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Atmospheric Chemistry and Physics Discussions

Interactive comment on "From quantum chemical formation free energies to evaporation rates" *by* I. K. Ortega et al.

Anonymous Referee #1

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Ortega and co-workers report a very interesting theoretical work facing the first stages of nucleation between sulfuric acid and ammonia or dimethylamine (DMA). The work is rigorous and well done and deserves publication in Atmospheric Chemistry and Physics. However, there are some comments I would like to address the authors.

In page 5, Conformational sampling section, the authors state that "the energies of all conformations are computed, and those with the lower energies are saved". The authors should clarify at which level these energies are computed.

Page 6, Method benchmark section. (a) I guess that one of the headers of Table 3 (B3LYP/CBSB7+RICC2 should read B3RICC2. (b) The Gibbs free energy of formation of sulfuric acid dimer written in the text (-7.91 kcal/mol, second line below Table 2), does not match with the number written in the Table (-7.89 kcal/mol). This should be

fixed.

It is very interesting the fact that the key factor for the stability of the cluster is the proton transfer. However, this fact in not clearly reflected, neither in the cluster names in Figure 1 nor in the reaction in Tables 3 and 4. I would suggest the authors, indicating in Tables 3 and 4, which reactions involve proton transfer. In connection to this point, it is also not clear whether the evaporation and fission processes are associated to acid base reactions, and I think this is an important point. Has this any effect in the cluster fragmentation in over-critical clusters?.

There are two Tables "3". The table in page 9 should read Table 5.

In the last paragraph of page 11, the authors compare the DMA evaporation rate of the (H2SO4)4(CH3)2NH cluster 2.83âĂć10-4 s-1 with the fission rate. . ., 35.29 s-1. The value 2.83âĂć10-4 s-1 does not match with the value in table of page 9 (2.72âĂć10-4 s-1). The authors should indicate the Tables these numbers come from.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 27327, 2011.