

A JOINT EXPERIMENTAL THEORETICAL STUDY OF NITRIC ACID-WATER COMPLEXES

SOTIRIS S. XANTHEAS, PATRICK R. MCCURDY AND WAYNE HESS, *Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, 906 Battelle Boulevard, PO Box 999, MS K8-91, Richland, WA 99352, USA.*

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.