Chemical Bonding -- Lewis Theory **(Chapter 9)**

Ionic Bonding

1. Ionic Bond

Electrostatic attraction of positive (cation) and negative (anion) ions

$$\text{Neutral Atoms} \xrightarrow[\text{(IE and EA)}]{e^- \text{ transfer}} \text{cation} + \text{anion}$$

$$\text{cation} + \text{anion} \xrightarrow{\text{(Lattice Energy)}} \text{Ionic Compound}$$

Lattice Energy: energy released when gaseous ions combine to form crystalline solid (an ionic compound)

e.g., LE of NaCl is 787 kJ/mole:

$$Na^+{}_{(g)} + Cl^-{}_{(g)} \longrightarrow NaCl_{(s)} + 787\ \text{kJ}$$

2. Octet Rule

In forming ionic compounds, atoms tend to gain or lose electrons in order to achieve a stable valence shell electron configuration of 8 electrons.

Group I metals	$\longrightarrow$	+1 cations (Li^+, Na^+, etc.)
Group II metals	$\longrightarrow$	+2 cations (Mg^{2+}, ca^{2+}, etc.)
Al (group III)	$\longrightarrow$	Al^{3+}
Group VII (17)	$\longrightarrow$	-1 anions (F^-, Cl^-, Br^-, etc.)
Group VI (16)	$\longrightarrow$	-2 anions (O^{2-}, S^{2-}, etc.)
Group V (15)	$\longrightarrow$	-3 anions (N^{3-}, P^{3-})

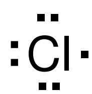
e.g., $Na\ \ 2s^2\,2p^6\,3s^1 \longrightarrow Na^+\ \ 2s^2\,2p^6$ {~ Ne}

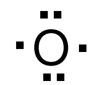
$Cl\ \ 3s^2\,3p^5 \longrightarrow Cl^-\ \ 3s^2\,3p^6$ {~ Ar}

3. Lewis Symbols

simple notation for showing number of valence electrons

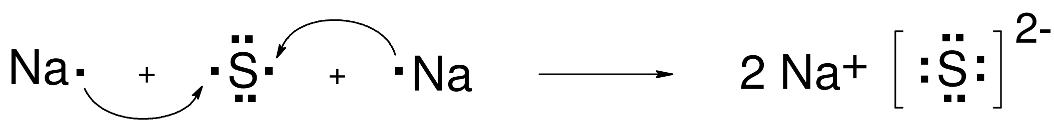
Cl	**O**
group VII (7 valence e^-)	group VI (6 valence e^-)
$3s^2\ 3p^5$	$2s^2\ 2p^4$





e.g., Use Lewis Symbols to illustrate the formation of a compound of sodium and sulfur

Na_2S Na^+ combined with S^{2-}

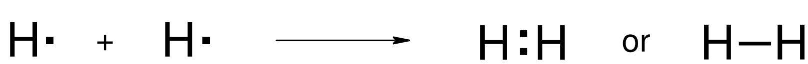


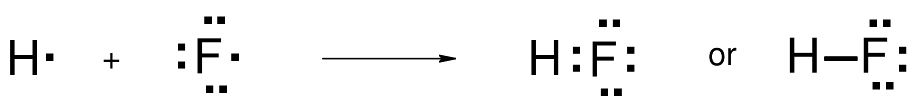
Covalent Bonding

1. Covalent Bond Formation

results from sharing of one or more pairs of electrons between 2 atoms

Examples:

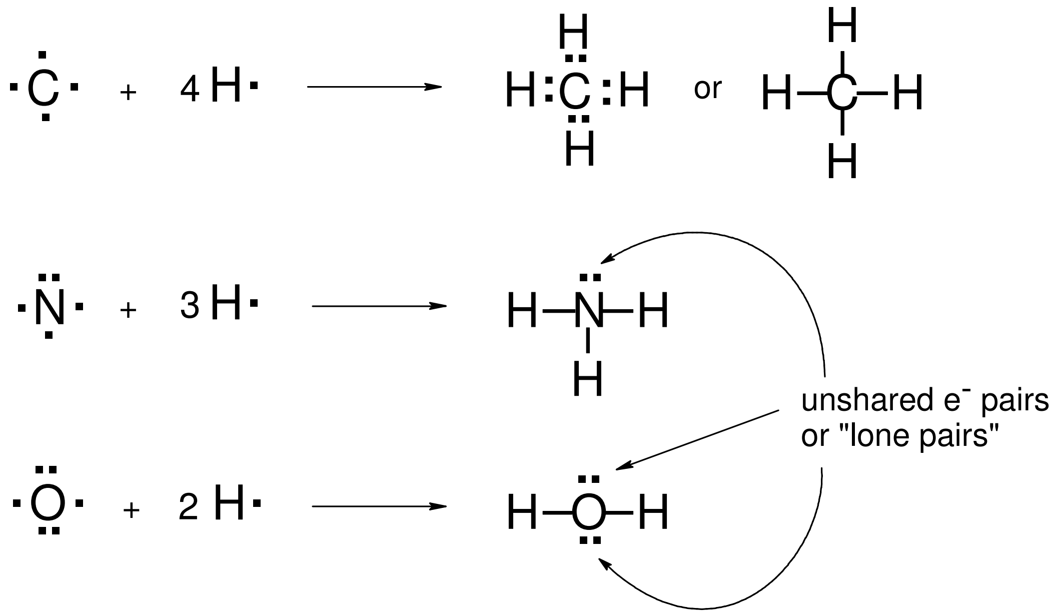




2. Octet Rule -- for covalent bonding

In forming covalent bonds, atoms tend to share sufficient electrons so as to achieve a stable outer shell of 8 electrons around both atoms in the bond.

Examples:



3. Multiple Bonds -- "double" and "triple" bonds

double bond: sharing of 2 pairs of electrons between two atoms
triple bond: sharing of 3 pairs of electrons between two atoms

Bond Energy / Bond Strength →

Type of Bond:	single	double	triple
Bond Order:	1	2	3

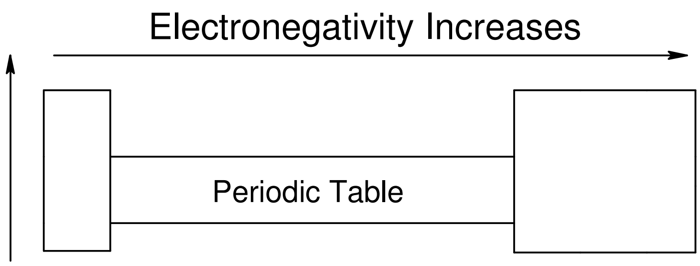
← Bond Distance

Examples:

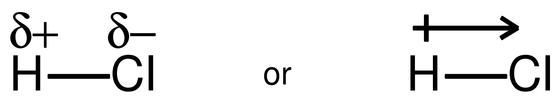
Examples:	O_2	{ O=O double bond }
	N_2	{ N≡N triple bond }
	CO_2	{ two C=O double bonds }

4. Electronegativity and Bond Polarity

electronegativity tendency of an atom *in a molecule* to attract electrons to itself



e.g., Cl is more electronegative than H, so there is partial charge separation in the H-Cl bond:



the H-Cl bond is described as "***polar***" and is said to have a "***dipole***"

the entire HCl molecule is also polar as a result

more complex molecules can be polar or nonpolar, depending on their 3-D shape (Later)

Lewis Electron Dot Formulas

1. **General Procedure** -- stepwise process

   - Write the skeletal structure (which atoms are bonded?)
   - Count ***all valence electrons*** (in pairs)
   - Place 2 electrons in each bond
   - Complete the octets of the terminal atoms
   - Put any remaining electron pairs on the central atom, or
   - Use multiple bonds if needed to complete the octet of the central atom
   - Show formal charges and resonance forms as needed

   Apply the **OCTET RULE** as follows:

   - H never has more than 2 electrons (i.e., one bond)
   - 2nd row elements (e.g., C, N, O) ***almost always*** have an octet and ***never have more than 8 electrons*** (sometimes Boron has only 6)
   - 3rd row and higher elements can have more than 8 electrons but ***only after the octets of any 2nd row elements are completed***

2. Formal Charge -- the "apparent" charge on an atom in a covalent bond

   = (# of valence e^- in the isolated atom) – (# of bonds to the atom)
   – (# of unshared electrons on the atom)

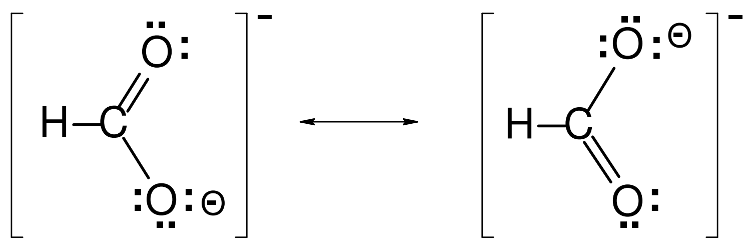
   { minimize formal charges whenever possible }

   Write Lewis Dot Formulas: NH_3 NH_4^+ SF_2 SF_4

3. Resonance

When multiple bonds are present, a single Lewis structure may not adequately describe the compound or ion -- occurs whenever there is a "choice" of where to put a multiple bond.

e.g., the HCO_2^- ion is a "***resonance hybrid***" of two "***contributing resonance structures***"



the C-O bond order is about 1.5 (average of single and double bonds)

Examples

Write Lewis Electron Dot Structures (including formal charges and/or resonance as needed) for the following compounds and ions.

PF_3 HCN SF_5^- NO_2^- $SOCl_2$ O_3

HNO_3 H_2CO N_3^-

Bond Energies and Heats of Reaction (ΔH)

Bond Energy is the energy required to break a chemical bond.

Tabulated values (Table 9.3) are ***average*** bond energies in units of kJ / mole.

Bond-breaking is endothermic, bond-making is exothermic.

ΔH for a reaction can be estimated from bond energies as follows. (Counting ALL bond energies as positive values!)

$$\Delta H° \approx \sum BE \text{ (bonds broken)} - \sum BE \text{ (bonds formed)}$$

Problem

Use data in Table 9.3 to estimate $\Delta H°$ for the reaction.

$$CH_2{=}CH_2 + H_2O \longrightarrow CH_3{-}CH_2{-}OH$$

Bonds Broken		Bonds Formed	
C=C	612	C-C	348
H-O	463	C-H	412
$\sum$ =	1,075	C-O	360
		$\sum$ =	1,120

$\therefore \Delta H° \approx 1{,}075 - 1{,}120 \approx -45$ kJ/mole

This estimate compares well with the value calculated from Standard Heats of Formation (Chapter 6).

Use tabulated $\Delta H°_f$ values from textbook:

$$\Delta H° = \sum \Delta H°_f \text{ (products)} - \sum \Delta H°_f \text{ (reactants)}$$

$$\Delta H° = (-278) - [(+51.9) + (-285.9)] = -43 \text{ kJ/mole}$$