Abstract Submitted
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Full-dimensional close-coupling study of rovibrationally inelastic scattering of SiO-H_2[1] B. YANG, University of Georgia, X. WANG, Emory University, P. ZHANG, Duke University, P. C. STANCIL, University of Georgia, J. M. BOWMAN, Emory University, N. BALAKRISHNAN, University of Nevada Las Vegas, R. C. FORREY, Penn State University — Molecular collisional excitation rate coecients are required to interpret spectra of molecular gas not in local thermodynamic equilibrium. Silicon monoxide (SiO) has been detected in a variety of astronomical sources and is of astrophysical importance. Its rovibrational level populations are perturbed by collisions with He, H and H_2. The corresponding collisional rate coefficients and their temperature dependence are largely unknown. Theoretical scattering calculations are the primary source of such rate coefficients. In this work a full-dimensional (6D) potential energy surface (PES) of SiO-H_2 was calculated using the high-level CCSD(T)-F12B method and fitted using an invariant polynomial approach in 6D. We performed the first full dimensional quantum close-coupling scattering calculations for SiO in collision with H_2 on the 6D PES. Pure state-to-state rotational excitation transitions from SiO($v_1 = 0$, j_1=0-10) are computed. For rovibrational transitions, state-to-state and total quenching cross sections and corresponding rate coefficients from several low-lying rotational levels in the first excited vibrational level of SiO are calculated for both para-H_2 and ortho-H_2 collisions.

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Phillip Stancil
University of Georgia

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