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Atmospheric Chemistry and Physics
Discussions

Interactive comment on "Role of Base Strength, Cluster Structure and Charge in Sulfuric Acid-Driven Particle Formation" *by* Nanna Myllys et al.

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This work is based on quantum chemical calculations and kinetic simulation as well as ESI-MS experiments to study the aerosol nucleation abilities for various composition and charge states. The cluster binding patterns with size dependence, the nucleation barrier analysis, the cluster relative concentrations ratio and the formation rates are properly analyzed. The strong binding of guanidine comparing with the other bases is highly emphasized and properly validated. This work provides important insights to the different base contributing nucleation abilities and has shown significant evidences from the view of structure, thermodynamics and kinetics. So I recommend it to be

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Discussion paper

published in Atmos. Chem. Phys. with minor revisions.

Specific comments:

1) In 3.3, for the conclusion that “This indicates that the enhancing effect of bisulfate in particle formation becomes more remarkable for weaker bases, since the presence of bisulfate removes the thermodynamic barrier of cluster growth (which does not exist in the case of guanidine)”, it is unreasonable to draw this since the analysis for figure 6 only points to the stronger nucleation abilities with the increase of alkalinity for the case of bisulfate. If “the enhancing effect of bisulfate” could be known, it should be compared with different acids with the same base, like comparing figure 6 with figure 2. Whether or not the enhancing effect of bisulfate is more remarkable for weaker bases could also be figured out through comparing figure 6 with figure 2.

2) For the simulation of formation rates with the aid of ACDC, the boundary condition setting is crucial so the boundary conditions for all the systems should be added on the supplementary information.

3) The overestimation of new particle formation rates with constant base source is a very important conclusion. More descriptions about the constant base concentration case as well as the validity of simulation settings should be given.

Technological errors:

1) I am wondering if the free energies shown on figure 6 are standard Gibbs free energies or the actual concentration-dependent ones. If it’s the former case, please correct it to match the figure caption.

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