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Role of the van der Waals interaction in atom-diatom reaction dynamics at low temperatures[1] PHILIPPE F. WECK, NADUVALATH BALAKRISHNAN, University of Nevada Las Vegas, Las Vegas, NV 89154, JOAO BRANDAO, CARLA ROSA, WENLI WANG, Universidade do Algarve, 8005-139 Faro, Portugal — Quantum-mechanical scattering calculations are reported for the $O(^3P) + H_2$ collision at energies close to the reaction threshold with emphasis on the sensitivity of the reaction dynamics to the van der Waals interaction. The dynamics has been investigated using the lowest $^3A''$ GLDP potential energy surface developed by Rogers et al. [J. Phys. Chem. A **104**, 2308 (2000)] and its recent BMS1 and BMS2 extensions by Brandão et al. [J. Chem. Phys. **121**, 8861 (2004)] which explicitly include the van der Waals interaction. Quasiclassical trajectory calculations on all three potential energy surfaces are also reported to explore the validity of this method near the reaction threshold and to assess the importance of quantum effects at low temperatures.

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