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Extreme Potential Energy Surface Sensitivity for Rotational Quenching of Water via Hydrogen Atom Impact[1] BENHUI YANG, PHILLIP STANCIL, University of Georgia — Quantitative determinations of inelastic cross sections and rate coefficients for H_2O-H collisions are of interest for astrophysical models, while the water-H interaction is crucial for molecular dynamics simulations of hydrogen atom collisions on crystalline and amorphous ices. In this work, rotational energy transfer of H_2O due to H collisions was studied using an explicit quantum close-coupling approach for collision energies between 10^{-6} and 1000 cm^{-1} with para-H_2O initially in levels $1_{1,1}$ and $2_{2,0}$, and ortho-H_2O in levels $1_{1,0}$ and $2_{2,1}$. Total quenching cross sections and rate coefficients are obtained on two different potential energy surfaces typically adopted in molecular dynamics simulations. The quenching cross sections are found to differ significantly over the full range of considered energies. Elastic cross also show large discrepancies in the cold to ultracold regimes, but agree for collisions energies greater than 10 cm^{-1}, where agreement is also found with relative total scattering experiments.

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