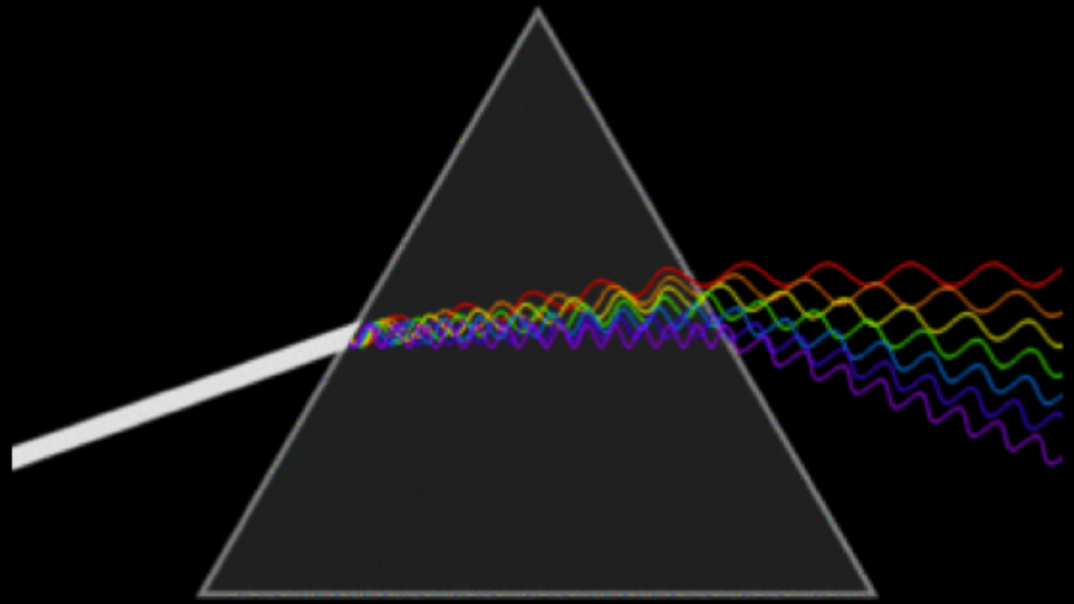


CH301 Unit 2

REVIEW TWO: QUANTUM THEORY SOLUTIONS,

ELECTRON CONFIGURATIONS, TRENDS

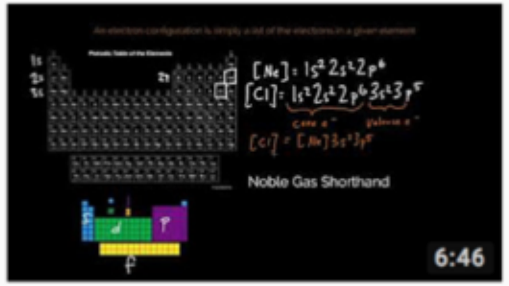
Foundations for these topics:

YouTube videos:

Lesson Two: Quantum Numbers (Atomic Theory)

Jimmy Wadman • 91 views • 2 months ago

In this lesson, we will discuss the quantum numbers and how they relate to the modern atomic model.



Lesson Two: Electron Configurations (Atomic Theory)

Jimmy Wadman • 52 views • 2 months ago

In this lesson, we will highlight the basic rules for **electron configurations**. Later on, we will focus on a few specific exceptions to ...

What is Quantum Mechanics?

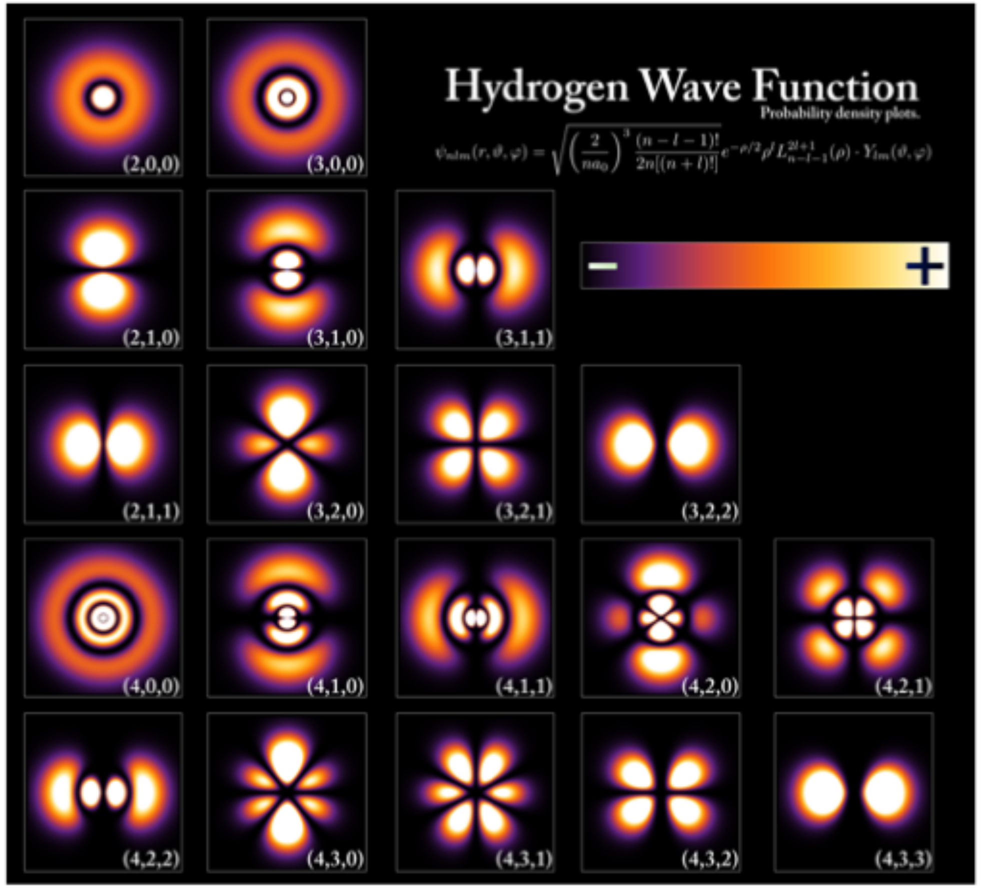
- Quantum mechanics helps us explain the currently accepted model of the atom using the following empirically derived postulates:

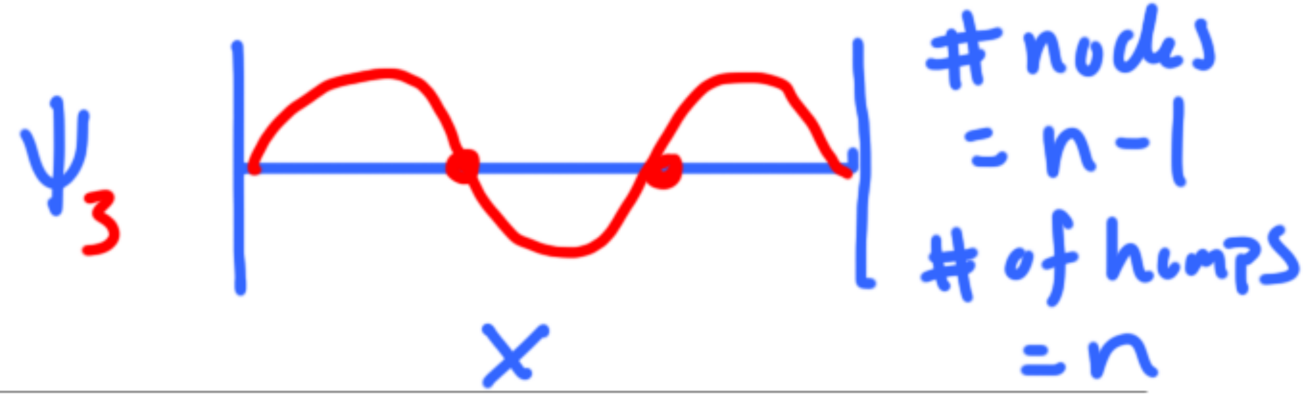
1. Electrons exist in **discrete, quantifiable energy states**.
   - Absorption/Emission spectra: The line spectra for a given gas has characteristic wavelengths
2. Electrons and light (photons) exhibit **wave-particle duality**.
   - Photoelectric effect: Light can act like particles
   - X-Ray diffraction: Small particles (electrons) can act like waves
3. The position and momentum of electrons can only be described with statistical **probabilities** when electron orbitals are quantified as wave functions
   - 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)
   - We use the quantum numbers for "electron accounting" in electron configurations and diagrams

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.**





Particle in a Box

- The Schrödinger Equation gives us insight to the **energy of an electron** and the **probability of finding that electron** (location, correlates with shape) in a given range of three dimensional space.
- Particle in a Box is useful because it conceptualizes the simplest demonstration of the Schrödinger equation (1 particle, 1 dimension, no potential energy):
  - Given any n-value, where can I find the particle? Where is there zero probability of finding the particle?
- The Radial Distribution Function helps bring it all together in three-dimensional space by answering:
  - Where are my electrons most likely to be found?

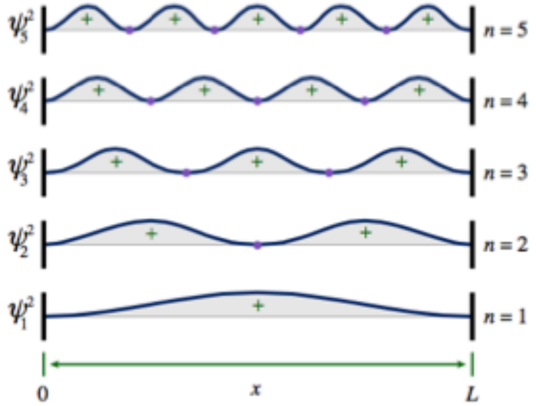
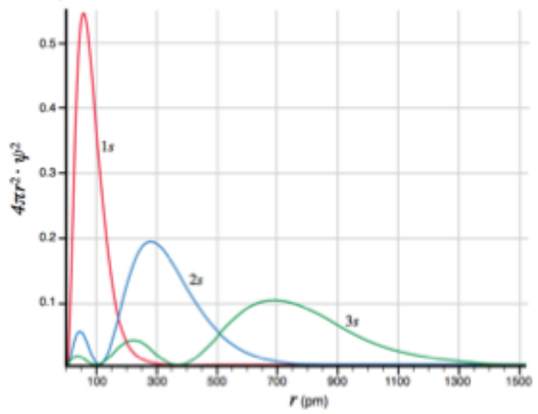


figure 2



Humps = Maximum Probability
Nodes = Zero Probability

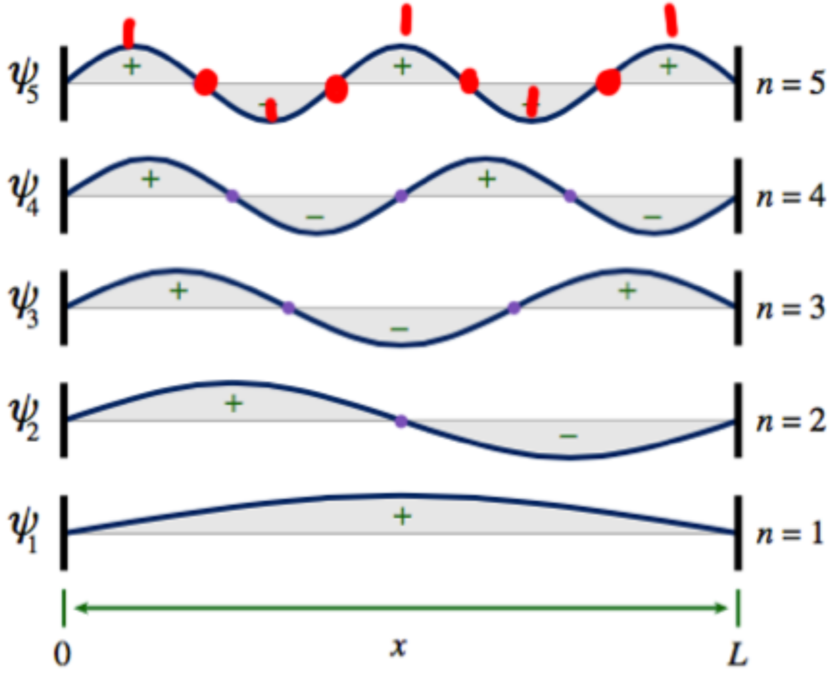
Particle in a Box

Some helpful rules:

- # of full wavelengths = n/2
- # of distributions ("humps") = n
- # of nodes = n-1

- 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)

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}\right)x$$



Multiply by Ψ to get all positive values

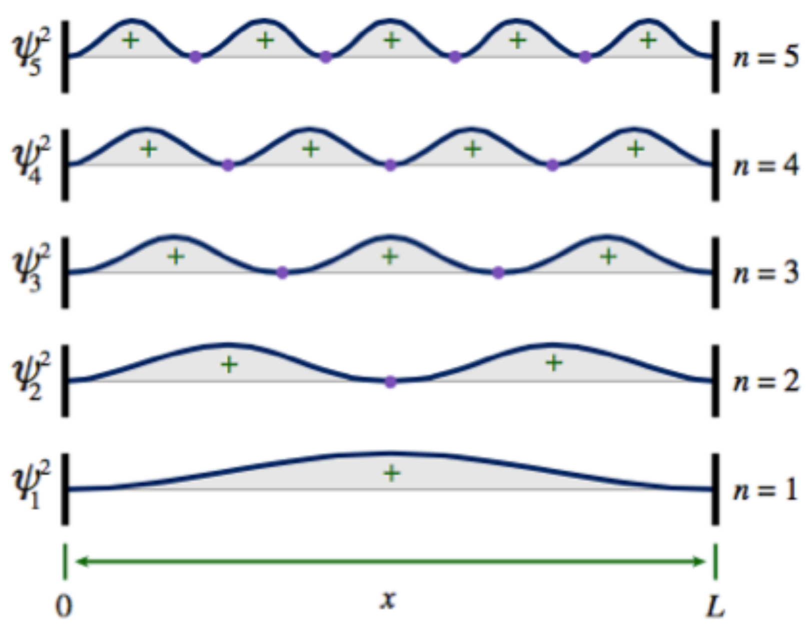


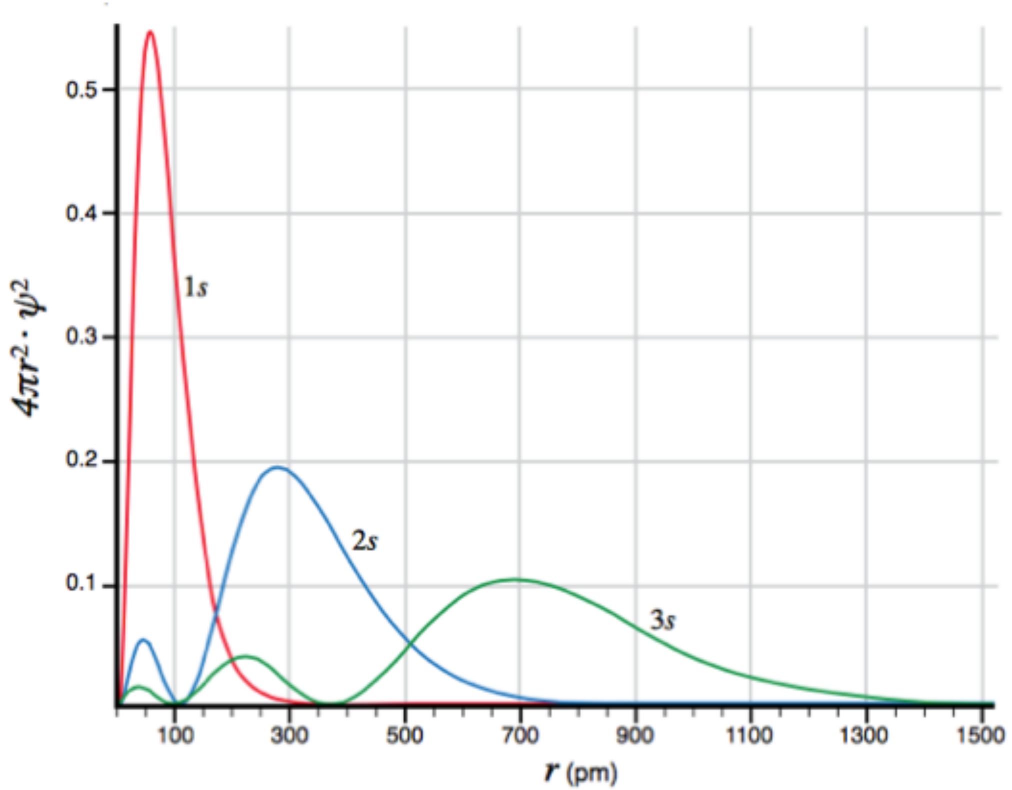
figure 2

Node: any time the sinusoidal function crosses from (-) to (+) or (+) to (-). 0 chance of finding an electron.

# of humps = n
# of nodes = n-1

Radial Distribution

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



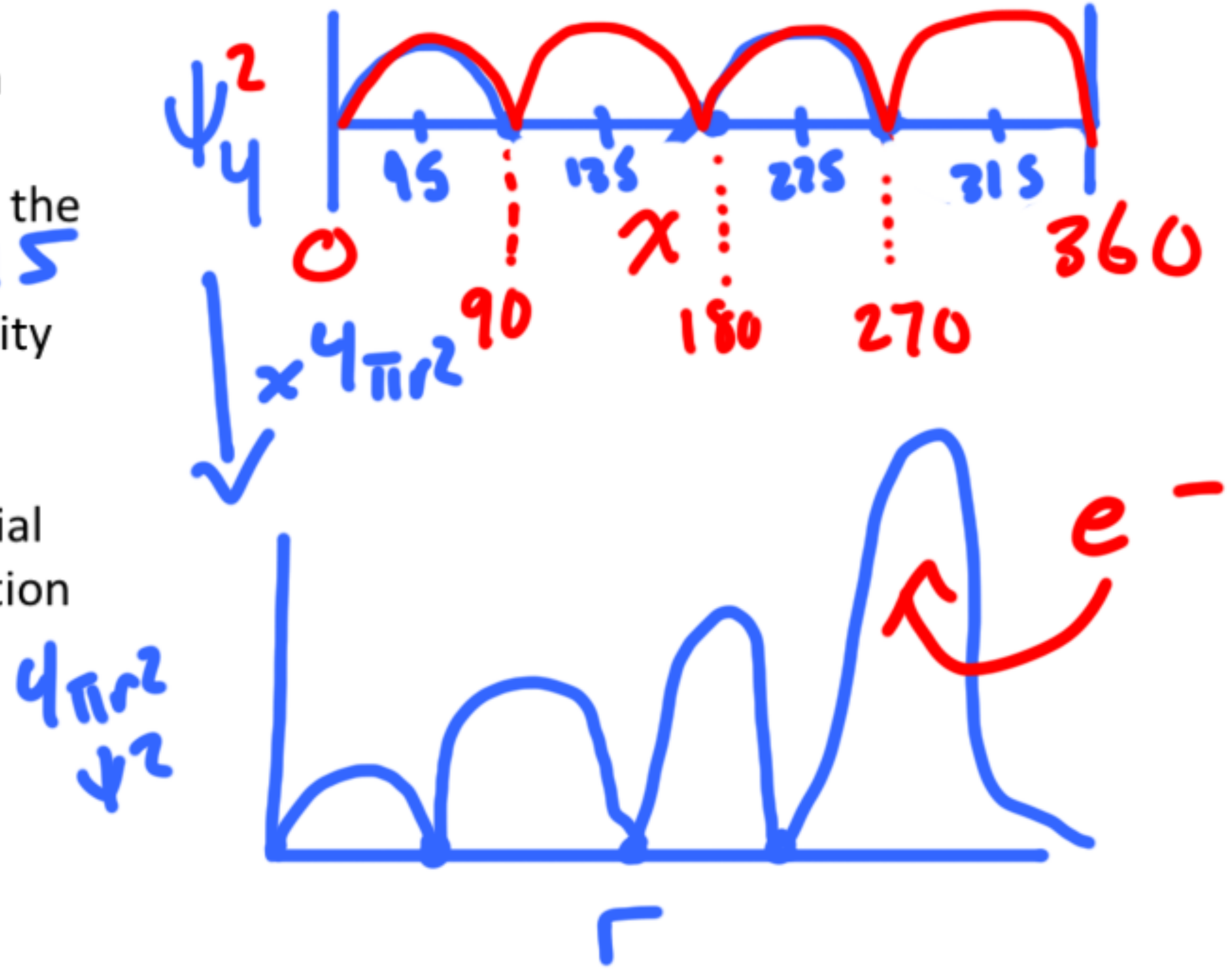
- Radial distribution curves show the same number of nodes as particle in a box, but they also show the actual probability of finding an electron in **three-dimensional space**.
- The number of distributions is equal to the n-value. It is always most probably that electrons are found in the furthest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

PIB to Radial Distribution Example

Suppose you have a single particle confined to a one-dimensional "box" of length 360 pm.

1. At what distances are you most likely to find the particle if n = 4? 45, 135, 275, 315
2. At what distances do you have zero probability of finding this particle? 90, 180, 270
3. Lastly, if this particle is a hydrogen atom electron in the 4s orbital, what does the radial distribution function tell you about the location of the electrons?

4 humps → highest probability in 4th hump

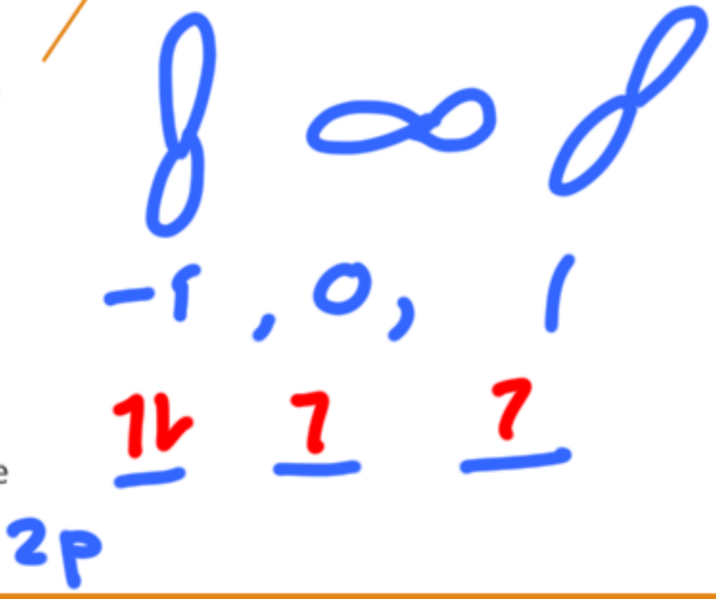


Quantum Numbers

- The Quantum Numbers (n, ℓ, m_l, and m_s) stem from the solutions of the Schrödinger Equation and represent the following:
  1. **Principal 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
     - **How do we get the shape? What ℓ represents is the number of angular nodes. Knowing this can help determine the fundamental shape of even the most complicated orbitals (f, g, h, i, etc.)***
  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

$\ell = 0$, s
$\ell = 1$, p
$\ell = 2$, d
$\ell = 3$, f

Angular Nodes = ℓ



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:

Principal 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

l=0, s l=2, d l=4, g
l=1, p l=3, f l=5, h

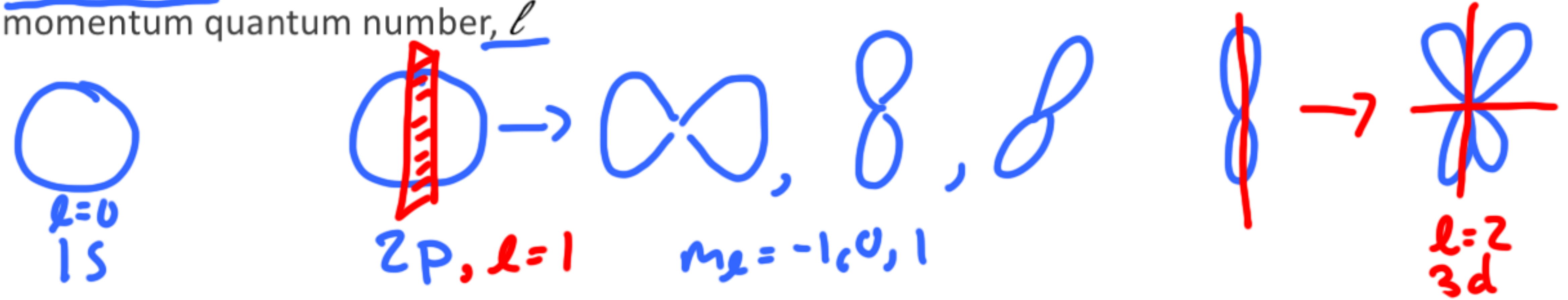
Note: our radial distribution function example (4s) gave us the spherical nodes

Simplifying Nodes and Complex Orbitals

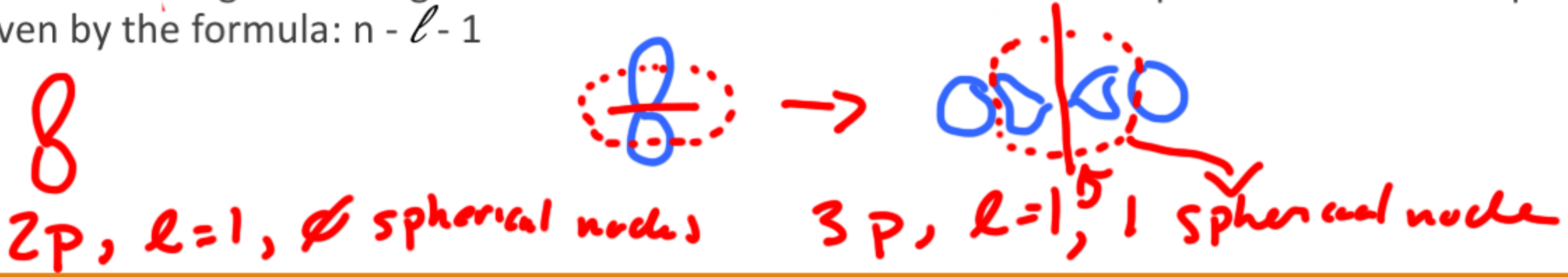
7h → 5 angular nodes

A quantum orbital can have **angular** or **spherical** nodes:

1. Angular nodes dictate the fundamental shape. The number of angular nodes is given by the angular momentum quantum number, ℓ (l=5)



2. Spherical nodes give us insight into variations of the fundamental shape. The number of spherical nodes is given by the formula: n - ℓ - 1



Quantum Numbers in Use

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:

$$[P] = 1s^2\, 2s^2\, 2p^6\, 3s^2\, 3p^3$$

$n = 2$

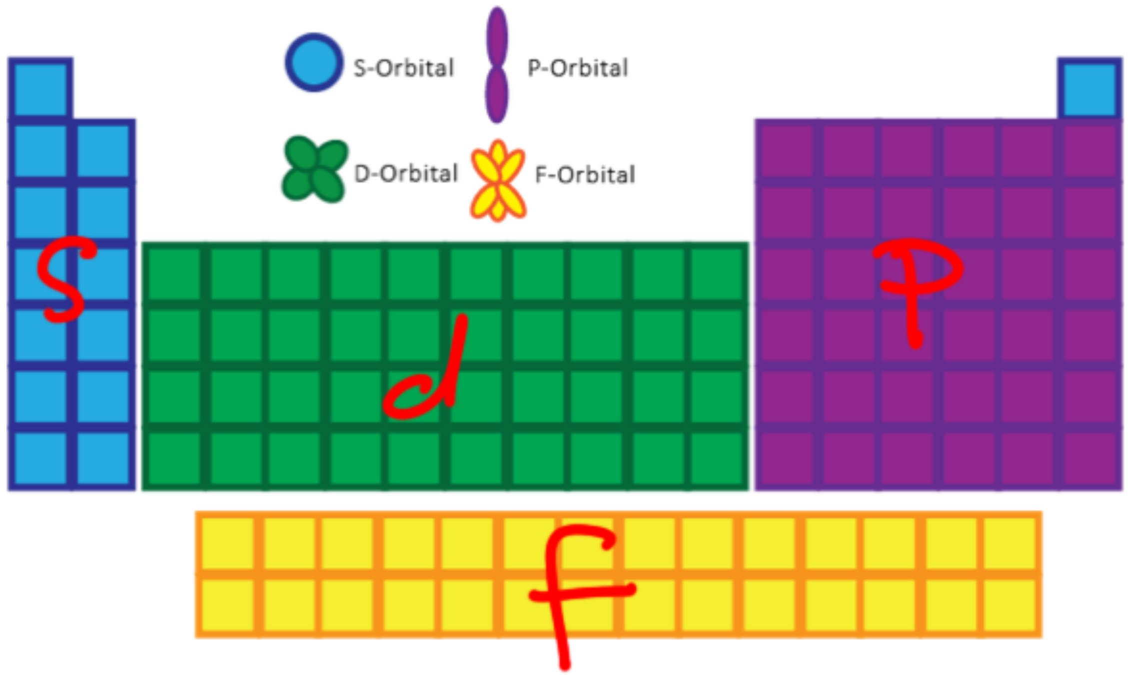
$l = 1$

3 orbitals, each with 2 electrons

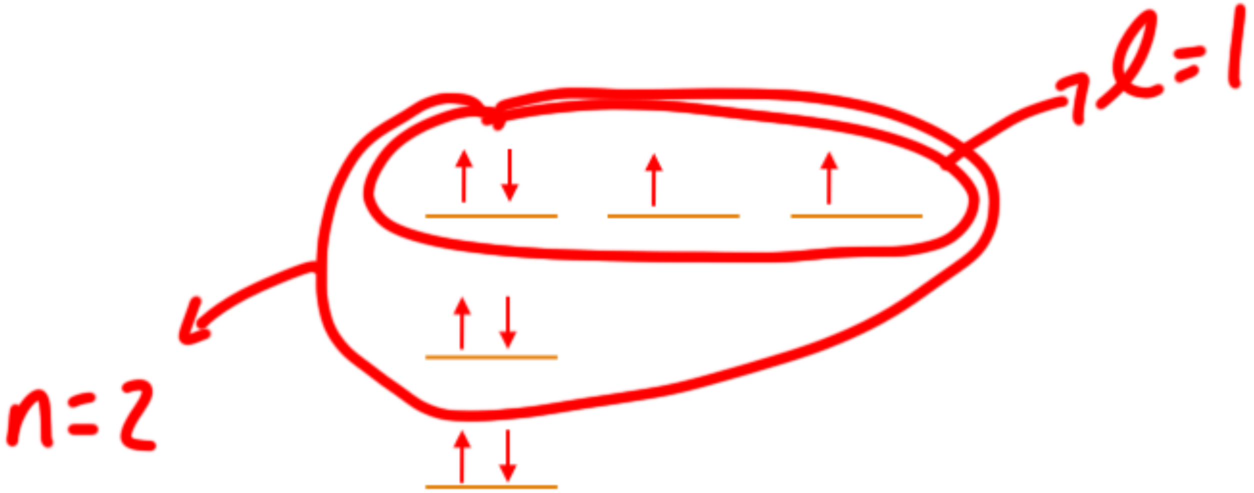
- $m_l = -1, 0, 1$
- $m_s = +1/2, -1/2$

Quantum Numbers: Why

The Periodic Table can be divided into **blocks** that represent the shape of the highest energy electron orbitals

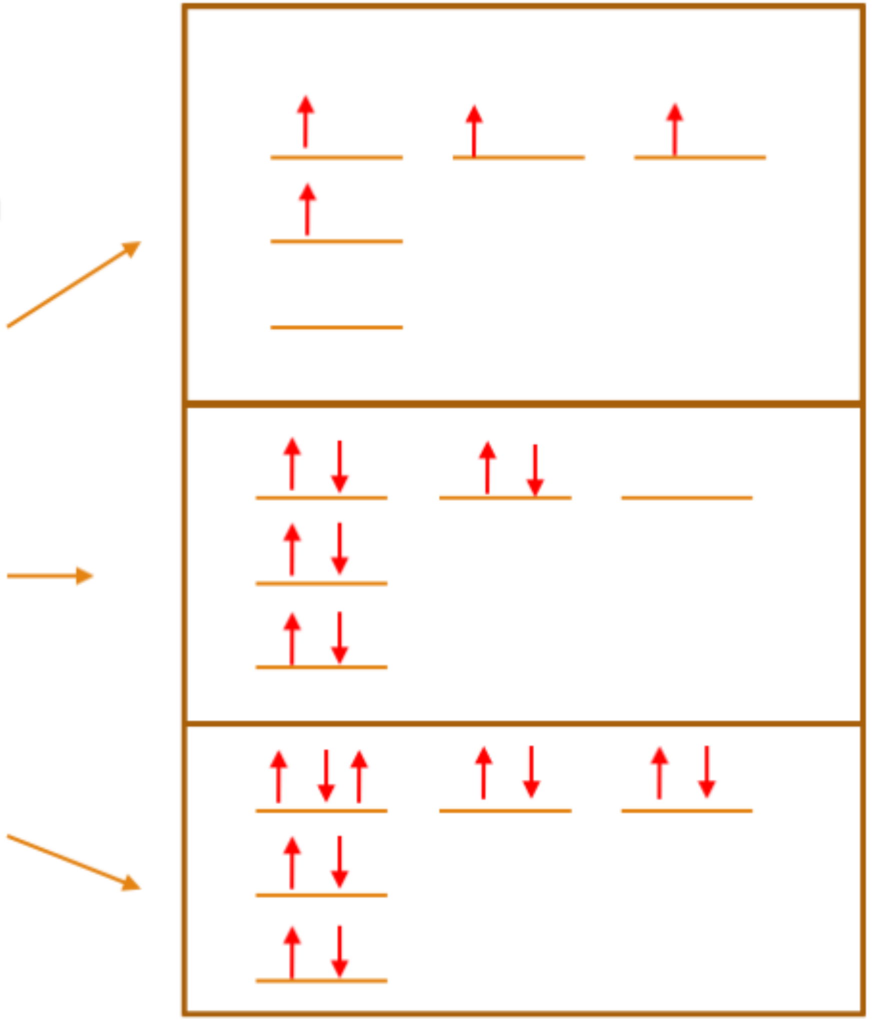


Electron configurations and their diagrams can be used to show the quantum numbers that describe the electron.



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

Exception One: 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

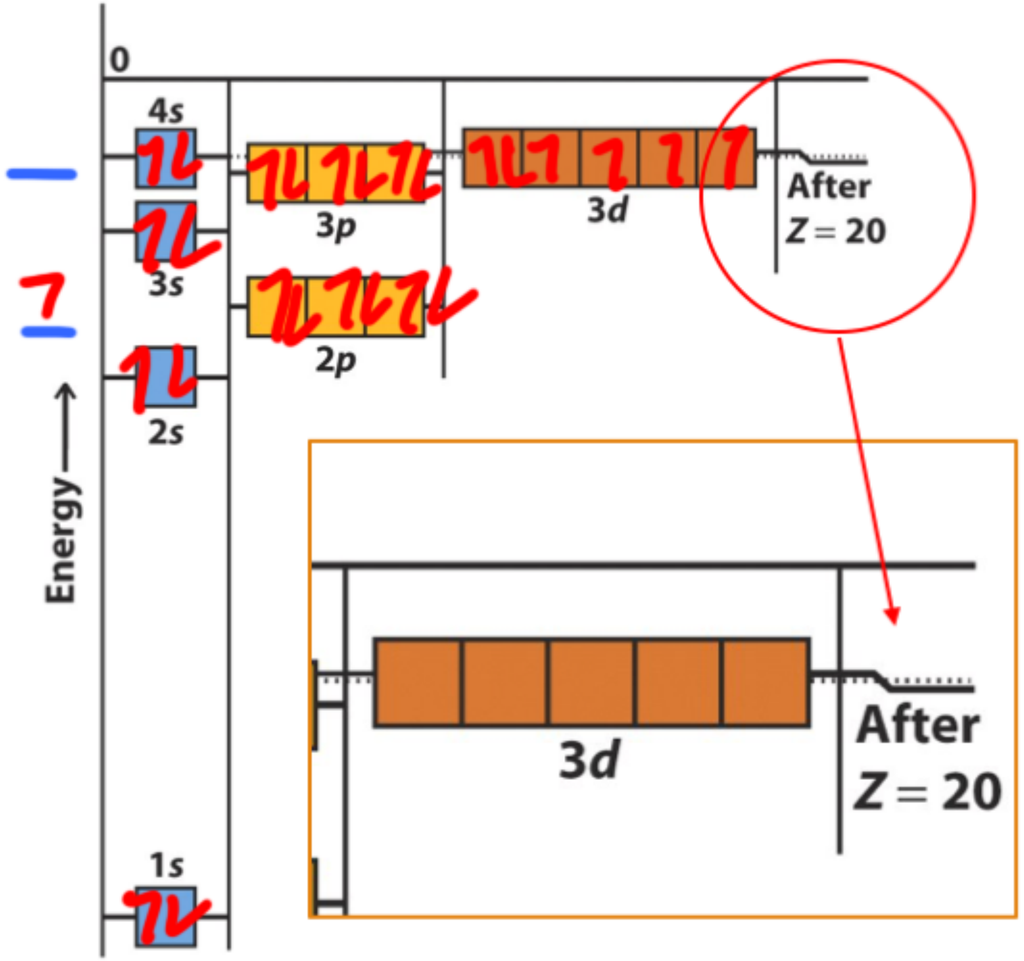
- Remove e^- from highest n-value first!

Exception Two: Filling versus "Unfilling"

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

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

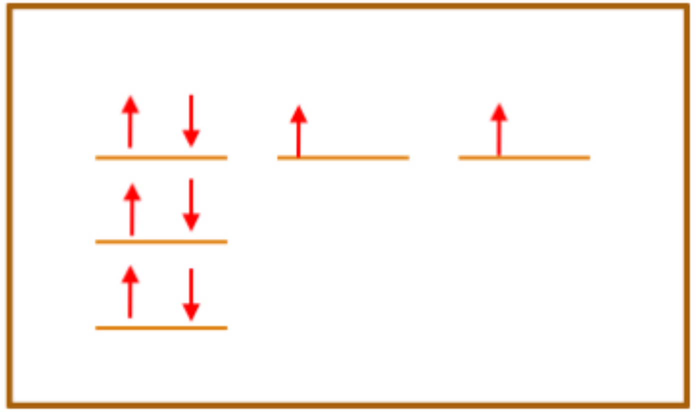
Why?



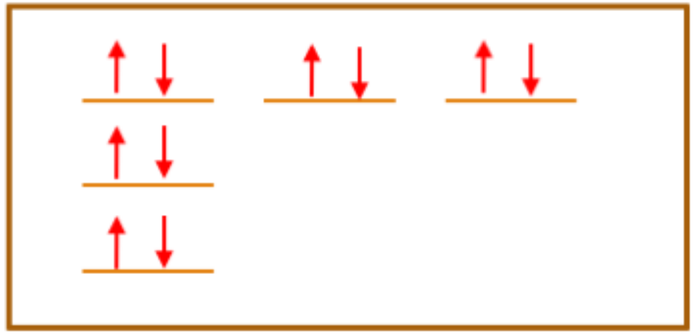
- When filling, use the "Aufbau" Order
- When "unfilling," use the "Energy" Order
  - What's the rule? Unfill the HIGHEST n value FIRST

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 from a magnetic field**
  - Remember: “di” means “two” or ”double” in Latin. Think two electrons in each orbital.
  - All odd number atoms are paramagnetic, but not all even number atoms are diamagnetic
  - FYI: in order for this to happen, the element needs ALL filled subshells. This is really easy to identify on the periodic table.

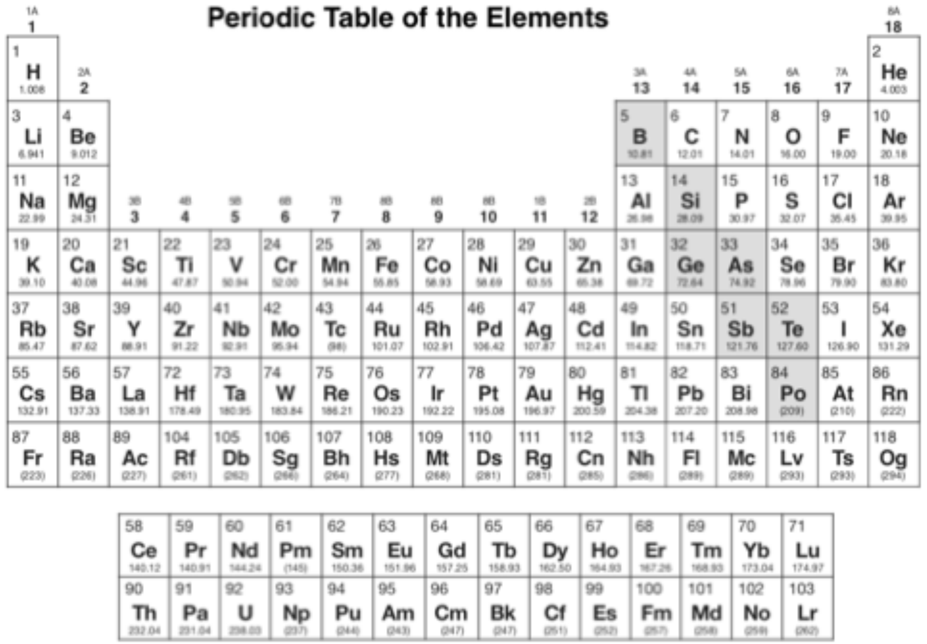


Electron Configuration Exam Questions

For the chlorine anion that is isoelectric with argon,

a. What is the electron configuration? Shorthand notation? Diamagnetic or paramagnetic?

b. How many quantum number sets can be used to describe the highest energy electrons of chloride?

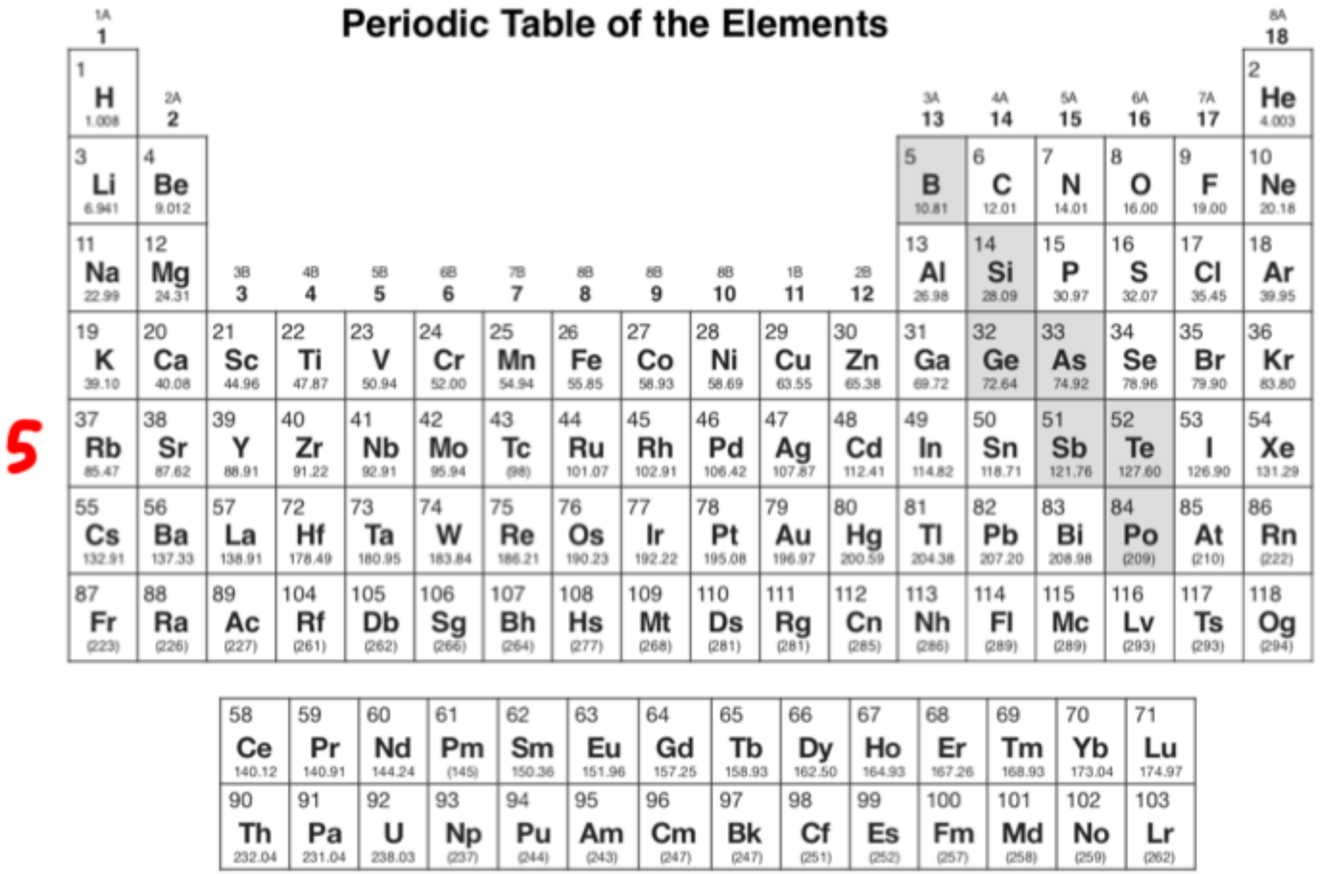


all paired

$[Cl^-] = 1s^2 2s^2 2p^6 3s^2 3p^6$

$6e^-$, 6 Q.N. sets

Electron Configuration Exam Questions



Write the electron configurations of:

a. [In]: $[Kr]\,5s^2 4d^{10} 5p^1$

b. [Zr^{2+}]: $[Kr]\,4d^2$

c. [Mo]: $[Kr]\,5s^1 4d^5$

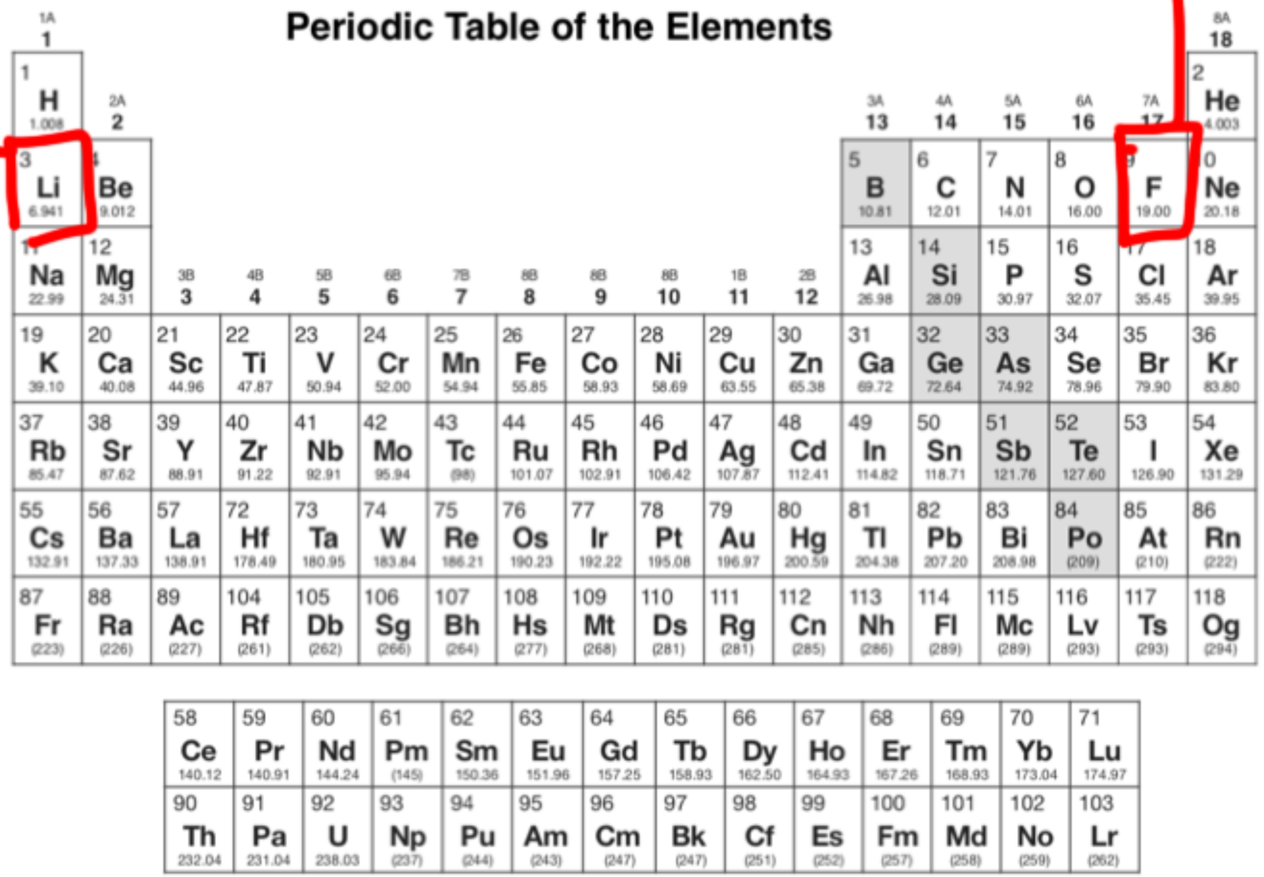
Low ionization Energy

High electron affinity

$Li^+ + F^-$

$\hookrightarrow LiF$

Moving into Trends + Bonding

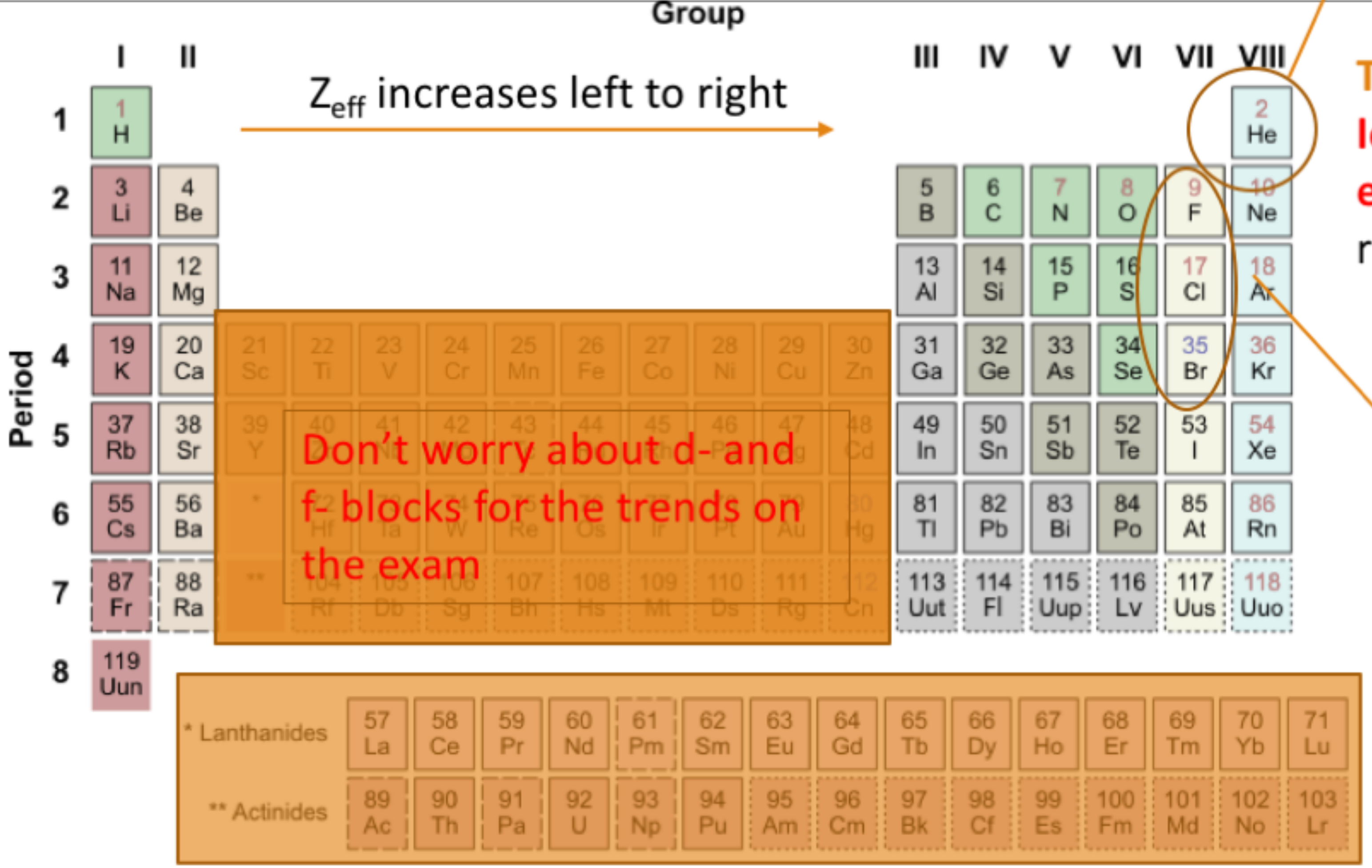


- In chemistry, we are primarily concerned with the **valence electrons**
- The periodic trends in ionization energy, electron affinity, Z-effective, and atomic radius help to explain the behavior of valence electrons
- An element with a **very low ionization energy** is likely to form a **cation** in our atmosphere
- An element with a **very high electron affinity** is likely to form an **anion** in our atmosphere

Periodic Trends

Helium has the maximum ionization energy

Shielding Increases going down



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

The halogens have the highest electron affinity

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