Unusual Hydrogen Bond Diversity in Ammonium Halide Nanoclusters

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Aerosolized ammonium chloride is an environmental contaminant that can form in polluted marine atmospheres when both NH_3 and HCl are present. Small ionic or neutral nanoparticles of ammonium halides (F, Br and Cl) are studied and their energetic and bonding properties analyzed. "Mag-walking" simulated annealing Monte Carlo calculations are an effective and unbiased way to rapidly locate thermally important minimum-energy structures of molecular clusters and small nanoparticles. These structures can then be subsequently refined and analyzed using *ab initio* and/or density functional theory calculations. Proton transfer between NH_3 and HX is driven by the addition of a third polarizable body in the case of X=(Br,Cl), resulting in ionic clusters. The situation appears to be considerably more complex for X=F clusters, which are unusual systems in that three distinct types of hydrogen bonds are observed nonuniformly as a function of cluster size.