Abstract Submitted
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Rovibrational inelastic scattering in the CO-H_2 complex[1] R.C. FORREY, Penn State University at Berks, B. YANG, University of Georgia, N. BALAKRISHNAN, University of Nevada Las Vegas, PENG ZHANG, Duke University, X. WANG, Emory University, P.C. STANCIL, University of Georgia, J.M. BOWMAN, Emory University — Rovibrational inelastic collisional rate coefficients for the CO-H_2 system have significant application in interstellar astronomy. In an attempt to address this need, we present quantum coupled-channel calculations of rovibrational state-to-state and total cross sections and rate coefficients. Full dimensional close-coupling (CC) and coupled-states (CS) approximation scattering calculations were carried out on a full-dimensional (6D) potential energy surface (PES), which was obtained using the high-level CCSD(T)-F12B method and fitted using an invariant polynomial approach in 6D. Pure state-to-state rotational excitations from CO(v_1 = 0, j_1=0, 1) were benchmarked with crossed molecular beam measurements. For rovibrational transitions, quenching cross sections and rate coefficients were calculated for the vibrational quenching of rovibrationally excited CO and H_2. The resulting data are compared with experimental results and previous calculations which used 4D PESs and various decoupling approximations, where available. Work is on-going to extend the computations to high-lying initial rovibrational levels though CC calculations in 6D require enormous computational resources.

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