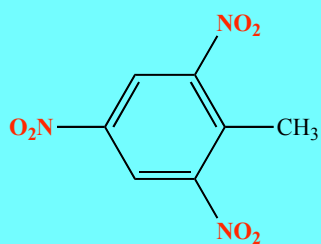


## Bonding and Structure of Organic Molecules



## Molecular Structure

What is molecular structure?

Why study molecular structure?

- Physical properties:  $\text{H}_2\text{O}$  bp  $100^\circ\text{C}$  versus  $\text{CH}_3\text{OH}$  bp  $65^\circ\text{C}$
- Chemical properties:  $\text{H}_2\text{SO}_4$  (strong acid) versus  $\text{H}_2\text{O}$  (weak acid)
- Biological properties: Enzyme specificity; DNA replication
  
- *Review general chemistry topics as needed*

## Covalent Bonding

Electron count on atoms controls... Covalent bonds  $\longrightarrow$  Sigma bonds ( $\sigma$ )  
 Lone pairs Pi bonds ( $\pi$ )  
 Formal charges

**Covalent bond:** Sharing of an electron pair via orbital overlap

**Orbital:** Mathematical description of a volume of space in which there is a certain probability of finding an electron of a certain energy

**Lone pair** (nonbonded pair): Pair of electrons assigned to just one atom

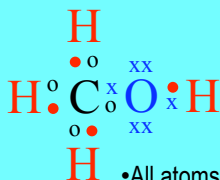
**Formal charge:** The charge on an atom in a Lewis structure if the bonding was perfectly covalent and the atom has exactly a half-share of the bonding electrons.

## Covalent Bonding

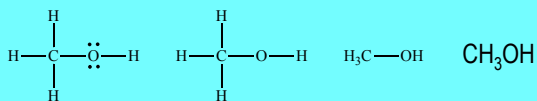
Example: Methyl alcohol  $\text{CH}_3\text{OH}$

Atom	Electron configuration	Valence shell electron count
H	$1s \uparrow$	$1 \xrightarrow{\text{Gain 1 electron}}$
C	$2s \uparrow\downarrow \quad 2p_x \uparrow \quad 2p_y \uparrow \quad 2p_z$	$4 \xrightarrow{\text{Gain 4 electrons}}$
O	$2s \uparrow\downarrow \quad 2p_x \uparrow\downarrow \quad 2p_y \uparrow \quad 2p_z \uparrow$	$6 \xrightarrow{\text{Gain 2 electrons}}$

Lewis structure



Alternate representations



- All atoms have full valence shells
- Oxygen has two lone pairs
- No atoms have formal charges *Formal charge tutorial on course web site*

## Electrons in Bonds

In covalent bond are electrons shared equally?

C : O versus C: O versus C :O

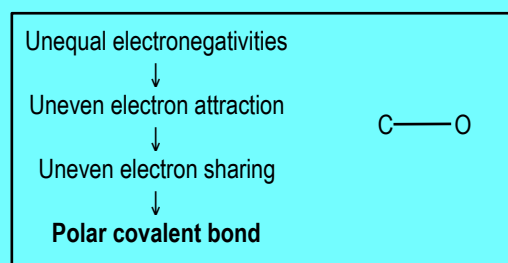
**Electronegativity:** An atom's ability to attract electrons to itself

•Higher EN value = stronger electron attraction

H 2.1			
C 2.5	N 3.0	O 3.5	F 4.0
	P 2.1	S 2.5	Cl 3.0
			Br 2.8
			I 2.5

Electronegativity Trends

•EN decreases with periodic table distance from F



## Polar Covalent Bonds

Bond polarity depends on...

•**EN:**  $\Delta EN$  causes in  $\delta^+$  and  $\delta^-$

$\Delta EN < 1.7$ : Bond is more covalent than ionic

$\Delta EN > 1.7$ : Bond is more ionic than covalent

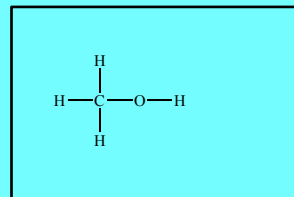
$\Delta EN$  0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2 2.4



Increasing polarity (increasing ionic character)

•**Bond length:** Longer bonds amplify  $\delta^+$  and  $\delta^-$

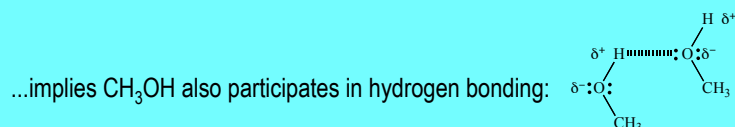
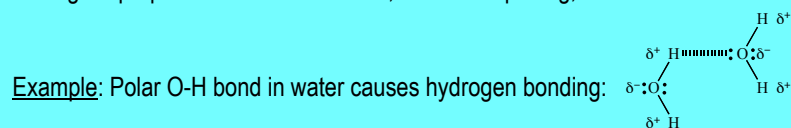
C-H ( $\Delta EN = 0.4$ ) less polar than S-H ( $\Delta EN = 0.4$ )



## Consequences of Polar Covalent Bonds

The effects of polar covalent bonds are widespread...

- Physical properties: Boiling point, solubility, etc.
- Chemical properties: Many reaction initiated by interaction of polar bonds
- Biological properties: Protein structure, DNA base pairing, etc.



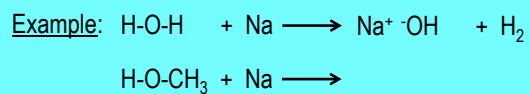
**Similar bonding arrangements cause similar properties**

## Functional Groups



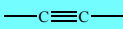

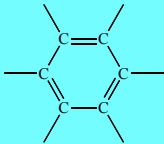
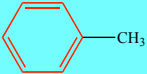
Similar bonding arrangements cause similar properties

**Functional group:** A group of atoms whose bonding is the same from molecule to molecule.


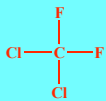
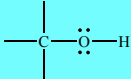
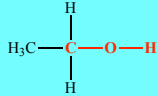
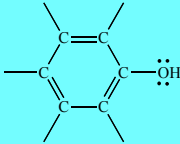
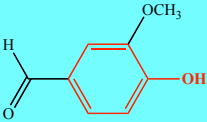
- Value:
- Predict molecular properties
  - Basis for nomenclature



## Functional Groups

Name	General Structure	Example
Alkene		Ethylene <i>Tomato ripening hormone</i>
		
<ul style="list-style-type: none"> <li>• Unspecified bonds can be anything</li> <li>• C-C and C-H bonds are not usually considered functional groups</li> </ul>		
Alkyne		Acetylene <i>Welding gas</i>
		
Benzene ring		Toluene <i>Solvent</i>
		
<ul style="list-style-type: none"> <li>• Larger functional groups are not said to contain smaller functional groups</li> </ul>		

## Functional Groups

Name	General Structure	Example
Alkyl halide Haloalkane	 X = F, Cl, Br, I	Dichlorodifluoromethane <i>Freon 12; a CFC</i>
		
Alcohol		Ethanol <i>Yeast fermentation product</i>
		
Phenol		Vanillin <i>Natural flavoring agent</i>
		
<ul style="list-style-type: none"> <li>• Functional groups in close proximity may interact</li> <li>• Molecules frequently contain multiple functional groups</li> </ul>		

## Functional Groups

Name	General Structure	Example
Ether		Ethyl ether (ether) Solvent; anesthetic 
Epoxide		Epichlorohydrin Epoxy resin component 
Thiol		3-Methyl-1-butanethiol Present in skunk musk 
Disulfide		Protein structural unit 

## Functional Groups

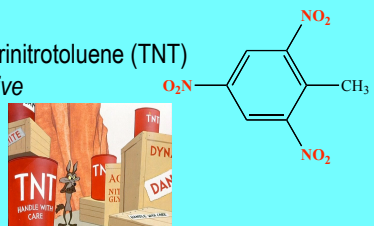
Name	General Structure	Example
Amine		Putrescine Present in rotting meat 
Ketone		Acetone Solvent 
•Carbonyl (C=O) not a functional group by itself		
Aldehyde		Benzaldehyde Artificial flavor 
Carboxylic acid (Carboxyl group)		Acetic acid Present in vinegar 

## Functional Groups

Name	General Structure	Example
Ester		Methyl methacrylate <i>Forms plexiglass</i>
Amide		Peptide bond <i>In proteins</i>
Acid chloride		Phosgene <i>Chemical weapon</i>
Acid anhydride		Acetic anhydride <i>Used in aspirin synthesis</i>

## Functional Groups

Name	General Structure	Example
Imine		Rhodopsin <i>Essential for vision</i>
Nitrile		Acetonitrile <i>Solvent</i>
Nitro		2,4,6-Trinitrotoluene (TNT) <i>Explosive</i>



## Functional Groups

What Should I Be Able to Do With Functional Groups?

- Identify in molecules
- Draw molecules containing specific functional groups
- Etc.