Abstract Submitted
for the DAMOP13 Meeting of
The American Physical Society

The effect of Vibrational excitation of molecular hydrogen on the dynamics of reaction between O(^1D) and H_2 at ultracold temperatures[1]

G.B. PRADHAN, N. BALAKRISHNAN, University of Nevada Las Vegas, B.K. KENDRICK, Los Alamos National Laboratory — The effect of vibrational excitation of H_2 molecule on the reactivity of O(^1D)+H_2 reaction is explored. A time-independent quantum mechanical approach based on hyperspherical coordinates combined with the potential energy surfaces of Dobbyn and Knowles has been used for the calculation. Energy dependent cross section, probability, and rate coefficients are computed for elastic, inelastic, and reactive channels over collision energies ranging from the ultracold to thermal regimes. Our calculations show that total reaction probabilities, cross sections, and rate coefficients are almost independent of the initial vibrational quantum number of the H_2 molecule. The collision outcome is strongly influenced by the intermediate H_2O complex formed in the reaction than the initial vibrational quantum number. However, the OH vibrational distribution is found to be sensitive to the initial vibrational level of the H_2 molecule. For all three vibrational levels of H_2 the reaction is found to populate high rotational levels of OH.

[1]This work was supported in part by NSF grant PHY-1205838 (N.B.).

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Date submitted: 22 Jan 2013 Electronic form version 1.4