

Tunneling vibrational motion in van der Waals complexes

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Quantum tunneling have a significant impact on chemical reactions, particularly in low-temperature conditions and low-energy collisions. In molecular systems with multiple minimum-energy configurations, the wave functions localized at each potential minimum can overlap, causing the vibrational wave functions to become delocalized and spread over the multiple configurations. As a result, the vibrational energy levels that would be degenerate without such wave function mixing are split into multiplets. This splitting is a clear indication of the quantum tunneling effect and can be used to evaluate potential energy surfaces relevant to tunneling dynamics, such as proton tunneling and hydrogen-bonding rearrangements. Molecular clusters and van der Waals complexes containing helium atoms are useful systems for studying the tunneling effect, as helium is the second lightest atom after hydrogen and the intermolecular interactions involving helium are relatively weak.