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Full-dimensional vibrational quenching of CO in collisions with H_2[1] BENHUI YANG, University of Georgia, PENG ZHANG, Duke University, XIAOHONG WANG, Emory University, P. STANCIL, University of Georgia, J. BOWMAN, Emory University, N. BALAKRISHNAN, University of Nevada Las Vegas, R. FORREY, Penn State University — We report a six-dimensional (6D) potential energy surface (PES) for the CO-H_2 collision system calculated using the explicitly correlated coupled-cluster (CCSD(T)-F12B) method as implemented in MOLPRO2010.1 and fitted using an invariant polynomial method. In the fit of the 6D PES, the total polynomial expansion power was restricted to 6 and expansion coefficients were obtained using standard weighted least-squares optimization for potential energies up to 10,000 cm^{-1}. Close-coupling scattering calculations have been performed on the new 6D PES for rotational and vibrational quenching of CO in collisions with H_2 using the TwoBC code. Cross sections for $j = 0 \rightarrow 1$ pure rotational transition in CO, convoluted with a Gaussian kinetic energy distribution, show better agreement with measurement than that obtained on a recently available 4D PES. State-to-state and total quenching cross sections and rate coefficients for the vibrational quenching in CO($v_1 = 1, j_1 = 0$)+H_2($v_2 = 0, j_2 = 0$) $\rightarrow$ CO($v_1' = 0, j_1'$)+H_2($v_2' = 0, j_2' = 0$) collisions, for $j_1' = 0, 1, \cdots, 25$ are presented and compared with experimental results and previous calculations using 4D and 5D PESs and various decoupling approximati

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