A JOINT EXPERIMENTAL THEORETICAL STUDY OF NITRIC ACID-WATER COMPLEXES

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We present a joint theoretical experimental study of the solvation and dissociation of nitric acid in water. First principles electronic structure calculations assist in identifying spectroscopic features of the solvated nitric acid-water clusters and their transition upon formation of Solvent Separated Ion Pairs (SSIPs). The theoretical results are used to interpret experimental FTIR spectra of matrix isolated nitric acid-water clusters formed by incrementally increasing the amount of water in the matrix.