Chemical Bonding

Why Do Atoms Stick Together?

Valence Electrons and Chemical Bonds

- Valence electrons are the electrons in the outermost occupied shell of an atom

<u>Examples</u>

Hydrogen: $1s^1$	1 valence electron
Helium: $1s^2$	1 valence electrons
Carbon: $1s^2\,2s^2\,2p^2$	4 valance electrons
Sulfur: [Ne] $3s^2\,3p^4$	6 valence electrons

Valence Electrons and Chemical Bonds

<u>Examples</u>

Hydrogen: $1s^1$	H·
Helium: $1s^2$	He:
Carbon: $1s^2\ 2s^2\ 2p^2$	·Ċ· (with one dot below)
Sulfur: [Ne] $3s^2\ 3p^4$	:Ṡ: (with one dot below)

Valence Electrons and Chemical Bonds

- Atoms usually want to have a filled valence shell
- They will give away, steal, or share electrons with other atoms in order to fill their valance shell
- When atoms do this, chemical bonds form as a result

Valence Electrons and Chemical Bonds

- The Noble gases (He, Ne, Ar, Kr, Xe, and Rn) have filled valence shell, so they do not need to share electrons with other atoms in order to be happy
- The Noble gases are unreactive—they don't form chemical bonds with other atoms

Types of Chemical Bonds

- Ionic Bonds—result when electrons are exchanged between atoms forming ions
  - An ion is a chemical species with an electrical charge, either positive or negative
  - The electrostatic attraction holds the ions together

Types of Chemical Bonds

- Ionic Bonds

<u>Examples</u>

Chlorine: [Ne] $3s^2\ 3p^5$:Ċ̤l:

Cl has 7 valence electrons—it wants 8

Cl often “steals” an electron from another atom in order to fill its valence shell

Cl now will have 17 protons and 18 electrons resulting in a negatively charged ion, Cl^- ([Ne] $3s^2\ 3p^6$)

Types of Chemical Bonds

- Ionic Bonds

<u>Examples</u>

Sodium: [Ne] $3s^1$ Na·

Na has 1 valence electron—it wants 8 in its outer shell

Na is willing to give away an electron in order to have a filled valence shell

Na now will have 11 protons and 10 electrons resulting in a positively charged ion, Na^+ ([He] $2s^2\ 2p^6$)

Types of Chemical Bonds

- Ionic Bonds

Examples

The Na^+ ion is attracted to the Cl^- ion to form the ionic compound:

NaCl (table salt)

Types of Chemical Bonds

- Covalent Bonds—result when electrons are shared between atoms to form a bond

The Octet Rule

- Atoms want to have a filled valence shell—for the main group elements, this means having filled s and p orbitals. Hence the name "octet rule" because when the valence shell is filled, they have a total of eight valence electrons.
- We use "dot structures" to represent atoms and their electrons.

Lewis Dot Structures

- Dots around the elemental symbol represent the valence electrons.

Examples

Hydrogen ($1s^1$)	H·
Carbon ($1s^2$ $2s^2$ $2p^2$)	·Ċ· (with one dot above and one below)
Chlorine ([Ne] $3s^2$ $3p^5$)	:C̈l· (with two dots above and two below)

Lewis Dot Structures

- None of the atoms in the previous example contained full valence shells.
- When creating bonds, atoms may share electrons in order to complete their valence shells.

Lewis Dot Structures

Examples

H_2 molecule:

H needs two e^-'s to fill its valence shell. Each hydrogen atom shares its electron with the other in order to fill their valence shells.

H· + ·H ⇒ H:H

Lewis Dot Structures

Examples

H_2 molecule: H:H

The result is a "covalent bond" in which two electrons are shared between nuclei and create a chemical bond in the process.

When two e-'s are shared, it makes a "single" bond.

Lewis Dot Structures

Examples

F_2 molecule:

F has seven valence e^-'s, but wants eight e^-'s to fill its valence shell.

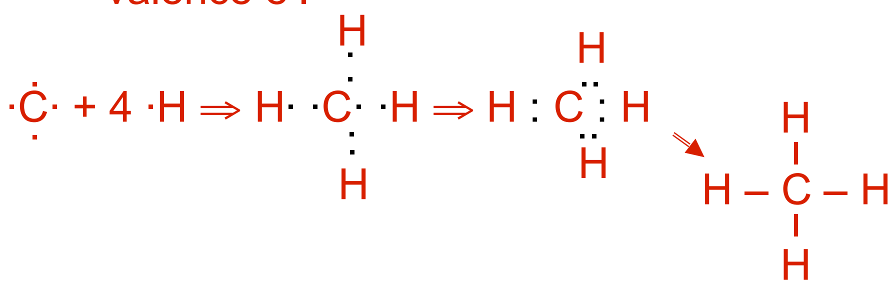
A line is often used to represent shared electrons.

Lewis Dot Structures

Examples

CH_4 molecule:

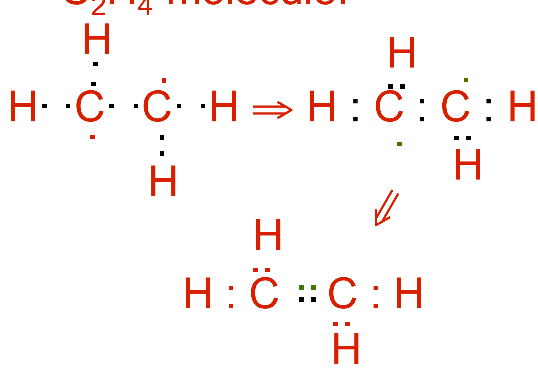
C has four valence e^-'s; H has one valence e^-.



Lewis Dot Structures

Examples

C_2H_4 molecule:

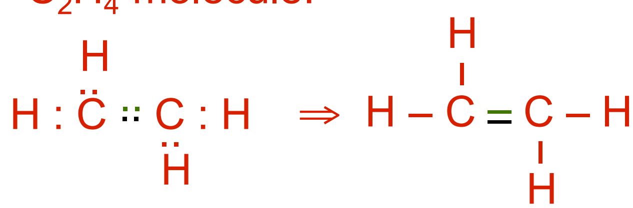


Is this complete—do all atoms have filled valence shells?

Lewis Dot Structures

Examples

C_2H_4 molecule:

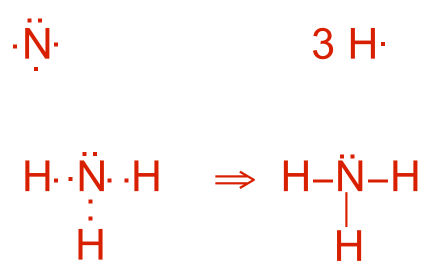


Sharing of four electrons between two nuclei results in a “double” bond.

Lewis Dot Structures

Examples

NH_3 molecule:

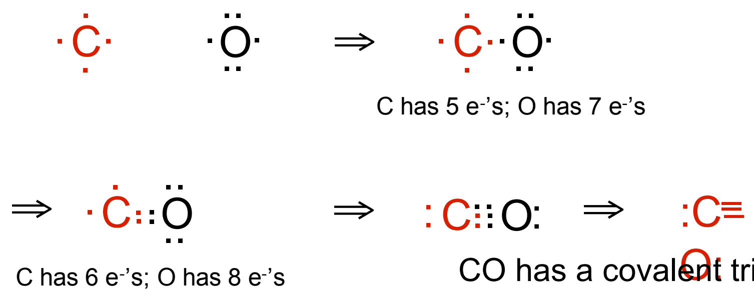


Not all electrons in a Lewis dot structure need to be part of a chemical bond—some electrons may be in the form of “lone pairs”

Lewis Dot Structures

Examples

CO molecule:



CO has a covalent triple bond—6 e^-'s are shared to form the bond

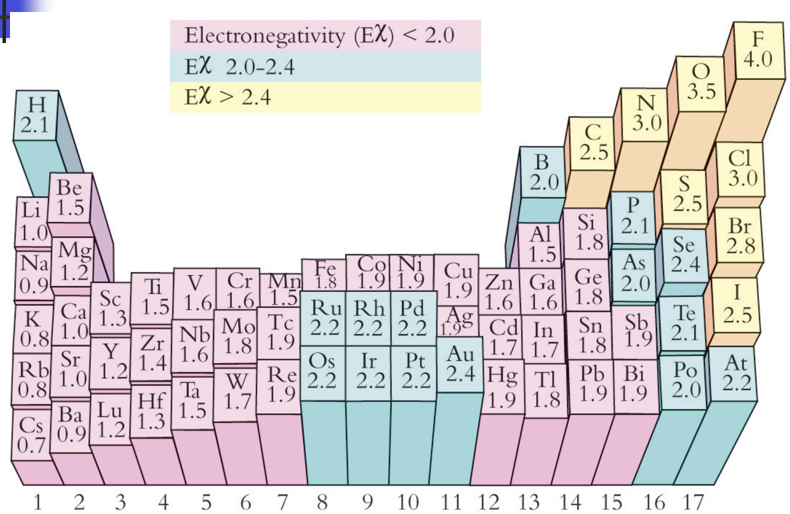
Electronegativity and Bonding

- When nuclei share electrons to form a covalent chemical bond, the electrons are not necessarily shared equally—a shared electron may spend more time closer to one of the nuclei.
- The *electronegativity* of the nuclei determines how the electron is shared.
- Electronegativity is a measure of how strongly a "bound" electron participating in a chemical bond is attracted to a nucleus.

Electronegativity and Bonding

- Electronegativity is related to electron affinity and ionization energy.
- Electronegativity (denoted by the greek symbol χ) is highest for elements in the upper right hand side of the Periodic Table and increases from left to right and from bottom to top.

Electronegativity and Bonding



Polar Covalent Bonds

- When two elements with different electronegativities bond, the resulting covalent bond will be *polar*, *i.e.*, the shared electrons will spend more time closer to the nucleus with the higher χ, so that end of the bond will be slightly more negative, and the other end will be slightly more positive.

$$\overset{\delta+}{H} - \overset{\delta-}{F}$$

χ=2.1 χ=4.0

Polar Covalent Bonds

- The molecule has a polar bond meaning the electrical charge is not equally distributed between the nuclei involved in the chemical bond. The molecule also has a *dipole moment*—an uneven distribution of electrical charge.

$$\overset{\delta+}{H} - \overset{\delta-}{F}$$

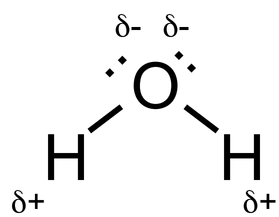
χ=2.1 χ=4.0

Polar Covalent Bonds

Other Examples

Water: H_2O is a bent molecule with two pairs of unshared e^-'s in p orbitals.

Is water a polar molecule?



$\chi(O) = 3.5$

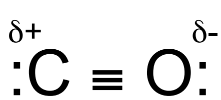
$\chi(H) = 2.1$

Polar Covalent Bonds

Examples

Carbon monoxide: CO

Is CO a polar molecule?



$\chi(O) = 3.5$

$\chi(C) = 2.5$

Polar Covalent Bonds

<u>Examples</u>

Carbon dioxide: CO_2 is a linear triatomic molecule.

Is CO_2 a polar molecule?

$$\overset{\delta-}{\ddot{\underset{..}{O}}} = \overset{\delta+}{C} = \underset{\delta-}{\ddot{\underset{..}{O}}}$$

$\chi(O) = 3.5$

$\chi(C) = 2.5$

Bond Lengths

- The bonding between atoms can have a significant effect on the bond distance between atoms.
- Multiple bonds between two atoms have shorter bond lengths compared to single bonds involving the same elements:

Bond Lengths

Examples

	average bond lengths			
single bond	C-C	154 pm	C-O	143 pm
double bond	C=C	133 pm	C=O	120 pm
triple bond	C≡C	120 pm	C≡O	113 pm

Bond Energies

- The bond energy is the amount of energy it takes to pull two atoms apart and break the chemical bond.
- For some diatomic gas phase species, we know the bond energies exactly through measurement.

Bond Energies

- For polyatomic molecules, we can calculate the average bond energy for a given type of bond by measuring bond energies in a wide variety of molecules containing that specific type of bond and averaging the results.
- Just as in bond lengths, the type of bonding has a dramatic effect on the bond energy in molecules.
- Multiple bonds are much harder to break than are single bonds.

Bond Energies

Examples

	Average bond energy (kJ mol^{-1})		
	single bond	double bond	triple bond
C-H	416		
C-C	356	598	813
C-O	336	750	1073
C-N	285	616	866
N-N	160	418	946
N-O	201	605	
C-S	272	575	

Bond Energies

Example: Calculate the reaction enthalpy for the combustion of methane

Step 1—Write balanced chemical equation:

$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$

Step 2—Determine energy needed to break bonds:

4 C-H bonds: 4 x 416 kJ/mol	= 1664 kJ/mol
2 O=O bonds: 2 x 498 kJ/mol	= 996 kJ/mol
total energy to break bonds	= 2660 kJ/mol

Bond Energies

Example: Calculate the reaction enthalpy for the combustion of methane

Step 3—Determine energy released in forming new bonds:

2 C=O bonds: 2 x -750 kJ/mol	= -1500 kJ/mol
4 O-H bonds: 4 x -467 kJ/mol	= -1868 kJ/mol
total energy to form bonds	= -3368 kJ/mol

Step 4—Determine enthalpy of reaction:

$\Delta H_{rxn} = E_{break\ bonds} + E_{form\ bonds}$

$= 2660$ kJ/mol – 3368 kJ/mol = -708 kJ/mol

$\Delta H_{rxn} = -802$ kJ/mol (literature value)