

National Training School in Theoretical Chemistry

4 Lectures in Chemical Reaction Dynamics

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Summary

In these lectures, I will present an introduction to quantum scattering theory and to the quantum theory of chemical reaction rates, at a level that will hopefully be accessible to students with a good working knowledge of bound state quantum mechanics but little or no previous knowledge of continuum wave functions.

In order to do this in four lectures, I will present the entire theory in the context of a simple one dimensional barrier transmission problem, and leave to further reading how the final result (Miller's flux-side correlation function expression for the reaction rate coefficient) can be applied to more general reactions.