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The Transition State in a Noisy Environment THOMAS BARTSCH, TURGAY UZER, Georgia Institute of Technology — Classical transition state theory is the cornerstone of reaction rate theory. It postulates a partition of phase space into reactant and product regions, which are separated by a dividing surface that reactive trajectories must cross. In order not to overestimate the reaction rate, the dividing surface must be chosen so that no reactive trajectory crosses back into the product region. Whereas most chemical reactions take place in a randomly fluctuating environment, as, e.g., a liquid, conventional transition state theory is not well equipped to handle this case because the no-recrossing condition is difficult to enforce in the presence of noise. To generalize the formalism of transition state theory to reactive systems driven by noise, we introduce a time-dependent dividing surface that is randomly moving in phase space so that it is crossed once and only once by each reactive trajectory.

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