Understanding these reactions really means getting acquainted with the molecules as if they were your friends and knowing what their nature is and what they will do...

~ Henry Eyring

**Molecular Orbitals**

- Orbitals are electron probability standing waves
- Shape of orbital depends on forces (charge) & energy
- New standing wave patterns (new shapes) when there are multiple nuclei
- Molecular orbitals
  - Follow same rules as atomic orbitals:
    - 2 e⁻/orbital (opposite spins)
    - Fill lowest energy orbitals first

**Thermite**

- Fe₂O₃ + 2Al → Al₂O₃ + 2Fe
- Very large energy release (molten Fe)!
- Only goes with hot fuse
- Raise the screen to do this!

**Where did the energy come from?**

A. The atoms’ electrons jumping to lower energy levels
B. The atoms becoming less organized
C. Iron is in the 3rd row while aluminum is in the 2nd. When they switch places they release energy.

**Classify Elements According to Reactivity**

- Don’t react at all
  - He, Ne
- React with great difficulty
  - Ar, Kr, Xe
- Form diatomic gases
  - H₂, N₂, O₂, F₂, Cl₂
- Very reactive
  - Li, Na, K, Rb, Cs
- Most metals
- Many of the diatomic gases above

**Molecular Orbitals & Bonding**

- When atoms get close, MO’s can form
- If the electrons are lower in energy in the resulting MO’s than they were in the atomic orbitals, bonds form
Why do some things form bonds, whereas others don’t?

A Thermodynamic View of Bonding

Bond formation is favorable if it leads to decreased energy for the system, and/or increased entropy for system + surroundings

3 ways to do it
- Lots of atoms share lots of electrons: metals
- Nonmetals “take” electrons from metals: ionic materials
- Nonmetals share electrons with each other: covalent materials

Conservation of Matter: Balancing Chemical Reactions

Matter is not created or destroyed in chemical reactions
This is reflected in the way we write them

Which way of writing the reaction of hydrogen with oxygen to make water best complies with conservation of matter and describes what happens?

1. \( H_2 + O_2 \rightarrow H_2O \)
2. \( H_2 + \frac{1}{2}O_2 \rightarrow H_2O \)
3. \( 2H_2 + O_2 \rightarrow 2H_2O \)

Electrolysis

Can run the reaction backward:
- \( 2H_2O \rightarrow 2H_2 + O_2 \)
Pumping energy back into the system
For each water molecule that reacts, how many molecules of \( H_2 \) are produced?
Same question, for \( O_2 \)?

Reactions Take Time

Going in the direction \( 2H_2 + O_2 \rightarrow 2H_2O \), reaction is fast
Or is it? What if you don’t have a match?
Electrolysis clearly takes time
Clock reaction (oscillating clock demo)
Really a complex set of racing reactions
When one set leads, yellow
When the other leads, purple
Reactions Go at Different Speeds

• Cellulose + O₂ → CO₂ + H₂O
  • Dead tree in forest
  • Wood in fire
  • Sawdust in explosion

Why?

What Governs Speed of a Reaction?

• Definition: rate that reactants are consumed, or products are produced

Factors:
• Physical state of reactants
• Collision rate
• Energetic requirements
• Entropic (organization) requirements

Collision Rate Limits Reaction

• Reactants must get close for electron clouds to interact

What controls collision rate?
• Temperature (because it is a reflection of molecular speed)
• Physical state
• Pressure (for gases) or concentration (for liquids)

Which factor has the biggest effect on reaction rate?

1. The amount of energy released when reactants are transformed into products
2. The temperature of the reacting system
3. The monetary value of the products
4. The amount of disorder created when reactants are transformed into products

Effect of Energy

• The net energy released (or consumed) does not affect rates
• The energy required to reach the transition state (“activation energy”) has large effect

Transition state
• The critical arrangement of atoms where the reacting system “decides” whether or not to make products
• Typically involves breaking and/or formation of bonds

Effect of Entropy

• Reactants frequently must have a certain orientation at the transition state, or reaction will not occur
• This corresponds to order in the transition state: entropy of activation
Our Handwarmers

- What has more entropy, a solid or a liquid?
  - 2 things to think about....
    1. Structure
    2. Energy

Let's Blow Some Stuff Up

- $H_2$
- $H_2 + O_2$
- $H_2 + O_2$ w/ Pd/C catalyst

Equilibrium

- Reactions go in both directions:
  - Reactants  Products
- You've already seen this in the $H_2 + O_2$ reaction
- This dynamic balance is called “chemical equilibrium”

Catalysts

- Decrease energy or increase entropy of activation without themselves being consumed; speed up rate
- $H_2O_2$ decomposes spontaneously
- Much faster in presence of Br$^-$ (or MnO$\text{2}$)
- Catalyst makes new, lower energy route possible

Why do we need to use a match to explode the $H_2 + O_2$ balloon?

A. Products of combustion of the match catalyze reaction of $H_2 + O_2$
B. Heat from the match provides the required energy of activation
C. We need the match to pop the balloon and expose the $H_2$ to the $O_2$
D. Matches contain small amounts of palladium (Pd)

Meaning of Equilibrium

- When forward and reverse rates are equal, amount of reactant & product no longer changes
- Equilibrium is the state of lowest energy, entropy; everything moves toward it