Review of:

Enhancing effect of dimethylamine in sulfuric acid nucleation in the presence of water – a computational study.

V. Loukonen, T. Kurtén, I.K. Ortega, H. Vehkamäki, A. A. H. Pádua, K. Sellegri, and M. Kulmala

General Comment:

The manuscript compares the effect of ammonia and dimethylamine on the hydration of clusters containing 1-2 sulfuric acid molecules. The authors use up to date computational methods according to the size of the system and the aim of the study. The results show that dimethylamine enhances the addition of sulfuric acid to the clusters more efficiently than ammonia when the clusters contain no water or more than two water molecules. On the other hand, it is also shown that the clusters containing two sulfuric acid molecules and one dimethylamine will remain unhydrated in the range of RH studied.
The present paper fits the scope of ACP and it continues the series of publications in this journal related to the thermochemistry of sulfuric acid clusters in the atmosphere. For these reasons I believe that it should be published after revising some minor points listed below.

Comments for Introduction:

1. The authors mentioned the fourth assessment report of the IPCC from 2007. As far as this reviewer knows, there has been a new version from 2009. They should refer to the newest one.

Comments for Computational Details:

1. Pg. 2324, line 23: the authors wrote “Part of the initial structures …” while a few lines later (Pg. 2325, line 1) the authors wrote “… to generate initial guesses for all the structures”. It is not clear how they finally generated the initial guesses. If they used different methods, then they should specify why and for which ones.
2. Pg. 2325, line 11: the authors describe 10 initial structures as a “fair set”. Why ten? Is there any clue for that?
3. Pg 2326, line 9: the authors use the scaling procedure in order to correct for anharmonic effects. How procedures like “hindered rotor” or simply free rotor approximations would compare? It would be nice to see at least one comparison (for the smaller systems).
4. Page 2326, line 24: “… those arising from the different methods and basis sets used …” The sentence is quite confusing as written because it seems that they used different electronic-structure methods in order to evaluate the scaling factors. In my opinion the sentence would be more clear as “… and those inherent to the method and basis set used”.
5. Pg. 2327, line 5: although the different scaling factors (s_{ZPE}) are listed in the Supplementary Information, it would be very useful to have at least a few of them in the text and see there directly the comparison with the more standard scaling factors published by *Radom et al.*
6. Pg. 2327, line 17: This referee is aware of the impossibility to obtain scaling factors for the big clusters. However I can not see why the differences in the scaling factors would get smaller as the size of the cluster grows. Taking into account that the number of weak interactions increases with the size of the cluster and thus the anharmonicity of the system, I do not think that the scaling factors stabilize.

Comments for Results and Discussion

1. Pg. 2333, line 13: The authors speak about the T-dependence but they never introduced this variable in their study. Therefore that statement should be removed where mentioned.
2. Pg. 2333, line 19: which would be the most typical RH in the troposphere? Is that 50%? What about the temperature? Definitely, 298K is too high for the troposphere. I would rather say, the most tropospherically reasonable T is lower.
3. Pg. 2334, line 18: the authors stated that RH = 45% is low. In which context? In the troposphere?
4. Pg 2336, line 8: In line with the comment 2, I do not consider that T = 298 K and RH = 50% are the most representative for the tropospheric conditions. However, I believe their conclusions can be extrapolated in order to get some atmospheric relevant clues, but probably mentioning the real T and RH conditions in the troposphere.