

Role of Quantum Tunneling in Peptide Bond Formation

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An insight in the mechanism of peptide bond formation/break is obtained from analysis of dipeptide reaction starting from the example of two alanine amino acids. Analysis is based on combination of two approaches: (i) Tracing the system's potential energy profile as a function of the reaction coordinate obtained via, the transition state (TS) search. The reaction coordinate increment is contributed by a proton transfer, playing role in peptide bond formation. (ii) Wave packet dynamics of protons. A sequence of reaction steps from TS search demonstrates importance of proton transfer for formation of the peptide bond. The details of proton transfer are explored by wave packet dynamics on the basis of *first principles* potential energy surfaces. The activation energy of the reaction lower than the energy of the TS state is predicted as a quantized feature of proton-transfer dynamics.