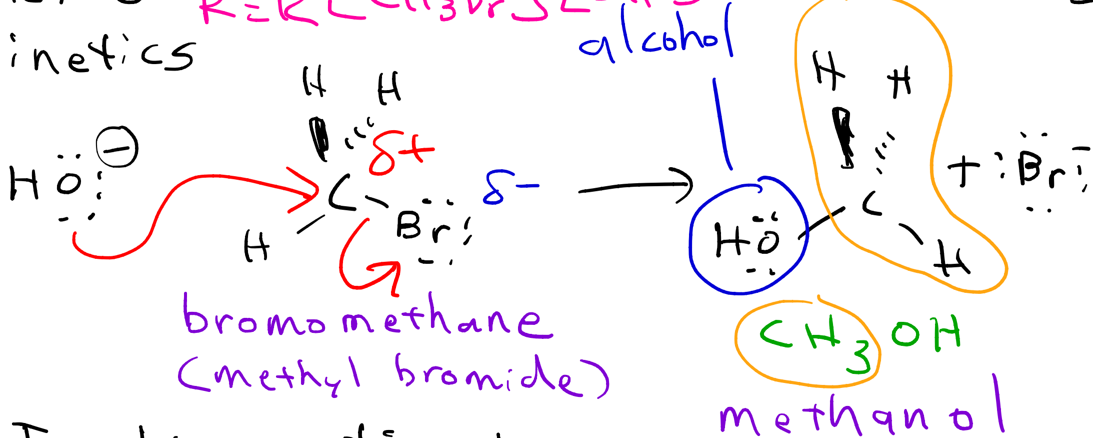
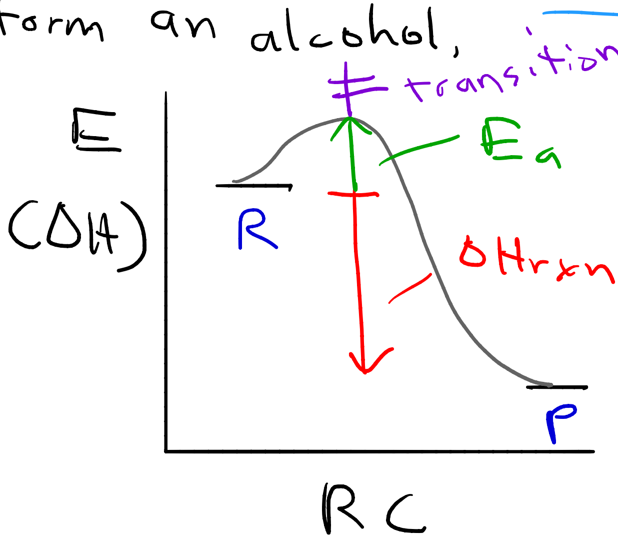
5/18/20

Kinetics

$R = k[CH_3Br][OH^-]$

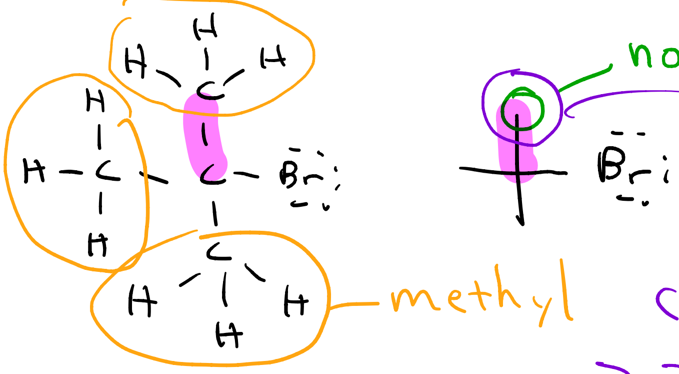


In this reaction, hydroxide and bromomethane react simultaneously to form an alcohol.



Activation energy – The energy necessary for the reaction to be successful.

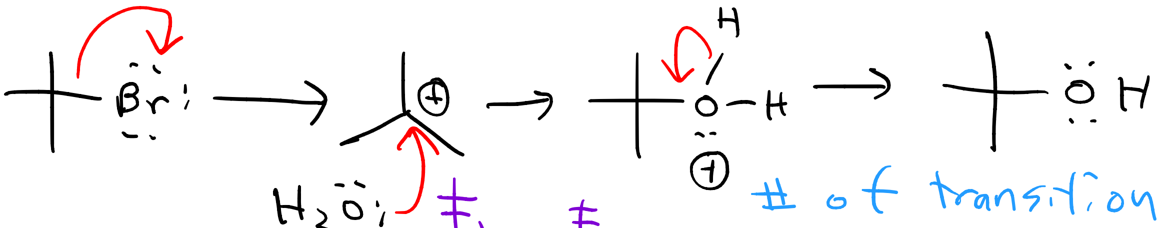
The reaction coordinate is a simplication of a multidimensional graph that represents the most likely (most energetically favorable) pathway through a reaction.



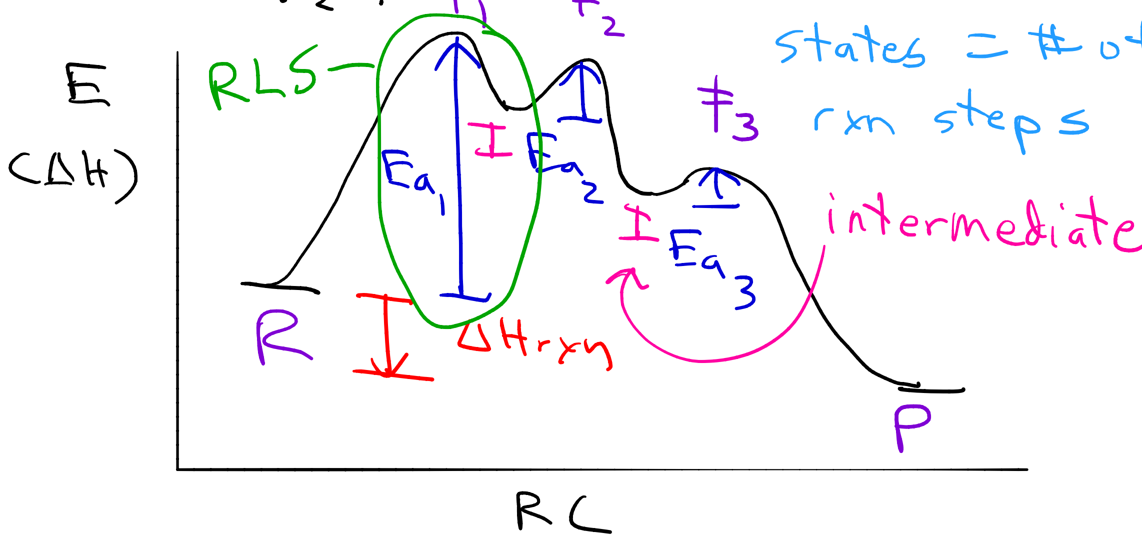
no label = carbon

only one bond written to the circled carbon → 3 hydrogens

$(CH_3)_3CBr$



# of transition states = # of rxn steps



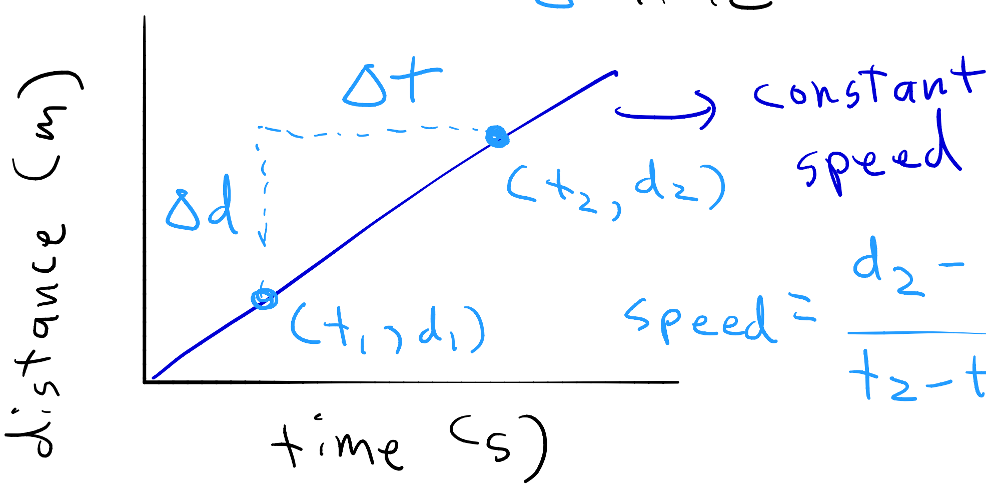
In this reaction, an alcohol forms by a process that involves multiple steps.

mechanism - the step-by-step way a reaction occurs

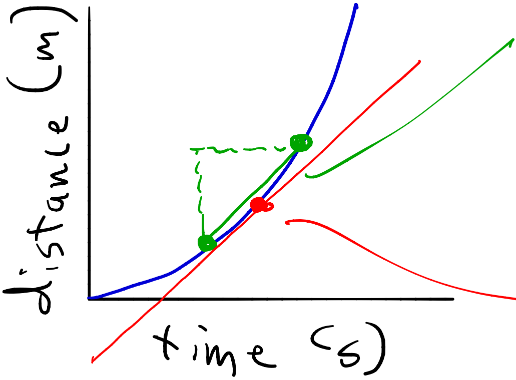
- A reaction can be composed of one or more fundamental steps, such as a bond forming, a bond breaking, or electron transfer.

- In many cases, the rate of an overall reaction depends on only one fundamental step, which is known as the rate-limiting step (RLS). This step is usually the one with the highest activation energy and/or the highest-energy transition state.

Rate — speed = $\frac{\Delta \text{ distance}}{\Delta \text{ time}}$



$$\text{speed} = \frac{d_2 - d_1}{t_2 - t_1}$$



average rate - calculated only using the initial and final states

instantaneous speed

$$= \frac{\Delta d}{\Delta t} = \frac{0}{0} = ???$$

$$y = x^2$$

$$f(t) = t^2$$

$$y = f(x) = x^2$$

slope at an instantaneous point

$$\text{speed} = \lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{(x+\delta) - (x)}$$

$$= \lim_{\delta \to 0} \frac{(x+\delta)^2 - (x)^2}{\delta}$$

$$= \lim_{\delta \to 0} \frac{(x^2 + 2x\delta + \delta^2) - (x^2)}{\delta}$$

$$= \lim_{\delta \to 0} \frac{2x\delta + \delta^2}{\delta} = \lim_{\delta \to 0} = 2x + \delta = 2x$$

Rate of reaction

$$\text{Rate} = \frac{\Delta\,\text{Concentration}}{\Delta\,\text{time}}$$

average

$$\text{Rate} = \frac{\delta[\,]}{\delta t}$$

instantaneous

Rate law

Example (Reaction I)

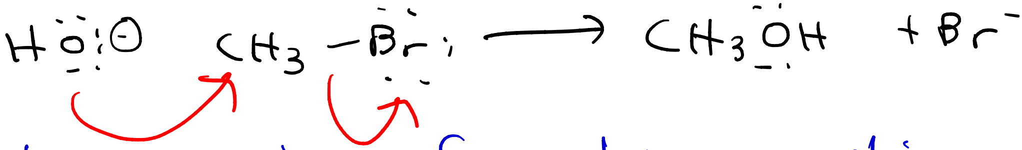
$$R = k\,[CH_3OH][OH^-]$$

k: rate constant

The rate law generally only contains those substances that participate in the RLS.

The rate of reaction depends on the number of successful collisions of molecules involved in a fundamental step.

Reaction I



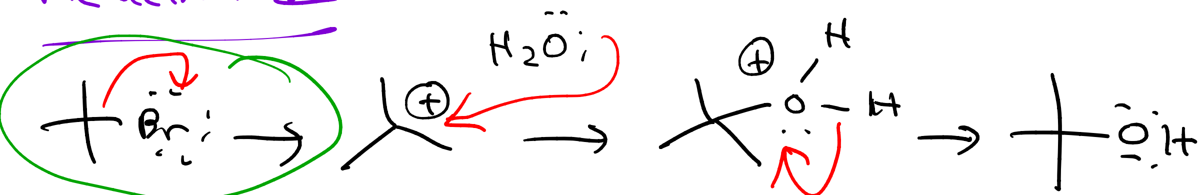
The rate law for this reaction contains both reagents, since both reagents are involved simultaneously in the only rxn step.

$$R = k[CH_3Br][OH^-]$$

Bimolecular Nucleophilic Substitution (S_N2)

two molecules involved at the same time

Reaction II



The rate law for this reaction contains only one reagent because it is the only one involved in the RLS

$$R = k[(CH_3)_3CBr]$$

Unimolecular Nucleophilic Substitution (S_N1)

only one molecule involved