

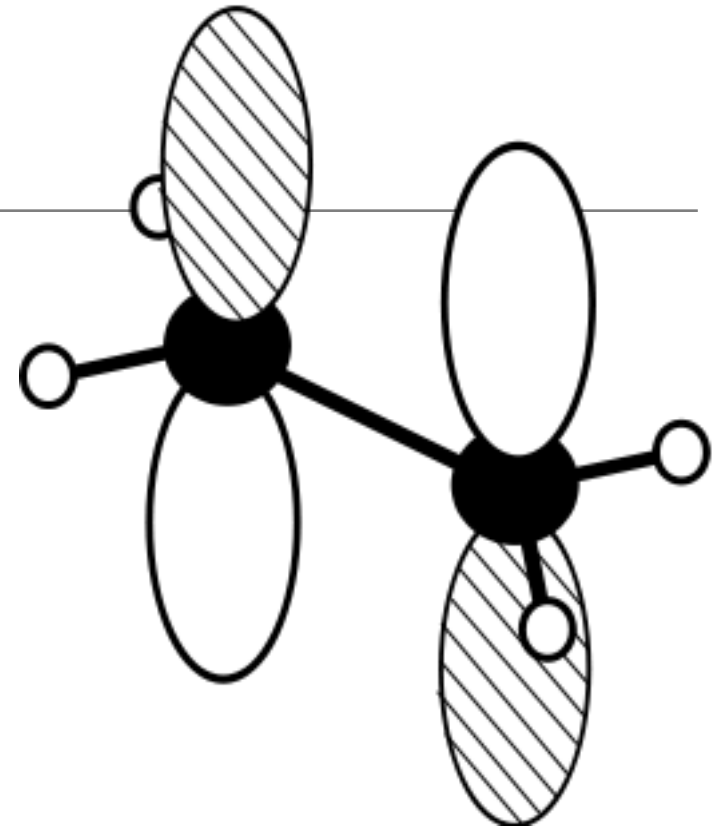
Note: Due to recent changes the exam 2 material for these slides ends at Ionization Energy Exceptions. You can omit Lewis Structures through General Formal Charge Rules.

CH301 Unit 2

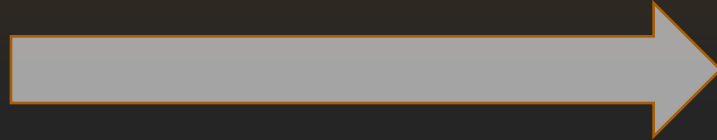
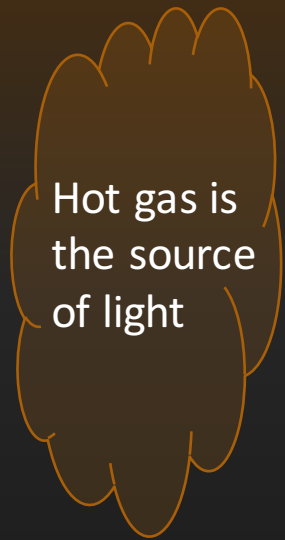
QUANTUM NUMBERS AND ELECTRON CONFIGURATIONS

Goals for Today

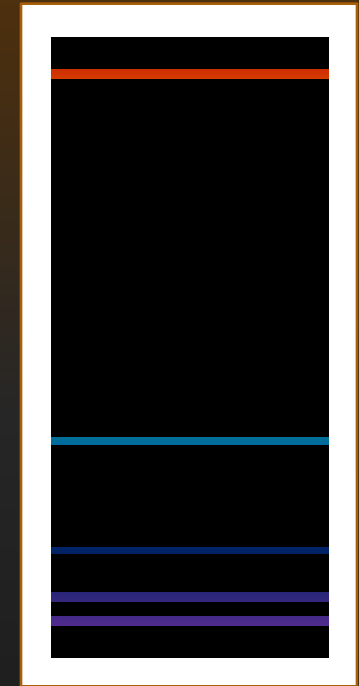
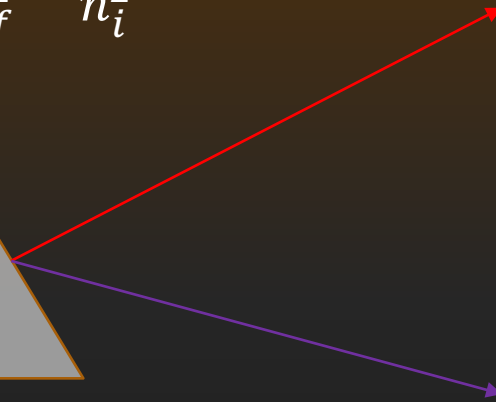
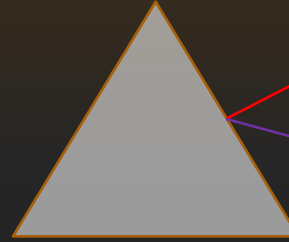
- Clarify some Rydberg Concepts
 - Absorption vs. emission
- Particle in a box to Quantum numbers
 - Wave functions, radial distribution, possible quantum numbers
- Electron configurations
 - Basic principles and exceptions
- If possible, introduce Lewis Structures



EMISSION

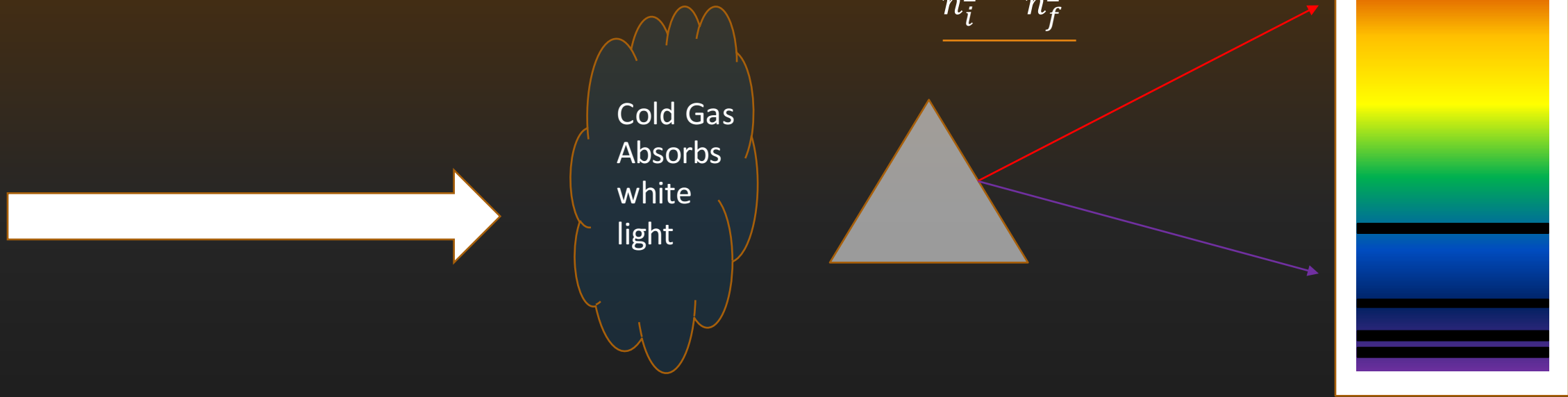


$$\Delta E = R \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$



- 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



- 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

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

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

-
- 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

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

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

-
- 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.

RYDBERG EQUATION TO WAVELENGTH, FREQUENCY

$$|\Delta E| = E_{\text{photon}} = h\nu$$
$$c = \lambda\nu$$

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

-
- 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

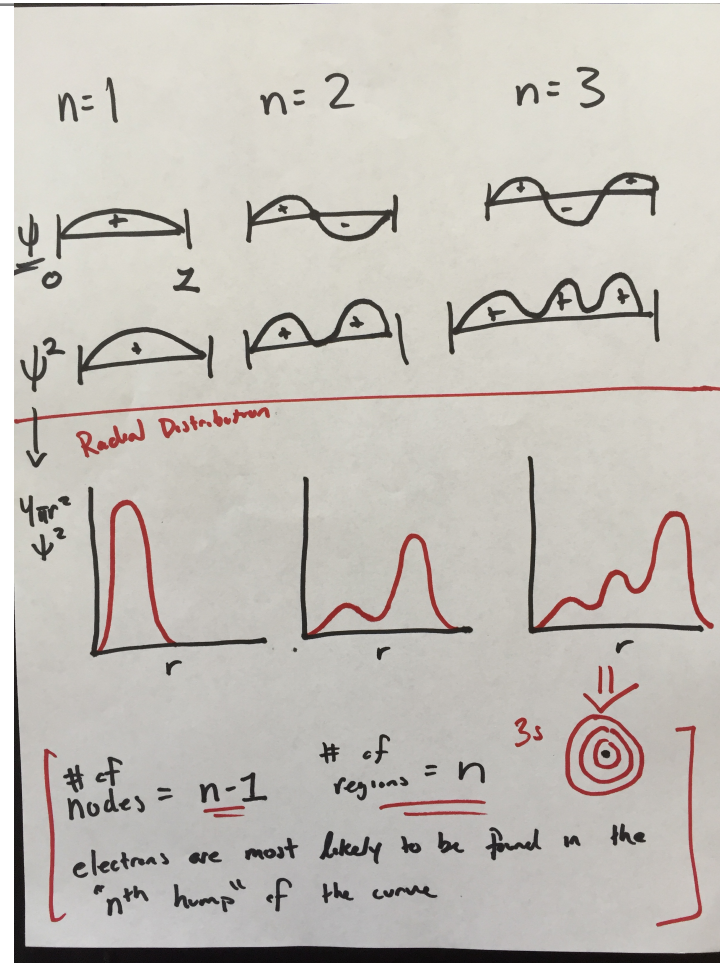
OR IF YOU WOULD RATHER:

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

$$R = 3.3 \times 10^{15} \text{ Hz}$$

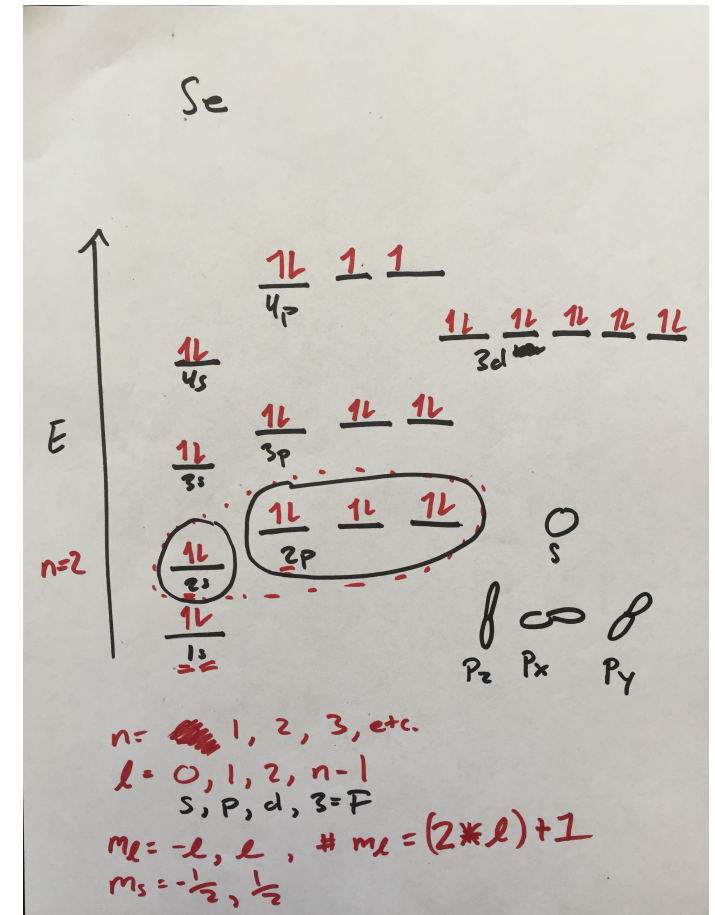
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- The frequency is proportional to the absolute value of the difference between n_f^2 and n_i^2
 - But REMEMBER: absorption leads to an increase in energy (low n to high n), emission leads to a decrease in energy (high n to low n)

Particle in a Box to Radial Distributions



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



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

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, to infinity

note: as far as electron configurations are concerned in real life, our periodic table goes up to $n = 7$

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 $3d^4$.

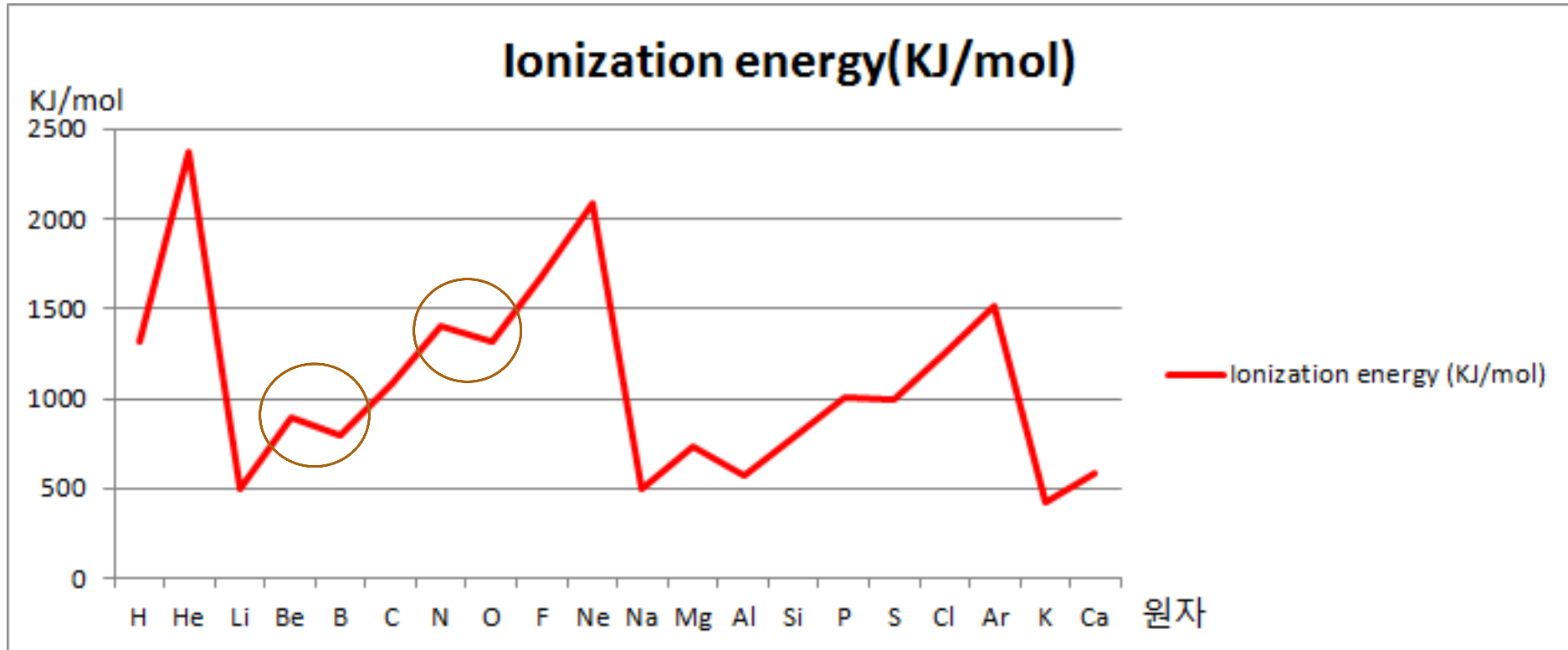
Electron Configurations: Exceptions

- 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]4s¹3d⁵
 - Cu = [Ar]4s¹3d¹⁰

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

Ionization Energy Exceptions



Recognize that it is difficult to remove an electron from half-filled p orbitals or filled s orbitals

Unit Three Material

Lewis Structures

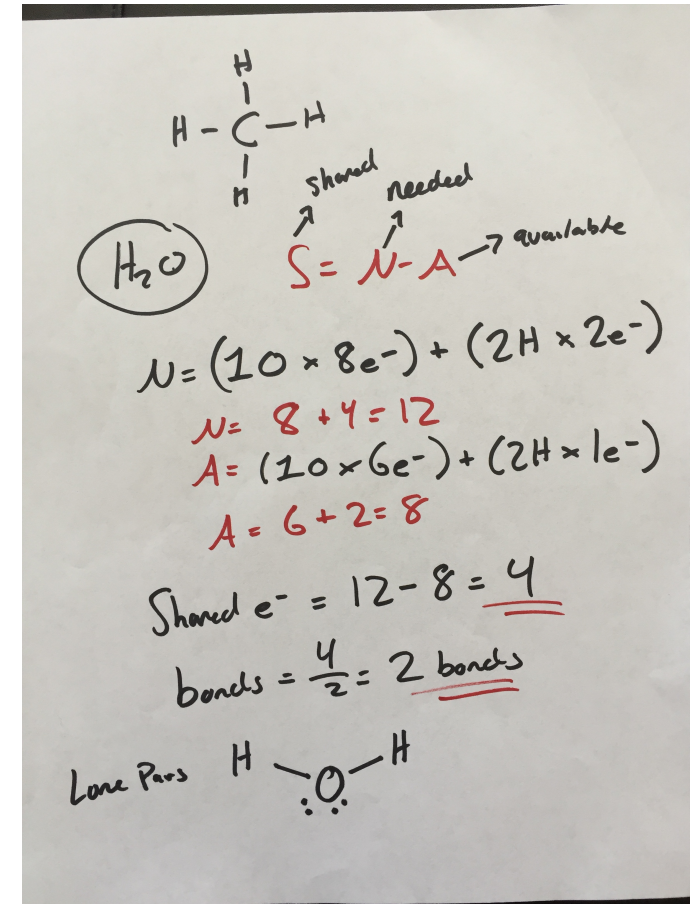
- Lewis structures are the main form of drawing molecules. There are two important equations to know when drawing Lewis Structures:

$$S = N - A$$

- The number of shared electrons is equal to the total electrons **needed** to fill the valence minus the electrons **available**
- You can then calculate the number of bonds by dividing the shared electrons by two

$$FC = \text{Valence} - (\text{lone electrons} + \text{bonds})$$

- The formal charge of any atom in a molecule is equal to the the valence electrons of the atom (as seen on the periodic table) minus the “things it’s touching” in the Lewis structure (the lone electrons and the number of bonds)



General Formal Charge Rules

- Formal charge defines the distribution of charge throughout a molecule. More specifically, it is used to show the charge on each atom in a molecule.
- The formal charge of a molecule is the sum of the individual formal charges of the atoms in the molecule. Formal charges should be minimized in your Lewis Structures.

Element	-1 Charge	Neutral	+1 Charge
Carbon	3 bonds*	4 bonds	5 bonds*
Nitrogen	2 bonds	3 bonds	4 bonds
Oxygen	1 bond	2 bonds	3 bonds

* In this class carbon is nearly always neutral (4 bonds);

General Formal Charge Rules

