TOWARDS A QUANTUM DYNAMICAL STUDY OF THE H_2O+H_2O INELASTIC COLLISION: REPRESENTATION OF THE POTENTIAL AND PRELIMINARY RESULTS

STEVE ALEXANDRE NDENGUE, RICHARD DAWES, *Department of Chemistry, Missouri University of Science and Technology, Rolla, MO, USA*.

Water, an essential ingredient of life, is prevalent in space and various media. H_2O in the gas phase is the major polyatomic species in the interstellar medium (ISM) and a primary target of current studies of collisional dynamics. In recent years a number of theoretical and experimental studies have been devoted to H_2O-X (with X=He, H_2, D_2, Ar, ...) elastic and inelastic collisions in an effort to understand rotational distributions of H_2O in molecular clouds. Although those studies treated several abundant species, no quantum mechanical calculation has been reported to date for a nonlinear polyatomic collider. We present in this talk the preliminary steps toward this goal, using the H_2O molecule itself as our collider, the very accurate MB-Pol surface to describe the intermolecular interaction and the MultiConfiguration Time Dependent (MCTDH) algorithm to study the dynamics. One main challenge in this effort is the need to express the Potential Energy Surface (PES) in a sum-of-products form optimal for MCTDH calculations. We will describe how this was done and present preliminary results of state-to-state probabilities.