Abstract Submitted
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A full-dimensional study of H2+H2 collisions: coupled-states versus close-coupling formulation[1] ROBERT C. FORREY, ALEX BOHR, STEPHEN PAOLINI, Penn State University at Berks, N. BALAKRISHNAN, University of Nevada Las Vegas, P.C. STANCIL, University of Georgia — Kinetic models often require a complete set of rate coefficients for H_2+H_2 collisions in order to interpret results from spectroscopic observations or to make quantitative predictions. Recent progress in full-dimensional quantum dynamics using the numerically exact close-coupling (CC) formulation has provided good agreement with existing experimental data for low-lying states of H_2 and increased the number of state-to-state cross sections that may be reliably determined over a broad range of energies. Nevertheless, there exist many possible initial states (e.g. states with high rotational excitation) that still remain elusive from a computational standpoint even at relatively low collision energies. In these cases,the coupled-states (CS) approximation offers an alternative full-dimensional formulation. We assess the accuracy of the CS approximation for H_2+H_2 collisions by comparison with benchmark results obtained using the CC formulation. The results are used to provide insight into the orientation effects of the various internal energy transfer mechanisms. A statistical CS approximation is also investigated and cross sections are reported for transitions which would otherwise be impractical to compute.

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