CH301 Unit 2

EXAM REVIEW

Disclaimer:

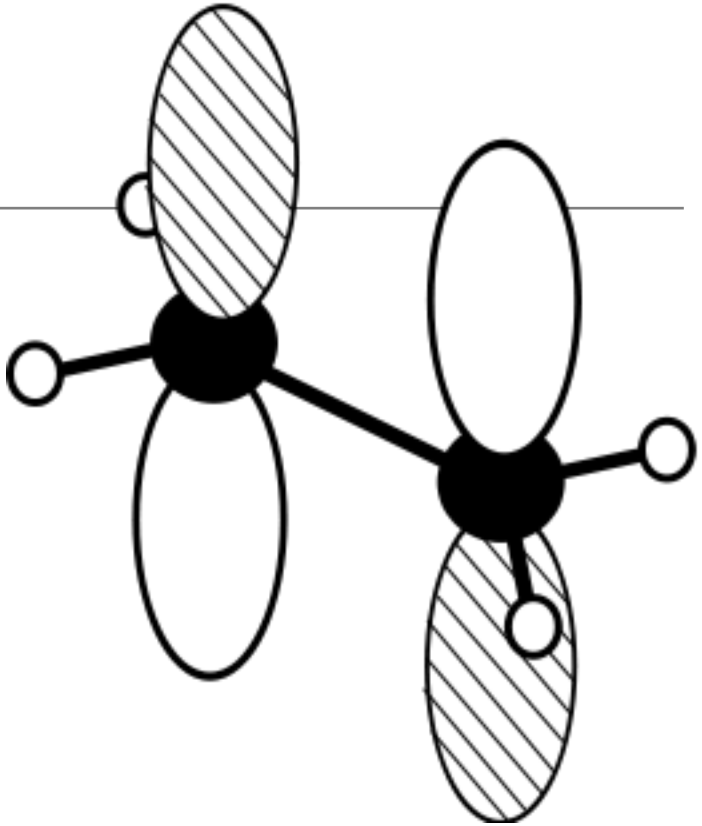
THIS REVIEW IS MEANT FOR T/TH CLASSES, AND THEREFORE DOES NOT COVER ALL THE MATERIAL ON THE M/W/F EXAMS. THIS REVIEW DOES NOT COVER COVALENT BONDING, LEWIS DOT STRUCTURES, ELECTRONEGATIVITY, RESONANCE, ETC.

Goals for Today

- Study Tips
- Exam Review
  1. Electromagnetic Spectrum
  2. Quantum Mechanics
  3. Electron Configurations
  4. Periodic Trends
  5. Introduction to Bonding
  6. Nomenclature

The **theme** of today: commit yourself to understanding what is actually going on, and you will be much more likely to succeed on the exam

Don’t lose sight of the story we are telling with this unit. Quantum mechanics is the study of discrete energy levels that can be used to define the interaction between matter and light. Understand why it was developed (failures of classical mechanics) and what it means to us today.



Reflections on Exam One

There are two main reflections I have heard from students last exam:

1. I did all the work (I took the LE seriously, I reworked the homework, I took notes on g-chem, I studied lecture notes, and then I searched for old exams online) and I made a really good grade.
2. I worked hard and I thought I did enough, but I did not make a good grade. It takes a lot of work to do well in UT chemistry courses, and sometimes it takes a big step up from the effort you put into high school to get the grades you are used to making.
    - Redo all the homework problems, create an outline of the course material putting all the equations and relationships into your own words, and then seek out additional practice problems from old exams posted on the web.
    - Don't let yourself miss out on points you deserve: knowing the equations is usually just one step to getting the correct answer. Be familiar with units, nomenclature, and conversions.

Wadman Study (Cram) Schedule

1. When you get home: create a thorough outline of the topics covered in class
    - If you kept up with the G-chem site and took good notes, make another one with an added dimension (add color coding, highlighting, etc.)
    - Adding color increasing the effective time of engagement with the material
2. Work through the blank homework assignments provided and g-chem problem sets **without looking at the solutions** until you feel like you can go to sleep with confidence in the material
3. Designate thirty minutes to an hour before going to sleep (and getting at least 8 hours of sleep!) for doing something relaxing / unrelated to chemistry
4. The day of the exam, continue working through problem sets (old exams?) and referring to your outline for help.
    - If your outline is not sufficient for answering a questions, add to it!
5. Eat well throughout the day of the exam
6. If you do well on the exam, save that outline for the final!

Learning Objectives – Unit 2

- Perform quantitative calculations based on the relationship between wavelength, energy, and the speed of light.
- Identify and rank the different types of radiation which comprise the electromagnetic spectrum.
- Explain why classical mechanics doesn't describe electromagnetic radiation.
- Describe the photoelectric effect and relate the energy and/or intensity of the photons to the work function and kinetic energy of the ejected electrons.
- Explain the origin of atomic and emission spectra and relate these spectra to discrete energy levels.
- Apply the Rydberg formula to predict the energy of transitions between fixed energy levels in the hydrogen atom.
- Explain that quantum mechanics is a mathematical model, the solutions of which yield wave functions and energies.*
- List the possible combinations of quantum numbers that are allowed.
- State the atomic orbital names based on quantum numbers.
- Explain that a wave function can be used to calculate a radial distribution function that describes the probability of an electron as a function of distance away from the nucleus
- Distinguish between one-electron systems and multi-electron systems.
- Apply the Aufbau principle to determine the configuration for any atom or ion.
- Relate the electronic configuration of an element to its position on the periodic table.
- Recognize that there are exceptions to the Aufbau principle and predict where on the periodic table these are likely to occur.
- Apply Hund's Rule and the Pauli Exclusion Principle to determine electron configuration using an orbital diagram (electrons in individual orbitals with spins).
- Fill an electron atomic orbital diagram and determine whether the element is paramagnetic or diamagnetic.
- Apply the shell model of multi-electron atoms to describe the concept of core vs. valence electrons.
- Describe the organization of the periodic table and the characteristics of elements in different regions of the table.
- Describe the concept of electronic shielding and effective nuclear charge (Zeff) and their relationship to trends in ionization energy, atomic radii, and ionic radii.
- Identify metals and non-metals, and predict the types of compounds (ionic/covalent) that will form from different elements.
- Distinguish between molecules, ions, and atoms.
- Predict the anion or cation that a main-group element is likely to form.
- Relate Coulomb’s law to ionic radii, ionic charge, and lattice energy.

Introduction to Bonding

IONIC BONDING, LATTICE ENERGY, CHARGE DENSITY

Formation of an Ionic Bond

- An ionic bond is formed by the transfer of electrons from one atom to another. This happens in three thermodynamic phases:
- **The release of an electron by a metal:**

$$Na \rightarrow Na^+ + e^-$$

- **The gain of an electron by a nonmetal:**

$$Cl + e^- \rightarrow Cl^-$$

- **The formation of a crystal lattice by the metal and nonmetal:**

$$Na^+ + Cl^- \rightarrow NaCl$$

Properties of Ions and Ionic Compounds

- **Charge Density**: the distribution of an ion's charge over a given space

$$\rho = \frac{q}{r}$$

  - This equation states that the **charge density** (rho) is equal to the **charge** (q) divided by the **radius** (r)
  - Or we can say that the charge density is **directly** proportional to the charge and **inversely** related to the radius.

- **Lattice Energy**: the energy required to break the bonds of an ionic compound

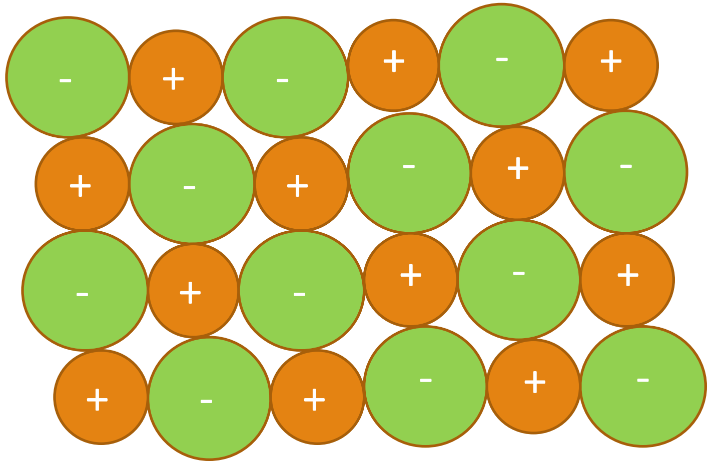
$$\Delta H_{lattice} \propto \frac{q_1 q_2}{r}$$

  - This equation states that the **lattice energy** (ΔH) of an ionic compound is proportional to the product of the **charges** divided by the **radius**
  - Or we can say that the lattice energy is **directly** proportional to the charges and **inversely** proportional to the radius.
  - When you are asked to compare lattice energies, you should first rank based on charge and then rank based on radius

Visualizing Lattice Energy

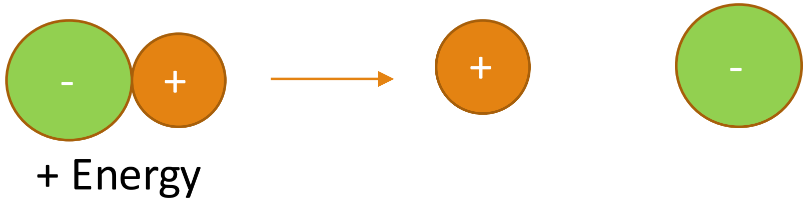
- Lattice Energy: the energy required to break the bonds of an ionic compound

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



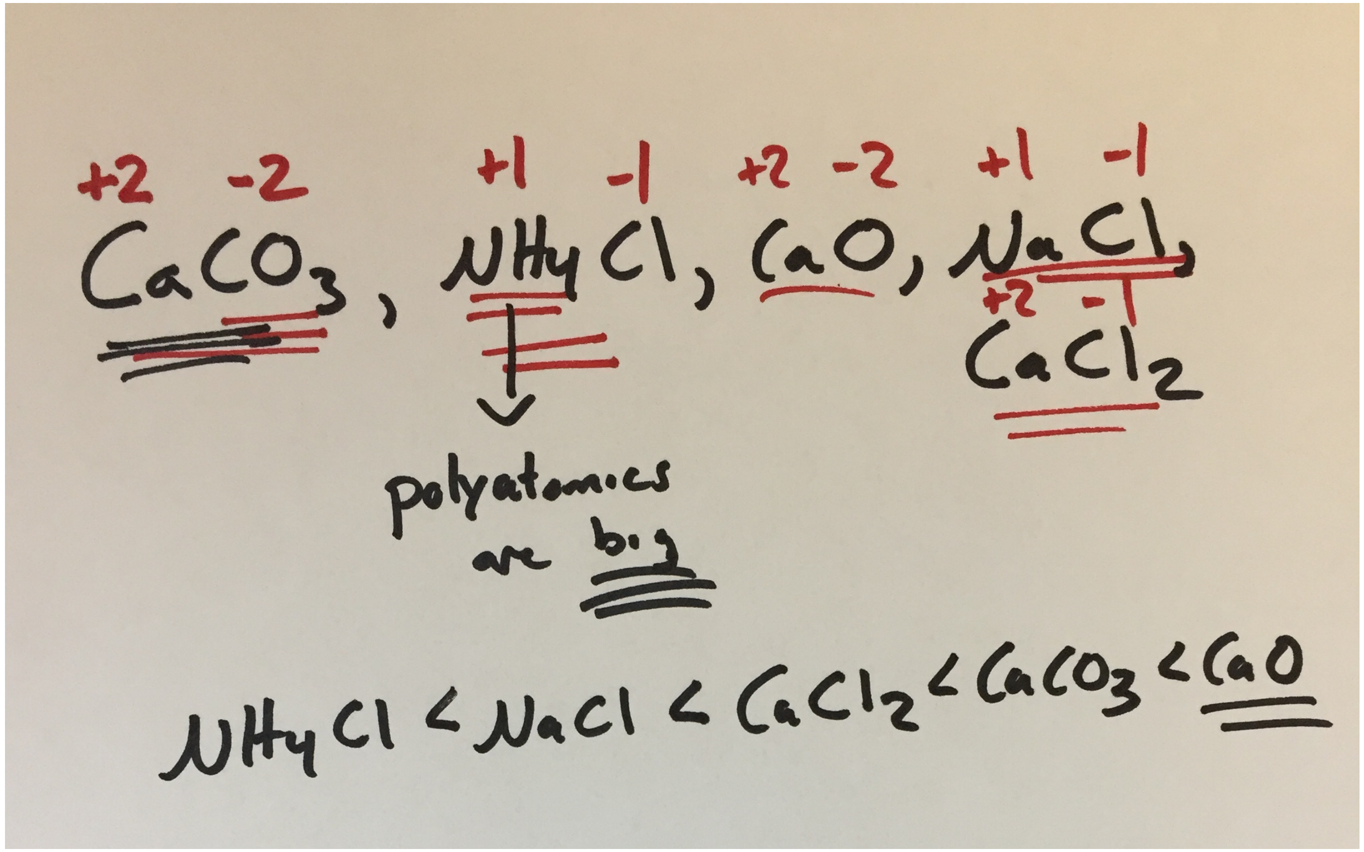
- This describes the energy of the following reaction:

$$NaCl \rightarrow Na^+ + Cl^-$$



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**



$\overset{+2}{Ca}\overset{-2}{CO_3}$, $\overset{+1}{NH_4}\overset{-1}{Cl}$, $\overset{+2}{Ca}\overset{-2}{O}$, $\overset{+1}{Na}\overset{-1}{Cl}$,

$\overset{+2}{Ca}\overset{-1}{Cl_2}$

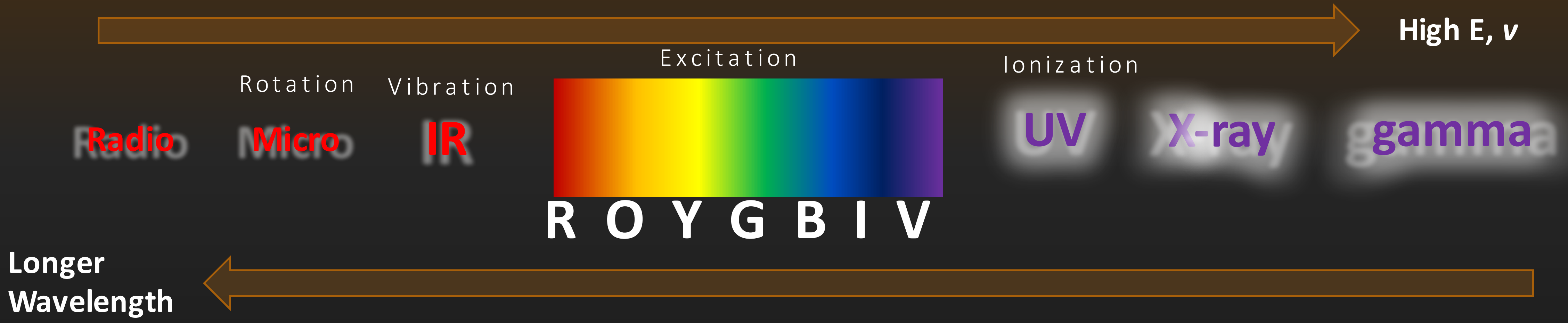
polyatomics are big

$NH_4Cl < NaCl < CaCl_2 < CaCO_3 < CaO$

Electromagnetic Radiation

THEORY, CALCULATIONS, PHOTOELECTRIC EFFECT, DISCRETE ENERGY LEVELS (ABSORPTION/EMISSION & RYDBERG)

THE ELECTROMAGNETIC SPECTRUM



High E, ν

Rotation Vibration Excitation Ionization

Radio **Micro** **IR** **UV** **X-ray** **gamma**

R O Y G B I V

Longer Wavelength

- Understand the relative energies, wavelengths, and frequencies of characteristic radiation types AND what this means for their interaction with matter.
- Microwaves: enough energy to begin rotating a molecule
- IR: enough energy to begin vibrating a molecule
- Visible (400-700nm): enough energy to begin exciting electrons
- UV and beyond: begins the full ionization (breaking) of electrons/bonds

Quantifying Light

- Modern physics defines light as photon particles exhibiting wave-like properties:

$$c = \lambda\nu$$

  - This equation states that the **speed of light** (c) is equal to the **frequency** (ν) times the **wavelength** (λ)
  - Or you could say that wavelength and frequency are inversely proportional
  - The speed of light is a constant and therefore independent of frequency and wavelength
    - That is to say that if you change frequency, you will change wavelength and vice versa to keep $c = 3\text{x}10^8$m/s

- You can also calculate the energy per photon:

$$E_{photon} = \mathrm{h}\nu \quad \text{or} \quad E_{photon} = \mathrm{h}\frac{c}{\lambda}$$

  - This equation states that the **the energy of a photon** is directly proportional to **frequency**
  - You can multiply your E_{photon} by Avogadro's number (N_A) to get energy per mole

Quantifying Light: Photoelectric Effect

- The photoelectric effect is a revolutionary experiment that demonstrates that light and matter can interact based on the equation:

$$E_k = h\nu - \phi$$

or

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

Note: you can think of this like a piece-wise function where

If $E_{photon} < \phi$, $E_k = 0$

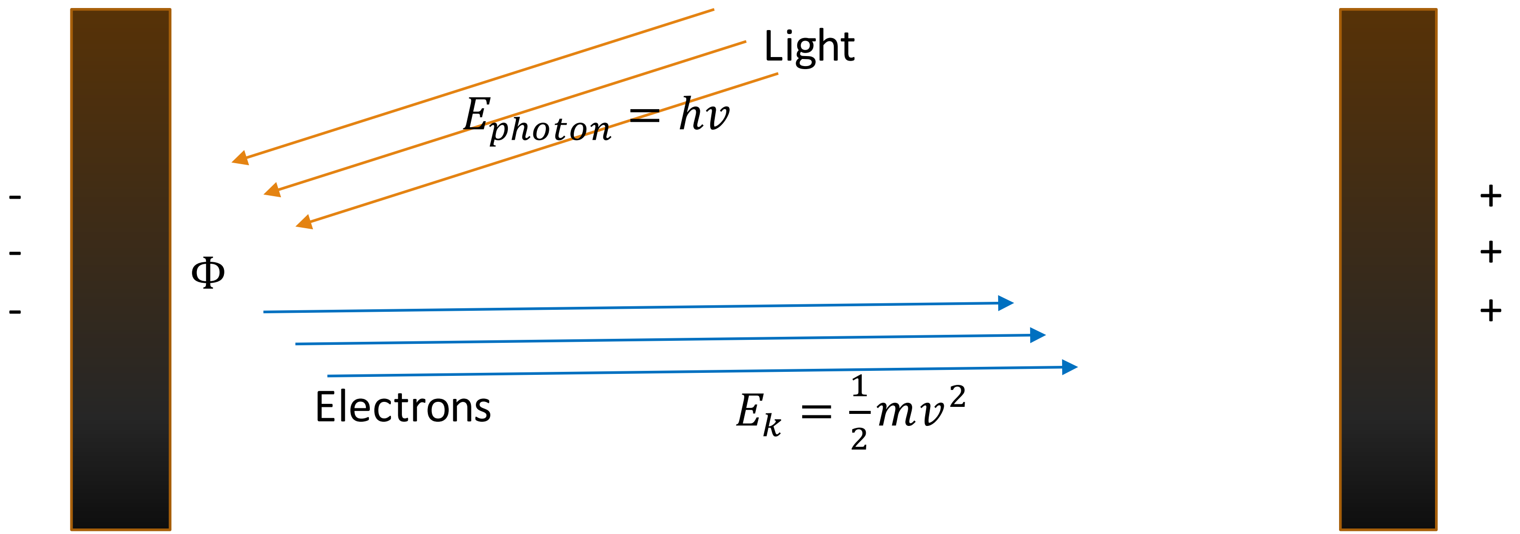
If $E_{photon} >= \phi, E_k = h\nu - \phi$

- This equation states that the **kinetic energy of an electron released** (E_k) is equal to the difference between the **photon energy of the incident light** (hv) minus the **work function of the metal** (ϕ)
- This equation only works if E_{photon} (hv) is greater than the work function. Until your $E_{photon} = \phi$, your energy is going into potential energy. After you reach ϕ, all of your photon energy will contribute to the kinetic energy

Quantum Mechanics: Photoelectric Effect

- The postulates of quantum mechanics were demonstrated by a series of important experiments between 1885-1930’s.
- **Photoelectric Effect**: a metal will eject electrons if a beam of light reaches a threshold energy
  - Proves that matter (the electrons of a metal) can interact with light

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



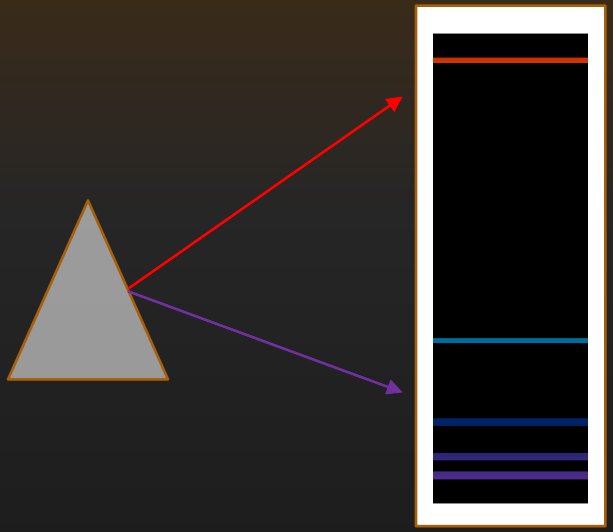
Key points:

- If an electron is not ejected, your light does not have sufficient energy (you must decrease wavelength / increase frequency)
- Increasing the intensity will result in more electrons ejected if the threshold is reached. If the threshold is not reached, increasing the intensity will do nothing

EMISSION:

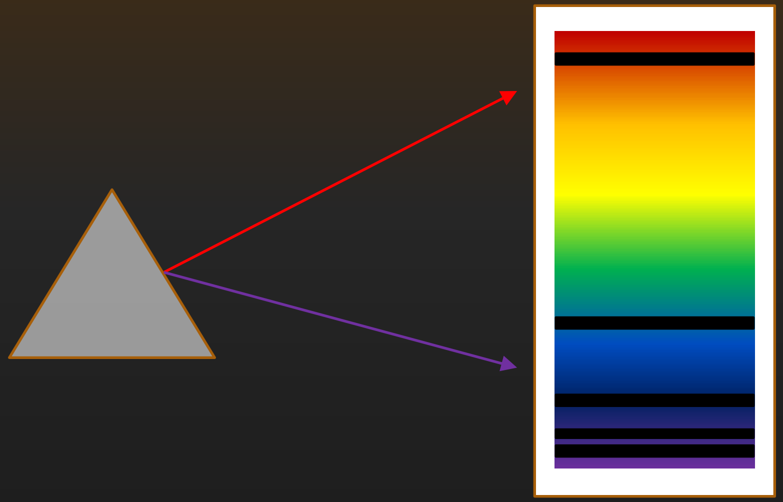
- HIGH N TO LOW N

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



ABSORPTION

- LOW N TO HIGH N



- The absorption and emission lines were an early experimental indicator that electrons emit characteristic frequencies
- Emission lines show a few colored lines on a black background.
- Absorptions lines show a few black lines on a rainbow background.
- The absorption and emission spectrums of a given element are the exact opposites

RYDBERG EQUATION TO WAVELENGTH, FREQUENCY

$$|\Delta E| = E_{photon} = hv$$

$$c = \lambda v$$

$R = 2.18 \times 10^{-18}$J

- YOU CAN CALCULATE THE WAVELENGTH OR FREQUENCY USING THE ABSOLUTE VALUE OF THE ENERGY CHANGE
- THIS IS THE WAVELENGTH OF LIGHT ABSORBED OR EMITTED GIVEN ANY ENERGY DIFFERENCE BETWEEN TWO N VALUES

Quantum Theory

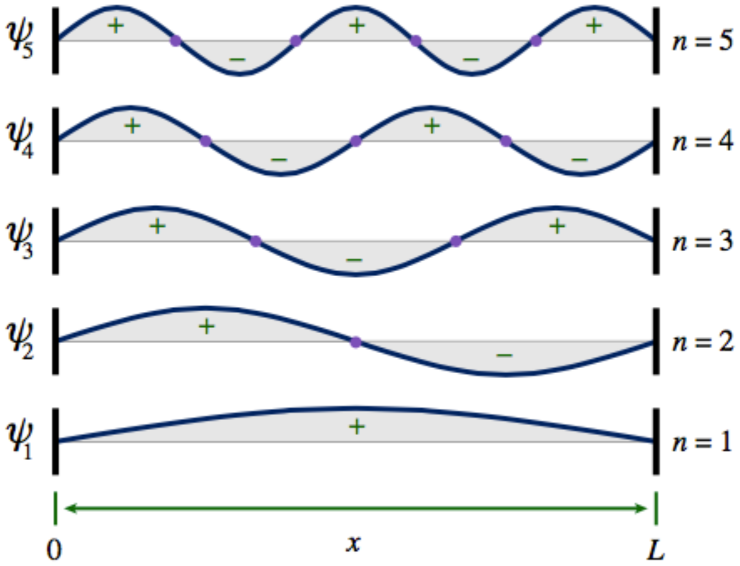
WAVE FUNCTION SOLUTIONS, ELECTRON CONFIGURATIONS

Particle in a Box

- The Schrödinger Wave Function gives us insight to the energy of an electron and the probability in finding that electron in a given range of three dimensional space. However, it is easier to conceptualize the wave function with a single-electron atom (hydrogen) in one dimension.
- Particle in a Box is useful because it answers two straightforward questions:
  - Given any n-value, where can I find the electrons? Where is there zero probability of finding an electron?

Particle in a Box

- Given any n-value, where can I find the electrons?
  - Where the graph gives you a non-zero value
- Where is there zero probability of finding an electron?
  - At the nodes (y=0)



Multiply by Ψ to get all positive values

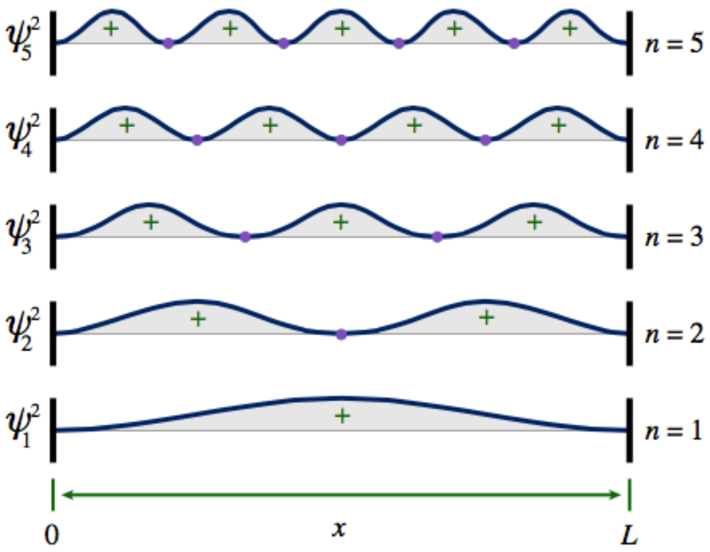
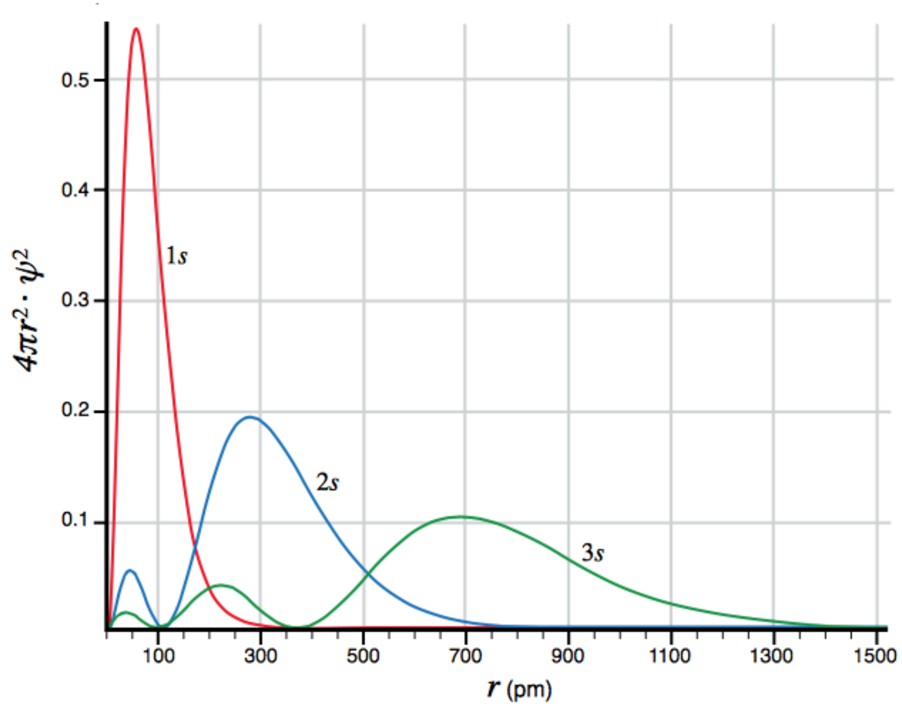


figure 2

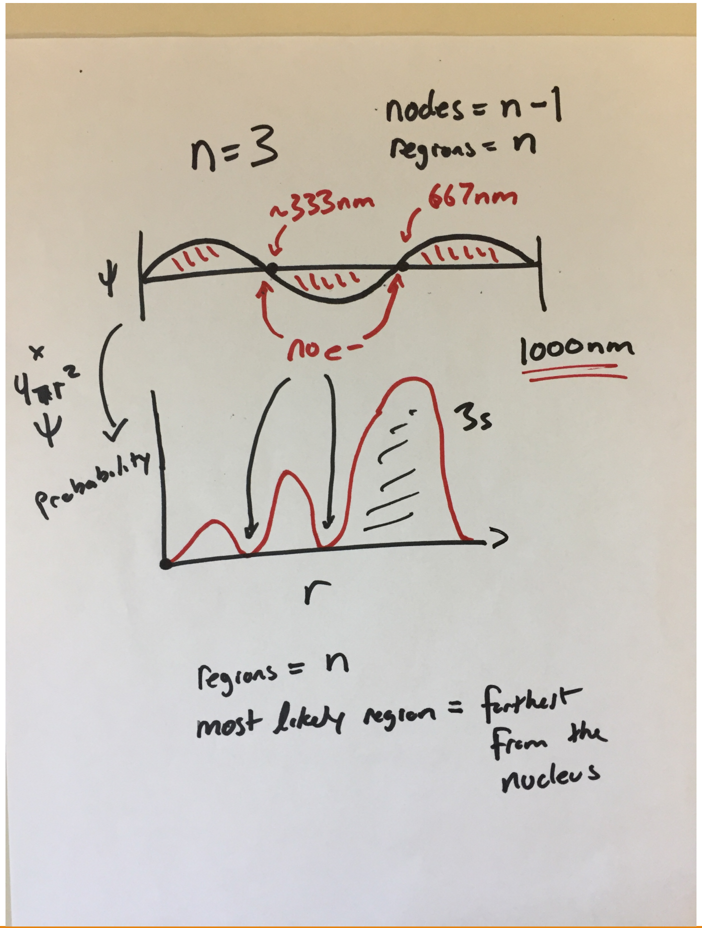
Radial Distribution

- If we further apply this concept, we can answer the more specific question: where are the electrons **most likely** to be found?



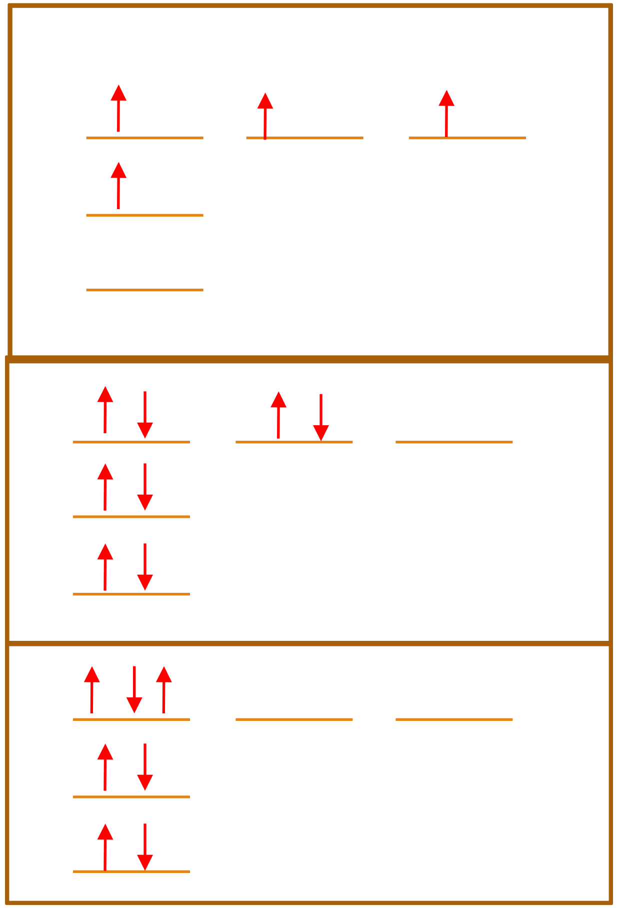
- Radial distribution curves show the **same nodes** as particle in a box, but shows the actual probability of finding an electron in **three-dimensional space**.
- The number of “humps” is equal to the n-value. It is always most probably that electrons are found in the furthest hump from the nucleus (r=0)

PIB to Radial Distribution Example



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's rule:** 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

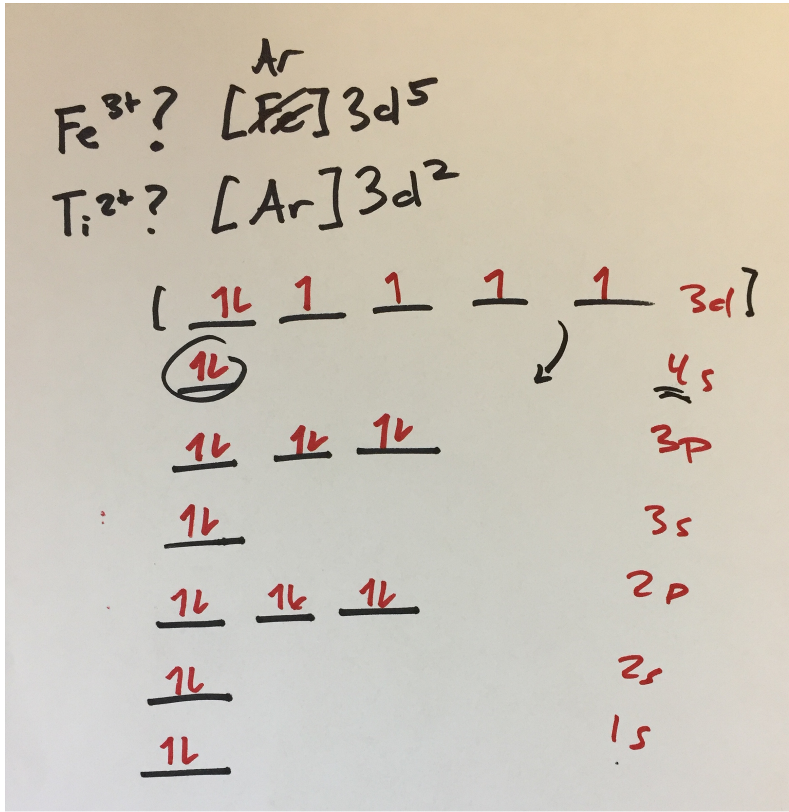
Quantum Numbers

- The Schrödinger Wave Function gives us insight to the energy of an electron and the probability in finding that electron in a given range of three dimensional space.

- The Quantum Numbers (n, l, m_l, and m_s) stem from the solutions of the wave function 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
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

Electron Configuration Examples



Fe^{3+}? $[\overset{Ar}{\cancel{Fe}}]3d^5$

Ti^{2+}? $[Ar]3d^2$

[↑↓ ↑ ↑ ↑ ↑ 3d]

↑↓ 4s

↑↓ ↑↓ ↑↓ 3p

↑↓ 3s

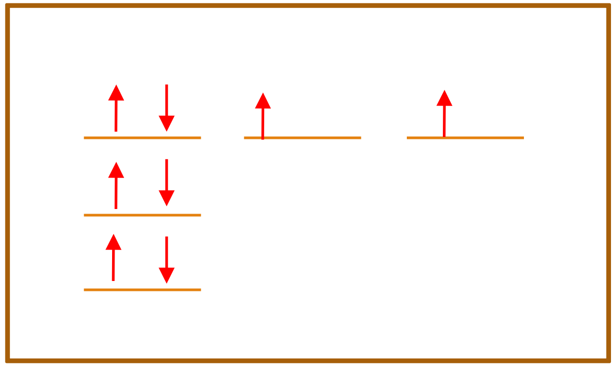
↑↓ ↑↓ ↑↓ 2p

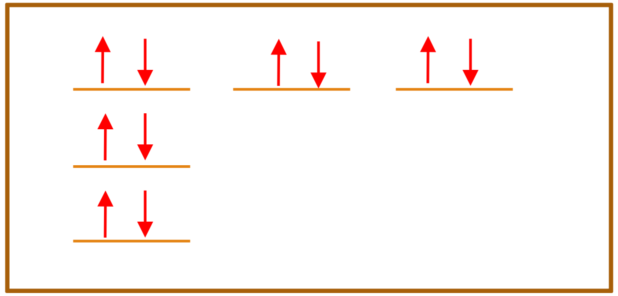
↑↓ 2s

↑↓ 1s

Magnetic Susceptibility

- **Paramagnetic:** If an atom or molecule has unpaired electrons, it will be attracted to a magnetic field
  - Remember: “un”-para = unpaired.
- **Diamagnetic:** if an atom or molecule has all paired electrons, it will be repelled by a magnetic field
  - Remember: “di” means “two” or ”double” in Latin. Think two electrons in each orbital.
  - All odd number atoms are diamagnetic, but not all even number atoms are paramagnetic





Note: these are all examples of these rules violated

Periodic Table Trends

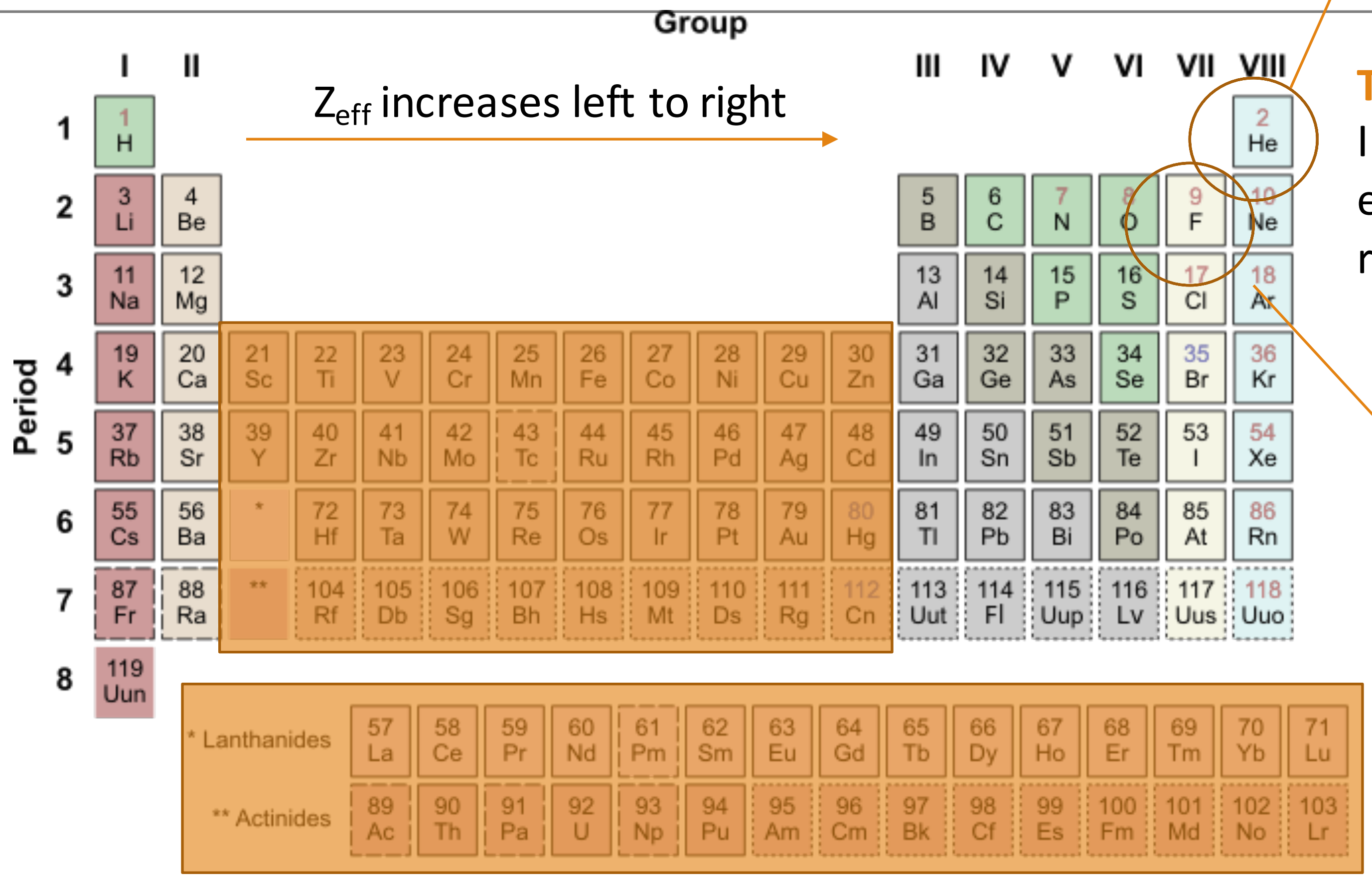
IONIZATION ENERGY, Z EFFECTIVE, ATOMIC RADIUS, ELECTRON AFFINITY

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 the outer electrons by the nucleus**
  - Trend: increases as you go to the top right

Periodic Trends

Helium has the maximum ionization energy



Z_{eff} increases left to right

Shielding Increases going down

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 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 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																	

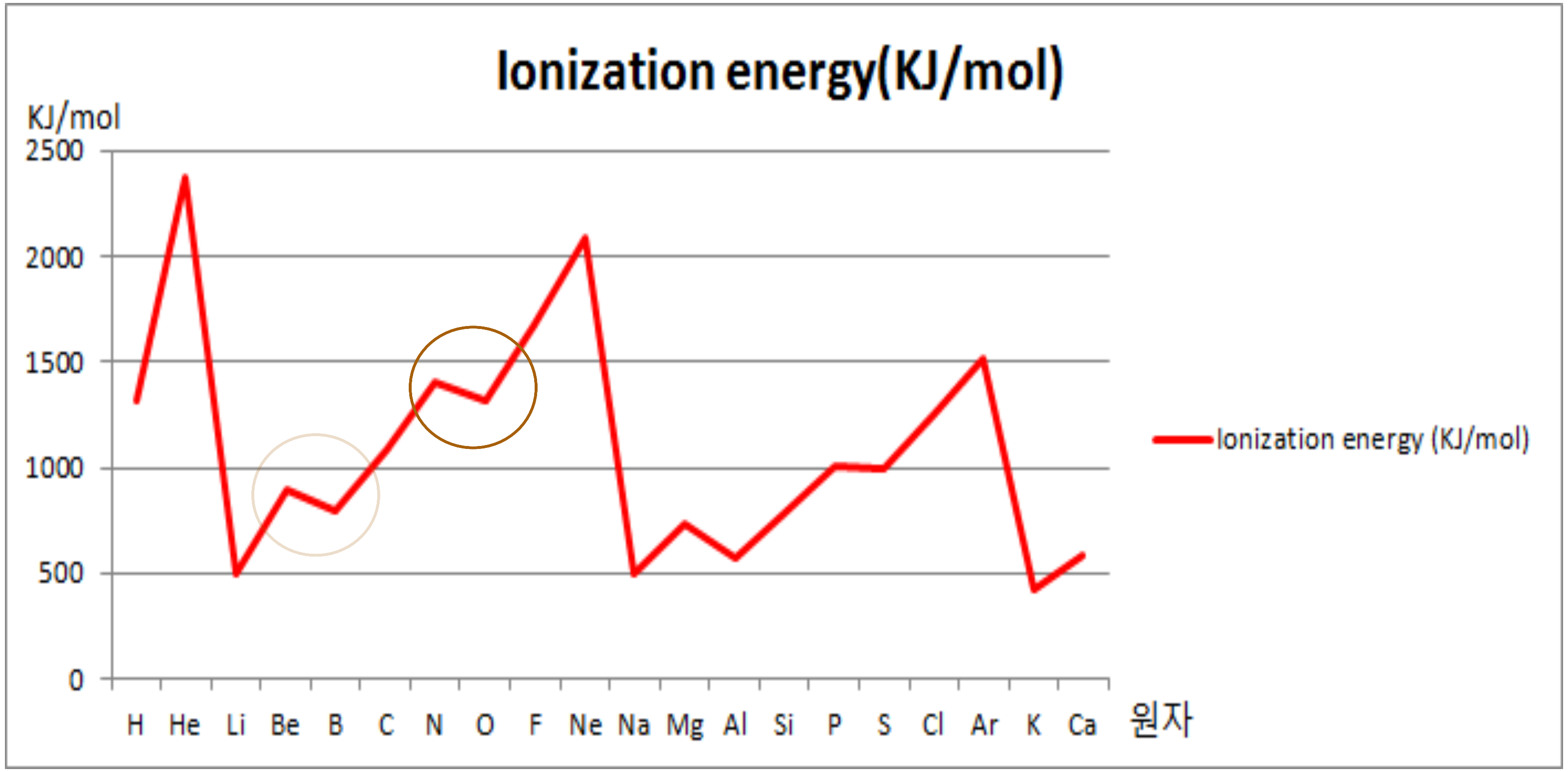
* Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
** Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

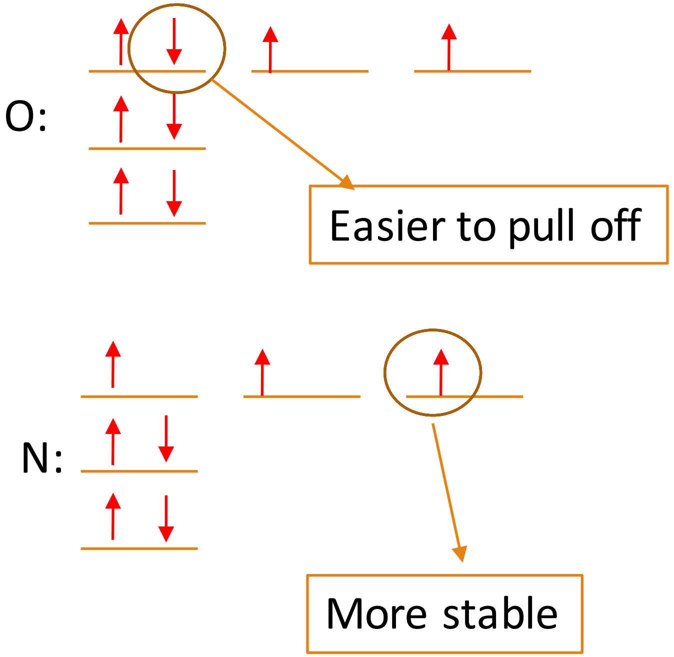
TOP RIGHT: High Ionization energy, high electron affinity, small radius

Fluorine has the maximum electron affinity

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

Ionization Energy Exceptions





Easier to pull off

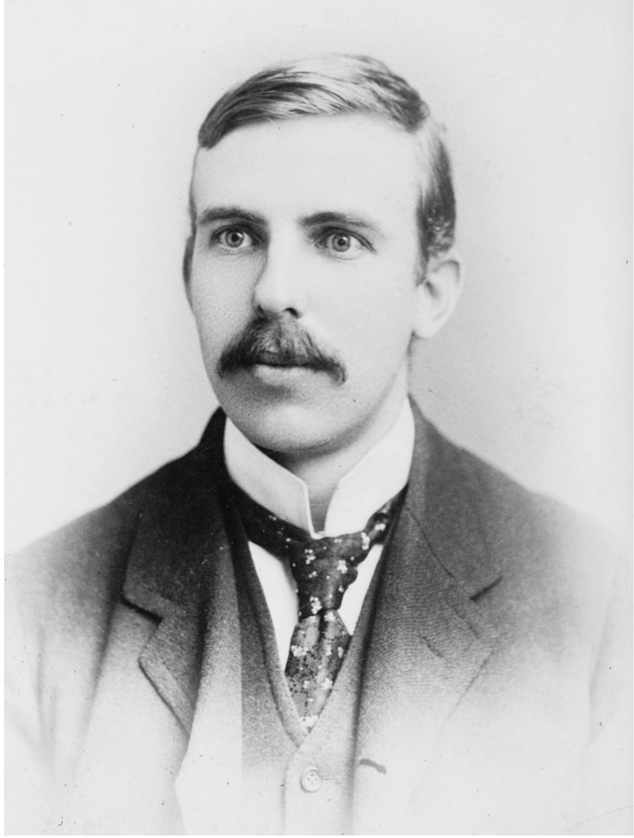
More stable

The ”special” stability of a fully filled s or p orbital, or a half-filled p orbital, causes exceptions to the trend of ionization energy

Extra Slides

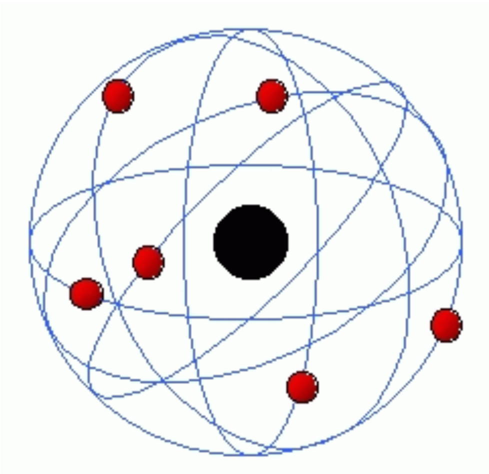
Classical Atomic Theory

- The classical theory of an atom is an important contribution to science that is still taught today even though it is extremely wrong.
- The following points are the main pillars of classical atomic theory
  1. The atom consists of three fundamental particles: protons, neutrons, and electrons
  2. Electrons whirl around the nucleus like planets around the sun, and (like all things in the universe) are governed by Newtonian laws of motion
  3. Light is a wave and exhibits only wave-like behavior



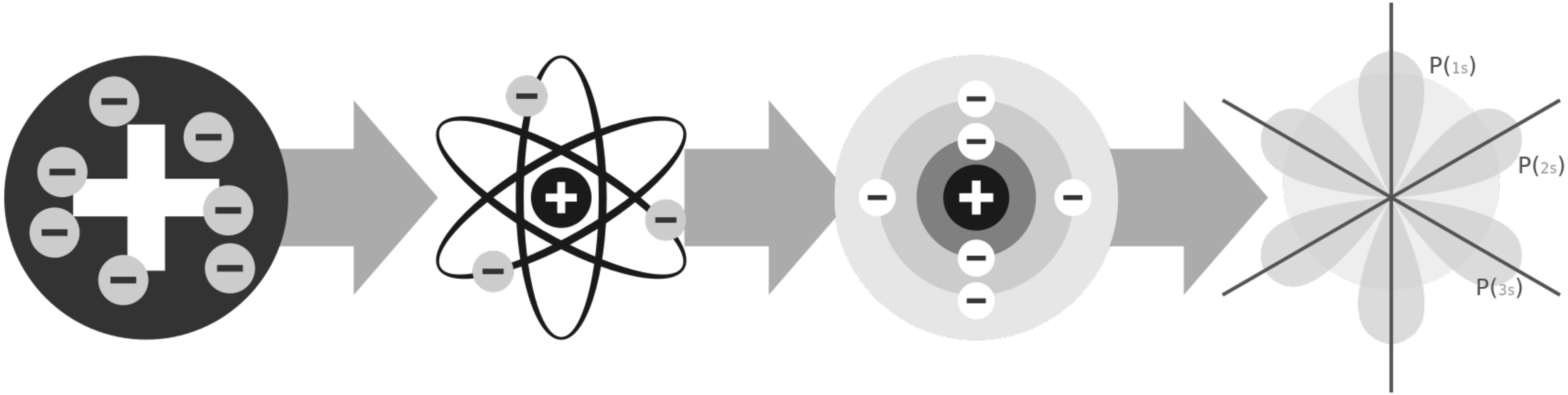
Classical Atomic Theory

- However, there were known failures in these models that, until technology caught up to theoretical physics, could not be explained:
  1. If electrons truly abided by the laws of classical motion, they would lose their energy and collapse in on the nucleus – this would happen on a human time-scale in the blink of an eye
  2. The UV catastrophe showed that blackbodies emit characteristic wavelengths at low wavelengths, whereas the current laws predicted that the absorption would approach infinity before the visible spectrum-range
  3. The spectrum of hydrogen absorption and emission showed indescribable patterns that conflicted with the idea that light and electrons could not interact



Not covered by MWF classes; likely to not be tested by TTH classes

The History of the Modern Atomic Model



Classical Theory

Quantum Theory

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**.
  2. Electrons and light (photons) exhibit **wave-particle duality**.
  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.
     - Furthermore, this demonstrates that electrons exist in “clouds” and not circular orbits

Classical Vs. Quantum Mechanics

Classical Mechanics

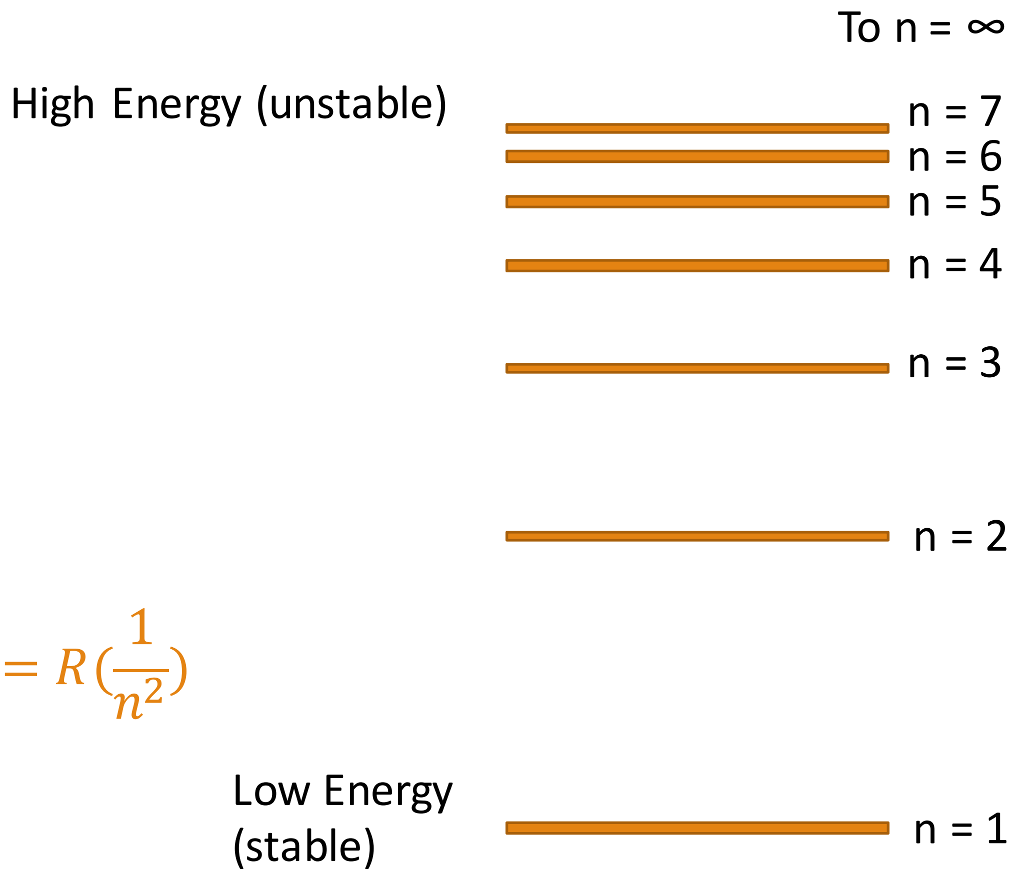
- Three fundamental particles: protons, neutrons, and electrons
- Light is a wave
- Electrons and light do not interact
- Electrons orbit the nucleus
- Position and momentum are predictable

Quantum Mechanics

- Many subatomic particles and growing
- Light exists as tiny packets of energy called photons. Photons exhibit particle-like behavior.
- Electrons and light interact
- Electrons exist in a “cloud” outside the nucleus and are confined to energy levels (n) of various shapes (l)
- Position and momentum are not simultaneously predictable
- Everything with momentum has a quantifiable wavelength

Rydberg Energy Levels

- You can understand Rydberg n-values by adhering to the following 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 potential energy of a given energy state is proportional to the inverse square of the whole number integer n
  3. The greatest energy difference between two consecutive numbers is 1 and 2.



To n = ∞

High Energy (unstable)

n = 7

n = 6

n = 5

n = 4

n = 3

n = 2

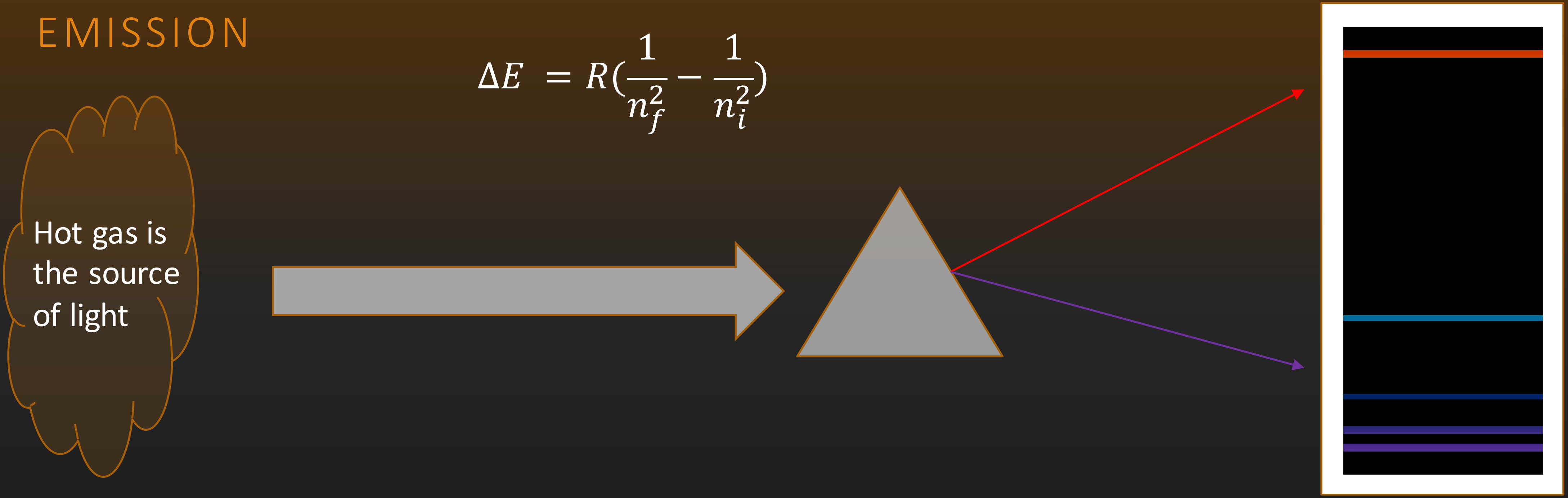
$$E_n = R\left(\frac{1}{n^2}\right)$$

Low Energy (stable)

n = 1

EMISSION

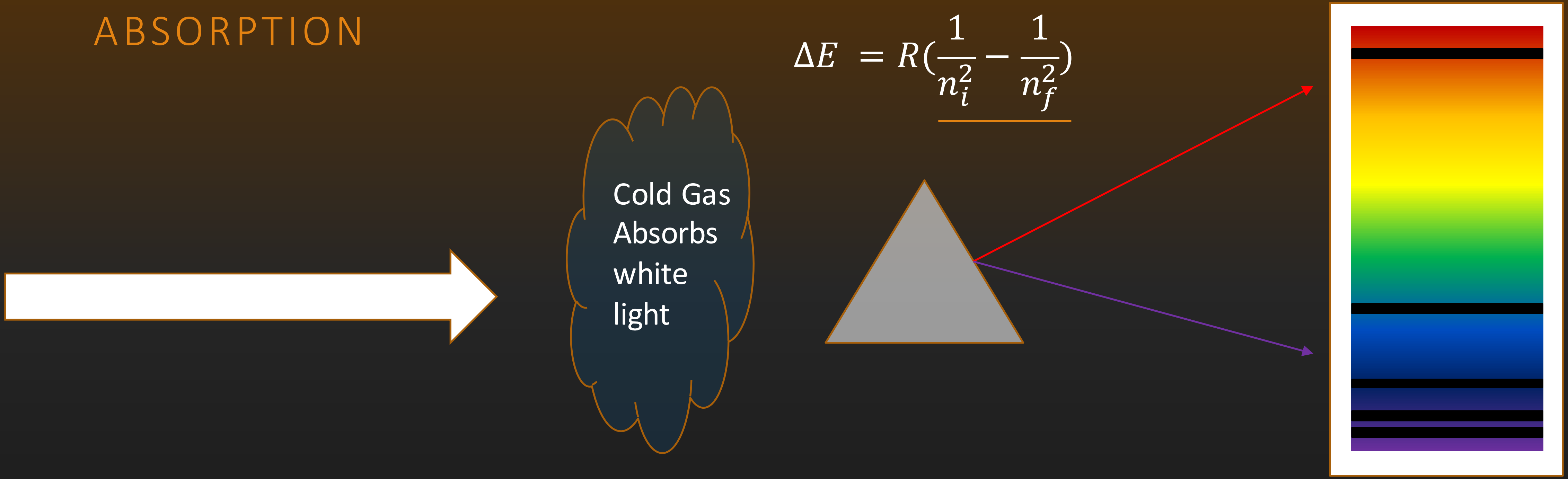
$$\Delta E = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$



Hot gas is the source of light

- YOU SEE ONLY THE CHARACTERISTIC FREQUENCIES OF HYDROGEN EMISSION
- THE LIGHT EMITTED HAS THE ENERGY OF THE FREQUENCIES SEEN IN THE COLORED LINES. THIS CORRESPONDS TO ELECTRONS FALLING FROM A HIGH N TO A LOWER N

ABSORPTION



Cold Gas Absorbs white light

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

- YOU WILL SEE THE CONTINUOUS ("WHITE LIGHT") SPECTRUM MINUS THE CHARACTERISTIC FREQUENCIES OF HYDROGEN
- THE LIGHT ABSORBED IS "LAUNCHING" THE ELECTRONS FROM A LOW N VALUE TO A HIGHER N VALUE. THIS ABSORPTION REQUIRES ENERGY THAT CORRESPONDS TO THE FREQUENCIES OF LIGHT THAT ARE MISSING

RYDBERG EQUATION: EMISSION

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

R = 2.18 X 10^{-18}J

- THIS EQUATION SHOWS THE ENERGY OF A PHOTON RELEASED BY A TRANSITION BETWEEN TWO ENERGY LEVELS WITH THE CONDITION THAT YOU ARE UNDERGOING EMISSION
- IN OTHER WORDS, THIS EQUATION ONLY WORKS AS WRITTEN IF YOUR ELECTRON IS FALLING FROM A HIGH ENERGY STATE TO A LOWER ONE (IN OTHER WORDS $N_F < N_I$)
- YOU WILL GET A POSITIVE ENERGY CHANGE, BUT UNDERSTAND THAT THIS IS THE ENERGY OF YOUR PHOTON. YOUR ELECTRON IS DECREASING IN ENERGY BY THIS MUCH.

RYDBERG EQUATION: ABSORPTION

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

R = 2.18 X 10^{-18}J

- THIS EQUATION SHOWS THE ENERGY OF A PHOTON RELEASED IN THE TRANSITION BETWEEN TWO ENERGY LEVELS WITH THE CONDITION THAT YOU ARE UNDERGOING ABSORPTION
- IN OTHER WORDS, THIS EQUATION ONLY WORKS AS WRITTEN IF YOUR ELECTRON IS JUMPING FROM A LOW ENERGY STATE TO A HIGHER ONE (IN OTHER WORDS $N_F > N_I$)
- BECAUSE YOU SWITCHED THE PLACEMENT OF YOUR N-VALUES, YOU WILL AGAIN GET A **POSITIVE** ENERGY CHANGE.

Quantum Numbers

- 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, …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

Electron Configurations: Exceptions

- D-block and f-block elements prioritize filling their half-way or fully filled subshells if they are one electron away.
- This is because it is more stable to have $4s^1$ and $3d^5$ than it is to have $4s^2$ and $3d^4$.

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.

- The electron configurations are therefore:
- Cr = $[Ar]4s^1 3d^5$
- Cu = $[Ar]4s^1 3d^{10}$