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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Formation of binary ion clusters from polar vapours: Effect of the dipole-charge interaction" *by* A. B. Nadykto and F. Yu

Anonymous Referee #2

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MS-NR: ACPD2003-080 Title: Formation of binary ion clusters from polar vapours: Effect of the dipole-charge interaction Authors: A. B. Nadykto and F. Yu

General comments: This paper presents an improved theoretical treatment of the interaction of polar molecules with charged clusters by incorporating the charge-dipole interaction into the Kelvin-Thomson equation. The goal of this work is to improve the prediction of cluster ion-ligand thermodynamics. This work presents a useful advance in the simple theory presently used to predict cluster ion thermodynamics in ion-induced nucleation models.

Specific comments: 1. The authors show that including the charge-dipole interaction reduces the vapor pressure over the clusters and reduces the size of the critical clus-

ter in the nucleation of ions containing H2SO4 and H2O. This paper would benefit significantly by comparing the predictions of the new theory with the known thermodynamics of cluster ions. For example, a direct comparison between the predictions and experimental thermodynamics of H+(H2O)n and HSO4-(H2SO4)m would be very meaningful. Nucleation rates are extremely sensitive to the thermodynamics of cluster growth, and it is not clear if the theory presented in this work can accurately predict thermodynamics for cluster ions relevant to the atmosphere. 2. The authors compare critical cluster sizes predicted by their new theory to the critical cluster sizes predicted by the standard Thomson equation. These comparisons are interesting, but are only part of the story. The rate of nucleation is an exponential function of the barrier height, and it is important to also compare the heights of the nucleation barriers predicted by the two theories. 3. It would be useful to present general expressions for the Gibbs free energy change for the addition of a molecule to an arbitrary cluster based on the extended Thomson theory.

Technical corrections: 1. p. 4930, line 2: condensed is misspelled. 1. Equation (7): "mu" should be "pi". 3. p. 4931, line 2: infinity is a subscript. 4. Equation (11): first two quotients should have "b" subscripts? 5. p. 4932, line 1: eqn(12)=eqn(10)+eqn(11), not just the 2nd lines.

Interactive comment on Atmos. Chem. Phys. Discuss., 3, 4927, 2003.