Today

Sections 5.5 - 5.13
How alkenes react

Kinetics, thermodynamics, reaction coordinate diagrams, and catalysis

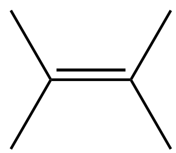
Next Class

Test 2

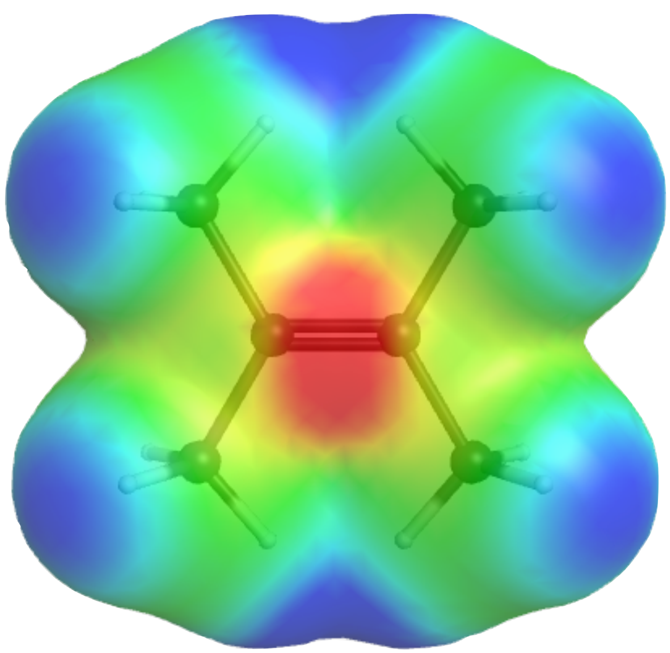
Test 2 on Chap 3 and 4 and Sections 5.1, 5.2, and 5.4 (be able to identify and name functional groups from class on Oct 26) on Friday, November 4.

Review session 7:30 pm Thursday, November 3 in Wilson 130.

alkenes



all atoms connected to the sp^2 C atoms at the ends of the db must lie in the same plane



alkenes are e^- rich

4 e^-'s between to C atoms

and

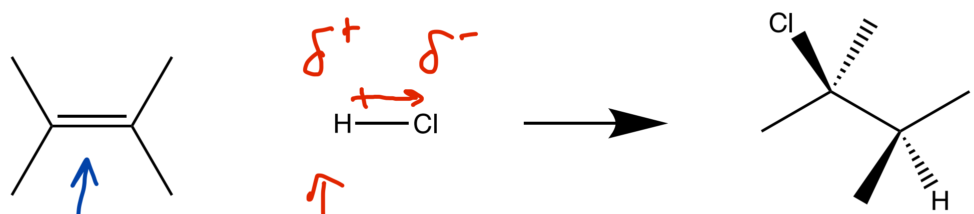
2 of the e^-'s are in a π bond that sticks out away from the nuclei

alkenes are nucleophilic

Nucleophiles: e^- rich, have electrons that are 'easy' to get at and can be donated to make a bond

Electrophiles: e^- deficient and therefore e^- loving, are attracted to the electrons of a nucleophile and can accept the nucleophiles e^-'s to form a bond

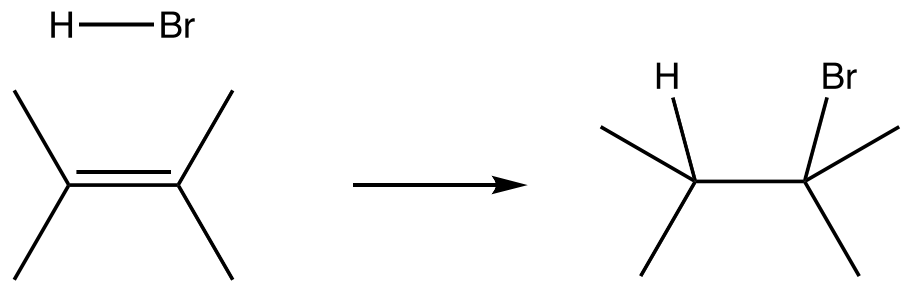
e^- loving

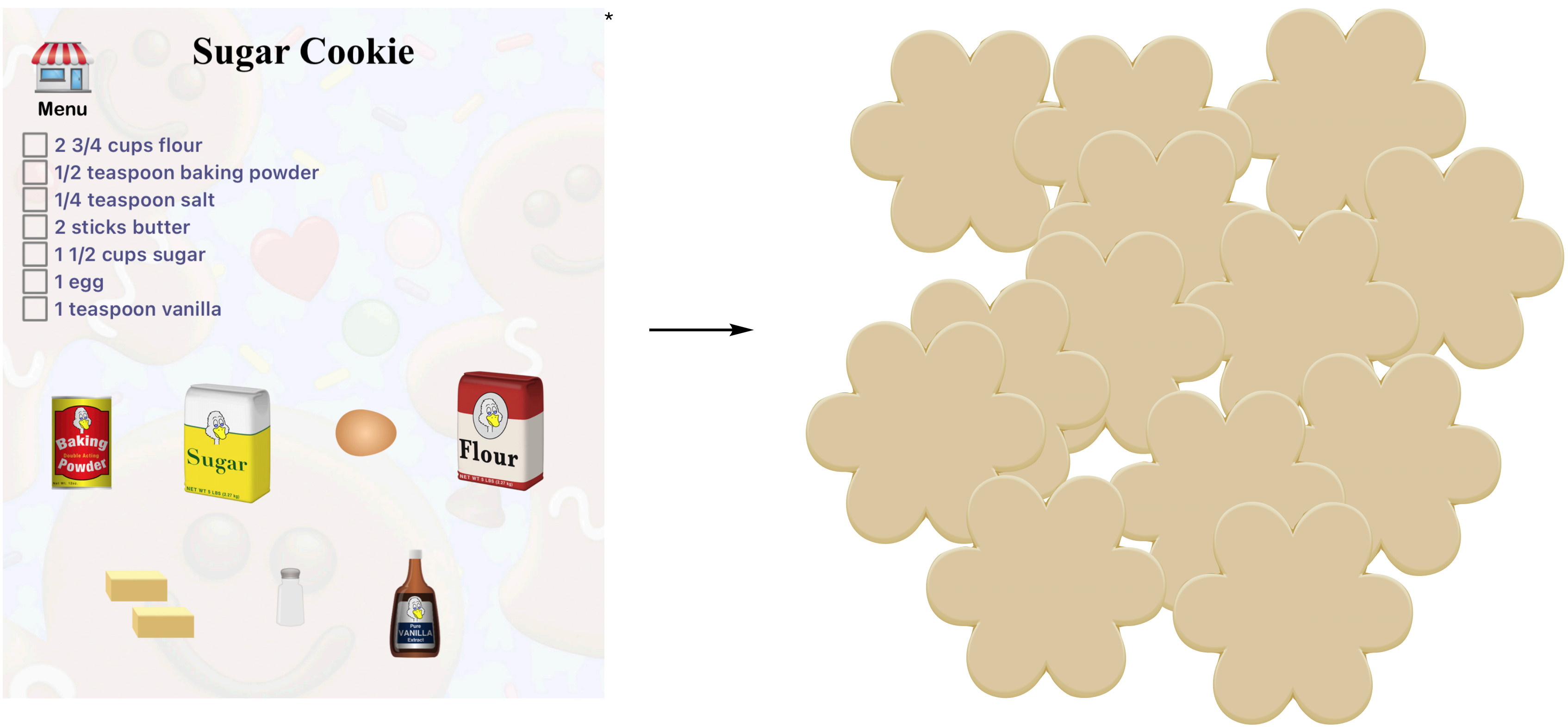


electron rich nucleophile

this ⊕ part means the H-Cl can play the role of the electrophile

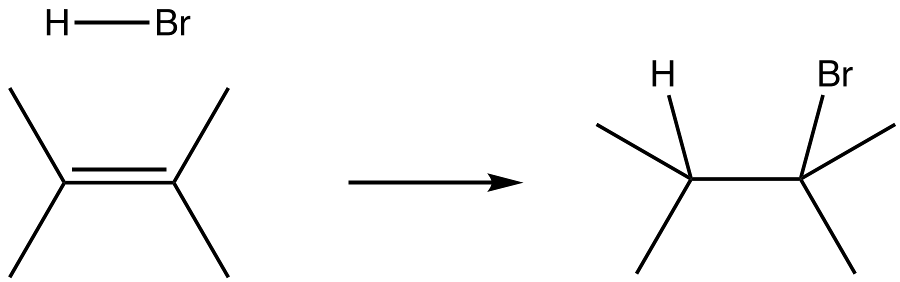
Ok, H^+ part is attracted to the e^- rich alkene, but how does the Cl get on the product? How does this rxn work?

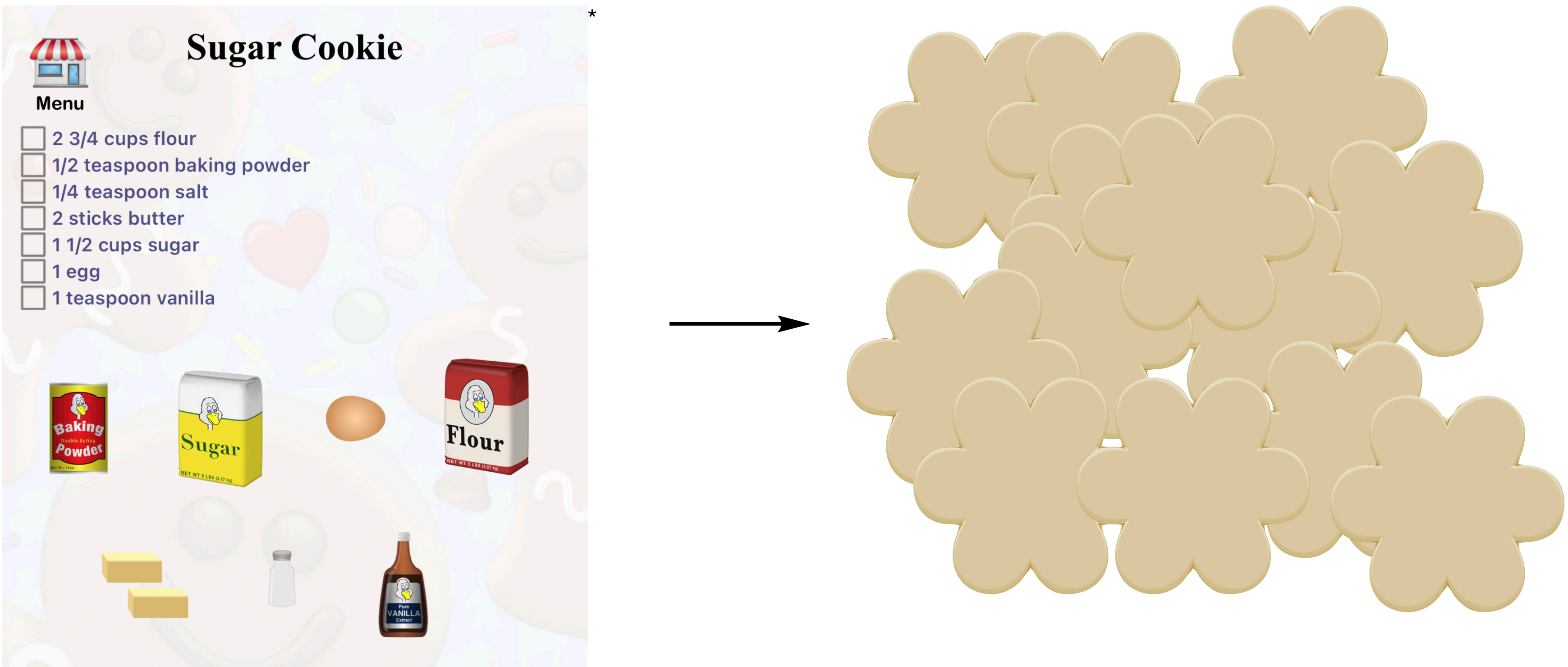




*CookieDoodle https://apps.apple.com/us/app/cookie-doodle/id342128086

Balanced chemical equations are like ingredient lists





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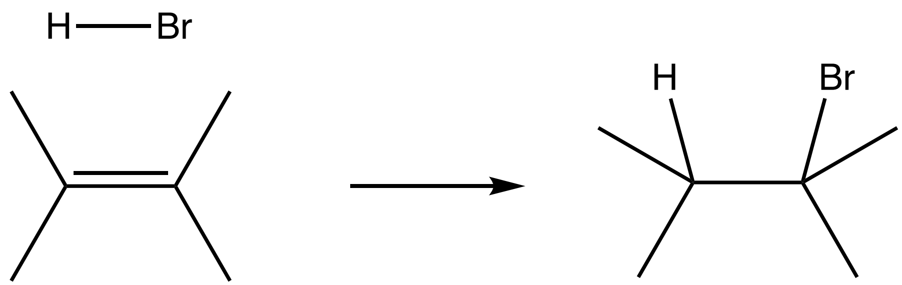
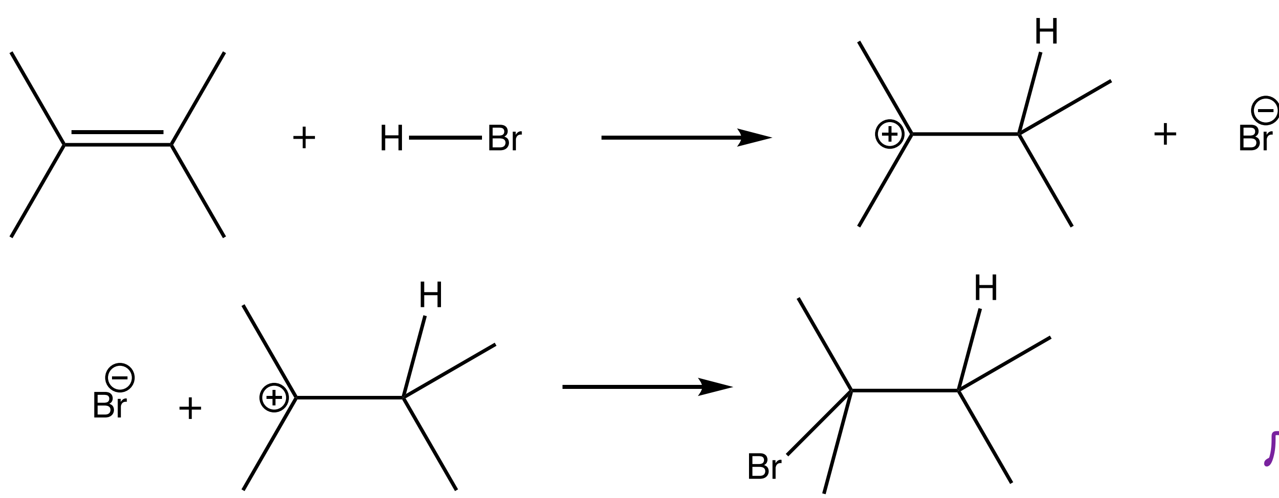
*CookieDoodle https://apps.apple.com/us/app/cookie-doodle/id342128086

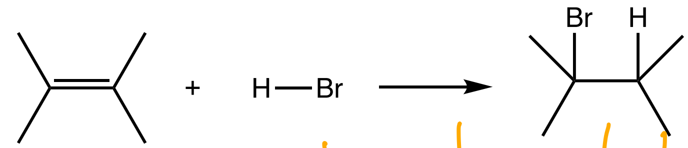
Mechanism one: this is a 1 step reaction where two reactants collide and form the product, which is created in one step.



Mechanism two: This is a two step reaction In this mechanism the reactants collide and form two intermediates, and the intermediates react to form the product



Mechanisms are like the recipe instructions; mechanisms are how a reaction occurs



transition state

* Reactant(s) are consumed during a reaction. appear on the left of the arrow

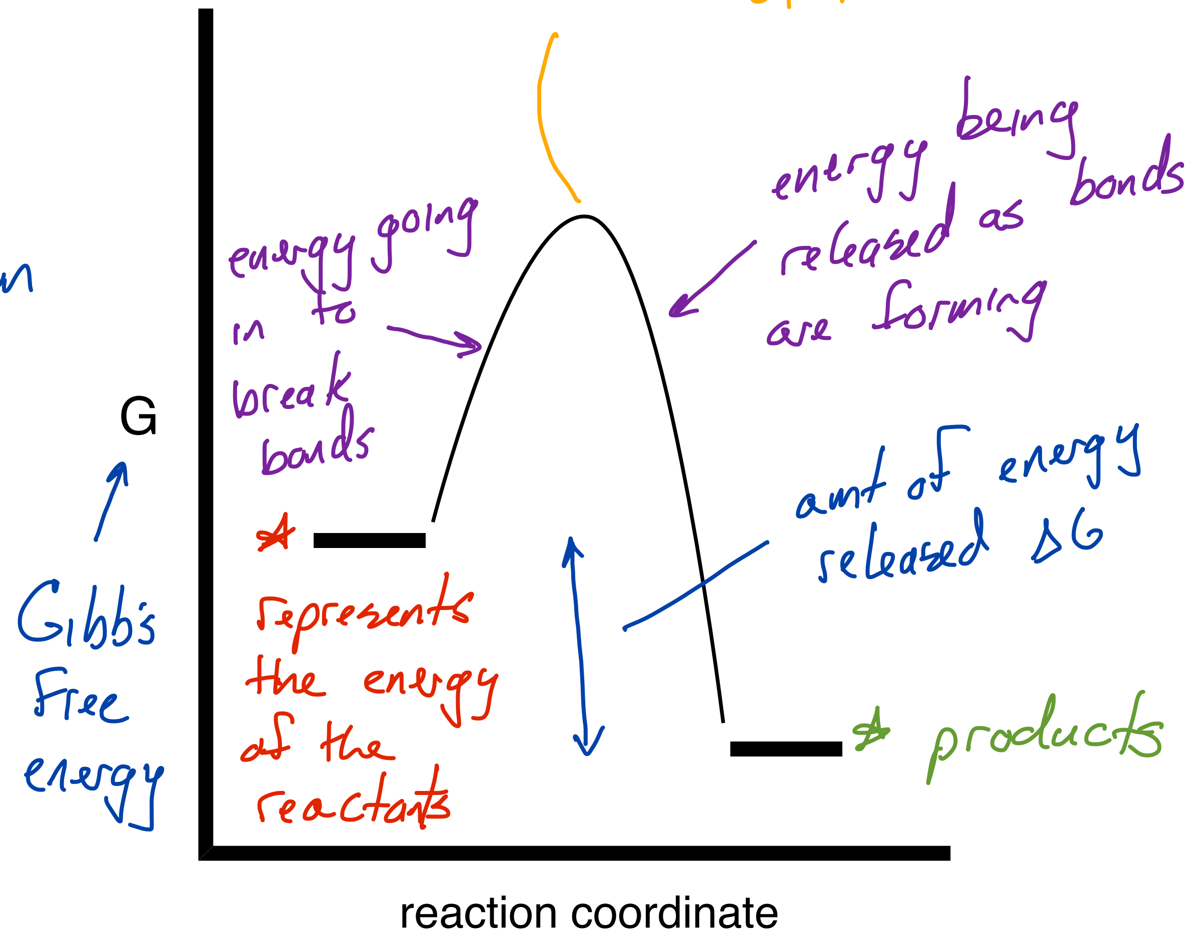
* Product(s) created during a reaction appear on the right of the arrow

Transition State

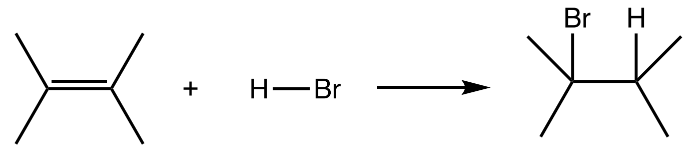
highest energy point on path from reactant to product

Intermediate

no intermediate in this 1-step mechanism



extent of reaction



ΔG is a measure of the amount of energy absorbed or released during a rxn.

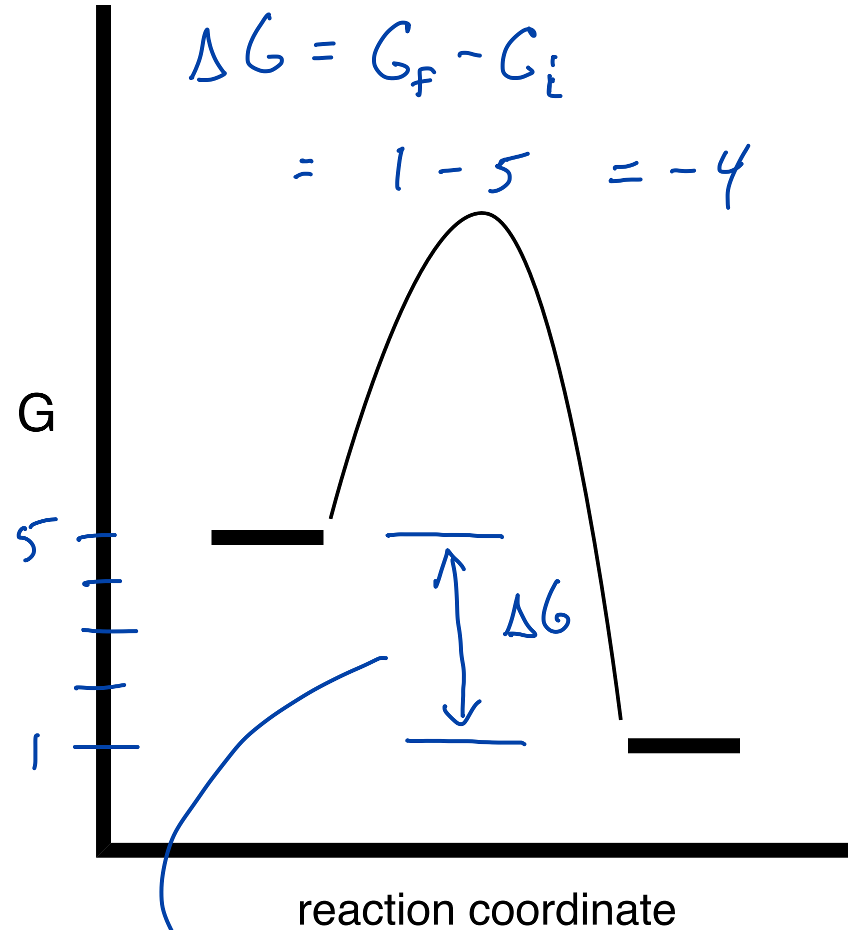
$\Delta G < 0$ favorable reaction

K large or small K's represent reactions with favorable equilibrium constants?

$K = \frac{[prod]}{[react]}$ large

$\Delta G = G_f - G_i$

$= 1 - 5 = -4$



amount of energy released in this rxn

Relationship between ΔG° and K

$\Delta G^\circ = -RT \ln K$ if $K > 1$

$\ln K$ ⊖ or ⊕?

$10^y = x$ $\log_{10} x = y$

$\log_{10} .1 = -1$ $\log_{10} 1 = 0$ $10^0 = 1$

Draw a reaction coordinate diagram for a one-step mechanism that has an unfavorable ΔG (a small K)

uphill

ΔG > 0 an unfavorable ΔG is a reaction that "runs uphill" energetically speaking.
It has a ⊕ ΔG

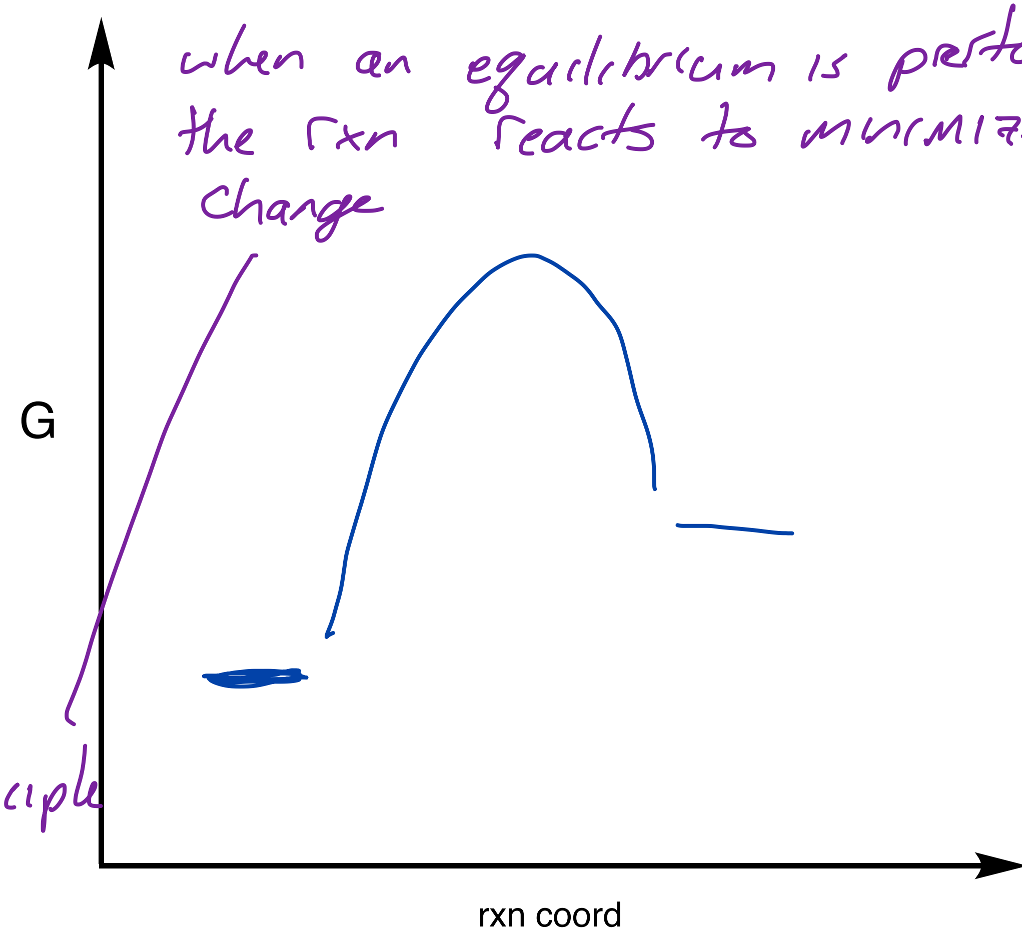
K is small .... how could I make as much C as possible? Le Châtlier's Principle

$$A + B \rightleftharpoons C + D$$

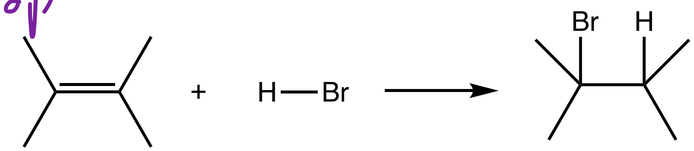
add more A or more B

or remove a product to encourage more to form

when an equilibrium is perturbed the rxn reacts to minimize the change



This is a proposed mechanism.

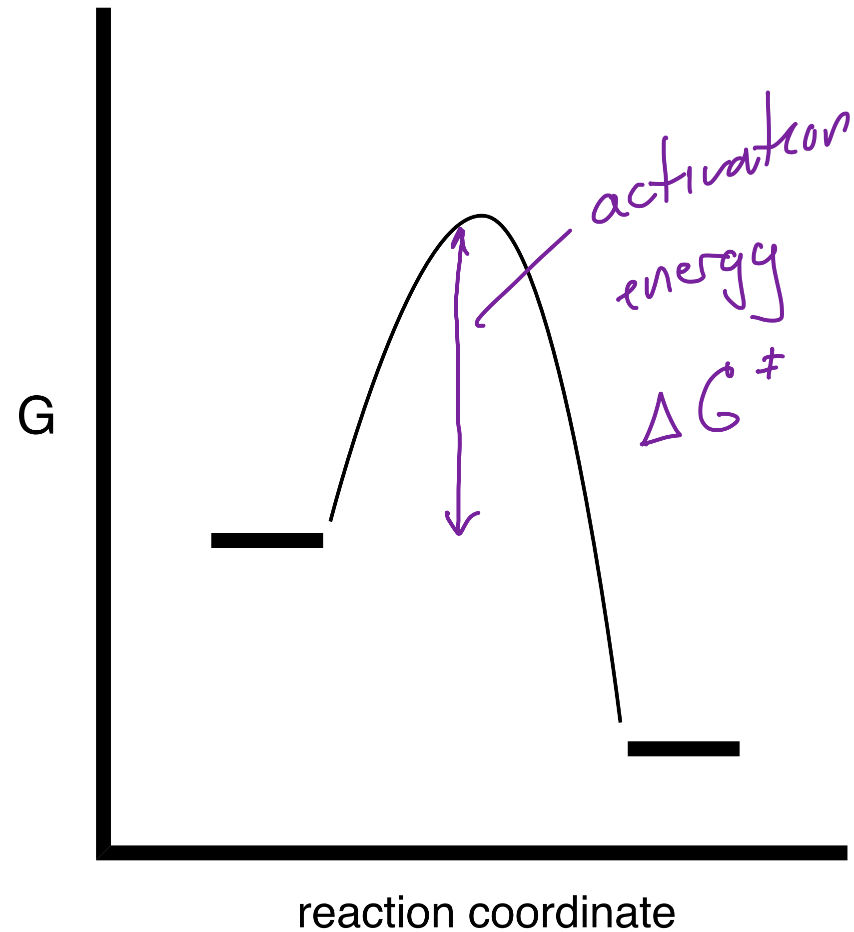


Activation Energy (Kinetics), $\Delta G^{\ddagger}$

rate of a reaction

amount of energy required to overcome the activation energy barrier (to get past the transition state)

high $\Delta G^{\ddagger}$ means that the reaction will be slower than rxns with low $\Delta G^{\ddagger}$ when the rxns are run under similar conditions



$C_{(d)} \rightarrow C_{(graphite)}$

Reaction Coordinate Diagrams: Kinetics

proposed Mechanism

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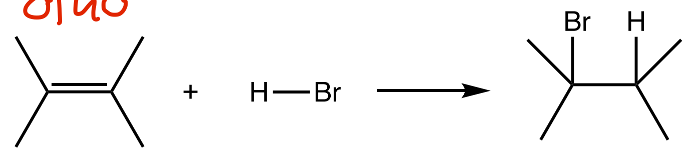
$\Delta G^{\ddagger}$ + ΔG are not related to each other



rate of a reaction

ave

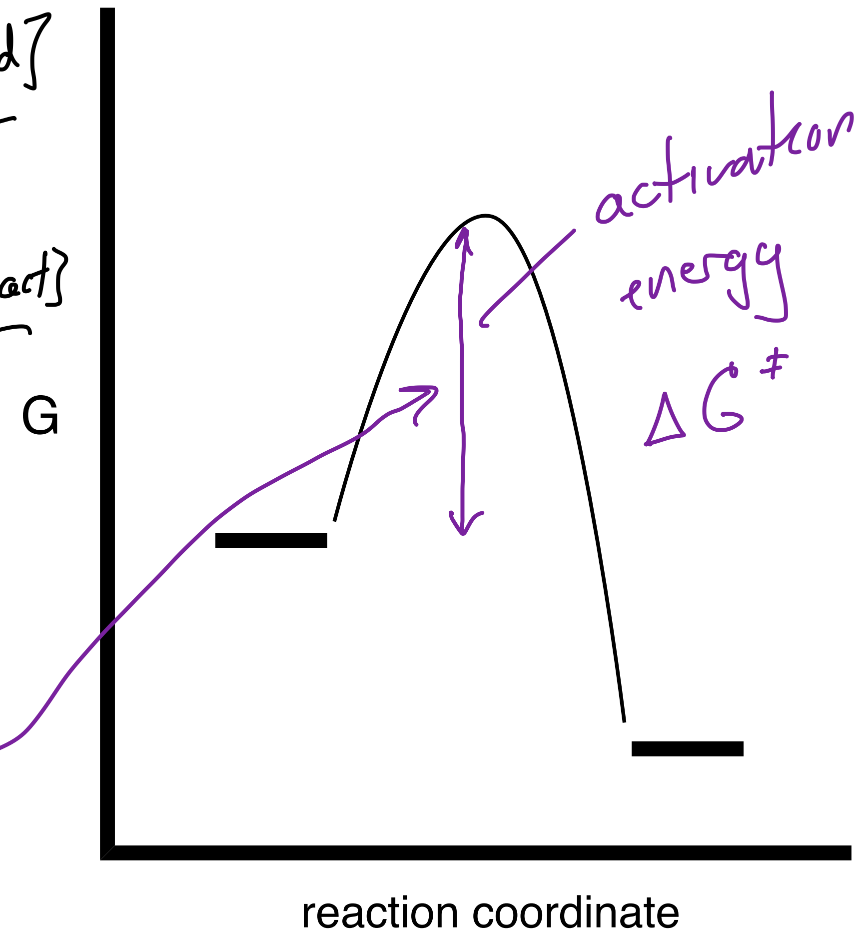
$$\text{rate} = \frac{\Delta[\text{prod}]}{\Delta t}$$

instantaneous

$$\text{rate} = \frac{d[\text{prod}]}{dt}$$

$$\text{rate} = -\frac{\Delta[\text{react}]}{\Delta t}$$

$$\text{rate} = -\frac{d[\text{react}]}{dt}$$



activation energy

$\Delta G^{\ddagger}$

Mechanisms predict a hypothetical rate law

$$\text{rate} = k\,[\,{>}{=}{<}\,][\text{H-Br}]$$

Fancy lowercase k is the rate constant and it is related to

K

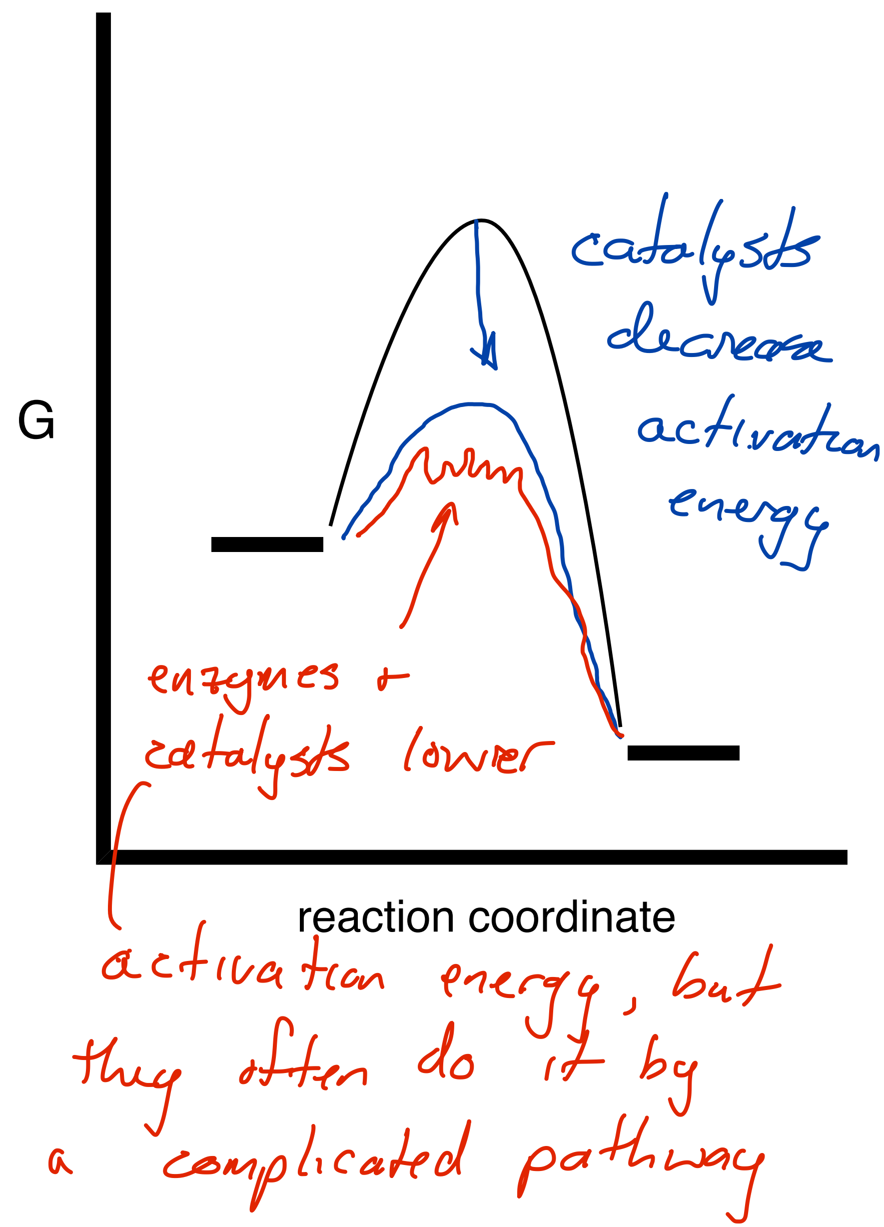
K k

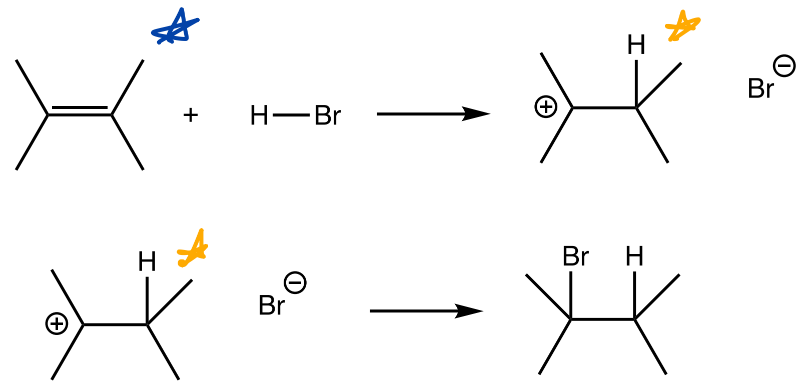
Large $\Delta G^{\ddagger}$... k large or small? Slow reaction

k would be small to lower value of $[{>}{=}{<}][\text{H-Br}]$

Draw the path for a catalyzed version of the reaction

catalysts - speed up reactions and are not consumed by a reaction





Reactant

Product

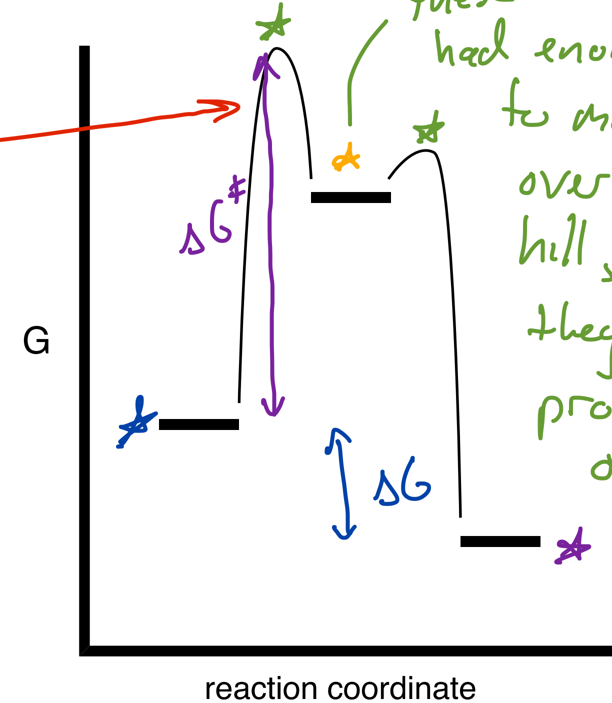
Transition State

More than 1 step more than one transition state

In this reaction, this 1st step is the rate determining step.

Intermediate

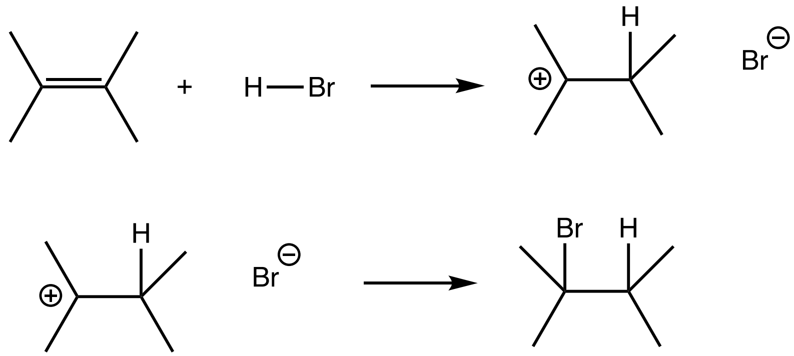
Are molecules or ions that form during a reaction and are consumed by the end of the react

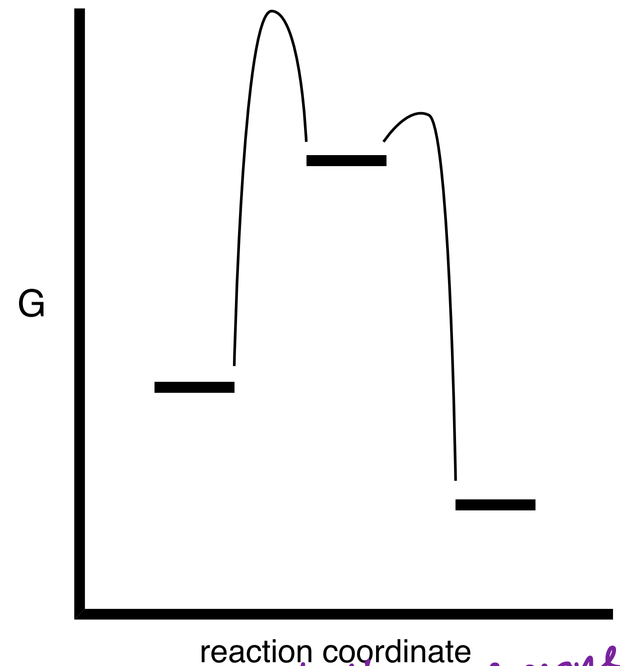


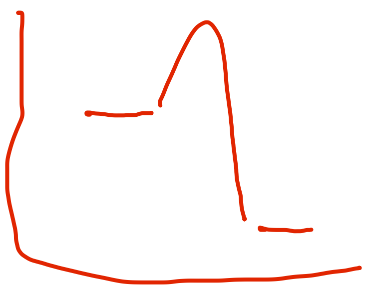
these intermediates had enough energy to make it over the 1st hill, so they have no problem overcoming the 2nd activation energy barrier

the largest activation energy barrier is the one that controls the rate of the reaction

Hammond Postulate TS resembles the molecule it is closer to in energy







this bond is breaking

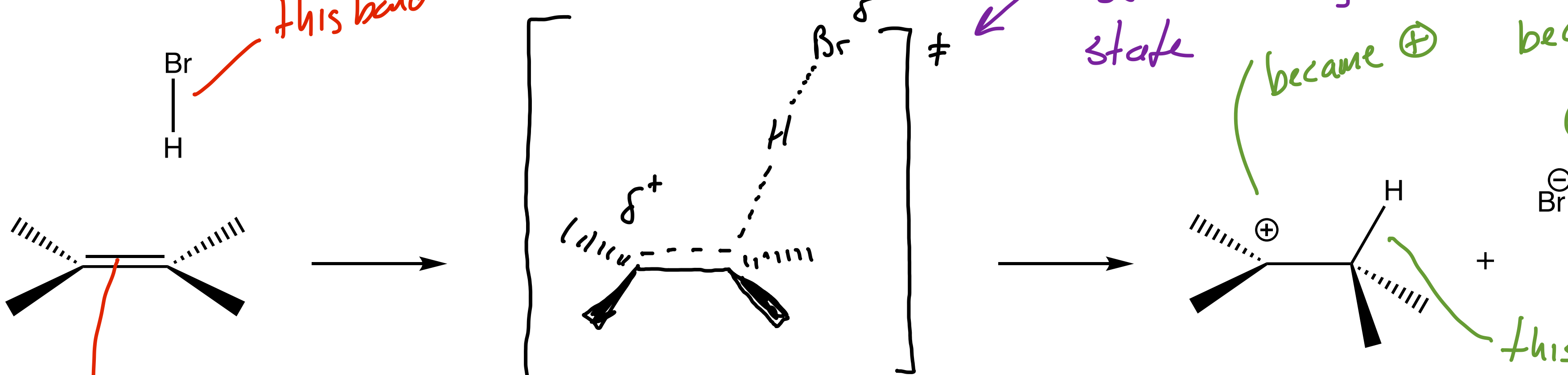
this π bond is breaking

this tells everyone you are drawing a transition state

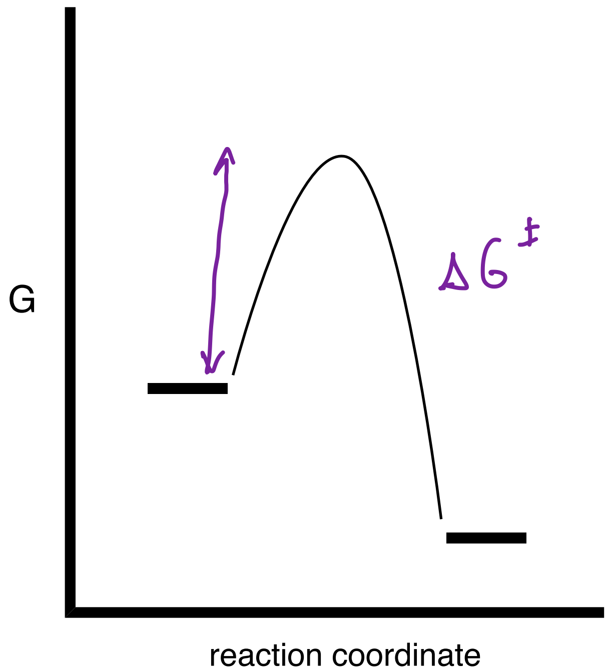
became ⊕

became neg

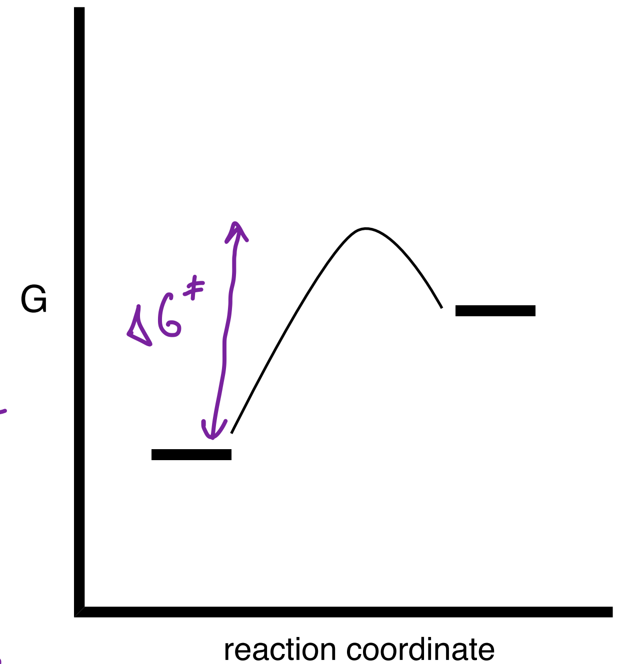
this bond is forming



$FC_c = 4 - 3 = +1$



these are the same so even though one has a more favorable K, they have the same intrinsic rate

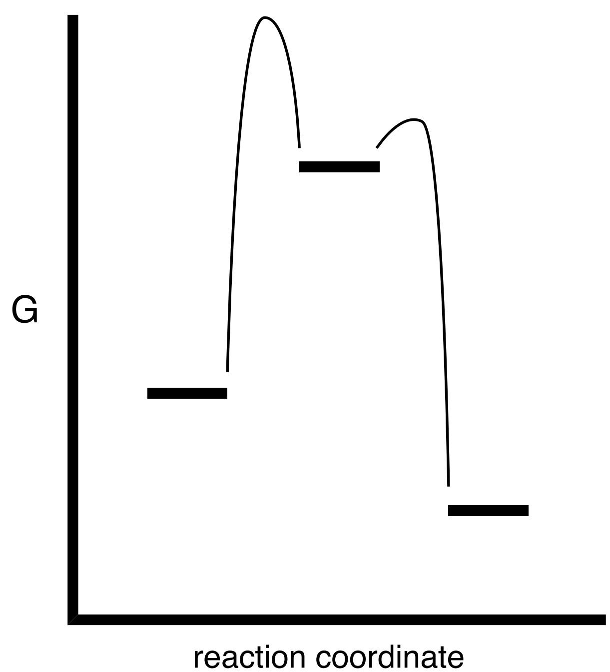


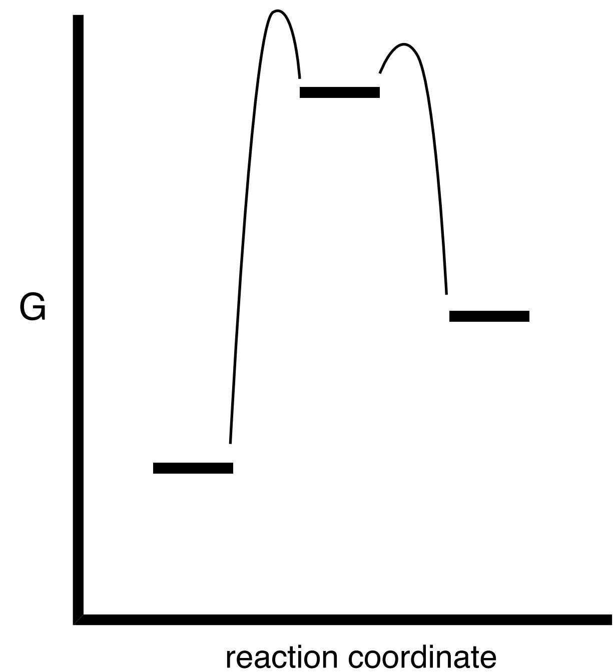
more favorable ΔG, $\Delta G < 0$

larger K

less favorable ΔG, $\Delta G > 0$

smaller K


G
reaction coordinate


G
reaction coordinate

Today’s Office Hours Postponed to 12:30 to 2:00.

On Monday, we will be looking at section 5.5 - 5.12