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Quantum dynamics of energy transfer for H collisions with water[1]
BENHUI YANG, University of Georgia, CHEN QU, Emory University, P. STANCIL, University of Georgia, J. BOWMAN, Emory University, N. BALAKRISHNAN, University of Nevada, Las Vegas, R. FORREY, Penn State University, Berks Campus — Modeling of molecular emission spectra from the interstellar medium requires the calculation of rate coefficients for excitation by collisions with abundant species. Water is an abundant molecule in a variety of astrophysical environments, and has been the focus of countless theoretical astrophysical studies and observations. In this work we report a full-dimensional (6D) potential energy surface (PES) and scattering calculations for the H_2O-H collision system. The 6D PES was calculated using the high-level ab initio RCCSD(T)-F12b method. A two-component invariant polynomial method was applied to fit the PES analytically in 6D. The pure rotational state-to-state cross sections and rate coefficients from selected initial states of H_2O were compared with previous theoretical results. We also consider the calculation of rovibrational state-to-state cross sections and rate coefficients of H_2O in collision with H for the fundamental vibrational modes of water, ν_1 (symmetric stretching), ν_2 (bending mode), and ν_3 (antisymmetric stretching).

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