

(28) Today

Sections 6.1 – 6.5

Sections 6.7 – 6.10

Next Class (29)

Sections 6.7 – 6.10

Chap 7

() Second Class from Today

Test 3 on Chap 5 and 6.1 - 6.5

Third Class from Today (30)

Chap 7

Reworked Test 2 due Wednesday, November 20.

On a separate piece of paper provide answers for any question for which you did not receive full credit. I do NOT need the test itself back.

Describing a Reaction: **Equilibria**, Rates, and **Energy Changes**

Section 6.7

Gibbs Free Energy $\Delta G < 0$ large K products are favored releases energy

$$\Delta G^\circ = \Delta H^\circ - T \Delta S^\circ$$

ΔH change in enthalpy... under very specific conditions ΔH
can be thought of as heat

$\Delta H < 0$ release heat

exothermic

release energy make a reaction
favorable

$\Delta H > 0$ absorbing heat

endothermic

ΔS change in entropy a measure of randomness/probability

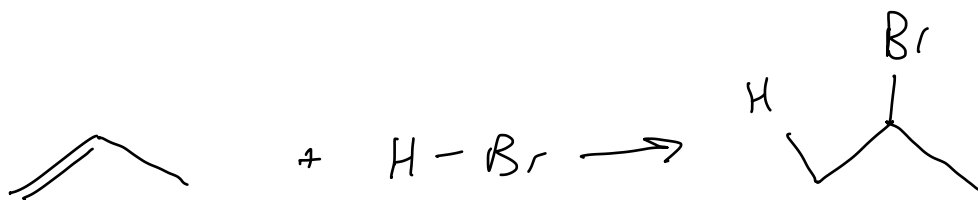
$\Delta S > 0$

increasing entropy

increasing randomness/disorder

encourage a reaction to occur

$\Delta S < 0$



$$\Delta S < 0$$

entropy is
decreasing

$$\Delta G = \Delta H - T \Delta S$$

$$\Delta G = \Delta H - T (-)$$

$$\Delta G = \Delta H + (+)$$

If this is a spontaneous rxn ... ΔH must be < 0

relationship between (equilibria and energy changes) and rates

That's right ... there isn't one

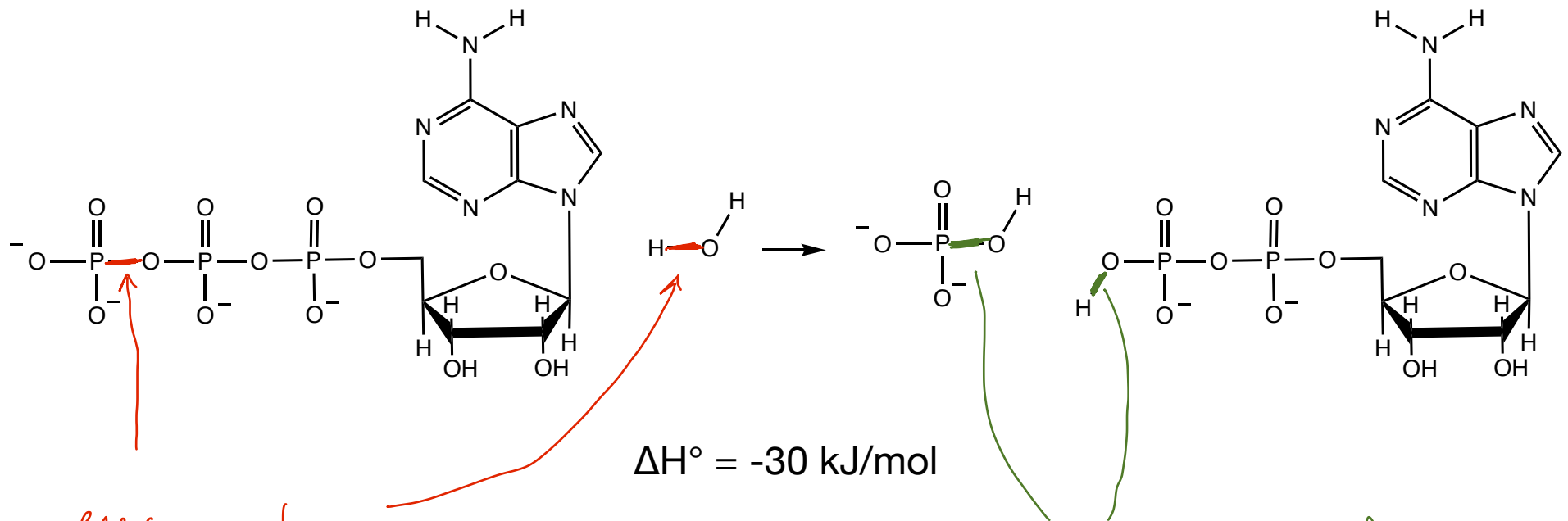
rate does not depend on K (equilibrium const)

It depends on

concentration of reactants

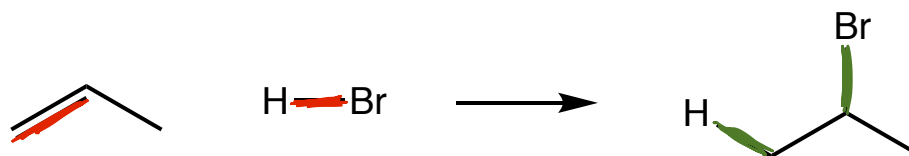
higher concentration means more chances for reactants to collide

the activation energy ... not every collision is successful ...
bonds have to break for a reaction to occur then the
activation energy will depend on the strength of the
bonds being broken



energy in to
break this bond

energy is released
when we make these
bonds



ΔH_{BDE} is the amount of enthalpy required to break a bond

ΔH_{rxn} = energy in to break C to C π bond
 energy in to break H to Br bond

+ 312 kcal/mol + 366 kcal/mol

energy out/released when C-H bond forms

- 421 kcal/mol

energy out/released when C-Br bond forms

- 294 kcal/mol

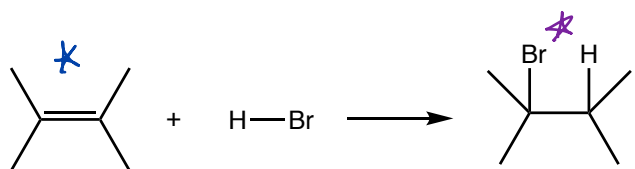
ΔH_{rxn} = 678

- 715

ΔH_{rxn} = - 37 kcal/mol

Putting It All Together in a Reaction Coordinate Diagram

Section 6.9, 6.10



***** Reactant(s)

***** Product(s)

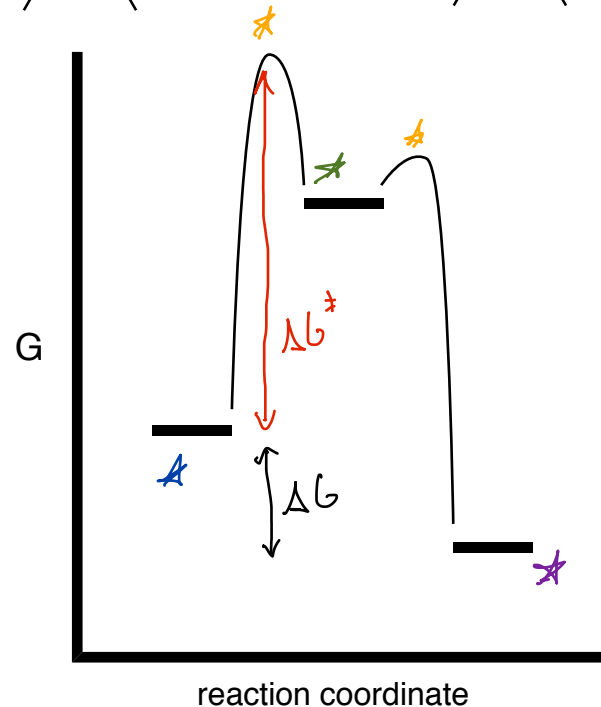
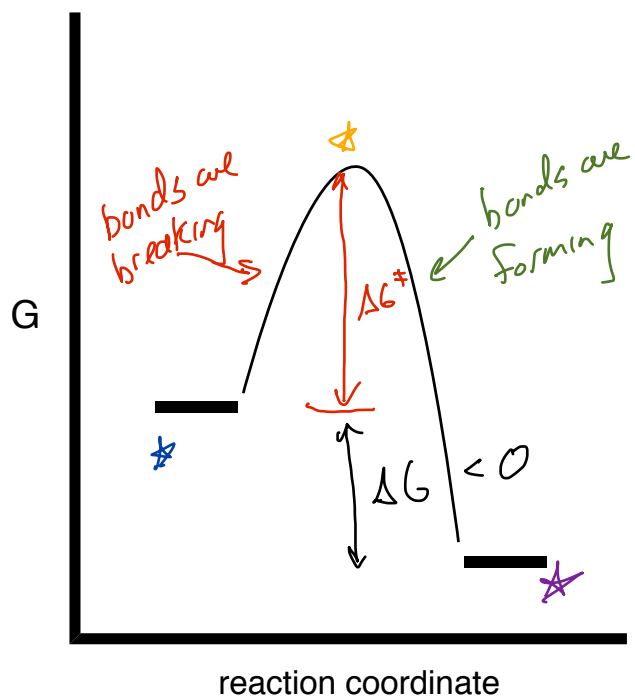
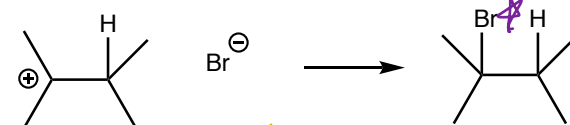
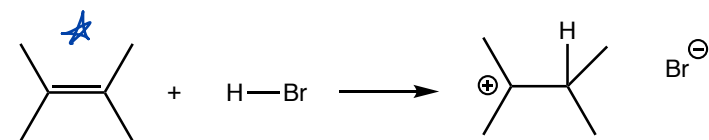
***** Transition State(s)

***** Intermediate(s)

***** Activation Energy ΔG^\ddagger
rate of a reaction
(kinetics)

ΔG (thermodynamics)
K (thermodynamics)

$$\Delta G = G_F - G_I$$



***** Transition state is the highest energy pt on the path from reactants to products... old bonds are partially broken and new bonds are partially formed

***** Intermediates are chemicals that are formed & consumed during a rxn

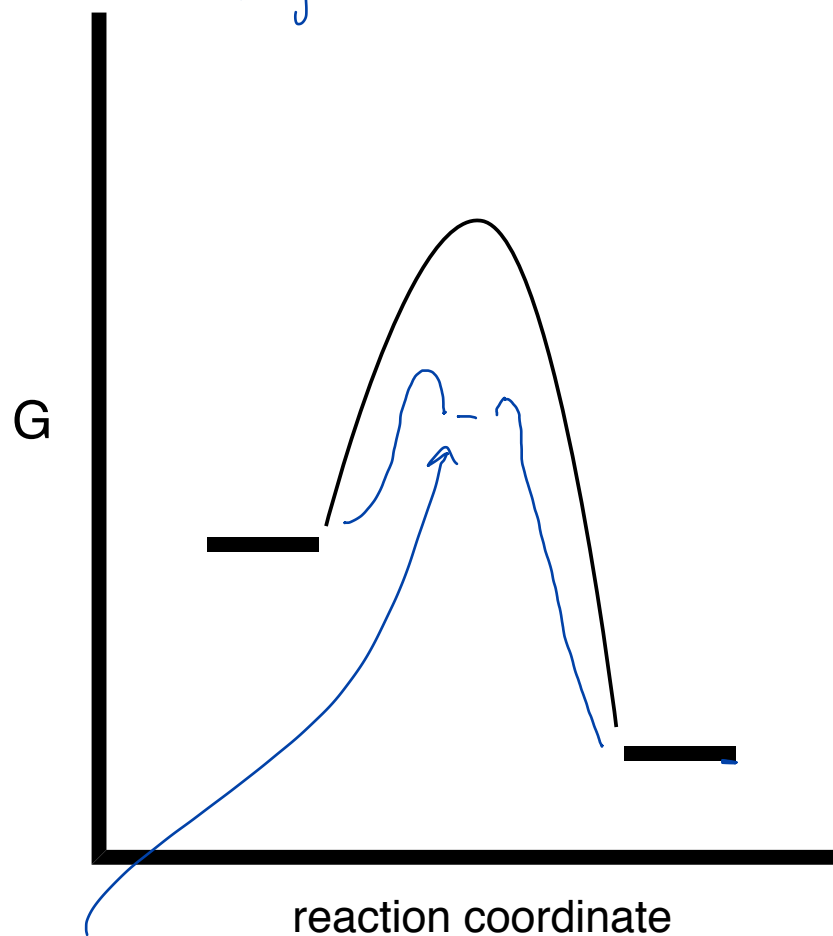
Catalysis

catalysts do not change the thermodynamics of a rxn

catalysts lower the activation energy typically by altering the mechanism of the reaction

Section 6.9, 6.10

uncatalyzed 1 step rxn
catalyzed reaction

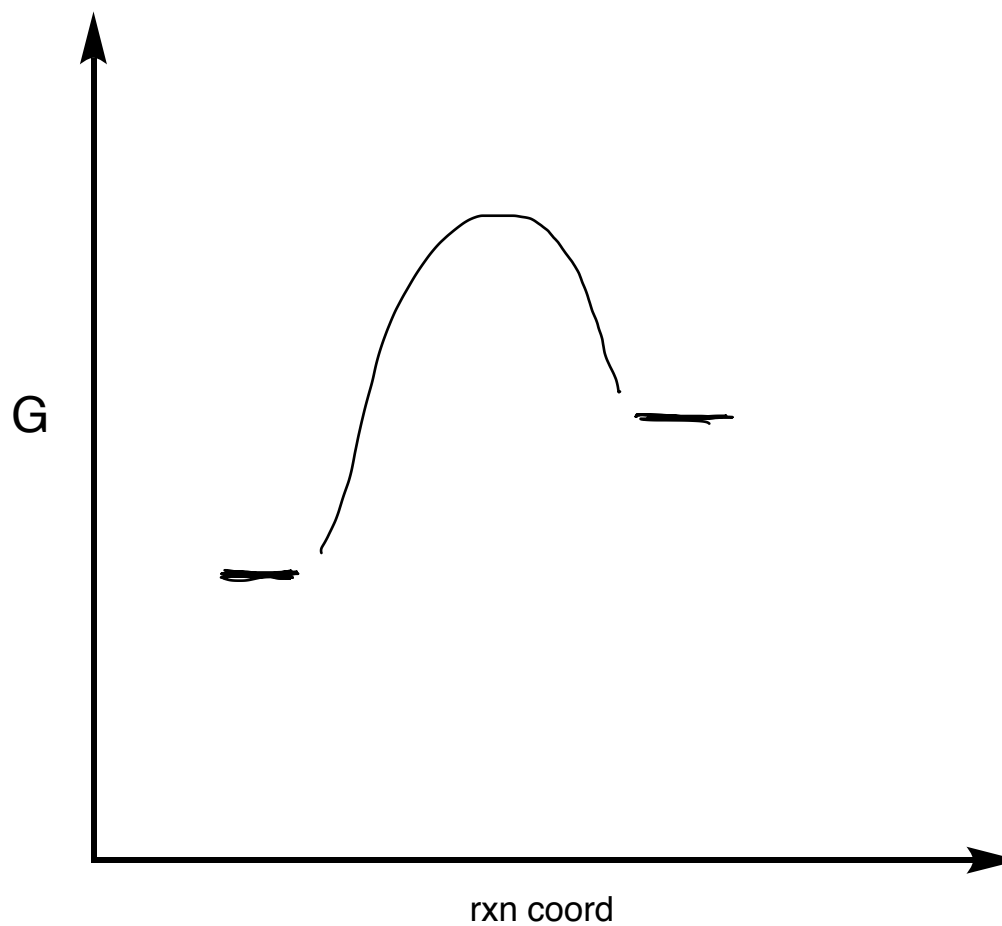


number of intermediates depends on the mechanism of the catalyst

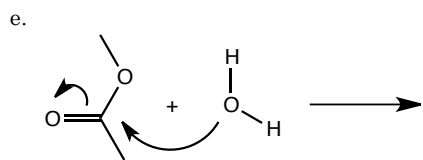
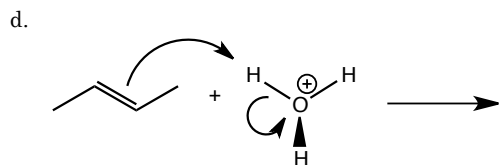
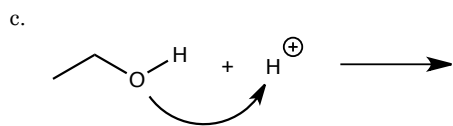
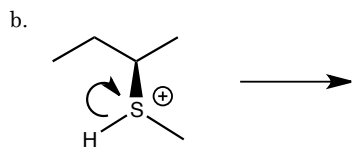
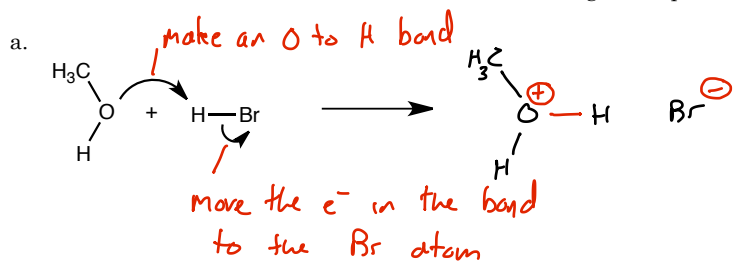
Draw a reaction coordinate diagram for a one-step mechanism that has an unfavorable ΔG (a small K)

Practice

positive ... products higher in E



Draw the molecules or ions that result from the following arrow pushing.



Draw electron pushing arrows for the following mechanisms.

