MAG-WALKING SIMULATED ANNEALING MONTE CARLO STUDY OF NANO-SOLVATED AMMONIUM CHLORIDE. Sangjoon Lee, Steven L. Topper and Robert Q. Topper. Department of Chemistry, The Cooper Union for the Advancement of Science and Art, New York, NY 10003

Airborne ammonium chloride nanoparticles are formed by the reaction of ammonia and hydrogen chloride in the presence of water. Although it is known that the formation can be affected by the humidity, temperature, and the presence of dissolved organic matter, less is known about the mechanism for aerosol particle growth. In the present study, the minimum energy structures of nano-solvated ammonium chloride (surrounded by 2-8 water molecules) were determined using the mag-walking simulated annealing Monte Carlo method. Implemented via the TransRot software, mag-walking uses either a small, optimized stepsize or (randomly) a larger, magnified fixed stepsize, and can be tuned to either find the global minimum structure or, where relevant, higher-energy structures of interest. The method and parameters were benchmarked through the successful replication of literature global minimum energy values of water clusters using the TIP3P, TIP4P, and TIP4P/2005 empirical pair potentials. In future work, we plan to use ab initio calculations to predict thermodynamic properties, reaction energetics, and infrared spectra of nano-solvated ammonium chloride.