CHEM135 - 3415

Ash Dorsey
ash@ash.lgbt

Contents

Dimensional Analysis

Many problems can be solved by looking at the units and trying to divide everything.

Units can be multiplied and divided just like variables.

$$\text{undesired unit} \times \frac{\text{desired unit}}{\text{undesired unit}}$$

Prefix	**Symbol**	**Multiplier**
tera	T	10^{12}
giga	G	10^{9}
mega	M	10^{6}
kilo	k	10^{3}
deci	d	10^{-1}
centi	c	10^{-2}
milli	n	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}
femto	f	10^{-15}

$1\ \mathrm{gal} = 3.785\,411\,784\ \mathrm{L}$, $1\ \mathrm{m} = 10^{10}\,\text{Å}$

1. How many pm are in $532\ \mathrm{nm}$?

$$532\ \mathrm{nm} \times \frac{10^{-9}\ \mathrm{m}}{1\ \mathrm{nm}} \times \frac{1\ \mathrm{pm}}{10^{-12}\ \mathrm{m}} = 532\,000\ \mathrm{pm}$$

2. Convert $27.8\ \mathrm{L}$ to cm^3. How many in^3 is this? Given: $1\ \mathrm{mL} = 1\mathrm{cm}^3; 1\ \mathrm{in} = 2.54\ \mathrm{cm}$

Plan: $\mathrm{L} \to \mathrm{mL} \to \mathrm{cm}^3$

$$27.8\ \mathrm{L} \times \frac{10^3\ \mathrm{mL}}{1\ \mathrm{L}} \times \frac{1\mathrm{cm}^3}{1\ \mathrm{mL}} = 2.78 \times 10^4\ \mathrm{cm}^3$$

$$2.78 \times 10^4\ \mathrm{cm}^3 \times \left(\frac{1\ \mathrm{in}}{2.54\ \mathrm{cm}}\right)^3 = 1.70 \times 10^3\ \mathrm{in}^3$$

3. Passenger planes, such as the Boeing 747, tend to use a specific fuel blend of kerosene and gasoline called Jet-A aviation turbine fuel, with a density of $0.820\frac{\mathrm{g}}{\mathrm{cm}^3}$ If the plane is fueled with $175\,000\ \mathrm{L}$ of Jet-A fuel, what is the mass of the fuel in kg?

$$\mathrm{L} \to \mathrm{mL} \to \mathrm{cm}^3 \to \mathrm{g} \to \mathrm{kg}$$

$$170\,000\ \mathrm{L} \times \frac{10^3\ \mathrm{mL}}{1\ \mathrm{L}} \times \frac{1\,\mathrm{cm}^3}{1\ \mathrm{mL}} \times \frac{0.820\ \mathrm{g}}{1\,\mathrm{cm}^3} \times \frac{1\ \mathrm{kg}}{1\,000\,\mathrm{g}} = 1.44 \times 10^5\ \mathrm{kg}$$

4. For this problem, consider a $1.0 \times 1.0\ \mathrm{in}$ square of aluminum foil with a thickness of $0.016\ \mathrm{mm}$. One Al atom is spherical with a diameter of 1.50Å. Estimate the number of Al atoms in this square of aluminum foil, assuming the aluminum foil is composed of 100% Al. Given: $1\ \mathrm{in} = 2.54\ \mathrm{cm}$

$\frac{1.0\ \mathrm{in}\ \times 1.0\ \mathrm{in}\ \times 0.016\ \mathrm{mm}}{1\ \mathrm{Al\ sheet}} \times \left(\frac{2.54\ \mathrm{cm}}{1\ \mathrm{in}}\right)^2 \times * \frac{1 \cdot 10^{-2}\ \mathrm{m}}{1\ \mathrm{cm}})^2 \times \frac{10^{-3}\ \mathrm{m}}{1\ \mathrm{mm}} \times \left(\frac{10^{10}\text{Å}}{1\ \mathrm{m}}\right)^3 \times \frac{1\ \mathrm{Al\ atom}}{\frac{4}{3}\pi((1.50\text{Å}))^3} = 5.84 \times 10^{21}\ \mathrm{Al\ atoms}$

5. The US has an area of about $9 \times 10^6\ \mathrm{km}^2$. How deep would the US be covered with marbles (diameter = $1.00\ \mathrm{cm}$) if you had the same number of marbles as the number of aluminum atoms from the reality check question on the previous slide? How deep is this relative to the length of a football field (i.e., how many football fields deep of marbles would you have)?

$$\frac{\frac{4}{3}\pi(0.5\ \mathrm{cm})^3}{9 \times 10^6\ \mathrm{km}^2} \times 5.84 \times 10^{21} = 3.398\,37 \times 10^{-1}\ \mathrm{km}$$

Avogadro's number

Avogadro's number is the number of atoms in one mole. It's about $6.023 \times 10^{23}\frac{\mathrm{entities}}{\mathrm{mol}}$

Example

An $8\ \mathrm{oz}$ glass of water contains about $13\ \mathrm{mol}$ of water. How many molecules of water does the glass hold?

$13\ \mathrm{mol} \times 6.023 \times 10^{23}\frac{\mathrm{atoms}}{\mathrm{mol}} = 7.8 \times 10^{24}\ \mathrm{molecules\ of\ water}$

Module 2: Solar Cells

Energy

Fossil Fuels

Most energy in the world comes from fossil fuels, which are formed from the decomposition of long-dead plants and animals.

Why go solar?

- The sun is abundant
- Solar energy is renewable and clean
- Despite the initial cost, solar energy is really cheap.

Solar cells capture energy from the sun and convert that energy into electricity.

With your group, brainstorm questions that you need answered to understand how questions work.

Main questions:

1. How does light produce electrons to make electricity?
   - What is light, and how does it behave?
   - What are electrons, and how do they behave?
   - Which electrons in an atom are ejected?
     - How are electrons structured in the atom?
2. What makes a good solar cell material?
   - Solar cells are primarily composed of silicon
   - Why silicon?
   - How do the electrons know where to go?

Chapter 2: Atoms

We know:

- Ordinary matter can be broken up into smaller components called **atoms**.
- There are 92 different types of atoms that naturally exist, but we can make more. (See the periodic table).

Nuclear Theory of the atom

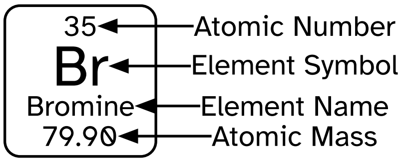
- Atoms comprise a small, dense nucleus surrounded by mostly empty space.
- The nucleus contains protons and neutrons, accounting for most of the mass and all of the positive charge
- The empty space surrounding the nucleus contains small, negatively charged electrons

Subatomic Particles

Particle	Mass (kg)	Charge (C)	Relative Charge
Proton	$1.672\,62 \times 10^{-27}$	$1.602\,18 \times 10^{-19}$	$+1$
Neutron	$1.674\,93 \times 10^{-27}$	0	0
Electron	$9.109\,38 \times 10^{-31}$	$-1.602\,18 \times 10^{-19}$	-1

Periodic Table

Atomic number: Number of protons in the nucleus, this defines the element
Element symbol: one or two-letter abbreviation
Element name: not always present
Atomic mass: mass in amu or $\frac{\mathrm{g}}{\mathrm{mol}}$ of one atom of a particular element.



Isotopes

All atoms have the same number of protons but not the same number of neutrons. For example, Bromine has 44 or 46 neutrons. ${}^{79}_{35}\mathrm{Br}$ or Bromine-79 and ${}^{81}_{35}\mathrm{Br}$ or Bromine-81

${}^{\mathrm{A}}_{\mathrm{Z}}Y$ Y is the element, A is the number of protons and neutrons, and Z is the number of protons.

Atomic Mass

Atomic mass is calculated by taking the weighted average mass of the atom's isotopes as they occur in nature.

Ions

The number of electrons in a neutral atom equals the number of protons in its nucleus. When the number of electrons does not equal the number of protons, the result is an ion. Positively charged ions are called cations, and negatively charged ions are called anions.

What does an atom look like?

- Atoms comprise a small, dense nucleus surrounded by mostly empty space.
- The nucleus contains protons and neutrons, accounting for most of the atom's mass and all of its positive charge
- The empty space surrounding the nucleus contains small, negatively charged electrons.

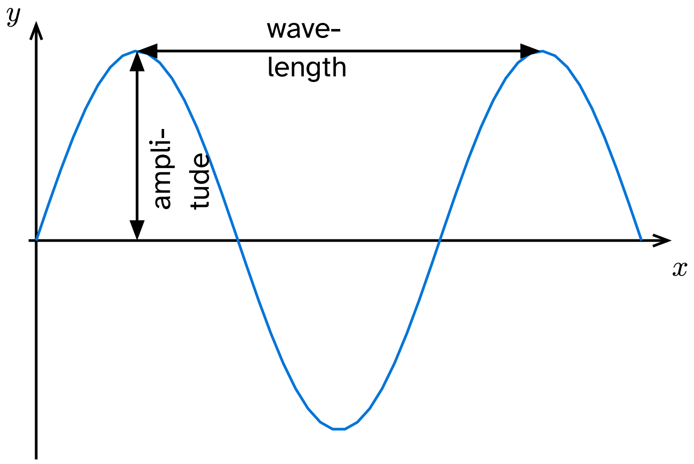
Quantum Theory

- Classical Mechanics: describe the behavior of things on the macroscopic scale
- Quantum Theory: describe the behavior of things on the microscopic scale
  - Wave-particle duality
  - Schrodinger's cat
  - indeterminacy of the position of electrons

Wavey light

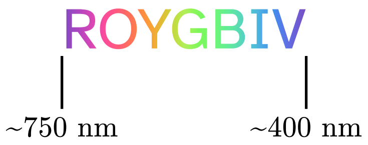
- Light is a type of electromagnetic radiation, meaning it has an electric and magnetic component
- Light can be visualized as perpendicular waves of these two fields propagating through space.

Light as a wave is a <u>classical</u> theory.



Amplitude determines brightness: with higher amplitude comes higher brightness.

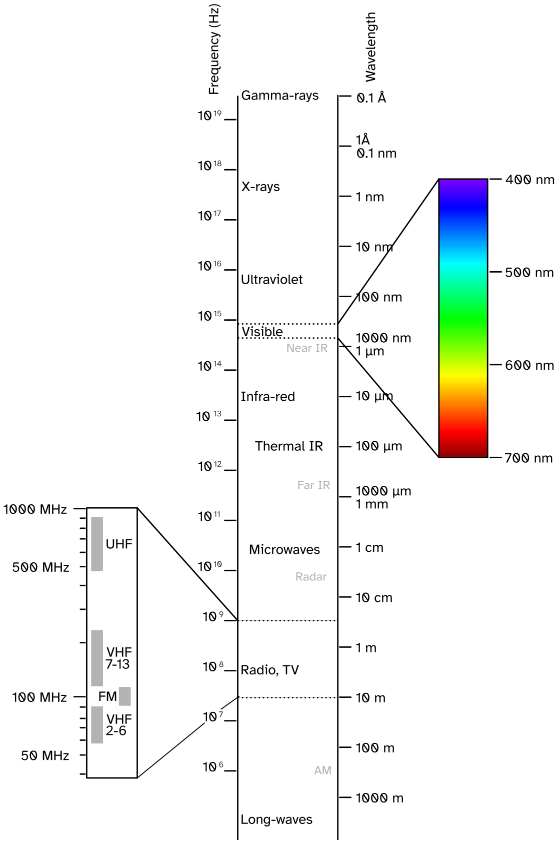
Wavelength determines the color of light.



ν is frequency, λ is wavelength

$$\underbrace{\nu}_{\text{nu}} = \frac{c}{\lambda}$$

Electromagnetic Spectrum



Example

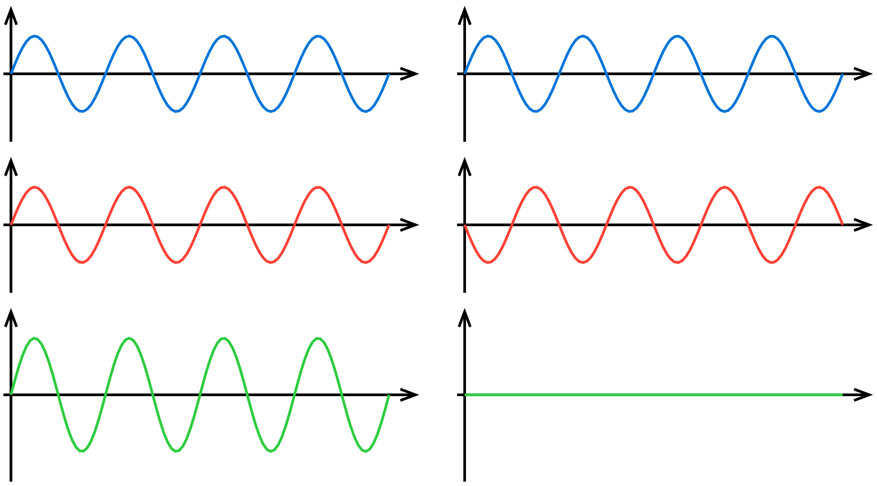
Calculate the frequency of red light: We know $\lambda = 750\ \text{nm}$

$$\nu = \frac{c}{750.\ \text{nm}} = \frac{299\,792\,458\frac{\text{m}}{\text{s}}}{750.\ \text{nm}} \times \frac{10^{9}\ \text{nm}}{1\ \text{m}} = 4.00 \times 10^{14}\ \text{Hz}$$

Interference

When a wave encounters another wave, they interfere:

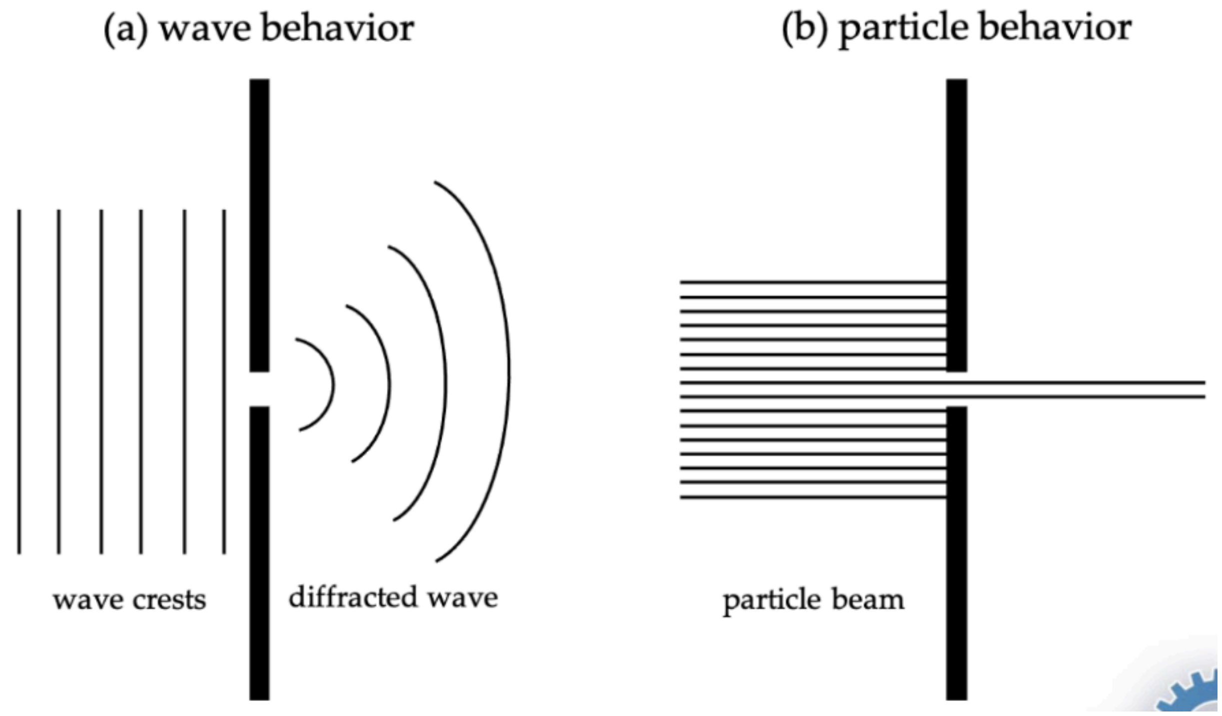
- Constructive interference: One wave's peak aligns with another wave's peak. They are in phase and have a higher combined amplitude
- Destructive interference: One wave's peak aligns with another wave's trough. They are out of phase, which results in a lower combined amplitude



Diffraction

When traveling waves encounter a barrier with a small opening (about the same size as its wavelength), they will bend as they pass through the opening.

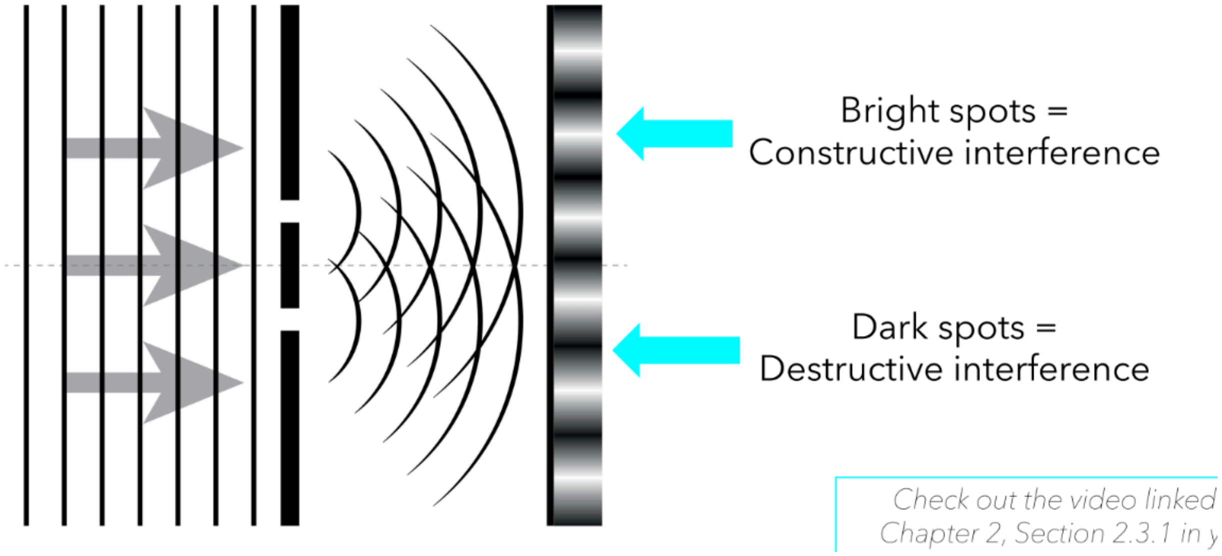
Particles don't diffract, this behavior is unique to waves.



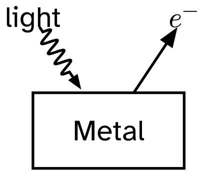
Particle Light

Experiments with light

The double-slit experiment shows that light is a wave resulting in an interference pattern.



Photoelectric effect

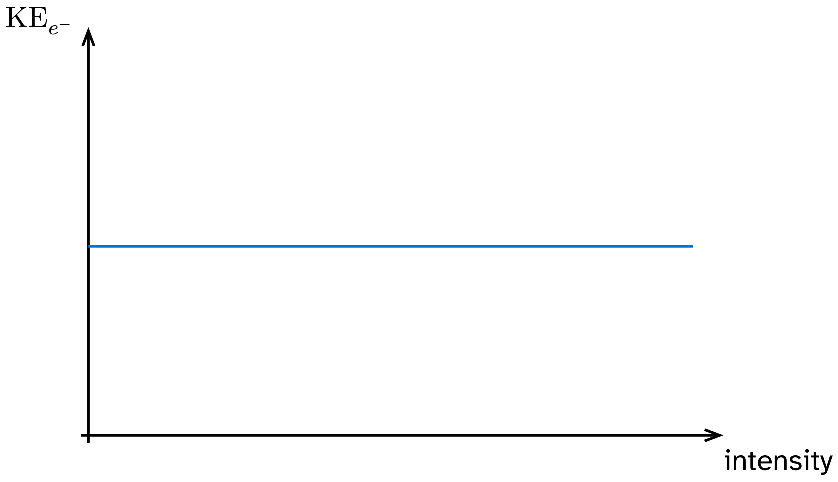


What is happening? Energy from the light is transferred to electrons in the metal until $E_{\text{transferred}} > E_{\text{binding}}$. The more the energy transferred, the greater the KE_{e^-}.

If light is a wave, as classical mechanics states, $E_{\text{wave}} \propto A_{\text{wave}}$

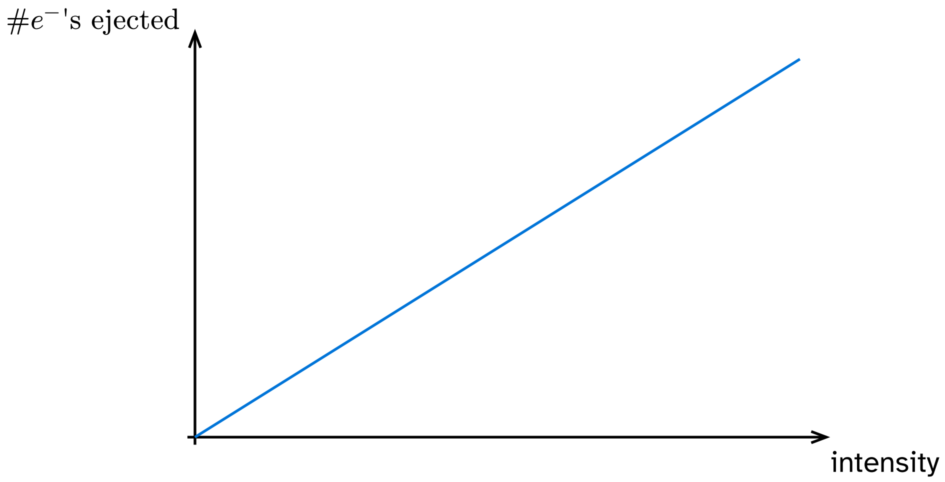
<u>Prediction</u>: If we increase the intensity of light, we will see greater, KE_{e^-}.

<u>Actual Results:</u> (A)



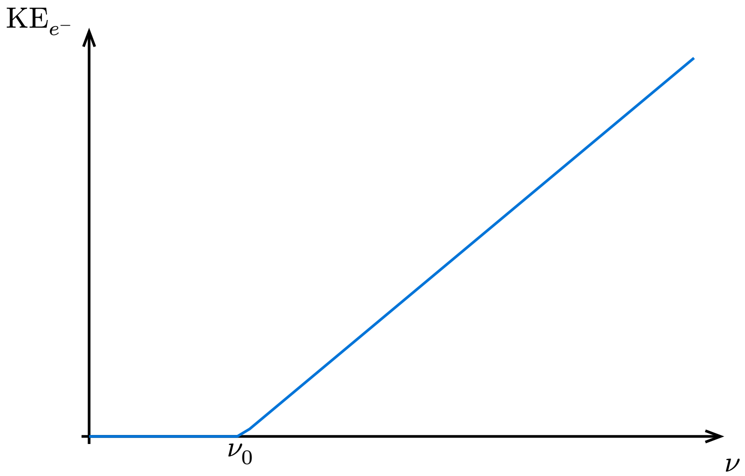
$\therefore E_{\text{light}} \not\propto A_{\text{wave}}$, light is not behaving as a wave.

(B)



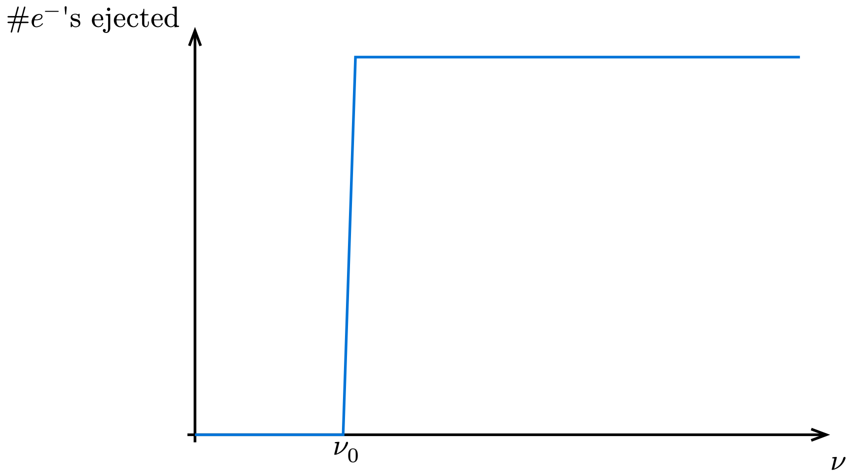
$\therefore \#e^-\text{'s} \propto \text{intensity}$

(C)



$\therefore E_{\text{light}} \propto \nu$

(D)



$\therefore E_{\text{light}} \propto \nu$

Light is behaving as a particle in these experiments.

Conclusions:

Via plot C, $E_{\text{particle of light}} \propto \nu$ (color)

Via plot B, $\# \text{ particles of light} \propto \text{intensity}$

One particle of light can kick out **one** e^- $\Rightarrow$ the higher the intensity, the more particles of light $\Rightarrow$ the more particles of light, the more electrons that can be ejected (if $\nu > \nu_0$)

Photoelectric Effect

Einstein confirmed the previous theory: light behaves as a particle. (little packets of energy).

Those particles are called photons.

$$E_{\text{photon}} = h\nu$$

$$h = 6.26 \times 10^{-34} \text{ J} \cdot \text{s}$$

$$E_{\text{photon}} = h\nu \text{ and } \nu = \frac{c}{\lambda} \Rightarrow$$

$$E_{\text{photon}} = \frac{hc}{\nu}$$

Example

Calculate the velocity of a photoelectron when potassium metal is irradiated with a green light with a wavelength of 527 nm. The binding energy for potassium is 2.29 eV.

Given: $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}, m_e = 9.109 \times 10^{-31} \text{ kg}$

$$\underbrace{E_{\text{in}}}_{\text{light}} = \underbrace{E_{\text{out}}}_{\text{electron}}$$

$$\underbrace{E_{\text{photon}}}_{h\nu} = \underbrace{E_{\text{binding energy}}}_{\Phi} + \underbrace{\text{KE}_{e^-}}_{\frac{1}{2}m_{e^-}v^2}$$

$$h\nu = \Phi + \text{KE}_{e^-}$$

$$\frac{hc}{\lambda} - \Phi = \text{KE}_{e^-}$$

$$\frac{hc}{\underbrace{527 \text{ nm}}_{\text{need to be m}}} - \underbrace{(2.29 \text{ eV})}_{\text{need to be J}} = \text{KE}_{e^-}$$

$$\Phi = 2.29\cancel{eV} \times \frac{1.602 \times 10^{-19} \text{ J}}{1\cancel{eV}} = 3.668\,58 \times 10^{-19} J$$

$$\frac{(6.626 \times 10^{-34} \text{ J} \cdot \text{s})(2.998 \times 10^{8} \frac{\text{m}}{\text{s}})}{5.27 \times 10^{-7} \text{ m}} - 3.668\,58 \times 10^{-19} \text{ J} = 1.008\,218\,98 \times 10^{-20} \text{ J}$$

$$1.008\,218\,98 \times 10^{-20} \text{ J} = \frac{1}{2}m_{e^-}v^2 = \frac{1}{2}(9.109 \times 10^{-31} \text{ kg})v^2$$

$$\sqrt{v} = \sqrt{2.213\,68 \times 10^{10} \frac{m^2}{s^2}}$$

$$v = 1.49 \times 10^{5} \frac{\text{m}}{\text{s}}$$

BONUS POINT: check sig figs on a physical piece of paper, particularly around the subtraction.

Tangent about material properties and threshold frequency

What happens if $\nu = \nu_0$ (threshold frequency)? The photon has exactly enough energy to overcome the binding energy, so it dislodges the electron, resulting in a 0 velocity electron, $\text{KE}_{e^-} = 0$.

$$\text{KE}_{e^-} = 0 \Rightarrow h\nu_0 = \Phi$$

Different metals have different Φ and different ν_0, but they are related by the above equation.

Questions

A Light source emits a total of 2.03×10^{-17} J of light with a wavelength of 980 nm. How many photons are emitted?

$$\frac{2.03 \times 10^{-17} \text{ J}}{\frac{hc}{980 \text{ nm}}} = 100.109 \approx 1.00 \times 10^{2}$$

What are electrons?

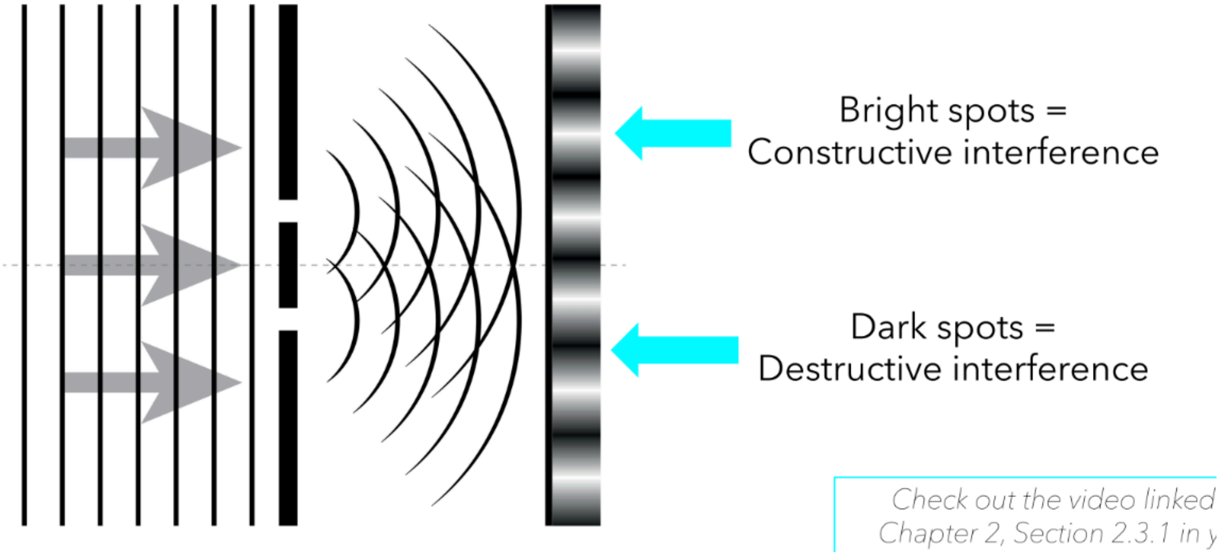
Are electrons particles?

Maybe.

We know that electrons are tiny pieces of matter with a mass on the order of 10^{-31} kg and a negative charge on the order of 10^{-19} C. But maybe they're also waves?

Double-slit experiment

After performing the same experiment as we did on photons, it also showed wave-like properties.



And it's not just electrons—all matter behaves as a wave, but it only matters when stuff is tiny.

Indeterminacy

Weird quantum property!

If you do the same thing twice in classical physics, the outcome will be the same. When you throw a football twice in the same way, it results in the exact same distance and path.

But for quantum particles, it's indeterminate. If you do the same thing twice, the same thing *could* happen twice or could not. It's a field of probabilities, a probability distribution map.

Atomic Orbitals

Atomic orbitals are where the electrons are likely to exist in the atom. In order to figure out what these orbitals look like, we need to treat matter as a wave. To do so, solve the Schrödinger Equation:

$$\hat{H}\psi = E\psi$$

Because the solutions to this equation are distinct (see the slides for the equation), electrons in the atom can only have certain energies, and therefore, energy is quantized.

Quantum Numbers

We need **3** quantum numbers to describe atomic orbitals: $n, \underbrace{l}_{\text{lowercase L}}, m_l$

Principal Quantum Number: n

An integer that determines the overall **size** and **energy** of the orbital. The greater the n, the larger the orbital, and the greater its energy.

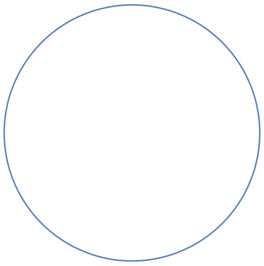
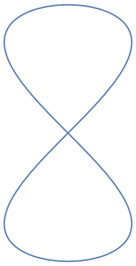
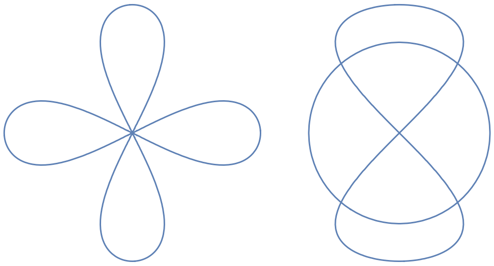
$$n \in \mathbb{N}^{>0} \qquad / \qquad 0 < n$$

$n = 1$ is the closest to the nucleus and has the lowest energy.

Angular Momentum: l

An integer that determines the **shape** of the orbital.

$$l \in \{0, 1, 2, ..., n-1\} \qquad / \qquad 0 \leq l < n$$

Value of l	**Letter Designation**	**Shape(s)**
0	s	
1	p	
2	d	
3	f	Too complex, see plots later on in the slides

Example

$$n = 2 \Rightarrow l \in \{0, 1\}$$

Magnetic Quantum Number: m_l

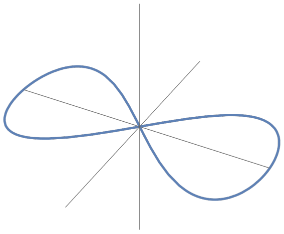
An integer that specifies the **orientation** of the orbitals in 3D space.

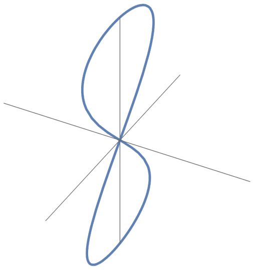
$$m_l \in \{-l, ..., l\}$$

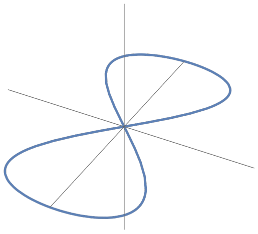
Example

$$n = 2 \Rightarrow l \in \left\{ \underbrace{0}_{M_l \in \{0\}}, \underbrace{1}_{M_l \in \{-1,0,1\}} \right\}$$

Therefore, 3 different orientations: on the x-plane, y-plane, and z-plane







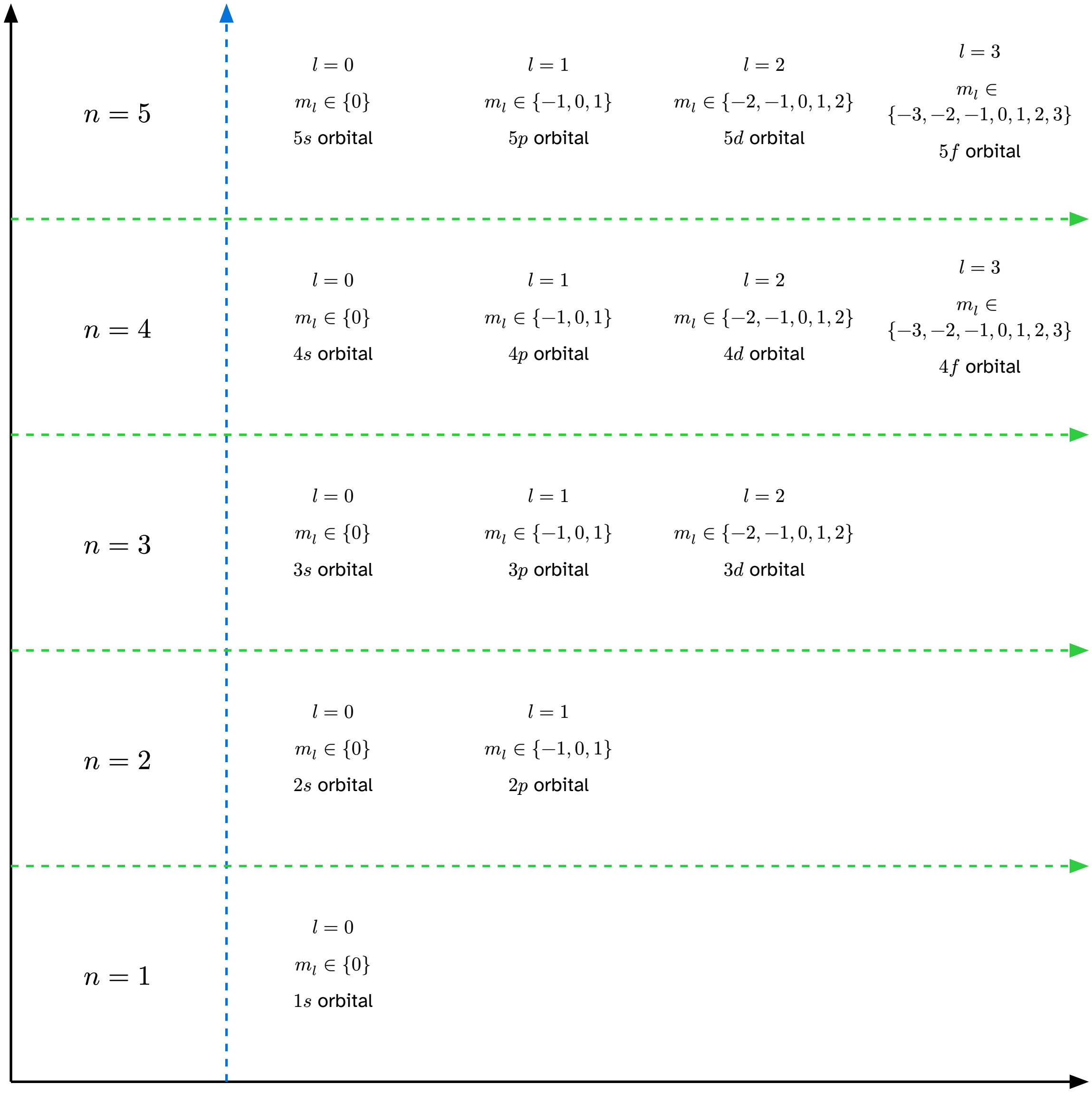
Spin Quantum Number m_s

Specifies the orientation of the electron spin.

$$m_s = \underbrace{+1/2}_{\text{spin up}} \lor m_s = \underbrace{-1/2}_{\text{spin down}}$$

Putting n, l, m_l together

- Principal level (shell) given by n.
- Sublevels given by l.
  - the number of sublevels in a principal level $= n$
  - the number of orbitals in a sublevel = $2l + 1$
  - the number of orbitals in a principal level $= n^2$



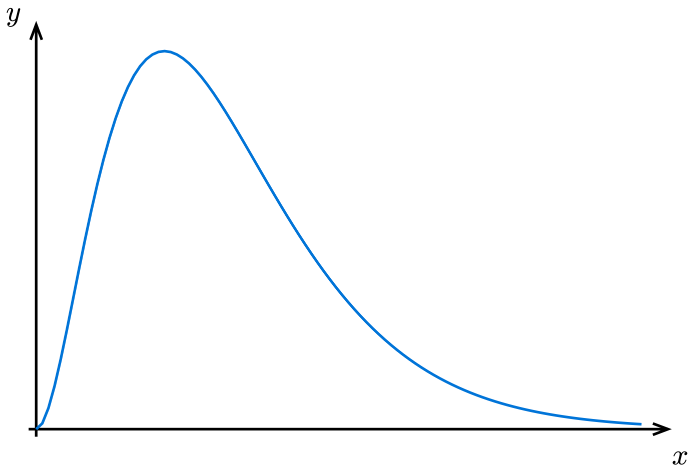
$n = 5$	$l = 0$ $m_l \in \{0\}$ $5s$ orbital	$l = 1$ $m_l \in \{-1, 0, 1\}$ $5p$ orbital	$l = 2$ $m_l \in \{-2, -1, 0, 1, 2\}$ $5d$ orbital	$l = 3$ $m_l \in$ $\{-3, -2, -1, 0, 1, 2, 3\}$ $5f$ orbital
$n = 4$	$l = 0$ $m_l \in \{0\}$ $4s$ orbital	$l = 1$ $m_l \in \{-1, 0, 1\}$ $4p$ orbital	$l = 2$ $m_l \in \{-2, -1, 0, 1, 2\}$ $4d$ orbital	$l = 3$ $m_l \in$ $\{-3, -2, -1, 0, 1, 2, 3\}$ $4f$ orbital
$n = 3$	$l = 0$ $m_l \in \{0\}$ $3s$ orbital	$l = 1$ $m_l \in \{-1, 0, 1\}$ $3p$ orbital	$l = 2$ $m_l \in \{-2, -1, 0, 1, 2\}$ $3d$ orbital	
$n = 2$	$l = 0$ $m_l \in \{0\}$ $2s$ orbital	$l = 1$ $m_l \in \{-1, 0, 1\}$ $2p$ orbital		
$n = 1$	$l = 0$ $m_l \in \{0\}$ $1s$ orbital			

By the way, you don't have to draw the 3d plots, those are typically just boxes. Those plots *are* to scale.

$2d$ orbitals don't exist because $2d$ means that $n = 2$ and $l = 2$, but that is not possible because $l < n$, and if not, it is not a solution to the Schrödinger Equation.

Visualizing orbitals

There are two ways that you will commonly see atomic orbitals visualized: density of dots and radial distribution functions Here is a radial distribution function for the 1s orbital:



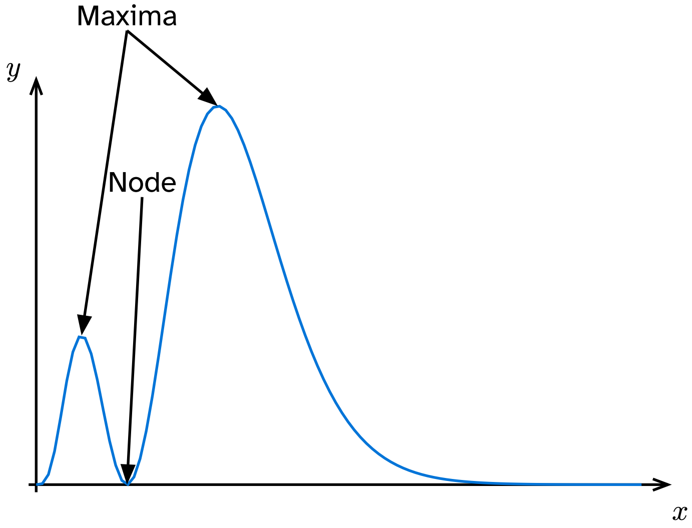
Maxima: distance from the nucleus (radius) where we will most likely find the electron in that orbital. The taller the peak, the more likely we are to find the electron there.

Nodes: radii where we cannot find the electron in that orbital.

General note: the closer an electron can get to the nucleus, the lower its energy.

In general, atomic orbitals have $n - l - 1$ radial nodes.

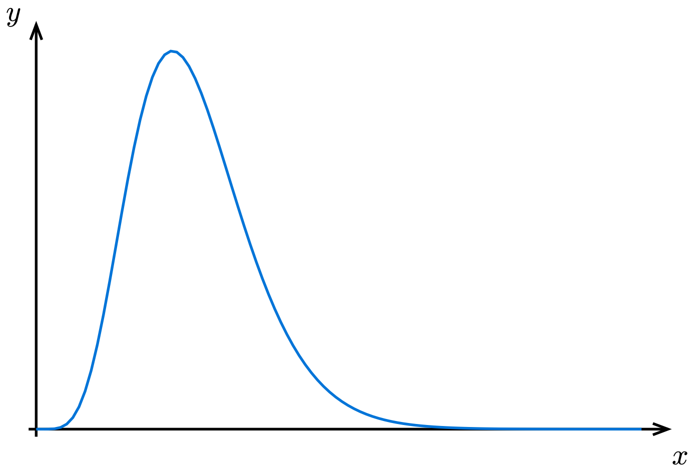
So a $3p$ orbital would have $n = 3, l = 1$, radial nodes $= 3 - 1 - 1 = 1$



Question

How many radial nodes does a 3d orbital have?

$$n = 3, l = 2, \text{radial nodes} = 3 - 2 - 1 = 0$$



Shapes

See the slide show for shapes or see small versions in the chart above

Chapter 3: The Periodic Table

Remember spin.

When electrons are placed in a strong magnetic field, they behave like tiny magnets.

Remember from physics: when an electric charge moves in a loop, it creates a magnetic field.

Scientists guessed that electrons must be spinning because they behave like tiny magnets, ergo, spin quantum number m_n.

Spin up:

$$m_n = +\frac{1}{2} \text{ or } \upharpoonleft$$

Spin down:

$$m_n = -\frac{1}{2} \text{ or } \downharpoonright$$

Pauli Exclusion Principle

No two electrons can have the same 4 quantum numbers; therefore, there are two spin-paired electrons per orbital.

n: size
l: shape
m_l: orientation
m_n: spin

Spin-paired electrons are when two electrons are in the same “box”.

Summary

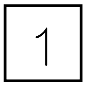
$\underbrace{1}_{\text{from } n}\underbrace{s}_{\text{from } l}, 2s, 2p, 3s, 3p, 3d, \ldots$

Aufbau Principle

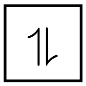
Electrons will fill orbitals beginning with the lowest energy orbital.

Example

Hydrogen (H): $1e^-$ (via the atomic number)

- Electron Configuration: $1s^1$
- Orbital diagram: 

Helium (He): $1e^-$ (via the atomic number)

- Electron Configuration: $1s^1$
- Orbital diagram: 

But for Lithium (Li), we now need to show that the s orbitals are lower energy than the p orbitals.

Coulomb's law

Coulomb's law describes the attractions and repulsions between charged particles.

- For like charges, potential energy is positive and reduces when they get further apart
- For opposite charges, potential energy is negative and becomes more negative when they get closer
- The strength of the interaction increases as the size of the charges increases
- The strength also increases as the charges get closer

$$F = \frac{kq_1q_2}{r^2}$$

Electrons in multielectron atoms feel two forces:

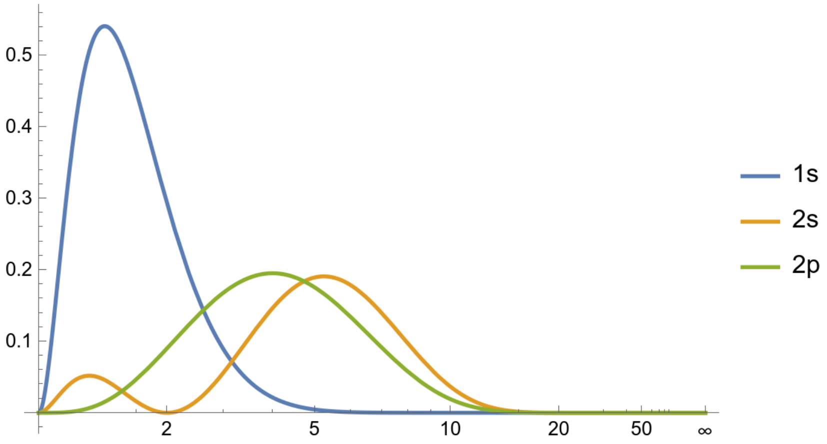
1. attraction from the positively charged nucleus
2. repulsion from other electrons.

$$\underbrace{Z_{\text{eff}}}_{\text{effective nuclear charge}} = \underbrace{Z}_{\text{number of protons in nucleus}} - \underbrace{S}_{\text{number of shielding electrons}}$$

For the example of the $2s$ electron in lithium, $Z_{\text{eff}} = 3 - 2 = 1$, so it's feeling a $+1$ charge. On the other hand, the inner 2 electrons in the $1s$ orbital are feeling more charge, $+3$ charge.

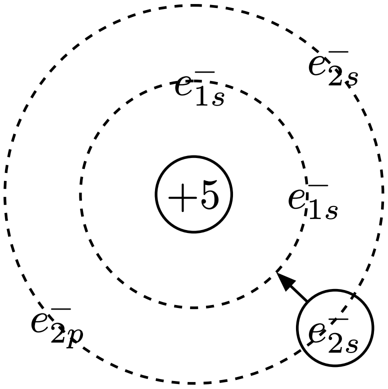
If an electron could penetrate, it would have a lower charge, so why wouldn't it do so? The shape of the orbitals could prohibit it?

Prediction: If the $2s$ orbital has lower energy than $2p$, we expect to see more penetration when in the $2s$ orbital.



See the small peak of the $2s$ (orange) near the peak of the $1s$ (blue)? That means that the $2s$ electrons could penetrate the $1s$ orbitals.

But look at the $2p$ distribution: there is no peak near the peaks of lower functions. That means that there is no significant probability of penetration of a $2p$ electron into a lower energy orbital.



The fact that the electron could penetrate from the $2s$ orbital and couldn't from the $2p$ orbital means that the $2s$ orbital has a lower energy level. This leads to sublevel splitting and is why $s < p < d < f$

Valence electrons

All electrons in the highest principal level in an atom are defined as valence electrons. For transition elements, any elements in a partially filled d-sublevel (or partially filled f-sublevel for lanthanides or actinides) are also considered to be valence electrons.

Which electrons are ejected?

The valence electrons are ejected to create electricity in a solar cell.

Why silicon?

Electron configurations and properties

- Noble gases (8A)
  - 8 valence electrons (except for He, with 2) ⟶ full outer quantum levels
  - particularly unreactive and stable

- Halogens (7A)
  - one electron short of noble gas configuration (ns^2np^5 configuration)
  - tend to gain one electron to form 1- ion
- Alkali Metals (1A)
  - one electron beyond noble gas
  - tend to lose an electron to form a 1+ ion
- Alkaline Earth Metals (2A):
  - two electrons beyond noble gas configuration
  - tend to lose two electrons and form 2+ ion

Example

$$\underbrace{\mathrm{F}^-}_{\text{gained one electron}}$$

$$\text{neutral F} = 9e^-$$

$$+e^- = 10e^- \therefore 1s^2 2s^2 2p^6 \rightarrow \text{same as Ne}$$

$$\underbrace{\mathrm{Na}^+}_{\text{lost one electron}}$$

$$\text{neutral Na} = 11e^-$$

$$-e^- = 10e^- \therefore 1s^2 2s^2 2p^6 \rightarrow \text{same as Ne}$$

$$\text{Because both have the same electron configuration, they are isoelectronic}$$

Transition elements

For a transition element, always remove electrons from the highest n level first.

$$\mathrm{Cu}^+ : \text{neutral Cu} : \underbrace{\underbrace{[\mathrm{Ar}]}_{\text{up one and over to the right on the periodic table}} [4s^1 3d^{10}]}_{\text{to make Cu}^+\text{, need to lose } 1e^-} \therefore \mathrm{Cu}^+ : [\mathrm{Ar}]3d^{10}$$

$$\mathrm{Cd}^{2+} : \text{netural Cd: } [\mathrm{Kr}]4d^{10}$$

Periodic Trends: atomic radius

As you go down a group on the periodic table atomic radius increases.

- n increases as you go down a group
- orbital size increases with n
- The principal level the valence electrons are in is increasing
- As you go across the periodic table from left to right, the atomic radius decreases.
  - As you move to the right across a row, you will remain in the same n shell
  - You are adding protons to the nucleus
  - But the number of core electrons stays the same
  - Therefore, the electrons on the outer shell are feeling more pull because of the higher charge in the center, so the atomic radius decreases.

Ionic Radii

When atoms form anions, electrons are added to the valence shell. This makes the rest of the electrons that were already in the shell spread out more, which makes the anions bigger than the corresponding atom.

When atoms form cations, electrons are removed from the valence shell. This makes the rest of the electrons that were already in the shell get more space, and so can come closer together, which makes the cations smaller than the corresponding atom.

Within the same isoelectronic species, cations are smaller than neutral atoms, and neutral atoms are smaller than anions. The greater the charge, the greater the effect.

Ionization Energy

Making a cation (+) from a neutral element:

The first ionization energy is the energy required to remove an electron from a neutral element in the gas phase:

$$X(g) + \text{energy} \to X^+(g) + e^-$$

The energy it takes to remove an electron from an element in the gas phase is called the ionization energy.

Metallic Properties

Metals generally are malleable, ductile, with a high melting point, and conduct electricity and heat well.

- Metals tend to form cations
- The first ionization energy (IE_1) is the energy needed to form a cation. The greater IE_1 is, the harder it is to lose electrons.

Metallic character, as a result of the ionization energy, runs opposite to the ionization energy.

Insulators and conductors

Nonmetals ⟶ Insulators, bad conductors of electricity

Metals ⟶ conductors, good conductors of electricity

Why silicon?

Silicon is a metalloid, in between metals and nonmetals. This tends to mean that it is a semiconductor.

- Practically: it's the 2nd most abundant element on Earth, after oxygen.
- Silicon is cheap
- Silicon has a long lifetime.

Bonds

Bond Type	Type of atoms bonding	Behavior of valence electrons in the bond
Ionic	Metal and nonmetal	Electrons are transferred between the atoms to form a cation-anion pair

Covalent	Nonmetal and nonmetal	electrons are shared between the two atoms
Metallic	Metal and metal	communal sharing of electrons between all atoms in the material to form a “sea” of electrons

Module 2 In-Class Activity: Solar Cells

Part 1: Why is silicon a good choice for a solar cell material

Silicon, as an atom, is a metalloid, and as a material, is a semiconductor.

To conduct electricity, metals have mobile electrons that can move wherever they want to because they have a “sea” of electrons (from the valence electrons of the metal atoms) → metals are conductors.

The valence band of conductors touches the conduction band. For semiconductors, the valence and conductor bands are slightly further apart, and for insulators, its even further apart. (I highly recommend watching the latest Veritasium videos about blue LEDs). The distance between the bands is called the band gap

In order for an electron to move, it must enter the conduction band.
- Valence band: where the valence electrons are
- Conduction band: empty orbitals closest in energy to the valence orbitals (*this is a slight lie)

Element	Band Gap (eV)	Classification
C	~5	Insulator
Si	1.11	Semiconductor
Ge	0.66	Semiconductor
Sn	0.08	Conductor
Pb	~0	Conductor

Recall that solar cells work by capturing energy from the sun and turning that energy into electricity that we can use to power things.

This means that we would actually like to have the electron inside the material: let the internal photoelectric effect come to the rescue.

We want the electron to be mobile inside the material: this means that you need to put enough energy in to overcome the band gap.

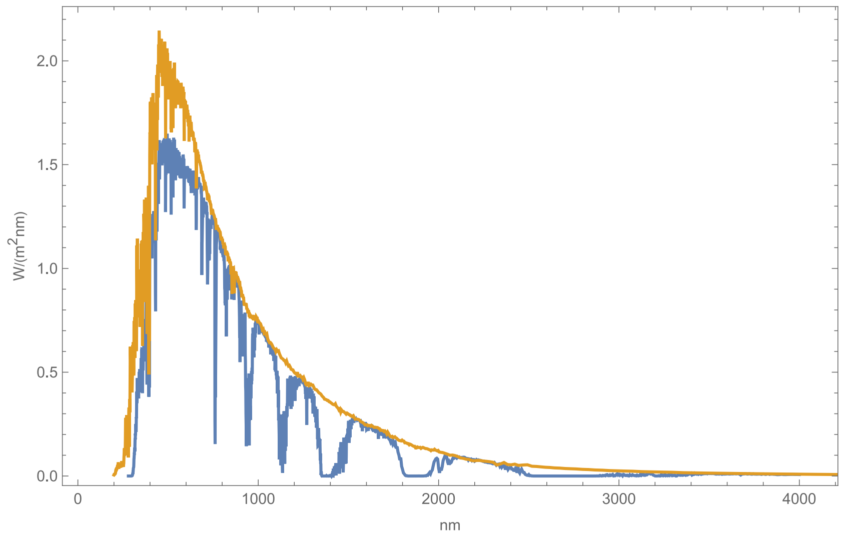
$E_{\text{photon}} > E_{\text{band gap}}$

For silicon to be effective, it needs to capture most of the sun.

Let’s solve for the wavelength:

$$\frac{hc}{\lambda} > 1.11\ \mathrm{eV}$$
$$\lambda < 1\,120\ \mathrm{nm}$$

Being less than 1120 nm is most of the sun’s spectrum:



Therefore, silicon is acceptable as a solar cell material.

Conductors won't work because the electron don't go to a specific place, it just heats up the whole material.

How do the electrons know where to go in a solar cell?

Doping

To increase the conductivity of a semiconductor, impurities are purposefully added to their crystal structure.

Solar cells often have layered structures:

p-type layer
n-type layer

N-type semiconductors have extra electrons because they have added electron-rich impurities, and those extra electrons go into the conduction band.

Conversely, p-type semiconductors have fewer electrons by adding electron-deficient impurities, which results in "holes" in the valence band.

To be stable, the electrons move to fill holes, by moving from the n-type layer to the p-type layer. This results in a positive charge for the impurity in the n-type layer, and a negative charge for the impurity in the p-type layer.

Now, when electrons are produced by the silicon, they go towards the positive charge because they're attracted to it.

This movement of electrons creates an electric potential, allowing the solar panel to power electronic devices.

Part 2: What atoms would work best to dope the silicon layers in a solar cell?

1. Which of the following would be the best choice to dope silicon in the n-type layer?
- Boron
- Carbon
- Thallium
- Phosphorus
- Arsenic

We need an element with $4 + 1 = 5$ valence electrons, preferably one of a similar atomic mass to silicon. Therefore, phosphorus is a good choice, because it has 5 valence electrons but only one more atomic weight.

2. Which of the following would be the best choice to dope silicon in the p-type layer?
- Boron
- Carbon
- Thallium
- Phosphorus
- Arsenic

We need an element with $4 - 1 = 3$ valence electrons, preferably one of a similar atomic mass to silicon. Aluminum would be nice, but it is usually only $3+$, and we need it to be $1-$. Smaller and less toxic is better, so go with boron rather than thallium.

When doping, you want something that is a similar size to limit the disruption of the crystal structure and hopefully less toxic to avoid other harms (you won't need the toxicity information on the exam)

Module 3

Chapter 4

Bonding

Bond Type	**Type of atoms bonding**	**Behavior of valence electrons in the bond**
Ionic	Metal and nonmetal	Electrons are transferred between the atoms to form a cation-anion pair
Covalent	Nonmetal and nonmetal	electrons are shared between the two atoms
Metallic	Metal and metal	communal sharing of electrons between all atoms in the material to form a "sea" of electrons

Ionics bonds happen because metals typically become cations and nonmetals typically become anions. The attraction between them is the ionic bond.

Naming

Formula Unit

The basic unit of an ionic compound is the formula unit, the smallest, electrically neutral collection of ions. For example with Al and O, Al is +3 and O is 2-. This becomes $\mathrm{Al_2O_3}$ to be neutral because $2 \times (3\,+) + 3 \times (2\,-) = 0$.

$$\mathrm{Ca} \wedge \mathrm{O} \Rightarrow \mathrm{Ca}^{2+} \wedge \mathrm{O}^{2-} \Rightarrow \mathrm{CaO}$$

Ionic Naming

The only ions you need to know are in the “ions to know” document on canvas.

$$\mathrm{Cr}^{3+} + \mathrm{Br}^{-1} \to \mathrm{CrBr}_3 \to \underbrace{\text{Chromium}}_{\text{Cr}}\underbrace{\text{(III)}}_{3+}\ \underbrace{\text{bromide}}_{\text{Br}}$$

$$\mathrm{CuO} \to \mathrm{Cu}^{1+} + \mathrm{O}^{1-} \to \mathrm{Cu}^{2+} + \underbrace{\mathrm{O}^{2-}}_{\text{oxygen must be 2-}} \to \text{Copper(II) oxide}$$

Convalent Bonding

Two or more nonmetals. These form covalent bonds.

$$\mathrm{NI}_3 \to \text{nitrogen triiodine}$$
$$\mathrm{P}_4\mathrm{S}_{10} \to \text{tetraphosphorus decasulfide}$$

Binary Acid

Hint: do the discussion worksheet.

Exam, no class.

Biodegradable Polymers

Polymers

Polymers are molecules composed of repeated units.

Polymers are everywhere in everyday life:
- DNA
- Absorbable sutures
- Cotton
- Kevlar
- Styrofoam
- Plastic water bottles

Biodegradeable

Things that can be decomposed by living organisms, like bacteria, form natural byproducts such as carbon dioxide and nitrogen.

Why care about whether things are biodegradable or not?

Take plastics as an example of a polymer.

Pollution due to single-use plastics is a serious global problem:
- Plastics are made from fossil fuels: a nonrenewable, limited resource

- They take hundreds of years to decompose
- Once recycled, it is hard to recycle again.
- Improperly disposed of plastics can have major negative impacts on natural ecosystems

Biodegradable Polymers

- Can be made from renewable components found in plants or other natural resources
- when disposed, degrades on the timescale of a few months to years
- no harmful pollutants are released

Two Examples

Polypropylene (PP):

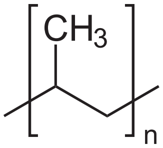
- Non-biodegradable
- Used in things like plastic car bumpers, plastic medical syringes, plastic bottle caps
- derived from fossil fuels

Polylactic Acid (PLA)

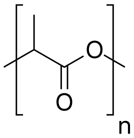
- biodegradable
- used in things like plastic cutlery, medical implants such as stents, food packaging
- derived from plant starches and sugar cane

Compare and Contrast the Structures

Polypropylene (PP):



Polylactic Acid (PLA):



Oxygens are on the PLA, what does that mean?

Focus Questions

- Q1: How do we interpret the structure of a polymer?
  1. How can atoms bond together to form molecules?
  2. What are organic molecules and how do we represent them?
  3. How do we predict and draw the structures of molecules in general?
  4. How do molecules look in 3D?
  5. How do polymers form from monomers?
- Q2: How do polymers degrade?
  1. How does the structure of a polymer influence its interactions?

Organic Compounds

Both PP and PLA are organic compounds.

A molecule is classified as organic if it contains primarily carbon and hydrogen.

What's so special about carbon, anyway?

What is special about carbon

Carbon is element #6 on the periodic table, with 6 protons, 6 total electrons, and 4 valence electrons.

It needs 4 more electrons to get a noble gas configuration. Because it isn't a metal, it primarily participates in covalent bounding (shares valence electrons).

Carbon "wants" to make 4 covalent bonds.

Bond-line structures

Single Bonds

Carbon can form a single bond:

$$C^{2\ \text{electi}\underline{\text{ons}}\ \text{shared}}C$$
$$C – C – C – C$$

C C C C

→

   H H H H
H C C C C H
   H H H H

→

Double Bonds

C=C-C

→

H H H
C=C-C H
H   H

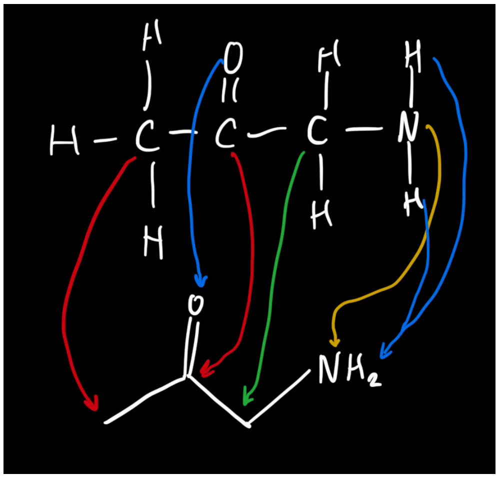
→

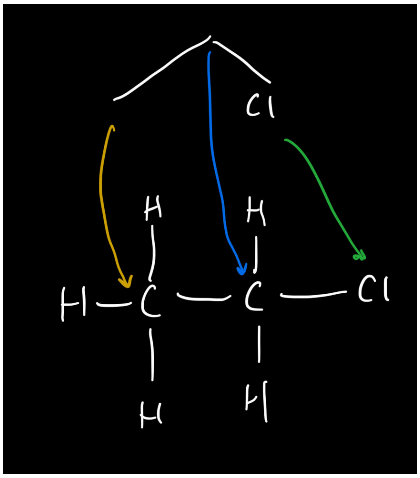
Rules

1. All carbon atoms are implied.
2. Hydrogen atoms bonded to carbon atoms are implied. You know the amount because all carbons "want" to form 4 covalent bonds.
    3. This is *only* relevant for bonds to carbon

4. Any atom other than carbon or hydrogen is written explicitly
5. Lone pairs are normally omitted
6. The geometry of the molecule is represented by the angles in the bond-line structure
    - Single and double bonds zigzag
    - Triple bonds are straight

More examples





Clicker Question

What is the molecular formula of the molecule shown on the document camera?

Answer: C_6H_{14}

Naming Simple Hydrocarbons

$$\underbrace{\text{prefix}}_{\text{number of cations (the parent chain)}}\underbrace{\text{suffix}}_{\text{type of C-C bond}}$$

Prefix

Number of carbon atoms	Prefix

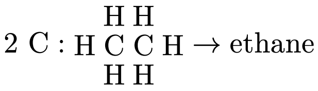
1	meth-
2	eth-
3	prop-
4	but-
5	pent-
6	hex-
7	hept-
8	oct-
9	non-
10	dec-

Suffix

Type of carbon-carbon bonds	**Suffix**
All $\mathrm{C}-\mathrm{C}$ single bonds	-ane
At least one $\mathrm{C}=\mathrm{C}$ double bond	-ene
At least one $\mathrm{C}\equiv\mathrm{C}$ triple bond	-yne

Examples

$$1\ \mathrm{C}: \mathrm{CH}_4 \rightarrow \text{methane}$$



$$2\ \mathrm{C}: \begin{matrix} & \mathrm{H} & \mathrm{H} & \\ \mathrm{H} & \mathrm{C} & \mathrm{C} & \mathrm{H} \\ & \mathrm{H} & \mathrm{H} & \end{matrix} \rightarrow \text{ethane}$$

Parent Chain

The parent chain is the longest continuous chain of carbon atoms.

Substituent group

A group attached to the a parent chain

Beyond Simple Hydrocarbons: Naming with Functional Groups

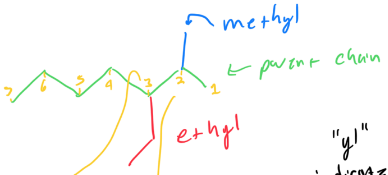
prefix-infix-suffix

Prefix	Number of Carbons
Infix	Type of C-C bond (same as before, but without an e)
Suffix	Functional Group

Naming

Functional group	**Suffix**
Alcohol	-ol
Aldehyde	-al

Ketone	-one
Carboxylic acid	-oic acid
Amine	-amine



"yl" indicates a substituent group attached to the parent chain

3-ethyl-2-methylheptane

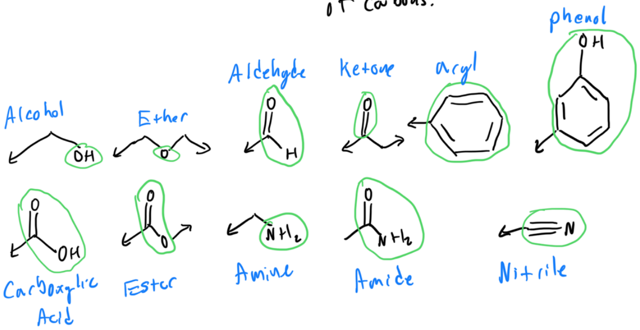
2 carbons

1 carbon

7 carbon single bonds in the parent chain

Parent Chain:

Longest continous chain of carbons.

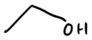


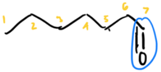
2 carbons

Ethanol ⇒

alchol

single bonds



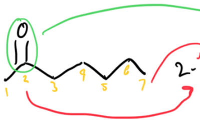


7 carbon

single bonded

heptanal

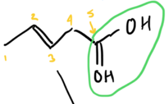
aldehyde



ketone

2-heptanone

single bonds



pentenoic acid

double bond

pent-3-enoic acid

𝟘 Which functional groups are present in the molecule amphotericin B?

- All of the above

Molar Mass

Molar mass is the mass in grams of one mole of a compound or formula unit. This is also called molecular weight or formula mass.

$$\text{molar mass} = \sum n_i \cdot (\text{atomic mass})_i$$

Example: H_2O

$$\begin{aligned} H_2O &= (2 \text{ mols H})(\text{atomic mass H}) + (1 \text{ mol O})(\text{atomic mass O}) \\ &= (2)(1.008) + (1)(16.00) \approx 18.02 \text{ g/mol} \end{aligned}$$

Practice

A sample of the explosive TNT ($C_7H_5N_3O_6$) has a mass of 650.5 g. How many moles of TNT are in this sample? How many molecules is this?

$$(7)(12.01) + (5)(1.008) + (3)(14.01) + (6)(16.00) = 227.14$$

$$650.5 \text{ g TNT} \times \frac{1 \text{ mol TNT}}{227.14 \text{ g TNT}} = 2.864 \text{ mol TNT}$$

$$2.865 \text{ mol TNT} \cdot \frac{6.022 \times 10^{23} \text{ molecules TNT}}{1 \text{ mol TNT}} = 1.725 \times 10^{24}.$$

Practice

What mass of carbon is in the 650.5 g sample of TNT?

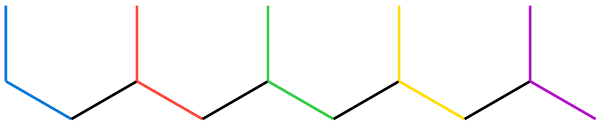
$$(7)(12.01) + (5)(1.008) + (3)(14.01) + (6)(16.00) = 227.14$$

$$650.5 \text{ g TNT} \times \frac{1 \text{ mol TNT}}{227.133 \text{ g TNT}} \times \frac{7 \text{ mol C}}{1 \text{ mol TNT}} \times \frac{12.01 \text{ g C}}{1 \text{ mol C}} = 240.8 \text{ g C}$$

Back to Polymers

Polymers are molecules composed of repeating units. Polymers are made by forming chemical bonds between monomers.

PP:



Why do atoms bond?

In general, energy drives bond formation. The potential energy of the atoms bonded together is lower than the potential energy of the isolated atoms.

If we wanted to calculate this potential energy, we would need to consider
- Nucleus-nucleus repulsions
- electron-electron repulsions

- nucleus-electron attractions

Returning to types of bonds

In ionic and covalent bonds, are electrons always perfectly shared or transferred completely?

No! Consider bond polarity:

There is a continuum of bond types *between* perfect sharing and perfect transferring, with unequal sharing existing in the continuum.

Polar covalent bonds are covalent bonds where electrons are unequally shared.

In these bonds, one atom pulls the electrons more strongly than the other, resulting in partial ionic charges on each atom.

Electronegativity

nonpolar covalent: $0 \leq \delta\ \mathrm{EN} \leq 0.4$
polar covalent: $0.4 \leq \delta\ \mathrm{EN} \leq 2$
ionic: $2 < \delta\ \mathrm{EN}$

Lewis Model

The Lewis model is one of the simplest bonding theories—we will get to more advanced models later.

Bonding theories are central to chemistry because their structure often determines the properties of compounds.

In the lewis model, it's about forming octets: groups of 8 valence electrons.

There are two exceptions: Hydrogen and Helium because Helium is Hydrogen's associated noble gas, but Helium is in the 1s orbital.

Strengths and Lengths of Chemical Bonds

$$\text{triple bonds} \underset{\text{stronger}}{\overset{\text{shorter}}{\leq}} \text{double bonds} \underset{\text{stronger}}{\overset{\text{shorter}}{\leq}} \text{single bonds}$$

Concrete Example:

$$C - C \Rightarrow 346\ \mathrm{KJ/mol}$$
$$C = C \Rightarrow 602\ \mathrm{KJ/mol}$$
$$C \equiv C \Rightarrow 835\ \mathrm{KJ/mol}$$

How to Draw a Lewis Structure

1. **Calculate the total number of valence electrons in the structure**: Simply sum the valence electrons of each atom in the molecular formula. If drawing the structure of an ion, add or subtract valence electrons according to its charge.
2. **Arrange the atoms in space**: The least electronegative atom will occupy a central position, and the more electronegative atoms will occupy terminal positions, with the exception of hydrogen, which is always a terminal atom.

3. **Connect all terminal atoms to the central atom using a single bod** and then deduct the electrons used in single bonds from the total number of valence electrons.
4. **Include remaining available valence electrons as lone pairs**, first adding to terminal atoms, then adding the remaining to the central atom.
5. **Form multiple bonds by moving lone pair electrons to be bonding pairs as needed to have an octet.** (Hydrogen and helium should have a duet)
6. **Check**, make sure you have the correct total number of electrons in your final structure.

Example: CO2

1. CO_2 ⇒ $4 \cdot 1 + 6 \cdot 2 = 16$ valence electrons.

2. Arrange Atoms in Space

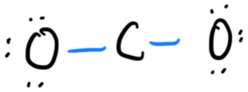
O C O

3. Add in single bonds to central atom.

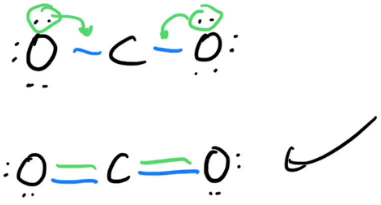
$16 - 2 \cdot 2 = 12$ e^- back

$O-C-O$

4. Include Remaining e^- as lone pairs, starting with terminal atoms.

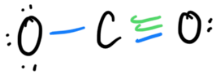


5. Form multiple bonds to form octets



preferred structure

Alternatively,



Example: CO, Clicker

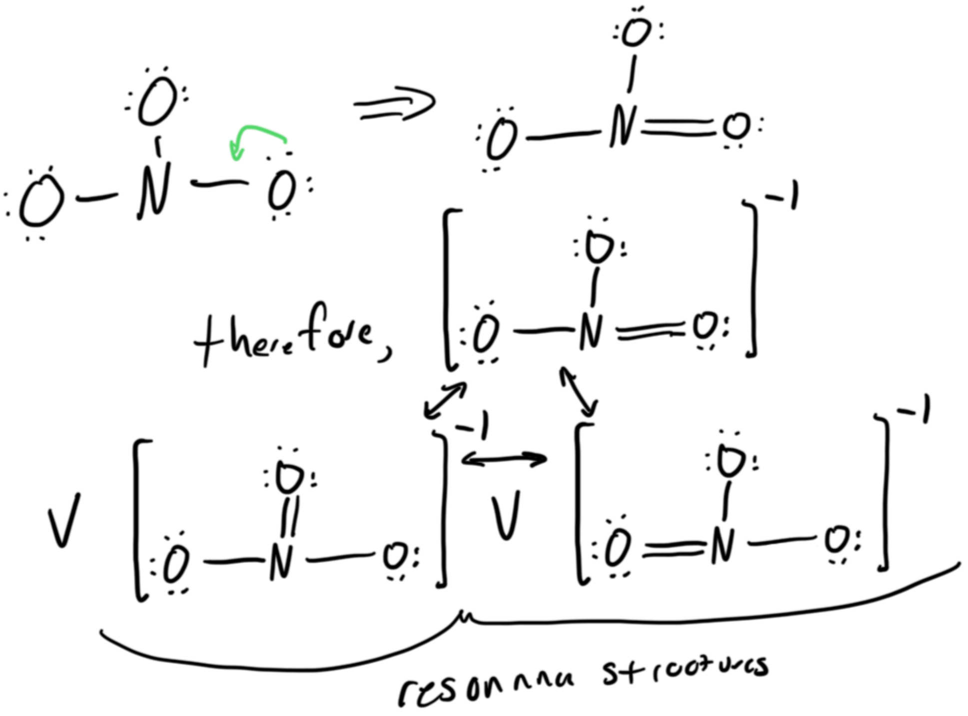
What type of bond is in carbon monoxide?

$$\begin{gathered}\text{CO} \Rightarrow 4\cdot 1 + 6\cdot 1 = 10\\ 8\cdot 1 + 8\cdot 1 = 16\\ 16 - 10 = 6 \Rightarrow \frac{6}{2} = 3 \Rightarrow \text{triple bond}\end{gathered}$$

C. Triple

Example: Nitrate, an ion

$$NO_3^- \Rightarrow 5\cdot 1 + 6\cdot 3 + 1 = 24$$

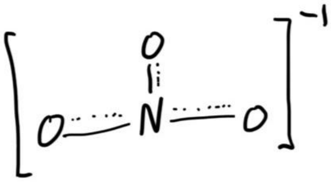


Resonance Structures

Two or more Lewis structures with atoms in the same location but different electron arrangements.

Resonance Hybrid Structure

In reality, electrons are not stuck in bonds between these atoms but are <u>delocalized</u> due to the resonance.



Formal Charge

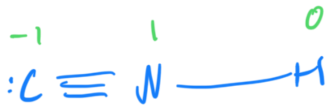
Why is one particular structure the best structure for $\mathrm{CO_2}$?

Formal charges are fictitious charges to help us decide between competing Lewis structures.

What would be the charge on each atom if all electrons in bonds were shared equally (assume no electronegativity)?

The formal charge on an atom is the number of valence electrons on the periodic table minus the nonbinding electrons and half the bonding electrons.

$$\text{Formal charge} = \#\text{ valence } e^- - \#\text{ nonbinding } e^- - \frac{1}{2}(\#\text{ bonding } e^-)$$



$C: 4 - 2 - \frac{1}{2}(6) = -1$

$N: 5 - 0 - \frac{1}{2}(8) = 0$

$H: 1 - 0 - \frac{1}{2}(2) = 0$

$N: 5 - 2 - \frac{1}{2}(6) = 0$

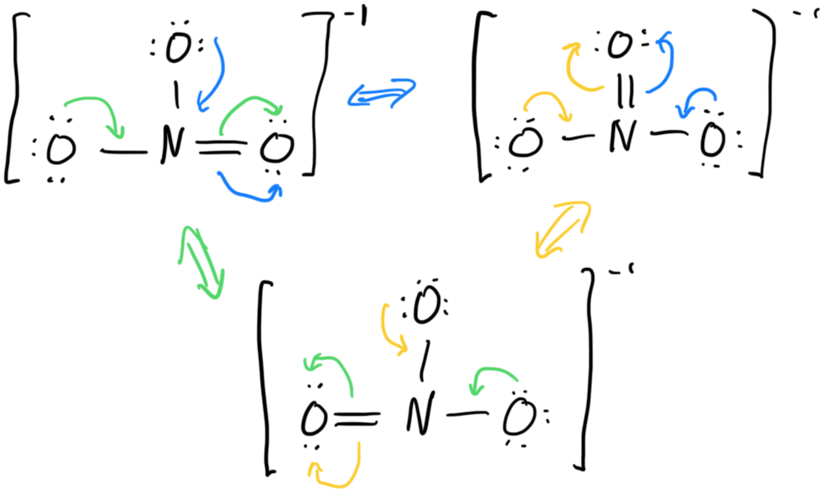
$C: 4 - 0 - \frac{1}{2}(8) = 0$

$H: 1 - \frac{1}{2}(2) = 0$

1. The sum of all formal charges in a molecule must equal the charge of the molecule or ion, respectively.
2. The best formal charge is zero on all atoms. If zero formal charge is not possible on all atoms, the closer to zero, the better.
3. When a formal charge of zero on all atoms is not possible, any negative formal charge should go on the less electronegative atom(s).

How to find the number of resonance structures

You can just try to count it or, perhaps, use curved arrows:



Alternative to indicate ions in Lewis structure

You can use nonzero formal charges. The sum of the formal charges will be the total charge of the ion.

Example

$N: 5 - 0 - \frac{1}{2}(8) = 1$

$O: 6 - 6 - \frac{1}{2}(2) = -1$

$O: 6 - 4 - \frac{1}{2}(4) = 0$

$O: 6 - 6 - \frac{1}{2}(2) = -1$

$\Sigma = -1$

(only add nonzero values to the structures)

Draw Lewis Structures

Free Radicals

Example: NO

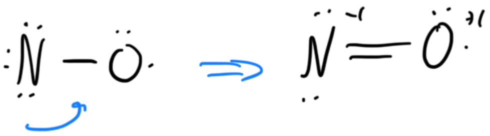
$$\text{NO} \Rightarrow 5 \cdot 1 + 6 \cdot 1 = 11\ e^- \Rightarrow$$

We will have an unpaired electron in the structure, making it a free radical.

$N: 5 - 3 - \frac{1}{2}(4) = 0$

$O: 6 - 4 - \frac{1}{2}(4) = 0$

OR



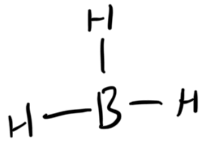
$N: 5 - 4 - \frac{1}{2}(4) = -1$

$O: 6 - 3 - \frac{1}{2}(4) = 1$

Incomplete Octets

Example BH_3

$BH_3 \Rightarrow 3\cdot 1 + 1\cdot 3 \Rightarrow 6e^-$



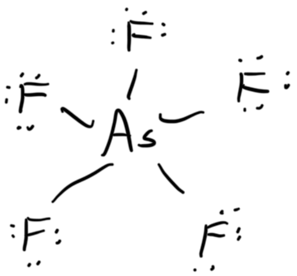
Expanded Octents

Greater than an octet of electrons around a central atom

- Common
- Only elements in the 3rd row of the periodic table and below can have expanded octets (up to 12-14 electrons are typical)

Example: $\mathrm{AsF_5}$

$AsF_5 \Rightarrow 5\cdot 1 + 5\cdot 7 = 40e^-$



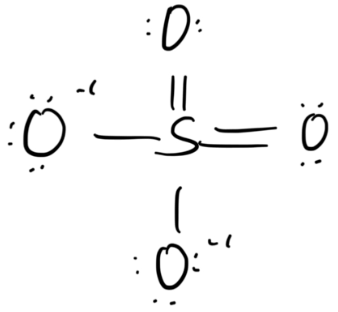
5F : 1As

∴ more than 1 octect is necessary

Example: $\mathrm{SO_4^{2-}}$

SO_4^{2-}

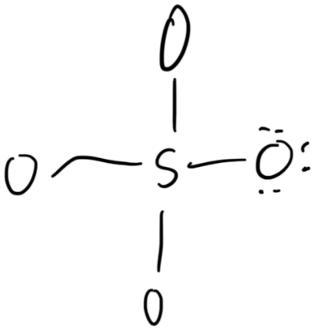
$6 + 6 \cdot 4 = 30 - 4 \cdot 2 = 22 + 2 = 24$



$O: 6 - 4 - \frac{1}{2}(4) = 0$

$S: 6 - 0 - \frac{1}{2}(12) = 6$

$O: 6 - 6 - \frac{1}{2}(1) = -1$



$S: 6 - 0 - \frac{1}{2}(8) = 2$

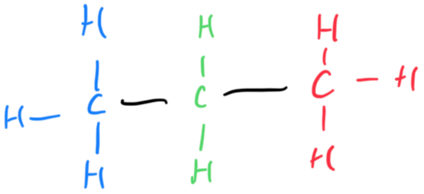
$O: 6 - 6 - \frac{1}{2}(2) = -1$

It has 6 equivalent resonance structures; rotating doesn't reduce the total.

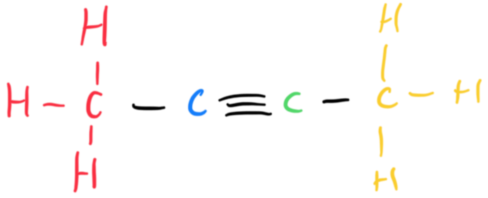
Organic Structures

See examples

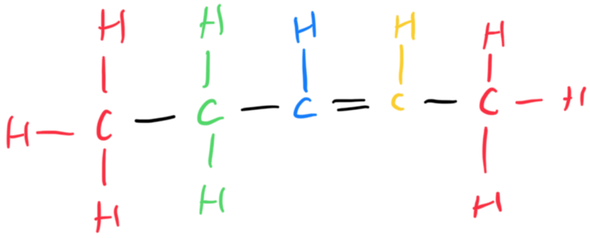
$CH_3CH_2CH_3$



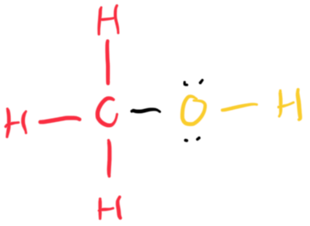
CH_3CCCH_3



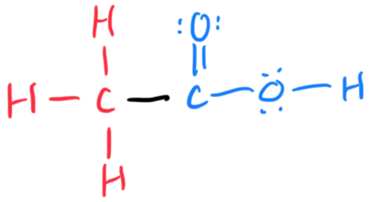
$CH_3CH_2CHCHCH_3$



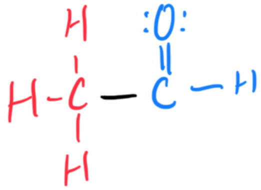
CH_3OH alcohol



$CH_3 COOH$



$CH_3 COH$



Common Patterns for Lewis structures

Carbon typically has 4 bonds and 0 lone pairs for 0 formal charge.

Oxygen typically has 2 bonds and 2 lone pairs for 0 formal charge.

Nitrogen typically has 3 bonds and 1 lone pair for 0 formal charge.

Hydrogen typically has 1 bond and 0 lone pairs for 0 formal charge.

How do molecules look in 3d?

Why does the zig-zag exist/

Lewis Theory predicts that there are regions of space around an atom that contain electrons.

VSEPR Theory (Valence Shell Electron Pair Repulsion Theory) uses the knowledge from Lewis Theory to predict how molecules look in 3D.

Specifically, because electrons are negatively charged, bonds try to be as far apart as possible from each other.

The regions of space around a central atom that are occupied by electrons are called electron groups.

Electron Group Geometries

- Electron groups repel each other and spread out
- The number of electron groups will determine the geometry.
- The shapes formed are called electron group geometries

5 basic geometries

- Two electron groups → linear
- Three electron groups → Trigonal Planar
- Four electron groups → Tetrahedral
- Five electron groups → Trigonal bipyramidal
- Six electron groups → Octahedral

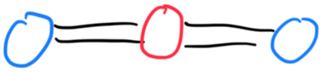
CO_2

:O=C=O:

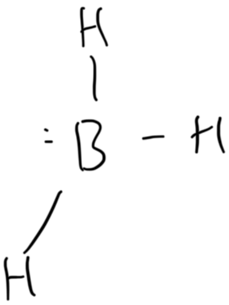
2

Linear

180°



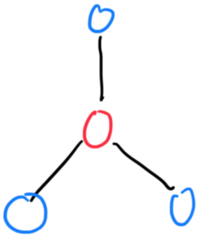
BH_3



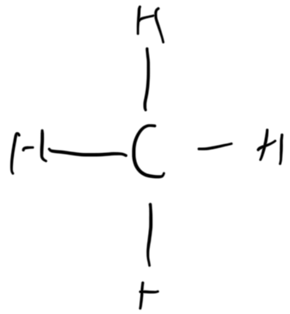
3

Trigonal planar

120°



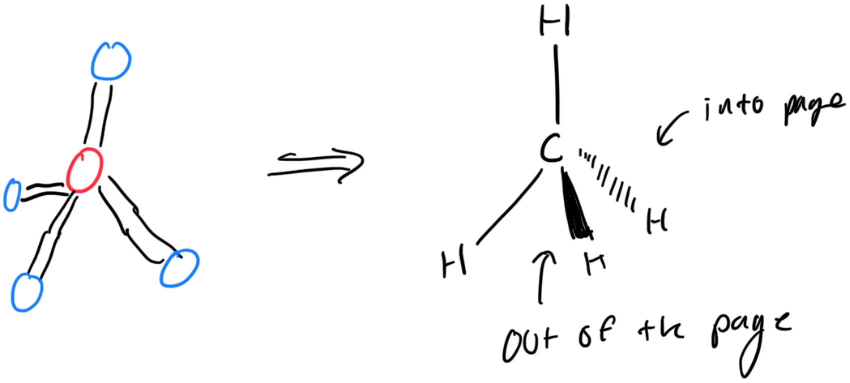
CH_4



4

Tetrahedral

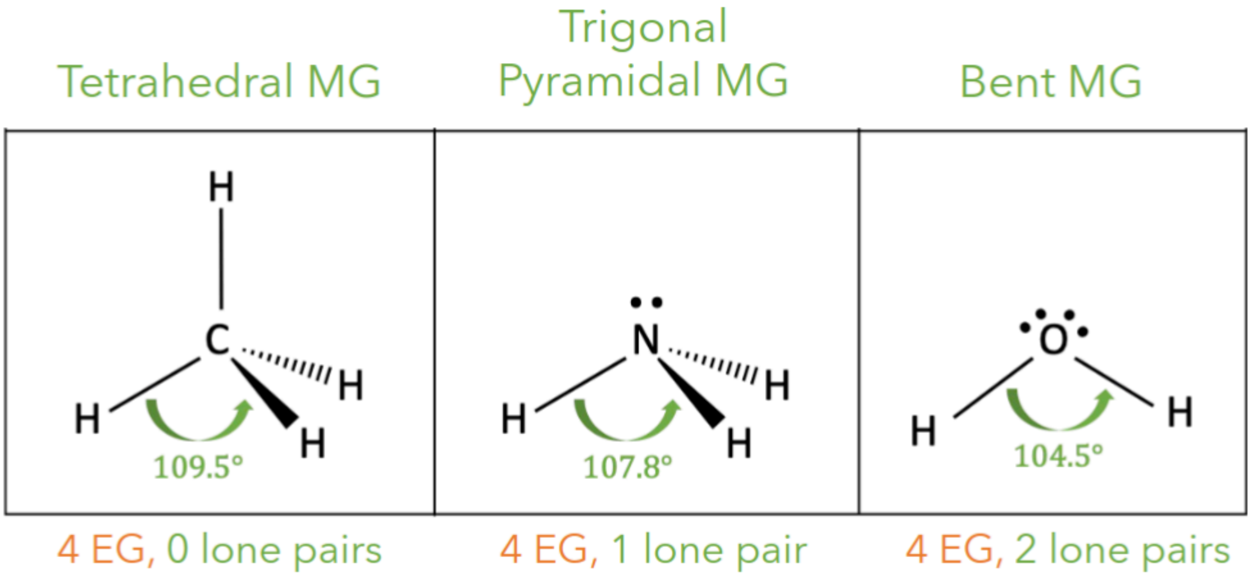
109.5°



Flaws

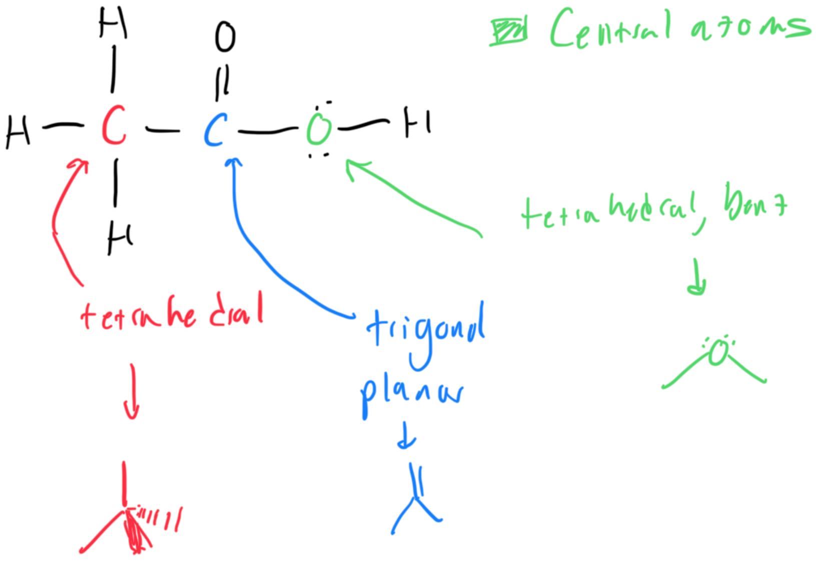
But those VSEPR shapes assume that there are no lone pairs! That isn't necessarily the case!

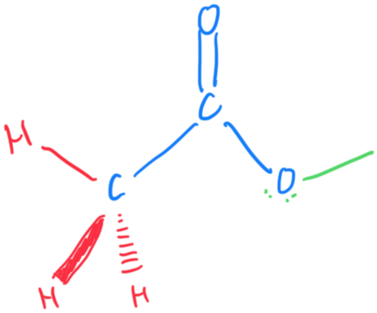
For example, tetrahedral electron geometry results in tetrahedral pyramidal molecular geometry with one lone pair and bent molecular geometry with two.



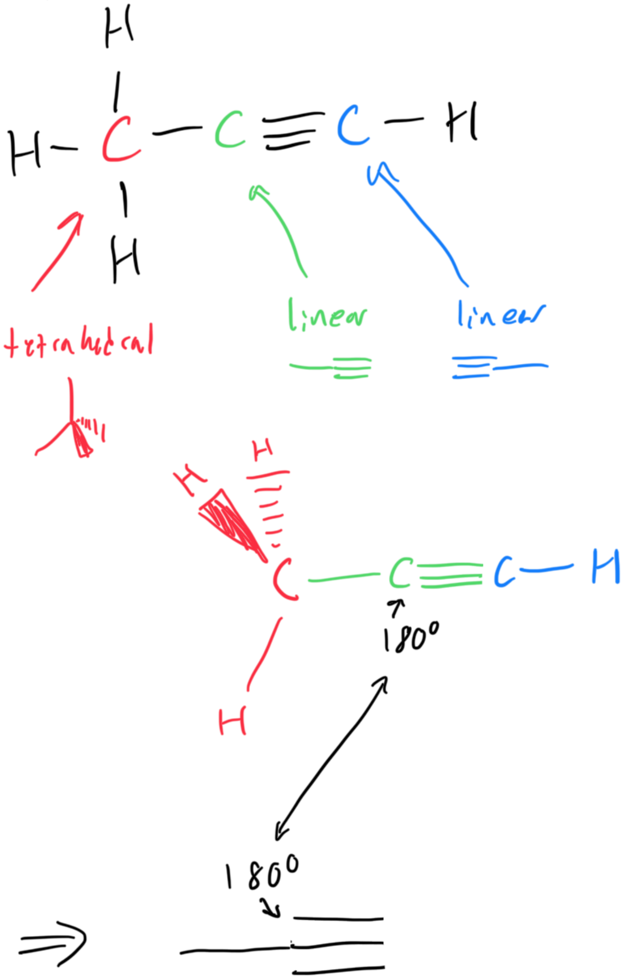
Examples

CH_3COOH : Acetic Acid

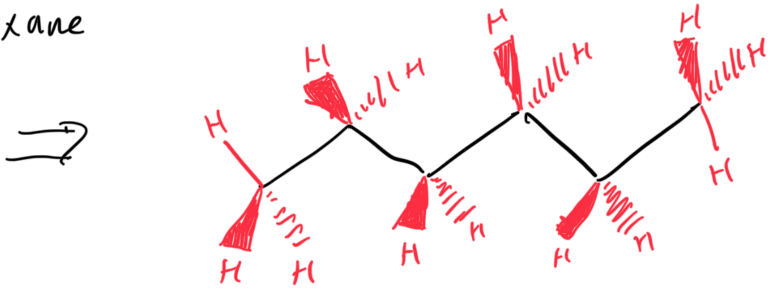




propyne:



Hexane



Still, we are missing something

Lewis Theory and VSEPR Theory still aren't explaining all aspects of electrons. They don't use atomic orbitals to explain things and, consequently, ignore quantum mechanics.

VSEPR Theory and Lewis Theory ignore the fact that electrons have wave-like properties. Introducing Valence Bond Theory to use those properties!

Valence Bond Theory

Chemical bonds result from the overlap of orbitals between 2 atoms.

The overlap results in the sharing of electrons between these two atoms.

For $\mathrm{H_2}$, because the s-orbitals overlap, you would write that as $\mathrm{H}\ (s) - \mathrm{H}\ (s)$.

Overview

As we saw in $\mathrm{H_2}$, overlapping standard atomic orbitals usually do not explain the VSEPR shapes. Instead, we will use hybrid orbitals.

Hybrid orbitals result from summing the mathematical functions that describe two or more of the atomic orbitals on one atom.

This results in a new region of space where the electron is likely to be found.

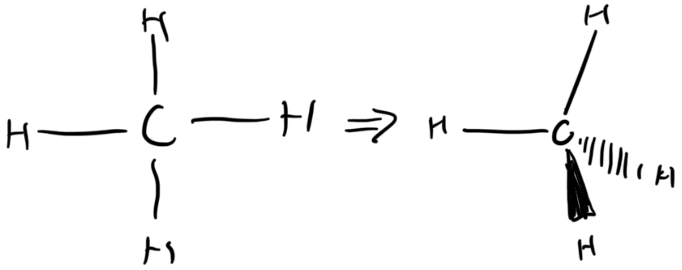
- The number of atomic orbitals combined must equal the number of hybrid orbitals formed
- The name of the hybridization tells you which orbitals were combined.

Number of electron groups	Electron Group Geometry	Hybridization
2	Linear	sp
3	Trigonal Planar	sp^2
4	Tetrahedral	sp^3
5	Trigonal Bipyramidal	sp^3d
6	Octrahedral	sp^3d^2

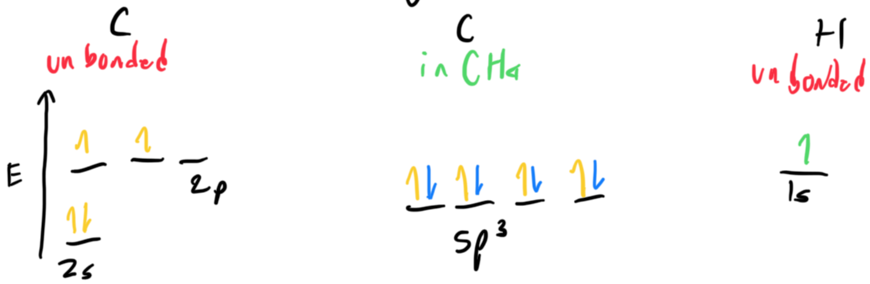
Guidelines

1. We will assume that all atoms (with the exception of hydrogen) form hybrid orbitals according to the number of electron groups that they have in the Lewis structure. The particular hybridization of an atom will be determined using the table above.
2. Hydrogen atoms will remain unhybridized and will bond through their s atomic orbital directly
3. The number of hybrid orbitals formed will equal the number of atomic orbitals mixed.
4. Chemical bonds will result from the overlap of half-filled orbitals (atomic or hybrid) between the two bonding atoms.

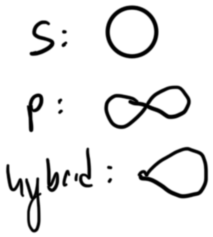
Example

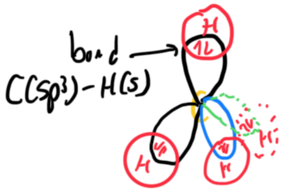


4 electron groups ⇒ sp^3 hybridization



Orbital Shapes





into the page

out of the page

sp^2 hybridization

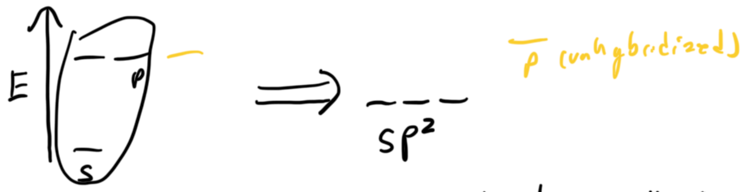
σ-bond

An orbital overlap is a head-to-head overlap of orbitals along the bonding axis. It can form between any two orbital types: hybrid orbital to hybrid orbital, hybrid orbital to standard atomic orbital, or standard atomic orbital to standard atomic orbital.

π-bond

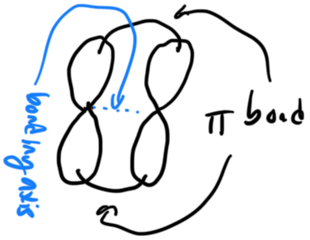
Overlap of orbitals parallel to each other but perpendicular to the bonding axis. Only p and d orbitals can participate in π bonding.

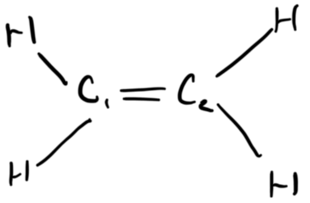
Bond Type	Composition
Single bond	one σ bond
Double bond	one σ bond, one π bond
Triple bond	one σ bond, two π bonds



2 types of orbitals results in

2 types of possible bonds





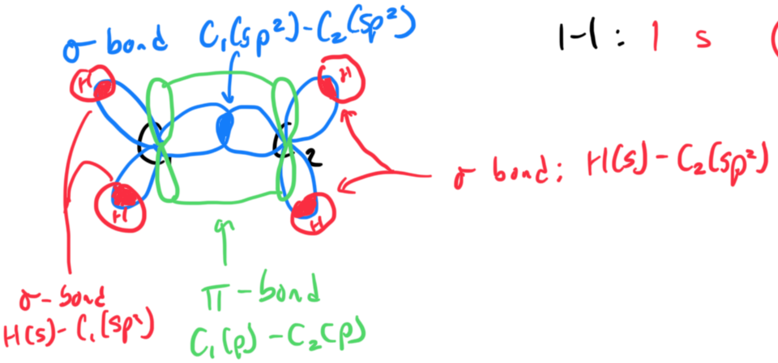
C_1: 3 sp^2 ⬭

1 p ∞

C_2: 3 sp^2 ⬭

1 p ∞

H : 1 s ○



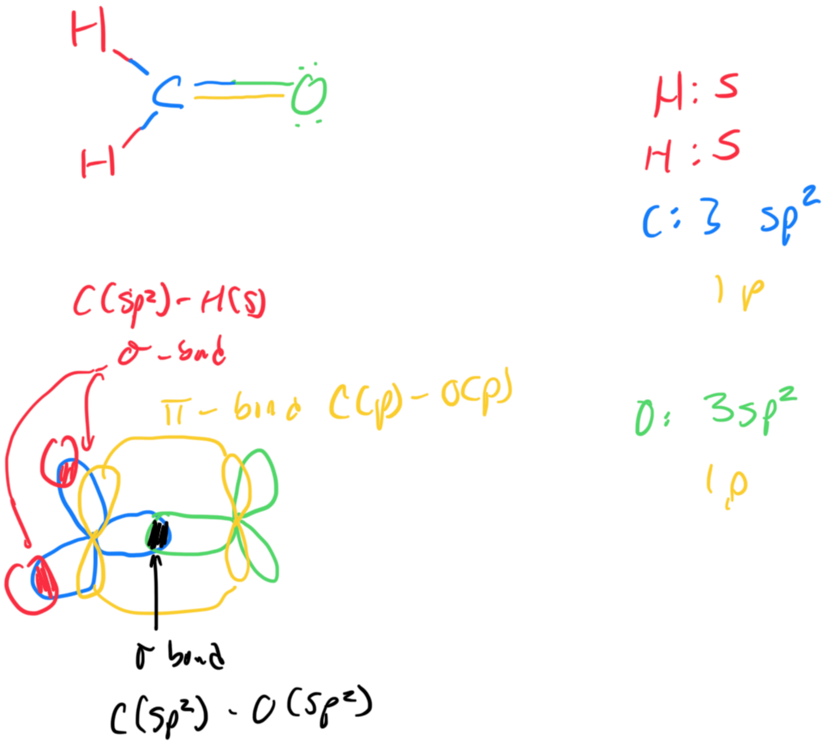
Because the π bonds are more rigid in terms of rotation, you cannot rotate the molecule about π-bonds—in contrast to σ-bonds.

sp hybridization

With two unhybridized p-orbitals, you can now make a triple bond, as you can now form two π-bonds.

“Homework” for next class

Draw the Lewis structure for $\mathrm{CH_2O}$ and list all orbital overlaps. (maybe extra credit).

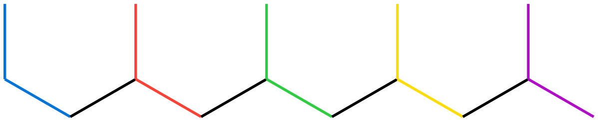


Note:

- Hybrid orbitals cannot participate in π bonding
- Hybrid orbitals overlap in σ bonds or can house lone pairs.

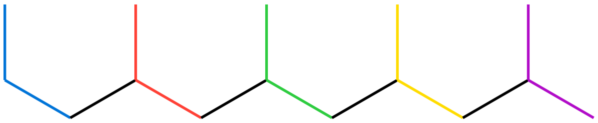
Our Polymers

PP



PLA

TODO: (this is PP right now)



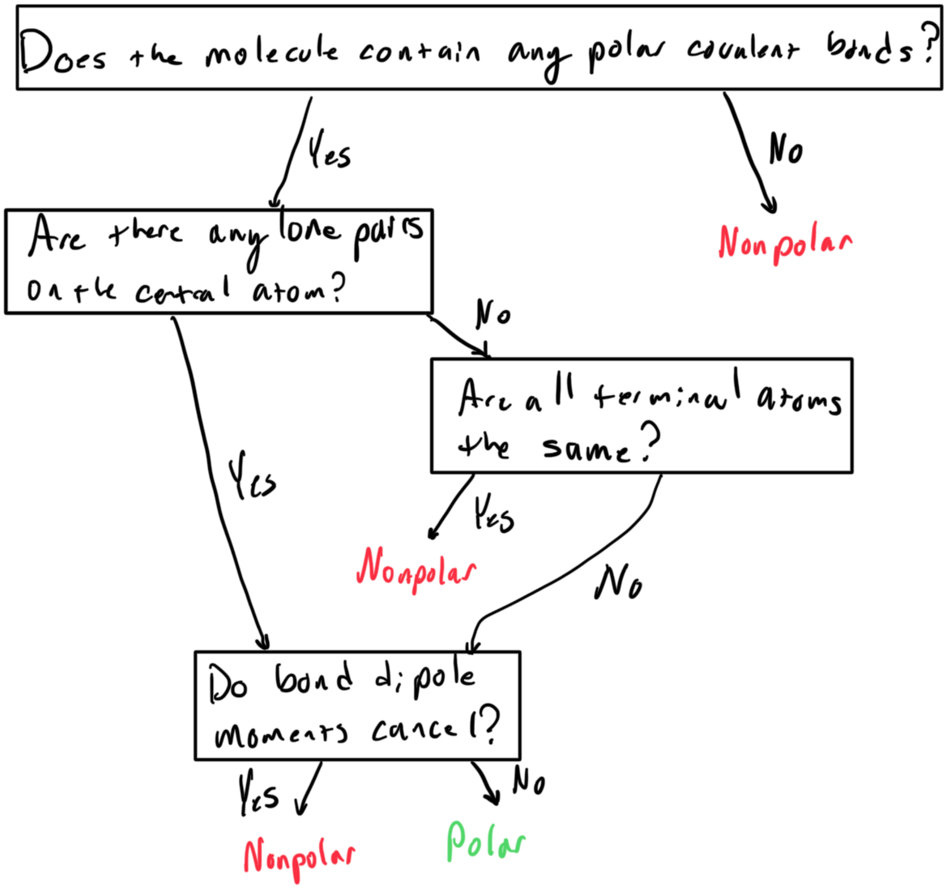
To convert between PP monomers and the full PP polymer, you have to make a double bond into the bond between the monomers.

To synthesize PLA, you make a bond to form the ester between monomers. This forms an H_2O, creating a condensation reaction. This also means the converse: to biodegrade, it needs water to break down.

This forms the first step of biodegradation: forming shorter chains through hydrolysis. It can be done without biological influences.

Why would happen? Well, remember that chemical bonds can be polar.

Molecular Dipole Moments



Dipole Moment Vector

- Direction indicates which element is more electronegative, where electrons tend to go towards.
- The length represents ΔEN

head is more electonegatve

plus is less electonegtne

$\overset{+\!\!\longrightarrow}{\text{H-Cl}} \Rightarrow \Delta EN = 3.0 - 2.1 = 0.9$

dipole moment vecter

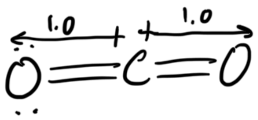
$\overset{\delta-}{\text{H}} - \overset{\delta+}{\text{Cl}}$ ∴ H-Cl H-Cl

is better than

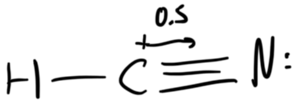
H-Cl Cl-H

becase like charges repel

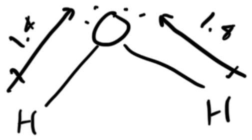
C-H bonds are considered to be nonpolar covalent bonds.



∴ nonpolar

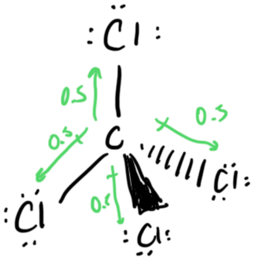


∴ polar

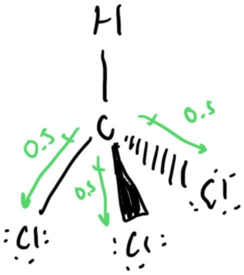


∴ polar

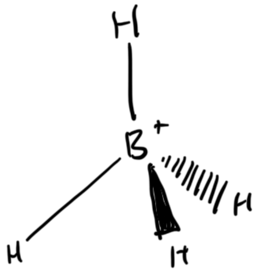
net vector ↑ 1.7



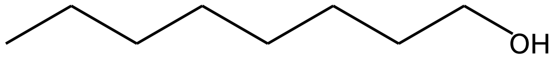
∴ non polar
all bond pull symetrically



polar
net moment ↓



Structurally nonpolar
but, because it's an
ion, treat it as polar

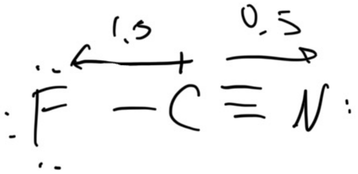


Amphipathic

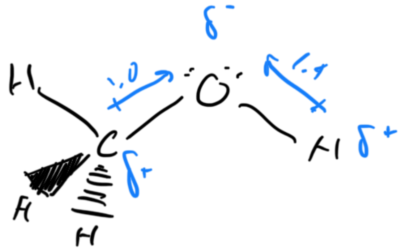
It is called this if it has both a polar and nonpolar component

Examples

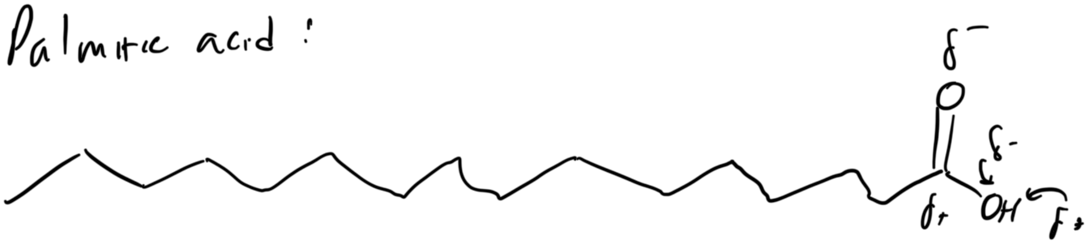
FCN:

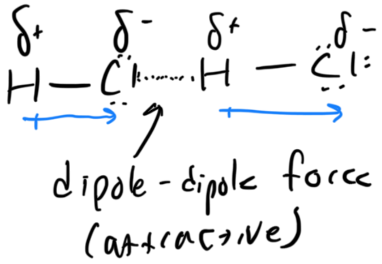


Methanol ⇒ CH_3OH



Palmitic acid :





Because PP is nonpolar and PLA is polar, the reaction between water and PLA is more favorable than the reaction between water and PP because water is also polar.

Intramolecular forces

The chemical bonds which have strong attractions between atoms in a molecule are intermolecular forces.

Intermolecular forces

The weaker forces between molecules are the intermolecular forces.

Types of intermolecular forces

- Polar Interactions
  - Ion-ion
  - Ion-dipole
  - dipole-dipole
    - Hydrogen bonding is the strongest form of dipole-dipole bonding
- Nonpolar Interactions
  - Dispersion
- Nonpolar-polar interactions
  - Dipole-induced dipole

Dipole-dipole interaction

An attractive force between two molecules with permanent dipoles.

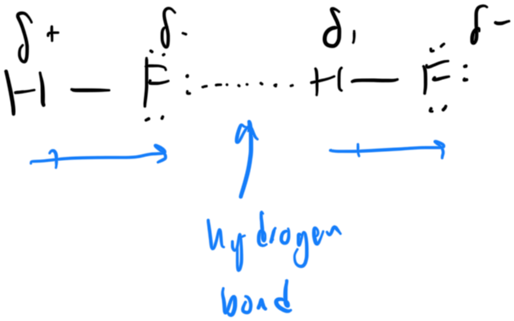
The $\partial -$ and $\partial +$ attract each other and so interact and attract.

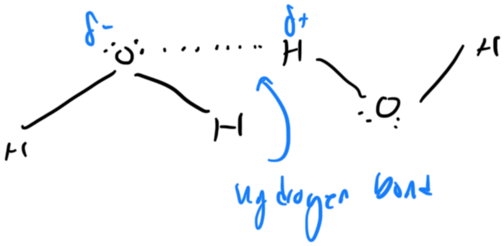
Hydrogen Bonding

If fluorine, oxygen, or nitrogen with a lone pair is near a hydrogen that is covalently bonded to fluorine, oxygen, or nitrogen, that is a hydrogen bond.

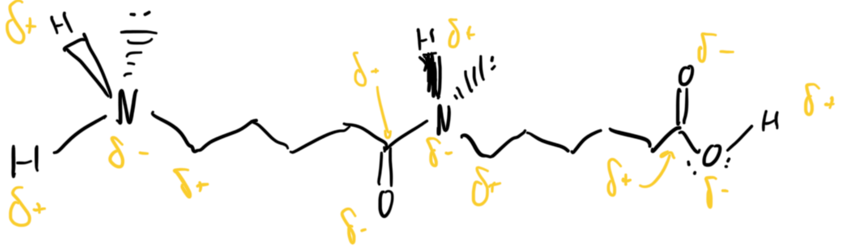
It is just a particularly strong type of dipole-dipole interaction.

The acceptor is nonhydrogen, and the donor is hydrogen.





Polar Polymer



<u>polar polymer</u>

because there are polar parts all over the place, not just at the end like an amphiporhic melecule

H-bonding and properties

The boiling point is the temperature of the liquid-gas phase transition.

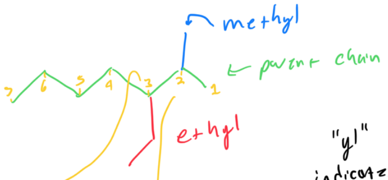
Why would H_2O, HF, and NF_3 have such high boiling points? Because of hydrogen bonds!

PLA polymers

The oxygens have $\partial -$, and the carbons connected have $\partial +$, and they will have dipole-dipole interactions. The alcohol groups will have hydrogen bonds.

Of the functional groups, esters, amides, and ethers are common linkages found in biodegradable polymers due to their ability to hydrolyze under the right conditions.

Note that not all polymers with ester, amide, or ether linkages will be biodegradable. Sometimes, they do not at all, and sometimes, it just takes too long.



3-ethyl-2-methylheptane

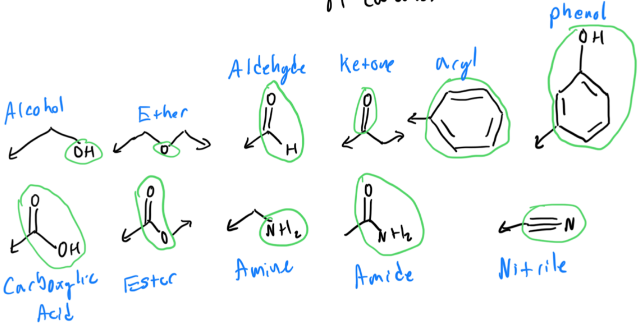
2 carbons

1 carbon

"yl" indicates a substituent group attached to the parent chain

7 carbon single bonds in the parent chain

Parent Chain:
Longest continous chain of carbons.



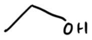
2 carbons

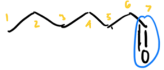
Ethanol

alchol

single bonds

⇒



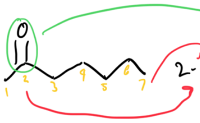


7 carbon

single bonded

heptanal

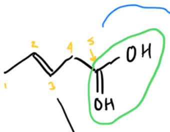
aldehyde



Ketone

2-heptanone

single bonds



pentenoic acid

double bond

pent-3-enoic acid

Why doesn't PP hydrolyze? Now, we need to know more about nonpolar intermolecular forces to analyze what will happen.

Intermolecular Nonpolar Forces

- Dispersion: actually present in all atoms and molecules, but most important for nonpolar ones
  - Weakest interaction for polar molecules
  - Varying strength for nonpolar molecules depending on size and area of interaction
- Dipole-induced dipole: interaction between a molecule with a permanent dipole and a nonpolar molecule
  - Weaker than dipole-dipole

Dispersion

Attraction between two molecules due to a momentary shift in electron density.

For example, if you have atoms that are vaguely close to each other, the electrons will interact and force each other away as like charges repel, causing a momentary shift in electron density.

They can be stronger between large molecules but weak between two small molecules.

Strength of dispersion forces

The strength of dispersion depends on polarizability. The larger the molecule, the more polarizable. The greater the surface area of interaction, the stronger the dispersion.

For example, in a tetrahedral bond, pentane will have a higher polarizability than pentane that is straight because it has a higher surface area.

Dipole-induced dipole

Like dispersion, electrons repel other electrons, and protons attract other protons, but the force is stronger because the charge differential can be higher.

PP

PP will only interact with water using the dipole-induced dipole intermolecular force, which is far weaker than the dipole-dipole force. PLA will have far stronger forces with water, which allows it to be broken down by water because the stronger interactions are more favorable.

Intermolecular force	Present between	Approximate strength ($\mathrm{kJ}\ /\ \mathrm{mol}$)
Ion-dipole	An ion and a molecule with a permanent dipole	$30 - 100 +$
Hydrogen bonding	Molecules with H bonded to F, O or N	$10 - 40$
Dipole-dipole	Two molecules with permanent dipoles	$5 - 25$
Dispersion	All molecules	$0.05 - 40$

Sutures

Sutures are what are used to stitch wounds.

- Absorbable ones are those that naturally break down in your body
- Non-absorbable ones don't break down and must be removed.

Monofilament/braided

Braided is stronger but more abrasive.

In-class activity

Hydrogen bonds are everywhere, and some of the partial positive carbons also bond despite their distance.

Combustion

With your group, make a bulleted list of questions that you need answered to answer the focus question, “How does gasoline make your car go?”:

1. Why does gasoline explode?
2. Why use gasoline over other substances like diesel or hydrogen gas?

The questions they provide are:

1. Where does the gas go?
2. What is gasoline?
3. What does it mean to “burn” fuel? What is actually happening?
4. How is energy from “burning” the gas in the car used to make the car move?

First of all, what is C_8H_{18}? It can be many different types of isomers, including octane.

Gasoline is a mixture of hydrocarbons. It is mixed with air in the cylinder of the car and then has a reaction, giving out energy.

Combustion reaction

They are reactions in which a substance reacts with O_2 to produce one or more oxygen-containing compounds.

- Combustion of a hydrocarbon always results in H_2O and CO_2. Carbon dioxide is always a gas, and water is usually a gas.
- They are exothermic reactions (produce heat as a product.)

Activity 1

1. Write the balanced reaction for the combustion of liquid octane.

$$\mathrm{C_8H_{18}} + \quad \mathrm{O_2} \rightarrow \quad \mathrm{CO_2} + \quad \mathrm{H_2O}$$

$$\text{Assume 1 for octane}$$

$$1\mathrm{C_8H_{18}} + \quad \mathrm{O_2} \rightarrow 8\mathrm{CO_2} + 9\mathrm{H_2O}$$

$$\text{But } \mathrm{O_2} \text{ can't work here, so multiply all by 2 and now } \mathrm{O_2} \text{ can work.}$$

$$2\mathrm{C_8H_{18}} + 25\mathrm{O_2} \rightarrow 16\mathrm{CO_2} + 18\mathrm{H_2O}$$

2. How many moles of oxygen are needed to completely react with $0.028\ \mathrm{mL}$ of octane?

$$0.028\ \mathrm{mL} \times \frac{0.702\ \mathrm{g}}{1\ \mathrm{mL}} \times \frac{1\ \mathrm{mol}}{114.23\ \mathrm{g}} \times \frac{1}{2} \times 25 = 0.021\,5\ \mathrm{mol}$$

3. The cylinder in your car engine contains 1.45×10^{-4} moles of octane and 2.20×10^{-3} moles of oxygen O_2. What mass in grams of CO_2 can be produced?

$$\begin{aligned} C_8H_{18}: &\quad 1.45 \times 10^{-4} \text{ mol octane} \times \frac{1}{2 \text{ mol octane}} = 7.25 \times 10^{-5} \\ O_2: &\quad 2.20 \times 10^{-3} \text{ mol oxygen} \times \frac{1}{25 \text{ mol oxygen}} = 8.80 \times 10^{-5} \end{aligned}$$

$$\Rightarrow 7.25 \times 10^{-5} \text{ is the minimum base mols}$$

$$7.25 \times 10^{-5} \times 16 \text{ mol carbon dioxide} \times 44.01 \text{ g/mol} = 5.11 \times 10^{-2} \text{ g}$$

What does it mean to burn

Burning fuel just means that it is reacting in a combustion reaction. These reactions are exothermic (produce heat).

Thermochemistry

The study of energy changes in chemical reactions, particularly those involving heat.

Thermochemical reactions will have heat as a part of the equation:

$$2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O + \text{heat}$$

1st Law of Thermodynamics

Conversation of energy: energy is neither created nor destroyed.

It can be converted from one form to another:
- Potential energy → kinetic energy
- Chemical energy → heat

Breaking bonds requires an input of energy, and making bonds releases energy to its surroundings.

Heat and Work

Energy can be transferred as heat or work.

Heat is a transfer of energy due to a difference in temperature.

Heat transfers energy through a difference in temperature. Heat always flows from the warmer object to the cooler object.

Work is a transfer of energy due to a force exerted over a distance. In this class, we are interested in PV work (presumably pressure-volume?), work done due to the compression or expansion of a gas.

Heat

Endothermic process: heat enters the system, $q > 0$
Exothermic process: heat leaves the system, $q < 0$

Work

Work is done on the system, $w > 0$
The system does work, $w < 0$

Combustion engines generate a lot of heat. Some of that heat is used to power the car, but there is also wasted heat from both the combustion reaction and friction from the moving parts.

Coolant will distribute heat by moving it from the engine to the radiator. But why use (mostly) water?

Specific Heat Capacity

The quantity of heat required to raise the temperature of $1\ \mathrm{g}$ of a substance by $1°\mathrm{C}$.

$q = mC_s\Delta T$

Substance	Specific heat capacity C_s in $\frac{J}{\mathrm{g}\ °\ \mathrm{C}}$
Water (l)	4.184
Water (g)	2.08
Water (s)	2.11
Ethanol (l)	2.44
Copper (s)	0.385
⋮	

Practice

A $37.0\ \mathrm{g}$ cube of aluminum at $87.5°\mathrm{C}$ is placed in a cup containing $165\ \mathrm{g}$ of liquid water at $35.8°\mathrm{C}$. What is the temperature of the water after the aluminum cube has been added?

Solution

Because the aluminum is hotter, the heat will go from the aluminum to the water.

$$-q_{\mathrm{Al}} = q_{\mathrm{H_2O}}$$

$$-m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}\left(T_f - T_{i,\ \mathrm{Al}}\right) = m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}}\left(T_f - T_{i,\mathrm{H_2O}}\right)$$

$$-m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}T_f + m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}T_{i,\ \mathrm{Al}} = m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}}T_f - m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}}T_{i,\mathrm{H_2O}}$$

$$m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}T_{i,\ \mathrm{Al}} + m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}}T_{i,\mathrm{H_2O}} = m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}}T_f + m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}T_f$$

$$m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}T_{i,\ \mathrm{Al}} + m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}}T_{i,\mathrm{H_2O}} = \left(m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}} + m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}\right)T_f$$

$$\frac{m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}T_{i,\ \mathrm{Al}} + m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}}T_{i,\mathrm{H_2O}}}{m_{\mathrm{H_2O}}C_{s,\mathrm{H_2O}} + m_{\mathrm{Al}}C_{s,\ \mathrm{Al}}} = T_f$$

$$\boxed{37.7°\mathrm{C} = T_f}$$

Change in Enthalpy ΔH

Many chemical reactions are performed under constant pressure conditions, so the heat required or produced is equal to the change in enthalpy:

$q_p = \Delta H_{\mathrm{reaction/rxn}}$

Calculating ΔH_{rxn}

You can estimate it using bond energies (not used in this class).

Alternatively, calculate ΔH_f^o via the standard heats of formation.

This requires reactants to be in their standard states:

- Gas: pure gas at $1\ \mathrm{atm}$
- Liquid/solid: pure substance in the most stable form at $1\ \mathrm{atm}$ and $25°\mathrm{C}$
- Solution: the concentration is 1 molar ($\frac{\mathrm{mol}}{\mathrm{m}^3}$).

From this, you can calculate the $\Delta H^o_{\mathrm{rxn}}$:

$$\mathrm{CH_4}(g) + 2\mathrm{O_2}(g) \to 2\mathrm{H_2O}\ (g) + \mathrm{CO_2}(g)$$

$$\Delta H^o_{\mathrm{rxn}} = 2\Delta H^o_f(\mathrm{H_2O}) + \Delta H^o_f(\mathrm{CO_2}) - \left(\Delta H^o_f(\mathrm{CH_4}) + 2\Delta H^o_f(\mathrm{O_2})\right)$$

$$= 2\left(-241.8\frac{\mathrm{kJ}}{\mathrm{mol}}\right) + 1\left(-393.5\frac{\mathrm{kJ}}{\mathrm{mol}}\right) - \left(1\left(-74.6\frac{\mathrm{kJ}}{\mathrm{mol}}\right) + 2\left(0\frac{\mathrm{kJ}}{\mathrm{mol}}\right)\right) = -802.5\frac{\mathrm{kJ}}{\mathrm{mol}}$$

The negative symbol indicates that it is an exothermic reaction

We will get $802.5\ \mathrm{kJ}$ of heat if $1\ \mathrm{mol}\ \mathrm{CH_4}$ reacts with $2\ \mathrm{mol}\ \mathrm{O_2}$.

Therefore, the mols are for per mole of reaction.

This can be interpreted as:

$$\frac{-802.5\ \mathrm{kJ\ heat}}{1\ \mathrm{mol\ CH_4}} \text{ or } \frac{-802.5\ \mathrm{kJ\ heat}}{2\ \mathrm{mol\ O_2}} \text{ or } \frac{-802.5\ \mathrm{kJ\ heat}}{1\ \mathrm{mol\ CO_2}} \text{ or } \frac{-802.5\ \mathrm{kJ\ heat}}{2\ \mathrm{mol\ H_2O}}$$

So,

$$\mathrm{g\ O_2} \xrightarrow{\text{molecular weight}} \mathrm{mol\ O_2} \xrightarrow{\Delta H^o_{\mathrm{rxn}}} \mathrm{kJ\ heat}$$

$$6.47\ \mathrm{g\ O_2} \times \frac{1\ \mathrm{mol\ O_2}}{32\ \mathrm{g\ O_2}} \times \frac{-802.5\ \mathrm{kJ\ heat}}{2\ \mathrm{mol\ O_2}} = -81.1\ \mathrm{kJ\ of\ heat}$$

Activity 2

1. Using standard heats of formation, calculate the standard change in enthalpy for the combustion of liquid octane.

Balanced equation:

$$2\mathrm{C_8H_{18}}(l) + 25\mathrm{O_2}(g) \to 16\mathrm{CO_2}(g) + 18\mathrm{H_2O}(g)$$

Calculate $\Delta H^o_{\mathrm{rxn}}$:

$$\Delta H^o_{\mathrm{rxn}} = 16(-393.5) + 18(-241.8) - (2(-250.3) + 25(0)) = -10\,147.8 \approx -10.15 \times 10^3 \frac{\mathrm{kJ}}{\mathrm{mol\ rxn}}$$

2. If the fuel injector in your car sprays $0.028\ \mathrm{ml}$ of octane into the cylinder, how much heat is produced? For this question, assume the octane reacts completely.

$$0.028\ \mathrm{ml\ octane} \times \frac{0.702\ \mathrm{g\ octane}}{\mathrm{ml\ octane}} \times \frac{1\ \mathrm{mol\ octane}}{114.23\ \mathrm{g\ octane}} \times \frac{1\ \mathrm{mol\ rxn}}{2\ \mathrm{mol\ octane}} \times \frac{-10\,147.8\ \mathrm{kJ}}{1\ \mathrm{mol\ rxn}} = -0.87\ \mathrm{kJ\ of\ heat}$$

Chapter 9:

Properties of gases

- No definite shape or volume
- uniformly fills any container
- exerts pressure on surroundings via collisions
- change volume dependent on temperature and pressure.
- miscible: they mix together in any proportion
- much less dense than solids or liquids

$P = \frac{F}{A} = \frac{ma}{A}$

Ideal Gases

- The volume of the individual gas molecules is so small that compared with the overall volume of the container it's negligible
- The individual gas molecules/atoms do not interact with each other with intermolecular forces (they can still bounce off each other)

Unit	Pa	atm	torr	mmHg	inHg	psi
Pa	1	9.869×10^{-6}	7.501×10^{-3}	7.501×10^{-3}	2.953×10^{-4}	1.450×10^{-4}

$P_{\text{atm}} \propto m$ (pressure at any altitude is proportional to the mass of air above that location)

Atmospheric pressure at sea level is $1\ \text{atm}$. If the mass of the atmosphere at the elevation of the Mile High City is $4.38 \times 10^{18}\ \text{kg}$ and the surface area of the Earth is $5.1 \times 10^{14}\ \text{m}^2$, what is the atmospheric pressure (in atm) in Denver, CO?

$$P = \frac{ma}{A} = \frac{mg}{A} = \frac{(4.38 \times 10^{18}\ \text{kg})(9.8\frac{\text{m}}{\text{s}^2})}{5.1 \times 10^{14}\ \text{m}^2} \times \frac{1\ \text{atm}}{101\,325\ \text{Pa}} = 0.83\ \text{atm}$$

The gas laws

$$P = \text{pressure}$$
$$V = \text{volume}$$
$$n = \text{amount of substance}$$
$$T = \text{temperature}$$

Boyles Law: $P \propto \frac{1}{V}$
Charles's Law: $T \propto V$
Avogadro's Law: $n \propto V$

In sum: $PV = nRT$ where R is a constant (the ideal gas constant)

Forming the Ideal Gas Law

$$\begin{aligned} \text{Boyle's Law} &: P \propto \frac{1}{V} \\ \text{Charles's Law} &: V \propto T \\ \text{Avogadros's Law} &: n \propto V \\ \text{Amonton's Law} &: T \propto P \end{aligned}$$

Our goal is to put these together into one expression:

$$\begin{aligned} V \propto T \land n \propto V &\quad \Rightarrow V \propto nT \\ V \propto nT \land T \propto P &\quad \Rightarrow PV \propto nT \end{aligned}$$

$$PV = \mathbb{c}_1 nT$$

$$\Rightarrow \underbrace{\boxed{PV = nRT}}_{\text{Ideal Gas Law}}$$

$$R = 0.082\,06 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{°K}}$$

R is the universal gas constant

Example

Calculate the pressure of $1.2\ \text{mol}$ of methane gas in a $3.3\ \text{L}$ container at 25°C.

$$\begin{aligned} n &= 1.2\ \text{mol} \\ V &= 3.3\ \text{L} \\ T &= 25\text{°C} \approx 298\ \text{K} \end{aligned}$$

$$\Rightarrow P = \frac{nRT}{V} = (1.2\ \text{mol})\left(0.082\,06 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot \text{°K}}\right)\frac{298\text{°K}}{3.3\ \text{L}} = 8.9\ \text{atm}$$

$$\text{Initial State} : P_1 V_1 = n_1 R T_1$$

$$\text{Final State} : P_2 V_2 = n_2 R T_2$$

$$\Rightarrow R = \frac{P_1 V_1}{n_1 T_1} \land R = \frac{P_2 V_2}{n_2 T_2}$$

$$\Rightarrow \underbrace{\boxed{\frac{P_1 V_1}{n_1 T_1} = \frac{P_2 V_2}{n_2 T_2}}}_{\text{combined gas law}}$$

Clicker

$$\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2}$$
$$\frac{P_1}{T_1} = \frac{P_2}{T_2}$$
$$\frac{P_1}{T_1} = \frac{P_1 - \Delta}{T_2}$$
$$\frac{P_1T_2}{T_1} = P_1 - \Delta$$
$$P_1 - \frac{P_1T_2}{T_1} = \Delta$$
$$P_1\left(1 - \frac{T_2}{T_1}\right) = \Delta$$
$$13.5 \text{ psi} \times 0.046\,758 = \Delta$$
$$0.631\,235 \text{ psi} \neq 2 \text{ psi}$$

STP (Standard Temperature and Pressure)

$$T = 0°\text{C}$$
$$P = 1 \text{ atm}$$

Mixures of Gas

Compound	% composition (moles)
N_2	78%
O_2	21%
Ar	0.93%
Other (CO_2, Ne, CH_4, etc)	$< 0.07\%$

Dalton's Law of partial pressures

$$P_{\text{total}} = \sum_n \underbrace{P_n}_{\text{partial pressures}} = P_1 + P_2 + P_3 + \cdots + P_n$$

For example:

$$P_{\text{atm}} = P_{N_2} + P_{O_2} + P_{Ar} + \cdots$$

Partial Pressure due to one component in a mixture:

$$P_{N_2} = \frac{n_{N_2}RT}{V}$$

$$\frac{P_1}{P_{\text{total}}} = \frac{n_1}{n_{\text{total}}} = \underbrace{\chi_1}_{\text{mole fraction}}$$

The mole fraction is the ratio of the number of moles of a component in a mixture to the total number of moles.

$$\frac{P_1}{P_{\text{total}}} = \chi_1 \Longrightarrow P_1 = \chi_1 P_{\text{total}}$$

Example

Air is 21% O_2. If we have $1.00\ \text{L}$ of air at $298°\text{K}$ in Denver, CO ($P_{\text{atm}} = 0.83\ \text{atm}$):

1. What is P_{O_2}?

$$21\% \Rightarrow \chi_{O_2} = 0.21$$

$$P_{O_2} = \chi_{O_2} P_{\text{total}} = \chi_{O_2} P_{\text{atm}} = (0.21)(0.83\ \text{atm}) = \boxed{0.174\,3\ \text{atm}}$$

2. How many moles of O_2 are in the container?

$$n_{O_2} = \frac{P_{O_2} V}{RT} = \frac{(0.174\,3\ \text{atm})(1.00\ \text{L})}{\left(0.082\,06 \frac{\text{L} \cdot \text{atm}}{\text{mol} \cdot °\text{K}}\right)(298°\text{K})} = 0.007\,1\ \text{moles}\ O_2$$

Activity

1. Air is taken into your car's cylinder to an initial volume of $55.0\ \text{mL}$ at $298°K$ and atmospheric pressure. At sea level, how many moles of oxygen will then be present in the cylinder?

$$n_{O_2} = \frac{\chi_{O_2} P_{\text{atm}} V}{RT} = 4.72 \times 10^{-4}\ \text{mol}\ O_2$$

2. What volume of octane should be injected into the cylinder, given your calculation in question 1?

$$n_{O_2} \times \frac{2\ \text{mol octane}}{25\ \text{mol}\ O_2} \times \text{MW}_{\text{octane}} \times \frac{1}{d_{\text{octane}}} = 0.006\,15\ \text{mL}$$

Where does the gas go?

1. Air and fuel go into the combustion chamber through the input value
2. The spark plug ignites the air/fuel mixture, prompting a combustion reaction
3. The hot gas expands, moving the piston down.
4. Combustion products are expelled from the cylinder through the exhaust

Our simplifying assumptions

Ignore the intake and compression strokes and assume that air is taken into the cylinder at its minimum volume (55.0 mL) (the volume as it is in the power stroke). Assume the combustion reaction occurs instantaneously and produces heat at constant pressure.

Calculating the heat produced in the cylinder

From a previous activity,

$$\Delta H = -10\,147.8\ \frac{\text{kJ}}{\text{mol rxn}}$$

Furthermore, the cylinder contains:

$$4.72 \times 10^{-4} \text{ mol } \mathrm{O_2}$$

$$4.72 \times 10^{-4} \text{ mol } \mathrm{O_2} \times -10\,147.8 \ \frac{\text{kJ}}{\text{mol rxn}} = -0.192 \text{ kJ of heat}$$

What happens to the heat

Oxygen is the only thing that reacted with the gasoline—all the other parts of air and the combustion products are still left. Therefore, they will absorb the heat.

1. The combustion reaction produces heat
2. The heat is transferred to the remaining molecules: they absorb heat.
3. Those gas phase molecules experience an increase in temperature according to $q = mC_s\Delta T$
4. Using the combined gas law,

$$\frac{P_1V_1}{n_1T_1} = \frac{P_2V_2}{n_2T_2} \Rightarrow \frac{V_1}{T_1} = \frac{V_2}{T_2}$$

   Therefore, the gas increases in volume.

Activity

If there are $0.071\,7$ g of gas-phase molecules remaining in the cylinder after combustion, what change in volume does the cylinder experience when those molecules absorb the 0.192 kJ of heat from the combustion reaction, given that the specfic heat of these gas-phase molecules is $1.012\frac{\mathrm{J}}{\mathrm{g \cdot K}}$.

$$q = mC_s\Delta T \Rightarrow \frac{q}{mC_s} = \Delta T$$

$$\frac{V_1}{T_1} = \frac{V_1 + \Delta V}{T_1 + \Delta T} \Rightarrow \frac{V_1(T_1 + \Delta T)}{T_1} = V_1 + \Delta V$$

$$V_1 + \frac{V_1\Delta T}{T_1} = V_1 + \Delta V$$

$$\frac{V_1\Delta T}{T_1} = \Delta V$$

$$\frac{V_1 q}{mC_sT_1} = \Delta V$$

$$\begin{cases} q = 192 \text{ J} \\ V_1 = 55 \text{ mL} \\ m = 0.071\,7 \text{ g} \\ C_s = 1.012 \text{ J / g} \cdot \text{K} \\ T_1 = 298 \text{ K} \end{cases}$$

$$\Rightarrow \qquad \Delta V = 488 \text{ mL}$$

2. Now, take a step back and summarize in words with your group how gasoline makes your car go. Make a numbered list of events and associate them with any equations that you now know can be applied.
   1. Gasoline and air enter the combustion chamber
   2. A spark plug ignites the gasoline

3. The gasoline makes an explosion, thereby increasing the volume
    1. Can use stoichiometry, change in enthalpy, and the ideal gas law
4. The volume increasing turns the drive shaft
5. The drive shaft transfers power to the wheels, and the car moves forward.
6. The engine exhausts the waste products and brings new air and gasoline into the engine, and the process repeats.

Waste Water Treatment

Clean water

71% of the surface is covered with water, but less than 1% of that water can be used as drinking water.

Contaminated water is a problem: it can cause cholera, dysentery, and more.

But why isn't this a problem in the US? The US has regulated wastewater treatment, but other places may not.

The ground usually filters contaminants, but when the population gets too high, it cannot filter everything.

Why are there contaminants in the first place? Shit, tire wear, acid rain, pesticides, fertilizers, industrial waste, etc.

Where does wastewater go?

Wastewater treatment plants supplement what nature does: it removes enough contaminants that nature can take care of the rest.

Stage 1: Pretreatment

Its goal is to remove larger debris through screens and grit chambers. This is then collected and moved to a landfill.

Stage 2: Primary Treatment

After larger debris has been removed, the wastewater moves to primary clarifiers.

Water flows through these tanks so:

- Dense, larger particulate matter falls to the bottom (sludge)
- Less dense contaminants float to the top (scum)
- The remaining liquid in the center, effluent flows out for further treatment

But why do particular particulates float up?

Through density and intermolecular forces.

Intermolecular Forces

- Polar Interactions
    - Ion-ion
    - Ion-dipole
    - dipole-dipole
        - Hydrogen bonding is the strongest form of dipole-dipole bonding

- Nonpolar Interactions
    - Dispersion
- Nonpolar-polar interactions
    - Dipole-induced dipole

Ion-ion interactions

Ion-ion force: the attractive force between two ions of opposite charge. The ion force scales through Coulomb's Law:

$$F = \frac{kq_1q_2}{r^2}$$

Ion-dipole interaction

Ion-dipole force: the attractive force felt between an ion and a molecule with a permanent dipole.

Which of those is stronger?

It depends on the ionic compound you're trying to dissolve.

If something dissolves in water (soluble), the ion-dipole forces are stronger than the ion-ion forces, and if something doesn't dissolve in water (insoluble), the ion-ion force is stronger.

How does this affect clarifiers?

The nonpolar, less dense molecules will go to the top, and the nonpolar, denser molecules will go to the bottom.

The polar molecules will be more in the middle/effluent layer.

Clickers

Where would soap go? In between!

This is because dipole-induced dipole is the strongest IM force to water on the tail of the soap, but ion-dipole is the strongest on the head of the soap, so it straddles the border.

Stage 3: Secondary Treatment

Aeration basins break down dissolved organic matter into smaller molecules and ions such as $\mathrm{CO_2}$, nitrates and phosphates. This is done by having bacteria use the oxygen in the air to digest the dissolved organic materials.

Stage 4: Disinfection

Use chlorination, ozone treatment, or UV treatment to kill the bacteria in the water.

Class is online, recorded lectures.

Clicker Question

The double headed arrows represent intermoelecular forces between the indicated molecules/ion. Which interaction is strongest?

1. $\mathrm{Ba^{2+}} \leftrightarrow \mathrm{SO_4^{2-}}$
2. $\mathrm{Ba^{2+}} \leftrightarrow \mathrm{H_2O}$
3. $\mathrm{SO_4^{2-}} \leftrightarrow \mathrm{H_2O}$

4. $H_2O \leftrightarrow H_2O$
5. Two of these are strongest

1. is the strongest because $BaSO_4$ is insoluble, and therefore its intermolecular force ion-ion is stronger than hydrogen bonding.

Stage 5: Effluent Release

You simply release it into the natural environment. But is this enough? Is the water clean enough to not harm the environment?

Maybe not. After aerobic digestion in the secondary treatment processes, two of the primary products remaining are nitrates and phosphates, two inorganic ions.

NO_3^- and $PO_4^{3\text{-}}$

But if you dump a bunch of these in, it leads to problems like algae blooms. This:
- Blocks sunlight
- Can snuff out other aquatic plant life
- When algae die, they decay at the bottom of the water and leave oxygen dead zones in the water because bacteria consume the oxygen. These dead zones can kill fish and other aquatic life.

What reactions can happen in water

Example

Formation of ammonium nitrate.

$$NH_4NO_3$$

$$\underbrace{HNO_3(aq) + NH_3(g) \rightarrow NH_4NO_3(aq)}_{\text{molecular equation}}$$

A molecular equation is a formula where all of the components are in their neutral form.

Since ammonium nitrate is soluble, we can write its dissociation, similarly to all soluble ionic compounds:

$$NH_4NO_3(aq) \rightarrow NH_4^+(aq) + NO_3^-(aq)$$

We can do the same with the acid:

$$HNO_3(aq) \rightarrow H^+(aq) + NO_3^-(aq)$$

Remember to only break up soluble, aqueous, ionic compounds into ions. **Do not** break up solids, liquids or gases.

Therefore, we can make the equation:

$$\underbrace{H^+(aq) + NO_3^-(aq) + NH_3(g) \rightarrow NH_4^+(aq) + NO_3^-(aq)}_{\text{total ionic equation}}$$

We can simplify this by removing the duplicated ions:

$$\underbrace{\mathrm{H^+(aq) + NH_3(g) \rightarrow NH_4^+(aq)}}_{\text{net ionic equation}}$$

We did this by removing the spectator ion, $\mathrm{NO_3^-}$, ions that are on both sides of the ionic equation. To go from a total to a net ionic equation, eliminate these spectator ions.

Precipitation reaction

A precipitation reaction is a type of aqueous reaction in which one or more products are insoluble. The solid formed as a product in a precipitation reaction is called the precipitate.

Example

Mix a potassium iodide solution with a lead (II) nitrate solution.

$$\mathrm{KI\ (aq) + Pb(NO_3)_2(aq)}$$

Let's try switching the cation-anion pairs:

$$\mathrm{\rightarrow KNO_3 + PbI_2}$$

But are these results soluble?

$$\mathrm{\rightarrow KNO_3(aq) +} \underbrace{\mathrm{PbI_2(s)}}_{\text{precipitate}}$$

-

Then, we can balance the equations:

$$\mathrm{2\ KI\ (aq) + Pb(NO_3)_2(aq) \rightarrow 2KNO_3(aq) + PbI_2(s)}$$

This results in a total ionic equation of:

$$\mathrm{2K^+(aq) + 2I^-(aq) + Pb^{2+}(aq) + 2NO_3^+(aq) \rightarrow 2K^+(aq) + 2NO_3^+(aq) + PbI_2(s)}$$

And then to the net ionic equation, by removing spectator ions:

$$\mathrm{2I^-(aq) + Pb^{2+}(aq) \rightarrow PbI_2(s)}$$

Example

$$\mathrm{KI\ (aq) + NaCl\ (aq) \rightarrow KCl\ (aq) + NaI\ (aq)}$$

Total ionic equation:

$$\mathrm{K^+ + I^- + Na^+ + Cl^- \rightarrow K^+ + Cl^- + Na^+ + I^-}$$

There is no net ionic equation because everything is a spectator ion. Because of this, there is no reaction.

Acid-Base reaction

Definitions of acid:

Type	Acid Defintion	Base Defintion
Arrhenius	Produces one or more protons, H^+ ions, in aqueous solution.	Produces one or more hydroxide ions, OH^- ions, in aqueous solution.

Strong Acid

Completely ionized in water.

$$\mathrm{HNO_2 \rightarrow NO_2^- + H^+}$$

Weak Acid

Partially ionized in water.

$$\mathrm{HNO_2 \rightleftharpoons NO_2^- + H^+}$$

Examples

Acid-base reactions:

$$\underbrace{\mathrm{HCl}}_{\text{acid}}\mathrm{(aq)} + \underbrace{\mathrm{NaOH}}_{\text{base}}\mathrm{(aq)} \rightarrow \underbrace{\mathrm{NaCl}}_{\text{salt}}\mathrm{(aq)} + \underbrace{\mathrm{H_2O}}_{\text{water}}\mathrm{(l)}$$

This is called a neutralization reaction because no acids or bases are left, even though you start with some.

This results in a net ionic equation of:

$$\mathrm{H^+(aq) + OH^-(aq) \rightarrow H_2O\ (l)}$$

Monoprotic acids are acids that produce one mole of H^+ per mole of acid.

$$\underbrace{\mathrm{HCl\ (aq)}}_{\text{monoprotic acid}} \rightarrow \mathrm{H^+(aq) + Cl^-(aq)}$$

Polyprotic acids are acids that produce more than one mole:

$$\underbrace{\mathrm{H_2SO_4(aq)}}_{\text{polyprotic acid}} \rightarrow \mathrm{2H^+(aq) + SO_4^{2-}(aq)}$$

The general form of an acid-base neutralization reaction is $\mathrm{acid + base \rightarrow salt + water}$.

Example: Polyprotic acid

$$\mathrm{H_2SO_4(aq) + 2\ KOH\ (aq) \rightarrow K_2SO_4(aq) + 2H_2O\ (l)}$$

$$\mathrm{Acid: H_2SO_4(aq) \rightarrow 2H^+(aq) + SO_4^{2-}(aq)}$$

$$\mathrm{Base: 2\ KOH\ (aq) \rightarrow 2\ K^+(aq) + 2OH^-(aq)}$$

$$\mathrm{Salt: K_2SO_4(aq) \rightarrow 2K^+(aq) + SO_4^{2-}(aq)}$$

$$
\begin{aligned}
2H^+(aq) + SO_4^{2-}(aq) + 2\ K^+(aq) + 2OH^-(aq) \to 2K^+(aq) + SO_4^{2-}(aq) + 2H_2O\ (l) \\
\Rightarrow 2H^+(aq) + 2OH^-(aq) \to 2H_2O\ (l) \\
\Rightarrow H^+(aq) + OH^-(aq) \to H_2O\ (l)
\end{aligned}
$$

Back to the problem

Back to the problem of nutrient pollution, how can we remove the excess phosphate and nitrate from the wastewater to help reduce the environmental damage when the effluent is released?

With phosphate, you can add many different kinds of molecules to make a compound precipitate. You cannot do the same with nitrates because they are nearly always soluble. Instead, a process called denitrification is used, where microorganisms consume the nitrate and expel it as nitrogen gas.

How do antigen tests work?

COVID-19 at-home tests

COVID-19 at-home tests are a type of lateral flow antigen test.

- Lateral flow tests are simple tests that allow for rapid detection of a target substance in a liquid
- Some vocabulary:
  - Antigen: an easily identifiable biological molecule associated with the medical condition being tested for.
  - Antibody: molecules that bond to specific antigens.

When liquid moves through the test, there are two strips: one for the control and one for the test.

The test line will bond with the antigen, and the control line will bond with something that is definitely in the substance, so you can check that the flow was working correctly.

If the test line is colored, the antibodies bonded to the COVID-19 antigen: you have COVID-19.

If the test line is not colored, the antibodies did not bond to the COVID-19 antigen, so you probably don't have COVID-19.

Why do they stick

Through intermolecular forces, the antibodies "connect" to the antigen antigen through non-covalent interactions.

These interactions are reversible. So, we write the antibody-antigen binding process as a reversible chemical equation:

$$\mathrm{Ab} + \mathrm{Ag} \rightleftharpoons \mathrm{Ab} - \mathrm{Ag}$$

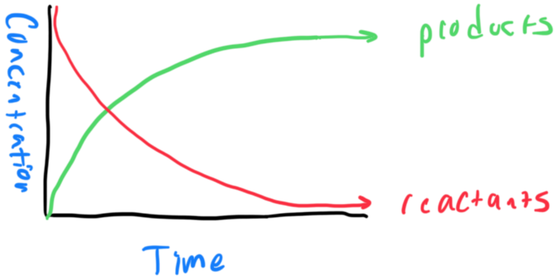
Chemical Equilibrium

It is the lowest energy state for a chemical reaction. There is no net change in the reactant or product concentration.

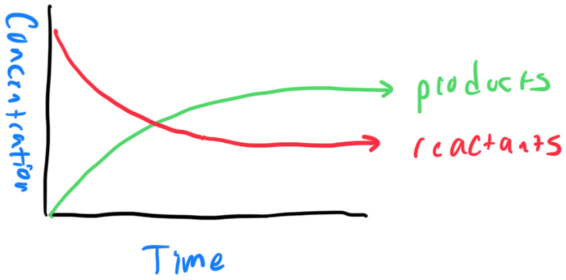
On a macroscopic scale, nothing is happening at chemical equilibrium, but reactions are still happening. It's just that both directions of the reaction are happening at the same rate.

- At equilibrium, the concentrations of reactants and products are constant over time. Note that the concentration of reactants does not necessarily equal the concentration of products.
- Some reactions will proceed to completion with all (or nearly all) reactants transformed into products, but some will not. The specific ratio of products to reactants at equilibrium is a characteristic of the particular reaction.
- The equilibrium constant K_{eq} indicates how far a reaction goes in the forward direction.

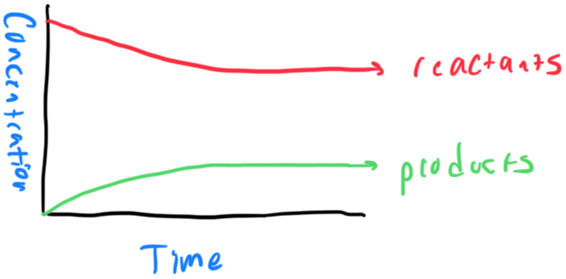
Equilibrium Constant



At equilibrium: $[\text{products}]_{\text{eq}} \gg [\text{reactants}]_{\text{eq}}$. The reaction is considered to have been completed because nearly all reactants have been converted to products. $\therefore K_{\text{eq}} \gg 1$.



At equilibrium: $[\text{products}]_{\text{eq}} > [\text{react}]_{\text{eq}}$. This reaction is *not* considered to have been completed because it is not a massive difference. $\therefore K_{\text{eq}} > 1$.



At equilibrium: $[\text{products}]_{\text{eq}} < [\text{react}]_{\text{eq}}$. This reaction doesn't go very far in the forward direction. $\therefore K_{\text{eq}} < 1$.

To quantify how far a reaction goes in the forward direction ("extent of reaction"), use the equilibrium constant K_{eq}.

$$K_{\text{eq}} = \frac{[\text{products}]_{\text{eq}}}{[\text{reactants}]_{\text{eq}}}$$

K_p is expressed as a ratio between partial pressures.

K_c is expressed as a ratio between concentrations.

K_a is the acid ioniziation constant.

K_{sp} is the solubility product constant.

In general:

$$a\text{A (g)} + b\text{B (g)} \rightleftharpoons c\text{C (g)} + d\text{D (g)}$$
$$a, b, c, d \in \mathbb{N}$$

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

Example

For HF in water:

$$\text{HF (aq)} \rightleftharpoons \text{H}^+\text{(aq)} + \text{F}^-\text{(aq)}$$
$$K_a = \frac{[\text{H}^+][\text{F}^-]}{[\text{HF}]^-}$$

Combustion of methane:

$$\text{CH}_4\text{(g)} + 2\text{O}_2(g) \rightleftharpoons \text{CO}_2(g) + 2\text{H}_2\text{O }(g)$$
$$K_c = \frac{[\text{CO}_2][\text{H}_2\text{O}]^2}{[\text{CH}_4][\text{O}_2]^2}$$

You can also do a similar thing with gases:

$$aA\ (g) + bB\ (g) \rightleftharpoons cC\ (g) + dD\ (g)$$

$$K_p = \frac{P_{\mathrm{C}}^c P_{\mathrm{D}}^d}{P_{\mathrm{A}}^a P_B^b}$$

For a combustion:

$$K_p = \frac{P_{\mathrm{CO_2}} P_{\mathrm{H_2O}}^2}{P_{\mathrm{CH_4}} P_{\mathrm{O_2}}^2}$$

$$K_p = K_c(RT)^{\Delta n}$$

$$\Delta n = \text{change in moles of gas}$$

For methane: $\Delta n = (2+1) - (2+1) = 0$ therefore $K_p = K_c$. This is only for methane and won't always be the case.

For example:

Units of K

They are unitless. The equilibrium constants are defined in terms of activity, which means that concentrations must always be in terms of molarity and pressure in atmospheres.

The value of K

How do you calculate it?

$$\mathrm{H_2(g) + I_2(g) \rightleftharpoons 2\ HI\ (g)}$$

Experiment 1:

$$K_c = \frac{[\mathrm{HI}]^2}{[\mathrm{H_2}][I_2]} = \frac{(1.98)^2}{(0.572)(0.012\,3)}$$

Experiment 2 + 3 (same numbers):

$$K_c = \frac{[2.78]^2}{(0.112)(0.112)}$$

The key point here is that K_{eq} is a constant for a particular reaction with a particular temperature, no matter the initial conditions.

Why do we care about this constant? It can give us an idea of who will win in the reaction and by how much.

If $K \ll 1$, there are far more reactants than products.

If $K \gg 1$, there are far more products than reactants.

If $K \approx 1$, the reaction goes about halfway.

$(K \approx 1 \Leftrightarrow K \in (0.01, 100))$

Examples

$$K_{\text{sp}} = 1 \times 10^{-54}$$

This means that the reaction almost won't happen, and will likely go in the reverse direction.

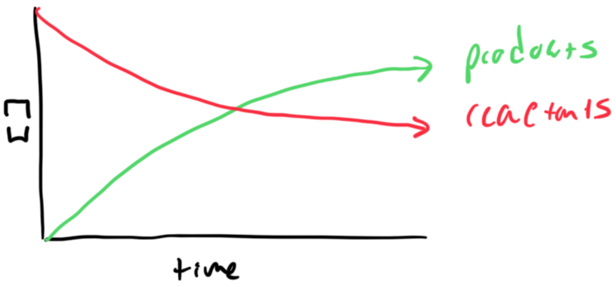
$$K_c = 2.4 \times 10^{47}$$

This means that the reaction is going to happen, and go to completion.

$$K_c = 50$$

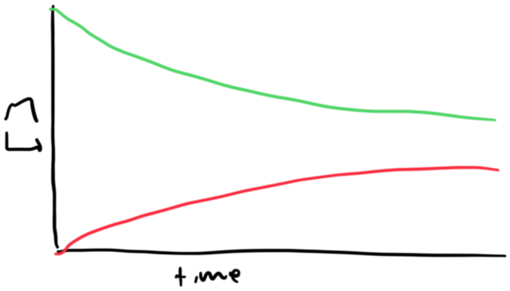
This means that the reaction will happen, but will not go to completion.

Trial 1



Our reaction proceeds foward.

Trial 2:



Our reaction proceeds backward.

Trial 2:

$$K_c = \frac{[\text{HI}]^2}{[\text{H}_2][\text{I}_2]} = 6.2 \times 10^2$$

$$Q_c = \underbrace{\frac{[\text{HI}]^2}{[\text{H}_2][\text{I}_2]}}_{\text{plug in initial conditions}} = \frac{(3.0)^2}{(0)(0)} \to \infty \text{ because } Q > K, \text{the reaction must go in reverse}$$

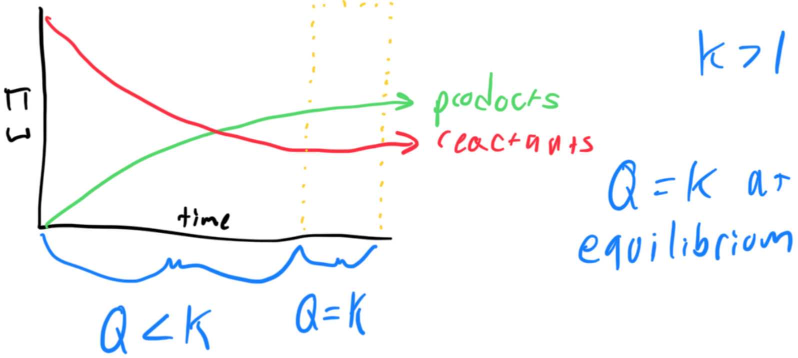
$$Q_c = \underbrace{\frac{[\mathrm{HI}]^2}{[\mathrm{H_2}][\mathrm{I_2}]}}_{\text{plug in initial conditions}} = \frac{(3.0)^2}{(0)(0)} \to \infty \text{ because } Q > K, \text{the reaction must go in reverse}$$

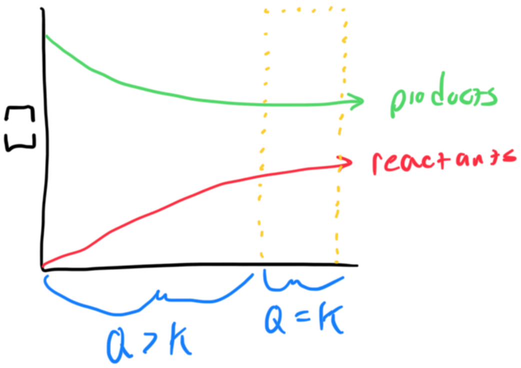
Going in reverse means more reactants are needed to reach equilibrium.

Trial 3:

$$Q_c = \frac{(1.0)^2}{(1.0)(1.0)} = 1 \Rightarrow \underbrace{1}_{Q} < \underbrace{620}_{K}, \text{therefore the reaction will go forwards}$$

Q is not a constant and changes as the reaction goes towards equilibrium:





Solids

So far, we have only examined reactions in which all reactants and products are in the gas phase. What happens if there are solids or liquids in the reaction?

Consider the dissolution of barium hydroxide in water:

$$\mathrm{Ba(OH)_2(s)} \rightleftharpoons \mathrm{Ba^{2+}(aq)}$$

Back to the at-home COVID tests

The antibodies “latch on” to the antigen through reversible non-covalent interactions.

$\mathrm{Ab} + \mathrm{Ag} \rightleftharpoons \mathrm{Ab} - \mathrm{Ag} \Longleftrightarrow \frac{[\mathrm{Ab} - \mathrm{Ag}]}{[\mathrm{Ab}][\mathrm{Ag}]}$

Basically, A was the only thing that had ions actively attracting, and D had objects directly in the way. A had ions repelling, and so:

B, C, A, D

Because B had the strongest bonds, it wanted to move forward the most, so it’s the largest.

What is the solution that you place your sample in for a COVID test?

The solution is a buffer. A buffer is a solution that resists changes in pH when an acid or base is added. It keeps the sample at physiological pH, the pH of your body, ~7.4.

This solves the problem that if conditions are changed too far, the antibody might change shape and, therefore, not match the antigen.

This raises the question of what pH is.

Brønsted-Lowry

Acids are a H^+ donor, and bases are a H^+ acceptor.

Example

$$\mathrm{HCl\ (aq)} \rightarrow \mathrm{H}^+\mathrm{(aq)} + \mathrm{Cl}^-\mathrm{(aq)}$$

This proton will quickly attach to a water molecule, forming the hydronium ion:

$$\mathrm{H_2O\ (l)} + \mathrm{H}^+\mathrm{(aq)} \rightarrow \mathrm{H_3O}^+\mathrm{(aq)}$$

You can then see the dissociation of hydrochloric acid in water as an acid-base reaction with water:

$$\mathrm{HCl\ (aq)} + \mathrm{H_2O\ (l)} \rightarrow \mathrm{Cl}^-\mathrm{(aq)} + \mathrm{H_3O}^+\mathrm{(aq)}$$

$$\underbrace{\mathrm{HCl\ (aq)}}_{\text{acid}} + \underbrace{\mathrm{H_2O\ (l)}}_{\text{base}} \rightarrow \underbrace{\mathrm{Cl}^-\mathrm{(aq)}}_{\text{conjugate base}} + \underbrace{\mathrm{H_3O}^+\mathrm{(aq)}}_{\text{conjugate acid}}$$

This is because the base could become HCl, and therefore is a base.

Another example

$$\mathrm{NH_3(aq)} + \mathrm{H_2O}\ (l) \rightleftharpoons \mathrm{NH_4^+(aq)} + \mathrm{OH}^-\mathrm{(aq)}$$

In this reaction, water is the acid because it becomes OH^- and donates a proton to the ammonia molecule.

As you can see, water can act as *either* an acid or a base.

Discovering pH

For a generic acid HA: We know it is this reaction because HA is an acid.

$$\mathrm{HA\ (aq) + H_2O\ (l) \rightleftharpoons A^-(aq) + H_3O\ (aq)}$$

$$K_a = \frac{[\mathrm{A^-}][\mathrm{H_3O^+}]}{[\mathrm{HA}]}$$

This is equivalent to:

$$\mathrm{HA\ (aq) \rightleftharpoons H^+(aq) + A^-(aq)}$$

$$K_a = \frac{[\mathrm{A^-}][\mathrm{H^+}]}{[\mathrm{HA}]}$$

Strong acids: they dissociate completely. Therefore, the reaction is $\mathrm{HA\ (aq) \to H^+(aq) + A^-(aq)}$. At equilibrium, $[\text{products}] \gg [\text{reactants}] \Rightarrow K_a \gg 1$

Weak acids: they dissociate partially. $\mathrm{HA\ (aq) + H_2O\ (l) \rightleftharpoons A^-(aq) + H_3O\ (aq)}$. At equilibrium, $[\text{reactants}] > [\text{products}] \Rightarrow K_a < 1$

Therefore, the stronger the acid, the more the ionization, the greater the K_a.

Autoionization of water

$$\mathrm{H_2O\ (l) + H_2O\ (l) \rightleftharpoons H_3O^+(aq) + OH^-(aq)}$$

$$\underbrace{K_w}_{\text{ion-product constant for water}} = [\mathrm{H_3O^+}][\mathrm{OH^-}]$$

At $298\ \mathrm{K}$, $K_w = 1 \times 10^{-14}$. Therefore, $[\mathrm{OH^-}] = [\mathrm{H_3O^+}] = 10^{-7}\ \mathrm{M}$.

$\mathrm{pH} = -\log_{10}([\mathrm{H+}])$

So for water:

$$\mathrm{pH_{water}} = -\log(10^{-7}) = 7$$

$\mathrm{pOH} = -\log([\mathrm{OH^-}])$

$$\begin{gathered} 10^{-14} = [\mathrm{H^+}][\mathrm{OH^-}] \\ -\log(10^{-14}) = -\log([\mathrm{H^+}][\mathrm{OH^-}]) \\ 14 = -(\log([\mathrm{H^+}]) + \log([\mathrm{OH^-}])) \\ 14 = -\log([\mathrm{H^+}]) - \log([\mathrm{OH^-}]) \\ 14 = \mathrm{pH} + \mathrm{pOH} \end{gathered}$$

That equation only applies at $298\ \mathrm{K}$, due to how K_w was created.

pH

pH's of 0-7 are acidic, and 7-14 are basic.

Example

What are the $[\mathrm{H^+}]$ and $[\mathrm{OH^-}]$ in household ammonia, a solution with a pH of 11.70?

$$\begin{gathered}\mathrm{pH} = 11.70 \\ -\log([\mathrm{H}^+]) = 11.70 \\ \log([\mathrm{H}^+]) = -11.70 \\ [\mathrm{H}^+] = 10^{-11.70} = 1.995 \times 10^{-12}\ \mathrm{M}\end{gathered}$$

Calculate the concentration of $[\mathrm{OH}^-]$:

$$\begin{gathered}K_w = [\mathrm{H}^+][\mathrm{OH}^-] = 10^{-14} \\ \frac{10^{-14}}{1.995 \times 10^{-12}} = 5.012 \times 10^{-5}\ \mathrm{M}\end{gathered}$$

Log significant figures

When taking the log, the resulting number should go to the same number of decimal places as the original value had significant figures

Acid K_a and $\mathrm{p}K_a$

Larger K_a's mean stronger acids, and therefore, smaller $\mathrm{p}K_a$'s mean stronger acids.

Larger K_a's also mean that there is greater $[\mathrm{H_3O^+}]$ at equilibrium. Greater $[\mathrm{H_3O^+}]$ means you have a smaller pH, and it is therefore more acidic.

Faking COVID tests

Students faked COVID tests using soda, energy drinks or fruit juice. This works because those liquids are all very acidic, and the acid destroys the antibodies so that they no longer bind only to the COVID-19 antigen. As a result, the antibodies bond to the gold nanoparticles which make the colored line, yielding a fake positive.

Gas exhaust

What would you expect to be in the exhaust? $\mathrm{CO_2, H_2O, N_2, O_2, unreacted\ gasoline}$. This is not all, though: CO and NO_x are also in the reaction.

Greenhouse gases are molecules that, when present in the upper atmosphere of the earth, reflect heat back down to the surface, resulting in an overall warming of the plant's surface. This includes $\mathrm{CO, CO_2, H_2O}$ and NO_x

These alternative products exist because of incomplete combustion. Poor mixing of gasoline and $\mathrm{O_2}$ and/or a nonideal ratio of $\mathrm{O_2}$ to gasoline results in a reaction that is not complete and forms other products like soot and carbon monoxide.

Focus Questions

1. What is the spark plug doing?
2. What is the mechanism for this reaction?

Combustion reactions

$$\mathrm{2C_8H_{18}(l) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O\ (g) + heat}$$

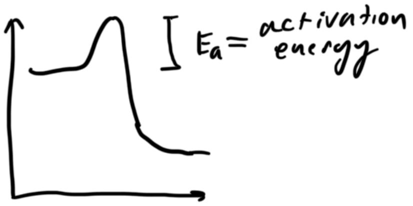
Because this reaction produces heat, it is considered exothermic.

Energy profile diagram

Can it be this?:

No! This means that as soon as octane meets oxygen, it will react. That is not the case, so this diagram is wrong.

Here is a more realistic plot:



Notice that the plot is overall downhill in terms of energy: it makes energy. However, it still requires energy to get started, and this energy is needed to break bonds.

In a car, the purpose of the spark plug is to give the energy needed to overcome E_a, the activation energy.

Now, we know that activation energy is required for a reaction, and we need collisions between molecules.

Take this reaction: $A + B \to A—B$. A and B must collide frequently enough, and with enough E to react.

Factors that affect the rate of reaction

1. Physical state: homogenous reactions are faster than heterogenous ones
   - Molecules collide more when they are in the same phase
2. Concentration: The greater the concentration of the reactants, the faster the reaction will occur
   - More concentration creates more frequent collisions
3. Temperature: higher temperatures create faster reactions
   - increasing temperatures increases KE, which then increases the energy and frequency of collisions
4. Presence of a catalyst

Instantaneous rates

Instead of using the average rate as an approximation, just take the derivative/see the slope.

The steeper the slope, the faster the reaction is going. This generally means that as a reaction proceeds, it slows down. This is because the concentration of the reactants is decreasing as well.

The rate law

Take the reaction $A + B \to C$:

We know that $\text{rate} \propto [A] + [B]$

This is the formula:

$$\text{rate} = k[A]^m[B]^n$$

Note: A and B are reactants. Only include gases and aqueous compounds.

The units of k, the rate constant, vary, with the fact that rate has units of M/s. k is independent of $[A] + [B]$. It only changes with temperature and/or the presence of a catalyst for a particular reaction.

The exponents m/n are the partial reaction orders. They tell us how sensitive the rate is to changes in the reactant's concentration.

For example, take $m = 0$ as a possible value. This is described as the reaction being zero-order in A. This means that the rate of the reaction does not vary with the concentration of A.

For example, if the concentration of A doubles, the rate remains the same.

Take $m = 1$. Therefore, $\text{rate} \propto [A]^1$. The reaction is first order in A. For example, if you double the concentration of A, the rate of the reaction doubles.

Take $m = 2$. Therefore, $\text{rate} \propto [A]^2$. The reaction is second order in A. If $[A]$ doubles, the rate quadruples.

$m + n$ is the overall reaction order.

$m + n = 2$ is described as a “second-order overall reaction”.

In general, reaction orders can only be determined by experiment.

An example of how they can be found is the method of initial rates.

Example

$$\text{rate} = k[\text{H}_2]^m[\text{NO}]^n$$

$$\begin{gathered} 0.044\,6 = k(0.10)^n(0.10)^m \\ 0.179 = k(0.10)^n(0.20)^m \\ 0.134 = k(0.30)^n(0.10)^m \end{gathered}$$

Via W|A:

$$k \to 45.241\,6, n \to 1.001\,36, m \to 2.004\,84$$

Manually: First, find n:

$$\begin{cases} 0.044\,6 = k(0.10)^n(0.10)^m \\ 0.134 = k(0.30)^n(0.10)^m \end{cases} \Rightarrow \frac{0.134}{0.044\,6} = \frac{(0.30)^n}{(0.1)^n} \Rightarrow 3.004\,48 = (3.0)^n \Rightarrow n \approx 1$$

Then we will find m:

$$\begin{cases} 0.044\,6 = k(0.10)^n(0.10)^m \\ 0.179 = k(0.10)^n(0.20)^m \end{cases} \Rightarrow 4.013\,45 = 2^m \Rightarrow m \approx 2$$

Find k:

$$\begin{gathered} 0.044\,6 \text{ M/s} = k(0.10 \text{ M})^1(0.10 \text{ M})^2 \\ k = 44.6 \ 1/(\text{M}^2 \text{ s}) \end{gathered}$$

$$\text{Rate} = k[\text{H}_2][\text{NO}]^2$$

Another Example

$$\begin{cases} 5.37 \times 10^4 = k(0.10)^n(0.1)^m \\ 1.52 \times 10^5 = k(0.2)^n(0.1)^m \\ 1.07 \times 10^5 = k(0.1)^n(0.2)^m \end{cases} \Rightarrow \begin{cases} k = 1.681\,39 \times 10^7 \\ m = 0.994\,617 \approx 1 \\ n = 1.501\,08 \approx 1.5 \end{cases}$$

Therefore:

$$\text{rate} = \left(1.68 \times 10^7 \ \frac{1}{s\sqrt{M^3}}\right)[\text{Cl}_2]^{1.5}[\text{CO}]^1$$

Formula

First-order

$$\text{rate} = k[A]^1$$

$$\text{rate} = -\frac{\mathrm{d}[A]}{\mathrm{d}t}$$

$$\int_{[A]_0}^{[A](t)} -\frac{\frac{\mathrm{d}[A]}{\mathrm{d}t}}{[A]^1}\,\mathrm{d}t = \int_0^t k\,\mathrm{d}t$$

$$\Rightarrow \ln([A](t)) = -kt + \ln{[A]_0}$$

Therefore, the plot will have a y-axis of $\ln[A]$ and an x-axis of t.

The slope will be $-k$, and the y-intercept will be $[A]_0$.

Rearrange 1st order integrated rate law:

$$[A]_t = [A]_0 e^{-kt}$$

Second-order

$$\text{rate} = K[A]^2 = -\frac{\mathrm{d}[A]}{\mathrm{d}t}$$

$$\Rightarrow \int_{[A]_0}^{[A](t)} \frac{\mathrm{d}[A]}{[A]^2} = \int_0^t -k\,\mathrm{d}t$$

$$\Rightarrow \frac{1}{[A](t)} = kt + \frac{1}{[A]_0}$$

Now, to form a straight line, let the y-axis be $\frac{1}{[A]}$, and the x-axis to be t. This results in a slope of $+k$ and a y-intercept of $\frac{1}{[A]_0}$.

This means that if a plot of $\frac{1}{[A](t)}$ is straight, the reactant is in second order.

Half-life

First-order

The time it takes for the concentration of a reactant to decrease by half.

For a first-order reaction, this value is

$$t_{1/2} = \frac{0.693}{k}$$

This also leads to another way of identifying first-order reactions: if sequential half-lives are the same, it is first-order.

Second-order

$$t_{1/2} = \frac{1}{k[A]_0}$$

This means that

$$t_{1/2}(1) < t_{1/2}(2) < \cdots$$

Comparing 1st and 2nd order

Consider reactions that occur in a single step:

$$A \rightarrow \text{products}$$

1st Order	2nd Order
$t_{1/2}$ is always the same	Sequential half-lives, $t_{1/2}$, increases
$t_{1/2}$ has no dependence on $[A]$	Dependence on $[A]$, as [A] decreases, $t_{1/2}$ increases
Therefore, only 1 A molecule is required for a reaction: no collision is necessary	Therefore, 2 A molecules must collide for a reaction.

Identifying the order: Summary

	0th Order	1st Order	2nd Order
Linear Plot	$[A]$ vs t	$\ln[A]$ vs. t	$1/[A]$ vs. t
Units of k	$\frac{M}{s}$	$1/\mathrm{s}$	$1/(\mathrm{M\ s})$
Sequential half-lives	$t_{1/2}(1) > t_{1/2}(2) > \cdots$	$t_{1/2}(1) = t_{1/2}(2) = \cdots$	$t_{1/2}(1) < t_{1/2}(2) < \cdots$
Halflife expression	$t_{1/2} = \frac{[A]_0}{2k}$	$t_{1/2} = \frac{\ln(2)}{k} \approx \frac{0.693}{k}$	$t_{1/2} = \frac{1}{k[A]_0}$

Note that this math only applies to a reaction that is second-order in one reactant. The same math, in general, does not apply when a reaction is 2nd order overall but 1st order in two different reactants.

Zero-order reactions

- The rate of reaction is independent of concentration.
- $[A] = -kt + [A]_0$, $t_{1/2} = \frac{[A]_0}{2k}$

This has some flaws: It is unclear how a reaction with no reactants continues. This doesn't make sense with single-step reactions.

Elementary steps

The point of a reaction mechanism is to break a net reaction down into a series of steps, called elementary steps, where the stoichiometry represents an actual number of molecules colliding.

For any elementary step, we can predict the rate law using the stoichiometry as follows:

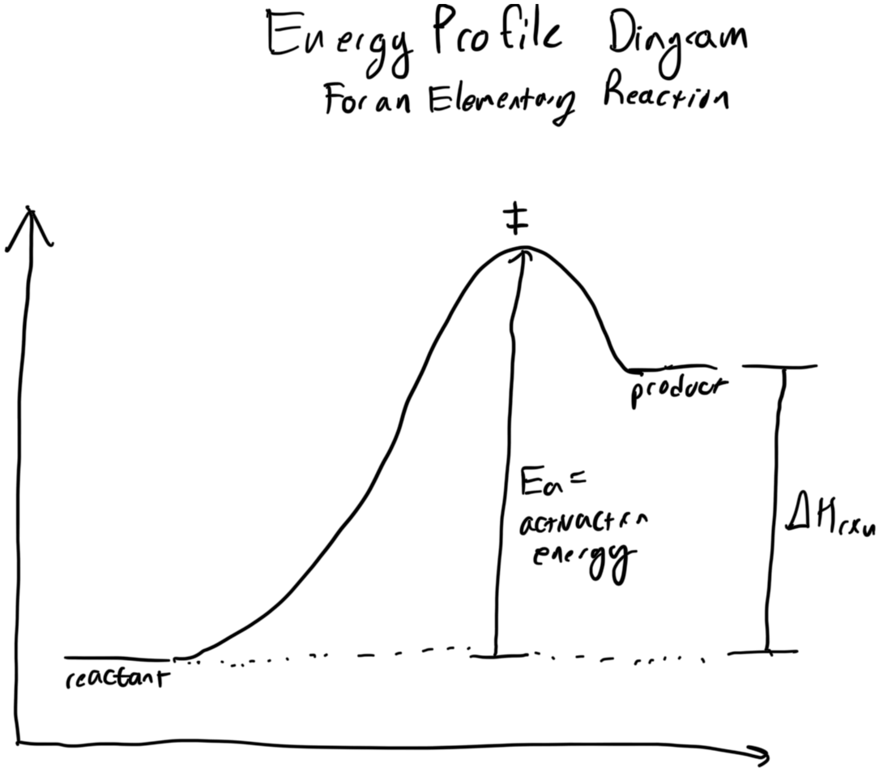
$$aA + bB \rightarrow cC + dD$$

$$\text{Rate} = k[A]^a[B]^b$$

Reaction	Molecularity	Rate law
$A \rightarrow \text{products}$	Unimolecular	$\text{Rate} = k[A]$

Reaction	Molecularity	Rate law
$A + A \rightarrow \text{products}$	Bimolecular	$\text{Rate} = k[A]^2$
$A + B \rightarrow \text{products}$	Bimolecular	$\text{Rate} = k[A][B]$
$A + A + A \rightarrow \text{products}$	Termolecular	$\text{Rate} = k[A]^3$
$A + A + B \rightarrow \text{products}$	Termolecular	$\text{Rate} = k[A]^2[B]$
$A + B + C \rightarrow \text{products}$	Termolecular	$\text{Rate} = k[A][B][C]$

Activation Energy



Activation energy in a simple $A \rightarrow B$ reaction means that molecules must collide with enough energy to react. This forms the “hill” to climb over, and the higher the hill, the longer it takes to “climb”.

The higher the activation energy, the slower the reaction. The number of hills equals the number of elementary steps in the mechanism. The step with the greatest activation energy will be slowest, and will be called the rate determining step (ROS), and it determines the rate of net reaction.

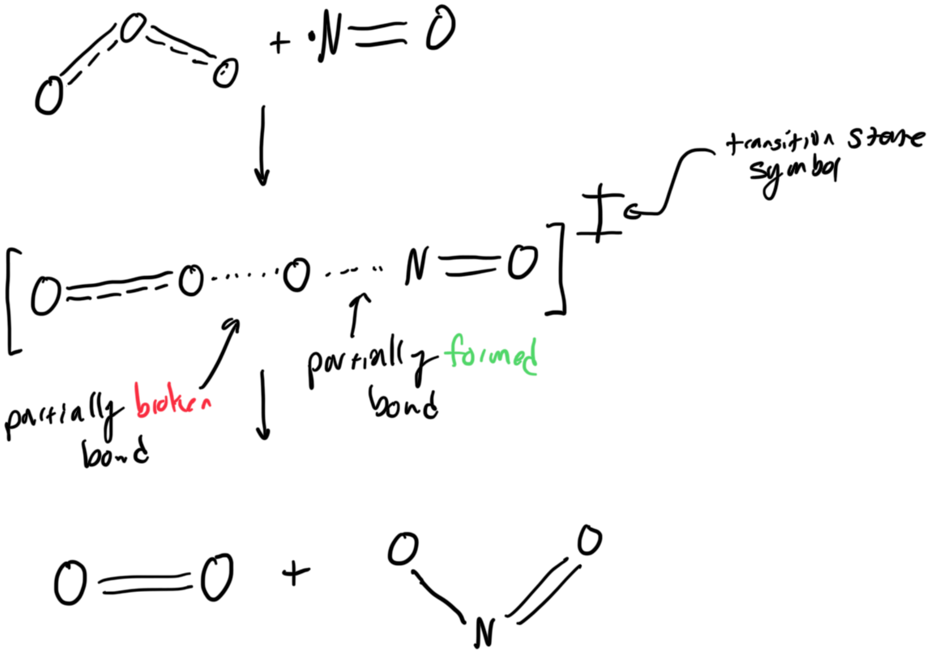
Transition States (‡)

They are high-energy activated complexes.

The number of maxima is equal to the number of transition states, which in turn is equal to the number of elementary steps in the mechanism.

Example

$$O_3\,(g) + NO\,(g) \rightarrow O_2\,(g) + NO_2\,(g)$$



Multi-step mechanisms

Most reactions occur in multiple steps. You can then write a reaction mechanism for any reaction, composed of a series of elementary steps:

For example:

$$\begin{aligned} \text{Net reaction} : A + 2B &\rightarrow 2C + D \\ \text{Proposed reaction:} & \\ A + B \overset{k_1}{\rightarrow} I + C &\qquad \text{Rate}_1 = k_1[A][B] \\ I + B \overset{k_1}{\rightarrow} C + D &\qquad \text{Rate}_2 = k_2[I][B] \end{aligned}$$

I is a reactive intermediate. This means that it does not appear in the overall net reaction. It is produced and then consumed in later steps. It is difficult to measure the concentration of any intermediate.

1. The elementary steps must sum to the overall balanced chemical reaction.

$$\begin{gathered} A + B + I + B \rightarrow I + C + C + D \\ \Rightarrow A + 2B + I \rightarrow I + 2C + D \\ \Rightarrow A + 2B \rightarrow 2C + D \checkmark \end{gathered}$$

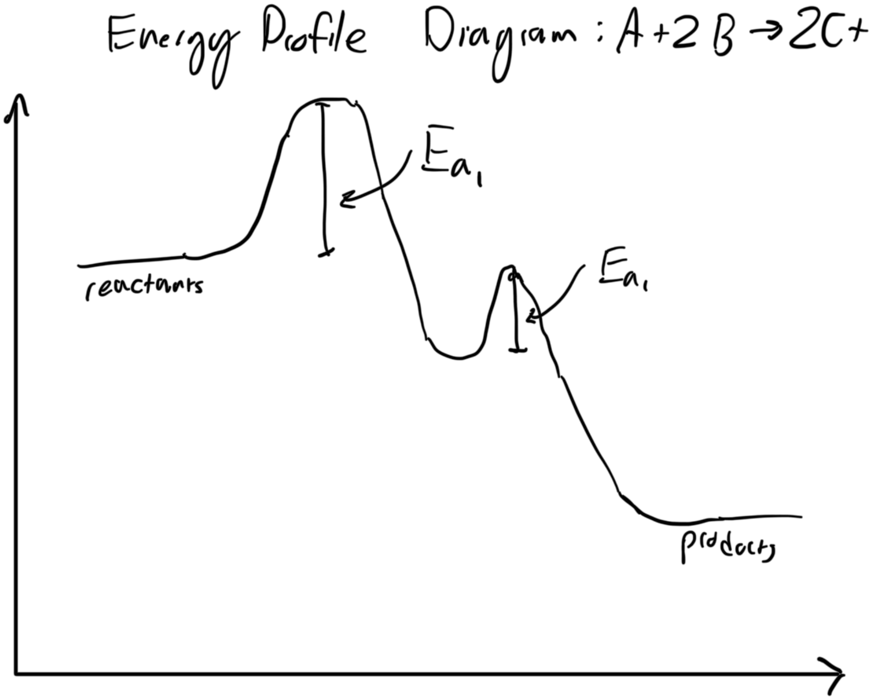
2. The rate law predicted by the mechanism’s rate-determining step must be consistent with the experimentally observed rate law.

Let’s just assume this to be true.

Since the mechanism has two steps, an energy profile diagram should show two transition states.

There are 2 options:

1. Step 1 is slower than step 2.

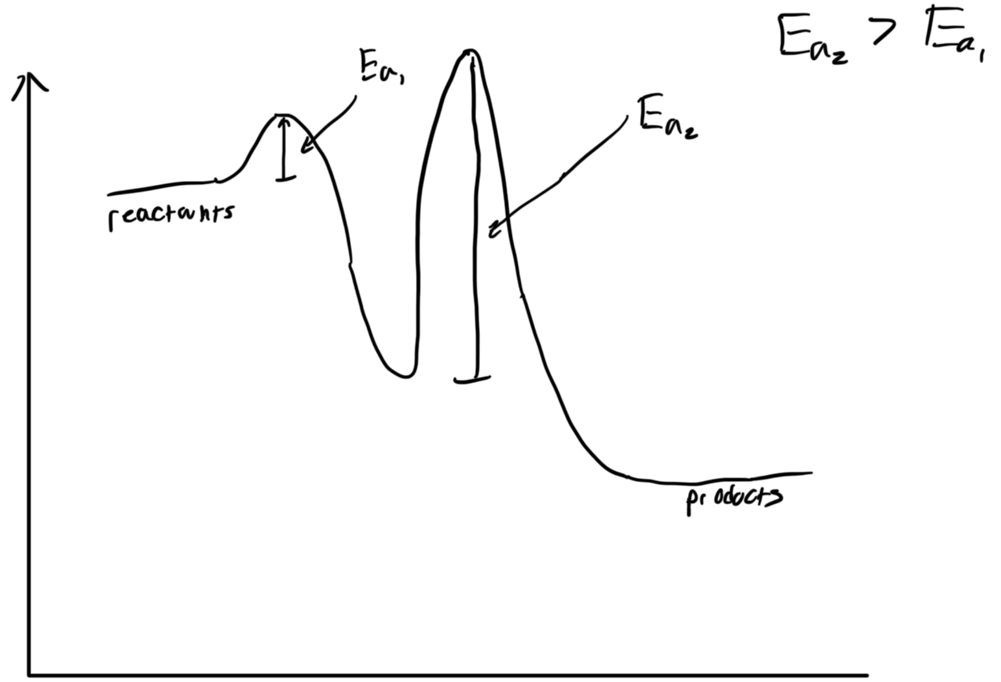
   

   This makes step 1 the rate-determining step, and therefore the predicted rate law is:

   $$\text{Rate} = k_1[A][B]$$

   If this matches what we see in an experiment, then we can say that this mechanism is possible.

2. Step 2 is slower than step 1.



This makes step 2 the rate-determining step. Therefore, our predicted rate law is:

$$\mathrm{Rate} = k_2[I][B]$$

We have these reactions:

Step 1: $A + B \underset{k_r}{\overset{k_f}{\rightleftharpoons}} I + C$

Step 2: $I + B \overset{k_2}{\rightarrow} C + D$

But $[I]$ is hard to measure, so you need to replace it with something you can measure.

We know $\mathrm{Rate}_f = \mathrm{Rate}_r$ at equilibrium, so:

$$k_f[A][B] = k_r[I][C]$$

$$[I] = \frac{k_f}{k_r}\frac{[A][B]}{[C]}$$

Then, overall:

$$\mathrm{Rate} = k_2\frac{k_f}{k_r}\frac{[A][B]}{[C]}[B] = \frac{k_2k_f}{k_r}[A][B]^2[C]^{-1}$$

Clicker

$A + B \rightarrow C$ as the slow elementary reaction means that the rate law is $\mathrm{rate} = k[A][B]$. Neither A nor B are intermediates, so this is simply the rate.

Using Kinetics to validate a mechanism

The point of predicting the rate law from the mechanism is to determine whether or not it is a valid mechanism for the reaction. Then, the point of the mechanisms is to understand how the reaction happens.

In order for a mechanism to be valid for a reaction:
- The elementary steps must sum to form the balanced equation
- The rate law predicted must be consistent with the rate law experimentally observed

The rate-determining step is the slowest step in the mechanism:
- You will either be directly told this or given an energy profile diagram. The highest activation energy step is the slow step.
- Alternatively, remember that the rate law predicted must be consistent with the rate law experimentally observed. From this, you can see which steps may be valid choices.

Example

$$A + B \underset{k_r}{\overset{k_f}{\rightleftharpoons}} I + C \qquad \text{(fast)}$$

$$I + B \overset{k_2}{\to} C + D \qquad \text{(slow)}$$

Therefore:

$$\text{rate} = k_2[I][B]$$

By equilibrium rates being equal:

$$k_f[A][B] = k_r[I][C]$$
$$\Rightarrow [I] = \frac{k_f}{k_r}\frac{[A][B]}{[C]}$$

Therefore:

$$\text{rate} = \frac{k_2 k_f}{k_r}\frac{[A][B]^2}{[C]}$$
$$\Rightarrow \text{rate} = k_{\text{exp}}[A][B]^2[C]^{-1}$$

The -1 means that as a product's concentration $[C]$ increases, the rate decreases, which jives with our understanding of rules of thumb for the speed of reactions.

There are examples on the slideshow for further practice.

Catalysts

Catalysts are substances that increase the rate of reaction but are not consumed in the process. They are consumed and then produced, as opposed to intermediates, which are produced and then consumed.

Chlorine

Chlorine is used as a catalyst to speed up the reaction of ozone. This is bad because we want stratospheric ozone to reflect the UV rays.

Unfortunately, CFCs were used in aerosols and refrigerants and then created chlorine atoms in the atmosphere. Those chlorine atoms then sped up the reactions of ozone.

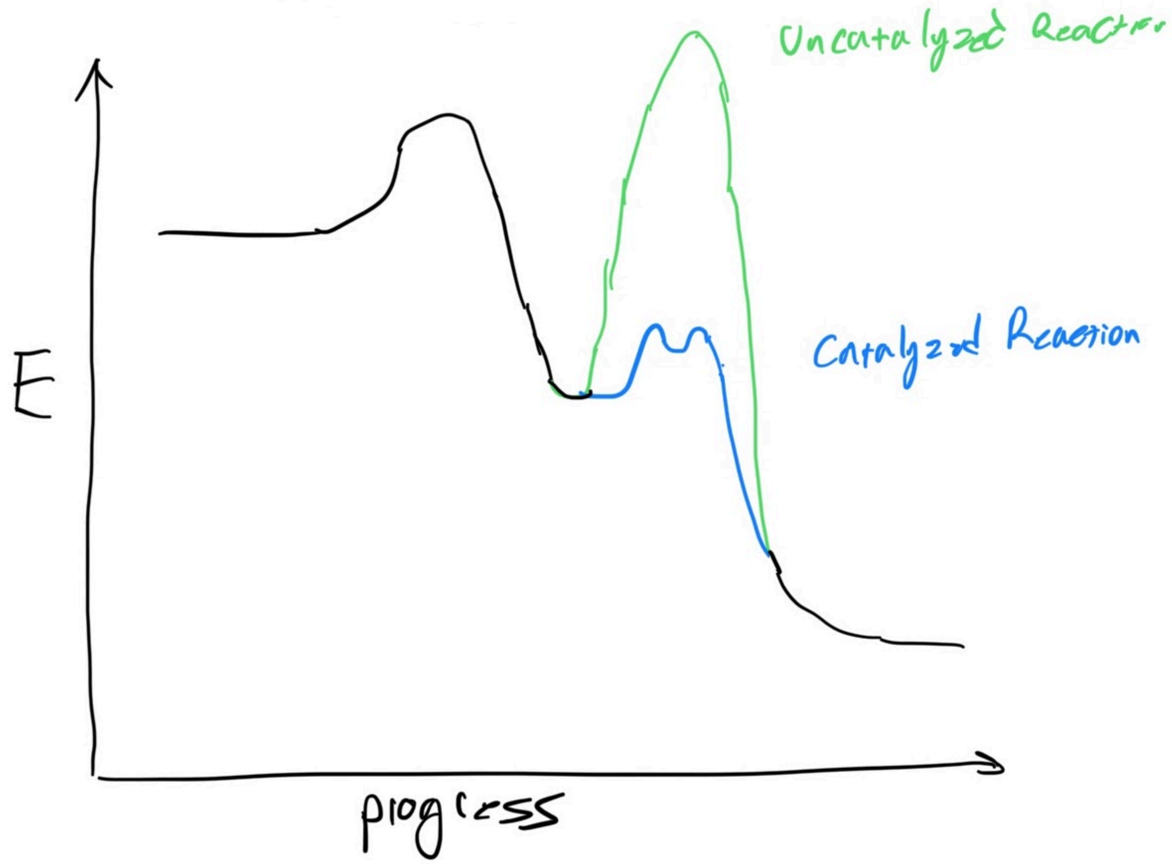
Example

$$2O_3(g) \rightarrow 3O_2(g)$$

$$\begin{aligned} O_3 &\rightleftharpoons O_2 + O && \text{fast} \\ O_3 + O &\rightarrow 2O_2 && \text{slow} \end{aligned}$$

It would be bad if this were fast because stratospheric ozone is good to have.

But oh no! Chlorine will speed this up by alternating the reaction and thereby decreasing the activation energy:



Mechanism of combustion reactions

It is most certainly not a simple reaction for gasoline due to the requirement of 27 molecules colliding at once.

In fact, it is believed to need over 6000 reactions to do the combustion reaction.

Let's simplify to methane:

$$\mathrm{CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O}$$

There are only a few hundred reactions now.

Anywho, the problem that happens when you have an incomplete reaction:

$$\mathrm{HCO + O_2 \rightarrow {\color{red}CO} + HO_2}$$
$$\mathrm{{\color{red}CO} + OH \rightarrow CO_2 + H}$$

Then you don't necessarily react all of the CO away.

We would like to reduce the harmfulness of products released from the car. We can do so by speeding up the reactions of:

$$\mathrm{2CO + O_2 \rightarrow 2CO_2}$$
$$\mathrm{2NO_2 \rightarrow N_2 + 2O_2}$$

This is done via a catalyst in the form of a catalytic converter.

Why does it work despite being solid? Because we also increased the surface area.

Clicker

We want the most heat per $\mathrm{CO_2}$ produced, so natural gas is the best, as it has the maximum negative number.

Focus Questions

What happened to the Statue of Liberty?
- What caused the color change?
- What caused the structural damage?

Batteries:
- How can we use a redox reaction to power something?
- How do rechargeable batteries work?

Redox Reactions

For example:

$$\mathrm{Zn}\ (s) + \mathrm{Cu^{2+}(aq)} \rightarrow \mathrm{Zn^{2+}} + \mathrm{Cu}\ (s)$$

As this reaction occurs, you can see the blue disappear from the liquid, as $\mathrm{Cu^{2+}}$ is blue, but $\mathrm{Zn^{2+}}$ is colorless.

This reaction occurs when electrons are transferred. Here, the electrons are transferred from copper to zinc.

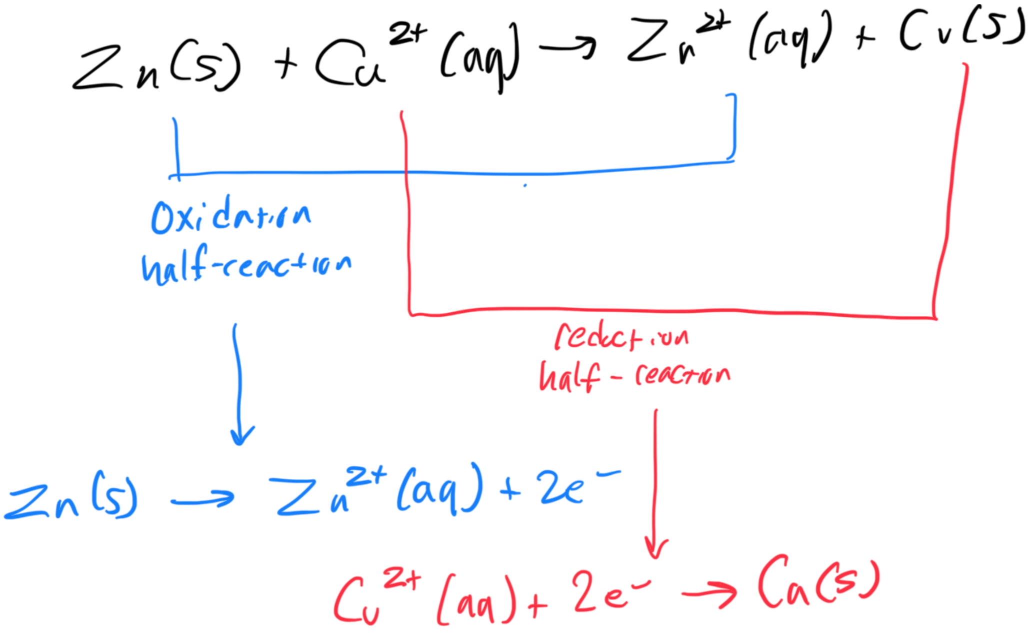
Oxidation-reduction reactions (redox reactions) are characterized by a transfer of electrons from one reactant to another.
- Many common redox reactions include reacting something with oxygen, such as rusting or combustion.

Redox reactions can be split:
The oxidation half-reaction:

- Loses electrons: electrons are a product
- Often increases the oxygen content
- Oxidation results in an increase in oxidation number

And the reduction half-reaction:

- Gains electrons: electrons are a reactant
- Often reduces oxygen content
- Oxidation results in a decrease in oxidation number



If you add the half-reactions, it should result in the same net reaction:

$$\text{Zn }(s) + \text{Cu}^{2+}(\text{aq}) + 2e^- \to \text{Zn}^{2+} + 2e^- + \text{Cu }(s)$$
$$\text{Zn }(s) + \text{Cu}^{2+}(\text{aq}) \to \text{Zn}^{2+} + \text{Cu }(s)$$

The electron flows from the $\text{Zn }(s) \to \text{Cu}^{2+}(\text{aq})$.

Zinc is oxidized, which is why it is called the reducing agent.

Copper ions are reduced, so they are called the oxidizing agent.

Spontaneity

The metal that is being oxidized is called the anode, and the metal that is being reduced is called the cathode.

Electrons flow from the anode to the cathode.

Check the standard reduction potentials to determine if a reaction will occur spontaneously.

It indicates how likely that half-reaction is to occur as a reduction in the redox reaction. The greater the E^o, the greater the probability of the reaction as a reduction.

For example:

$$\mathrm{F}_2(g) + 2e^- \rightarrow 2\mathrm{F}^- \mid E^o = 2.87 \text{ V}$$

Since 2.87 is a very positive number, it will likely occur as a reduction.

Alternatively,

$$\mathrm{Li}^+(\mathrm{aq}) + e^- \rightarrow \mathrm{Li}\ (s) \mid E^0 = -3.04 \text{ V}$$

This will not likely occur as a reduction. Instead, it will more likely occur as an oxidation reaction.

Example
Calculate the standard cell potential for the reaction:

$$2\mathrm{Fe}^{3+}(\mathrm{aq}) + 2\mathrm{I}^-(\mathrm{aq}) \rightarrow 2\mathrm{Fe}^{2+}(\mathrm{aq}) + \mathrm{I}_2(s)$$

$$E_{\text{cathode}} = 0.771 \text{ V}$$
$$E_{\text{anode}} = 0.535 \text{ V}$$
$$E_{\text{cell}} = E_{\text{cathode}} - E_{\text{anode}} = 0.236 \text{ V}$$

Since $0.236 \text{ V} > 0$, it is a spontaneous redox reaction.

Note that E^o is an intensive property: it does not depend on amount.

What caused the color change?

$$4\ \mathrm{Cu}\ (s) + \mathrm{O}_2(g) \rightarrow 2\mathrm{Cu}_2\mathrm{O}\ (g) + \mathrm{O}_2(g) \rightarrow \cdots$$

This is corrosion: the disintegration of a solid metal through a chemical reaction with its environment, often forming a metal oxide. Copper's patina is just the corrosion of copper.

Clicker

The most likely thing to happen when copper and iron interact is that copper is oxidized and iron is reduced. Therefore, iron will reduce.

$$\mathrm{Cu}^{2+}(\mathrm{aq}) + \mathrm{Fe}\ (s) \rightarrow \mathrm{Cu}\ (s) + \mathrm{Fe}^{2+}(\mathrm{aq})$$

$E_{\text{cell}} = 0.79 \text{ V}$

Because iron stops becoming a solid and instead becomes an ion, it is more likely to deteriorate.

This is not entirely correct, though, because copper ions are not copper solids.

Galvanic Corrosion

This is a type of corrosion where one metal preferentially degrades when in contact with another.

In the case of iron and copper, electrons flow from the iron to the copper. The electrons will then help with a reaction between water and oxygen from the environment. This is stated as:

$$2\text{ Fe }(s) + 2\text{H}_2\text{O }(l) + \text{O}_2(g) \to 2\text{Fe}^{2+}(\text{aq}) + 4\text{OH}^- \to 2\text{Fe(OH)}_2$$
$$4\text{Fe(OH)}_2 + \text{O}_2 + 2\text{H}_2\text{O} \to 4\text{Fe(OH)}_3$$
$$\text{Fe(OH)}_3 \to \text{FeO(OH)} + \text{H}_2\text{O}$$
$$\text{FeO(OH)} \to \underbrace{\text{Fe}_2\text{O}_3}_{\text{rust}} + \text{H}_2\text{O}$$

You don't need to know these reactions, but you should be able to understand why.

Module 8

This will be a final exam question.

Generating electricity through redox.

$\text{Zn} \to \text{Zn}^{2+} + 2e^-$ and $\text{Cu}^{2+} + 2e^- \to \text{Cu}$ are the two reactions going on.

The electrons are going over the wire from the zinc to the copper.

The salt bridge then balances the charge of the solution.

Anions go towards the anode, and cations go towards the cathode.

This is because anions are negatively charged to balance out the Zn^{2+}, and cations are positively charged to balance out the lack of anions because they have just moved.

In this reaction, $E_{\text{cell}} = 1.10\text{ V}$, so the reaction is spontaneous.

Standard Hydrogen Electrode

$2\text{H}^+ + 2e^- \to \text{H}_2$ with $E^o = 0\text{ V}$.

Relation to K_{eq}

$E_{\text{cell}} > 0\text{ V} \Leftrightarrow K_{\text{eq}} > 1$.

Conversely $E_{\text{cell}} < 0\text{ V} \Leftrightarrow K_{\text{eq}} < 1$.

Powering something with redox

If you start with all reactants, then you can harvest the energy. Otherwise, you're reversing time, or getting crazy lucky.

In order to use a redox reaction to power something you want:

- $K_{\text{eq}} \gg 0 \Leftrightarrow E^o_{\text{cell}} > 0$
- Start with $Q < K$, ideally as far as possible.

$$E^o_{\text{cell}} = E_{\text{cell}} - \left(\frac{RT}{nF}\right)\ln Q$$

At equilibrum, $Q = K$. Then, by another equation: $E_{\text{cell}} = \left(\frac{RT}{nF}\right)\ln K$. Therefore:

$$E^o_{\text{cell}} = \left(\frac{RT}{nF}\right)\ln K - \left(\frac{RT}{nF}\right)\ln K = 0\text{ V}$$

Lead-Acid Batteries

$$\mathrm{Pb}\ (s) + \mathrm{PbO_2}(s) + 2\mathrm{HSO_4^-}(\mathrm{aq}) + \mathrm{H^+}(\mathrm{aq}) \to 2\mathrm{PbSO_4}(s) + 2\mathrm{H_2O}\ (l)$$

Then, $E_{\text{cell}} = 2.02\ \mathrm{V}$. For $12\ \mathrm{V}$, use 6 of them in series.

To recharge this battery, you must make the redox reaction go in reverse: connect a power supply and then the electrons are replensished.