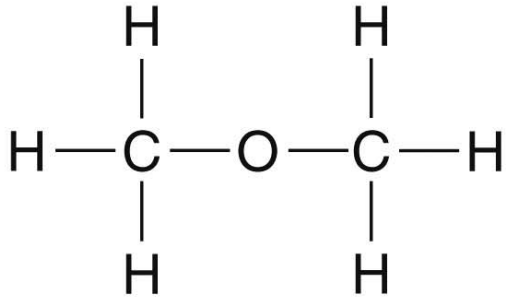
Chapter 1:
Electronic Structure and Bonding
Or
A Brief Review of General Chemistry
(Part 1) (Chapter 1.1-1.7)

1. The Structure of an Atom
2. Ionic and Covalent Bonds

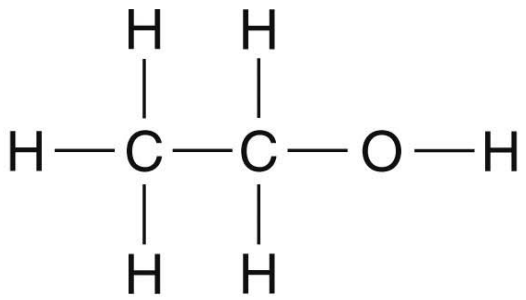
Review ideas from general chemistry:
atoms, bonds, molecular geometry

Electronic Structure and Bonding

In the mid 1800s, it was first suggested that substances are defined by a specific arrangement of atoms.



Dimethyl ether
Boiling point = −23°C



Ethanol
Boiling point = 78.4°C

Isomers or Constitutional Isomers have the same atoms but a with a different arrangement.

Electronic Structure and Bonding

- An **Electron Shell** is the set of orbitals with the same value of N.
  - E.g., 3s, 3p and 3d are subshells of 3
- The electrons in the outermost occupied shell are **valence electrons**.
- **Ground-state electron configuration** (lowest energy arrangement) of an atom lists orbitals occupied by its electrons
- **Noble gas configuration**: He, Ne, Ar, Kr, Xe, and Ra – The "Noble" Gases - are inert elements as their outer electron shells are filled making them very stable.
- Atoms tend to react in ways that enable them to achieve a more stable outer shell of 8 e-. This is called the **Octet Rule**.

Electronic Structure and Bonding

- If an element gives up (or donates) its electron easily – it is electropositive.

$$K - e^-$$

$$K\ (19)\ 1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$$

$$[Ar]4s^1 \longrightarrow K^+$$

- If an element accepts an electron easily – it is electronegative.

$$Cl + e^-$$

$$Cl\ (17)\ 1s^2 2s^2 2p^6 3s^2 3p^5$$

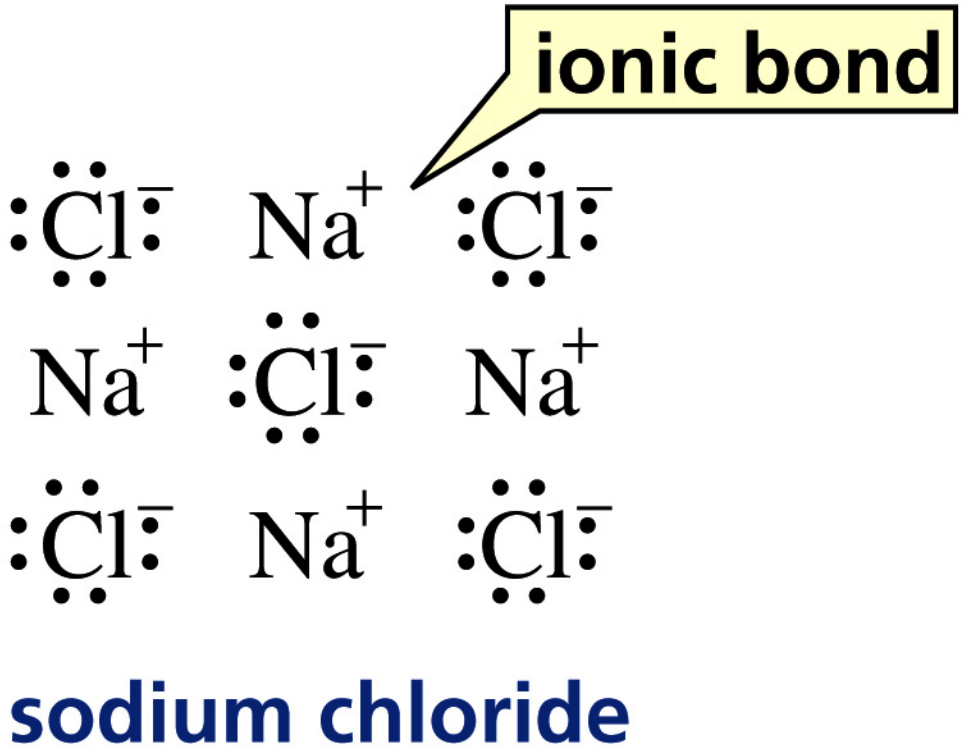
$$[Ne]3s^2 3p^5 \longrightarrow Cl^-$$

Electronic Structure and Bonding

- How do atoms form an octet?

- Atoms can obtain octets through gaining, losing or sharing electrons.
- An atom that gains an electron becomes a negatively charged anion.
- An atom that loses an electron becomes a positively charged cation.

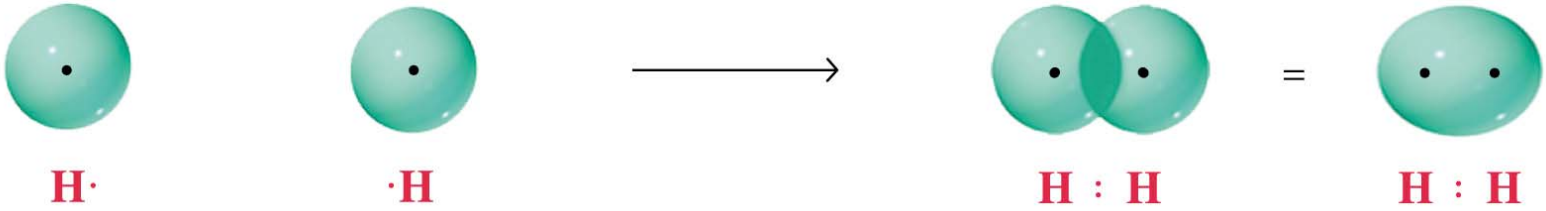
Electronic Structure and Bonding

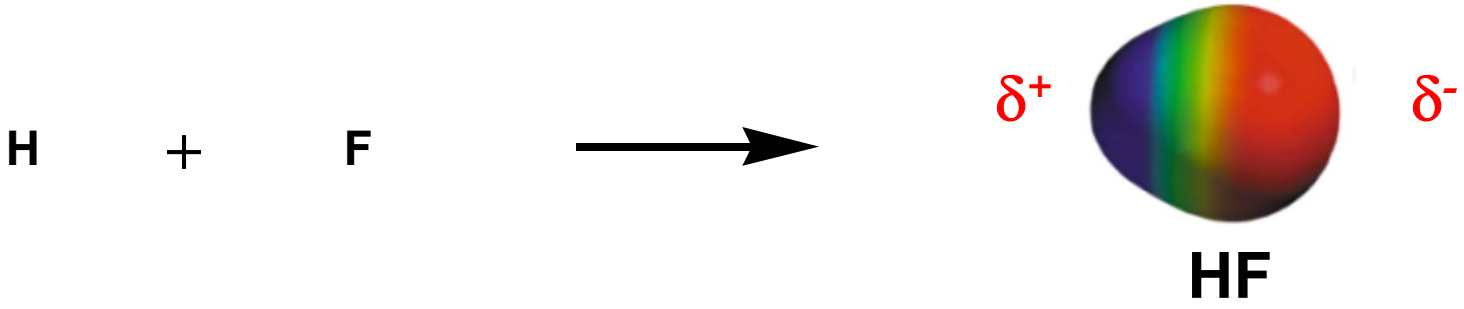


sodium chloride

Ionic compounds are formed when an electropositive element transfers electron(s) to an electronegative element.

Electronic Structure and Bonding





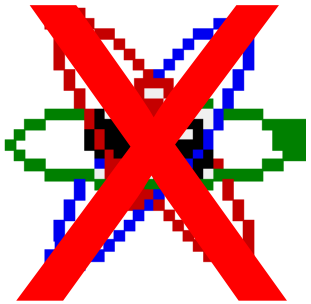
Range of Bond Types

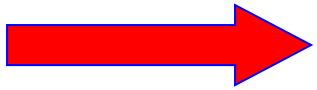
$K^+ Cl^-$ $\quad$ $\overset{\delta-}{O}—\overset{\delta+}{H}$ $\quad$ C—H, C—C

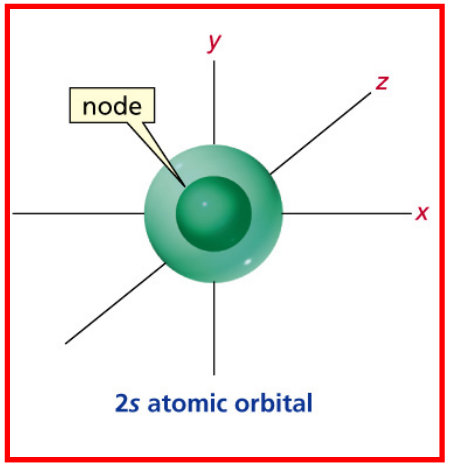
Ionic	Polar covalent	Nonpolar covalent
Difference in Electronegativity > 1.7	Difference in Electronegativity 0.5 – 1.7	Difference in Electronegativity < 0.5

Quantum Mechanics

- DeBroglie first proposed that matter should exhibit wavelike properties.
- Quantum mechanics uses the mathematical equation of wave motions to characterize the motion of an electron around a nucleus.
- The wave functions (or orbitals) developed by Schrödinger tell the energy of the electron and the volume of space around the nucleus where an electron is most likely to be found.



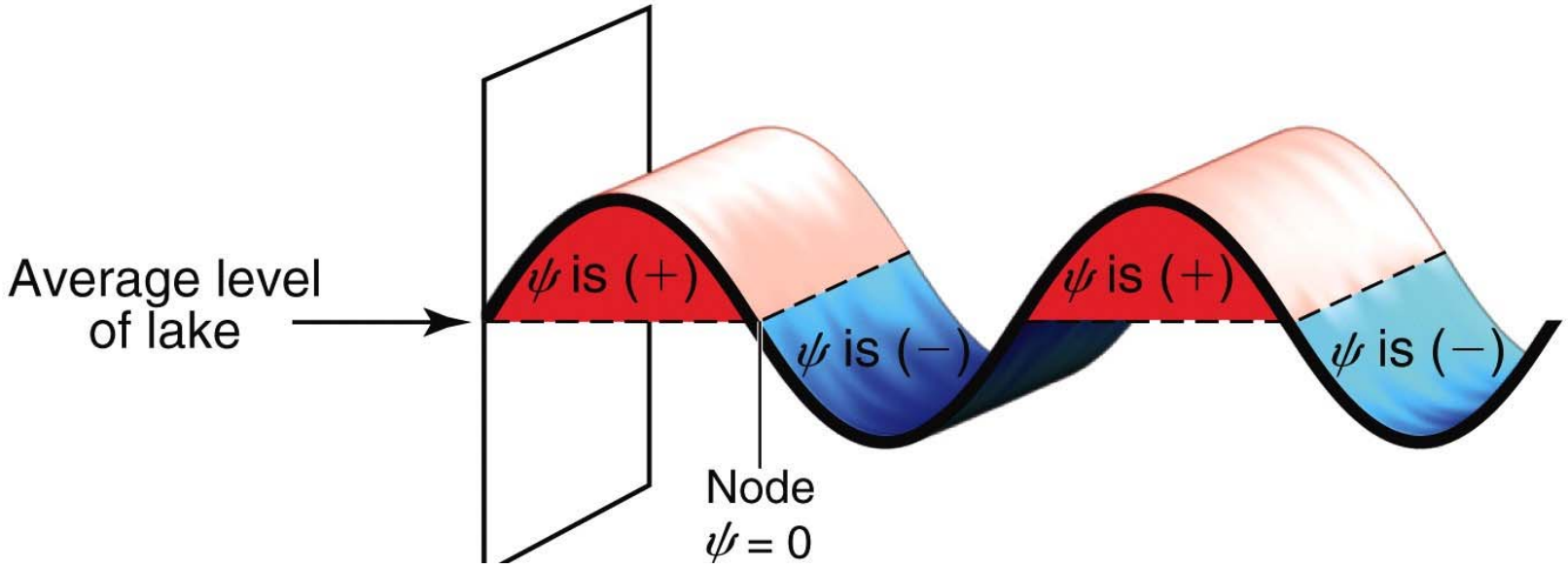




s and *p* orbitals most important in organic and biological chemistry

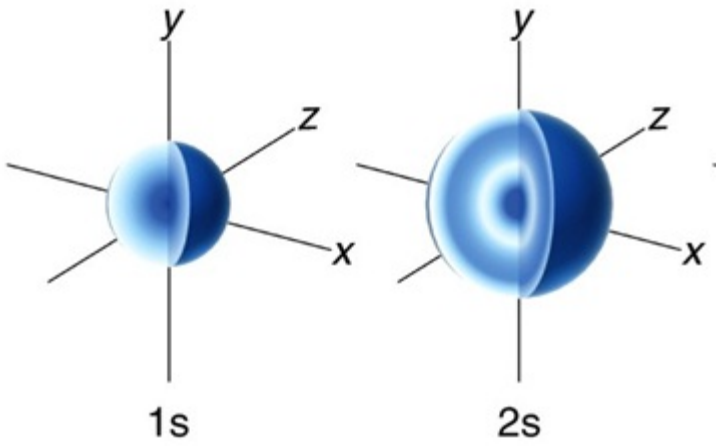
Quantum Mechanics

- Electrons behave as BOTH particles and waves.
- An orbital is a region where there is a calculated 90% probability of finding an electron.
- The theory does match experimental data, and it has predictive capability.
  - Like a wave, an electron's wavefunction can be (+), (-), or ZERO.



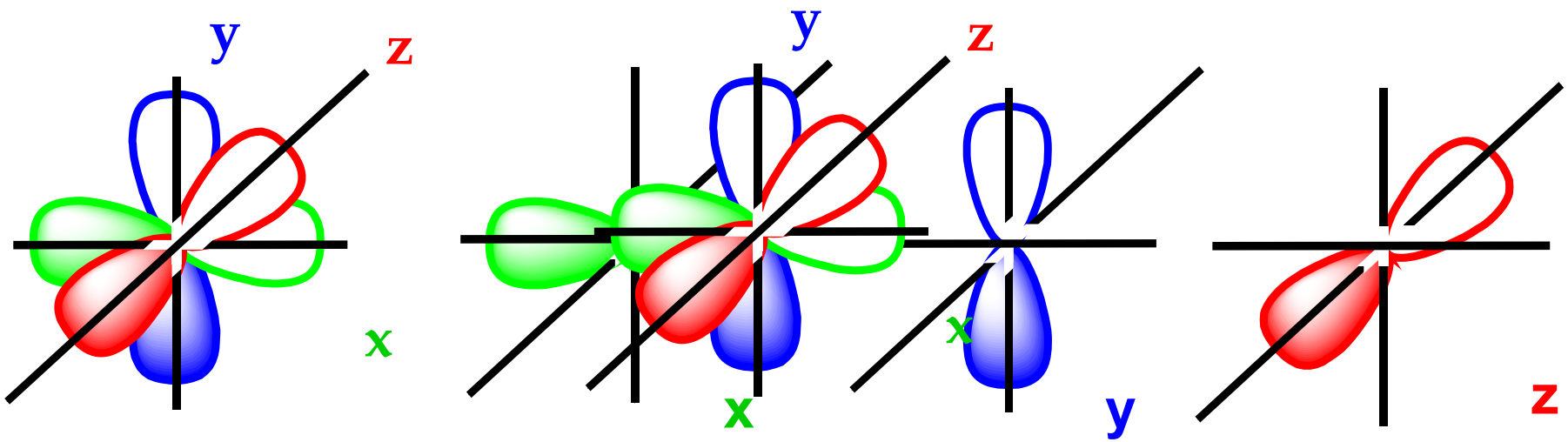
Quantum Mechanics

- Electrons are most stable (lowest in energy) if they are in the 1s orbital?
- The 1s orbital is full once there are two electrons in it.
- The 2s orbital is filled next. The 2s orbital has a node.



Electronic Structure and Bonding

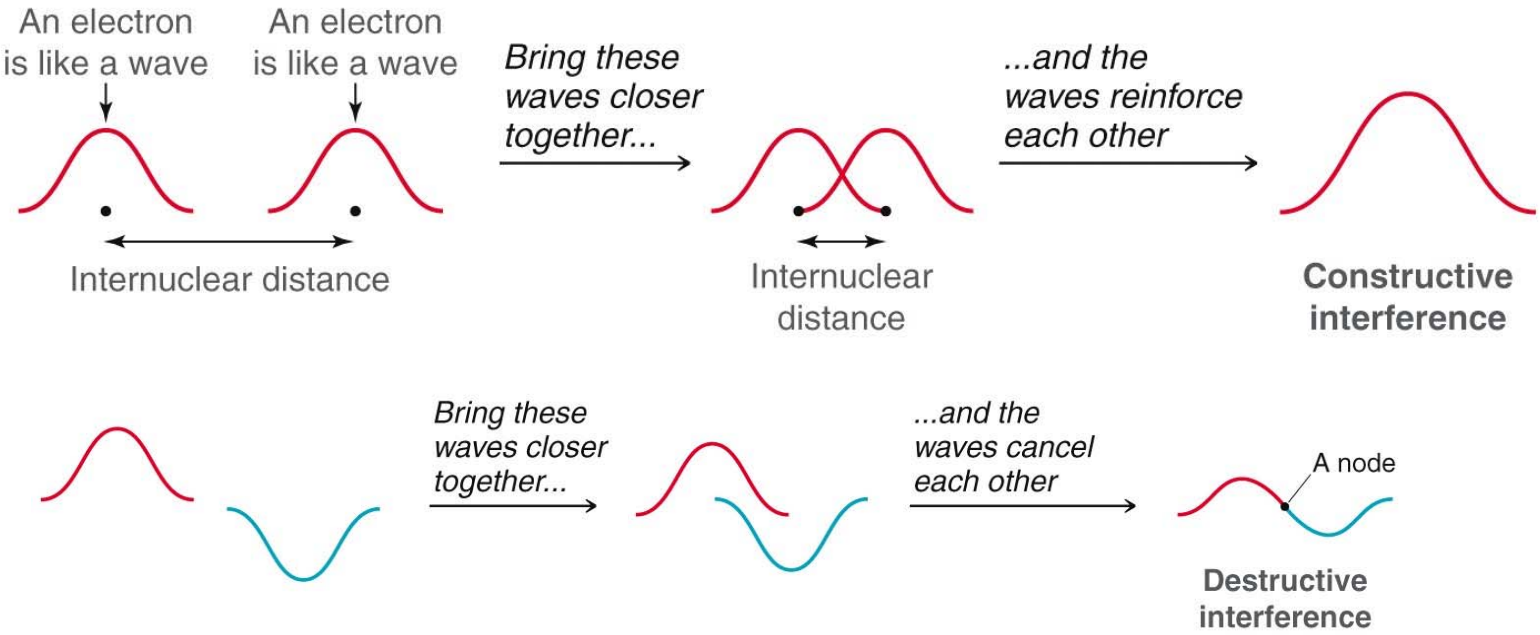
2p - Orbitals



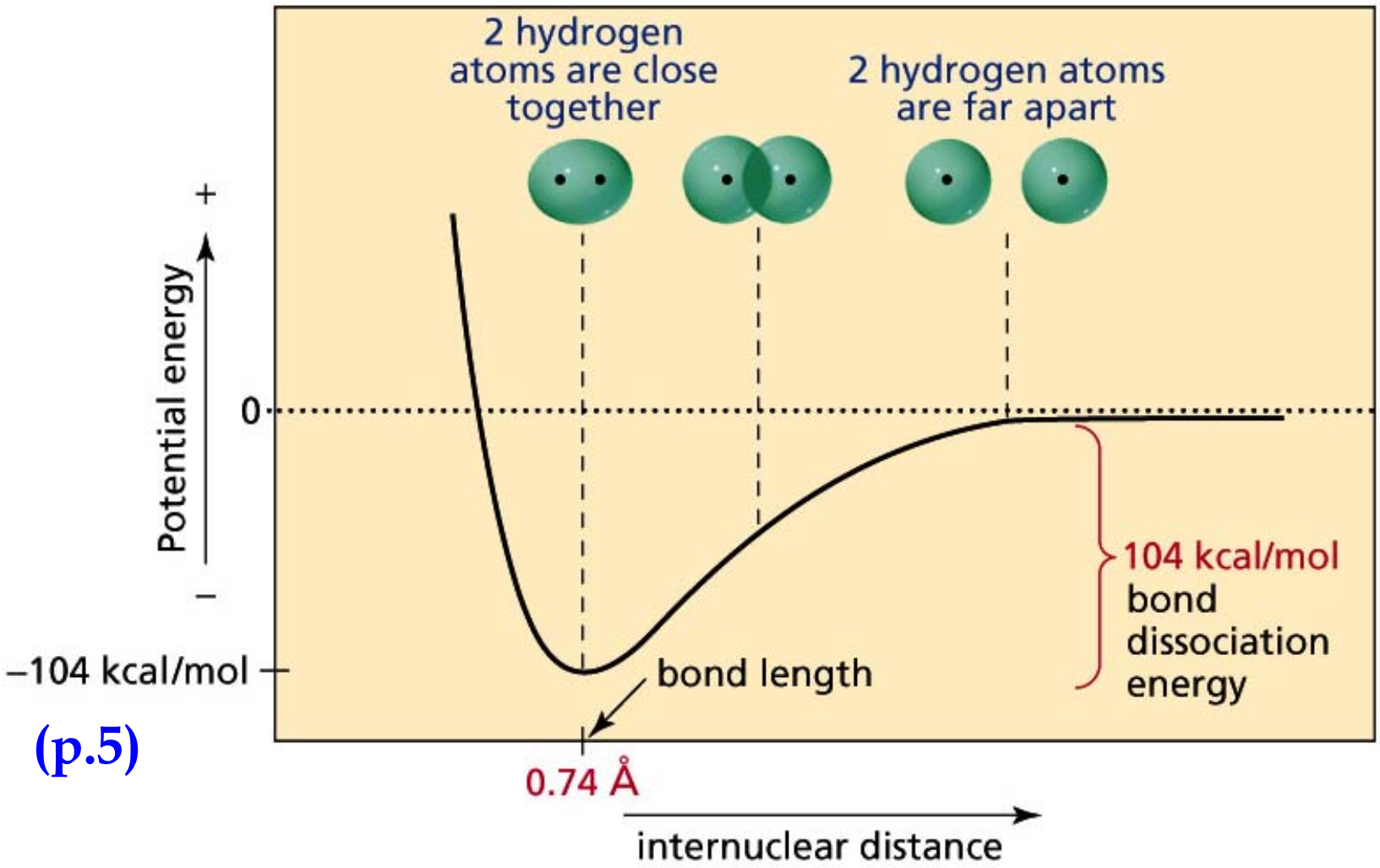
- Degenerate Orbitals are Orbitals of the same energy.
- Orbitals exist as mathematical constructs ALWAYS but only have meaning as we begin to fill with electrons.

Valence Bond Theory

- A bond occurs when atomic orbitals overlap. Overlapping orbitals are like overlapping waves.



- Only constructive interference results in a bond.



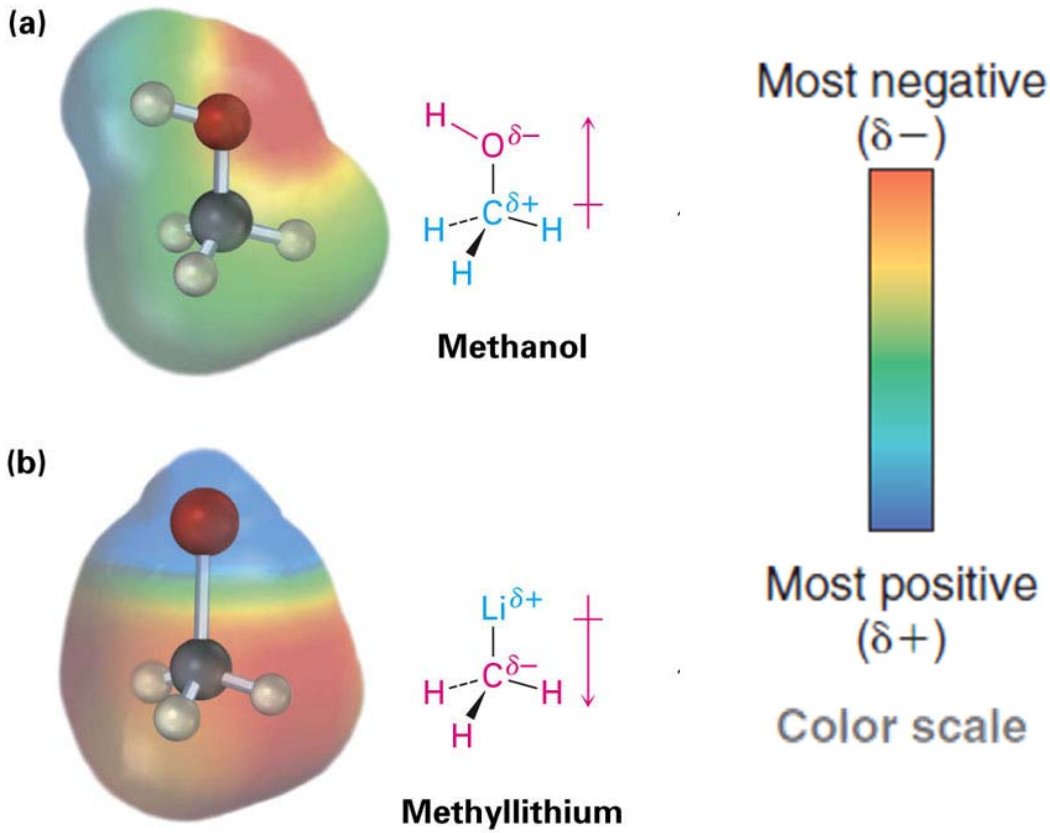
(p.5)

Organic compounds have **covalent bonds** from sharing electrons (G. N. Lewis, 1916)

Product has 436 kJ/mol less energy than two atoms: H–H has **bond strength** of 436 kJ/mol or 104 kcal/mol

Electrostatic Potential Maps

- **Electrostatic potential maps** show calculated charge distributions
- Colors indicate electron rich (red) and electron-poor (blue) regions
- Used to give a visual depiction of polarity.
- Arrows indicate direction of bond polarity (p.12)



For Next Time….

- Friday Sections 1.8 – 1.11
  - Monday Chapter 2 (2.1-2.7)
  - Wednesday Chapter 2 (2.8-2.11)

- Homework Practice Problems Chapter 1
  #8,12,15,37,39,43,45,48,49,53,56

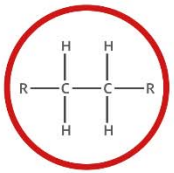
- If you will be needing Accommodations – please contact me as soon as possible.

Four semesters of organic chemistry made a pilot out of me. ~**Rick Perry**

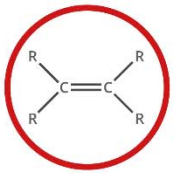
FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE BELOW, 'R' REPRESENTS A HYDROCARBON GROUP OR HYDROGEN, AND 'X' REPRESENTS ANY HALOGEN ATOM.

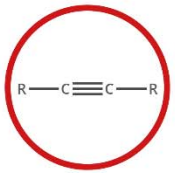
HYDROCARBONS · SIMPLE OXYGEN HETEROATOMICS · HALOGEN HETEROATOMICS · CARBONYL COMPOUNDS · NITROGEN BASED · SULFUR BASED · AROMATIC



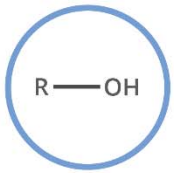
ALKANE
Naming: -ane
e.g. ethane



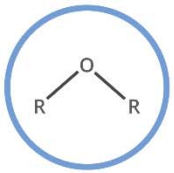
ALKENE
Naming: -ene
e.g. ethene



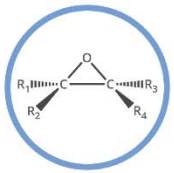
ALKYNE
Naming: -yne
e.g. ethyne



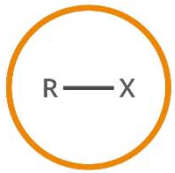
ALCOHOL
Naming: -ol
e.g. ethanol



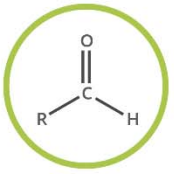
ETHER
Naming: -oxy -ane
e.g. methoxyethane



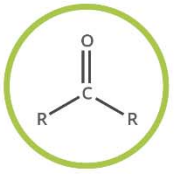
EPOXIDE
Naming: -ene oxide
e.g. ethene oxide



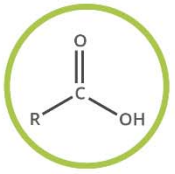
HALOALKANE
Naming: halo-
e.g. chloroethane



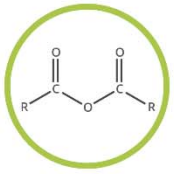
ALDEHYDE
Naming: -al
e.g. ethanal



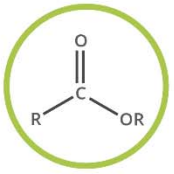
KETONE
Naming: -one
e.g. propanone



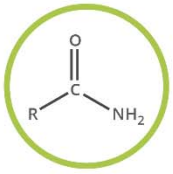
CARBOXYLIC ACID
Naming: -oic acid
e.g. ethanoic acid



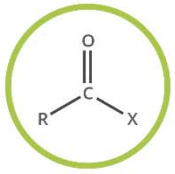
ACID ANHYDRIDE
Naming: -oic anhydride
e.g. ethanoic anhydride



ESTER
Naming: -yl -oate
e.g. ethyl ethanoate



AMIDE
Naming: -amide
e.g. ethanamide

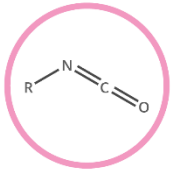


ACYL HALIDE
Naming: -oyl halide
e.g. ethanoyl chloride

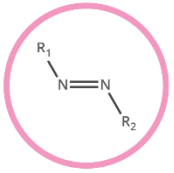
AMINE
Naming: -amine
e.g. ethanamine

NITRILE
Naming: -nitrile
e.g. ethanenitrile

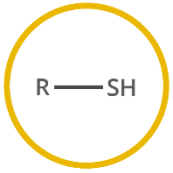
IMINE
Naming: -imine
e.g. ethanimine



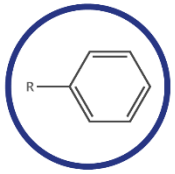
ISOCYANATE
Naming: -yl isocyanate
e.g. ethyl isocyanate



AZO COMPOUND
Naming: azo-
e.g. azoethane



THIOL
Naming: -thiol
e.g. methanethiol



ARENE
Naming: -yl benzene
e.g. ethyl benzene