Abstract Submitted
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Geometric phase effects in ultracold collisions of H/D with rotationally excited HD[1] BRIAN K. KENDRICK, Los Alamos National Laboratory, JAMES F. E. CROFT, JISHA HAZRA, N. BALAKRISHNAN, University of Nevada, Las Vegas — Quantum reactive scattering calculations for the H/D + HD($v = 4$, $j = 1, 2$)$\rightarrow$ H/D + HD(v', j') and H + H_2($v = 4$, $j = 1, 2$) $\rightarrow$ H + H_2(v', j') exchange reactions are presented for the ground electronic state of H_3. A numerically exact three-dimensional time-independent scattering method based on hyperspherical coordinates is used to compute rotationally resolved reaction cross sections and non-thermal rate coefficients for collision energies between 1 μK and 100 K. The geometric (Berry) phase associated with the D_{3h} conical intersection in H_3 is included using a $U(1)$ vector (gauge) potential approach. It is shown that the geometric phase leads to a significant (up to three orders of magnitude) enhancement or suppression of the ultracold reaction rate coefficients depending upon whether the interference between the reaction pathways encircling the conical intersection is constructive or destructive. The nature of the interference is governed by a newly discovered mechanism which leads to an effective quantization of the ultracold scattering phase shifts. Interesting behavior due to rotational excitation of the HD and H_2 is observed which might be exploited by experimentalists to control the reaction outcome.

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