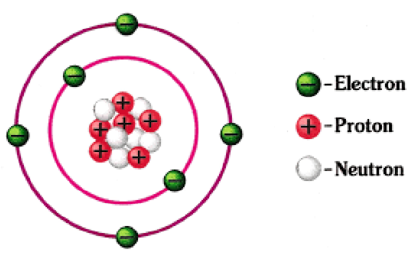
Electrons and Molecular Forces

Chemistry 30 – Ms. Hayduk

Atomic Structure

- **Atomic Number**
  - Number of protons in the nucleus
  - Defines the element
  - Used to organize the periodic table

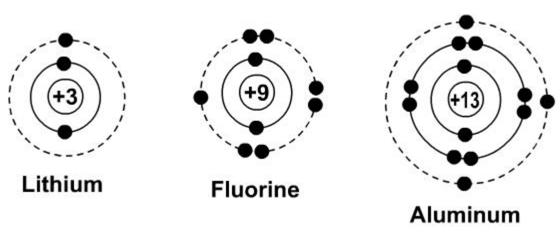


Bohr Model of the Atom

- Electrons can only move in specific energy levels (*n*)
- Larger values of *n* = high energy electron
- Each energy level = an orbit (circular path around nucleus)

Bohr Models

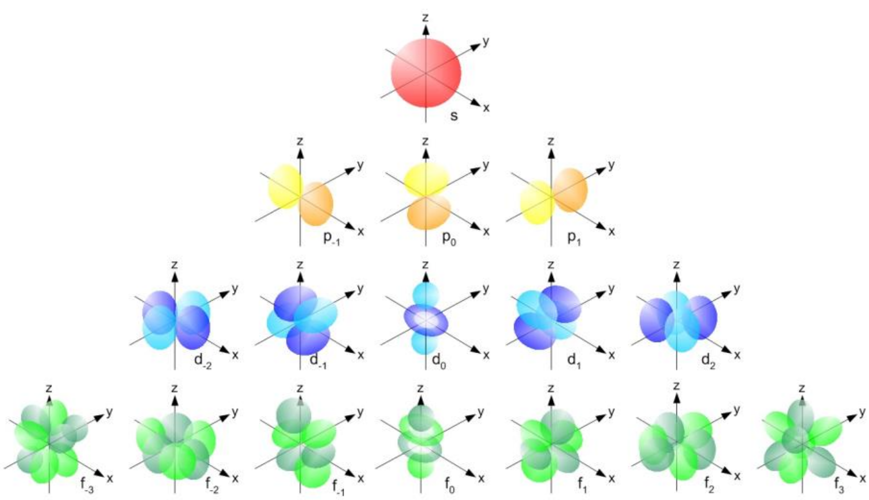
Energy Level (Orbit)	1	2	3	4
Number of Electrons	2	8	8	18



Quantum Mechanical Model

- Electrons exist at **quantized** energy levels (certain values with none "in-between") – "n"
- Electrons don't follow specific orbits
- 3D cloud around nucleus (atomic orbital) describes probable location
- Electrons have spin, clockwise or counter-, so only two can be in an orbital

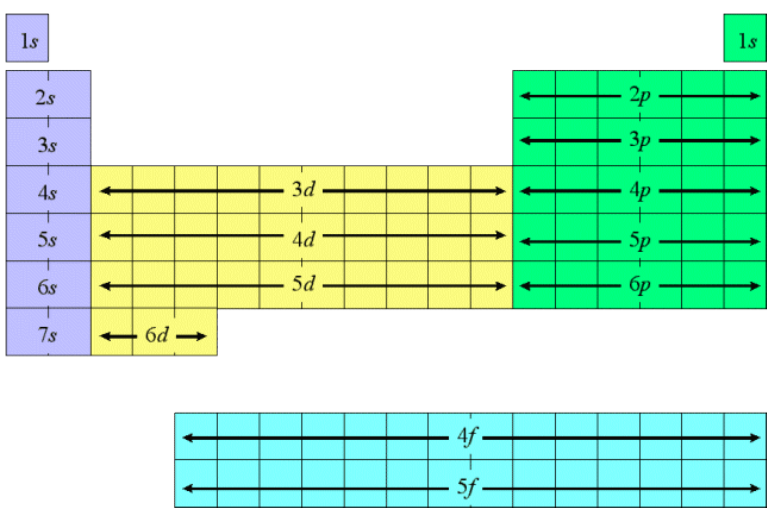
Orbital Shapes



Electron Configuration

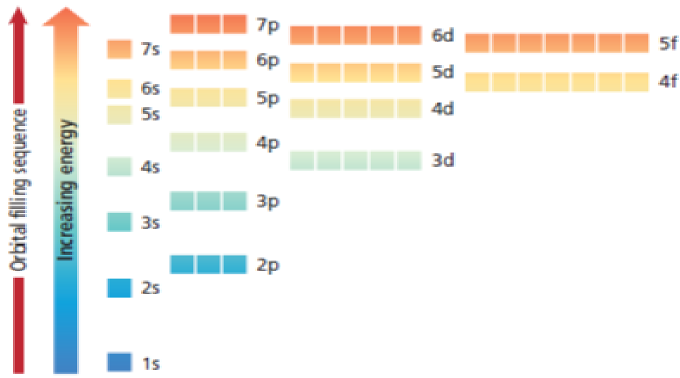
- Explains arrangement of atoms in lowest possible energy state (ground state)
- Can be in atoms or ions

Electron Configuration



Aufbau Principle

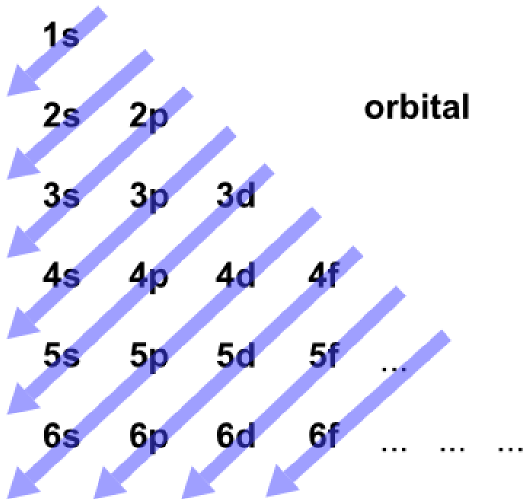
- electrons occupy the lowest energy orbitals first



Pauli Exclusion Principle

- Only two electrons, with opposite spins, can occupy an orbital

Orbitals



Examples: Electron Configuration

H

B

Na

Cl

Ag

Sn

Noble Gas Configuration

- Write the noble gas from the period above in square brackets, then continue electron configuration from that point
- Example:

Mg ($1s^2 2s^2 2p^6 3s^2$) becomes:

$[Ne]3s^2$

Examples: Noble Gas Config.

Ti

Cd

Cl

Ions

- Metals lose electrons from highest energy levels first, then largest orbital (f, d, p, s)
- Non-metals will gain electrons from in lowest energy levels first (lowest *n* with space available)
- Determine valence electrons by adding number of electrons in highest energy level

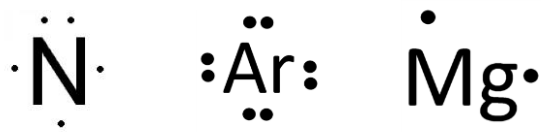
Example: Valence Electrons

1. How many valence electrons does Br have?

2. How many valence electrons does Zn have?

Valence Electrons

- Electrons in the outermost orbitals – available to bond
  - e.g. Oxygen [He]$2s^2 2p^4$ has six
- **Lewis Structure**: shows symbol and valence electrons



Examples: Lewis Diagrams

F

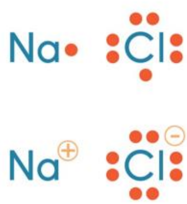
Ca

Pb

Nd

Ion Formation

- **Ion**: an atom that becomes charged by gaining or losing electrons to empty or fill an orbital



Ionic Bonds

- Formed when two or more ions with opposite charges are attracted together to form a compound
- Contain a metal (cation) and one or more non-metals (anion)
- Overall charge is zero

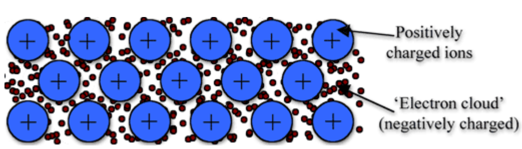
Example: Ionic Bonds

Na and Cl

Mg and O

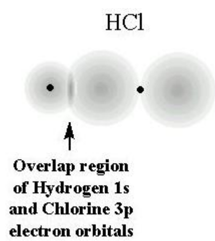
Metallic Bonds

- Metals form lattices where valence electrons move freely between atoms
- "Electron sea model"



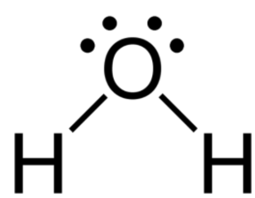
Covalent Bonds

- AKA molecular bonds
- Formed between non-metals, outer orbitals overlap to____________________________ between atoms



Lewis Structures

- Used to show 2D bonding shape of covalent molecules
- Bonds are lines (single —, double =, triple ≡), electron pairs are two dots



Rules

- Only for non-metals
- Atoms want to fill their orbitals
  - Often eight valence electrons
  - Can be more for d and f orbitals
- Hydrogen always has only one single bond, no lone pairs
- Central atom has the most unpaired electrons (often carbon), is least electronegative

Steps

1. Count # valence electrons in all atoms (add for negative ions, subtract for positive).
2. Draw symbol of central atom.
3. Draw single bonds between outer and central atom.
4. Draw lone pairs on outer atoms to fill orbitals. Leftover pairs go on central atom.
5. If central atom does not have four pairs, convert outer lone pairs to single/double bonds (only for C, N, O, P and S)

Examples: Lewis Structures

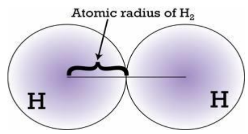
- F_2
- HCN
- NH_3
- SF_6

General Rule

- Periodic trends depend on the attraction between opposite charges (protons and electrons) and the repulsion of like charges
- Larger positive/negative charge difference increases attraction
- Distance decreases the attraction between opposite charges

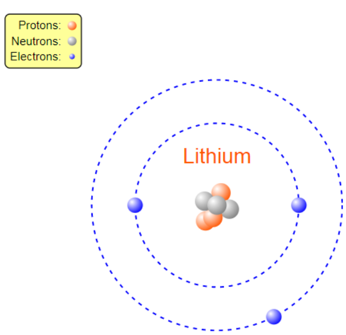
Atomic Radius

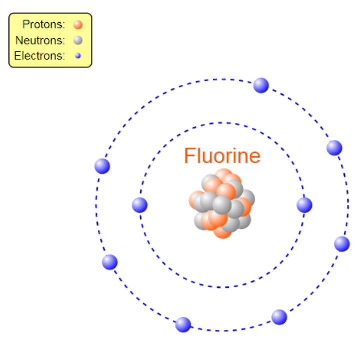
- Half the distance between adjacent nuclei of the same element



Atomic Radius

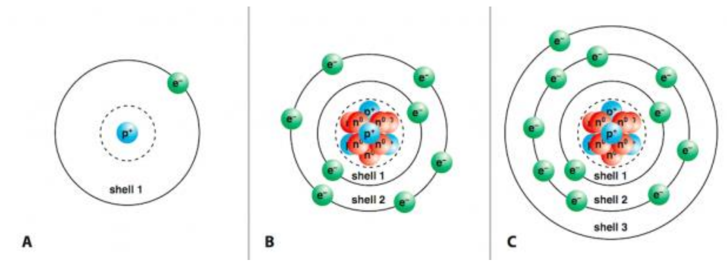
- ⇩across a period (larger nucleus, same number of energy levels)





Atomic Radius

- ⇧down a group (higher energy levels, electrons are further away, cannot be attracted as strongly)



Electronegativity

- Ability of an atom to attract electrons in a chemical bond
- 0 – 4.0 Paulings (0 for noble gases)
- High electronegativity = atom "wants" to gain electrons, low = wants to give away
- ⇧ across a period (larger nucleus pulls electrons in closer)
- ⇩ down a group (shielding)

Intramolecular Forces

- Describes how bonds are formed **inside** a compound (chemical bonds) – how electrons move between the atoms
- Strength depends on difference in electronegativity between elements
- Types: ionic, polar covalent, non-polar covalent, metallic

Bond Polarity

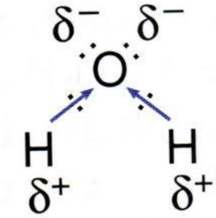
- Difference in electronegativity determines **polarity** of a bond
- **Polarity**: unequal sharing of electrons between two atoms
- Determines type of bond within a compound

Example: Bond Polarity

What is the electronegativity difference in a C-F bond?

Dipoles

- **Dipole**: area of positive or negative charge within a molecule
- Formed when electrons are held closer to one atom in a bond than the other
- Indicated by δ (delta) and the charge



Example: Dipoles

In a C-F bond, identify the dipoles.

Bonds and Electronegativity

- Ionic: complete transfer of electrons, EN difference > 2.0
- Covalent:
  - Non-Polar: equal sharing of electrons, EN < 0.5
  - Polar: unequal sharing, 0.5 <EN<1.6
- EN is 1.6-2.0: ionic if a metal is involved, otherwise polar covalent

Example: Intramolecular Forces

What type of intramolecular force is present in each bond?

Ca-F	C-H
N-N	Na-Cl
C-O	H-F

Ionic Compounds

- Solid, brittle, poor conductors in the solid state
- Regular crystal structure
- Dissolve in polar substances only (like dissolves like) to form electrolytes (solutions that conduct electricity)
- High melting point (as an example, sodium chloride melts at 801°C)

Non-Polar Compounds

- Can be solid, liquid or gas
- Often more flexible and soft
- Dissolve in non-polar substances (like dissolves like)
- Low melting and boiling points (many below zero)

Polar Covalent Compounds

- For solids, irregular crystal structure
- Can be solid, liquid or gas
- Can dissolve in polar substances and non-polar substances, (depending on structure) can form weak electrolytes (solutions that conduct electricity)
- Moderate melting and boiling points – compare to water

VSEPR Models

- Valence Shell Electron Pair Repulsion model
- Shows 3D shape of covalent molecules
- Helps to determine properties of molecule and substance
- Shape is based on one central atom (larger molecules can have multiple VSEPR shapes at different places)

Drawing VSEPR

1. Determine central atom
2. Draw Lewis diagram
3. Determine number of bonds and electron pairs (steric number) and number of lone pairs
4. Check VSEPR shape table to determine geometry

Examples: VSEPR

CH_4 XeF_4

NO_3^- CO_2

Polarity and Geometry

- Even if bonds are polar, the molecule overall may be non-polar
- If bonds are polar, check <u>symmetry</u>
- Look "along" each bond – if the molecules is the same on both sides, it is symmetric

Symmetry Rules

If all “X”s are the same:

- Basic geometry is symmetric
- Square planar is symmetric
- Linear is symmetric

If “X”s are different or any other geometry, as long as bonds are polar, molecule is polar.

Polarity and Geometry

Steps:

1. Check polarity of ALL bonds with central atom
   - If all are non-polar, molecule is non-polar
2. Check molecular shape
   - If shape is symmetric, molecule is non-polar

Examples: Molecular Polarity

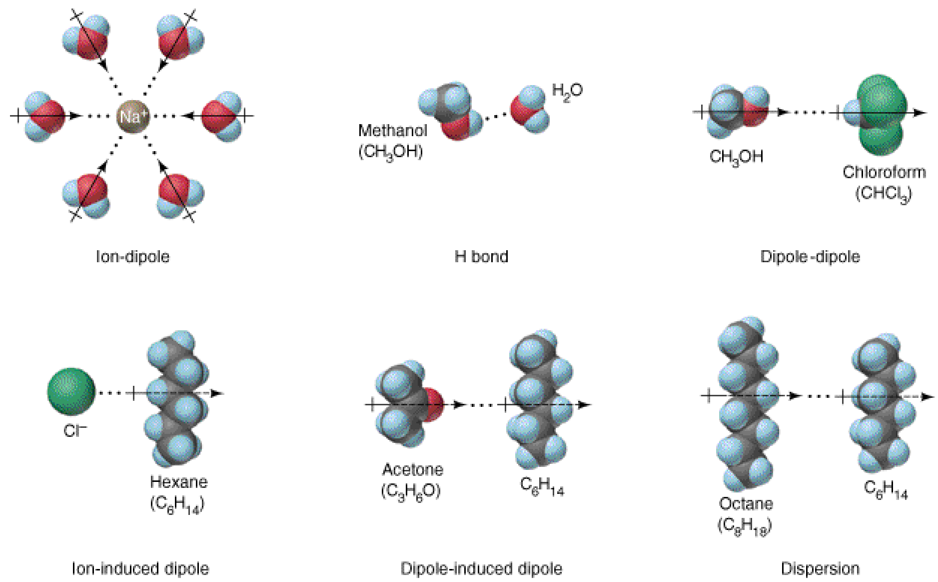
O_2

BrF_5

PF_5

Intermolecular Forces

- **Intramolecular forces**: describe attractive/repulsive forces within a molecular or compound (ionic or covalent)
- **Intermolecular forces**: describe how particles of the same substance are attracted to each other

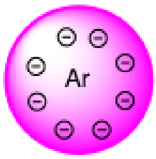


London Forces

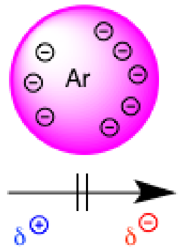
- Also called dispersion forces (Van der Waals forces)
- Caused by *instantaneous dipoles* caused by electron movement in a molecule
- Weak forces that exist for <u>all</u> molecules
- Increases in strength with molar mass

London Forces

if valence electrons are perfectly distributed, Ar has no dipole



on an instantaneous basis, there can be an imbalance of charges.



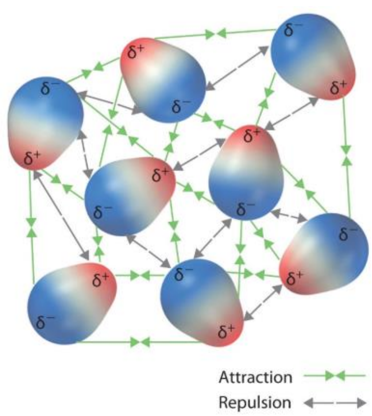
This is "long term average"

This creates a "temporary dipole"

These temporary dipoles attract

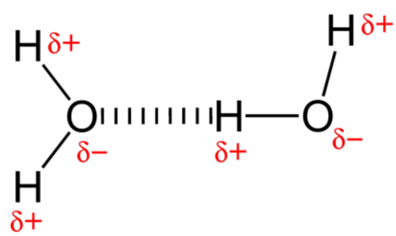
Dipole-Dipole Forces

- Attractions between charged points on polar molecules (dipoles)



Hydrogen Bonding

- Specific type of dipole-dipole force (stronger)
- Occurs when F, O or N is directly bonded to H
- Almost ionic in terms of EN difference



Strength of IMFs

Most	hydrogen bonding
	dipole-dipole
Least	London forces

All substances have London forces.

Polar substances have dipole-dipole forces, and some also have hydrogen bonding.

Strength of IMFs

- Substances will often have more than one type of intermolecular force
- When asked to identify IMFs for a substance, generally the strongest one is the most informative

Other Intermolecular Forces

- Ionic attraction, or lattice energy
  - Describes attraction between ions in a compound
  - Increases as ion charges increase (so +2 /-2 is stronger than +1/-1)
- Covalent network
  - Occurs in covalent solids (e.g. diamond)
  - Very strong, harder to break than ionic attraction

Example 1: IMFs

What IMFs does water have?

Example 2: IMFs

What IMFs does CCl_4 have?

Effect of Intermolecular Forces

Melting and Boiling Points

- Increases with stronger forces
- For substances with the same type of IMF, MP and BP will be higher with higher molar mass

Surface Tension

- Increases with stronger forces

Example: Boiling Points

Which would have a higher boiling point of:

HF or HCl?

CO_2 or NH_3?

Example: Surface Tension

When a drop of water is placed on a surface, it holds it shape. What causes it to do this?

Effect of Intermolecular Forces

Vapour Pressure

- Affects flammability, volatility
- How easily a substance will evaporate (become a gas)
- Vapour pressure is lower (less gas produced) with stronger IMFs

Density

- Increases with stronger IMFs – molecules are held more tightly together

Example: Vapour Pressure

Which would evaporate first, water (H_2O) or methanol (CH_3OH)?

Example: Density

Explain why the density of the halogens increases down the family.

Effect of Intermolecular Forces

Solubility

- "Like dissolves like" – BUT WHY?
- Polar/ionic solutes dissolve in polar solvents, non-polar solutes dissolve in non-polar solvents
- **Polar molecules have a stronger attraction to other polar molecules than to non-polar molecules, so they do not interact**

Effect of Intermolecular Forces

- Particles of **solute** will dissolve **IF** it is ***more* attracted** to the **solvent** particles than ***to itself***