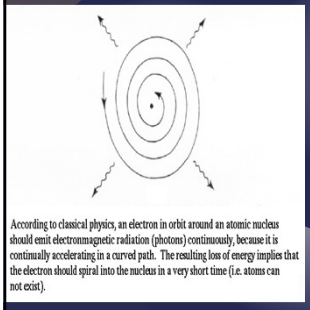
4.2 – WHERE are the electrons in the atom???? { QUANTUM NUMBERS

Bohr's Model Contradicts Common Sense



According to classical physics, an electron in orbit around an atomic nucleus should emit electromagnetic radiation (photons) continuously, because it is continually accelerating in a curved path. The resulting loss of energy implies that the electron should spiral into the nucleus in a very short time (i.e. atoms can not exist).

If only certain orbits with definite energies are allowed and the electrons constantly gives off radiation, wouldn't the electron eventually spiral into the nucleus?

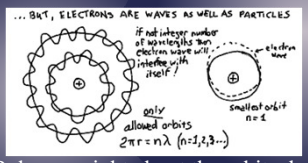
They had to change the way that they looked at the electron.

Louis de Broglie

Suggested:

- Electrons **were waves** confined to the space around the nucleus

Bohr's "orbits" have to have SPECIFIC ENERGIES

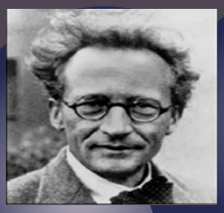


So, Bohr was right about the orbits, but electrons in each orbit travel with a specific wavelength.

SO they have to also have a specific frequency and therefore specific ENERGY! (E = $h\nu$.)

It is impossible to determine simultaneously both the position and velocity of an electron or any other particle.

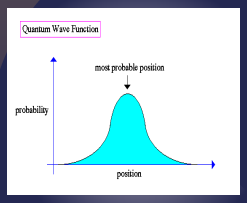
The Heisenberg Uncertainty Principle



Together with the uncertainty principle, the wave equation laid the foundation for modern quantum theory. **Quantum theory** mathematically describes the wave properties of electrons (and other small particles).

The Schrödinger Wave Equation (1926)

Solutions to the equations = Wave Functions

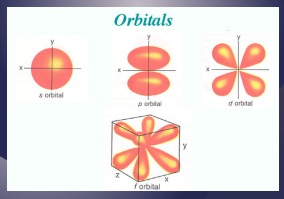


Schrodinger used wave functions to give only the probability of finding an electron at a given place around the nucleus.

The electrons do not travel around the nucleus in neat orbits, as Bohr had thought.

Orbitals

Instead of simply "orbits" like the planets, the electrons exist in certain regions called orbitals. An **orbital** is a three dimensional region around the nucleus that indicates the probable location of an electron.

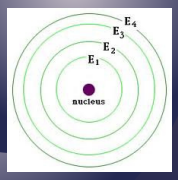


Atomic Orbitals and Quantum Numbers

- We use "quantum numbers" to describe the energy level, shape of orbital, and orientation of the different orbitals the electrons are likely to be in around the nucleus.

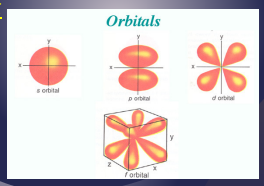
1st QN: Principal Quantum Number (n)

- Indicates the **main energy level (or shell)** occupied by the electron.
- Values of n are positive integers (1, 2, 3…)
- As n increases, the electron's energy and average distance from the nucleus increases.



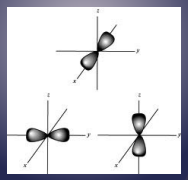
Angular Momentum Quantum Number (*l*)

- **Indicates the shape of the orbital.**
- **S sublevel**
- **P sublevel**
- **D sublevel**
- **F sublevel**
  - **We can assign these numbers, but we aren't going to…**



Magnetic Quantum Number (m)

- **Indicates the orientation of an orbital around the nucleus.**
- The values allowed are m = -l……0…….+l



- The 3 possible orientations of the P orbitals

Spin Quantum Number

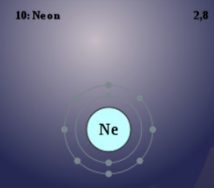
- Only two possible values, ±½
- **Tells you which direction the electrons are spinning ("up" or "down")**
- A single orbital can hold a maximum of two electrons, which must have opposite spins.

Section 4-3: Electron Configurations

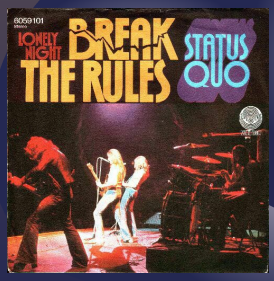
- Electron configuration: **The arrangement of electrons in an atom.**
- All systems in nature **assume the lowest possible energy state** ("Mama Nature don't like to sweat"). For atoms, this is the element's *ground-state electron configuration.*

Some background info…

- To simplify things, we show electrons in orbits around the nucleus (it's really 3-D orbitals).
- There can be a maximum of 8 electrons in the outer shell!!!
  - But only the noble gases (Group 18) are full (ex. Neon)



Rules Governing Electron Configurations



- The energy levels of the orbitals are determined and electrons are added to the orbitals one by one according to 3 basic rules:

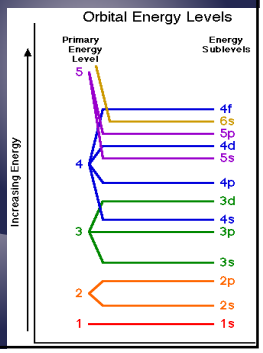
1. Aufbau principle
2. Pauli exclusion principle
3. Hund's rule

WRITE THESE DOWN

Aufbau ("Build-up") Principle

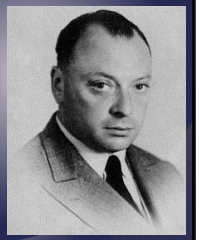
- An electron occupies the lowest-energy orbital that can receive it.

Note: Starting with the third main energy level ($n = 3$), the energies of the sublevels begin to overlap (see diagram on p. 105).



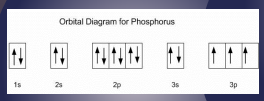
Pauli Exclusion Principle (1926)

- No two electrons in the same atom can have the same set of four quantum numbers. Thus electron pairs in orbitals must be of opposite spin.



Wolfgang Pauli:

Hund's Rule



Notice how the "3p" electrons are all up arrows before you start filling with down

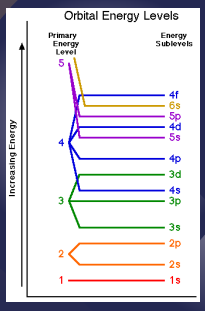
- Orbitals of equal energy are each occupied by one electron before any orbital is occupied by a second electron, and all electrons in singly occupied orbitals must have the same spin.
- The rule above minimizes electron-electron repulsion.

Four Ways of Representing Electron Configurations

1. Orbital Notation
2. Electron-Configuration Notation
3. Noble-Gas Notation
4. By the quantum numbers associated with each electron (you will NOT be held responsible for this on a test).

Terminology that you need to know follows:

Highest Occupied Level



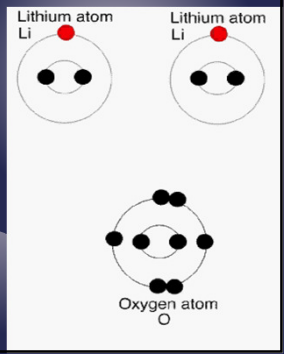
- The electron-containing main energy level with the highest principal quantum number.

AKA: The outermost shell/orbit

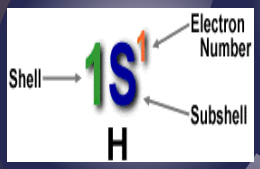
Inner-shell Electrons

Electrons that are not in the highest occupied energy level.

AKA: Everything that is NOT in the outer shell/orbit



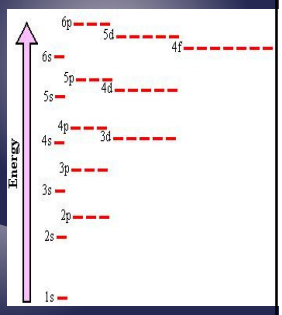
Electron-Configuration Notation



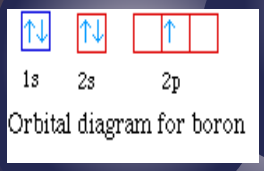
- We eliminate the lines and arrows and just show the number of electrons as a superscript to the sublevel designation.
- EXAMPLE: Calcium

Orbital Notation

- An unoccupied orbital is represented by a line. The lines are labeled with the principal quantum number and sublevel letter.
  - Why 1 line for s-orbitals?
  - Why 3 lines for p orbitals?
  - Why 5 lines for d orbitals?
  - Why 7 lines for f orbitals?
- EXAMPLE: Calcium



Arrows Denote Spin



Orbital diagram for boron

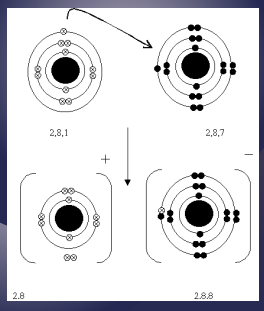
- We follow the filling rules noted previously and fill in the number of electrons needed.
- Even if an orbital is empty, you still need to draw it.
- Those with one electron have an up arrow, those with two electrons have both an up and down arrow to show electrons paired with opposite spin.

Now try writing the electron configurations for the following elements in both orbital notation and electron configuration notation
Use the "Steps to Writing E-Configuration" Packet!

- Magnesium - Mg
- Beryllium - Be
- Chlorine - Cl
- Iron - Fe

Noble Gas Configuration

- The outer main energy level is fully occupied, in most cases, by eight electrons (sometimes called "completing the octet").
- Which noble gas does not complete the octet?



Noble Gas Notation

Neon configuration

Na:	$1s^2\ 2s^2\ 2p^6\ 3s^1$	or	[Ne] $3s^1$
Mg:	$1s^2\ 2s^2\ 2p^6\ 3s^2$	or	[Ne] $3s^2$

- This is a shorthand method to show electron configurations, usually for atoms in the 3rd period and beyond. You show the nearest previous noble gas as the core, and then only denote the outermost (valence) electrons.

WARNING!!!

- The electron-configuration notation on your periodic table in the book is NOT in the proper order!!!
- Do not copy from the table, use the "yellow brick road"!!!

Weird Variations

- Chromium (Cr) expect $[Ar]4s^23d^4$, is $[Ar]4s^13d^5$
- Copper (Cu) expect $[Ar]4s^23d^9$, is $[Ar]4s^13d^{10}$

The reason is that mixes of half and/or fully filled orbitals are more stable (in a lower-energy state), than a fully or half filled orbital with a partially filled orbital.