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CN collisions with H_2 in full-dimension[1] BENHUI YANG, University of Georgia, N. BALAKRISHNAN, University of Nevada, Las Vegas, XIAOHONG WANG, Emory University, P. STANCIL, University of Georgia, J. BOWMAN, Emory University, R. FORREY, Penn State University — Rotational and vibrational rate coefficients of CN in collisions with H_2 are essential for modeling CN infrared spectra in interstellar gas. We report here full-dimensional potential energy surface (PES) and rovibrational scattering calculations for the CN-H_2 collision system. A full-dimensional (6D) PES was calculated using the high-level ab initio CCSD(T)-F12B method. The invariant polynomial method was applied to fit the PES analytically in 6D. Quantum coupled-channel calculations of rotational excitation cross section of CN(j_1=4) scattered by para-H_2(j_2=0, 2) and ortho-H_2 (j_2=1) were performed for collision energies ranging from 1.0 to 1500 cm^{-1}. State-to-state rate coefficients of CN(j_1=4) are computed for H_2 rotational states j_2=0-2. Comparison of the pure rotational cross sections and rate coefficients were made with previous available theoretical and experimental results. For the first time we present rovibrational quenching cross sections and rate coefficients of CN in collisions with H_2 on the new 6D PES.

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