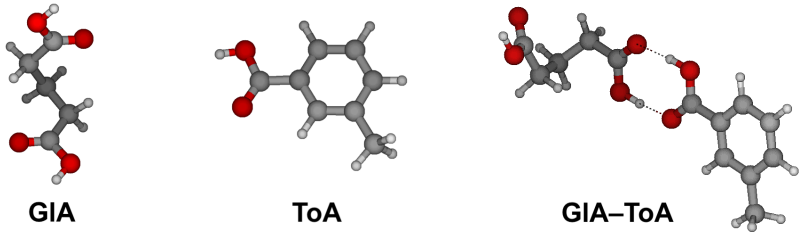

Figure 1. The global minimum free energy structures of GlA, ToA, and GlA–ToA are 0.7, 1.1, and 0.6 kcal/mol lower in DFT free energy, respectively, than structures reported by Zhang et al. Gray, white, and red spheres correspond to C, H, and O atoms, respectively.

five-carbon-chain GlA monomer, they employed a linear conformer that is 0.7 kcal/mol higher in DFT free energy. Previous studies have systematically demonstrated that the choice of monomer conformer can qualitatively affect calculated dimerization free energies (Kähärä et al., 2025). In the case of the ToA monomer, the reported structure is not even a true minimum, but rather a saddle-point structure corresponding to the internal rotation of a methyl group. This is confirmed by the presence of a low imaginary vibrational frequency corresponding to methyl rotation. This saddle-point structure is 1.1 kcal/mol higher in DFT free energy than the global minimum structure. Because cluster free energies are referenced to the isolated monomers, these two monomer sampling errors together lead to an artificial stabilization of the dimer of approximately 1.8 kcal/mol. In addition, DLPNO single-point energy corrections usually lead to $>$1 kcal/mol destabilization of this size dimers (Elm, 2019). However, there seem to be technical problems in DLPNO calculations which have been corrected in an erratum (Zhang et al., 2026b). It should be noted that even Zhang et al. performed some sampling for clusters, we found 0.6 kcal/mol lower DFT free energy GlA–ToA structure. This emphasizes the need to use systematic configurational sampling for both monomers and clusters.

2.2 Molecular cluster kinetics

Although the quantum chemical calculations are questionable on their own, the theoretical framework based on the cluster thermodynamics is even more concerning. Zhang et al. (2026a) concludes that organic acids form nanoparticles through hydrogen-bonding interactions, and justifies this conclusion solely based on the negative sign of the ΔG values computed using the standard reference pressure of 1 atm (instead of the actual Gibbs free formation energies using actual vapor concentrations). Even if the reported ΔG values were correct, they would still demonstrate that organic-acid clustering does not occur spontaneously anywhere close to the kinetic limit, but instead involves a free energy barrier. More precisely, the proposed nucleation mechanism cannot operate (i.e. form non-negligible amounts of nanoparticles) under the reported heat-wave conditions (or at any atmospherically relevant conditions).

At given conditions, a cluster is considered to be stable against evaporation when its collision rate with vapor molecules (or clusters) is equal to or higher than its evaporation rate. According to the law of mass balance, the formation of cluster $(i + j)$

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from clusters or molecules i and j as

$$i + j \rightleftharpoons (i + j) \tag{R1}$$

has the equilibrium constant K

$$K = \frac{C_{i+j}^{\mathrm{eq}}}{(C_i^{\mathrm{eq}})(C_j^{\mathrm{eq}})} = \frac{k_{\mathrm{B}}T}{p_{\mathrm{ref}}} \exp\left(-\frac{\Delta G}{k_{\mathrm{B}}T}\right), \tag{1}$$

where C_i^{eq} is the equilibrium concentration of species i, k_{B} is the Boltzmann constant, T is the temperature, ΔG is the Gibbs free energy of reaction (R1), and p_{ref} is the reference pressure at which ΔG is calculated (1 atm both here and in the study by Zhang et al.). At equilibrium and assuming detailed balance,

$$\gamma_{(i+j)\to i,j} C_{i+j}^{\mathrm{eq}} = \beta_{i,j} C_i^{\mathrm{eq}} C_j^{\mathrm{eq}}, \tag{2}$$

where $\gamma_{(i+j)\to i,j}$ is the evaporation rate constant and $\beta_{i,j}$ is the collision rate constant. From Eqs. (1) and (2), the evaporation rates of the clusters are obtained from the Gibbs free binding energies of the evaporating cluster and its products as

$$\gamma_{(i+j)\to i,j} = \beta_{i,j} C_{\mathrm{ref}} \exp\left(\frac{\Delta G_{i+j} - \Delta G_i - \Delta G_j}{k_{\mathrm{B}}T}\right). \tag{3}$$

The reference vapor concentration is obtained from the reference pressure as $C_{\mathrm{ref}} = p_{\mathrm{ref}}/(k_{\mathrm{B}}T)$.

Gibbs free binding energies ΔG, generally calculated at a standard reference pressure of 1 atm, yield insight into the relative cluster stabilities, but do not include the effect of the vapor-phase concentrations of the clustering species. The actual vapor-concentration-dependent Gibbs free energies of the clusters at given vapor concentrations C_n can be obtained as:

$$\Delta G_{\mathrm{actual}}(C_1, C_2, ..., C_{n_{\mathrm{tot}}}) = \Delta G - k_{\mathrm{B}}T \sum_{n=1}^{n_{\mathrm{tot}}} N_n \ln\left(\frac{C_n}{C_{\mathrm{ref}}}\right), \tag{4}$$

where N_n is the number of molecules of species n in the cluster. For a single species, Eq. 4 can be simply written as (Halonen, 2022):

$$\Delta G_{\mathrm{actual}}(C) = \Delta G - (N-1) k_{\mathrm{B}}T \ln\left(\frac{C}{C_{\mathrm{ref}}}\right). \tag{5}$$

The actual Gibbs formation free energies determine whether the cluster formation is thermodynamically favorable at given vapor concentrations.

2.2.1 Cluster evaporation occurs faster than new collisions

Using the standard detailed-balance approach, the evaporation frequency of the GlA–ToA complex with a reported $\Delta G = -7.7$ kcal/mol is on the order of 10^4 s^{-1}. To compete effectively with evaporation, the collision frequency between the complex and an incoming monomer would need to be comparable to the evaporation frequency. The collision-rate constant between A_2 and a new monomer, referred to as the dipole–dipole capture rate (k_D) by Zhang et al., is 3×10^{-10} cm^{-3} s^{-1}. The highest

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reported total organic-acid concentration ([OA]) is on the order of 2 ppb $\approx 5 \times 10^{10}$ cm^{-3}, which yields molecular collision frequencies of 15 s^{-1}. Computed collision and evaporation frequencies were further evaluated for all clusters containing up to six acid monomers, using the ΔG and k_D values from Zhang et al., which shows the evaporation frequencies to be approximately three orders of magnitude higher than the collision frequencies. This clearly demonstrates that none of the A_2–A_6 aggregates are stable against evaporation under the reported conditions (see Figure 2).

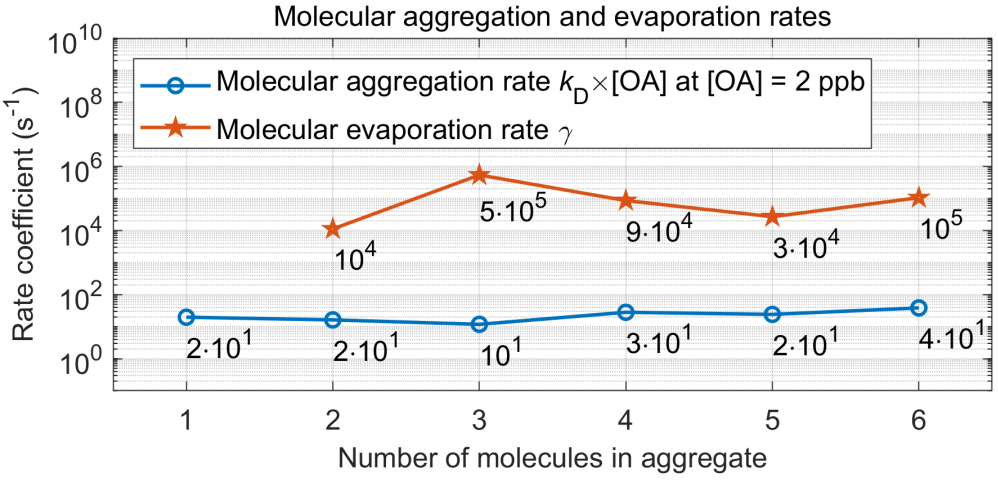

Figure 2. Molecular collision and evaporation frequencies for clusters consisting of 1–6 acid molecules. At a total [OA] of 2 ppb and at 298 K, the evaporation frequencies calculated from the Gibbs free energies provided by Zhang et al. exceed the collision frequencies by several orders of magnitude. Note that the use of corrected quantum-chemical data would further increase the evaporation rates.

Furthermore, the actual Gibbs free formation energies, calculated from the free energies reported by Zhang et al. (2026c) at an ambient total OA concentration of 2 ppb, demonstrate that the aggregate A_2–A_6 formation has a free energy barrier (see Figure 3), in contrast to the claim made in an original article. The actual Gibbs free formation energies account for the effect of the ambient monomer partial pressure, which is typically orders of magnitude lower than the reference pressure of 1 atm used in quantum chemical calculations (Vehkamäki and Riipinen, 2012).

2.3 Organic nanoparticle formation

New-particle formation simulations using the thermochemistry data by Zhang et al. (2026c) further demonstrate that the proposed mechanism yields negligible NPF rates at reported atmospheric conditions (see Figure 4). NPF was simulated using the Atmospheric Cluster Dynamics Code (ACDC) (Olenius et al., 2013; Olenius; McGrath et al., 2012) which generates the birth–death equations for a given set of clusters, and solves them explicitly by numerical integration. The birth–death equation for each cluster is written as

$$\frac{dC_i}{dt} = \frac{1}{2}\sum_{j<i}\beta_{j,(i-j)}C_jC_{(i-j)} + \sum_j \gamma_{(i+j)\to i,j}C_{(i+j)} - \sum_j \beta_{i,j}C_iC_j - \frac{1}{2}\sum_{j<i}\gamma_{i\to j,i-j}C_i + S_i - L_iC_i, \quad (6)$$

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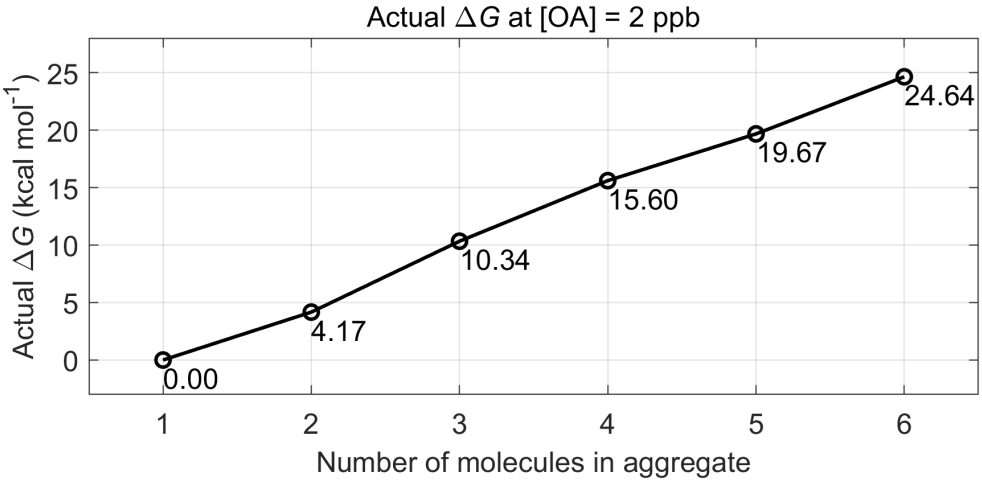

Figure 3. Actual Gibbs free formation energy at [OA]=2 ppb and 298 K, using the values from Zhang et al. for 1 atm reference pressure. Organic acid aggregate formation has a free energy barrier when the ambient acid concentration is accounted for. Note that the use of corrected quantum-chemical data would further increase the actual Gibbs free formation energies.

where C_i is the concentration of cluster i, $\beta_{i,j}$ is the collision rate coefficient between i and j, $\gamma_{(i+j)\rightarrow i,j}$ is the evaporation rate coefficient of cluster $(i+j)$, S_i is an external source term, and L_i is an external loss term, here corresponding to scavenging onto the surfaces of larger aerosol. The positive terms correspond to all collision and evaporation processes that create cluster C_i, and the negative terms to all processes in which the cluster is lost. The reference loss rate was set to 10^{-3} s^{-1}, corresponding to the lowest values of condensation sink in Fig. S11 by Zhang et al.; using an even lower value of 10^{-4} s^{-1} had no visible effect as such L values are negligible compared to the frequencies of the collision and evaporation processes.

To run new-particle formation simulations using the Gibbs free energies provided by Zhang et al., we lumped all monomers (GlA, ToA, 2-Methylglyceric acid, sulfuric acid, azelaic acid and tricarballylic acid) to represent general acid monomer OA and simulated a pseudo-1-component system. Instead of using concentrations for a specific acid, we thus used the total acid concentration [OA], which leads to overestimated collision and NPF rates. Collision rate coefficients between monomers and clusters were set to the k_{D} values given by Zhang et al. Coagulation rate coefficients between two clusters were calculated as hard-sphere collision rates assuming average molecular mass and density of 140 amu and 1.1 g cm^{-3}, following Zhang et al., leading to collision rates that are slightly higher than the k_{D} values. Additionally, allowing the larger (unstable) clusters consisting of more than six monomers to leave the simulation without re-evaporation also leads to overestimated NPF rates.

Even when using artificially stabilized clusters (excessively negative ΔG values by Zhang et al.) and assuming that the formed A_7 and larger clusters are not evaporating back to smaller sizes, the simulated NPF rate at 298 K and [OA]=2 ppb remains several orders of magnitude below the reported measured rates, and generally below values that can have a significant atmospheric impact. Because cluster stability decreases with increasing temperature according to $\Delta G = \Delta H - T\Delta S$, the NPF

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rate becomes even lower at elevated temperatures, including heat-wave conditions. These results clearly demonstrate that the proposed nucleation mechanism is not feasible.

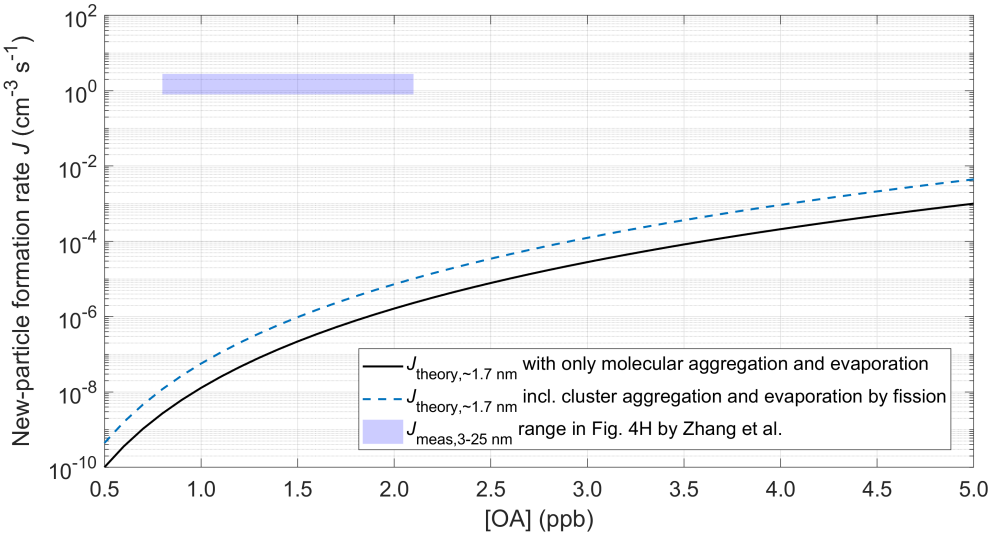

Figure 4. New-particle formation rate as a function of total organic acid concentration. Within the experimentally measured total [OA] range and at 298 K, the theoretical NPF rate of 1.7 nm particles is at most ca. 10^{-5} cm^{-3} s^{-1}, which is several orders of magnitude below the experimentally determined formation rates of 3–25 nm particles reported by Zhang et al. Note that the use of corrected quantum-chemical data would further reduce the simulated NPF rates.

2.4 Experimental limitations

In addition to the fundamental problems in the theoretical analysis, the experimental observations presented by Zhang et al. do not provide conclusive evidence for their hypothesis. While ambient observations cannot be reproduced independently, Zhang et al. report compositional measurements of small particles at substantially higher sensitivities than those previously achieved by other groups (Stolzenburg et al., 2025; Smith et al., 2021), yet without presenting methodological innovations or instrumental developments that would plausibly enable such observations. The sensitivity calibration used to determine the detection limits of the thermal desorption–ion drift–chemical ionization mass spectrometry (TD-ID-CIMS) system, reported to range from 0.01 to 0.06 ng, was performed by depositing calibrants directly onto the electrostatic particle collector. The reported 0.5 ng collected mass for 3 nm particles also appears difficult to reconcile with a simple particle-number mass balance. For 3 nm spherical particles with a density of 1 g/cm^3, 0.5 ng corresponds to about 3.5×10^{10} particles. At 5 L/min for 3 h, this requires a concentration of roughly 4×10^4 cm^{-3} particles actually reaching the collector. If 10% of sampled particles are charged and 10% penetrate the inlet lines and size-classification device, the required ambient 3 nm particle concentration becomes 4×10^6 cm^{-3}. This is far above the reported nucleation-mode concentrations, which peak around 2×10^4 cm^{-3} for the entire

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range of 3–25 nm particles (N_{3-25}). Therefore, the claimed mass closure of sub-10 nm particles should be treated cautiously unless the authors provide more methodological details on the size-resolved closure for charging efficiency, transmission through inlet and classification device, particle losses, and actual 3 nm number concentration during the collection period. In general, Zhang et al. present numerous measurements that surpass what others have managed to achieve before, yet provide very little detail on how this was made possible. The insufficient reporting of methods and instrument performance, especially for the non-trivial density and hygroscopicity measurements at 10 nm and below, undermines confidence in the reliability of the reported data.

Lastly, it should be still noted that particle-phase observations of 3–10 nm particles do not provide direct information about the nucleation mechanisms (Mohr et al., 2019; Kulmala et al., 2014). Compounds detected in 3–10 nm particles may have formed through particle-phase chemistry or condensed during later growth stages, rather than participating in the initial nucleation process itself. The analytical selectivity of the employed TD-ID-CIMS approach toward acidic compounds complicates interpretation of the measurements in terms of volatility and nucleation chemistry. Furthermore, the gas-phase measurements were performed using PTR-MS, which is not sensitive to the lowest-volatility vapors relevant for nucleation. As a result, the study lacks direct measurements of the low-volatility gas-phase species most likely involved in initial cluster formation.

3 Conclusions

This comment demonstrates that carboxylic acid–carboxylic acid interactions are insufficiently strong to produce thermodynamically stable non-ionic clusters at room temperature or above. Even at very high organic acid concentrations and using thermodynamic data that favor cluster stability, evaporation frequencies exceed molecular collision frequencies by several orders of magnitude, indicating that nucleation proceeds through a substantial thermodynamic barrier rather than spontaneous self-assembly. Furthermore, the experimental observations do not provide conclusive evidence for the proposed mechanism. Considerably more methodological detail and quantitative validation — including a transparent, size-resolved assessment of charging efficiency, transmission efficiency, sampling losses, and particle-number closure — would be required to establish the reported particle compositions reliably.

Our molecular cluster kinetics simulations further demonstrate that sequential addition of neutral organic acid monomers produces negligible nanoparticle formation rates under atmospherically relevant conditions. These findings indicate that hydrogen-bond–driven nucleation of pure organic acids is unlikely to represent a significant atmospheric new-particle formation pathway. More broadly, they reaffirm that both thermodynamic stability and cluster kinetics must be considered when evaluating feasibility of atmospheric nucleation mechanisms and that molecular composition measurements alone cannot establish the molecular pathways responsible for the initial steps of particle formation. Consequently, mechanisms involving additional stabilizing species or alternative molecular interactions remain necessary to explain the formation of organic nanoparticles in the atmosphere.

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Data availability. The optimized structures and calculation output files of all relevant compounds that support the findings of the manuscript will be available in the Zenodo repository (DOI: 10.5281/zenodo.20556060).

Author contributions. NM performed the calculations and wrote the manuscript. TO and TK contributed to the theoretical insights; TO made the Figures 2–4. JK, DS, MR, JNS and ME contributed to the experimental insights. All authors proofread the manuscript.

Competing interests. The corresponding author has stated that none of the authors have any competing interests.

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https://doi.org/10.5194/egusphere-2026-3785
Preprint. Discussion started: 7 August 2026

References

Bannwarth, C., Ehlert, S., and Grimme, S.: GFN2-xTB — An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions, J. Chem. Theory Comput., 15, 1652–1671, https://doi.org/10.1021/acs.jctc.8b01176, 2019.

Chai, J.-D. and Head-Gordon, M.: Long-Range Corrected Hybrid Density Functionals with Damped Atom-Atom Dispersion Corrections, Phys. Chem. Chem. Phys., 10, 6615–6620, https://doi.org/10.1039/B810189B, 2008.

Elm, J.: An atmospheric cluster database consisting of sulfuric acid, bases, organics, and water, Acs Omega, 4, 10 965–10 974, 2019.

Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Petersson, G. A., Nakatsuji, H., Li, X., Caricato, M., Marenich, A. V., Bloino, J., Janesko, B. G., Gomperts, R., Mennucci, B., Hratchian, H. P., Ortiz, J. V., Izmaylov, A. F., Sonnenberg, J. L., Williams-Young, D., Ding, F., Lipparini, F., Egidi, F., Goings, J., Peng, B., Petrone, A., Henderson, T., Ranasinghe, D., Zakrzewski, V. G., Gao, J., Rega, N., Zheng, G., Liang, W., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Throssell, K., Montgomery, Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M. J., Heyd, J. J., Brothers, E. N., Kudin, K. N., Staroverov, V. N., Keith, T. A., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A. P., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Millam, J. M., Klene, M., Adamo, C., Cammi, R., Ochterski, J. W., Martin, R. L., Morokuma, K., Farkas, O., Foresman, J. B., and Fox, D. J.: Gaussian16 Revision A.03, 2016.

Halonen, R.: A consistent formation free energy definition for multicomponent clusters in quantum thermochemistry, J. Aerosol Sci., 162, 105 974, https://doi.org/https://doi.org/10.1016/j.jaerosci.2022.105974, 2022.

Kähärä, J., Franzon, L., Ingram, S., Myllys, N., Kurtén, T., and Vehkamäki, H.: Enhanced configurational sampling methods reveal the importance of molecular stiffness for clustering of oxygenated organic molecules, Physical Chemistry Chemical Physics, 27, 23 410–23 420, 2025.

Kulmala, M., Petäjä, T., Ehn, M., Thornton, J., Sipilä, M., Worsnop, D., and Kerminen, V.-M.: Chemistry of atmospheric nucleation: on the recent advances on precursor characterization and atmospheric cluster composition in connection with atmospheric new particle formation, Annual review of physical chemistry, 65, 21–37, 2014.

McGrath, M. J., Olenius, T., Ortega, I. K., Loukonen, V., Paasonen, P., Kurtén, T., Kulmala, M., and Vehkamäki, H.: Atmospheric Cluster Dynamics Code: a Flexible Method for Solution of the Birth–Death Equations, Atmos. Chem. Phys., 12, 2345–2355, https://doi.org/10.5194/acp-12-2345-2012, 2012.

Mohr, C., Thornton, J. A., Heitto, A., Lopez-Hilfiker, F. D., Lutz, A., Riipinen, I., Hong, J., Donahue, N. M., Hallquist, M., Petäjä, T., et al.: Molecular identification of organic vapors driving atmospheric nanoparticle growth, Nature communications, 10, 4442, 2019.

Myllys, N., Elm, J., Halonen, R., Kurtén, T., and Vehkamäki, H.: Coupled cluster evaluation of the stability of atmospheric acid–base clusters with up to 10 molecules, J. Phys. Chem. A, 120, 621–630, 2016.

Neese, F.: Software update: the ORCA program system—version 6.0, Wiley Interdisciplinary Reviews: Computational Molecular Science, 15, e70 019, 2025.

Olenius, T.: Atmospheric Cluster Dynamics Code, https://github.com/tolenius/ACDC.

Olenius, T., Kupiainen-Määttä, O., Ortega, I., Kurtén, T., and Vehkamäki, H.: Free energy barrier in the growth of sulfuric acid–ammonia and sulfuric acid–dimethylamine clusters, The Journal of chemical physics, 139, 2013.

Pedersen, A. N., Knattrup, Y., and Elm, J.: A cluster-of-functional-groups approach for studying organic enhanced atmospheric cluster formation, Aerosol Research, 2, 123–134, 2024.

https://doi.org/10.5194/egusphere-2026-3785
Preprint. Discussion started: 7 August 2026

Pracht, P., Grimme, S., Bannwarth, C., Bohle, F., Ehlert, S., Feldmann, G., Gorges, J., Müller, M., Neudecker, T., Plett, C., Spicher, S., Steinbach, P., Wesołowski, P., and Zeller, F.: CREST—A program for the exploration of low-energy molecular chemical space, The Journal of Chemical Physics, 160, 114 110, 2024.

Riplinger, C., Pinski, P., Becker, U., Valeev, E. F., and Neese, F.: Sparse Maps—A Systematic Infrastructure for Reduced-Scaling Electronic Structure Methods. II. Linear Scaling Domain Based Pair Natural Orbital Coupled Cluster Theory, J. Chem. Phys., 144, 024 109, https://doi.org/10.1063/1.4939030, 2016.

Smith, J. N., Draper, D. C., Chee, S., Dam, M., Glicker, H., Myers, D., Thomas, A. E., Lawler, M. J., and Myllys, N.: Atmospheric clusters to nanoparticles: Recent progress and challenges in closing the gap in chemical composition, Journal of Aerosol Science, 153, 105 733, 2021.

Stolzenburg, D., Sarnela, N., Bianchi, F., Cai, J., Cai, R., Cheng, Y., Dada, L., Donahue, N. M., Grothe, H., Holm, S., et al.: Incomplete mass closure in atmospheric nanoparticle growth, npj Climate and Atmospheric Science, 8, 75, 2025.

Vehkamäki, H. and Riipinen, I.: Thermodynamics and kinetics of atmospheric aerosol particle formation and growth, Chemical Society Reviews, 41, 5160–5173, 2012.

Zhang, R., Li, Y., Zhao, J., Aridjis-Olivos, B., Zhao, L., Kowalewski, V., Kabir, M., Johnson, N. M., Nielsen, E. R., Brooks, S. D., Zhang, Y., Vedlitz, A., Porter, W., North, S. W., Li, W., Young, M. W., Seinfeld, J. H., Wang, Y., and Wang, Y.: Quantum Chemical and Structural Data for the article "Detecting supramolecular organic nanoparticles during heat wave", Zenodo, https://doi.org/10.5281/zenodo.20210614, 2026a.

Zhang, R., Li, Y., Zhao, J., Aridjis-Olivos, B., Zhao, L., Kowalewski, V., Kabir, M., Johnson, N. M., Nielsen, E. R., Brooks, S. D., Zhang, Y., Vedlitz, A., Porter, W., North, S. W., Li, W., Young, M. W., Seinfeld, J. H., Wang, Y., and Wang, Y.: Erratum for the Research Article “Detecting supramolecular organic nanoparticles during heat wave”, Science, 393, eaej7556, https://doi.org/10.1126/science.aej7556, 2026b.

Zhang, R., Li, Y., Zhao, J., Aridjis-Olivos, B., Zhao, L., Kowalewski, V., Kabir, M., Johnson, N. M., Nielsen, E. R., Brooks, S. D., Zhang, Y., Vedlitz, A., Porter, W., North, S. W., Li, W., Young, M. W., Seinfeld, J. H., Wang, Y., and Wang, Y.: Detecting supramolecular organic nanoparticles during heat wave, Science, 391, eady5192, 2026c.