

Abstract Submitted
for the DAMOP05 Meeting of
The American Physical Society

The role of van der Waals interaction in $O(^3P)+H_2$ reaction at low temperatures¹ BALAKRISHNAN NADUVALATH, PHILIPPE WECK, University of Nevada Las Vegas, Las Vegas, NV 89154, JOÃO BRANDÃO, W. WANG, C. J. ROSA, Universidade do Algarve, Campus de Gambelas, 8005-139 FARO, Portugal — We report quantum scattering calculations of the $O(^3P)+H_2(v)$ reaction with an aim of determining sensitivity of the results to details of the interaction potential. We use two different analytic representations of the $^3A''$ potential energy surface (PES) - the GLDP surface reported by Rogers et al. (J. Phys. Chem. A **104**, 2308 (2000)) that provides a partial description of the van der Waals region and the more recent BMS1 and BMS2 PESs by Brandão et al. (J. Chem. Phys **121**, 8861 (2004)) which explicitly include the van der Waals part. The ab initio data of Rogers et al. form the basis of all three surfaces. We report cross sections and rate coefficients on the three PESs using accurate quantum calculations. We also perform quasiclassical trajectory calculations on all three surfaces to explore quantum effects at low temperatures.

¹This work was supported in part by NSF grant PHY-0245019, the Research Corporation, and the FCT under the POCTI/CTA/41252/2001 research project, cofinanced by the European community fund, FEDER.

Balakrishnan Naduvalath
University of Nevada Las Vegas

Date submitted: 28 Jan 2005

Electronic form version 1.4