STRUCTURE AND INFRARED SPECTRA OF NEW AEROSOL PARTICLE FORMATION SEED CLUSTERS

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One of the largest unknowns in the understanding of aerosol particles is the structure and growth process that drives new particle formation, particularly from a *molecular* point of view. These processes are dictated by the underlying interplay of hydrogen-bonding interactions of the organic molecules with water and water with itself. The presence of amine groups may further accelerate new particle formation; thus we model the vibrational spectra of clusters of several heterocyclic molecules complexed with water and ammonia. We model the OH and NH stretching regions of the clusters' IR spectra through a suite of approaches that have favorable computational scaling and cost compared to standard anharmonic approaches. This acceleration allows us to consider the numerous cluster candidates and provide assignments. Finally, the wealth of spectral data (both theoretical and experimental) allows us to test the performance of data-driven spectroscopic models.