SES14-2014-000085

Abstract for an Invited Paper
for the SES14 Meeting of
the American Physical Society

Full-dimensional quantum dynamics calculations of rovibrationally inelastic scattering of CO-H_2[1]

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The CO-H_2 collisional system is crucial in determining the physics and chemistry of interstellar environments due to the astrophysical importance of H_2 and CO. We calculated for the first time a full-dimensional (6D) potential energy surface (PES) for this system using the high-level CCSD(T)-F12B method. The PES was fitted using an invariant polynomial method in 6D. Quantum close-coupling calculations of rotational and vibrational quenching of CO in collisions with H_2 were carried out on the new 6D PES. The pure state-to-state rotational excitations from CO($v_1 = 0$, j_1=0, 1) were benchmarked with crossed molecular beam measurement for collision energies of 795 - 991 cm^{-1} and 3.3 - 22.5 cm^{-1}. The computed cross sections for $j_1 = 0 \rightarrow 1$ transition in CO and show better agreement with measurement than those obtained on a recently available 4D PES. For rovibrational transitions, state-to-state and total quenching cross sections and rate coefficients were calculated for the vibrational quenching in CO($v_1 = 1, j_1$)+H_2($v_2 = 0, j_2$) $\rightarrow$ CO($v_1' = 0, j_1'$)+H_2($v_2' = 0, j_2'$) collisions, $j_1 = 0, 2$ for para-H_2 and $j_1 = 1, 3$ for ortho-H_2. The results are compared with experimental results and previous calculations using 4D PESs and various decoupling approximations. Our calculation also confirmed that the contribution from a quasi-resonant channel, CO(v_1=1) + H_2(v_2=0, j_2=2) $\rightarrow$ CO(v_1'=0) + H_2($v_2' = 0$, j_2'=6), dominates the vibrational quenching of CO in collision with para-H_2 for $T \geq 50$ K.

[1]Work at UGA and Emory are supported by NASA grant No. NNX12AF42G, at UNLV by NSF Grant No. PHY-1205838, and at Penn State by NSF Grant No. PHY-1203228.