

Interactive comment on “Estimating the NH₃:H₂SO₄ ratio of nucleating clusters in atmospheric conditions using quantum chemical methods” by T. Kurtén et al.

Anonymous Referee #2

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The results of this paper shed light on the initial steps in the nucleation of H₂SO₄-NH₃ clusters in the atmosphere and further our understanding of central issues in atmospheric chemistry. The authors study ammonia addition reaction in H₂SO₄-NH₃ molecular clusters using ab initio methods. Their results indicate that the most probable NH₃:H₂SO₄ mole ratio in small molecular clusters under typical atmospheric conditions is around 1:2. The analysis is based on structure optimization calculations involving small non-hydrated clusters for which H₂SO₄-NH₃ binding is expected to be strongest.

The methodology, results, and discussion of this work are clearly presented. I have only one suggestion. I think the paper could be enriched by including a more detailed

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discussion of the reported differences in $\text{H}_2\text{SO}_4\text{-NH}_3$ mole ratios between small and larger particles. What physical or chemical factors are driving this “transition”? What favors the increase of ammonia concentration in the larger particles? What is the influence of "interfacial effects" on the composition and structure of the smaller clusters?

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 2937, 2007.

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