Chemistry 301

FINAL EXAM REVIEW

PLEASE LOOK OVER MIDTERM REVIEWS FOR COMPREHENSIVE TOPICS

Most Important Exam Announcement:

When the professor is passionate about teaching and you genuinely understand and enjoy the class

Exam Study (Greatest Hits)

0 FOLLOWERS

Surge
Above & Beyond • Surge

Gravity - Original Mix
Parker & Hanson • Gravity

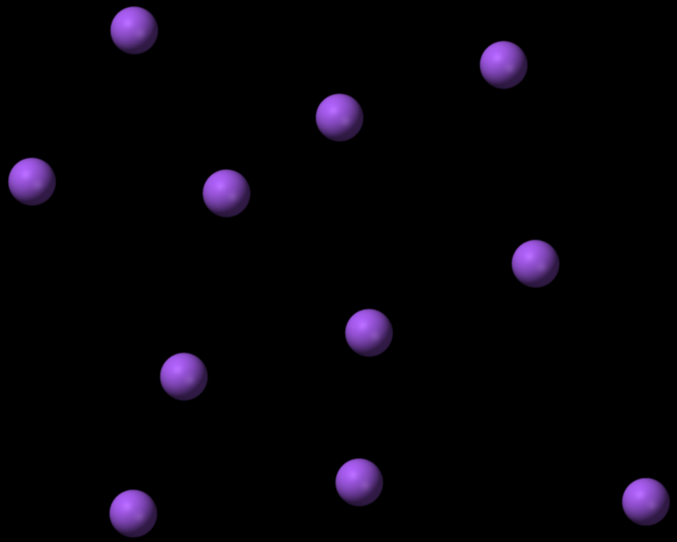
Filmic
Above & Beyond • Group Therapy

Other Exam Playlists:

Exam Study (Ambient)

Exam Study (Progressive)

Exam Study (Andrew Bayer Only)



Fundamentals

STOICHIOMETRY, NOMENCLATURE, UNITS

Basic Terminology in Reaction Stoichiometry

- **Mole:** a mole is basically a packet of atoms (6.02 x 10^{23} atoms to be exact)
  - We use the term “mole” because it is easier to work with in a lab.
  - The mass of each element is presented as its **molar mass** on the periodic table (g/mol)
  - Based on the phase of matter, a mixture will look different (condensed phases vs. gas phase)
    - **What is the difference? We now know that the condensed phases have potential energy in the form of IMF’s**
- **Limiting reagent:** the reactant that **runs out first**, thereby forcing the reaction to stop
- **Excess reagent:** a reactant that is added in high quantities so that another reactant runs out first
  - You will have a certain amount of this “excess reagent” left over once the limiting reagent runs out

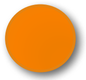
Molecules, Moles, and Mass

You are expected to know how to convert between molecules, moles, and molar mass.

Here's how you do it:

1. From Molecules to Moles
   - Remember: Avogadro's number ($N_A = 6.022 \times 10^{23}\ mol^{-1}$) represents the number of molecules in a mole.

$$\boxed{\frac{\#\ \text{molecules}}{N_A} = \#\ \text{moles}}$$



1 atom is one fundamental unit

2. From Moles to Molecules
   - On the exam, what if you forget if you multiply or divide by Avogadro's number? Remember, a mole is a "packet" of molecules. Converting from moles to molecules should always give you a **bigger number**

$$\boxed{\#\ \text{moles} \cdot N_A = \#\ \text{molecules}}$$

3. From Moles to Mass

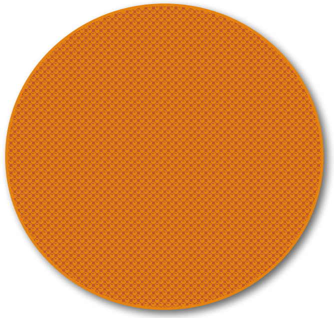
$$\boxed{\#\ \text{moles} \cdot \text{MW} = \text{mass}}$$

4. From Mass to Moles

$$\boxed{\frac{\text{mass}}{\text{MW}} = \#\ \text{moles}}$$

5. Molecular Weight

$$\boxed{\frac{\text{mass}}{\#\ \text{moles}} = \text{MW}}$$



1 mole is 6.022×10^{23} fundamental units

Chemistry Fundamentals: Stoichiometry

- Given the following generic, balanced chemical reaction:

$$A_{(g)} + 2B_{(g)} \text{-->} 3C_{(g)} + 4D_{(l)}$$

- **Simple ratio problems:** how many moles of B are required to make 7 moles of C?
  - This problem can be solved by simply understanding the stoichiometric ratio
- **Limiting Reagent, Gas Law Problems:** what is the total volume of your system when 10L of A are reacted with 10L B at STP. Assume this reaction goes to completion.
  - This problem should be solved by working out the reaction

***Do not include condensed states (liquids, solids) in the volume or pressure of the final solution**

Unit One Question

Calculate the mass of NH_3 that can be produced from 30.0g of N_2 and 5.0g H_2 in the following reaction:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

1. 42.5 g
2. 18.2 g
3. 36.4 g
4. 28.3 g
5. 63.8 g

$$\overset{30\,g}{N_2\,(g)} + \overset{5\,g}{3H_2\,(g)} \longrightarrow 2NH_3\,(g)$$

↳ $\frac{\text{moles}}{\text{rxn}}$, L/rxn, P/rxn, g/rxn

1) g → moles

$$30g\ N_2 \times \left(\frac{mol}{28g}\right) = 1.07\ moles$$

$$5g\ H_2 \times \left(\frac{mol}{2g}\right) = 2.5\ moles$$

2) How many reactions?

$$1.07\ moles\ N_2 \times \frac{rxn}{1\ mol} = 1.07\ rxn$$

$$\boxed{2.5\ moles\ H_2 \times \frac{rxn}{3\ mol} = 0.833\ rxn} \Rightarrow L.R.$$

3) Solve:

$$0.833\ rxn \times \frac{2\ mol\ NH_3}{rxn} = \underline{1.67\ moles\ NH_3}$$

$$\Downarrow$$

$$1.67\ moles\ NH_3 \times \frac{17g}{mol} = \boxed{28.3g\ NH_3}$$

Unit One Question

A 6.00L sample of C_2H_4 at 2.00 atm and 293K is burned in 6.00 L of oxygen gas at the same temperature and pressure to form carbon dioxide gas and liquid water. If the reaction goes to completion, what is the final volume of all gases at 2.00 atm and 293K?

$$C_2H_4(g) + 3O_2(g) \rightarrow 2H_2O(l) + 2CO_2(g)$$

1. 2.66 L
2. 12.00 L
3. 2.00 L
4. 8.00 L
5. 6.00 L

$$\overset{6.0L}{C_2H_{4(g)}} + \overset{6.0L}{3O_{2(g)}} \rightarrow \overset{\nearrow V=0L}{2H_2O_{(l)}} + 2CO_{2(g)}$$

$$6.0L\ C_2H_4 \times \frac{rxn}{1L} = \boxed{6\,rxn}\ \text{excess}$$

$$6.0L\ O_2 \times \frac{rxn}{3L} = \boxed{2\,rxn}\ \text{LR}$$

Produced

$$2\,rxn \times \frac{2L\,CO_2}{rxn} = 4L\,CO_2$$

Excess

$$\underset{\substack{\uparrow \\ \text{Initial} \\ \text{amount}}}{6L} - \underset{\substack{\uparrow \\ \text{amount} \\ \text{consumed}}}{\left(2\,rxn \times \frac{1L}{rxn}\right)} = \underset{\substack{\uparrow \\ \text{excess}}}{4L\ C_2H_4}$$

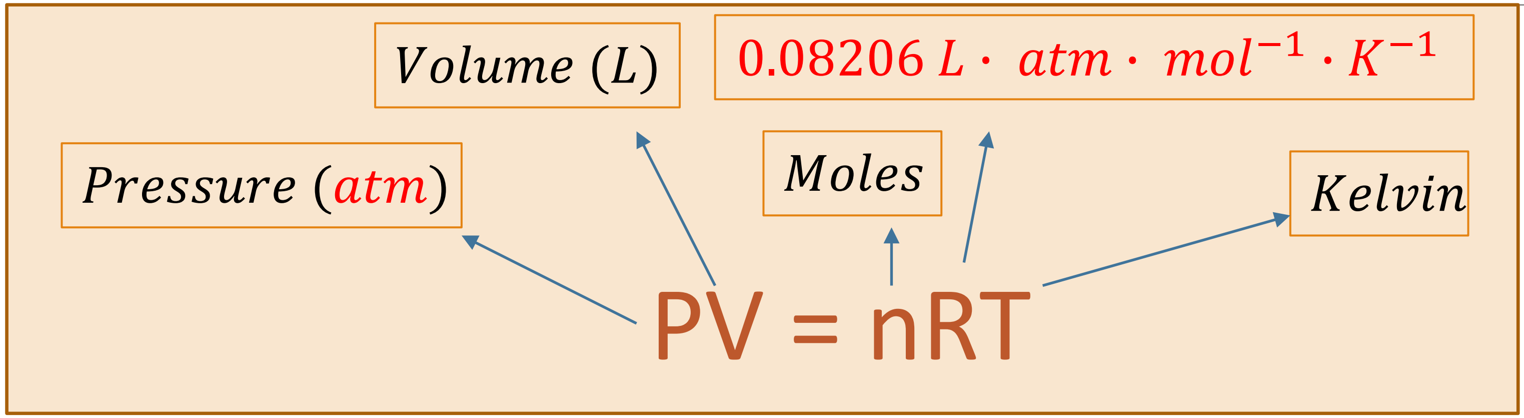
$$\text{total } V = 4L\,CO_2 + 4L\,C_2H_4$$
$$= 8L$$

Gas Laws

IDEAL, MIXTURES, KMT, NON-IDEAL

The equation that quantifies the state of a gas; solves for an unknown when the other variables are given

The Ideal Gas Law



$PV = nRT$

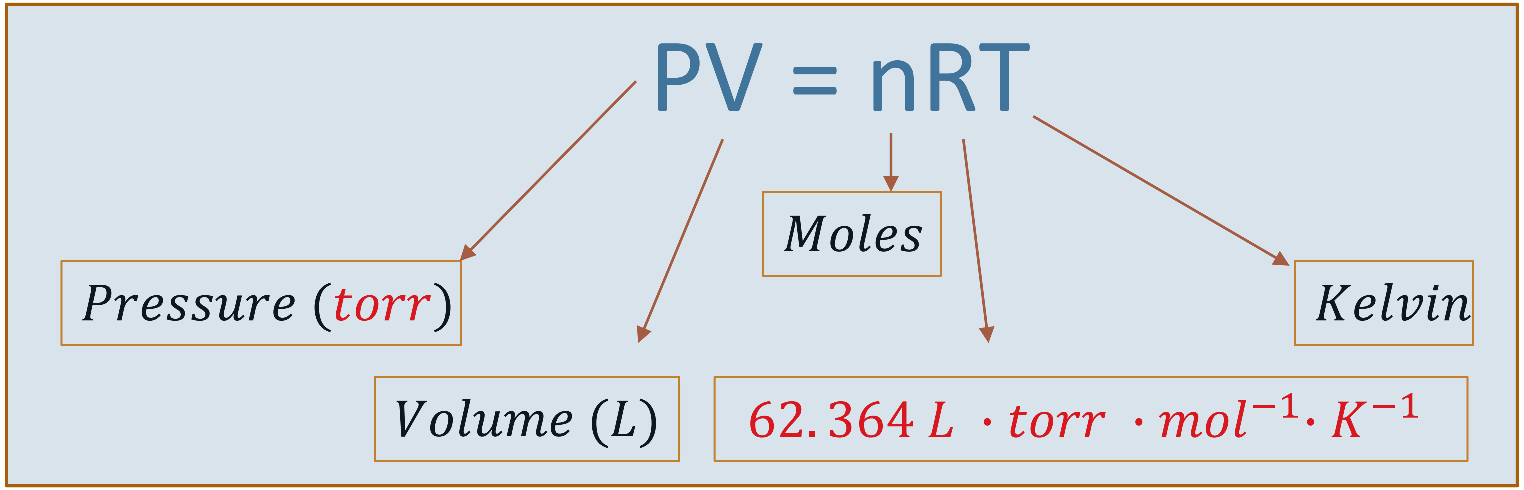
$Volume\ (L)$

$0.08206\ L\cdot\ atm\cdot\ mol^{-1}\cdot K^{-1}$

$Pressure\ (atm)$

$Moles$

$Kelvin$



$PV = nRT$

$Moles$

$Pressure\ (torr)$

$Kelvin$

$Volume\ (L)$

$62.364\ L\ \cdot torr\ \cdot mol^{-1}\cdot K^{-1}$

What do we see here?

- All units are the same except for pressure and R
- **The R you use for each problem depends on your pressure units**

The two mistakes students make:

- Using the wrong R-value
- **Using Celsius instead of Kelvin**

Note: P is pressure, ρ is mass density (m/V)

The Ideal Gas Law and Density

Choose one to memorize:

$$\rho = \frac{MW \cdot P}{R \cdot T}$$

↑

Solves directly for mass density (g/L)

$$\mathrm{MW} = \frac{\rho \cdot R \cdot T}{P}$$

↑

Solves directly for molecular weight (g/mol)

Two take-away conceptual points:

- All other conditions being equal in the ideal gas law equation (P, V, & T), **all ideal gases have the same number density;** number density depends on P, V, & T but NOT molecular weight
- All other conditions being equal in the ideal gas law equation (P, V, & T), **a heavier gas will have a greater mass density;** mass density depends on the molecular weight of the gas

$$MW \times \underbrace{(PV)}_{\checkmark} = \underbrace{(nRT)}_{\checkmark} \times MW$$

2 things:
1) Multiply by MW
2) Divide by volume

$$\begin{tikzcd} & MW \cdot P = \frac{m}{V} RT \arrow[dl] \arrow[dr] & \\ MW = \frac{\rho RT}{P} & , & \rho = \frac{MW \cdot P}{RT} \ * \end{tikzcd}$$

* NOT on formula sheet, but this is: $PV = nRT$

Unit One Question

What is the final pressure of hydrogen gas (H_2) if 4.5 mol Al reacts to completion with HCl in the following reaction, if the hydrogen gas occupies 14L at 300K

$$2Al(s) + 6HCl(l) \rightarrow 2AlCl_3(s) + 3H_2(g)$$

1. 11.9 atm
2. 0.233 atm
3. 1.07 atm
4. 0.0763 atm
5. 7.9 atm
6. 5.28 atm

$$\overset{4.5\text{ mol}}{\underline{\underline{2}\,\text{Al}(s)}} + \overset{\text{excess}}{6\text{HCl}(l)} \rightarrow 2\text{AlCl}_3(s) + \underline{\underline{3\text{H}_2}}(g) \nearrow \text{P?}$$

14L, 300K

$$4.5\text{ moles Al} \times \frac{\text{rxn}}{2\text{ moles}} = 2.25\text{ rxns}$$

$$2.25\text{ rxns} \times \frac{3\text{ moles H}_2}{\text{rxn}} = 6.75\text{ moles H}_2$$

✓ $$4.5\text{ moles Al} \times \frac{3\text{ mol H}_2}{2\text{ mol Al}} = \boxed{6.75\text{ moles H}_2}$$

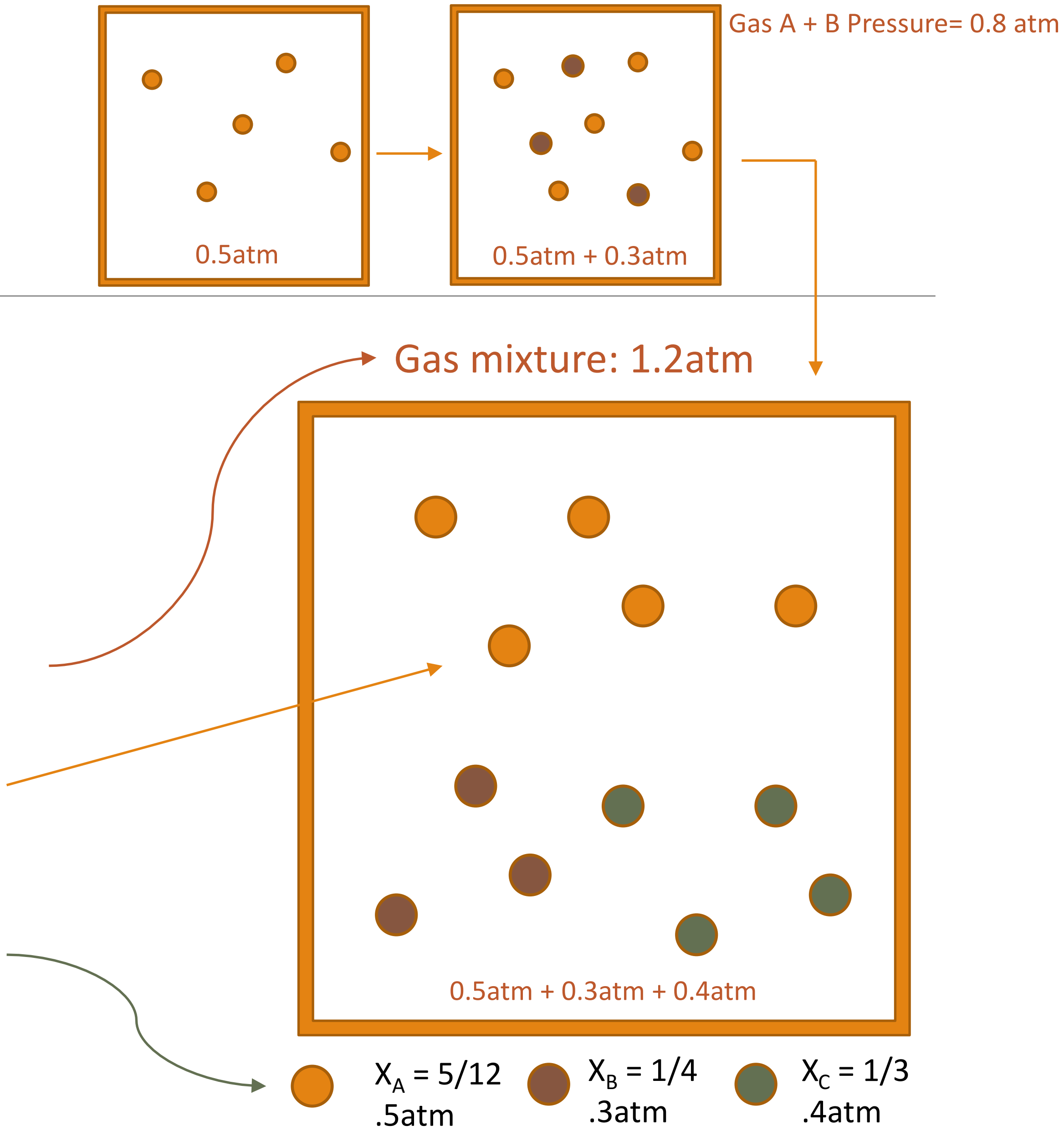
$$PV = nRT, \quad P = \frac{nRT}{V}$$

$$11.88\ \text{atm} = \frac{(6.75\ \cancel{\text{moles}})\left(0.08206\ \frac{\cancel{\text{L}}\cdot\text{atm}}{\cancel{\text{mol}}\cdot\cancel{\text{K}}}\right)(300\cancel{\text{K}})}{14\cancel{\text{L}}}$$

Partial Pressure

Partial pressure is a method for quantifying the pressures exerted by individual species in a gas mixture.

- Three terms are necessary for understanding partial pressures:
  1. **Total pressure** (P_{total}): the "actual" pressure of the system
  2. **Partial pressure** (P_i): the pressure exerted by a single species (i)
  3. **Mole fraction** (X_i): the ratio between the number of moles of a single species (i) and the total number of moles in the system



0.5atm

0.5atm + 0.3atm

Gas A + B Pressure= 0.8 atm

Gas mixture: 1.2atm

0.5atm + 0.3atm + 0.4atm

● $X_A = 5/12$ .5atm

● $X_B = 1/4$ .3atm

● $X_C = 1/3$ .4atm

Unit One Question

A 50/50 mixture (by mass) of nitrogen gas and carbon dioxide is made. What is the mole fraction of nitrogen in this mixture?

1. 0.44
2. 0.39
3. 0.73
4. 0.61
5. 0.27
6. 0.50
7. 0.56

50% 50%

$N_2 : CO_2$

50g : 50g

$$\chi_A = \frac{\text{moles}_A}{\text{moles}_{total}}, \quad \chi_{\underline{N_2}} = \frac{\text{moles}_{N_2}}{\underline{\text{moles}_{N_2} + \text{moles}_{CO_2}}}$$

not grams

$$N_2 = 50g \times \frac{1 \text{ mol}}{28 \text{ g}} = 1.79 \text{ moles } N_2$$

$$CO_2 = 50g \times \frac{\text{mol}}{44 \text{ g}} = 1.14 \text{ moles } CO_2$$

2.93 total

$$\frac{1.79}{2.93} = \boxed{0.61}$$

Standard Conditions (Memorize)

- STP is the default standard for gases
    - 0 degrees Celsius, 1atm (or 760 torr)
    - At STP, one mole of ideal gas occupies 22.4L
- STAP is a “modern” default for gases (less used)
    - 25 degrees Celsius (room temperature), 1 bar
- Thermodynamic room temperature, standard conditions
    - 25 degrees Celsius, 1 atm

Kinetic Molecular Theory

1. Gases are constantly moving in random directions
2. The distance between particles is large compared to the particle size
   - True ideal gases have relatively **no volume**
3. All particles have perfectly elastic collisions
   - There is no energy loss in the system to collisions; energy cannot be created or destroyed based on Newtonian Physics
4. No other forces act upon ideal gases
   - There are no attractive or repulsive forces that act upon ideal gas particles

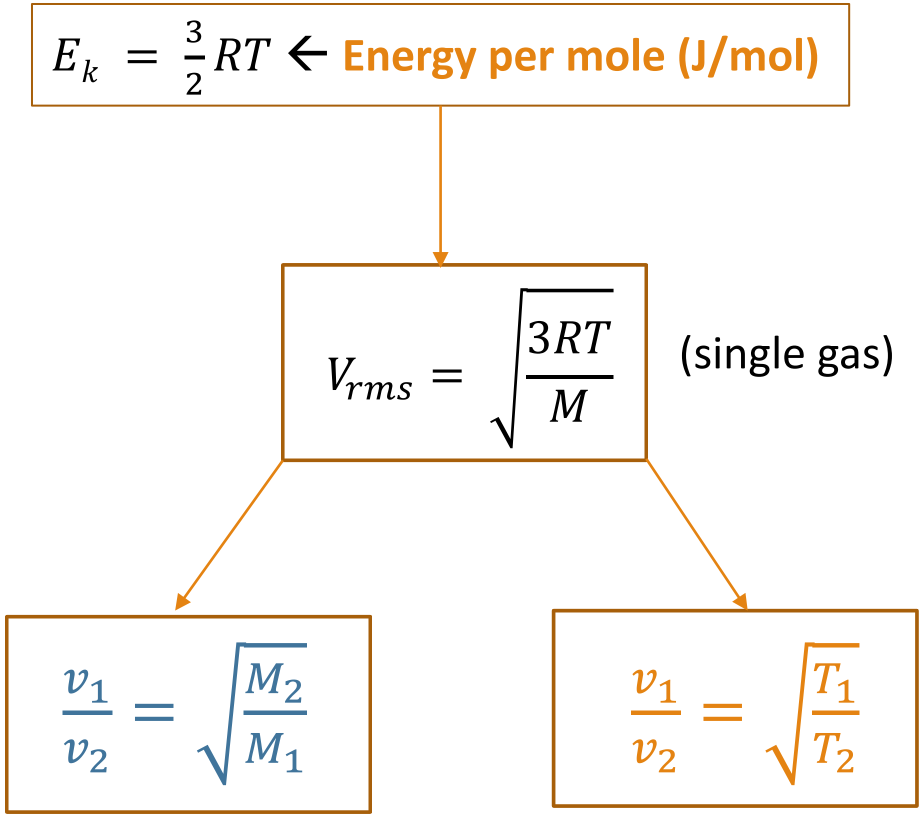
The ideal gas law fails us when these two assumptions do not hold true. Repulsions are caused by a low **available volume** (b); attractions are caused by significant **intermolecular forces** (a)

Main conclusions: the ideal gas law works because when these pillars of KMT hold true in a system. The ideal gas law is modeled best at **High Temperature** and **Low Pressure**

Kinetic Molecular Theory: Relationships

- Kinetic Molecules Theory gives us three key relationships that you should know as equations and by definition (in words)

1. **Kinetic Energy vs. Temperature**
    - Kinetic energy is dependent solely on the temperature of a gaseous system (direct relationship)
    - R = 8.314 J / mol K
    - Temperature in Kelvin
2. **Mass vs. Velocity**
3. **Temperature vs. Velocity**



$E_k = \frac{3}{2}RT$ ← **Energy per mole (J/mol)**

$$V_{rms} = \sqrt{\frac{3RT}{M}}$$

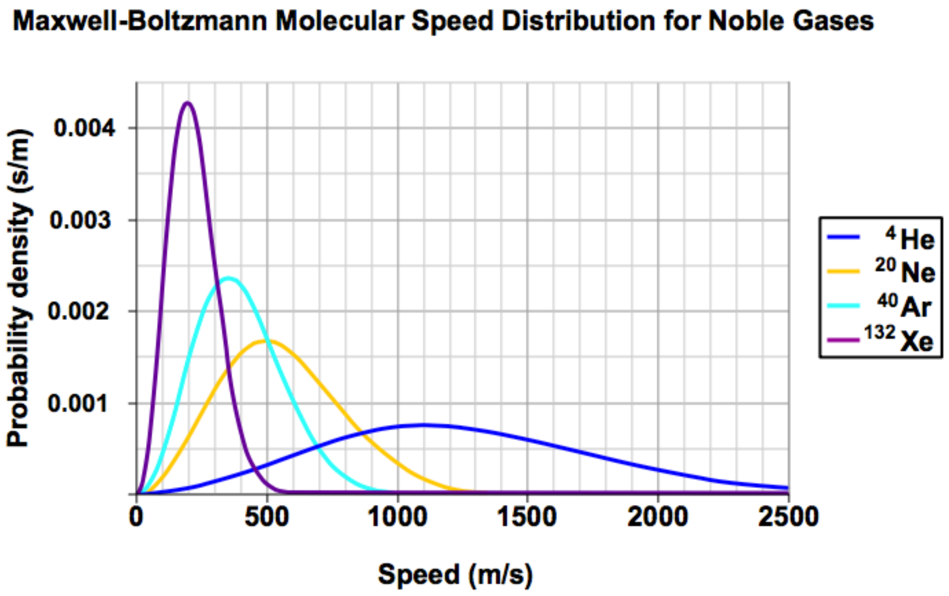
(single gas)

$$\frac{v_1}{v_2} = \sqrt{\frac{M_2}{M_1}}$$

$$\frac{v_1}{v_2} = \sqrt{\frac{T_1}{T_2}}$$

(ratio problems)

KMT: Mass vs. Velocity; Velocity vs. Temperature



- Some key features of this graph include:
  - Each curve looks like a unimodal distribution with a "tail" that approaches the limit infinite velocity (0 probability density)
  - Molecules are traveling at a variety of speeds but there is a clear average
  - The actual V_{rms} is slightly to the right of the peak

1. **Mass vs. Velocity (V_{rms})**
   - We can see that the heavier gases move slower and the lighter gases move faster
   - The faster the gas, the wider the distribution
2. **Velocity (V_{rms}) vs. Temperature**
   - If you were working with the same gas, a similar graph could be created by modifying temperature instead.
   - In this case, higher temperatures of the same gas result in faster speeds.

Pay very close attention to how the 1 and 2 match up in these relationships

KMT: Ratio Problems

When considering two gases, you can use the KMT equation to create a ratio:

1. **Mass vs. Velocity (V_{rms}) (same temperature, different molecule)**
   - Velocity is proportional to the inverse square root of mass.
   - **When temperature is constant, lighter particles move faster**

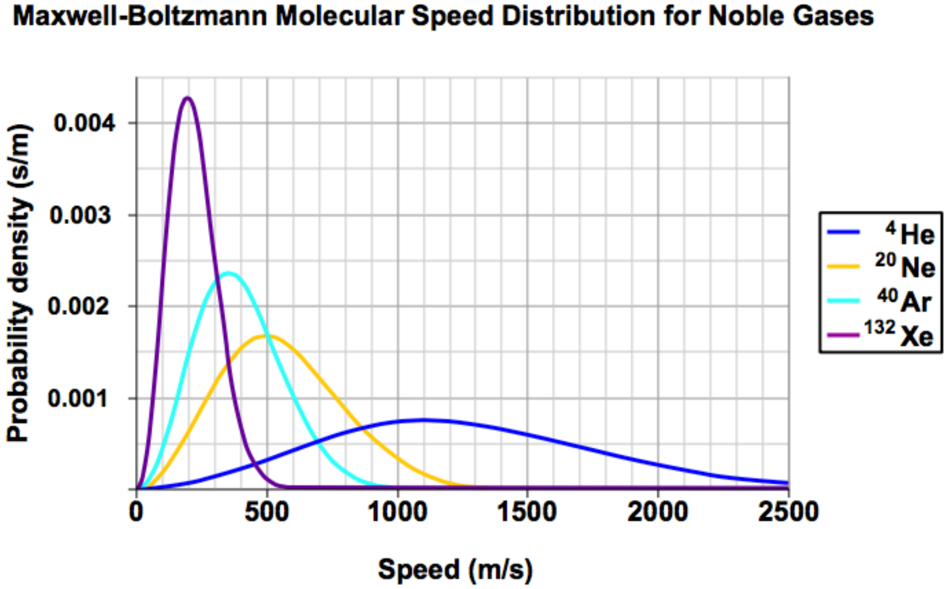
$$\frac{v_1}{v_2} = \sqrt{\frac{M_2}{M_1}}$$

2. **Velocity (V_{rms}) vs. Temperature (same molecule, different T)**
   - Velocity is proportional to the square of temperature
   - **When dealing with the same species gas, particles move faster at higher temperatures**

$$\frac{v_1}{v_2} = \sqrt{\frac{T_1}{T_2}}$$

Practice: What is the ratio of the effusion rates of SO_2 to Cl_2?

Maxwell-Boltzmann Distribution



- Given a Maxwell distribution, you should know:
  - Find the approximate **V_{rms}**
  - Be able to label **which gas is which** (or which temperature is which)
  - Understand the **relationships** between mass, velocity, and temperature
  - Understand how these relationships impact the **shape** of the curve

The Non-Ideal Gas Law

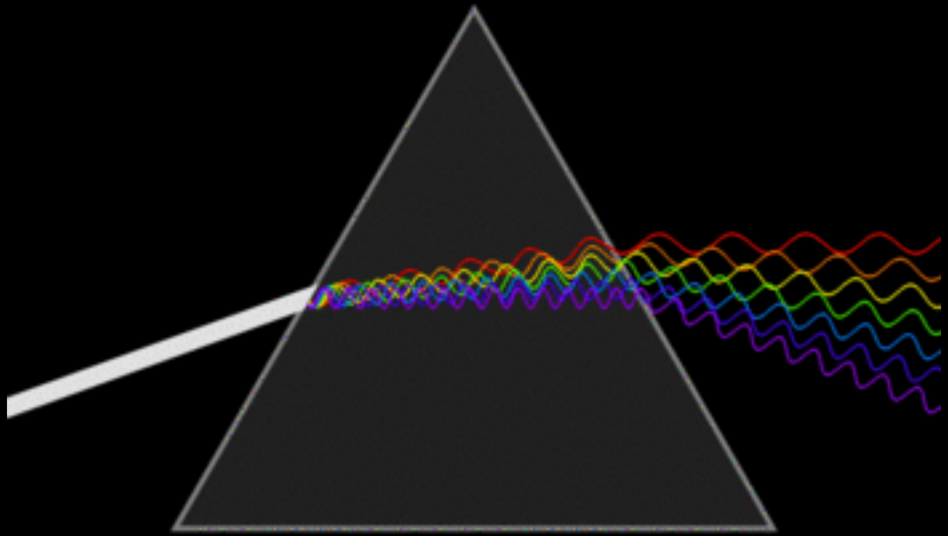
- **The Ideal Gas Law is adjusted for real gases in the following way:**

$$(P + \frac{an^2}{V^2})(V - nb) = nRT$$

- Important Notes:
  - The pressure expression $(P + \frac{an^2}{V^2})$ is equal to the **ideal pressure**. The P term is the **measured pressure**.
  - The volume expression $(V - nb)$ is equal to the **available volume**. The V term is the **volume of the container**.
- Key points:
  - Attractive forces decrease the pressure. **Stronger attractive forces give a larger “a” value**.
  - The size of the molecules decrease the available volume. **Larger molecules give a larger “b”**.
    - A larger b value correlates with more repulsions. Repulsions are an effect of the fact that two gas molecules can’t take up the same space – therefore, they repel each other

Favoring Non-Ideal Vs. Ideal Conditions

Ideal Conditions	**Non-Ideal Conditions**
High Temperature	Low Temperature
Low Pressure	High Pressure
High Volume	Low Volume
Small Molecules (small b term)	Large Molecules
No attractive forces (small a term)	High Attractive Forces (Intermolecular forces)
Small number of molecules	Large number of molecules

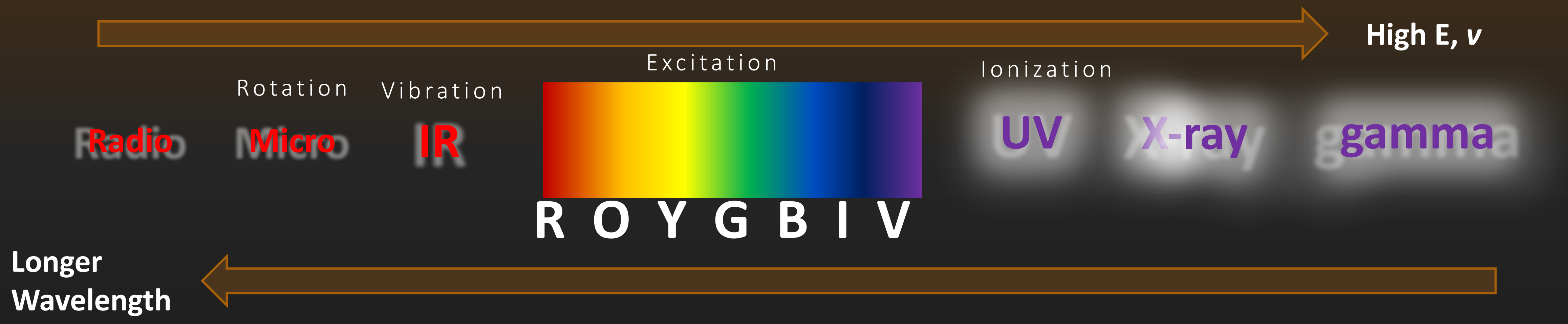


Atomic Theory

LIGHT, QUANTUM, ELECTRON CONFIGURATIONS, PERIODIC TRENDS

$c = \lambda\nu$; $E_{photon} = h\nu$; $E_{photon} = \frac{hc}{\lambda}$

THE ELECTROMAGNETIC SPECTRUM



High E, *ν*

Rotation Vibration Excitation Ionization

Radio Micro IR

R O Y G B I V

UV X-ray gamma

Longer Wavelength

- Microwaves: enough energy to begin rotating a molecule
- IR: enough energy to begin vibrating a molecule
- Visible (700nm to 400nm): enough energy to begin exciting electrons
- UV and beyond: begins the full ionization (breaking) of electrons/bonds

*: know how to make calculations
~~*: understand conceptually only~~
~~*: understand how to model the equation (PIB and RDF)~~

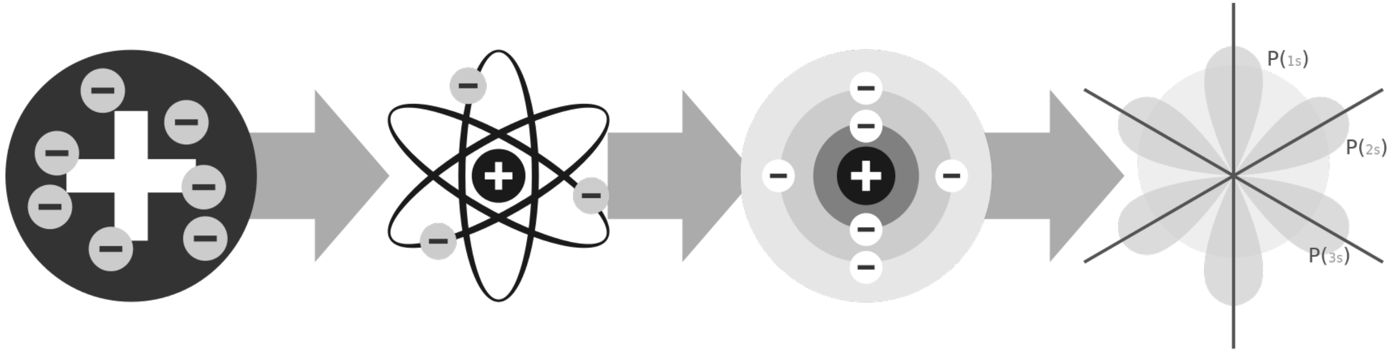
Quantum Mechanics: Evidence

1. Electrons exist in **discrete, quantifiable energy states**.
   - Absorption/Emission spectra: The line spectra for a given gas has characteristic wavelengths *
2. Electrons and light (photons) exhibit **wave-particle duality**.
   - Photoelectric effect: Light can act like particles (photons): *
     - Light of sufficient energy interacts with matter by ejecting electrons from a metal surface
   - ~~X-Ray diffraction: Small particles (electrons) can act like waves~~ *
     - ~~A perfect crystal will scatter incident x-rays into specific interference patterns~~
3. The location and behavior of electrons can be described only with **probabilities**.
   - The Schrödinger Equation: Uses an understanding of probabilities and uncertainty to give us useful information about the electrons of an atom, such as the 4 quantum numbers (n, l, m_l, and m_s) *

What is Quantum Mechanics?

- Quantum mechanics is the currently accepted model of the atom that describes the motion of subatomic particles and the interactions between them using the following empirically derived postulates:

1. Electrons exist in **discrete, quantifiable energy states** (Rydberg, absorption/emission)
2. Electrons and light (photons) exhibit **wave-particle duality** (photoelectric effect, ~~deBroglie~~)
3. The motion of electrons can be described only with **probabilities**. That is, only the position or momentum can be known with certainty at any given time (wave functions, ~~uncertainty principle~~)
    - Furthermore, this demonstrates that electrons exist in “clouds” and not circular orbits

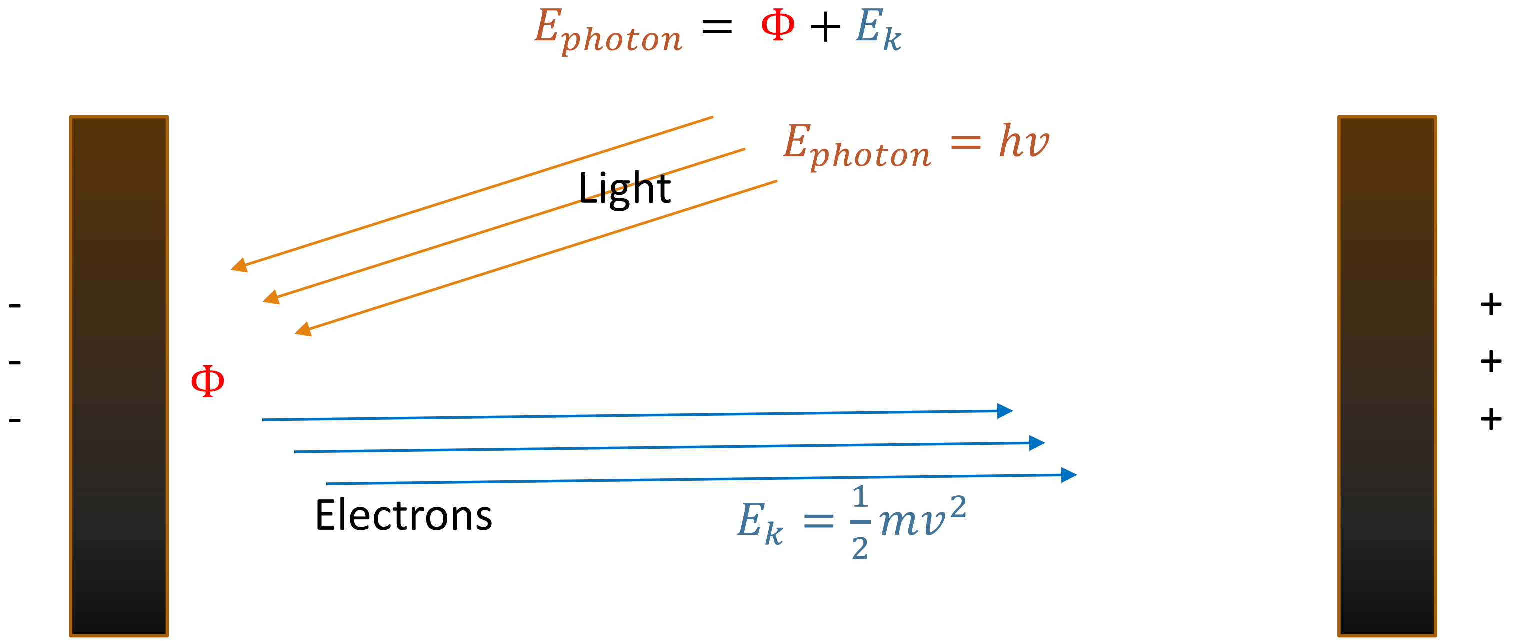


Classical Theory

Quantum Theory

Quantum Mechanics: Photoelectric Effect

- **Photoelectric Effect**: a metal will eject electrons if a beam of light reaches a threshold energy
  - Demonstrates how light can act as a particle when interacting with matter (the electrons of a metal)
  - Quantifies this interaction using the equations shown below:



$$E_{photon} = hv$$

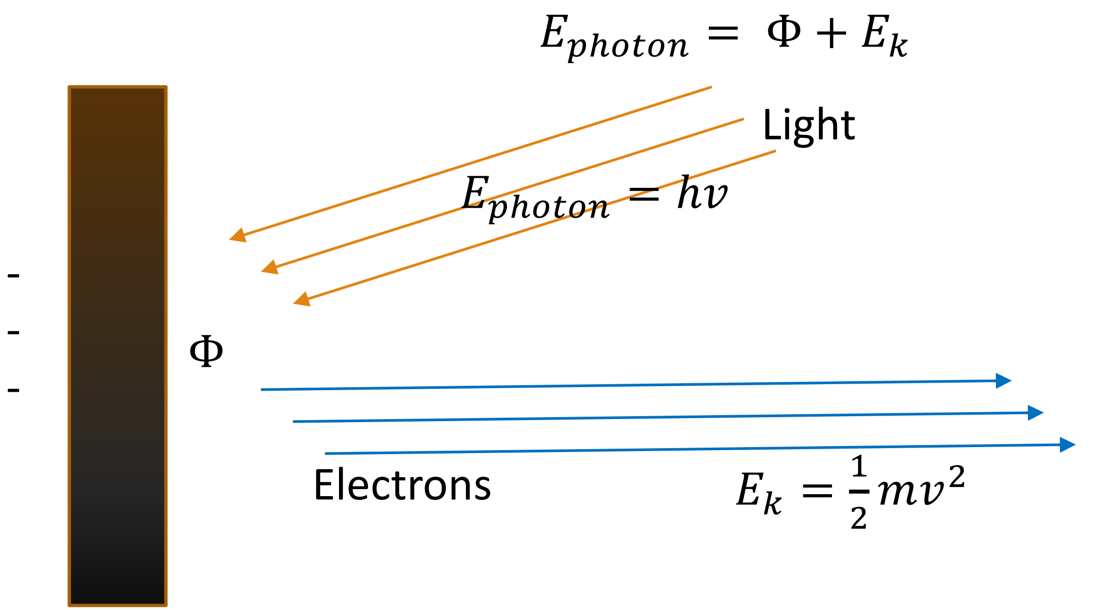
If threshold is met:

$$E_{photon} = \Phi + E_k$$

$$E_k = E_{photon} - \Phi$$

$$E_k = \frac{1}{2}mv^2$$

Quantum Mechanics: Photoelectric Effect



$$E_{photon} = \Phi + E_k$$

$$E_{photon} = hv$$

$$E_k = \frac{1}{2}mv^2$$

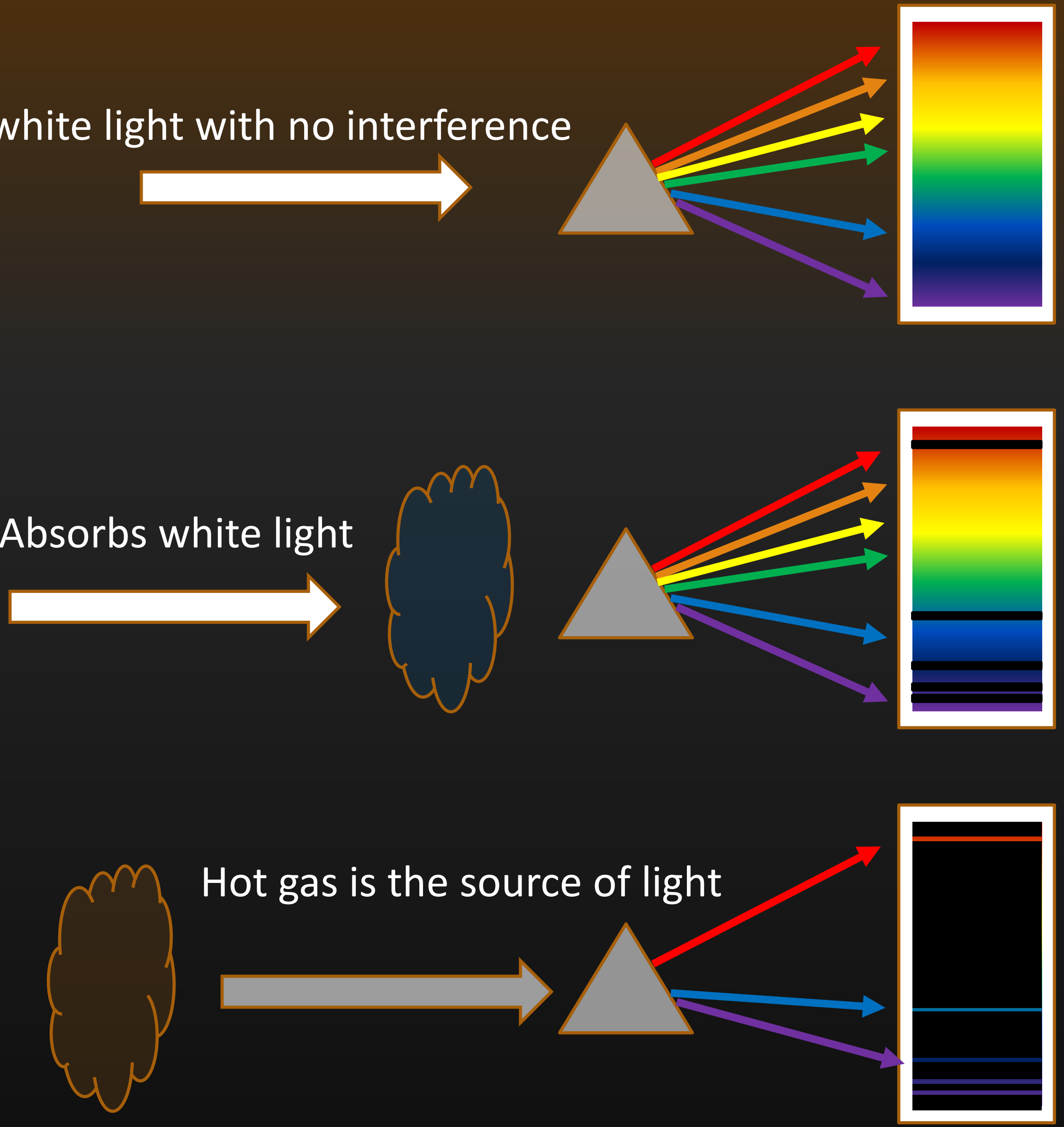
IF THE WORK FUNCTION IS REACHED:

- **Increasing intensity:**
  - Increases the number of emitted electrons
  - Has NO EFFECT on the kinetic energy/ velocity of the emitted electrons
- **Increasing the energy of the photon** (or increasing the frequency/decreasing the wavelength):
  - Increases the kinetic energy of the emitted electrons
  - Increases the velocity of the emitted electrons
  - Has NO EFFECT on the number of electrons

Unit the work function is reached ($E_{photon} < \Phi$):

- **Increasing intensity has no effect**
- Note: photon energy is **NOT additive in terms of reaching the work function**. Two 2.5eV photons does NOT equal 5eV overall.

Line spectra in various experiments



Pure white light with no interference

CONTINUOUS

Cold Gas Absorbs white light

ABSORPTION

Hot gas is the source of light

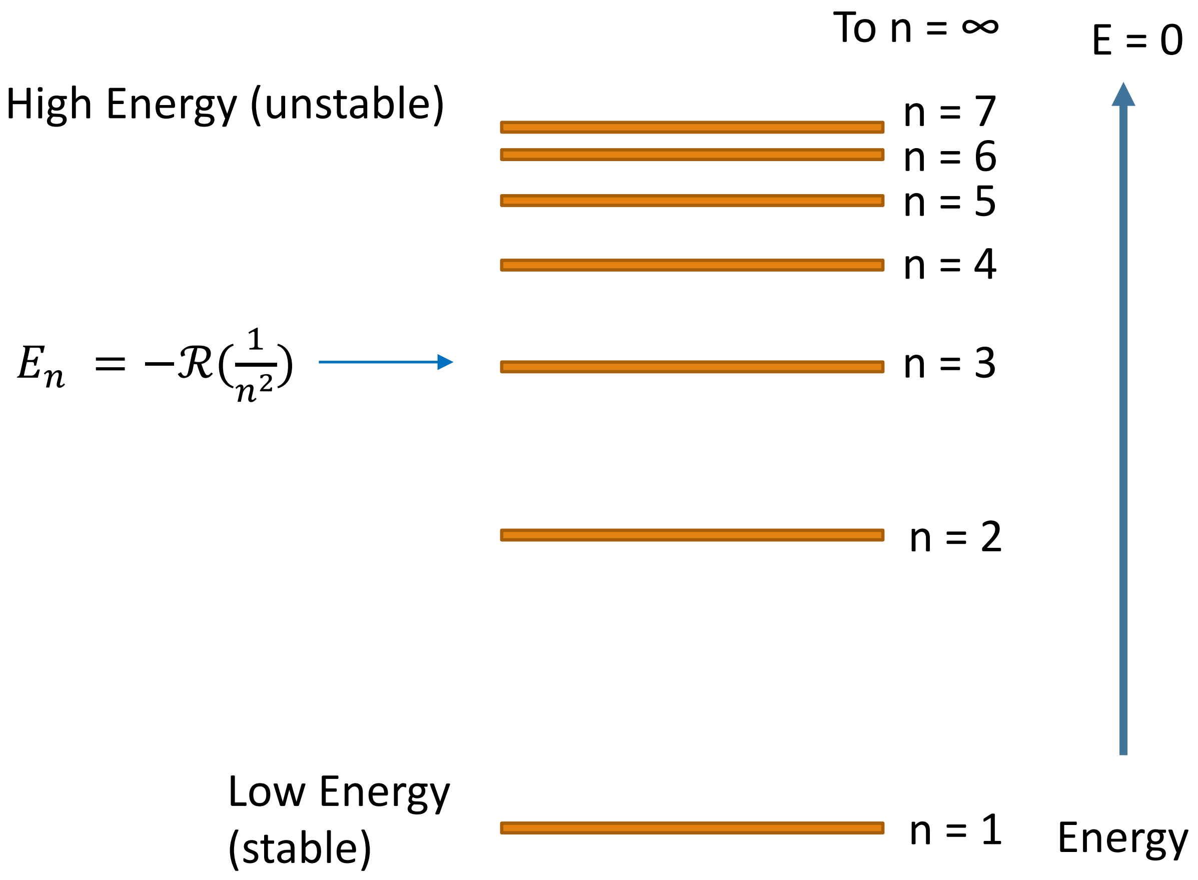
EMISSION

NOTICE HOW THESE ARE OPPOSITES FOR ANY GIVEN GAS. THIS IS EVIDENCE OF THE DISCRETE ENERGY LEVELS OF ELECTRONS

SPECIFIC GASES HAVE THEIR OWN DISCRETE ENERGY PATTERNS

Quantum Mechanics: The Bohr Model

- The Bohr Model of the atom explained that electrons exist in "energy states," which we now designate the letter "n."
- You can understand n values by following these rules:
  1. n values begin at 1 (closest to the nucleus) and go to infinity (completely out of the influence of the nucleus/ free in space)
  2. The lower n value means more stable (most negative potential energy)
  3. The greatest energy difference between two **consecutive** numbers is 1 and 2.
- This model works only for one-electron systems (the hydrogen atom), and collapses due to electron repulsions for more complex atoms



To n = ∞

E = 0

High Energy (unstable)

n = 7

n = 6

n = 5

n = 4

$$E_n = -\mathcal{R}\left(\frac{1}{n^2}\right) \longrightarrow$$

n = 3

n = 2

Low Energy (stable)

n = 1

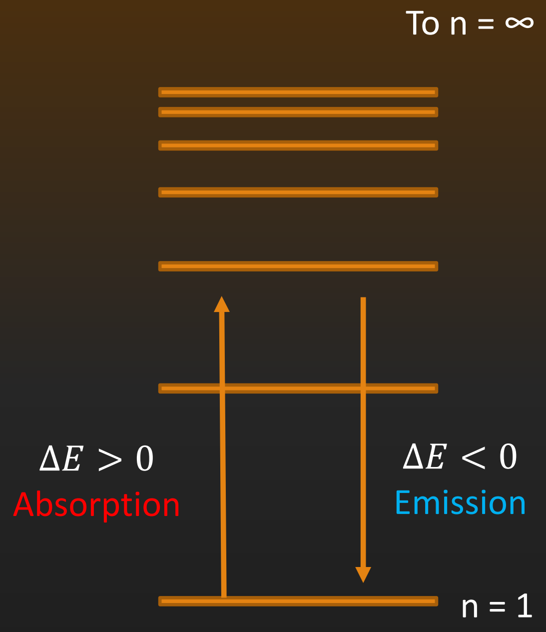
Energy

RYDBERG EQUATION

$$\Delta E = \mathcal{R}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

R = 2.18 X 10^{-18}J

$$|\Delta E| = E_{photon} = h\nu = \frac{hc}{\lambda}\ ^{*}$$



To n = ∞

$\Delta E > 0$
Absorption

$\Delta E < 0$
Emission

n = 1

Electron energy level transition	**Sign of ΔE**	**Absorption/Emission ($\|\Delta E\|$)** **(Cause/Effect)**
Low n to high n	Positive (increasing energy)	Light absorbed
High n to low n	Negative (decreasing energy)	Light emitted

* The energy, wavelength, and frequency of the light are always positive

Unit Two Question

Which transition between energy levels in a hydrogen atom corresponds to the shortest wavelength of light?

1. 2 to 3
2. 3 to 5
3. 5 to 6
4. 3 to 4
5. 2 to 5
6. 2 to 4

Unit Two Question

Which transition between energy levels in a hydrogen atom corresponds to the shortest wavelength of light?

1. 2 to 3
2. 3 to 5
3. 5 to 6
4. 3 to 4
5. 2 to 5
6. 2 to 4

Unit Two Question

What is the wavelength of the photon corresponding to the change from n = 2 to n = 5? Is this photon emitted or absorbed?

1. 434nm absorbed
2. 434nm emitted
3. 276nm absorbed
4. 276nm emitted
5. 1875nm emitted

$$E = R\left(\frac{1}{n_1^2} - \frac{1}{n_1^2}\right), \quad E = h\nu, \quad E = \frac{hc}{\lambda}$$

$$\downarrow$$

$$2.18\times10^{-18}\,\mathrm{J}\left(\frac{1}{2^2} - \frac{1}{25}\right) = 4.58\times10^{-19}\,\mathrm{J}$$

$$\frac{hc}{E} = \lambda = \frac{(6.626\times10^{-34}\,\mathrm{J\cdot s})(3\times10^{8}\,\frac{\mathrm{m}}{\mathrm{s}})}{4.58\times10^{-19}\,\mathrm{J}}$$

$$4.34\times10^{-7}\,\mathrm{m}\ \xrightarrow{\times10^{9}\,\frac{\mathrm{nm}}{\mathrm{m}}}$$

$$\boxed{\text{434 nm, absorbed}}$$

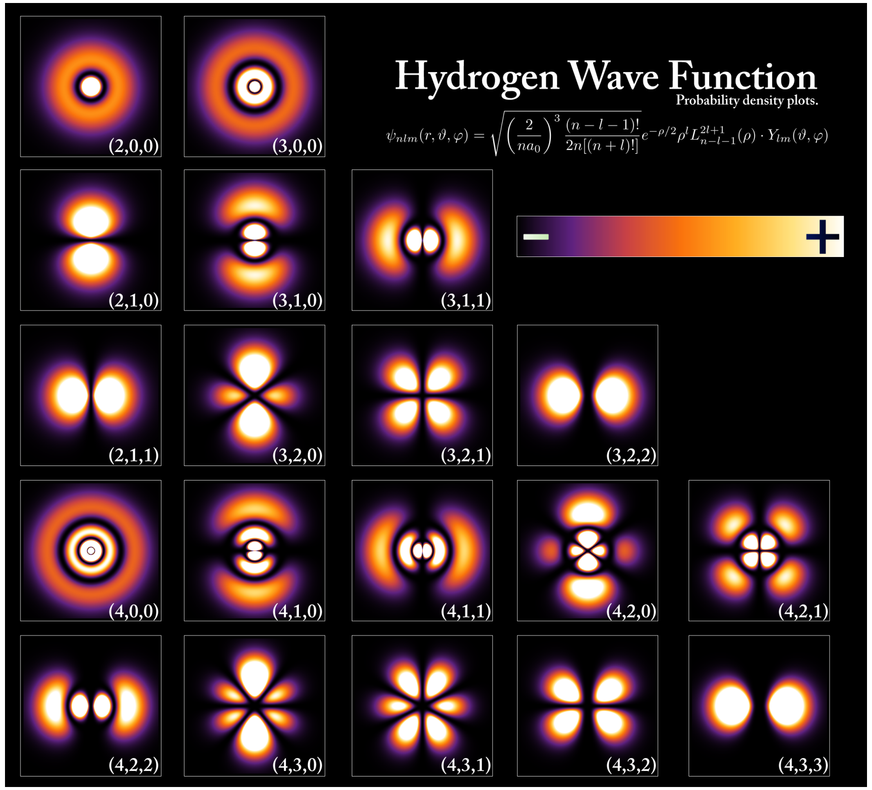
Absorbed? → Low to high n

Emitted? → High to low n

Conceptual look into the Schrödinger Equation

$$\underbrace{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}}_{\text{kinetic energy}} + \underbrace{V(x)\psi}_{\text{potential energy}} = \underbrace{E\psi}_{\text{total energy}}$$

- The Schrödinger Equation gives us infinite wave functions (solutions) for the Hydrogen atom.
- The wave functions are classified by the quantum numbers:
  - Principle Quantum Number, n (Energy)
  - Angular Momentum Quantum Number, l (Shape)
  - Magnetic Quantum Number, m_l (Orientation)
- **This ultimately tells us the energy of an electron and the probable location of that electron in three dimensional space.**



Quantum Numbers

- The Quantum Numbers (n, l, m_l, and m_s) stem from the solutions of the Schrödinger Equation and represent the following:

1. **Principle Quantum Number (n):** the size and energy of the shell; mostly corresponds to the row of the periodic table (exception: d, f block).
2. **Angular Momentum (l):** the shape of the subshell; corresponds to the region on the periodic table.
   - 0= s subshell; 1 = p subshell; 2 = d subshell; 3 = f subshell
   - Depending on the question, l can signify the shape OR the shape can signify l
3. **Magnetic (m_l):** the orbitals of the subshell; mathematically indicates the orientation of the subshell shape
   - The number of possible m_l values is equal to the number of orientations possible in space, which therefore represents the number of orbitals available
4. **Spin Magnetic (m_s):** the spin of the electrons in a subshell
   - Can equal ½ or - ½, but all that really matters is that no two electrons in the same orbital have the same value

Quantum Numbers: Rules

We are mostly interested in assigning possible quantum numbers to the electrons of a given species. To do this, we must understand the rules for assigning quantum numbers:

Principle Quantum Number (n) = 1,2,3, …to n = ∞

Angular Momentum (l) = 0,1,2,… to n-1

Magnetic (m_l) = -l to l

Spin Magnetic (m_s) = $\pm\frac{1}{2}$

Example:

If n = 4

l can equal 0,1,2,3

m_l can equal -3,-2,-1,0,1,2,3

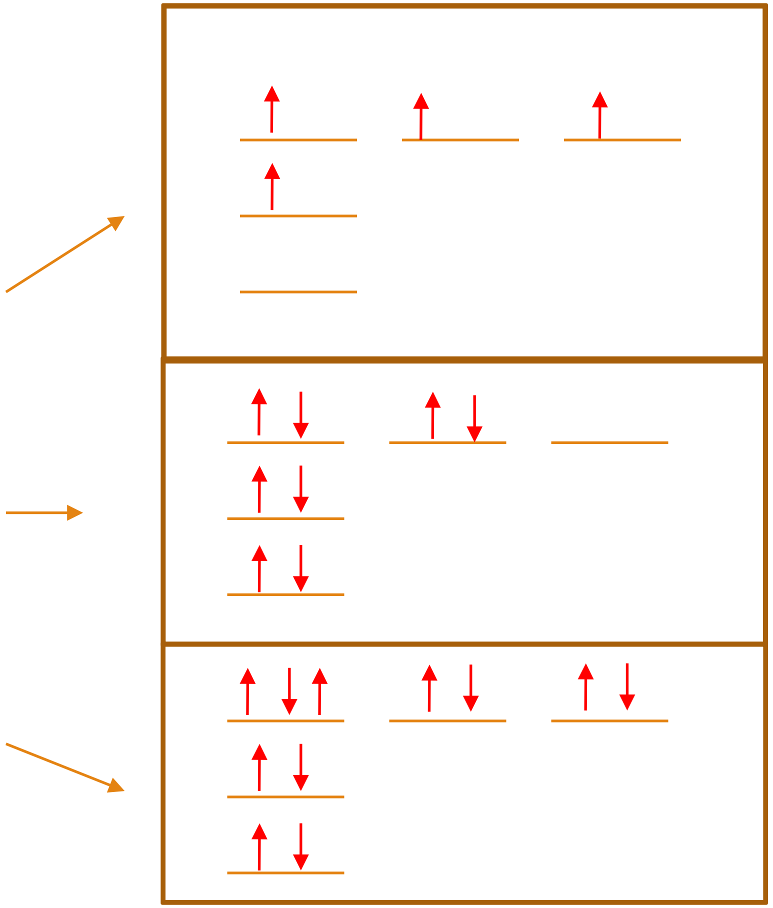
m_s = +/- 1/2

Ways to designate quantum numbers without saying it directly:

- "Highest energy electrons" = look at the last filled electrons. This will give you n and l.
- If we say 4s, we are giving you n (4) and l (s= 0)

Electron Configurations: Rules

- There are three main rules to abide by when filling out electron configurations. It is important to follow these rules when doing your own electron configurations and be able to identify the rule that an incorrect electron configuration breaks
- **Aufbau Principle:** fill electrons from the bottom (lowest energy) up
- **Hund's rule:** fill each orbital in a given subshell with a single electron before doubling up
  - Technically this refers to the idea that you should maximize the multiplicity of your configuration
- **Pauli's Exclusion Principle:** no electrons can occupy the same orbital with the same spin and a maximum of two electrons can exist in a single orbital



Note: these are all examples of these rules violated

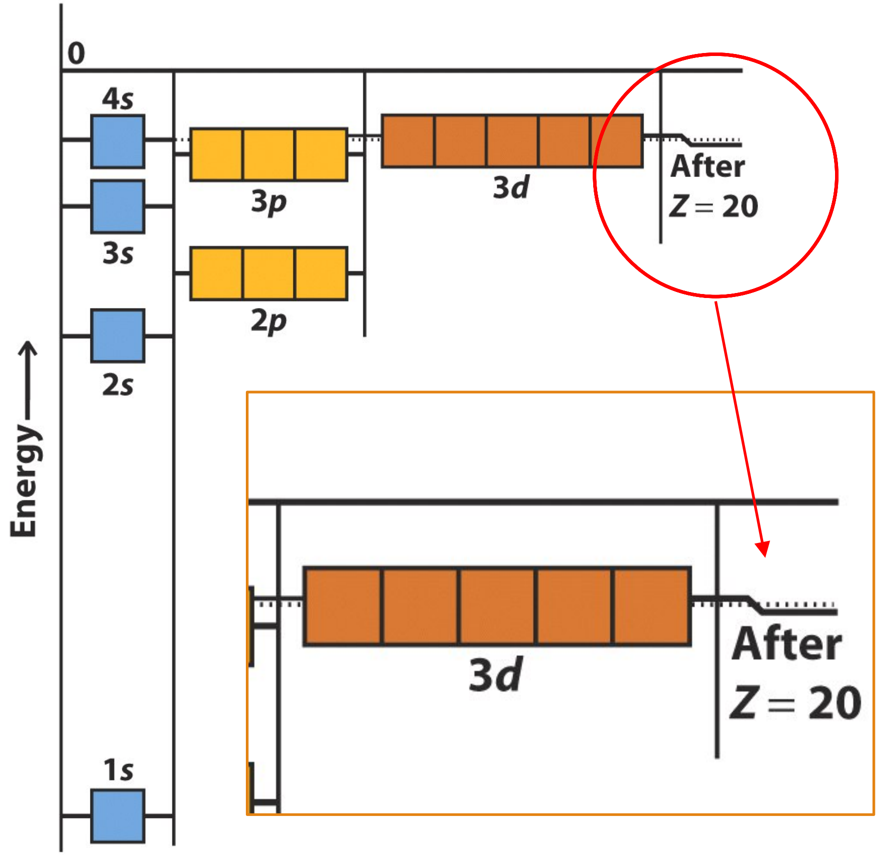
Filling versus "Unfilling"

$[Fe] = [Ar]4s^2 3d^6$

$[Fe^{2+}] = [Ar]3d^6$

Why?

- When filling, use the "Aufbau" Order
- When "unfilling," use the "Energy" Order
  - What's the rule? Unfill the HIGHEST n value FIRST



Ion Electron Configurations

- If you want to write the electron configuration of an ion, start with the neutral atom and then add (- charge) or remove (+ charge) electrons accordingly.
- Easy: O^{2-}

$$O : [He]2s^2 2p^4$$

$$O^{2-} : [He]2s^2 2p^6 \text{ or just } [Ne]$$

- Difficult: Zr^{2+} OR Ti^{2+} (from exam 2)

$$Zr : [Kr]5s^2 4d^2 \qquad Ti : [Ar]4s^2 3d^2$$

$$Zr^{2+} : [Kr]4d^2 \qquad Ti^{2+} : [Ar]3d^2$$

$$Ti^{3+} \ [Ar]3d^1$$

Electron Configurations: Exceptions

- D-block and f-block elements prioritize filling their half-way or fully filled subshells if they are one electron away.
- The most common examples of this are chromium and copper. You would expect to write chromium with 4 electrons in 3d and copper with 9 electrons in 3d. Instead, you borrow one electron from the 4s to fill the subshell.

Expected: Cr = [Ar]$4s^2 3d^4$

Expected: Cu = [Ar]$4s^2 3d^9$

- The actual electron configurations:

Cr = [Ar]$4s^1 3d^5$

Cu = [Ar]$4s^1 3d^{10}$

D-Block Exceptions

$[Cu] = [Ar]4s^1 3d^{10}$

$[Cr] = [Ar]4s^1 3d^5$

Why?

- The ½ filled s and fully filled d is more stable than the “non-exception” configuration
- The ½ filled s and ½ filled d is stable than the “non-exception” configuration

Know: Cu, Mo, Cr, Ag

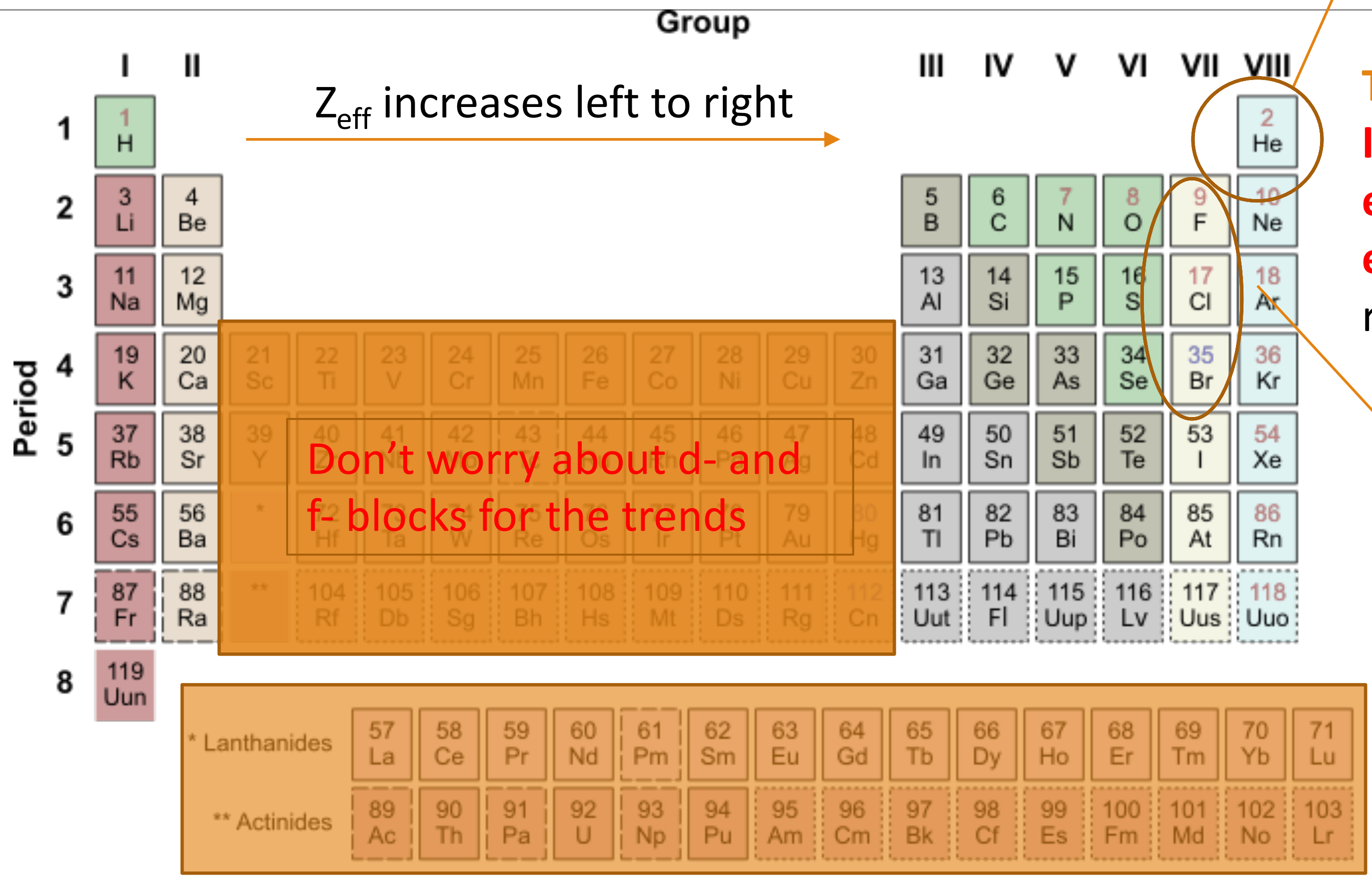
Basic Periodic Table Trends

- Ionization Energy: the energy required to **remove an electron** from an atom in the gas phase
  - Trend: generally increases going to the top right of the periodic table (*has notable exceptions)
  - Increases with each successive ionization (the second ionization energy is greater than the first, and so on)
- Electron Affinity: in much the opposite reaction, electron affinity is the energy released to **add an electron** to an atom in the gas phase
  - Trend: Electron affinity does not follow a stable trend; however, it generally trends toward the top right of the periodic table.
- Atomic Radius: size of the nucleus and its electrons (most of the size is in the space taken up by the electron clouds)
  - Trend: increases as you go to the bottom left where shielding is maximized and z_{eff} is minimized
- Z_{eff}: a measurement of the **pull of any given electrons (generally the valence) by the nucleus**
  - Trend: increases as you go from left to right
  - Remember: Z_{eff} = Atomic Number – Core Electrons
- **Electronegativity: how much an atom wants to pull the electron density in a covalent bond (leads to polarity)**
  - **Trend: increases as you go to the top right.**

Periodic Trends

Shielding Increases going down

Z_{eff} increases left to right



Group

Period	I	II											III	IV	V	VI	VII	VIII
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40	41	42	43	44	45	46	47	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	Hf	Ta	W	Re	Os	Ir	Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo
8	119 Uun																	

* Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
** Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Don't worry about d- and f- blocks for the trends

Helium has the maximum ionization energy

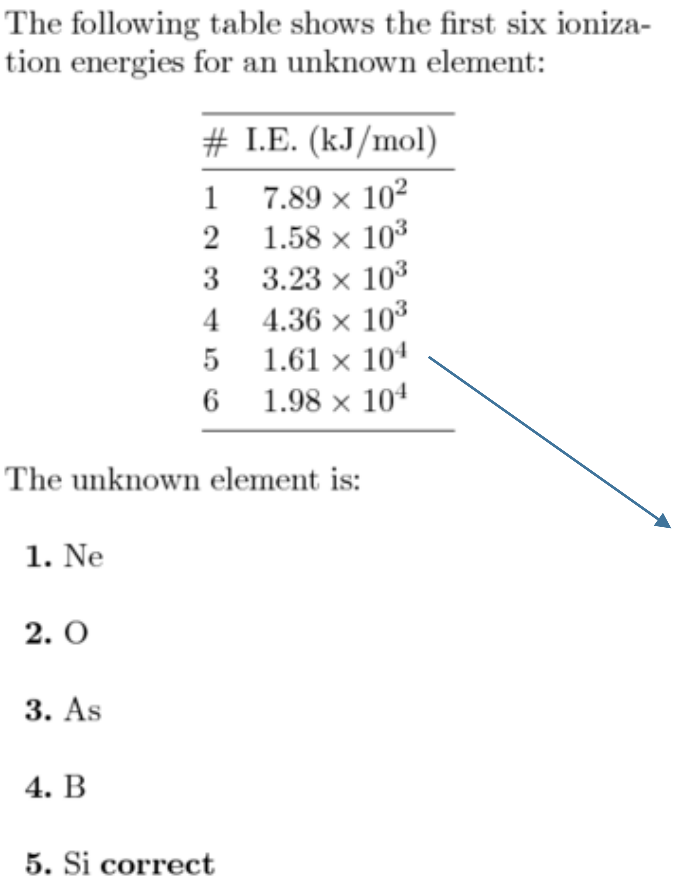
TOP RIGHT: **High Ionization energy, high electron affinity, high electronegativity,** small radius

The halogens have the highest electron affinity

Bottom Left: Low ionization energy, low electron affinity, low electronegativity, **large radius**

Note: all Si atoms in these equations are in the gas state

Successive Ionization Energies



The following table shows the first six ionization energies for an unknown element:

#	I.E. (kJ/mol)
1	7.89×10^2
2	1.58×10^3
3	3.23×10^3
4	4.36×10^3
5	1.61×10^4
6	1.98×10^4

The unknown element is:

1. Ne

2. O

3. As

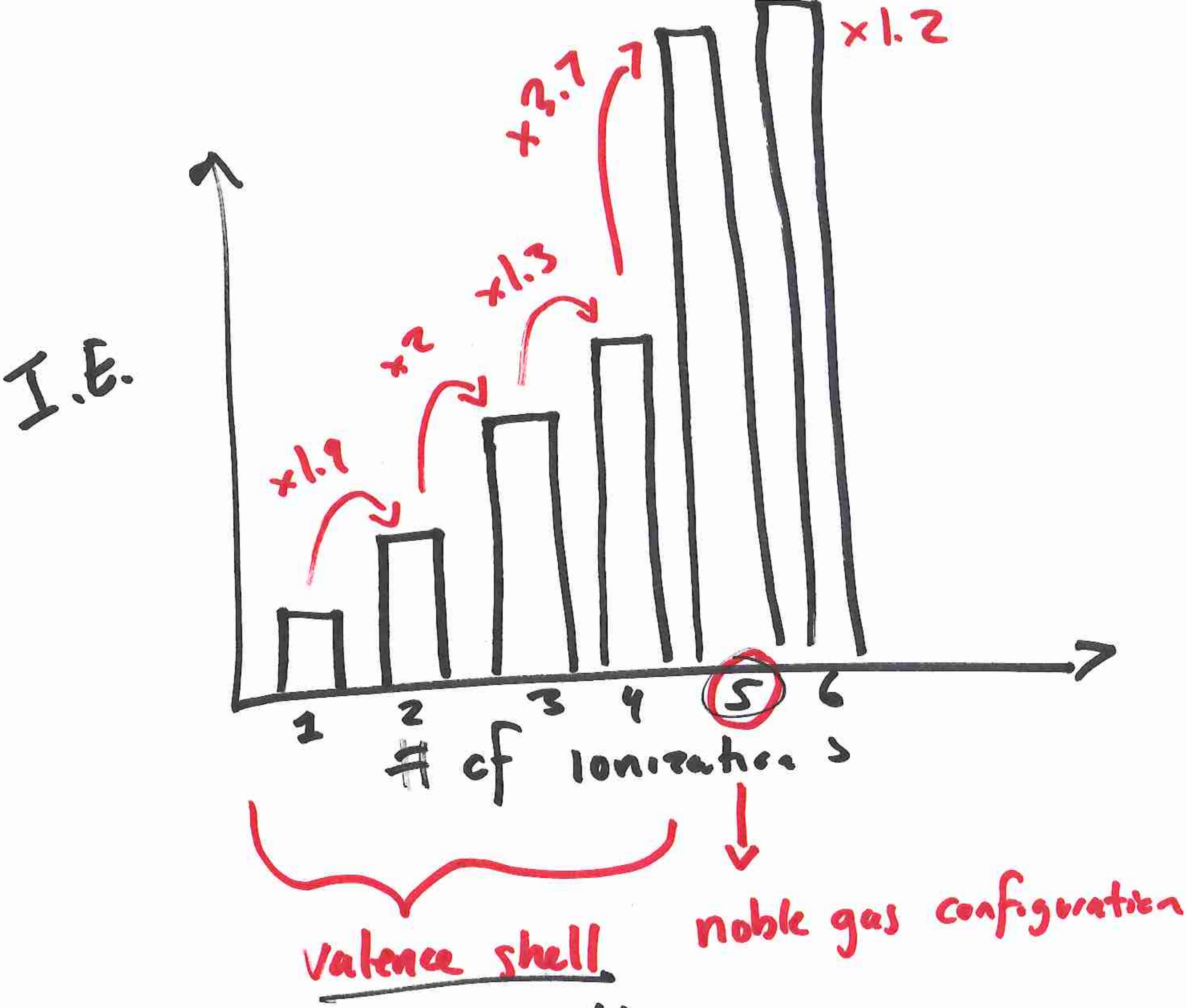
4. B

5. Si **correct**

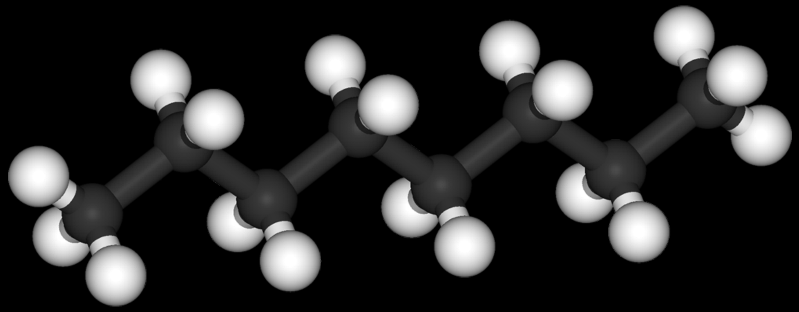
Energy increases for each successive ionization energy for the same atom

Big jump in IE means Si^{4+} is most likely the noble gas configuration

1. $\mathrm{Si} \rightarrow Si^{+} + e^{-}$
2. $Si^{+} \rightarrow Si^{2+} + e^{-}$
3. $Si^{2+} \rightarrow Si^{3+} + e^{-}$
4. $Si^{3+} \rightarrow Si^{4+} + e^{-}$
5. $Si^{4+} \rightarrow Si^{5+} + e^{-}$
6. $Si^{5+} \rightarrow Si^{6+} + e^{-}$


I.E.
x1.9
x2
x1.3
x3.7
x1.2
1
2
3
4
5
6
# of ionizations
valence shell
noble gas configuration

group # = 4



Bonding

LEWIS STRUCTURES, VSEPR, VB, MO

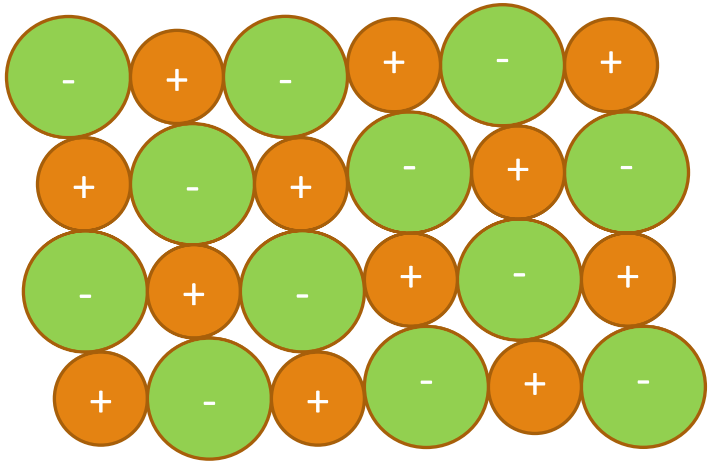
Lattice Energy

Is lattice energy positive or negative?

- Depends on how you're measuring it. But use the absolute value.
- **Lattice energy indicates the amount of energy necessary to overcome the negative potential energy binding the charges of an ionic compound**

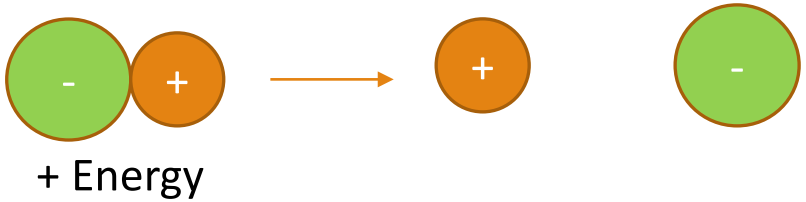
- Lattice Energy: is directly proportional to the charges of the ions (q_1 and q_2) and inversely proportional to the size of the ions (r)

$$\Delta H_{lattice} \propto \frac{q_1 q_2}{r}$$



- This describes the energy required for the following reaction:

$$NaCl(s) \rightarrow Na^{+}(g) + Cl^{-}(g)$$
$$NaOH\ (s) \rightarrow Na^{+}(g) + OH^{-}(g)$$



When Ranking Lattice Energies:

1. Prioritize **charge first**
2. If two ionic compounds have the same charge, the **smaller one will have a higher energy**
3. Polyatomic ions are **big**

Lattice Energy Problem

List the following in terms of increasing lattice energy:

+1, -1	+2, -2	+1, -2	+1, -1	+2, -2	+1, -1
LiF,	MgO,	Na_2SO_4,	$LiBr$,	$MgSO_4$,	NH_4Br

1. Rank based on charge:

LiF,
$LiBr$,
NH_4Br

Na_2SO_4

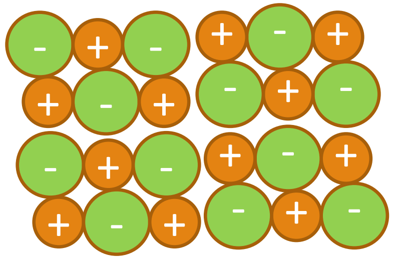
MgO,
$MgSO_4$

2. Settle everything else based on size:

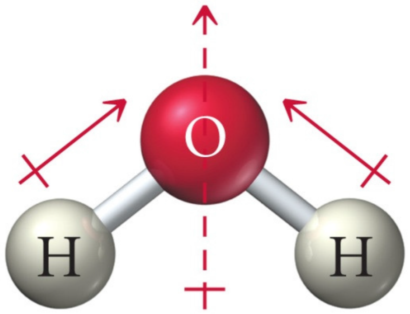
NH_4Br, $LiBr$, LiF, Na_2SO_4, $MgSO_4$, MgO

Ionic vs. Covalent Bonds

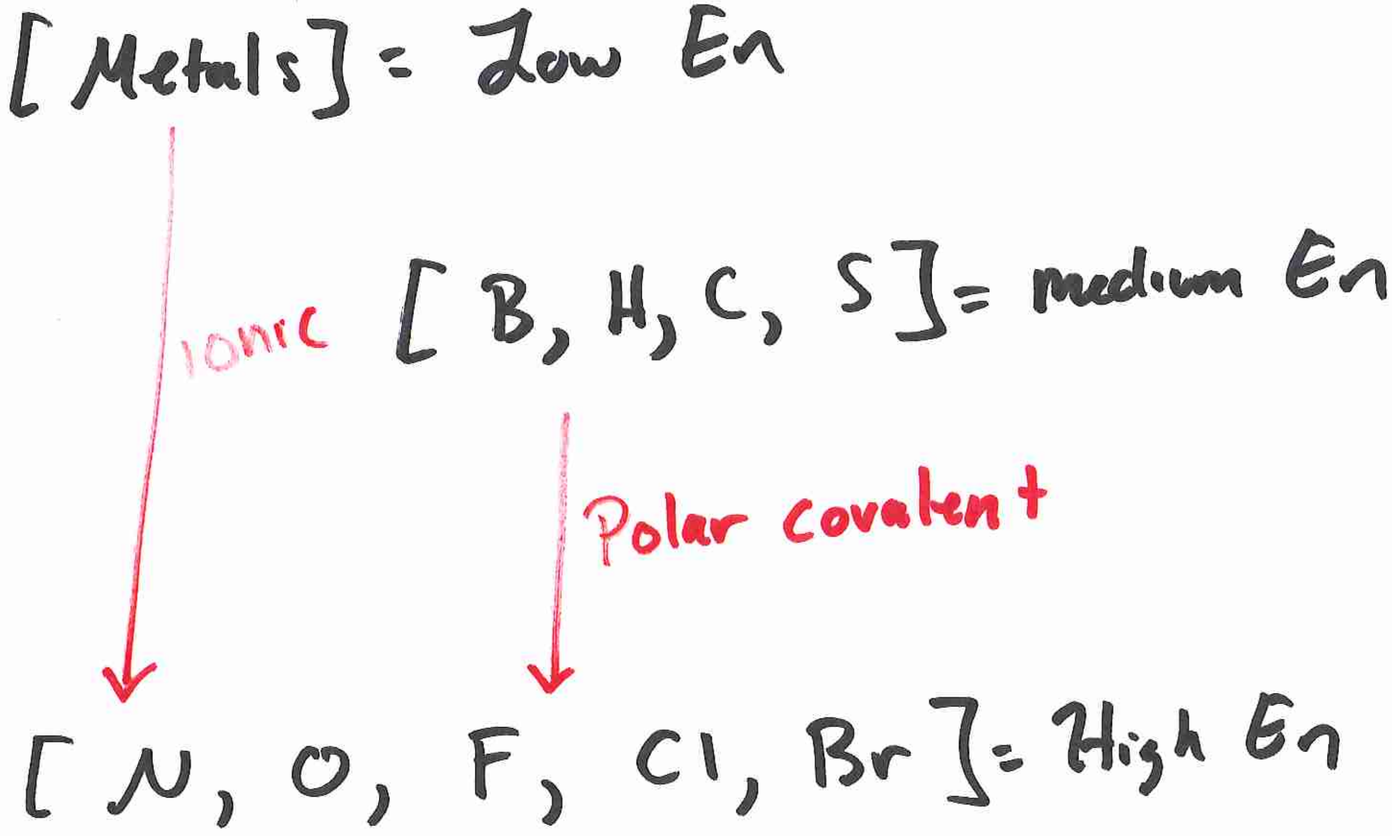
- **Ionic bonds** are the electrostatic interaction between discrete fully positive and fully negative charges.
  - Ionic bonds are quantified by lattice energy
  - Ionic compounds are almost always a metal (+) and nonmetal (-)
  - The ions can be elements or polyatomic ions (which are, themselves, covalent compounds)
  - Results in an alternating lattice of positive and negative charges



- **Covalent bonds** are the sharing of electrons between two species
  - Covalent bonds are quantified by bond length, bond strength, bond order, and polarity (Δen)
  - Covalent bonds result from the electrostatic interaction between partial charges (∂^+, ∂^-)
  - Results in molecules



Polarity Cheat Sheet



[Metals] = Low En

ionic

[B, H, C, S] = medium En

Polar covalent

[N, O, F, Cl, Br] = High En

* Anything to itself, non-polar

Lewis Structure Formal Charge Foundations

Element	-1 Charge	Neutral	+1 Charge
Hydrogen		1 bond	
Carbon*	3 bonds, 1 LP (rare)	4 bonds	
Nitrogen	2 bonds, 2 LP (rare)	3 bonds, 1 LP	4 bonds
Oxygen	1 bond, 3 LP	2 bonds, 2 LP	3 bonds, 1 LP
Halogens**	0 Bonds, 4 LP	1 bond, 3 LP	

This chart represents a "best guess" to draw out simple Lewis Structures. The formal charges are calculated based on a full octet and no exceptions.
*Carbon almost always has four bonds. Some notable exceptions are CO, CN^-, CNO^-
**Represents halogens as a peripheral atom, not a central atom. In other words, this applies to the fluorine in ClF_3 but not the chlorine.

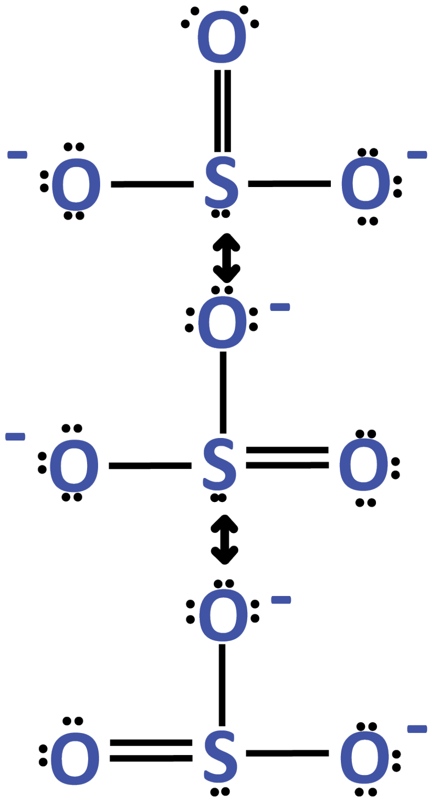
FC = Valence – (lone electrons + bonds)

FC = Valence – ("things it's touching")

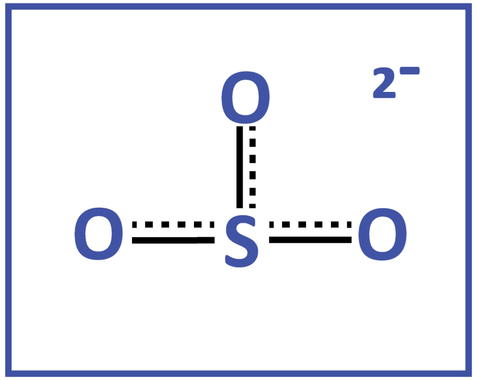
Bonding and Lewis Structures

- Resonance: multiple acceptable Lewis Structures are available for a given compound, meaning that the compound actually exists as the average of all acceptable structures
- Delocalized electrons: in the case of resonance, electrons are not confined to a single bond. Instead the electron charge is distributed over multiple bonds. We call this delocalization.
- **If you have multiple acceptable Lewis Structures in resonance, your actual structure will have the bonding character of the average. Example: Sulfite (SO_3^{2-})**

$$B.O. = \frac{total\ \#\ of\ bonds\ in\ resonance}{total\ \#\ of\ bonding\ regions\ in\ resonance}$$



"Acceptable" Structures: double and single bonds

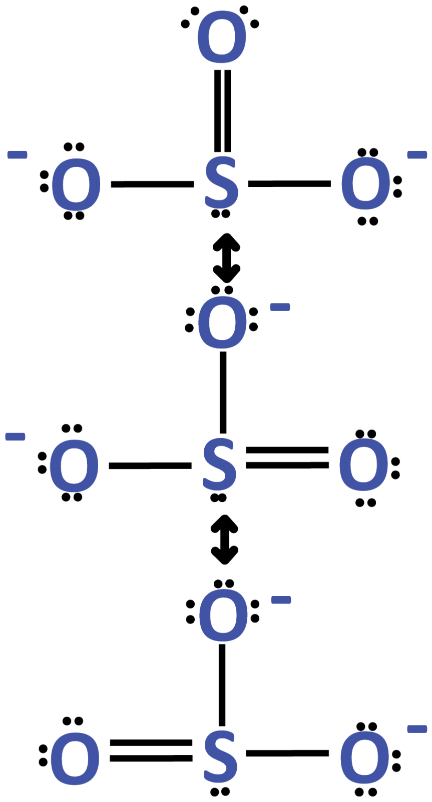


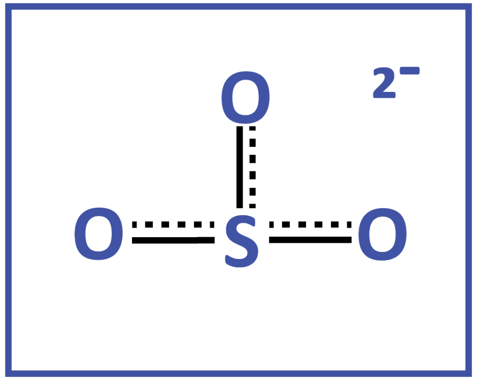
Correct Structure: three 1.33 bonds

Rules for an Acceptable Structure

- What constitutes an “acceptable” Lewis Structure?

   1. The negative charge is placed on only the electronegative or peripheral atoms, unless no better structure is possible (for example, CO and CN$^-$). Positive charges on the central atom are possible; however….
   2. Any individual charge should not exceed +/- 1
   3. Put your charges on as few atoms as possible
   4. Carbon, nitrogen, oxygen, and fluorine cannot disobey the octet rule
   5. **Your structure accurately reflects the number of available electrons in your atoms**





Exam Three Question

What is the formal charge on the central atom for the following molecules:

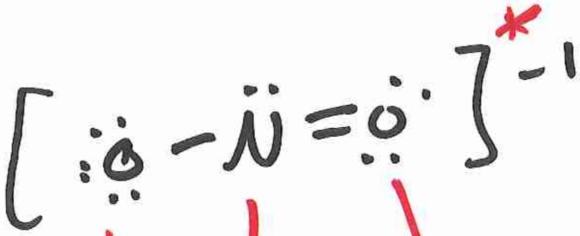
CN^-, NO_3^-, NO_2^-

FC = Valence – (lone electrons + bonds)

FC = Valence – (“things it’s touching”)

4-5=-1

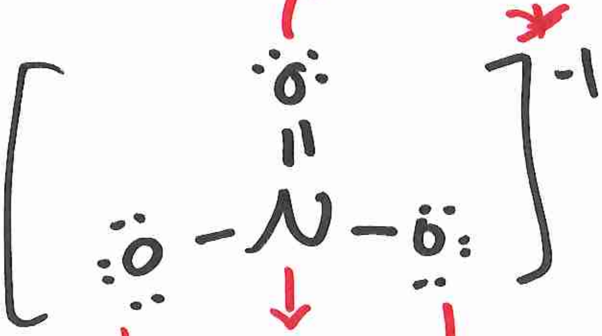
5-5=0



6-7=-1

5-5=0

6-6=0



6-6=0

5-4=1

6-7=-1

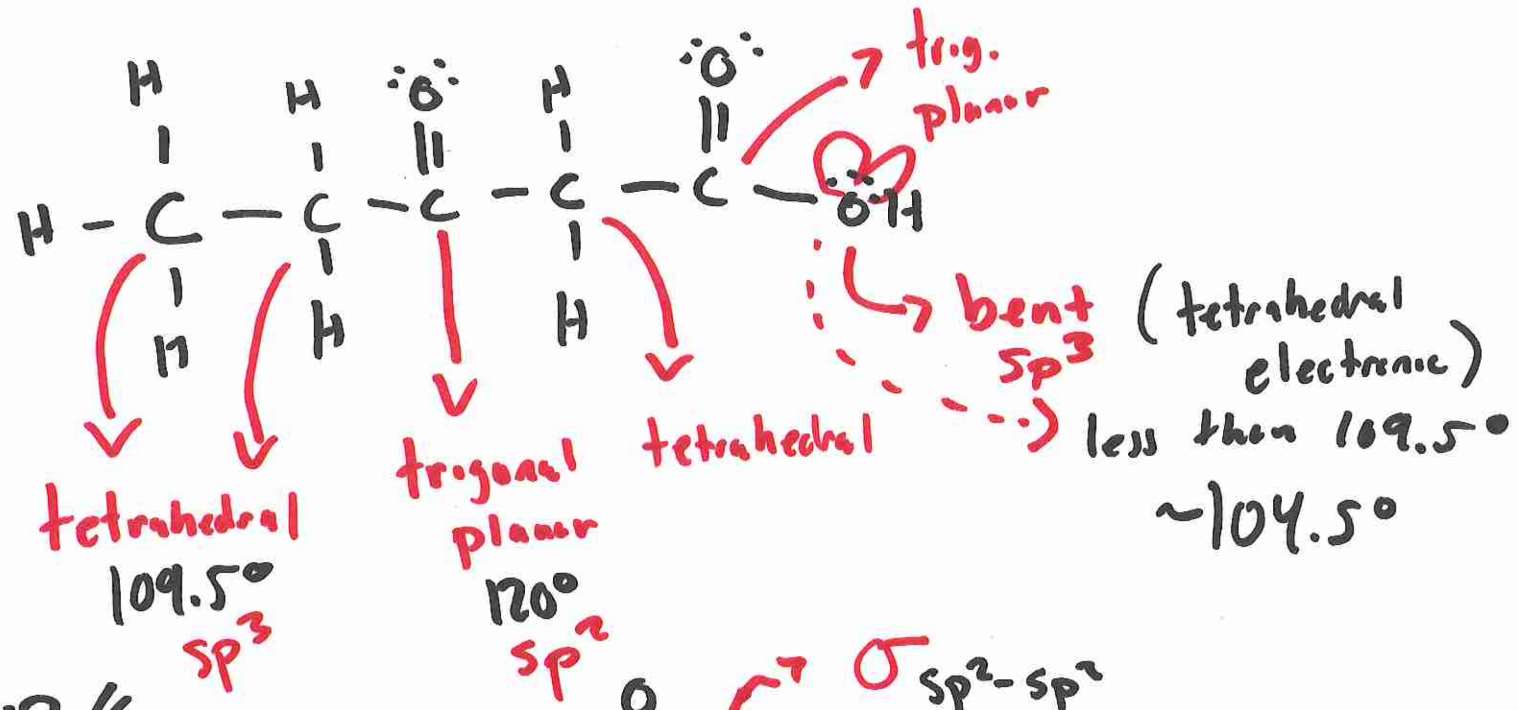
6-7=-1

* Resonance Structures *

Always Check Structure w/
Available # of electrons

$CH_3CH_2COCH_2COOH$,

✓ 1) VSEPR
✓ 2) VB
✓ 3) IMF's



$C{=}O$: $\sigma_{sp^2-sp^2}$, π_{2p-2p}

VB//

σ : 15

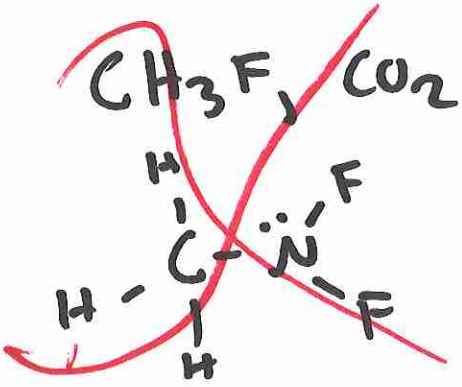
π : 2

IMFs//

Always Dispersion, Dipole-Dipole, H-bonding

N−H,

F−H



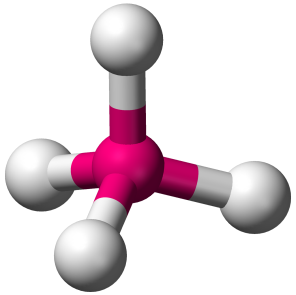
Bonding Theories Compared

- VSEPR Theory:
  - Shapes: molecular and electronic geometries
  - Explains bond angles
  - Focuses on the electron "regions"
  - Depends on the number of electron-dense regions (bonding and lone-pair regions)

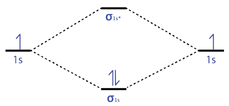
- Valence Bond Theory
  - Hybrid Orbitals: sp, sp^2, sp^3, sp^3d, sp^3d^2
  - Sigma and pi bonds
  - Identifies the overlapping orbitals to "name" the bonds
  - Focuses on the electron "clouds"
  - Depends on the number of electron-dense regions

sp^3

- Molecular Orbital Theory
  - Diagrams
  - Answers three fundamental questions regarding your molecule: bond order, magnetism, HOMO-LUMO gap
  - Sigma and pi bonds and anti-bonds
  - Focuses on the electrons as "waves"
  - Depends on the number of electrons



These theories might seem like a lot of information, but if you tie them together and simplify their conclusions, they actually make a lot of sense and don't require too much memorization.



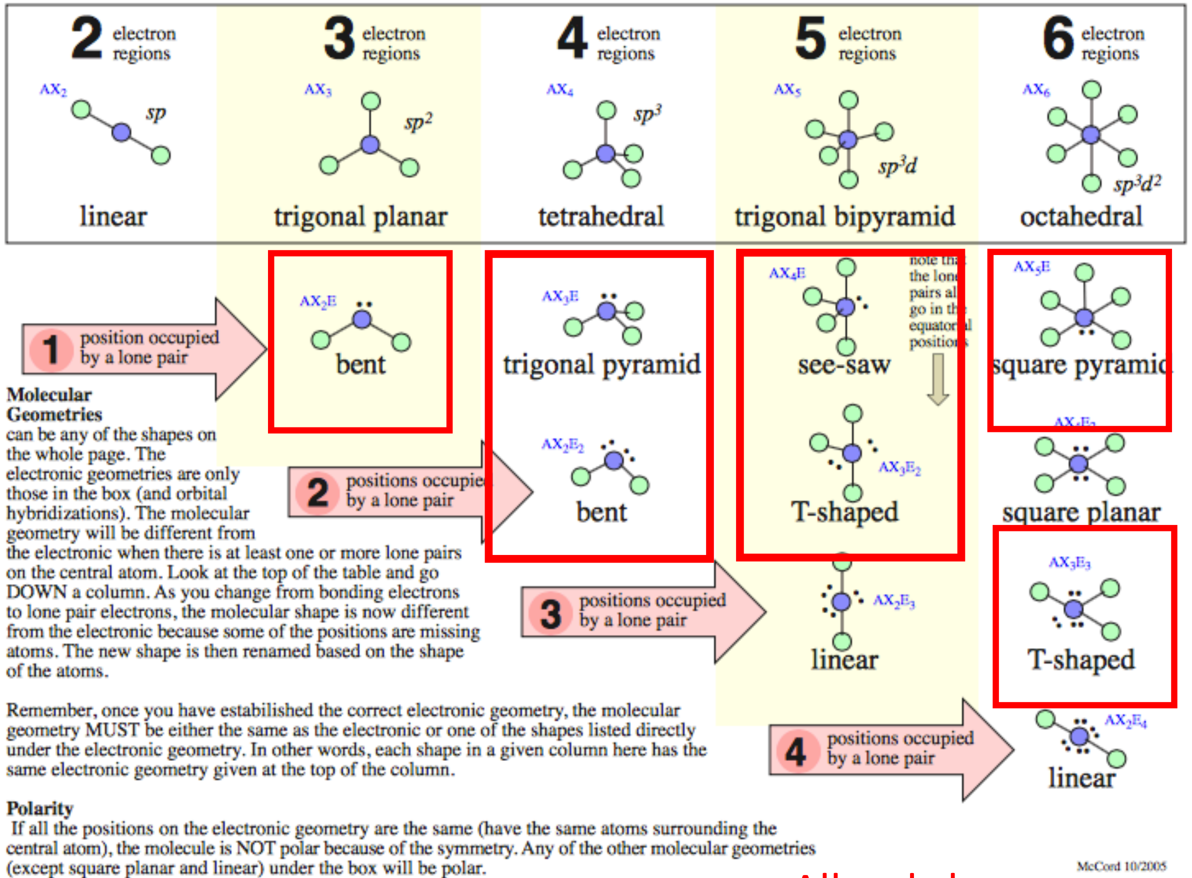
MO Diagram for H_2

Note: none of this means anything if your Lewis Structure is drawn incorrectly!

Valence Shell Electron Pair Repulsion

- **The basis of VSEPR is that electron-rich regions will achieve the lowest possible energy state by minimizing repulsions (maximizing the angles to spread out)**
- VSEPR gives us two different 3D geometries: **electronic geometry and molecular geometry**.
  - **Electronic geometry**: the shape of all electron-rich regions around a central atom, determined by counting the bonding AND lone pair regions
  - **Molecular geometry**: the shape of only the bonding regions around a central atom, determined by the electronic geometry and the (only) bonding regions
- The VSEPR shape is essential for the “actual” shape of the molecule, which gives us insight into the molecule’s bond angles and polarity.

Valence Bond Geometries



Molecular Geometries can be any of the shapes on the whole page. The electronic geometries are only those in the box (and orbital hybridizations). The molecular geometry will be different from the electronic when there is at least one or more lone pairs on the central atom. Look at the top of the table and go DOWN a column. As you change from bonding electrons to lone pair electrons, the molecular shape is now different from the electronic because some of the positions are missing atoms. The new shape is then renamed based on the shape of the atoms.

Remember, once you have estabilished the correct electronic geometry, the molecular geometry MUST be either the same as the electronic or one of the shapes listed directly under the electronic geometry. In other words, each shape in a given column here has the same electronic geometry given at the top of the column.

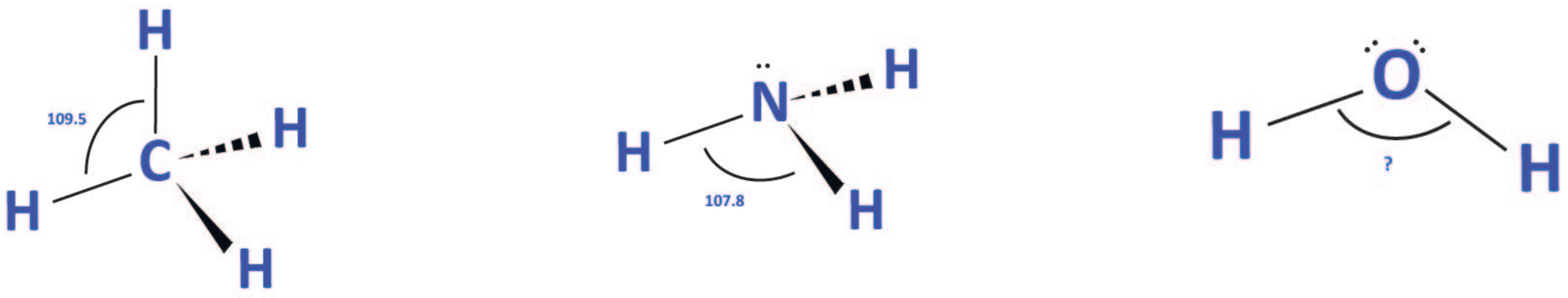
Polarity
If all the positions on the electronic geometry are the same (have the same atoms surrounding the central atom), the molecule is NOT polar because of the symmetry. Any of the other molecular geometries (except square planar and linear) under the box will be polar.

All red shapes are polar

- Polarity in a molecule occurs when there is a permanent dipole moment on the molecule. This can be identified by a few rules:
  - **A perfectly symmetrical molecule will always be nonpolar if its bonds are to the same atom.**
    - Examples: CO_2, SO_3, SF_6, PCl_5, CCl_4 are non-polar molecules even though they have polar bonds
  - **A central atom bound to different peripheral atoms will always be polar, as long as there is at least one polar bond.**
    - Examples: CH_3Cl, CHF_3, PCl_4F
  - **Molecular geometries with lone pairs are polar (even if the bonds are non-polar), except in linear and square planar geometries**
    - Examples: H_2O, NH_3, H_2S, O_3

VSEPR: The Effect of Lone Pairs

- Lone pairs occupy more space on the central atom than a bonding pair of electrons, meaning they end up being more repulsive than bonding regions
- The electron density of lone pairs **is ALL on the one central atom** – not shared between two– as in a conventional bond
- **The extra repulsive strength of the lone pair tweaks the bond angles of the central atom, making them smaller than expected for a pure geometry**



Exam Three Question

The best predicted shape and bond angle of SbH_3 is:

1. Trigonal pyramidal, 109.5
2. Tetrahedral, 109.5
3. Trigonal pyramidal, 107
4. Trigonal planar, 120

Follow-up: What are the IMF's present in this molecule?

Valence Bond Summary

Hybrids

# of Electron-Dense Regions	Hybridization
2	sp
3	sp^2
4	sp^3
5	sp^3d
6	sp^3d^2

Advanced: the more your practice, you will see that:

1. Sigma bonds are almost always overlapping hybrid orbitals (with the exception of hydrogen's pure 1s)
2. Pi bonds are always overlapping valence p-orbitals.

Types of Bonds

Single Bonds: 1 sigma bond

Double Bonds: 1 pi bond and 1 sigma bond

Triple Bonds: 2 pi bonds and 1 sigma bond

Bonding Names Overview

Remember on the exam that naming bonds and identifying the “overlapping” orbitals does not have to be a challenging question. Simplify what you know:

Single Bonds: 1 sigma bond

Double Bonds: 1 pi bond and 1 sigma bond

Triple Bonds: 2 pi bonds and 1 sigma bond

Sigma bonds are the **end-on-end (on axis)** overlap between hybrid orbitals (or pure 1s in the case of hydrogen because hydrogen doesn’t hybridize)

- Sigma bonds form on the inter-nuclear axis

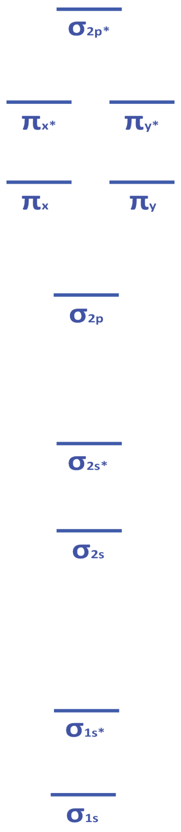
Pi bonds are the **side-by-side (off axis)** overlap between p orbitals

- Pi bonds form above and below the inter-nuclear axis

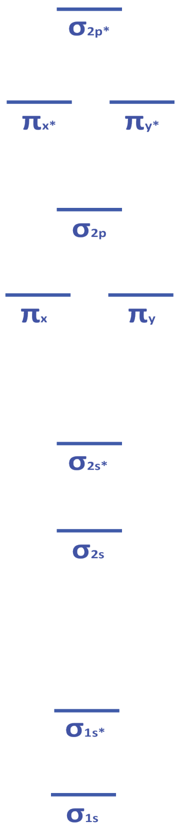
MO Theory: The one with the "Diagrams"

- **MO Theory is a quantum mechanical model for bonding that merges pure atomic orbitals into molecular orbitals**
- This theory is important because it gives us the following conclusions that VB and VSEPR cannot:
  - Stability can be described by bond order (**BO = bonding electrons – antibonding electrons**)
    - Bonding electrons aid in stability
    - Antibonding electrons lead to instability
  - Magnetism can be identified by the presence of paired or unpaired electrons in the highest occupied orbital
    - Diamagnetic: paired electrons, repelled from magnetic field
    - Paramagnetic: unpaired electrons, attracted to magnetic field
  - And of course, HOMO-LUMO…

You must memorize the diagrams to the right, their labels, and the pure atomic orbitals that go into making them.



O_2, F_2



Li_2 through N_2

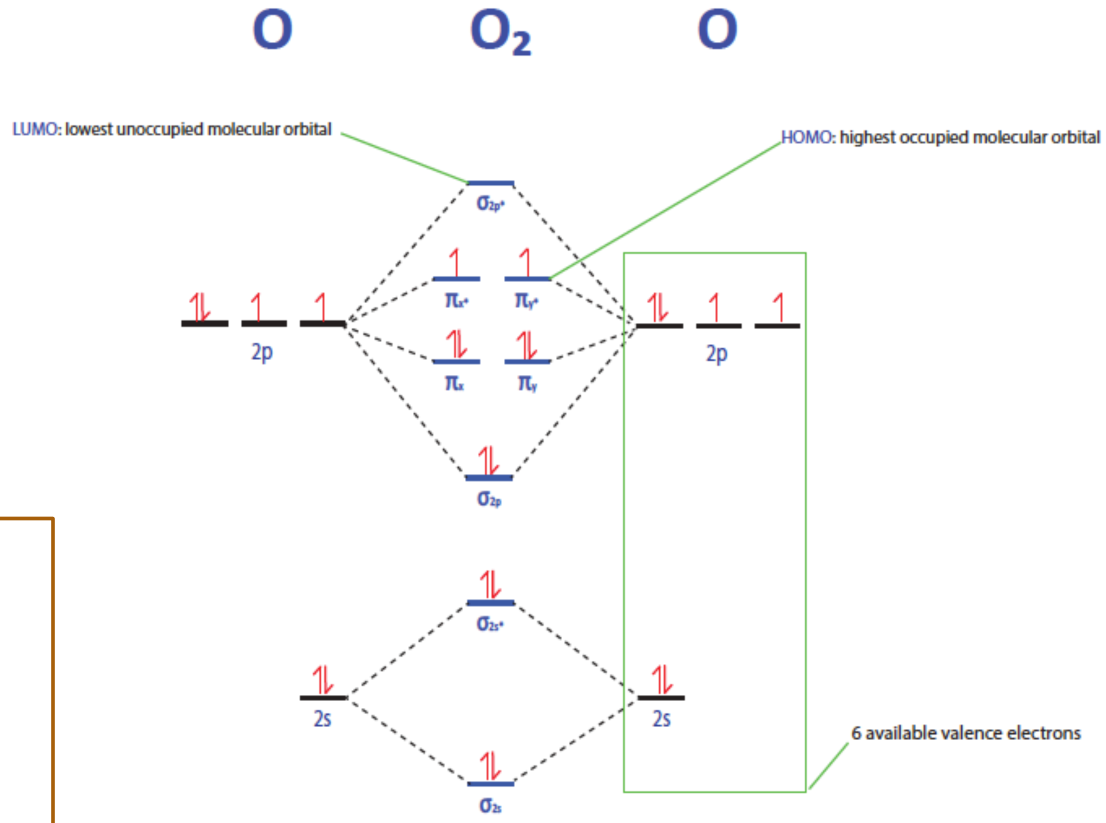
Molecular Orbital Theory: HOMO-LUMO

- One of the most important conclusions in molecular orbital theory is the energy difference between the **Highest Occupied Molecular Orbital (HOMO)** and the **Lowest Unoccupied Molecular Orbital (LUMO)**.
- This energy gap is important because it corresponds to energy of the photon emitted when an excited electron falls back down to ground state. **This can be applied to far more complicated molecules/materials**
- Because light is important here:

  Remember:

  IR….R.O.Y.G.B.I.V. …UV

  (---increasing energy, decreasing wavelength-->)



$$O_2 : \sigma_{1s}^{2}\ \sigma_{1s}^{*2}\ \sigma_{2s}^{2}\ \sigma_{2s}^{*2}\ \sigma_{2p}^{2}\ \pi_{2p}^{4}\ \pi_{2p}^{*2}$$

$$\text{B.O.} = \frac{\text{bonding} - \text{antibonding}}{2}$$

$$= \frac{\text{bonding} - \text{starred}}{2}$$

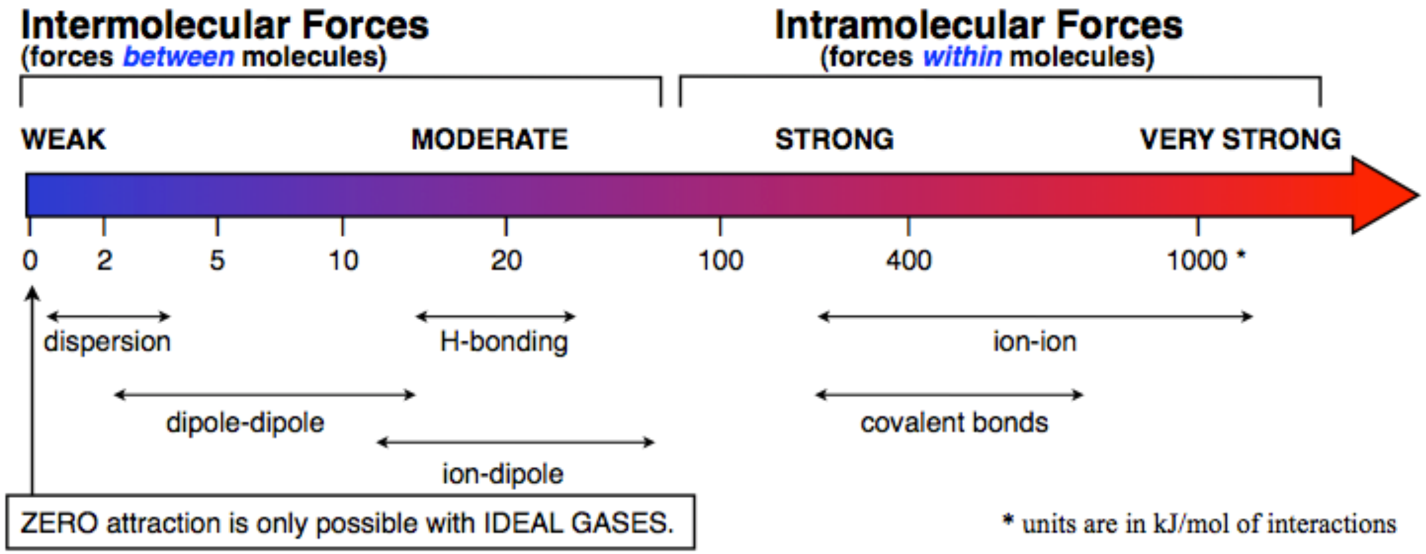
$$\frac{8-4}{2} = 2$$

Intermolecular Forces

IMF’S, LIQUID AND SOLID PROPERTIES

Intermolecular Forces

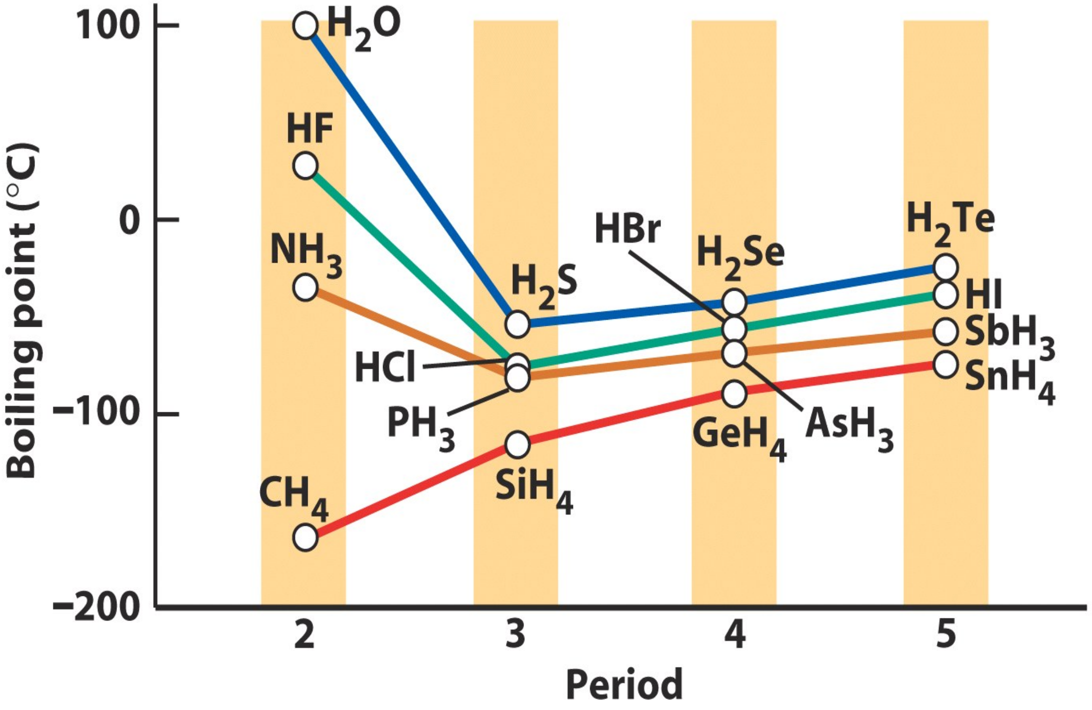
- Intermolecular forces (IMF's) are **electrostatic** interactions between molecules.
  - IMF's vary in strength, but are weaker than **intramolecular** forces (bonds)
  - Intermolecular forces are the electrostatic "glue" that hold molecules in condensed phases
- The three types of IMF's (in decreasing strength) are:
  1. Hydrogen bonding
  2. Dipole-dipole
  3. Dispersion forces
- And they depend on:
  1. Shape
  2. Polarizability (size)
  3. Temperature



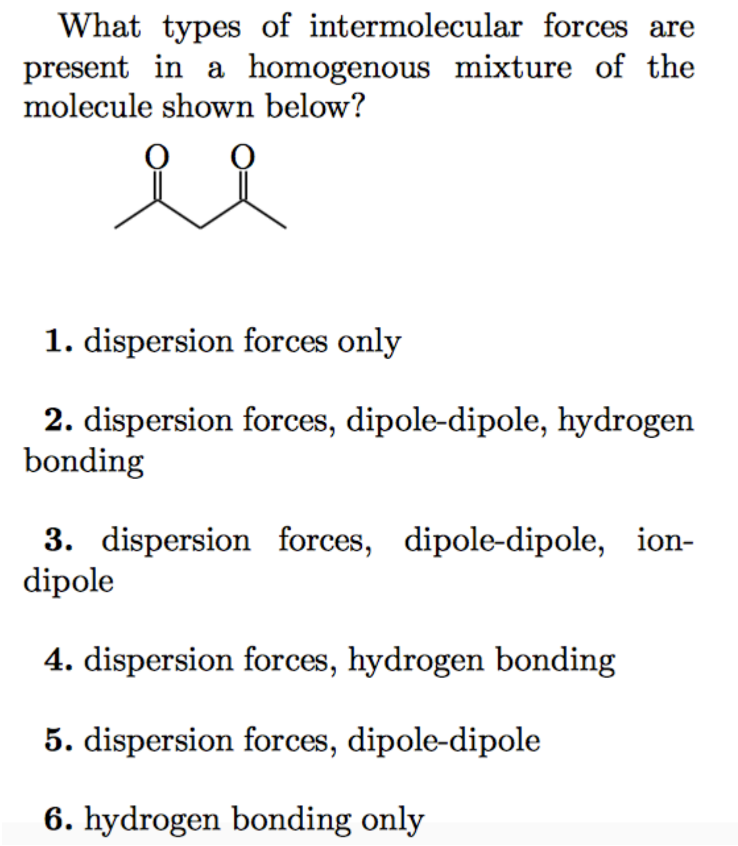
* units are in kJ/mol of interactions

IMF Comparisons

- The key features of this graph are as follows:
  - **Polarizability increases down a group (left to right on this chart)**
  - Shape changes across a period, leading to different polarity across a group (down up on this chart)
  - **Ammonia, hydrofluoric acid, and water break the trend in polarizability because they form hydrogen bonds. The red line follows the trend the best (no hydrogen bond)**



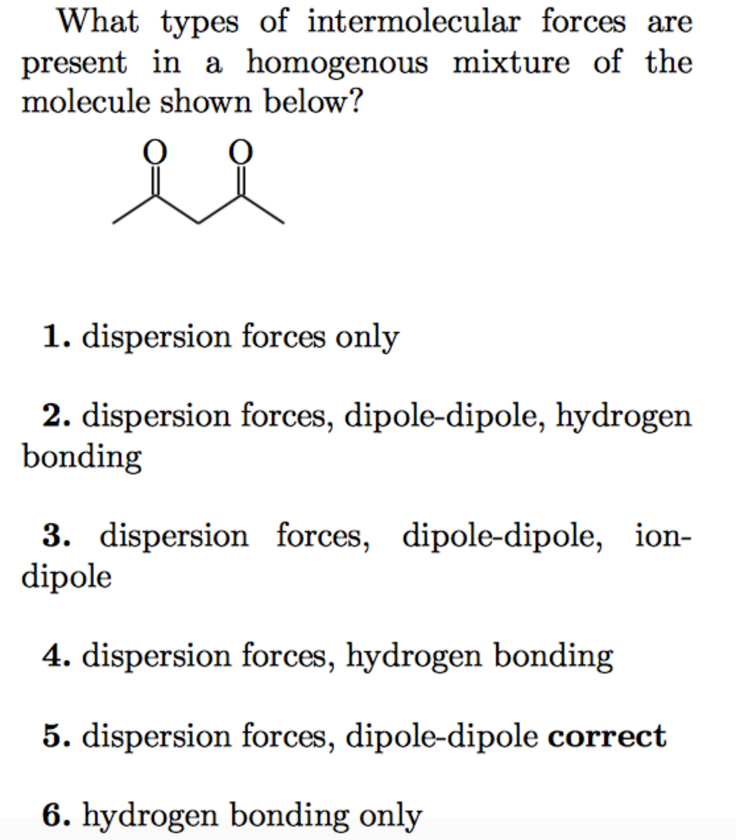
Exam Four Question



What types of intermolecular forces are present in a homogenous mixture of the molecule shown below?

1. dispersion forces only
2. dispersion forces, dipole-dipole, hydrogen bonding
3. dispersion forces, dipole-dipole, ion-dipole
4. dispersion forces, hydrogen bonding
5. dispersion forces, dipole-dipole
6. hydrogen bonding only

Exam Four Question



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1. dispersion forces only

2. dispersion forces, dipole-dipole, hydrogen bonding

3. dispersion forces, dipole-dipole, ion-dipole

4. dispersion forces, hydrogen bonding

5. dispersion forces, dipole-dipole **correct**

6. hydrogen bonding only

Liquid Properties Summary

Strong IMF - > High Viscosity, High BP, High Surface Tension

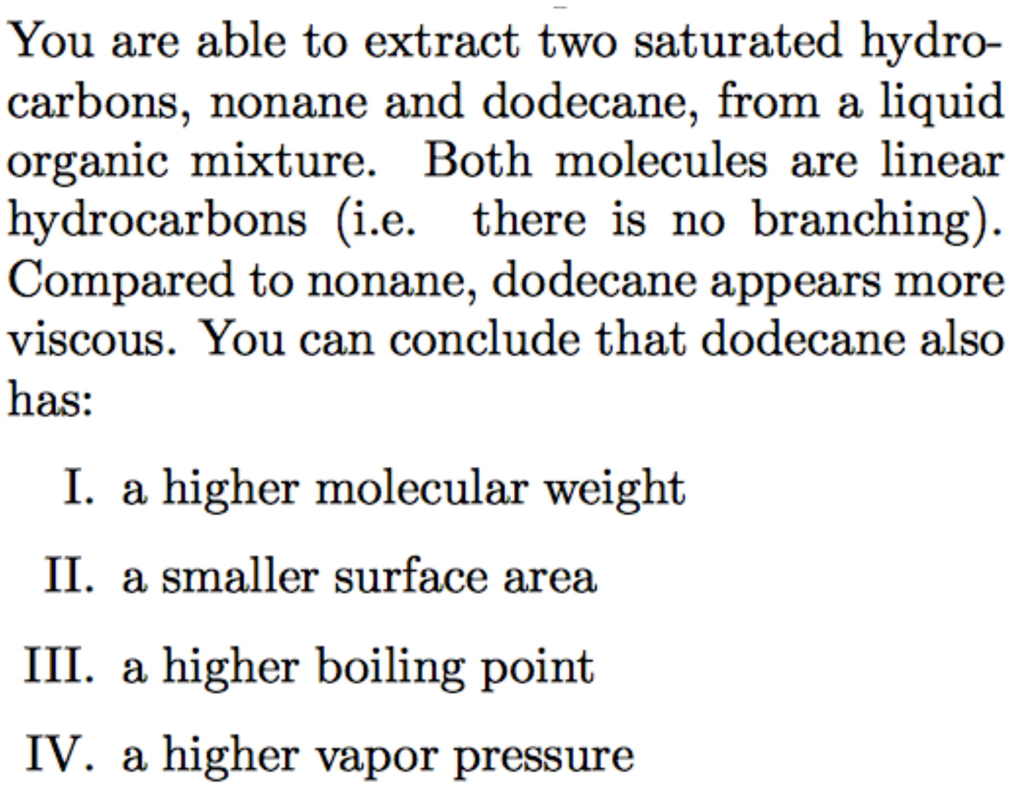
Weak IMF -> High Vapor pressure

High Temperature - > Lowers IMF Strength, Viscosity, and Surface Tension

High Temperature -> Raises Vapor pressure

(no effect on intrinsic properties, like boiling point, melting point, etc.)

Exam Four Question



You are able to extract two saturated hydrocarbons, nonane and dodecane, from a liquid organic mixture. Both molecules are linear hydrocarbons (i.e. there is no branching). Compared to nonane, dodecane appears more viscous. You can conclude that dodecane also has:

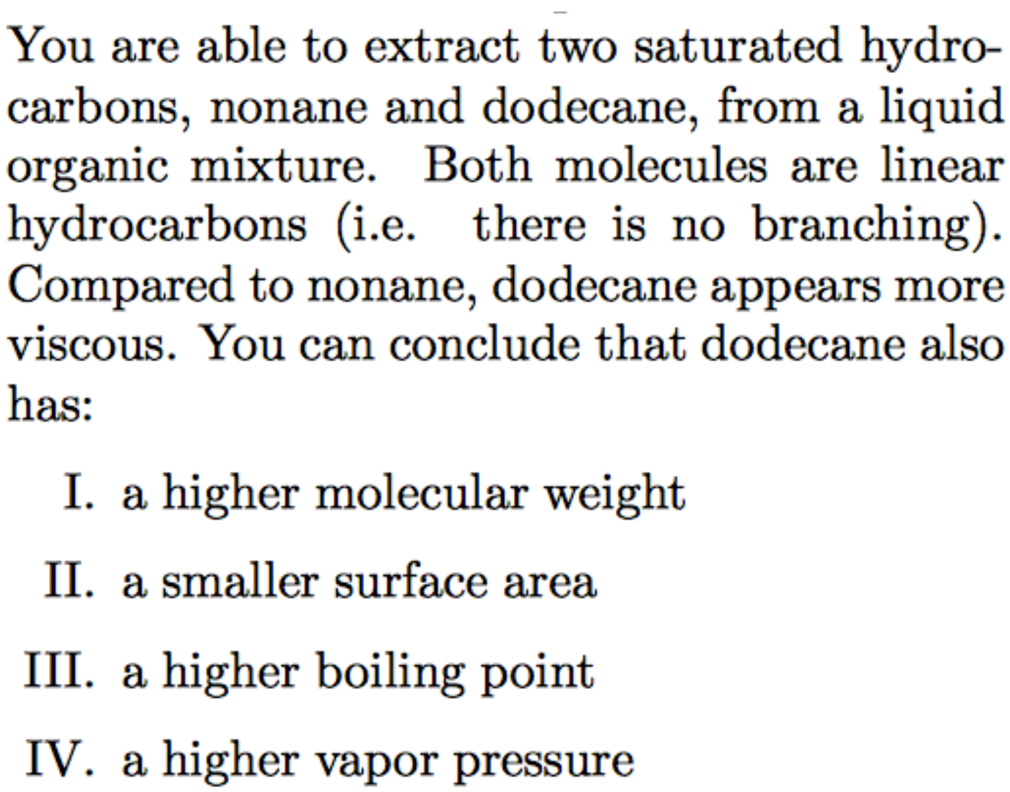
I. a higher molecular weight

II. a smaller surface area

III. a higher boiling point

IV. a higher vapor pressure

Exam Four Question



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I. a higher molecular weight

II. a smaller surface area

III. a higher boiling point

IV. a higher vapor pressure

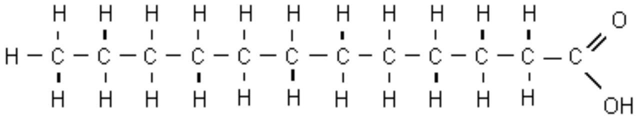
For a two linear hydrocarbons, the more viscous one has the higher IMFs. This correlates with a higher MW (larger surface area of overlap), higher polarizability, higher BP, higher surface tension **and lower vapor pressure.**

I and III only

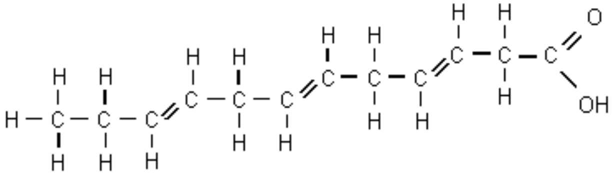
In-Depth Explanations

Dispersion forces scale with the size of a molecule, which correlates directly to polarizability

- **The larger the electron cloud, the larger the polarizability**
- **The larger the surface area (overlap), the larger the polarizability**
  - **”Stackability” is important here**



Saturated Fatty Acid



Unsaturated Fatty Acid

Lowest Polarizability, Lowest IMF’s

Gas: Cl_2

Liquid: Br_2

Solid: I_2

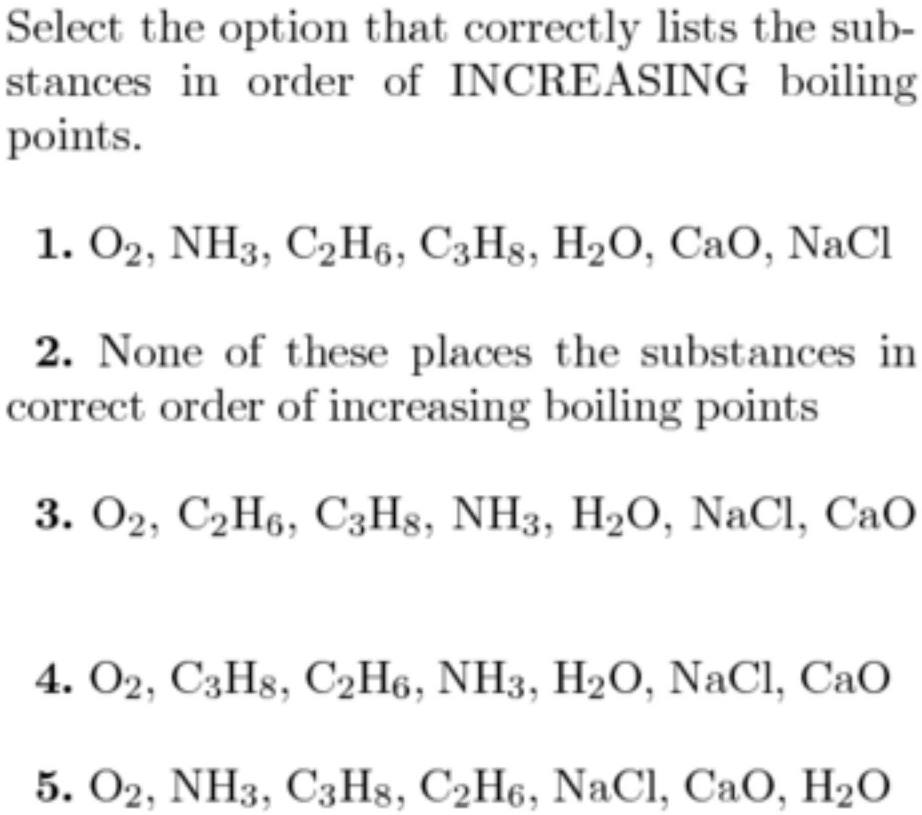
Highest Polarizability, Highest IMF’s

Comparing Solids

Class	**Examples**	**Characteristics**
Ionic	NaCl, KNO_3, $CuSO_4$	Hard, rigid, brittle; high melting/boiling points; those soluble in water give conducting solutions
Covalent Network	B, C, black P, BN, SiO_2	Hard, rigid, brittle; very high melting points; insoluble in water
Metallic	*s*- and *d*-elements	Malleable, ductile, lustrous; electrically and thermally conducting
Molecular	$BeCl_2$, S_8, P_4, I_2, ice, glucose	Relatively low melting/boiling points; brittle if pure

Class	**Electrons**	**Electrical Conductivity**
Ionic	Localized	Not a good conductor (only conducts electricity in aqueous solutions or when molten)
Network	Localized	Not a good conductor
Metallic	Delocalized	Good conductor
Molecular	Localized	Not a good conductor

Exam Four Question



Select the option that correctly lists the substances in order of INCREASING boiling points.

1. O_2, NH_3, C_2H_6, C_3H_8, H_2O, CaO, NaCl

2. None of these places the substances in correct order of increasing boiling points

3. O_2, C_2H_6, C_3H_8, NH_3, H_2O, NaCl, CaO

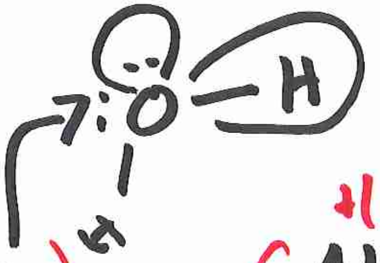
4. O_2, C_3H_8, C_2H_6, NH_3, H_2O, NaCl, CaO

5. O_2, NH_3, C_3H_8, C_2H_6, NaCl, CaO, H_2O

dispersion h-bond dispersion H-bond ionic

O_2, NH_3, C_2H_6, C_3H_8, H_2O, CaO, NaCl

↑BP ↑IMFs



(O_2
C_2H_6
C_3H_8),

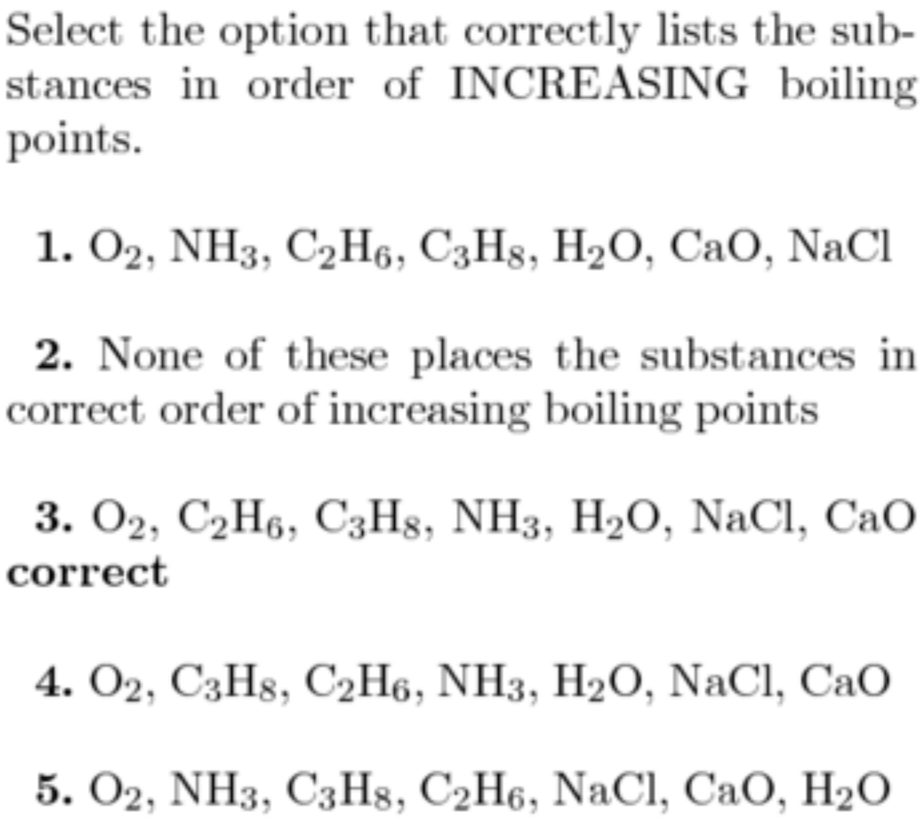
(H_2O
:NH_3
9),

(+1 -1
NaCl
+2 -2
CaO)

$O_2 < C_2H_6 < C_3H_8 < NH_3 < H_2O$

$< NaCl < CaO$

Exam Four Question



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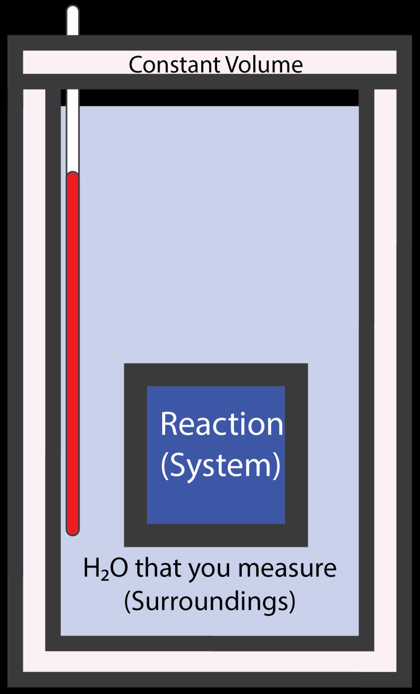
1. O_2, NH_3, C_2H_6, C_3H_8, H_2O, CaO, NaCl

2. None of these places the substances in correct order of increasing boiling points

3. O_2, C_2H_6, C_3H_8, NH_3, H_2O, NaCl, CaO
correct

4. O_2, C_3H_8, C_2H_6, NH_3, H_2O, NaCl, CaO

5. O_2, NH_3, C_3H_8, C_2H_6, NaCl, CaO, H_2O



Bomb Calorimeter

Thermodynamics

EXAM 5 TROUBLES, HEADS-UP
PLEASE LOOK OVER YOUR EXAM 5 AND MY EXAM 5 REVIEW FOR COMPREHENSIVE TOPICS

Basic First Law Calculations

$$\Delta U_{sys} = q + w$$

Work is the energy derived from organized molecular motion

w > 0 ; work energy in, work is done on the system (+), compression

w < 0 ; work energy out, work is done by the system (-), expansion

Heat is the energy derived from **random molecular motion** (always travels from high T to low T). Heat is transferred through conduction, convection, or radiation.

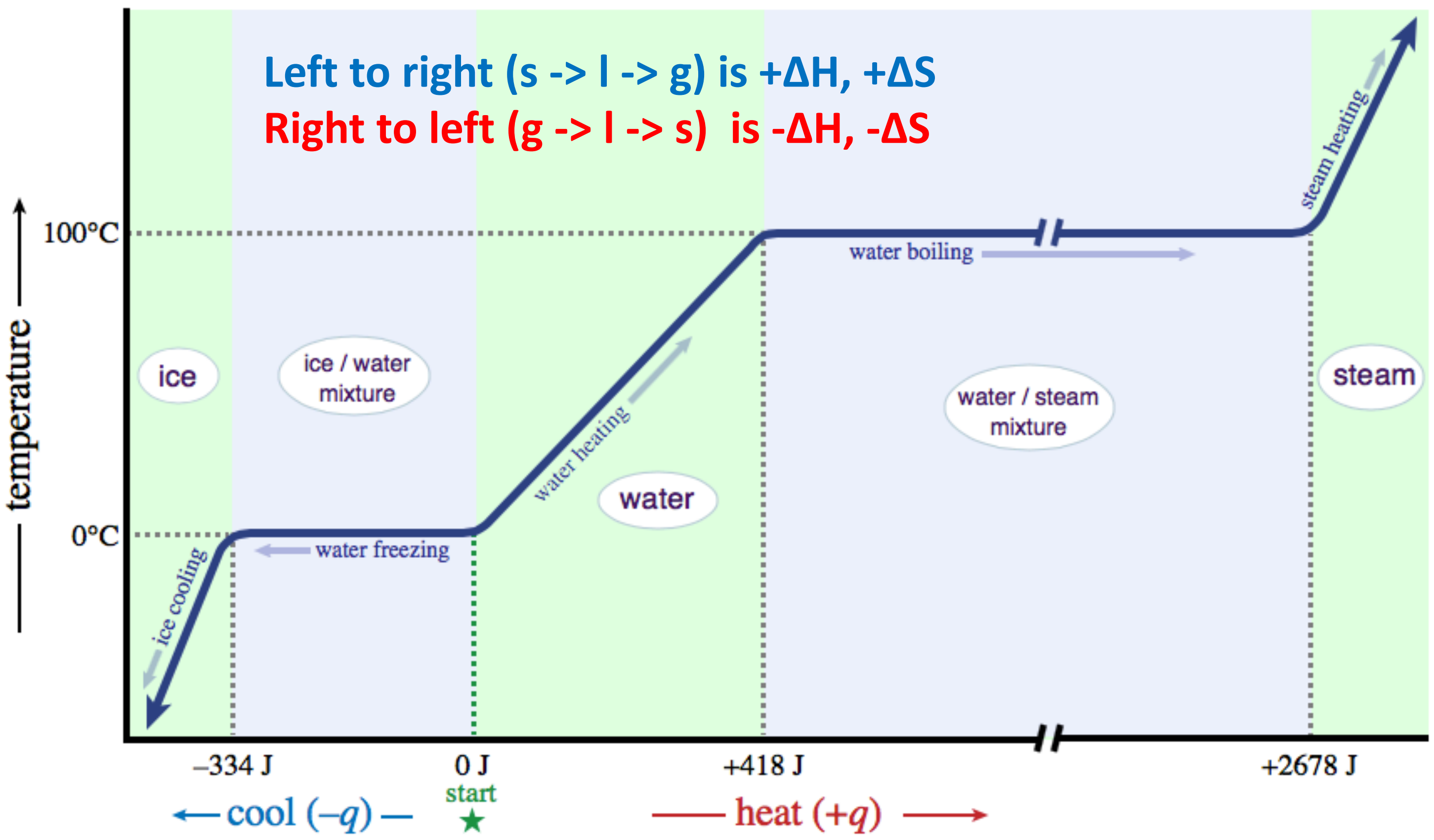
q > 0 ; endothermic (+), heat is absorbed

q < 0 ; exothermic (-), heat is released

At constant pressure…

$$\Delta U_{sys} = \Delta H - \Delta nRT$$

Heat Flow: Heating Curves



Left to right (s -> l -> g) is $+\Delta H$, $+\Delta S$

Right to left (g -> l -> s) is $-\Delta H$, $-\Delta S$

Heat of a Temperature Change

$q = mC_s\Delta T$

Heat of a Phase Change

$q = m\Delta H_{trans}$

Entropy of a temperature change

$\Delta S = mC_s\ln(T_f/T_i)$

Entropy of a phase change

$\Delta S = m\Delta H_{trans}/T$

Exam Five Question + Entropy

A 24mL sample of water at 41˚C is frozen and cooled to -18˚C. Calculate the heat of this process.

Now for the same process, calculate the change in entropy for the system.

Entropy of a temperature change

$\Delta S = mC_s\ln(T_f/T_i)$

Entropy of a phase change

$\Delta S = m\Delta H_{trans}/T$

Spontaneity: Entropy and Free Energy

- **The second law of thermodynamics states that the entropy of the universe is always increasing.**

$$\Delta S_{total} = \Delta S_{sys} + \Delta S_{surr}$$

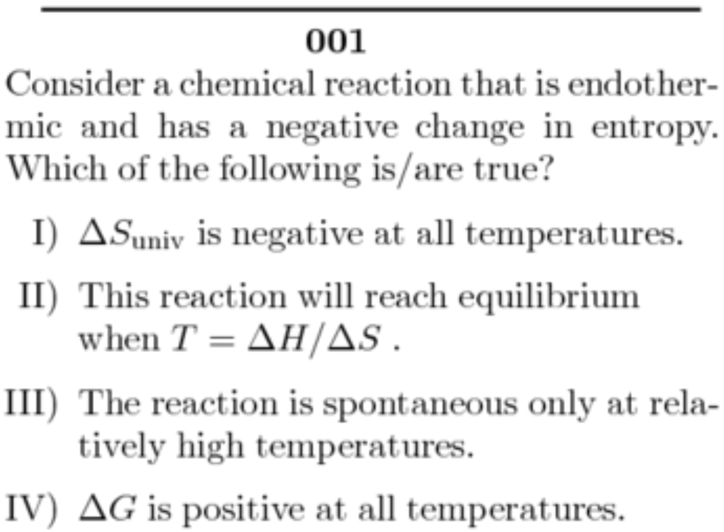
- This law gives us three conditions for **ΔS_{total}**:
  1. $\Delta S < 0$ (negative) ; your reaction is nonspontaneous
  2. $\Delta S = 0$ (zero) ; your reaction is at equilibrium / reversible
  3. $\Delta S > 0$ (positive) ; your reaction is spontaneous

- **The equation for the second law can be rewritten for free energy**

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

- This law gives us three conditions for **ΔG_{rxn}**:
  1. $\Delta G < 0$ (negative) ; your reaction is spontaneous
  2. $\Delta G = 0$ (zero) ; your reaction is at equilibrium
  3. $\Delta G > 0$ (positive) ; your reaction is nonspontaneous

Free Energy: Equilibrium Question



001

Consider a chemical reaction that is endothermic and has a negative change in entropy. Which of the following is/are true?

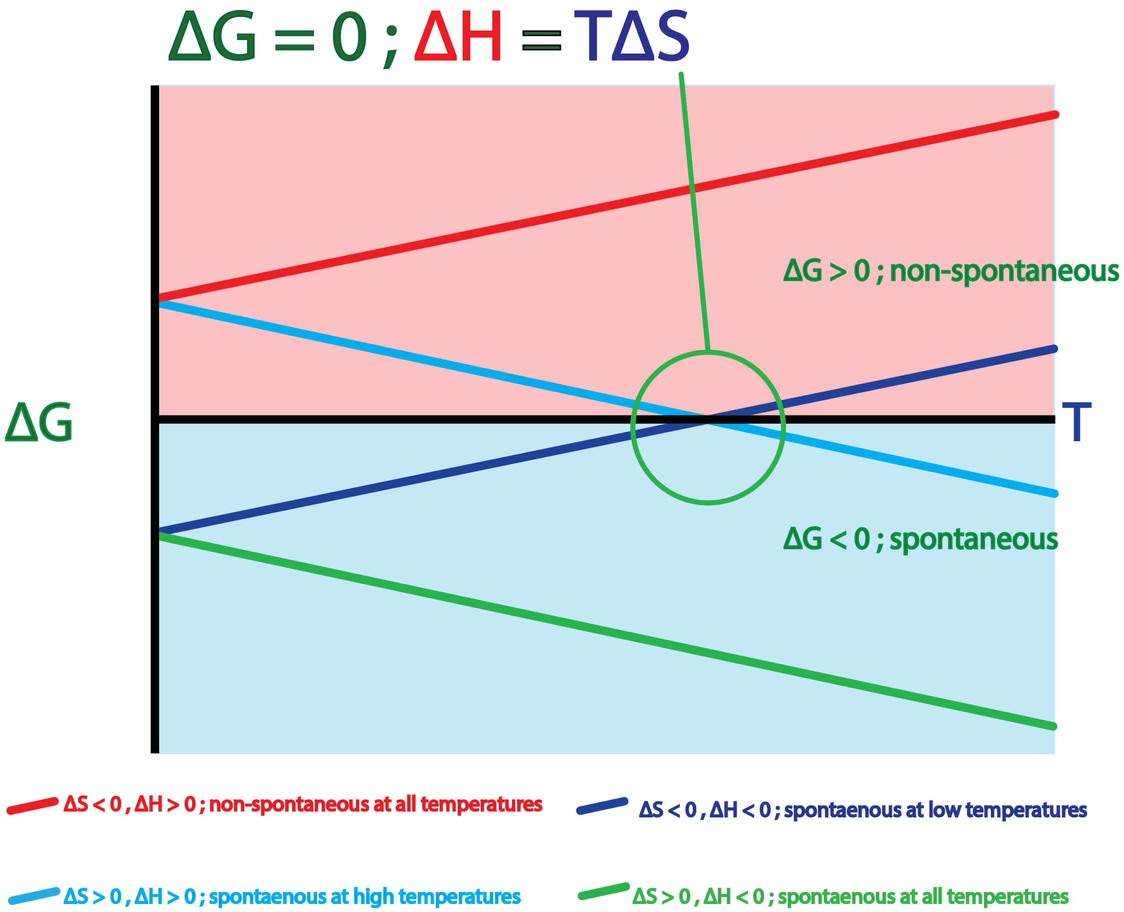
I) ΔS_{univ} is negative at all temperatures.

II) This reaction will reach equilibrium when $T = \Delta H/\Delta S$.

III) The reaction is spontaneous only at relatively high temperatures.

IV) ΔG is positive at all temperatures.

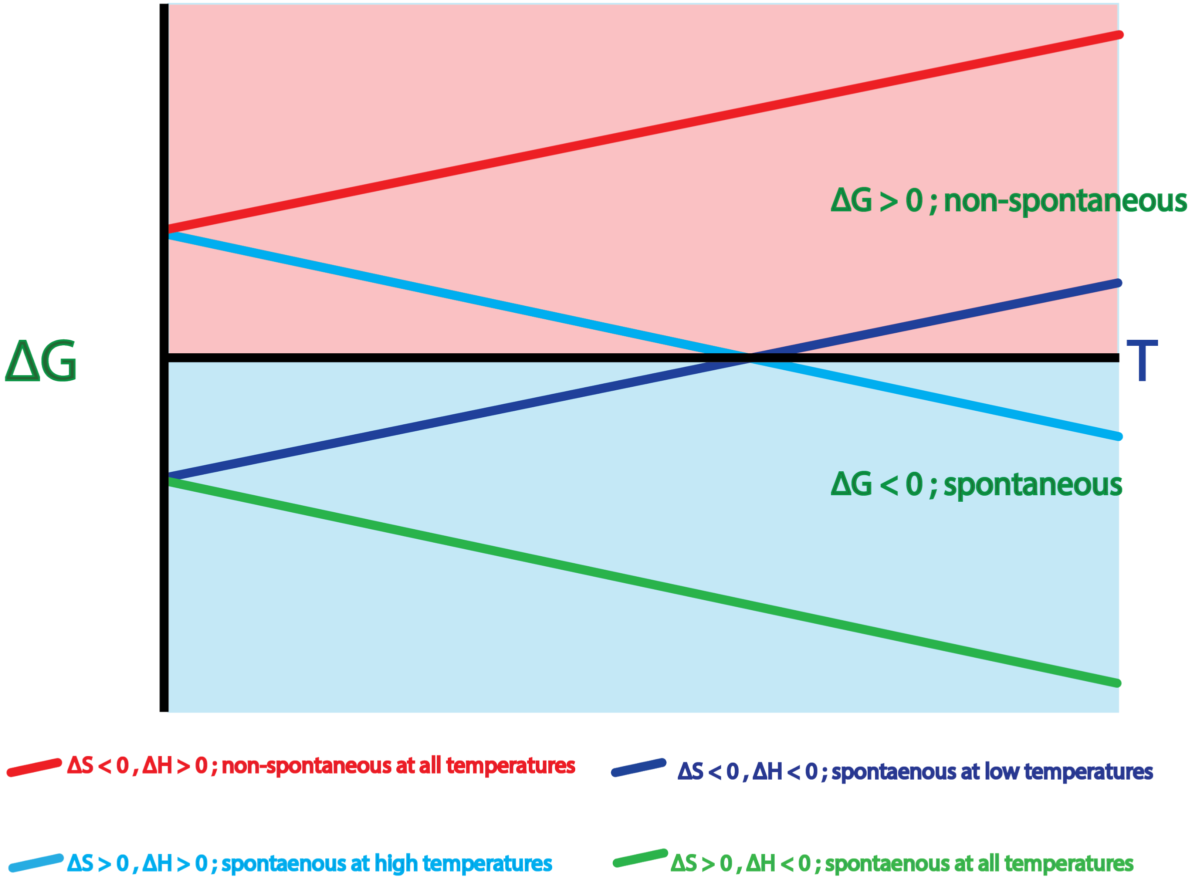
I and IV are correct



Free Energy: All Conditions Summary

ΔH	ΔS	Temperature Dependent?	Spontaneous?
-	+	No	Always
+	-	No	Never
-	-	Yes	Low T
+	+	Yes	High T

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



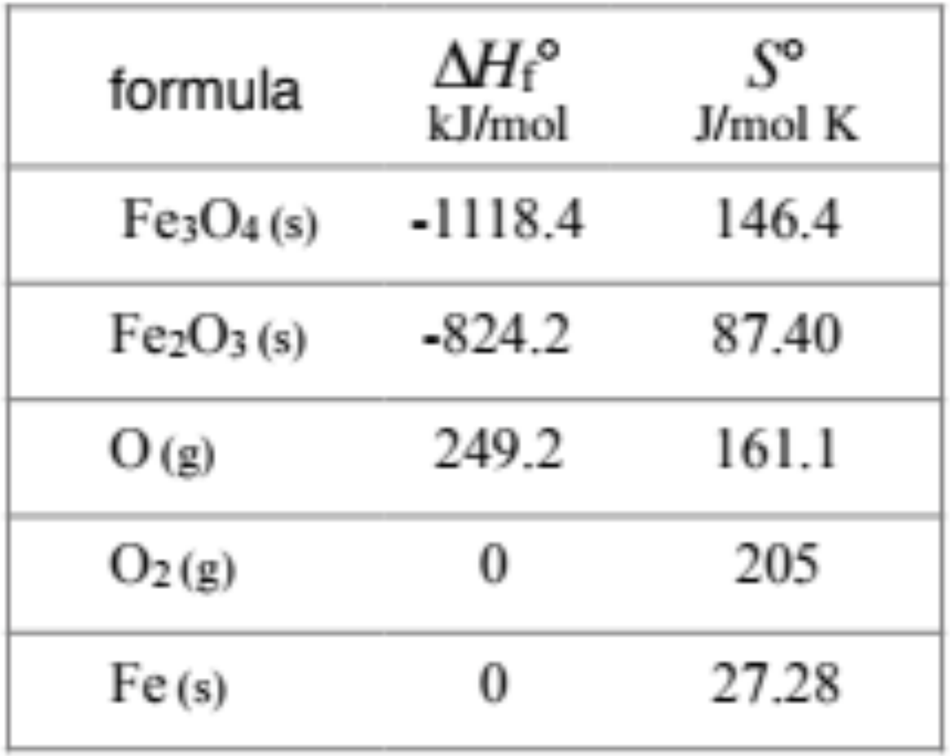
Free Energy and Equilibrium Questions

What is the ΔG°_f of Fe_2O_3?

At what temperature (if any) is this reaction first spontaneous?

Btw, what's the value of work for this reaction?

What's the change in internal energy?



formula	ΔH_f° kJ/mol	S° J/mol K
Fe_3O_4 (s)	-1118.4	146.4
Fe_2O_3 (s)	-824.2	87.40
O (g)	249.2	161.1
O_2 (g)	0	205
Fe (s)	0	27.28

$$2\,Fe_{(s)} + \frac{3}{2}O_{2}(g) \longrightarrow 1\,Fe_2O_3\,(s)$$

$$\Delta G^\circ_f = \Delta H^\circ_f - T\Delta S^\circ_{rxn}$$

$$\Delta H^\circ_f = \Delta H^\circ_{rxn} = -824.2 \text{ kJ/mol}$$

$$\Delta S^\circ_{rxn} = \sum n S^\circ_{products} - \sum n S^\circ_{reactants}$$

$$\left(87.40 \tfrac{J}{mol\,K}\right) - \left(2 \times 27.28 + 1.5 \times 205 \tfrac{J}{mol\,K}\right)$$

$$= -274.66 \tfrac{J}{mol\,K} = -0.27466 \tfrac{kJ}{mol\,K}$$

$$\Delta G = \overset{kJ}{-824.2} - \overset{K}{298}(\overset{kJ/K}{-0.27466})$$

$$= -742.35 \text{ kJ/mol}$$

$$\underbrace{\underset{\text{favorable}}{\Delta H = (-)} \quad , \quad \underset{\text{non-favorable}}{\Delta S = (-)}}_{\text{Spontaneous at Low Temperatures}}$$

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

first spontaneous when $\underline{\Delta G = -0.000000\ldots1}$

$$\underline{0} = \Delta H - T\Delta S$$

$$T\Delta S = \Delta H$$

$$T = \frac{\Delta H}{\Delta S} = \frac{-824.2\ kJ}{-0.2746\ kJ}$$

$$\boxed{\text{less then } 3001K}$$

H, U, G, S

$$\underbrace{2Fe(s) + \frac{3}{2}O_2(g) \rightarrow Fe_2O_3(s)}$$

Compression
$-\Delta n$, $+w$

work $= -\Delta nRT$

Δn → gas only

$+3716\text{ J} = -(-1.5)(8.314)(298)$

→ 3.716 kJ

q + w

$$\Delta U = \Delta H - \Delta nRT$$

$-824.4\text{ kJ} + 3.716\text{ kJ}$

$$\boxed{\Delta U = -820.48\text{ kJ}}$$