Orbitals and Electron Configuration

<u>Electron Orbitals</u>: three-dimensional regions around the nucleus which indicate the probable location of the electron in the electron cloud.

- Erwin Schrödinger used the hypothesis that electrons have a dual wave-particle nature to develop wave equations (or wave functions) to describe electrons. ($H\Psi = E\Psi$)
- Each individual orbital is located in a specific <u>main energy level</u> *and* <u>sublevel</u>
    - **<u>Main energy levels</u> or shells (n, the principle quantum number)**
        - the general amount of energy and distance from the nucleus a given electron in an orbital possesses.
        - Each period, or row, on the periodic table indicates a main energy level.
        - Indicated by numbers
    - **<u>Energy sublevels</u> or subshells (ℓ, the angular momentum quantum number):**
        - the different shapes of orbitals that exist within the same main energy level
        - Indicated by letters
- A maximum of 2 electrons can fit in a single orbital. ↑↓

<u>Electron configuration</u>: the arrangement of electrons in an atom

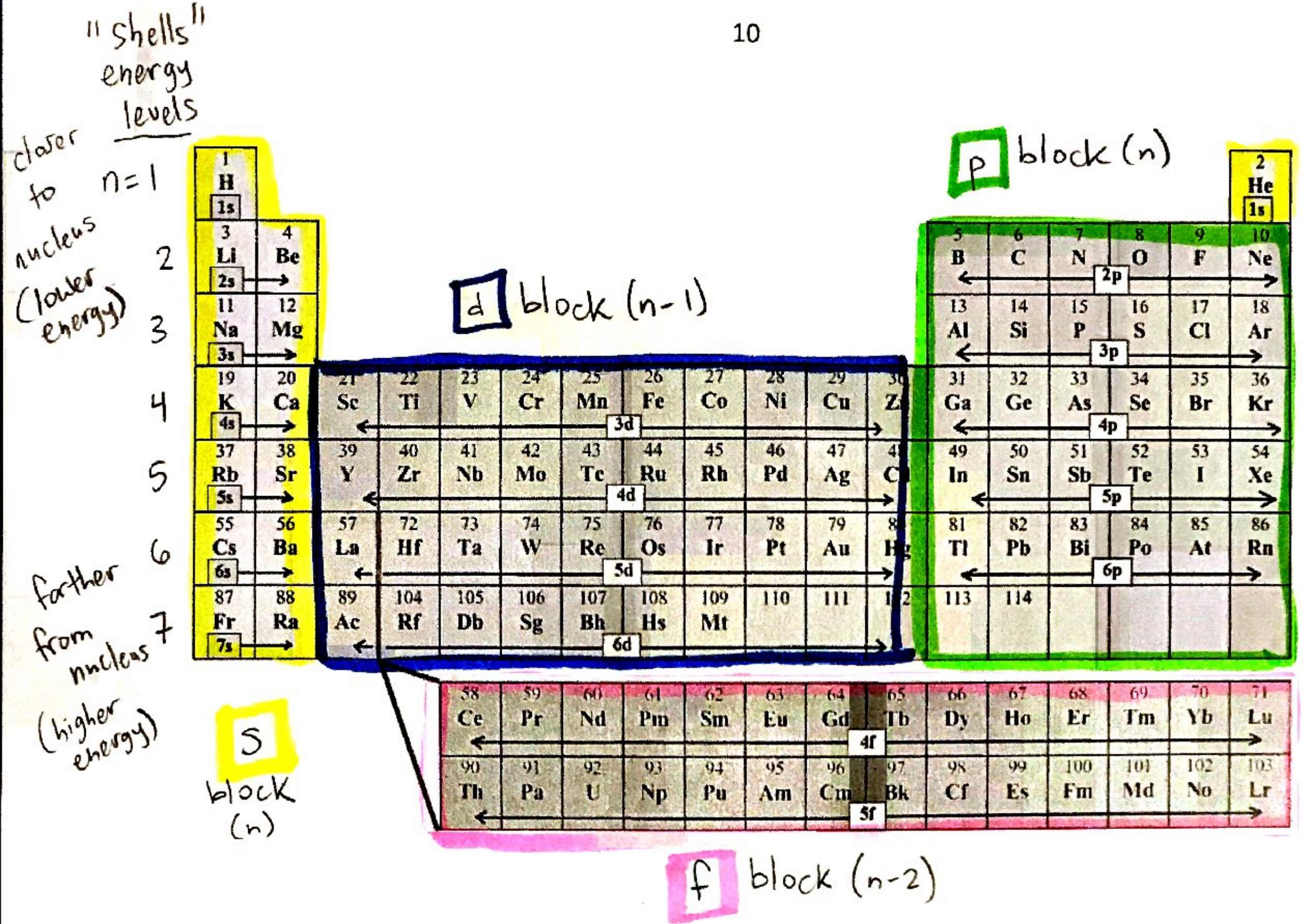
- Every single atom and ion has a specific <u>electron configuration</u> that tells you the exact level and sublevel of each electron it contains!

Energy Sublevels

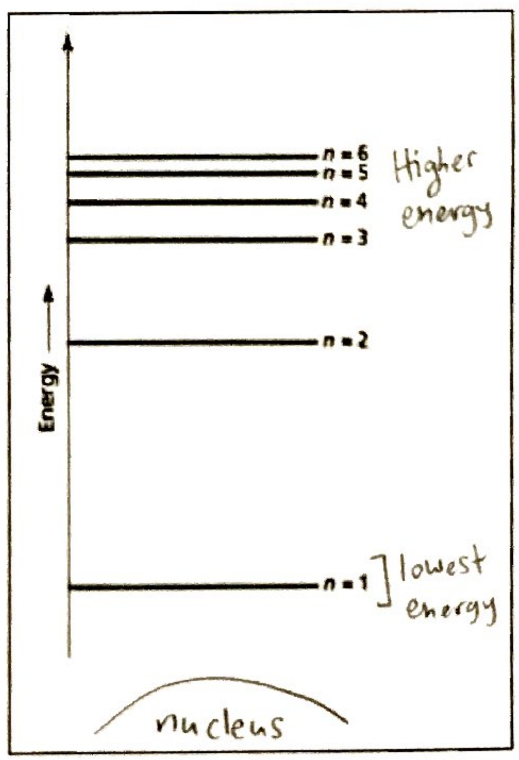
Orbital/sublevel name (*lowercase*)	Shape	How many orbitals in that sublevel? (per main energy level)	max # of e^-?
s	Sphere	1 = ↑↓	2
p	peanut	3 = ↑↓ ↑↓ ↑↓	6
d	daisy	5 = ↑↓ ↑↓ ↑↓ ↑↓ ↑↓	10
f	too freakin' complicated	7 = ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ ↑↓	14

How to remember the order of the energy sublevels:

Splendid people don't forget!

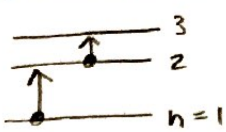


Note: as one moves further from the nucleus, the energy levels get closer together and there is a smaller difference in energy between the levels.



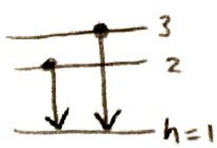
Electronic Transitions

a. Absorption: electron jumps UP to a higher energy level



gains energy!

b. Emission: electron drops DOWN to a lower energy level



releases energy!

Directions: Match each of the following electronic transitions with the most likely energy change.

Transition		Energy Change
1. n = 1 to n = 4	C.	A. red light emission
2. n = 5 to n = 4	A.	B. red light absorption
3. n = 4 to n = 1	D.	C. UV light absorption
4. n = 4 to n = 5	B.	D. UV light emission

(A, B: lower energy; C, D: higher energy)

Rules Governing How Electrons Fill Orbitals in the Ground State (lowest energy state)

The **Heisenberg Uncertainty Principle** states that it is impossible to determine simultaneously both the position and the velocity of an electron or any other particle. However, we are able to determine the *probable* location of an electron and determine how electron orbitals are filled, using the following rules:

1. **Aufbau Principle**: (German for "building up") states that, in the ground state (lowest energy state), an electron will occupy the lowest-energy orbital that can receive it.

   H: ↑ (1s) He: ↑↓ (1s) (NOT ↑ (1s) ↑ (2s))

2. **Pauli Exclusion Principle:** no two electrons can fit into the same orbital with the same spin (i.e. no two electrons can have the same set of four quantum numbers!) For the new AP CHEM exam, you do NOT have to answer questions about quantum numbers. So, basically, recognize that no two electrons can exist in the exact same orbital having the exact same spin.

   He: ↑↓ (1s) (NOT ↑↑ (1s)) Li: ↑↓ (1s) ↑ (2s) (NOT ↑↓↑ (1s))

3. **Hund's Rule**: (the good parent rule) states that orbitals of equal energy are each occupied by one electron before any orbital is occupied by a second electron, and all electrons in singly occupied orbitals must have the same spin. "Spin" is designated by an arrow: **spin up** = ↑ or ↿; **spin down** = ↓ or ⇂

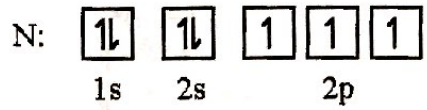
   N: ↑↓ (1s) ↑↓ (2s) ↑ ↑ ↑ (2p) (NOT ↑↓ (1s) ↑↓ (2s) ↑↓ ↑ _ (2p))

Practice! For each **ground state** orbital configuration shown below, identify which (if any) of the rules govern electron-filling have been violated (Pauli exclusion principle, Aufbau principle, and/or Hund's rule).

	1s	2s	2p			Violates?
1.	↑↓	↑↓↑				Pauli Exclusion Principle
2.	↑	↑				Aufbau Principle
3.	↑↓	↑↓	↑↓	↑	↑	✓
4.	↑↓	↑↓	↑↓			Hund's rule

Electron Configurations: The arrangement of electrons in an atom

A. **Orbital ~~Notation~~ Diagram:** uses arrows to represent electrons.



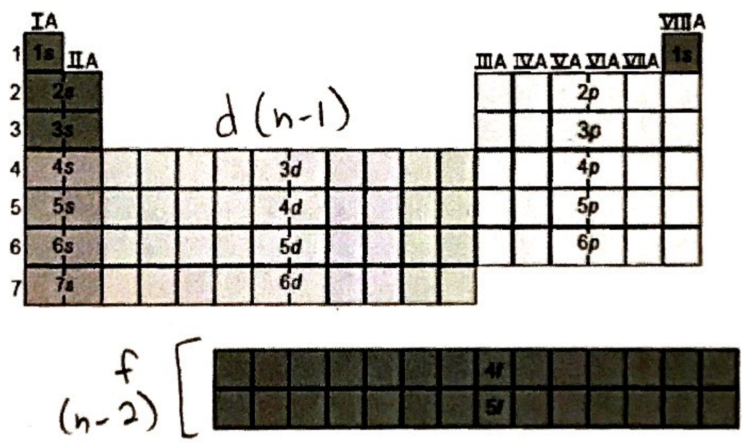
B. **~~Standard~~ Complete Electron Configuration:** Standard electron configurations eliminate the lines and arrows of orbital notation. The number of electrons in a sublevel is shown by adding a superscript.

Nitrogen: $1s^2 2s^2 2p^3$

C. **Noble Gas Electron Configurations:** A noble gas configuration is an electron configuration that utilizes a noble gas which has its valence level fully occupied. Noble gas configurations are often used to help shorten the electron configurations of those elements that contain large numbers of electrons.

Nitrogen: $[He] 2s^2 2p^3$
↑square brackets!

Adding Electrons: The periodic table holds the answer for the order in which electrons fill orbitals. Always start at hydrogen and then move through the periods (rows) until you arrive at the desired element.



The Order in Which Electrons FILL Energy Levels

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 5f^{14} 6d^{10}$

Removing electrons: Those pesky transition metals! } Remove valence s e^- first!

➔ When **REMOVING** electrons, once you get to scandium, the energy of the 3d orbitals becomes slightly less than that of the 4s, and that remains true across the rest of the transition series metals. Focus on the idea of ENERGY!

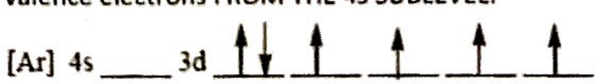
Example

The iron atom, Fe, has two valence electrons:

Fe atom = $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

When iron forms a cation, it FIRST loses its valence electrons FROM THE 4s SUBLEVEL:

Fe^{2+} cation = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$



It can then lose 3*d* electrons:

Fe^{3+} cation = $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$

Isoelectronic atoms and ions: the "iso" in "isoelectronic" means "Same", so isoelectronic atoms and ions have the same number of electrons.

Example:

- Write the electron configuration for S^{2-}: $1s^2 2s^2 2p^6 3s^2 3p^6$
- What noble gas is isoelectronic to S^{2-}? Ar
- List other atoms or ions that are isoelectronic to the S^{2-} ion: P^{3-}, Cl^-, K^+, Ca^{2+}

Yum, atoms! Let's practice.

Part I: The counting of electrons.

Si	Orbital Notation: 1s ↑↓ 2s ↑↓ 2p ↑↓ ↑↓ ↑↓ 3s ↑↓ 3p ↑ ↑ _	
	Electron Configuration: $1s^2 2s^2 2p^6 3s^2 3p^2$	Noble Gas Configuration: $[Ne] 3s^2 3p^2$
As	Orbital Notation: 1s ↑↓ 2s ↑↓ 2p ↑↓ ↑↓ ↑↓ 3s ↑↓ 3p ↑↓ ↑↓ ↑↓ 4s ↑↓ 3d ↑↓ ↑↓ ↑↓ ↑↓ ↑↓ 4p ↑ ↑ ↑	
	Electron Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^3$	Noble Gas Configuration: $[Ar] 4s^2 3d^{10} 4p^3$
Cl^-	Orbital Notation: 1s ↑↓ 2s ↑↓ 2p ↑↓ ↑↓ ↑↓ 3s ↑↓ 3p ↑↓ ↑↓ ↑↓	
	Electron Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6$	Noble Gas Configuration: $[Ne] 3s^2 3p^6$
Fe^{3+}	Orbital Notation: 1s ↑↓ 2s ↑↓ 2p ↑↓ ↑↓ ↑↓ 3s ↑↓ 3p ↑↓ ↑↓ ↑↓ 4s _ 3d ↑ ↑ ↑ ↑ ↑	
	Electron Configuration: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^0 3d^5$ (4s⁰: or leave out!)	Noble Gas Configuration: $[Ar] 3d^5$