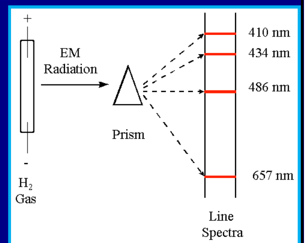
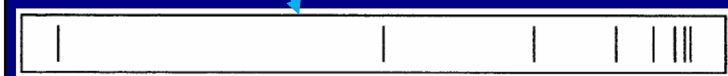
The Electronic Structure of the Atom

- Bohr based his theory on his experiments with hydrogen
- he found that when energy is added to a sample of hydrogen, energy is absorbed and reemitted as light
- When passed through a prism, a "line spectrum" is obtained



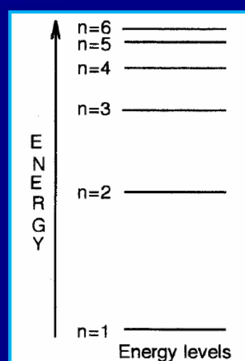


Bohr's Explanation:

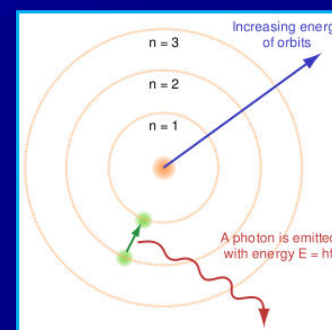
- The electron in hydrogen can only exist in specific energy states.
- These energy states are associated with specific circular orbits which the electron can occupy around the atom.
- When an electron absorbs energy, it moves from one orbit to another.
- The greater the energy, the farther the orbit is from the nucleus.

Energy Levels of Hydrogen:

- **Energy Level/Orbit**: the specific amount of energy of an electron in an atom
- The energy levels of hydrogen have the pattern shown ("n" is the number of the energy level)



- The **line spectrum** represents energy level differences occurring when an electron gives off energy by dropping from a high energy level to a lower one.
- Since there are specific energy levels the electrons can be in, there are only certain energy differences that occur
- The difference between two different energy levels is called a **QUANTUM** of energy



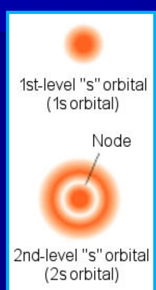
The Refined Theory:

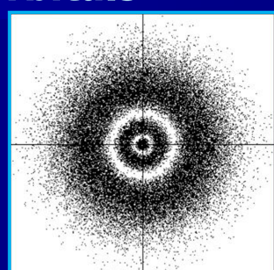
- after Bohr published his theories, several changes were made to his ideas.
- It was discovered that electrons don't travel in circular orbits!
- Instead, different electrons, depending on their energies, occupy particular regions of space called "orbitals".
- ORBITAL:
  - The actual region of space occupied by an electron in a particular energy level (based on probability of where an electron could be found)
  - **Each orbital can hold up to 2 electrons!**

Some Terminology:

- There are 4 types of orbitals that we discuss:
  - "s", "p", "d", and "f"
- Shell: the set of orbitals having the same "n" value
  - Ex. 3rd shell is made up of the 3s, 3p, and 3d orbitals
- Subshell: a set of orbitals of the same type
  - Ex. There are 3 "p" orbitals in the 2p subshell

Orbital Types and Shapes: "s orbitals"

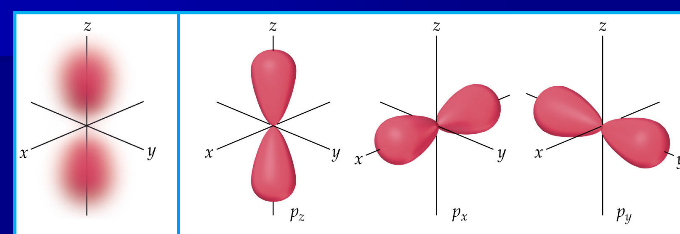




3n s orbital

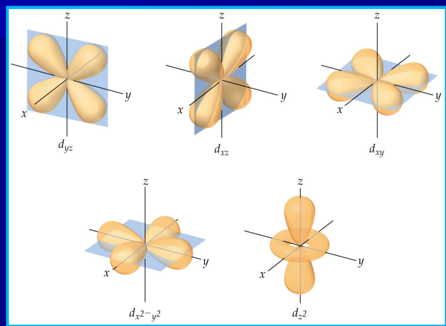
- In general, "s orbitals" are considered spherical
- There is only 1 s orbital in an s subshell
- ∴ an "s" subshell can hold 2 electrons

"p orbitals"



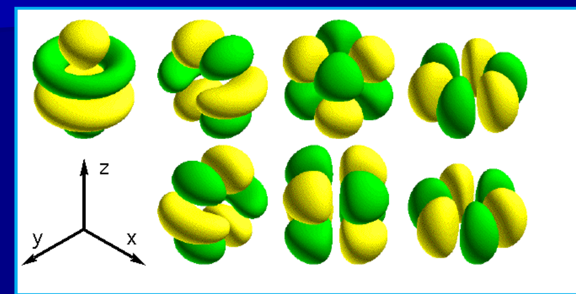
- Think balloon shapes!
- There are 3 "p" orbitals in every "p" subshell
- ∴ a "p" subshell can hold 6 electrons

“d orbitals”



- There are 5 “d” orbitals in every “d” subshell
- ∴ a “d” subshell can hold 10 electrons

“f orbitals”



- There are 7 “f” orbitals in every “ f ” subshell
- ∴ an “ f ” subshell can hold 14 electrons

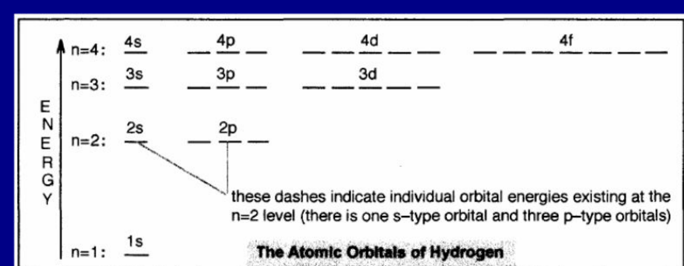
Rules governing which types of orbitals can occur:

- For a given value of “n”, n different types of orbitals are possible
- For n=1: only the s-type is possible
- For n=2: the s- and p-types are possible
- For n=3: the s-, p-, and d-types are possible
- For n=4: the s-, p-, d-, and f-types are possible.

- These rules come from the mathematical solutions for Schrödinger's wave equation

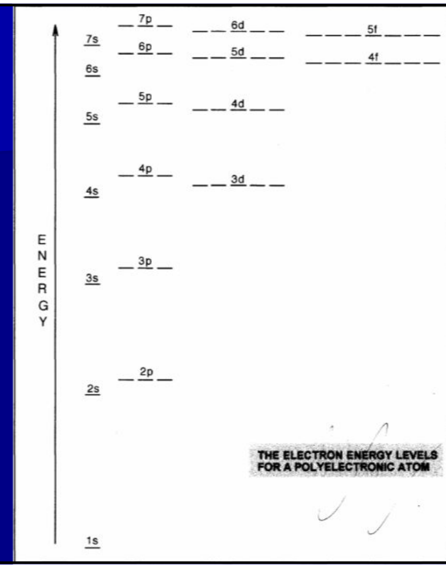
Energy Level Diagrams:

- Diagram showing the relative energy levels of all of the orbitals in the atom/ion
- Shown for hydrogen below:



Energy Level Diagram for Polyelectronic Atom

- Repulsion between electrons changes the energy of the different types of orbitals
- A new energy level diagram must be drawn that works for all atoms with more than 1 electron

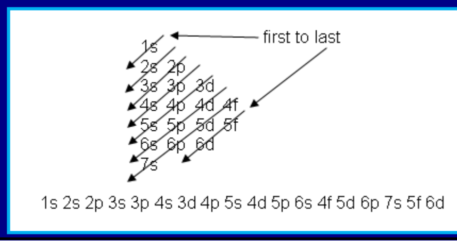


- 3 rules govern the order the orbitals are filled:
  - **Aufbau Principal**:
    - As atomic number increases, electrons are added to the available orbitals. To ensure lowest possible energy (ground state) for the atom, electrons are added to the LOWEST ENERGY ORBITALS FIRST.

- **Pauli Exclusion Principle**:
  - A maximum of TWO electrons can be placed in each orbital.
- **Hunds Rule**:
  - When electrons occupy subshells of equal energy, they must be singly occupied with electrons having parallel spins. 2nd electrons are then added to each subshell so each electron has opposite spin.

Energy Level Diagram Practice:

- Draw energy level diagrams for the following atoms:
  - Si, Tc, Ca, Zr, Ga
- Note: there is a trick to determining the order to fill orbitals without doing the full electron configuration

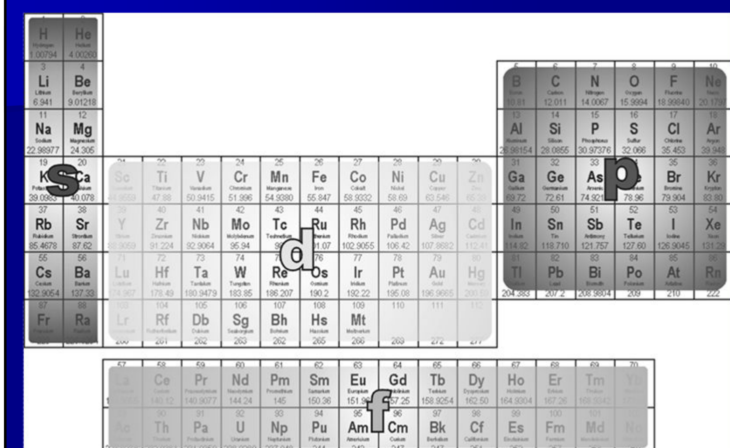


Electron Configurations:

- represents the orbitals that are occupied in an atom/ion and how many electrons are in each subshell
- like a simplified energy level diagram

Writing Electron Configurations for Neutral Atoms:

- The electron configuration of most elements can be easily determined by using the "orbital version" of the periodic table



Examples:

- Hydrogen:
  - $1s^1$
- Helium:
  - $1s^2$
- Lithium:
  - $1s^2\ 2s^1$
- Beryllium:
  - $1s^2\ 2s^2$
- Boron:
  - $1s^2\ 2s^2\ 2p^1$
- And so on…
  - Be: $1s^2\ 2s^2$
  - B: $1s^2\ 2s^2\ 2p^1$
  - C: $1s^2\ 2s^2\ 2p^2$
  - N: $1s^2\ 2s^2\ 2p^3$
  - O: $1s^2\ 2s^2\ 2p^4$
  - F: $1s^2\ 2s^2\ 2p^5$
  - Ne: $1s^2\ 2s^2\ 2p^6$

Practice Time:

- Predict the electron configuration of the following:
- Si:
  - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$
- Tc:
  - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^5$
- Ca:
  - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2$
- Zr:
  - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6\ 5s^2\ 4d^2$
- Ga:
  - $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^1$

Core Notation

- The electrons belonging to an atom can be broken into two subsets:
  1. The CORE electrons.
  2. The OUTER electrons.
- The CORE of an atom is the set of electrons with the configuration of the nearest noble gas having an atomic number LESS than that of the atom being considered.
- The OUTER electrons are all those outside the core. Since the core electrons are not involved in chemical reactions, they are excluded from the electron configuration.

Examples:

- Al: [Ne] $3s^2\ 3p^1$
- You try for…
  - Zr, Ga, Co
- Answers:
  - Zr: [Kr] $5s^2\ 4d^2$
  - Ga:[Ar] $4s^2\ 3d^{10}\ 4p^1$
  - Co:[Ar] $4s^2\ 3d^7$

- Two exceptions to the configurations of elements up to Kr:
  - Cr: [Ar] $4s^2\ 3d^4$ "$3d^4$" is actually [Ar] $4s^1\ 3d^5$
  - Cu: [Ar] $4s^2\ 3d^9$ "$3d^9$" is actually [Ar] $4s^1\ 3d^{10}$

A filled or exactly half filled d-subshell is especially stable.

- Because of this extra stability, an atom or ion that is one e^- short of a "d^5" or "d^{10}" configuration will shift an e^- from the s- subshell having the highest energy into the unfilled d- subshell.

Writing Electron Configurations for Ions

- **For Negative Ions: (anions)**
  - Add electrons to the last unfilled subshell, starting where the neutral atom left off.
- For Example:
  - O: [He] $2s^2$ $2p^6$
  - P: [Ne] $3s^2$ $3p^6$

For Positive Ions: (cations)

2 Rules to follow:

1. Electrons in the outermost shells (largest n value) are removed first.
2. If there are electrons in both the s and p orbitals of the outermost shell, the electrons in the p orbitals are removed first.

p-electrons **BEFORE** s-electrons **BEFORE** d-electrons

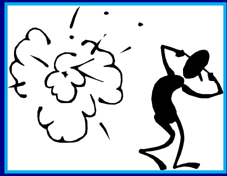
- Outermost electrons are removed preferentially since they are the least attracted to the nucleus

Examples:

- Sn^{2+}: [Kr] $5s^2$ $4d^{10}$ $5p^2$ - $2e^-$ → [Kr] $5s^2$ $4d^{10}$
- Sn^{4+}: [Kr] $5s^2$ $4d^{10}$ $5p^2$ - $4e^-$ → [Kr] $4d^{10}$
- V^{2+}: [Ar] $4s^2$ $3d^3$ - $2e^-$ → [Ar] $3d^3$
- Cu^+: [Ar] $4s^1$ $3d^{10}$ - e^- → [Ar] $3d^{10}$

Predicting the Number of Valence Electrons

- Valence Electrons:
  - Electrons that can take place in chemical reactions.
  - Are all the electrons in the atom **EXCEPT**:
    - Core electrons.
    - filled d- or f- subshells of electrons.



Examples:

- Al: [Ne] $3s^2$ $3p^1$ has 3 valence electrons:
  Just "$3s^2$ $3p^1$"
- Ga: [Ar] $4s^2$ $3d^{10}$ $4p^1$ has 3 valence electrons:
  Omit "$3d^{10}$" b/c filled
- Pb: [Xe] $6s^2$ $4f^{14}$ $5d^{10}$ $6p^2$ has 4 valence electrons:
  Omit "$4f^{14}$" and "$5d^{10}$" b/c filled
- Xe: [Kr] $5s^2$ $4d^{10}$ $5p^6$ has ZERO valence electrons:
  Noble gas configuration

Homework:

- Complete the Electron Configuration Worksheet