ROVIBRATIONAL LEVELS AND INELASTIC SCATTERING OF THE H_2O-Ar CLUSTER IN FULL AND REDUCED DIMENSIONALITY

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The Water-Argon cluster is an important system of fundamental and practical interest. It is for example known to be one of the simplest systems capable of manifesting "hydrophobic interactions" and as such is an ideal candidate for the study of those interactions. On the fundamental level, it is a model system for the description of the intermolecular potential, rovibrational states and inelastic scattering of an atom and an asymmetric top van der Waal complex and thus may serve as a test to perform similar work on other systems. Additionally, the description of the H_2O-Ar intermolecular interaction is an important initial step to a deeper understanding of the static and dynamical properties of condensed phases such H_2O doped in large $(Ar)_N$ clusters. We investigate in this work the H_2O-Ar cluster on a global potential energy surface recently generated. We thus compute the rovibrational energy levels of the cluster in the rigid rotor approximation and in full dimensionality using the MCTDH improved relaxation method and compare our results with available experimental measurements and previous calculations. Then, we present inelastic scattering cross-sections of H_2O+Ar collisions obtained in the rigid rotor approximation using time-independent method and time-dependent method, and compare where available results with previous calculations. Finally, we will discuss the extension of the scattering calculations to the full dimensional case and the prospect of studying rovibrational relaxation within accurate time-dependent quantum calculations on similar systems or clusters.