Abstract Submitted for the DAMOP05 Meeting of The American Physical Society

Close-Coupling study of vibrational-rotational quenching of CO by hydrogen atoms¹ B.H. YANG, P.C. STANCIL, University of Georgia, N. BAL-AKRISHNAN, University of Nevada Las Vegas — Accurate scattering calculations of rovibrational transitions for diatomic molecules induced by collisions of neutral species is a computationally challenging problem. In this work, quantum mechanical scattering calculations were performed for the rovibrational relaxation of CO in collisions with H atoms using the close-coupling approach for collision energies between 10^{-5} and 500 cm⁻¹. We adopted the H-CO interaction potential of Werner, Keller, and Schinke and computed state-to-state and total cross sections for the quenching of the v=1, j=0-2 levels of CO. Numerous resonances, as a consequence of the van der Waals potential, are observed and the cross sections are found to approach the Wigner relation in the limit of zero energy. Also, by averaging the cross sections over a Boltzmann distribution of velocities of the incoming atom, the quenching rate coefficients were obtained. The results will be compared with previous calculations which usually adopted a decoupling approximation.

¹This work was supported by NASA grant NNG04GG515. Some of the calculations were performed on the IBM p655 High Performance Computer of the UGA Research Computing Center.

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Date submitted: 11 Mar 2005

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