

Abstract Submitted  
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**Quantum Rovibrational dynamics of CS in collision with H<sub>2</sub>**<sup>1</sup> BEN-HUI YANG, University of Georgia, PENG ZHANG, Duke University, CHEN QU, Emory University, PHILLIP STANCIL, University of Georgia, J. BOWMAN, Emory University, N. BALAKRISHNAN, University of Nevada, Las Vegas, R. FORREY, Penn State University — Carbon monosulfide has been widely observed in a variety interstellar regions. An accurate prediction of its abundance requires collisional rate coefficients with ambient gases. Available collisional rate coefficients are limited to rigid-rotor calculations for a small range of rotational transitions in the vibrational ground state. In this work, we report the first six-dimensional (6D) PES for the CS-H<sub>2</sub> system. The PES was computed using high-level electronic structure theory and fitted using invariant polynomial method. Quantum scattering calculations were performed for rotational and rovibrational transitions of CS induced by H<sub>2</sub>. Cross sections for rotational transitions from  $j_1=0-5$  are compared with the results obtained within a rigid-rotor model. For rovibrational transitions, state-to-state and total quenching cross sections and rate coefficients were calculated for the vibrational quenching in  $\text{CS}(v_1 = 1, j_1) + \text{H}_2(v_2 = 0, j_2) \rightarrow \text{CS}(v'_1 = 0, j'_1) + \text{H}_2(v'_2 = 0, j'_2)$  collisions,  $j_1=0-5$ . Cross sections for collision energies in the range 1 to 5000 cm<sup>-1</sup> and rate coefficients ranging from 5 to 1000 K are presented for both para-H<sub>2</sub> ( $j_2=0$ ) and ortho-H<sub>2</sub> ( $j_2=1$ ) collision partners.

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