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Atmospheric Chemistry and Physics Discussions

Interactive comment on "The role of ammonia in sulfuric acid ion induced nucleation" *by* I. K. Ortega et al.

Anonymous Referee #1

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The authors present a new theoretical methodology consisting of a multi-step quantum chemical calculation to be applied on clusters of atmospheric relevance. They have checked their proposal on both ternary neutral and ion induced nucleation processes. Thus, the authors have studied the role of NH3 on the growth of neutral clusters (H2SO4)n(NH3)m, n = 2-4, m = 0-1 as well as the mechanism for the ion-induced nucleation (-HSO4)(NH3)m(H2SO4)n, n = 1-3, m = 0-1.

The level of theory used for optimization of structures and vibrational analysis, BLYP/DZP, was adopted only after a selection procedure intended to get the best accuracy/computational effort ratio. Electronic energy was single-point calculated upon the optimized structures at a high-level theory, RI-CC2/aug-cc-pV(T+d)Z, from which no noticeable basis-set size effect can be expected.

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Interactive Discussion
Discussion Paper

This is a research, theoretical in nature, that sheds light on some less studied mechanisms of gas-to-particle nucleation processes taking part in the formation of aerosols. Computational calculations have been wisely selected and the results, as far as they can be compared with experimental data, confirm first that ammonia plays an important role in enhancing the growth of neutral sulphuric acid clusters while if does not play any relevant role in enhancing ionic ones. The anharmonicity effects due to the isolated HSO4- ion are shown to diminish as the number of sulphuric acid units rises.

Although the authors claim that representative atmospheric conditions have been selected to perform thermodynamic calculations, no water molecules have been considered in the simulations although in typical atmospheric conditions a number of water molecules can be linked to sulphuric acid-ammonia. The authors justify this aspect, however, on the basis of the main goal of the paper. Notwithstanding, in order to check the reliability of the conclusions as concern more realistic atmospheric conditions the authors should consider in the future to take into account the presence of water molecules.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 5413, 2008.

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Interactive Comment