

## Chapter 1 - Structure and Bonding

### Atomic Structure

Electrons reside around the nucleus in discrete energy levels. These energy shells contain orbitals - a mathematical probability that an electron will exist in that space. Orbitals are described by quantum mechanics in distinct shapes. S orbitals are spherical and p orbitals are shaped like dumbbells. In this course, we will not need to deal with d and f orbitals.

Electron configurations describe how an atom fills its shells and orbitals with electrons. Remember the principles from general chemistry:

**Aufbau Principle** - the lowest energy orbital fills up first

**Pauli Exclusion Principle** - only two electrons can occupy an orbital and they must be of opposite spin

**Hund's Rule** - if two or more orbitals of equal energy are available they are filled with one electron of parallel spin until all are half filled. Only then will electrons be paired up. This is important in filling the three p orbitals

Valence electrons are those in the outermost energy shell of an atom.

### Bonding and Structure

The number of valence electrons determines the number of bonds an atom will make. The atom will try to fill its valence shell (octet rule).

**Ionic Bonds** - Atoms held together by electrostatic attraction (ions).

**Covalent Bonds** - Atoms share electrons between them - much stronger than ionic bonds.

**Ionization Energy** - The energy required to remove an electron from an isolated atom. Ionization energy generally increases (harder to remove electron) as you move to the right and up on the periodic table.

**Electron Affinity** - The tendency of an isolated atom to gain an electron. Electron affinity generally increases as you move to the right and up on the periodic table.

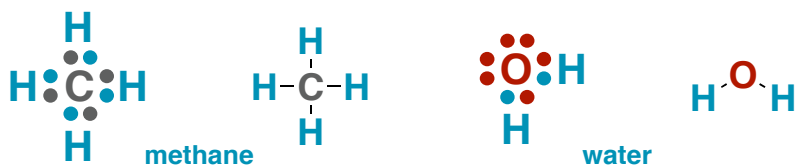
Na ( $1s^2 2s^2 2p^6 3s^1$ ) will easily give up an electron to achieve a filled energy shell.  $\text{Na}^+$  ( $1s^2 2s^2 2p^6$ ). F ( $1s^2 2s^2 2p^5$ ) will easily gain an electron to achieve a filled state,  $\text{F}^-$  ( $1s^2 2s^2 2p^6$ ). NaF will be an ionic compound.

Carbon ( $1s^2 2s^2 2p^2$ ) would have to gain or lose 4 electrons to achieve a filled shell and is therefore not easily ionized. Carbon forms covalent bonds rather than ionic bonds.

**Molecule** - a collection of atoms held together by covalent bonds.

**Lewis Structures** - represent the valence electrons around the atom by dots. Covalent bonds are shown with the two electron 'dots' shared between the atoms.

**Kekulé Structures** - Each covalent bond is represented by a single line indicating two shared electrons. Unshared (lone pairs) may or may not be shown.



**Valence Bond Theory** - Covalent bonds are formed by the overlap of atomic orbitals. Each atom maintains its atomic orbital, but shares the pair of electrons. The greater the overlap, the stronger the bond. When two orbitals overlap in a head to head fashion, this is called a sigma ( $\sigma$ ) bond.

**Bond Strength** - The energy required to pull two atoms apart (homolytically).

**Bond length** - the optimal distance between two atoms for the maximum overlap without the nuclear repulsion.

## Hybridization

The electronic configuration of carbon ( $1s^2 2s^2 2p^2$ ) would suggest that carbon could only make two or three bonds. We know that carbon forms four bonds to satisfy its octet in the second energy level and the structure is symmetrical with a tetrahedral arrangement of atoms bonded to it. In order to adopt this optimal bonding and geometry, carbon will “hybridize” and change its orbital configuration. The single s orbital and three p orbitals combine together (mathematically) to form four equal hybrid orbitals that we call  $sp^3$  orbitals. Thus, methane has a tetrahedral shape with  $109.5^\circ$  bond angles at each H-C-H angle. These are sigma ( $\sigma$ ) bonds.

