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Abstract

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Solvation effects on twenty-two homogeneous and heterogeneous clusters formed from m nitric acid molecules and n ammonia molecules were studied using density functional theory. Percent differences between the gas phase and solution phase values of critical geometric parameters were used to quantify the effects of water on hydrogen bonding and proton transfer in these clusters. The effects of water on proton transfer were further analyzed using a proton transfer parameter proposed by I.J. Kurnig and S. Scheiner. Trends in these structural data indicate that water has a weakening effect on hydrogen bonding, which becomes more prevalent with increasing cluster size, as well as a catalytic effect on proton transfer, which diminishes with increasing cluster size. The energies of formation, Gibbs free energies of solvation, and evaporation rates of these clusters were also calculated and observed to exhibit trends which are consistent with these findings. Solvation effects on two stepwise cluster growth processes were also studied and a detailed analysis of their energetics indicates that changes in the individual entropies of their reaction pathway structures are responsible for drastic changes in the activation barriers, which, in turn, translate to significant effects on the evaporation rates.