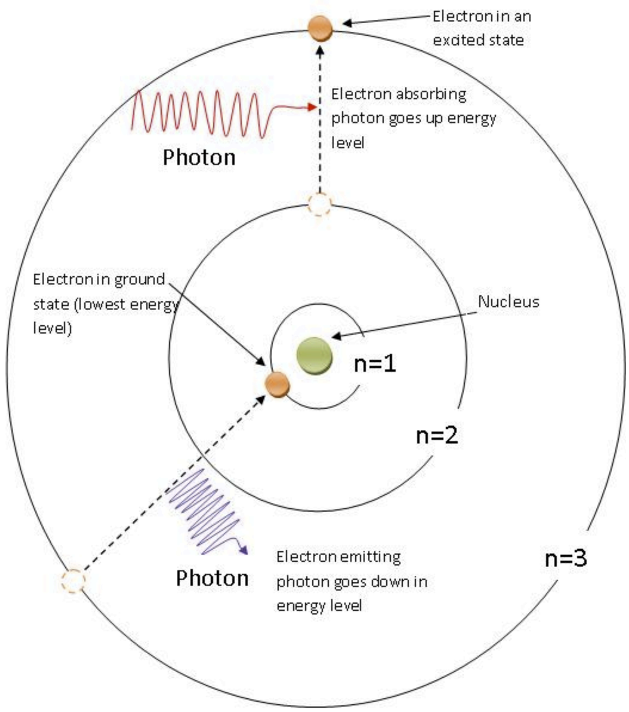
Notes 2.2: Quantum Mechanical Model of the Atom

Bohr's model works well for Hydrogen, but not the other elements.



Quick review:

- What is the general distribution of subatomic particles in an atom? (Think Rutherford)

- According to Bohr, where are electrons located?

A Quick History of the Quantum Mechanical Model

- Louis de Broglie: Electrons behave with **wave** and **particle** properties at the same time.

- Werner Heisenberg: It is impossible to know both the position and velocity of an electron simultaneously.
  - > Heisenberg's Uncertainty Principle
    - Position = particle nature
    - Velocity = wave nature
    - Can't be observed as a particle and a wave at the same time!

A Quick History of the Quantum Mechanical Model

- Erwin Shrodinger: Refined the wave-particle theory proposed by de Broglie.
  - > Developed an equation that treated an electron like a wave and predicted the **probable** location of an electron around the nucleus called the **atomic orbital.**

- ***The quantum mechanical model of the atom treats an electron like a wave.**

For a single particle in three dimensions:

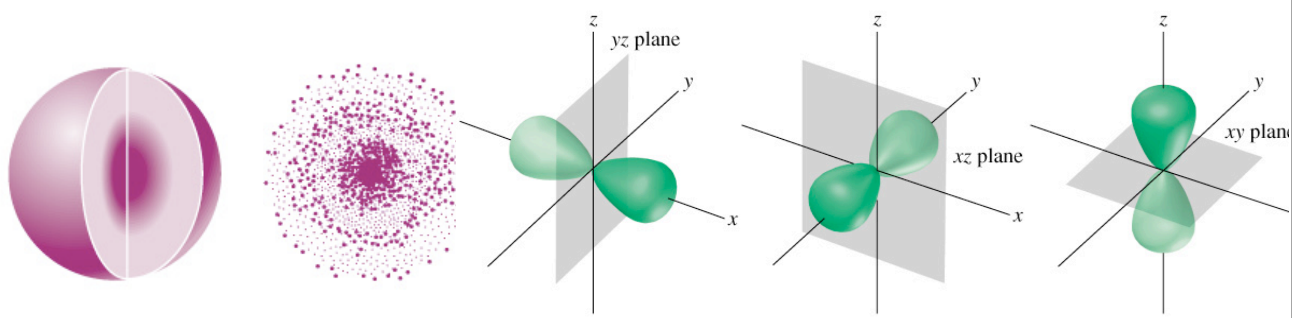
$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x,y,z)\psi$$

where

- ψ is the wavefunction, which is the amplitude for the particle
- m is the mass of the particle.
- $V(x,y,z)$ is the potential energy the particle has at each position.

Quantum Mechanical Model of the Atom

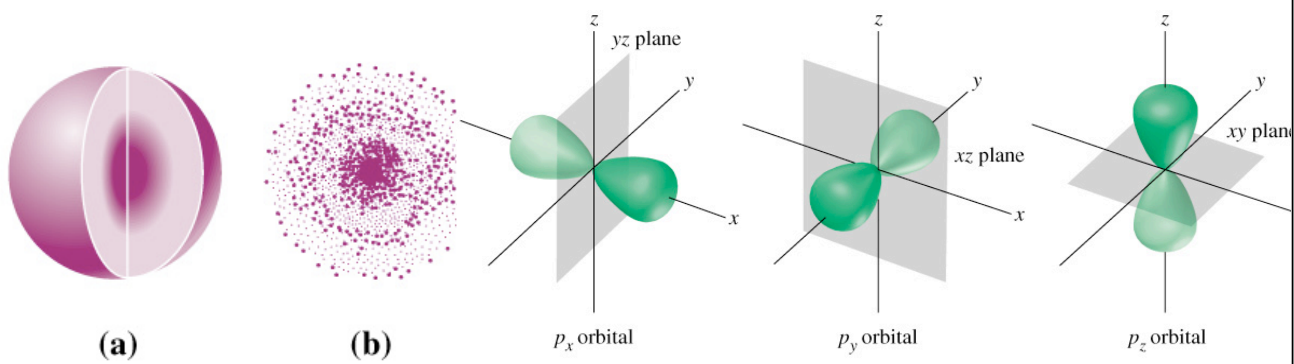
- Electrons are in a 3-D region around the nucleus called **atomic orbitals.**
  - > Electrons are NOT in circular orbits around nucleus like in Bohr model.
  - > The atomic orbital describes the probable location of the electron
  - > Similar to Bohr Model, electrons are limited to certain energy values (energy of an electron is quantized)



(a) (b) p_x orbital p_y orbital p_z orbital

Quantum Mechanical Model of the Atom

- There are different kinds of atomic orbitals that differ in the amount of energy and shapes (where the electron probably is).
- The atomic orbitals get filled by electrons in a certain order.



Lets imagine that electrons are like patrons at a hotel, and the atomic orbitals are like the rooms.

The hotel has different floors

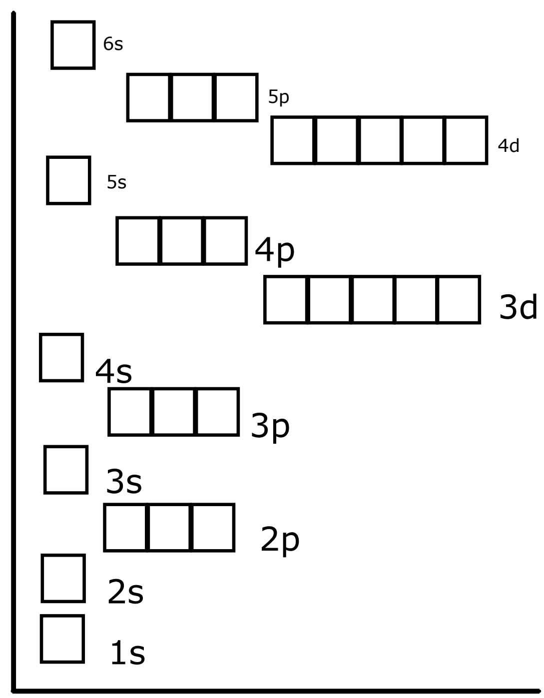
There are 4 different kinds of rooms.

S = Simple room

P = Posh room

D = Deluxe suite

F = Fancy-Shmancy Suite

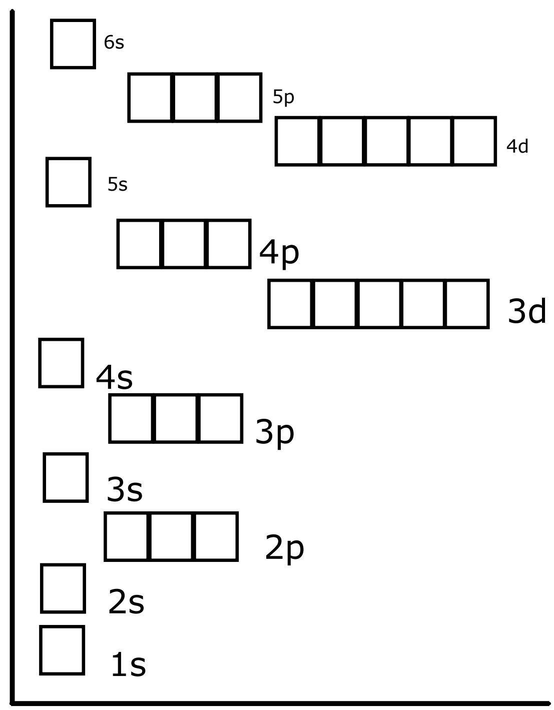


The owner of the hotel is VERY INSISTENT that the rooms get filled in a certain order. He has 3 rules.

1. **Aufbau rule:** Each electron must occupy the lowest level room available.

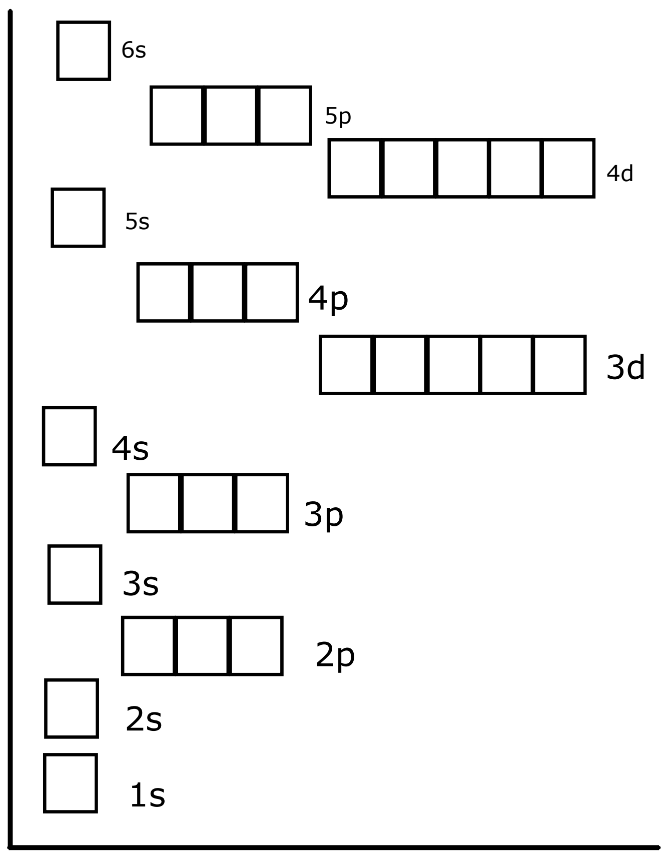
2. **Pauli rule:** Only a maximum of 2 electrons can stay in each room.   .

3. **Hund rule:** One electrons must occupy all of the rooms in the same level before pairing up. (Electrons want to avoid sharing rooms)



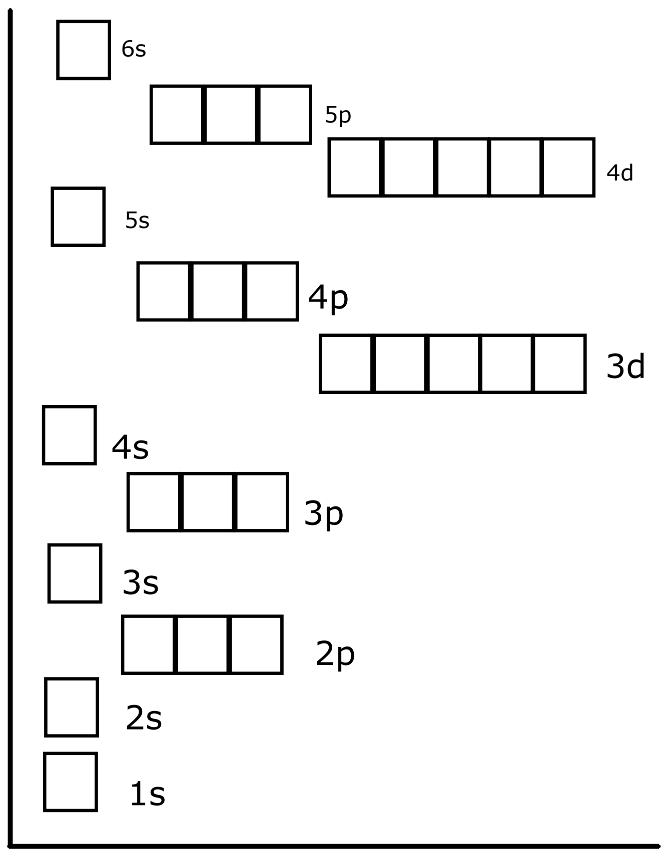
Lets practice filling up the hotel rooms with electrons.

How many electrons in Neon?



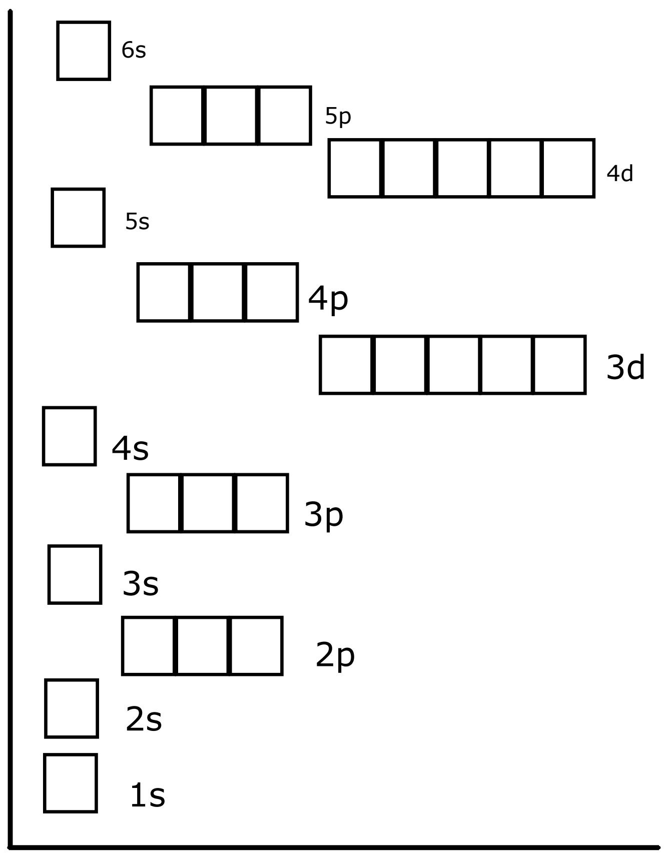
Lets practice filling up the hotel rooms with electrons.

How many electrons in Phosphorus?



Lets practice filling up the hotel rooms with electrons.

How many electrons in Zirconium?



Congratulations! You have just learned how to do Electron Configurations.

- Electron configuration is simply the arrangement of electrons in an atom.
- **electron configuration** is a list of all of the rooms that are filled from low to high.

For HW: Fill out 4 more orbital diagrams for the following elements: As, Si, Ca, and Cl and write out the electron configuration underneath.

Now, lets talk about what these numbers mean.

Electron Configuration and the Quantum Mechanical Model

- The quantum mechanical model describes the probable location of electrons in atoms by describing:
  - > Principal energy level
  - > Energy sublevel
  - > Orbital (in each sublevel)
  - > Spin

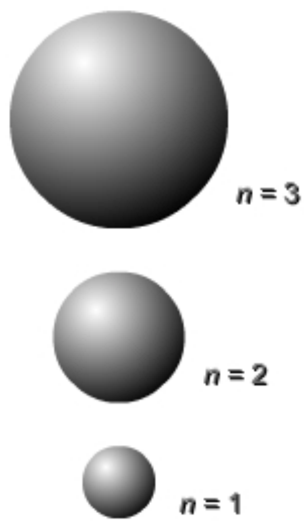
Describes the location of the electron within the atom

Describes the direction of spin

The electron configuration is like an "address" that tells us the probable location of each electron in the atom.

Principal Energy Level (n)

- **Principle energy level (n):** Indicates the relative size and energy of atomic orbitals. "Shells"
- **n=integers:** n= 1, 2, 3, etc.
- As n increases:
  - > orbital becomes larger
  - > electron spends more time farther away from nucleus
  - > electron's ar

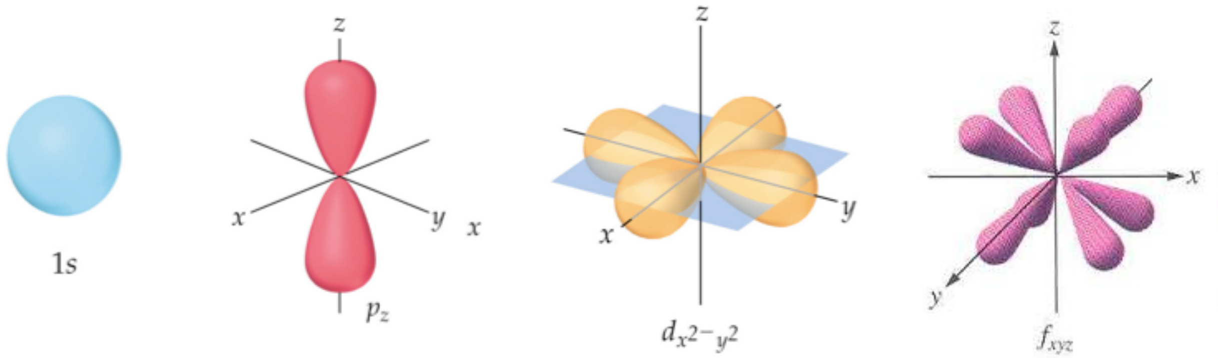


As the principle quantum number *n* increases, the size and energy of the orbital both increase, but the shape remains essentially the same.

http://www.chem.ox.ac.uk/vrchemistry/Machinery/html/page02.htm

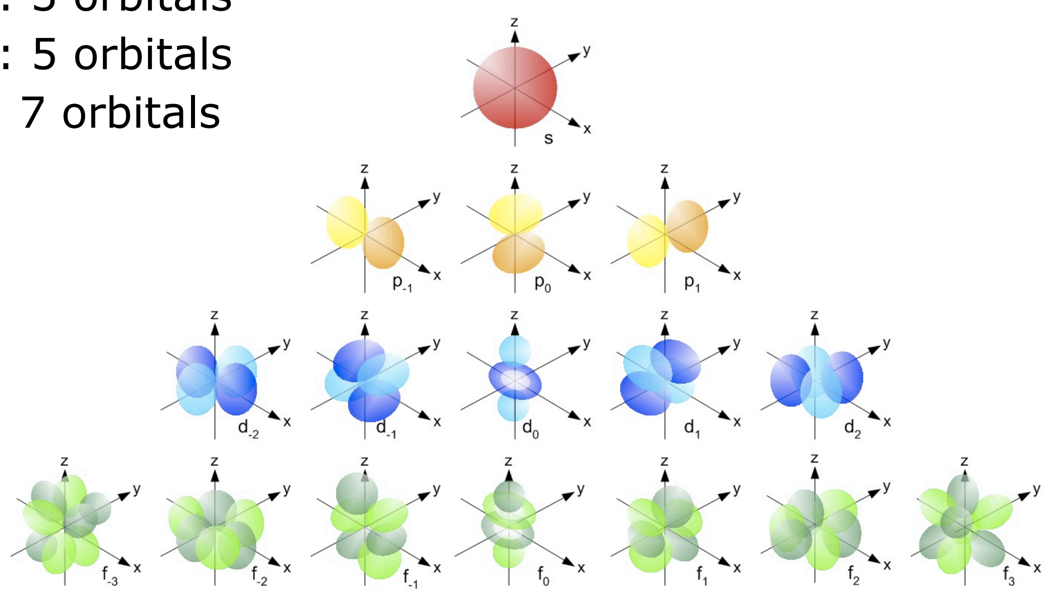
Energy sublevel

- Principal energy levels are broken down into sublevels.
- **Sublevels** define the orbital shape (s, p, d, f)
  - > n=1, 1 sublevel (s)
  - > n=2, 2 sublevels (s, p)
  - > n=3, 3 sublevels (s, p, d)
  - > n=4, 4 sublevels (s, p, d, f)



Orbitals

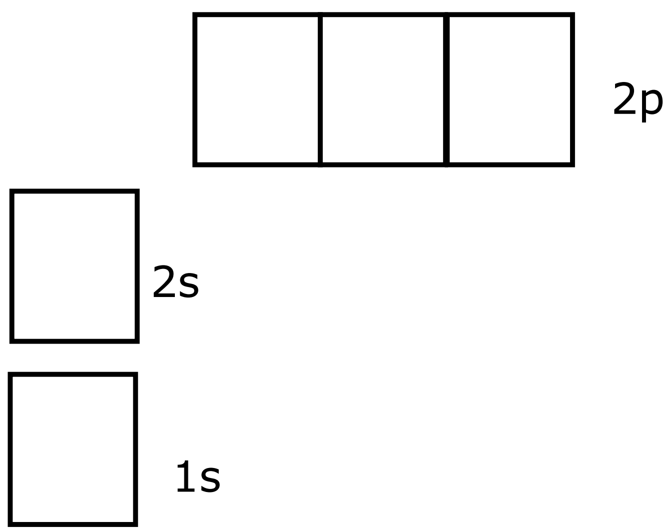
- **Orbitals:** Each sublevel has a different number of orbitals, each with a defined orientation.
  > s: 1 orbital
  > p: 3 orbitals
  > d: 5 orbitals
  > f: 7 orbitals



http://edtech2.boisestate.edu/lindabennett1/502/Periodic%20Table%20e%20config/electron%20configuration.html

Spin

- **Spin:** Electrons act like they are spinning on an axis
  - > Generates a magnetic field
  - > No two electrons in the same orbital can have the same spin



These 4 descriptions are "quantum numbers": Each electron in an atom has a unique set of these 4 quantum numbers that describe the orbital it is in (Principal energy level, sublevel, orbital) and its spin.

Summary:

- In each principal energy level, there are n^2 orbitals.
- In each principal energy level, there are a maximum of $2n^2$ electrons.

TABLE 5.1 Sublevels of the first four energy levels

Principal energy level	*Sublevel*	*Number of orbitals in sublevel*	*Total possible occupying electrons*	
1	*s*	1	2	
2	*s*	1	2	8
	p	3	6	
3	*s*	1	2	18
	p	3	6	
	d	5	10	
4	*s*	1	2	32
	p	3	6	
	d	5	10	
	f	7	14	

Electron Configuration

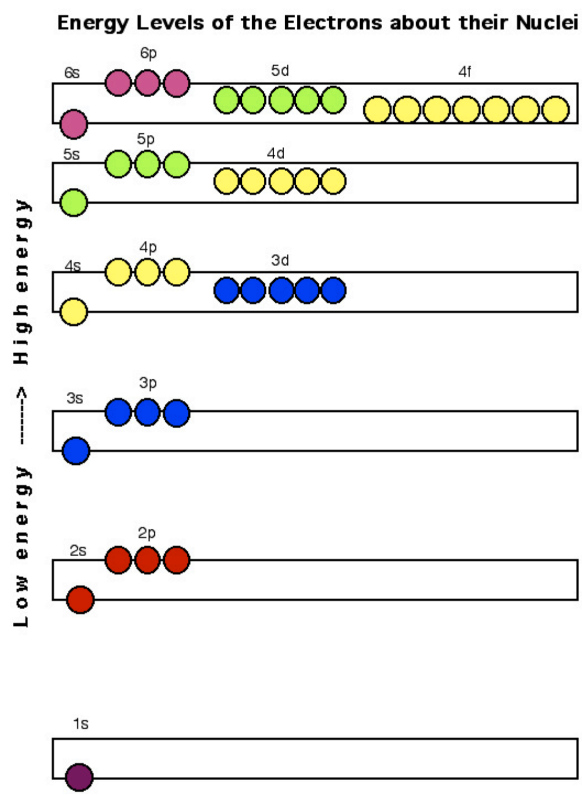
Describes the electron arrangement in atoms.

3 rules for electron configuration at ground state:

1. **Aufbau principle**: Each electron occupies the lowest energy orbital available.

2. **Pauli exclusion principle**: A maximum of 2 electrons may occupy a single atomic orbital, but only if they have opposite spins.

3. **Hund's rule**: a single electron with the same spin must occupy each orbital in a sublevel before they pair up with an electron with an opposite spin.



1 Sublevels define the

A Shape of the orbital

B What shell the electrons are on

C The spin of the electrons

D Spefic orientation of the orbital

2 The Aufbau rule states

A No more than two electrons can occupy each orbital

B Two electrons in the same orbital must have opposite spins

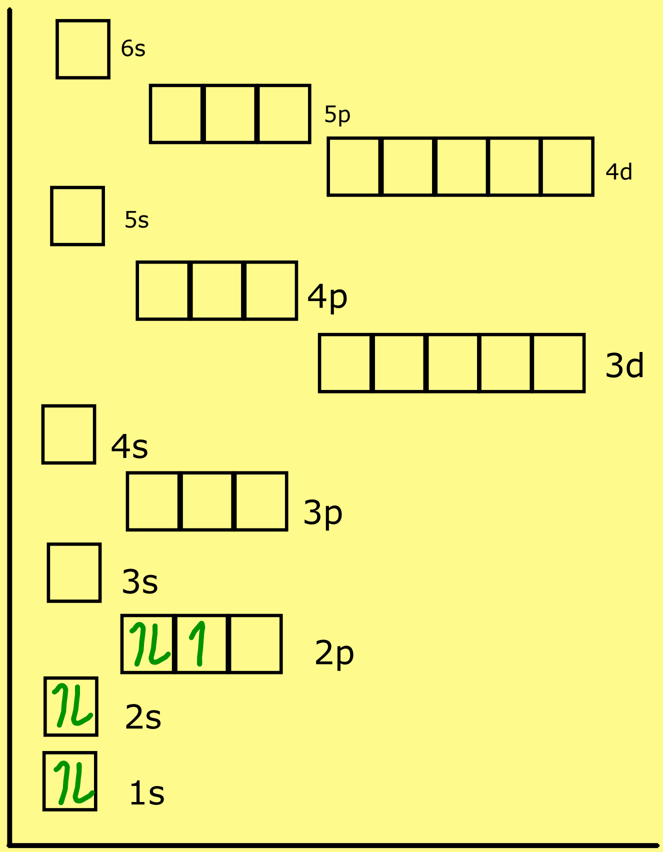
C One electron fills each orbital in a sublevel before pairing up.

D Orbitals must be filled from lowest energy to highest energy

3 Is the following orbital diagram completed correctly for Nitrogen?

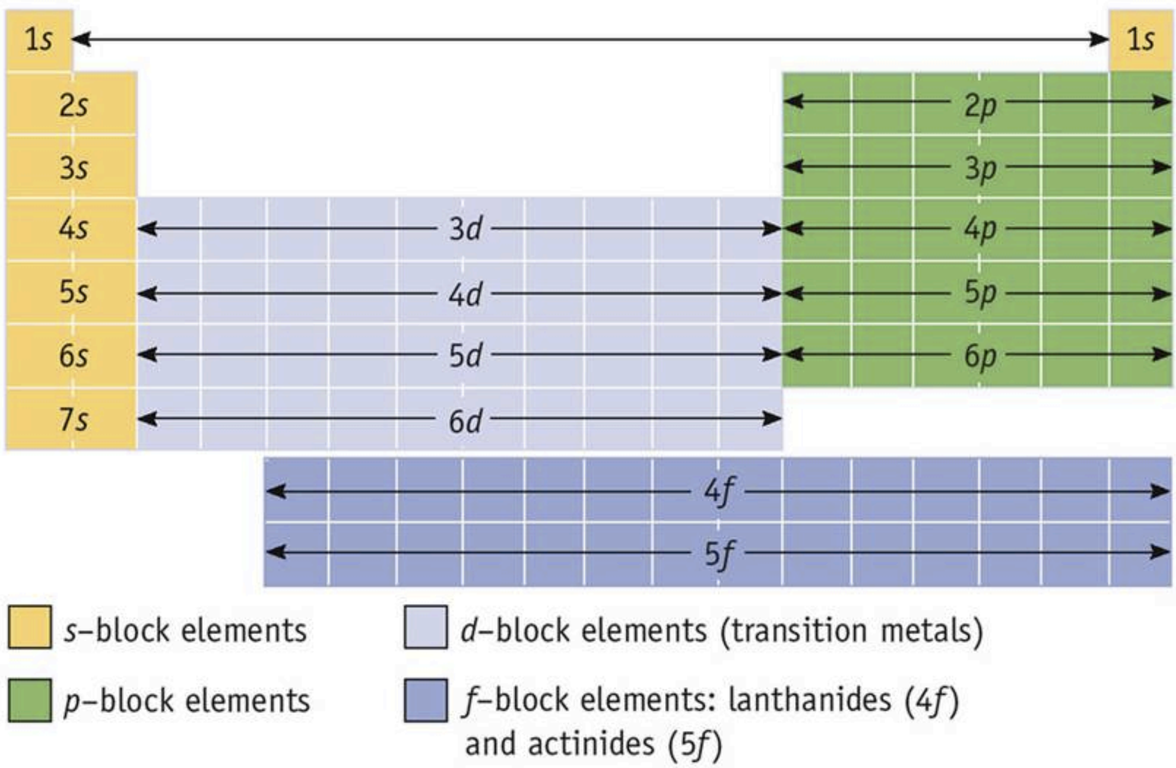
Yes

No

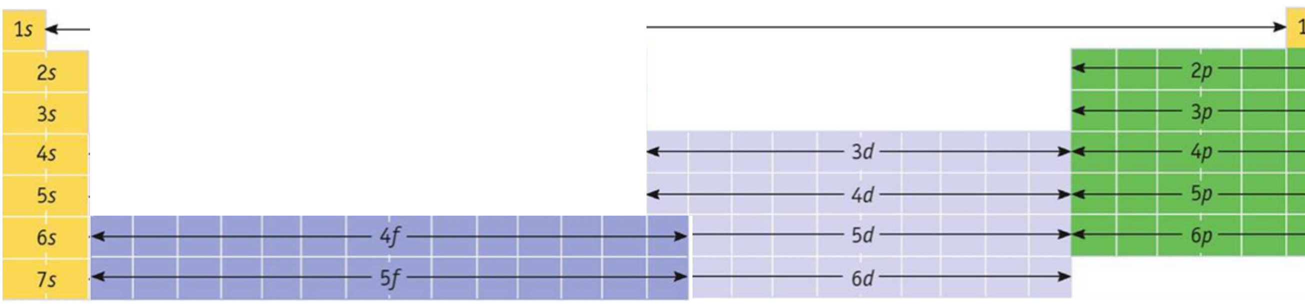


The Periodic Table and Electron Configuration

- The Periodic table is organized into 4 blocks.
- The 4 blocks correspond to the filling of the 4 quantum sublevels: s, p, d, f



October 24, 2014



Color in the blank periodic table into 4 blocks and label each SUBLEVEL using a black pen.

Color the filled in Periodic Table into 4 blocks.

- Then...
  > Take your orbital diagram (hotel) for Phosphorous and color the rooms with electrons:
    - "s" rooms YELLOW
    - "p" rooms GREEN
    - "d" rooms PURPLE

- How does the electron configuration and the periodic table MATCH UP??

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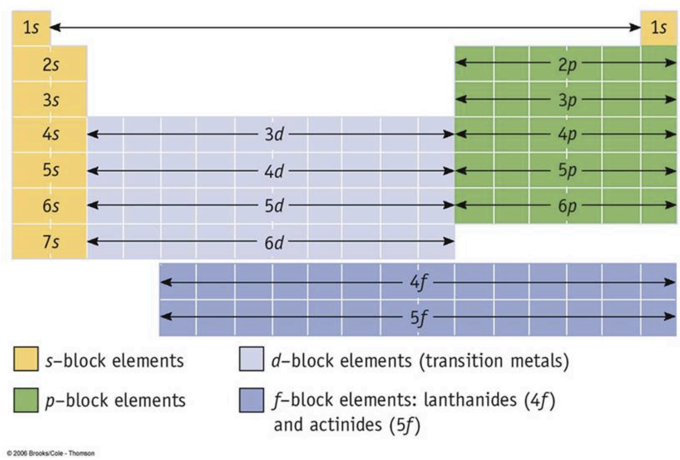
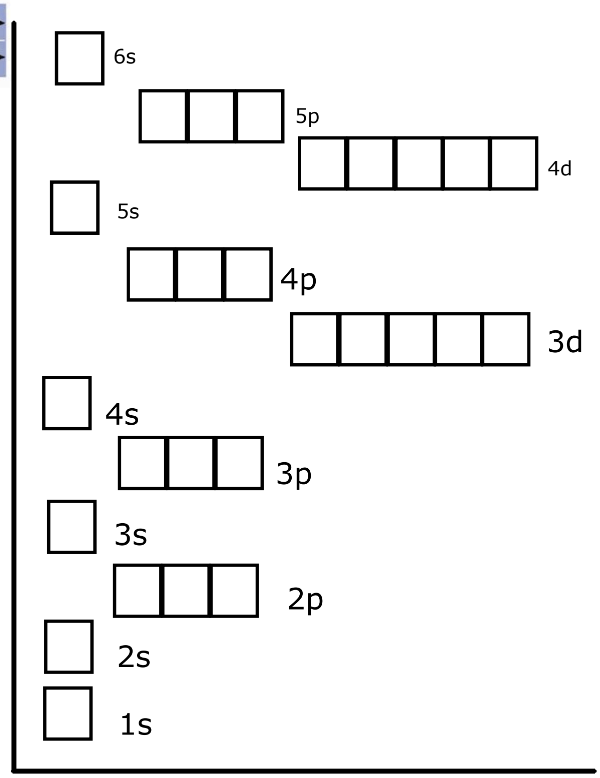
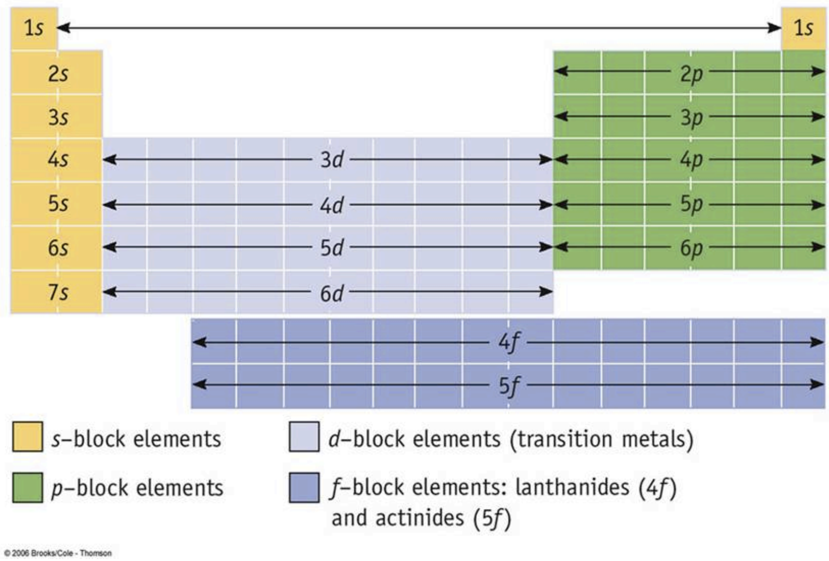




Electron Configuration and Noble-gas notation

- **Electron configuration**: List all sublevels in order of filling.
- Example:

- **Noble-gas notation:** Like a short cut! Put noble gas of previous period (row) in brackets, and then write electron configuration for the energy level being filled.
- Example:



Example: Write the electron configuration and noble gas notation for:

Selenium

Argon

Boron

Manganese

4 Which of the following shows the correct electron configuration for Fluorine?

A $1s^2 2s^2 2p^6$

B $1s^2 2s^2 2p^5$

C $1s^2 1p^6$

D $1s^2 1p^5$

5 Which of the following shows the correct noble gas notation for Sulfur?

A $[Ar]3s^{2}3p^{5}$

B $[S]3s^{2}3p^{4}$

C $[Ne]3s^{2}3p^{4}$

D $[Ne]3s^{2}3p^{6}$

Exceptions to Predicted Electron Configuration

- We follow 3 rules to fill out the electron arrangement in orbitals:
  - > Aufbau principle
  - > Pauli exclusion principle
  - > Hund's rule

- However, some elements are exceptions. Electron filling is out of order for groups 6 and 11
  - > s electron moves to the d sublevel in order to half fill or completely fill the d sublevel
  - > Half or completely full sublevels are more stable and therefore, at a lower energy level
  - > Cr: $[Ar]4s^1 3d^5$
  - > Cu: $[Ar]4s^1 3d^{10}$

Valence Electrons

- **Valence electrons:** Electrons that are in the highest principal energy level of an atom
  - > electrons in outermost orbitals
  - > Usually s and p orbitals
  - > These electrons are involved with forming chemical bonds.

Example: Which electrons are the valence electrons in:

- Selenium
- Argon
- Boron
- Manganese

Electron-dot diagram or electron-dot structure

- **Electron dot diagrams** shows an element with its valence electrons. Consists of:
  - > Element's symbol: Represents nucleus and inner-level electrons (core electrons, or non-valence electrons)
  - > Dots representing the atom's valence electrons
    - – Place dots one at a time on 4 sides of symbol before pairing.

- Example:
  - > Chlorine

Example:

Write the electron configuration notation, noble gas notation, and electron-dot diagram for

Carbon

Titanium

Silicon

Iodine

Zirconium