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Transition State Theory: The Phase Space Perspective[1]

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Transition State Theory (TST), which is at the basis of chemical reactivity calculations, assumes that once reactants pass through the Transition State, they cannot return. This "no-recrossing" rule serves to define the TS and is a necessary assumption in TST. Conventional transition states always lead to overestimates of the reaction rate because each intersection of the trajectory with the TS counts as a reactive event. Enforcing this no-recrossing condition beyond two degrees of freedom has been the major obstacle to applying TST in multidimensional systems. We will explain the solution of this problem based on dynamical systems theory.

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