Chapter 7

Chemical Reactions
Chemical Reactions Part 2 – Collision Theory

Collision Theory states that for a chemical reaction to occur the following conditions must be met:

1) Molecular collisions – reactants must collide with one another before any reaction can occur.

2) Activation energy – colliding reactants must possess a minimum total amount of energy ($E_a$ = activation energy) for the collision to result in a reaction.

3) Collision orientation – colliding reactants must come together in the proper orientation for a reaction to occur.

Let’s take a closer look at these conditions.

Molecular Collisions

When reactions involve 2 or more reactants, the reactants must come in contact with each other.

That is why most reactions occur in solution – liquid or gas.

Activation Energy: minimum energy that must be attained by reactants for a reaction to occur

Not ALL collisions result in a chemical reaction.
Collision Orientation

Even when the $E_a$ requirements are met, some collisions still do not result in product formation. The reactants must collide with sufficient energy (> $E_a$) and have the proper orientation.

Predict which collision has the proper orientation for the reaction:

$$\text{NO}_2(g) + \text{CO}(g) \rightarrow \text{NO}(g) + \text{CO}_2(g)$$

a)

b)

c)

What happens if the NO$_2$ and CO collide with the correct orientation, however, the collision energy is below the $E_a$?
Chemical Reactions Part 3 – Thermodynamics (Reaction Energy)

Energy: the capacity to do work or transfer heat

Bioenergetics: field of study concerned with the transfer of energy in reactions occurring in living cells

Units of Energy in Science and Nutrition

calorie: the amount of heat energy required to raise the temperature of 1 gram of water by 1°C

A muffin contains 350 Calories. How many Joules of energy does this muffin contain?
Heat Energy and Reaction Enthalpy

The First Law of Thermodynamics = Conservation of Energy
Energy can be neither created nor destroyed.

\[ \Delta H = \text{Heat of Reaction} = \text{heat given off or absorbed in a chemical reaction} \]

Exothermic and Endothermic Reactions – which way does the heat flow? Not ALL reactions release heat, some reactions need heat to occur.

Exothermic Reactions: A chemical rxn that gives off heat
the products are lower in chemical potential energy than the reactants

Endothermic Reactions: A chemical rxn that absorbs heat
the products are higher in chemical potential energy than the reactants

For the reverse reaction, we change the sign of \( \Delta H \).
Draw the complete Reaction Energy Diagram for each reaction.
Remember to label the axes and $\Delta H$ & include the reactants and products.
Classify the following reactions as Exothermic or Endothermic.

a) $\text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + \text{H}_2\text{O}(l)$ \hspace{1cm} $\Delta H = -213 \text{ kcal/mol}$

b) $\text{N}_2(g) + \text{O}_2(g) + 43 \text{ kcal} \rightarrow 2 \text{ NO}(g)$
Calorimetry: experimental technique to measure enthalpy changes

Calorie Content of Food

<table>
<thead>
<tr>
<th>Biomolecule</th>
<th>Foods Containing this Biomolecule</th>
<th>Cal/g</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbohydrates</td>
<td>Rice, potatoes, bread, vegetables, fruit, milk</td>
<td>4</td>
</tr>
<tr>
<td>Proteins</td>
<td>Fish, meat, dairy products, beans, legumes, milk</td>
<td>4</td>
</tr>
<tr>
<td>Fats</td>
<td>Oils, butter, margarine, animal fats, milk</td>
<td>9</td>
</tr>
</tbody>
</table>

Calculate the caloric content for each biomolecule using the nutritional label to the right.
Kinetics = Reactions Rates

Activation Energy: the minimum combined kinetic energy of reactants must possess for their collision to result in a reaction

Is Reaction A exothermic or endothermic?

Is Reaction B exothermic or endothermic?

Which reaction is faster?

Why?
Factors Affecting Reaction Rates

1. Concentration of the Reactants
2. Temperature
3. Catalyst

Concentration & Reaction Rates

Note how the $[N_2O_5]$ decreases over time in the reaction below.

$$2 \text{N}_2\text{O}_5(g) \rightarrow 4 \text{NO}_2(g) + \text{O}_2(g)$$

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>N$_2$O$_5$ Concentration (M)</th>
<th>Rate of Reaction (M/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.16</td>
<td>0.06</td>
</tr>
<tr>
<td>1</td>
<td>0.11</td>
<td>0.04</td>
</tr>
<tr>
<td>2</td>
<td>0.08</td>
<td>0.03</td>
</tr>
<tr>
<td>3</td>
<td>0.06</td>
<td>0.02</td>
</tr>
<tr>
<td>4</td>
<td>0.04</td>
<td>0.01</td>
</tr>
</tbody>
</table>
Temperature and Reaction Rates

Rule of Thumb: every 10°C increase in rxn temperature the rxn rate doubles

Since our bodies need to maintain a constant temperature, we can not use heat to increase biochemical pathways. A different strategy is needed.
Catalysts and Reaction Rates

Energy diagrams for three reactions

(a) exothermic rxn  (b) same exothermic rxn  (c) endothermic rxn with a catalyst

Catalyst: a substance that increases the rate of a chemical reaction without being consumed in the reaction.

How does a catalyst increase the rate of a chemical reaction?

The transition state is the particular arrangement of atoms in the reactants at the maximum energy level.

What is activation energy ($E_a$)?

Label the transition state energy and $E_a$ for graphs (b) and (c).

What happens to reactant molecules that have LESS energy than the energy of the transition state?

Enzymes are biochemical catalysts.
Chemical Rxns Part 5: Equilibrium Reactions and Le Chatlier’s Principle

Equilibrium:
when the forward and reverse reactions proceed at the same rate, the concentration of reactants and products no longer changes and the reaction has reached a state of equilibrium.

Reaction Rates & Equilibrium
For the reaction $HA \leftrightarrow H^+ + A^-$, plot the relative reaction rates of the forward and reverse reactions over time and label where the state of equilibrium begins.

Reactant and Product Concentrations & Equilibrium
For the reaction $HA \leftrightarrow H^+ + A^-$, plot the $[HA]$ and $[H^+]$ over time and label where the state of equilibrium begins.

What general statement can we make about the concentration of reactants and products at equilibrium?

At equilibrium, have the reactions stopped?
The state of equilibrium is often called “dynamic equilibrium”. Explain the meaning of the term “dynamic” in relationship to the reaction rates.

Most exothermic reactions are considered spontaneous, meaning the products are more stable (have lower energy) than the reactants. However, SPONTANEOUS does NOT necessarily equate to FAST. Draw a reaction energy diagram to explain this scenario. Overlay a second curve when a catalyst is present.
Changing Equilibrium Conditions

LeChatlier’s Principle: When a “stress” is applied to a system at equilibrium, the equilibrium shifts to relieve the “stress.”

What does “stress” mean?

Let’s see what happens when we add “stress” to a system at equilibrium.

\[
P_{\text{Cl}_3(g)} + \text{Cl}_2(g) \rightleftharpoons P\text{Cl}_5(g) + \text{heat}
\]

Original equilibrium: \[\begin{array}{ccc} \text{PCl}_3 & \text{Cl}_2 & \text{PCl}_5 \\ 5 & 7 & 5 \end{array} \]

new equilibrium: \[\begin{array}{ccc} \text{PCl}_3 & \text{Cl}_2 & \text{PCl}_5 \\ 5 & 7 & 5 \end{array} \]

What stress was added?

At the new equilibrium, what happened to the \([\text{PCl}_3]\)?

At the new equilibrium, what happened to the \([\text{Cl}_2]\)?

At the new equilibrium, what happened to the \([\text{PCl}_5]\)?

Which way did the equilibrium shift?

If we decrease the \([\text{PCl}_3]\), which way will the equilibrium shift?
What happens when we change the temperature?

\[ \text{PCl}_3(g) + \text{Cl}_2(g) \rightleftharpoons \text{PCl}_5(g) + \text{heat} \]

Is the reaction above exothermic or endothermic?

If we increase the temperature, are we adding or removing heat?

If we increase the temperature, do we favor the forward or reverse reaction?

If we increase the temperature of the reaction, which way will the equilibrium shift?

If we decrease the temperature, do we favor the forward or reverse reaction?

If we decrease the temperature of the reaction, which way will the equilibrium shift?

Draw the reaction energy diagram.
What happens when we change the pressure?

\[ \text{PCl}_3(g) + \text{Cl}_2(g) \rightleftharpoons \text{PCl}_5(g) + \text{heat} \]

How many moles of gas are present as reactants?

How many moles of gas are present as products?

If we increase the pressure, which way will the equilibrium shift?

Why?

Would a change in pressure affect the following reaction?

\[ \text{H}_2(g) + \text{Cl}_2(g) \rightleftharpoons 2 \text{HCl}(g) \]

Why?
Adding a catalyst

Do catalysts change the position of equilibrium?

What do catalysts change?

Show the effect of a catalyst for an exothermic reaction on a reaction energy diagram.

Plot the reaction rate versus time for the exothermic reaction above overlaying the reaction rates with and without a catalyst.
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