MCTDH ROVIBRATIONAL STATES AND STATE-TO-STATE INELASTIC SCATTERING CALCULATIONS ON THE H_2O-H_2 SYSTEM

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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. In this work we are following those studies and will present benchmark calculations of rovibrational states and resonances of the H_2O-H_2 cluster in the rigid rotor approximation using the MultiConfiguration Time Dependent Hartree (MCTDH) approach. We will also present the first state-to-state inelastic scattering results of the H_2O+H_2 process in the rigid rotor approximation using the MCTDH approach. These calculations will serve as a foundation for similar triatomic – linear molecule interactions which are usually computationally expensive using standard calculations methods.