Abstract Submitted
for the DAMOP05 Meeting of
The American Physical Society

Low energy He+H_2 collisions: Comparative study between two potential surfaces TECK-GHEE LEE, Physics Division, ORNL, C. ROCHOW, R. MARTIN, T.R. CLARK, R.C. FORREY, Physics Dept., Penn State University, N. BALAKRISHNAN, Chemistry Dept., University of Nevada, Las Vegas, P.C. STANCIL, Center for Simulational Physics, Physics Astronomy Dept., University of Georgia, A. DALGARNO, ITAMP, DAVID SCHULTZ, Physics Division, ORNL, GARY FERLAND, Physics & Astronomy Dept., University of Kentucky — The two most recently published potential energy surfaces (PESs) for the HeH_2 complex, the so-called MR (Muchnick and Russek) and BMP (Boothroyd, Martin, and Peterson) surfaces, are quantitatively evaluated and compared through the investigation of atom-diatom collision processes. The BMP surface is expected to be an improvement, approaching chemical accuracy, over all conformations of the PES compared to that of the MR surface. We found significant differences in inelastic rovibrational cross sections computed on the two surfaces for processes dominated by large changes in target rotational angular momentum. In particular, the $H_2(\nu = 1, j = 0)$ total quenching cross section computed using the BMP potential was found to be a factor of 1000 larger than that obtained with the MR surface. Detailed analysis has been performed to uncover the origin of the discrepancy.

Teck-Ghee Lee
ORNL

Date submitted: 28 Jan 2005 Electronic form version 1.4