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Geometric phase effects in ultracold chemistry[1] JISHA HAZRA, BALAKRISHNAN NADUVALATH, Department of Chemistry, University of Nevada, Las Vegas, BRIAN K. KENDRICK, Theoretical Division (T-1, MS B221), Los Alamos National Laboratory — In molecules, the geometric phase, also known as Berry's phase, originates from the adiabatic transport of the electronic wavefunction when the nuclei follow a closed path encircling a conical intersection between two electronic potential energy surfaces. It is demonstrated that the inclusion of the geometric phase has an important effect on ultracold chemical reaction rates. The effect appears in rotationally and vibrationally resolved integral cross sections as well as cross sections summed over all product quantum states. It arises from interference between scattering amplitudes of two reaction pathways: a direct path and a looping path that encircle the conical intersection between the two lowest adiabatic electronic potential energy surfaces. Illustrative results are presented for the O+OH→H+O_2 reaction and for hydrogen exchange in H+H_2 and D+HD reactions. It is also qualitatively demonstrated that the geometric phase effect can be modulated by applying an external electric field allowing the possibility of quantum control of chemical reactions in the ultracold regime.

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