Abstract Submitted
for the DAMOP06 Meeting of
The American Physical Society

State-to-state rotational transition in H_2+H_2 collisions at low temperatures[1] TECK-GHEE LEE, University of Kentucky and Oak Ridge National Laboratory, N. BALAKRISHNAN, University of Nevada–Las Vegas, R.C. FORREY, Penn State University, Berks-Lehigh Valley College, P.C. STANCIL, University of Georgia, DAVID R. SCHULTZ, Oak Ridge National Laboratory, GARY J. FERLAND, University of Kentuck — In previous meeting, we reported a quantum mechanical close- coupling study of He+H_2. This meeting, we present a quantum mechanical close-coupling study involving collisions between two hydrogen molecules in the energy range from ultracold to thermal regime. The two most recently published potential energy surfaces (PESs) for the H_2-H_2 complex, the so-called DJ (Diep and Johnson 2000) and BMKP (Boothroyd et al 2002) surfaces, are quantitatively evaluated and compared through the investigation of rotational transitions for the scattering of the two molecules. The BMKP surface is expected to be an improvement, approaching chemical accuracy, over all conformations of the PES compared to the rest of the older versions of H_2-H_2 potential surfaces. We found significant differences in inelastic rotational cross sections computed on the two surfaces for rotational excitations in ortho- and para-H_2. The discrepancy persists over a large range of energies from the ultracold to thermal and occurs for other low-lying initial rotational levels.

[1]This work is supported by NASA grants NNG05GD81G and JPL Spitzer Space Telescope

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Date submitted: 27 Jan 2006 Electronic form version 1.4