

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 #1

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The paper describes quantum chemical ab initio calculations for molecular clusters consisting of two sulfuric acid molecules with 0–4 ammonia molecules. Despite the fact that water molecules are not included in the calculation it is convincingly argued that these clusters give valuable information on the upper limit bonding energies for atmospheric clustering/nucleation of the ternary system. Because these neutral clusters are currently not accessible to any experimental technique for determination of the bond energies and ΔG values, these calculations are very valuable for determining the pathways of ternary H₂SO₄/NH₃/H₂O nucleation in the atmosphere and for the assessment of the detailed thermochemistry of ternary nucleation in model calculations. It is found that the most likely ratio of NH₃:H₂SO₄ in the clusters containing two sulfuric

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acid molecules is between 1:2 and 1:1 for typical atmospheric conditions. It is a very interesting finding of the paper that ammonium sulfate clusters $(\text{H}_2\text{SO}_4)_2(\text{NH}_3)_4$ with an $\text{NH}_3:\text{H}_2\text{SO}_4$ ratio of 2:1 are not formed in the atmosphere while ammonium sulfate is a typical component of large aerosol particles where properties are governed by the bulk phase.

The manuscript is well written and scientifically sound. The paper is well organized and all statements are justified. Rather conservative error analysis shows that the key statements hold even when large errors are assumed. The paper is suitable for publication in ACP.

Minor comment: Table 1: Reasons for the differences between the Delta G calculations by Kurtén et al., 2007, and Ianni and Bandy, 1999, should be discussed.

Technical correction: p. 2943, line 12, "...an unhydrated..."

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

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