Chasing the Magic

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Chemical Kinetics is the study of how fast chemical reactions occur

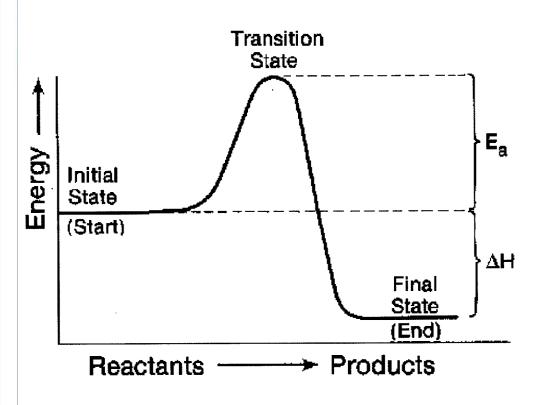
How do chemical reactions occur?

How does the reactant become a product?

Factors Affecting Kinetics

- 1) Physical state of the reactants
- 2) Concentration of the reactants
 - 3) Temperature of the reaction
 - 4) A catalyst presence or not

Transition State



Arrhenius equation

$$k = Ae^{-E_A/RT}$$

k - rate constant

 E_A – activation energy

T – temperature

R – gas law constant

Model Reactants & Products with Gaussian

Guess at the Transition State and model

From the model create a series of pictures of the reaction pathway

Animate the pictures of the reaction pathway

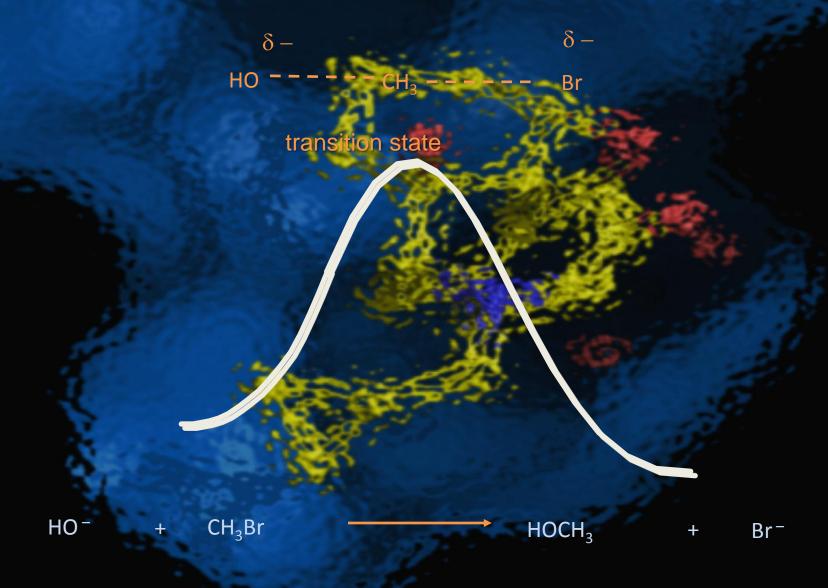
The Reaction

CH₃Br + HOH → CH₃OH + HBr

Transition State Guess

CH₃Br + HOH → CH₃OH + HBr

Bimolecular Mechanism



Current Status

Learning Curve on Gaussian now smaller

Implemented Model for reactants, Products, & T.S.

Target next week to have component pictures for animation