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Full-dimensional quantum rovibrational scattering of SO with H₂¹

BENHUI YANG, University of Georgia, PENG ZHANG, Duke University, CHEN QU, Emory University, PHILLIP STANCIL, University of Georgia, JOEL BOWMAN, Emory University, N. BALAKRISHNAN, University of Nevada, Las Vegas, ROBERT FORREY, Penn State University, Berks Campus — Molecular collisional rate coefficients are required to predict the abundance of molecular gas in the interstellar medium. SO has been widely observed in a variety of interstellar regions and its collisional rate coefficients with the dominant collision partner H₂ are of astrophysical importance. We present a quantum close-coupling study of rovibrationally inelastic scattering of SO with H₂. A six-dimensional (6D) potential energy surface (PES) was constructed with high-level ab initio calculations and an invariant polynomial fitting. The scattering calculations were carried out for both rotational and rovibrational transitions of SO induced by H₂. Cross sections for rotational transitions from $j_1=0-10$ of SO in the ground vibrational state were computed for collision energies ranging from 1 to 3000 cm⁻¹. The rotational rate coefficients are compared with previous theoretical results obtained within a rigid-rotor approximation. For rovibrational transitions, state-to-state quenching cross sections and rate coefficients were calculated for the vibrational quenching of SO from $(v_1 = 1, j_1)$, $j_1=0-5$. Cross sections for collision energies in the range 1 to 3000 cm⁻¹ and rate coefficients ranging from 5 to 600 K are presented.

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