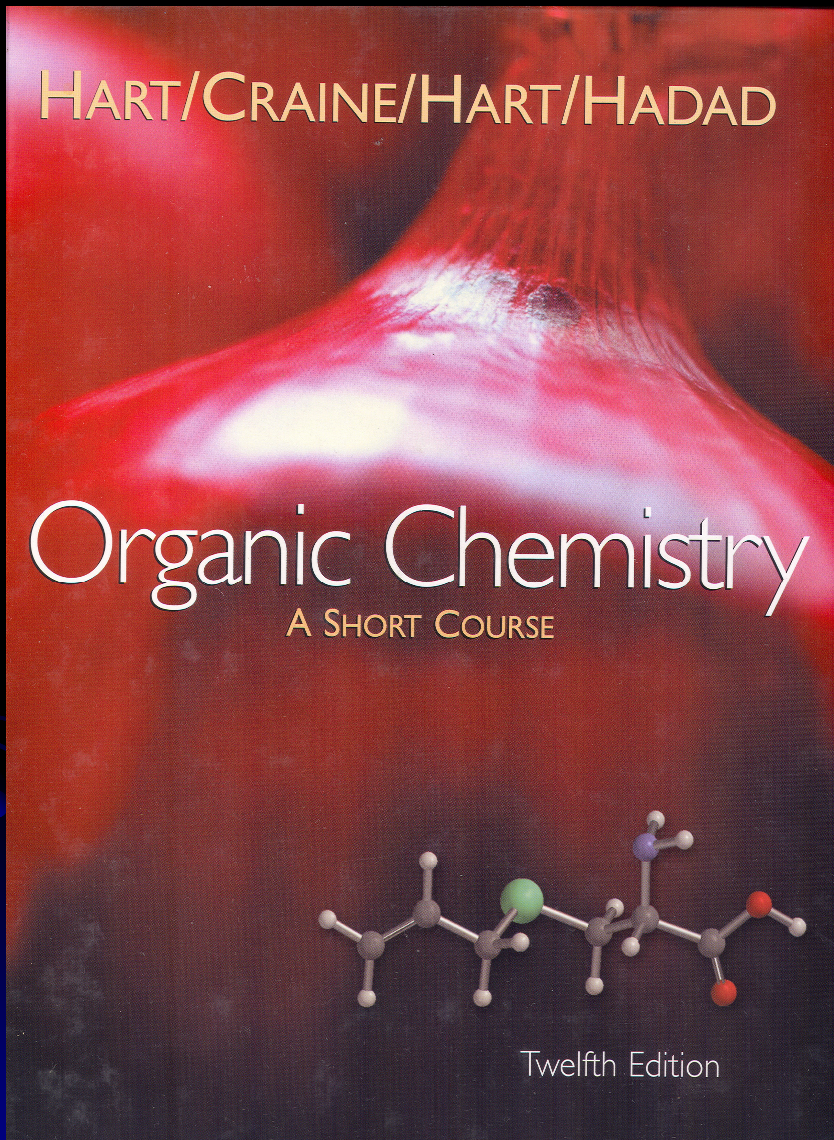

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Blackboard

$$\underset{\text{methyl butyrate}}{CH_3CH_2CH_2\overset{\overset{\large O}{\|}}{C}OCH_3} \qquad \underset{\text{propyl acetate}}{CH_3\overset{\overset{\large O}{\|}}{C}OCH_2CH_2CH_3}$$

Methyl butyrate and propyl acetate, organic flavor and fragrance molecules found in apples and pears, respectively, are structural isomers (Sec. 1.8).

1

Bonding and Isomerism

1.1 How Electrons are arranged in Atoms

Table 1.1 Numbers of orbitals and electrons in the first three shells

Table 1.1 **Numbers of orbitals and electrons in the first three shells**

Shell number	Number of orbitals of each type: *s*	*p*	*d*	Total number of electrons when shell is filled
1	1	0	0	2
2	1	3	0	8
3	1	3	5	18

Table 1.2 Electron arrangements of the first 18 elements

Table 1.2 **Electron arrangements of the first 18 elements**

Atomic number	Element	Number of electrons in each orbital				
		1s	*2s*	*2p*	*3s*	*3p*
1	H	1				
2	He	2				
3	Li	2	1			
4	Be	2	2			
5	B	2	2	1		
6	C	2	2	2		
7	N	2	2	3		
8	O	2	2	4		
9	F	2	2	5		
10	Ne	2	2	6		
11	Na	2	2	6	1	
12	Mg	2	2	6	2	
13	Al	2	2	6	2	1
14	Si	2	2	6	2	2
15	P	2	2	6	2	3
16	S	2	2	6	2	4
17	Cl	2	2	6	2	5
18	Ar	2	2	6	2	6

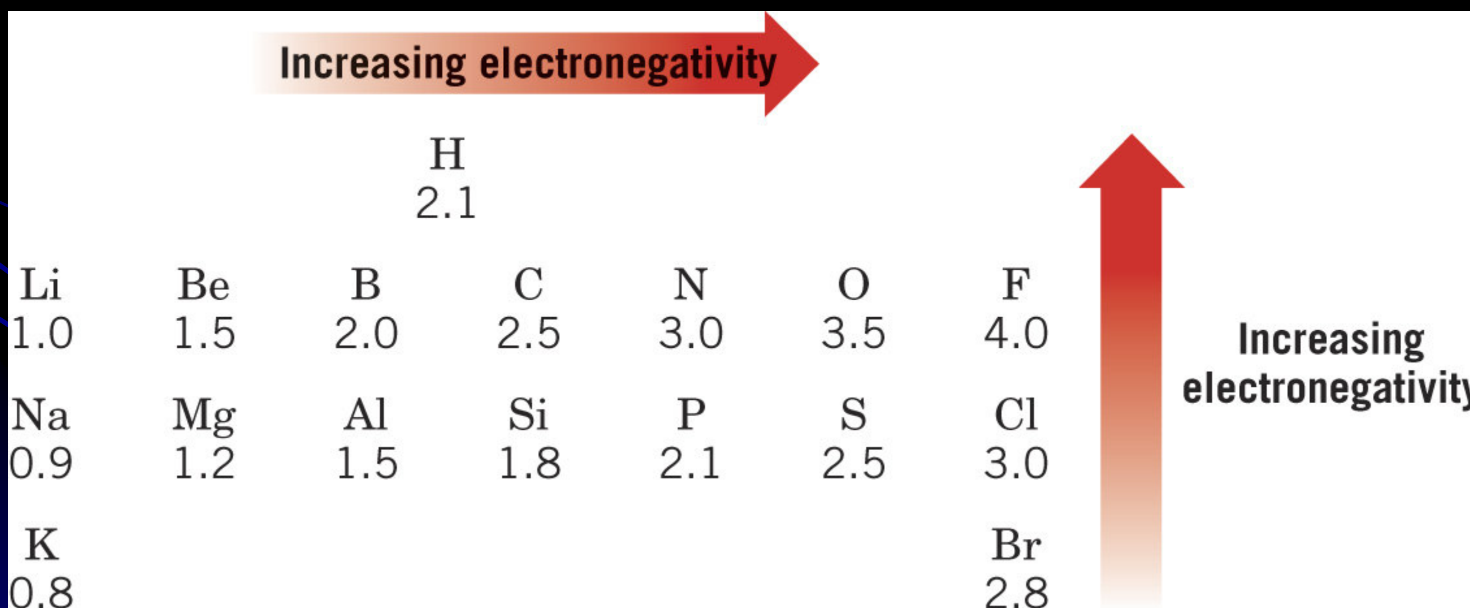
Table 1.3 Valence electrons of the first 18 elements

Table 1.3 Valence electrons of the first 18 elements

Group	I	II	III	IV	V	VI	VII	VIII
	H							He
	Li	Be	B	C	N	O	F	Ne
	Na	Mg	Al	Si	P	S	Cl	Ar

1.2 Ionic and Covalent Bonding

- Electronegativity
  - Electronegativity is the ability of an atom to attract electrons
  - It increases from left to right and from bottom to top in the periodic table (noble gases excluded)
    - Fluorine is the most electronegative atom and can stabilize excess electron density the best



- Ionic Bonds
  - When ionic bonds are formed atoms gain (electronegative) or lose electrons (electropositive) to achieve the electronic configuration of the nearest noble gas
    - In the process the atoms become ionic
  - The resulting oppositely charged ions (cations (+) & anions (-)) attract and form ionic bonds
  - This generally happens between atoms of widely different electronegativities
  - Example
    - Lithium loses an electron (to have the configuration of helium) and becomes positively charged
    - Fluoride gains an electron (to have the configuration of neon) and becomes negatively charged
    - The positively charged lithium and the negatively charged fluoride form a strong ionic bond (actually in a crystalline lattice)

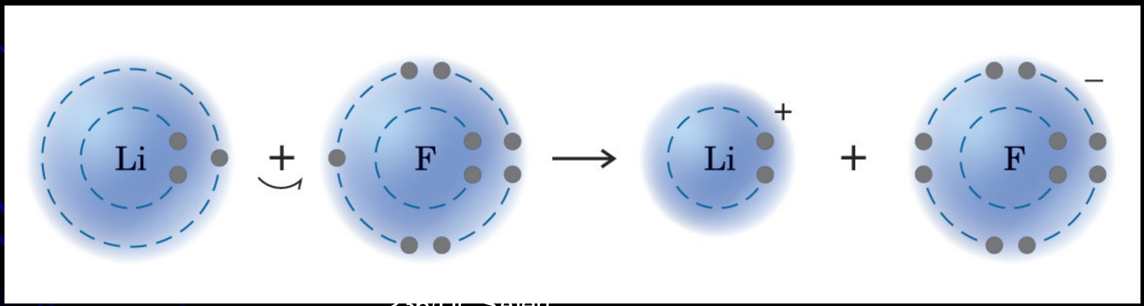
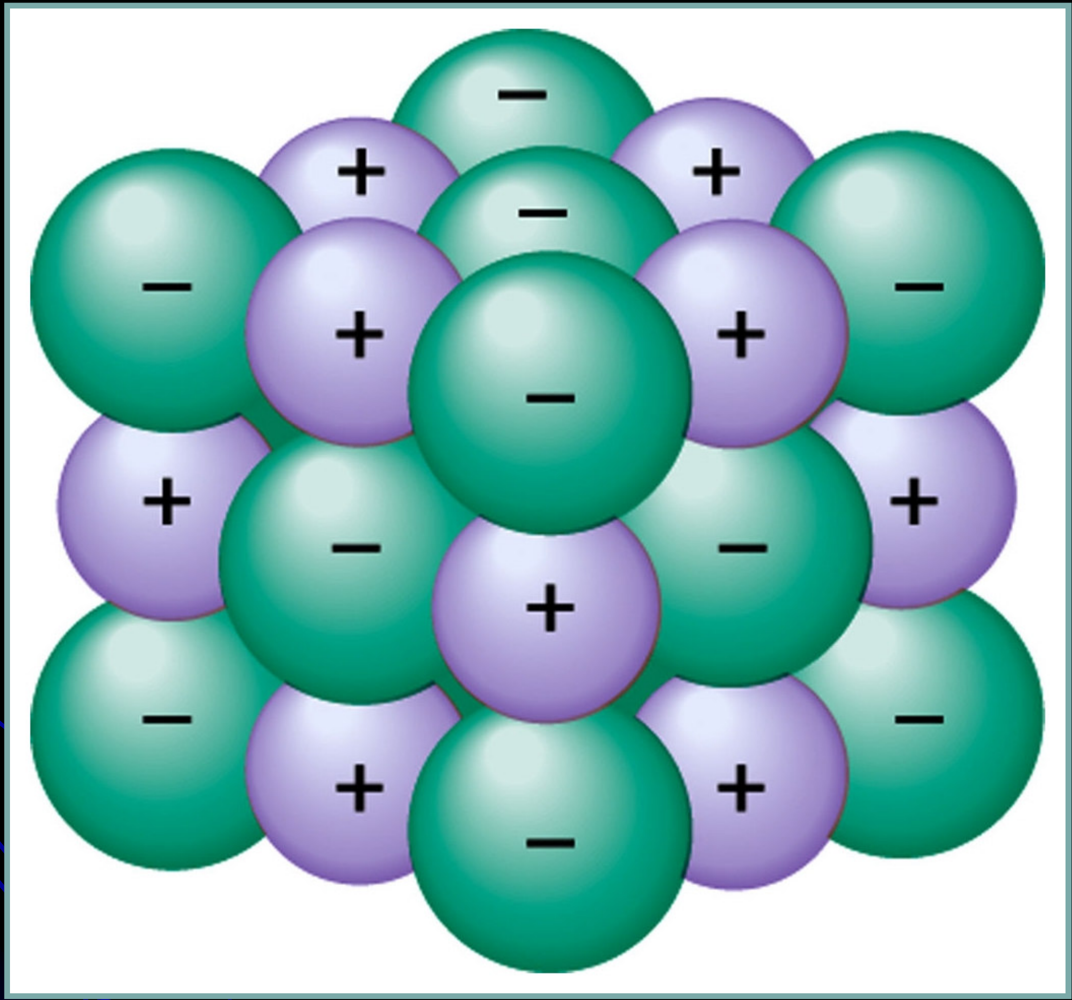
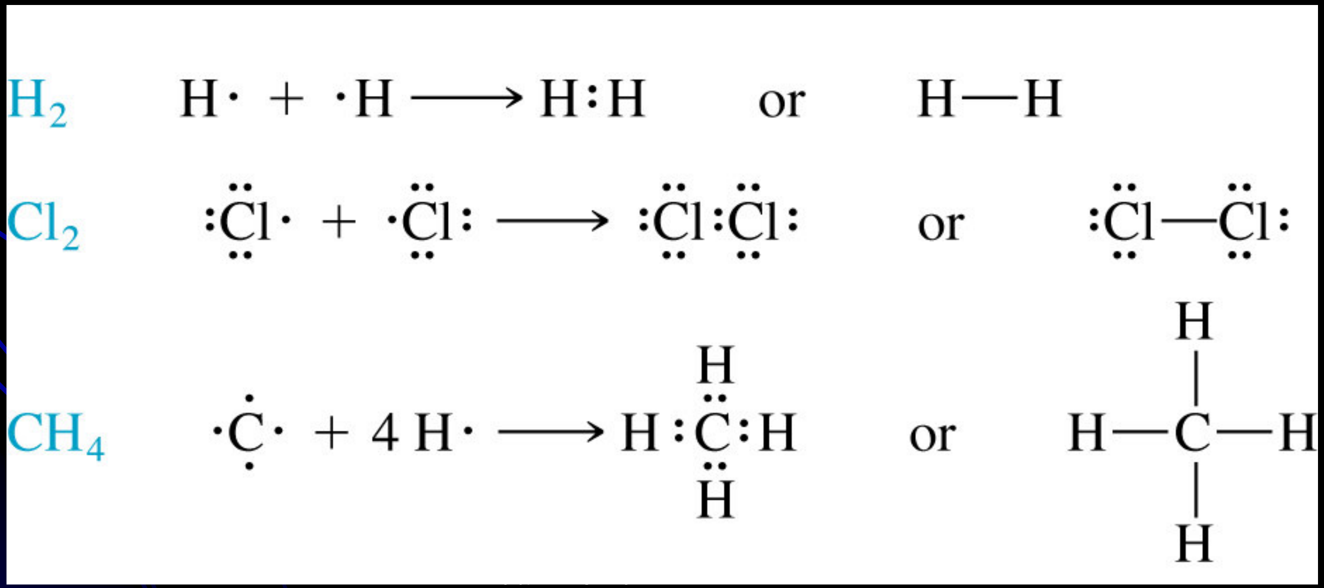


Figure 1.1 Sodium chloride is an ionic crystal

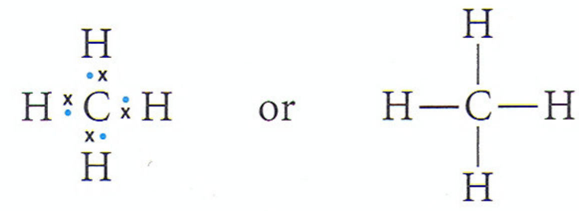


- Covalent Bonds
  - Covalent bonds occur between atoms of similar electronegativity (close to each other in the periodic table)
  - Atoms achieve octets by *sharing* of valence electrons
  - Molecules result from this covalent bonding
  - Valence electrons can be indicated by dots (electron-dot formula or Lewis structures) but this is time-consuming
  - The usual way to indicate the two electrons in a bond is to use a line (one line = two electrons)

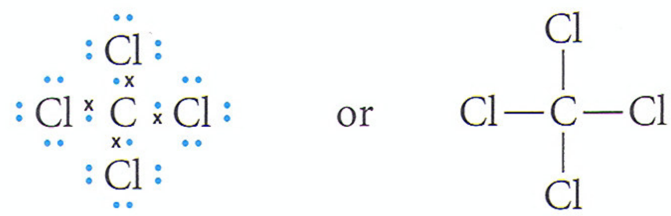


1.3 Carbon and the Covalent Bond

- Carbon is neither strongly electronegative nor strongly electropositive. Instead, it usually forms covalent bonds with other atoms by sharing electrons.



methane

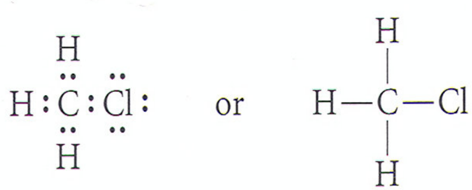


tetrachloromethane
(carbon tetrachloride)

EXAMPLE 1.5

Draw the structure for chloromethane (also called methyl chloride), CH_3Cl.

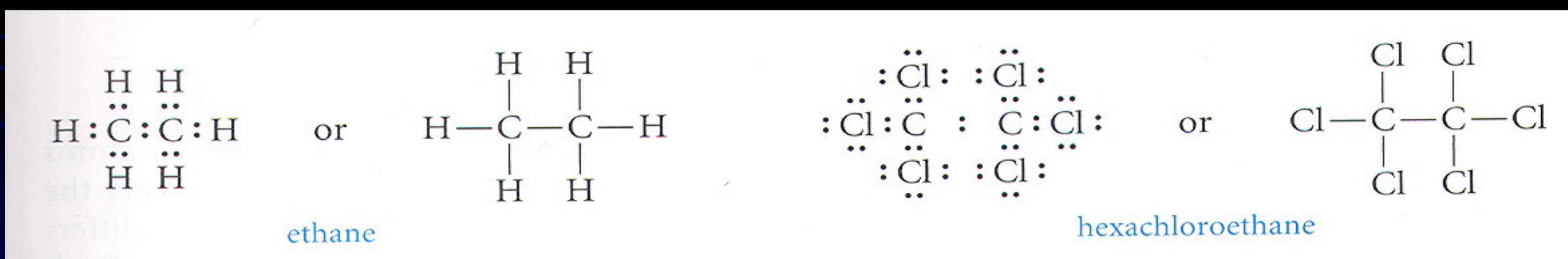
SOLUTION



PROBLEM 1.7 Draw the structures for dichloromethane (also called methylene chloride), CH_2Cl_2, and trichloromethane (chloroform), $CHCl_3$.

1.4 Carbon-Carbon Single Bonds

- Carbon atoms have the ability to share electrons not only with different elements but also with other carbon atoms. Carbon forms strong covalent bonds to other carbons and to other elements such as hydrogen, oxygen, nitrogen and sulfur.
- This property makes it possible for millions of organic compounds to exist (each with its unique chemical and physical properties). Only carbon has this ability.
- C-C chains could be very long. Branching and forming cyclic rings can also takes place. This accounts for the vast variety of organic compounds possible.
- Diversity and endless possibilities of carbon compounds makes it the element of life in all of its forms!



1.5 Polar Covalent Bonds

- Polar covalent bonds occur when a covalent bond is formed between two atoms of differing electronegativities
  - The more electronegative atom draws electron density closer to itself
  - The more electronegative atom develops a partial negative charge (δ-) and the less electronegative atom develops a partial positive charge (δ+)
  - A bond which is polarized is a dipole and has a dipole moment
  - The direction of the dipole can be indicated by a dipole arrow
    - The arrow head is the negative end of a dipole, the crossed end is the positive end

(positive end) $\longrightarrow$ (negative end)

Table 1.4 Electronegativities of some common elements

Table 1.4 **Electronegativities of some common elements**

Group

I	*II*	*III*	*IV*	*V*	*VI*	*VII*
H 2.2						
Li 1.0	Be 1.6	B 2.0	C 2.5	N 3.0	O 3.4	F 4.0
Na 0.9	Mg 1.3	Al 1.6	Si 1.9	P 2.2	S 2.6	Cl 3.2
K 0.8	Ca 1.0					Br 3.0
						I 2.7

< 1.0 1.5–1.9 2.5–2.9

1.0–1.4 2.0–2.4 3.0–4.0

Electronegativities of Common Elements

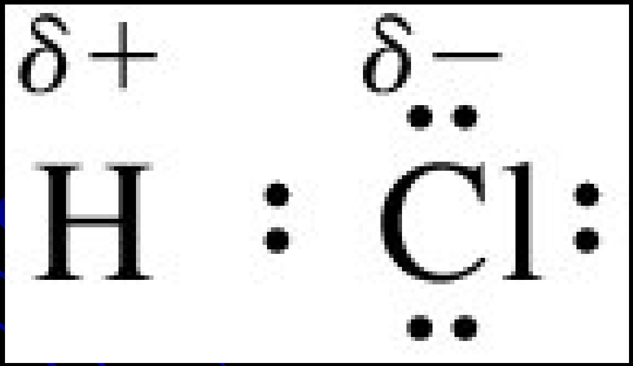
Increasing electronegativity

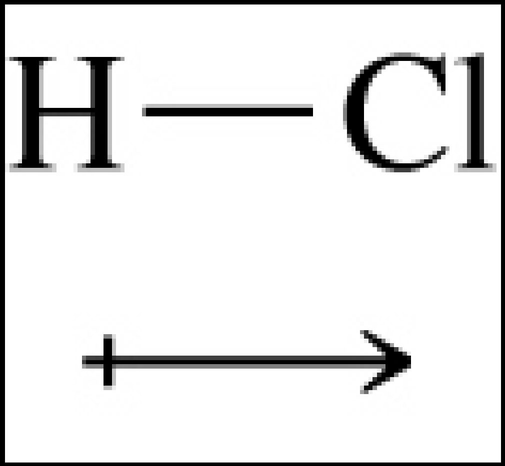
Increasing electronegativity

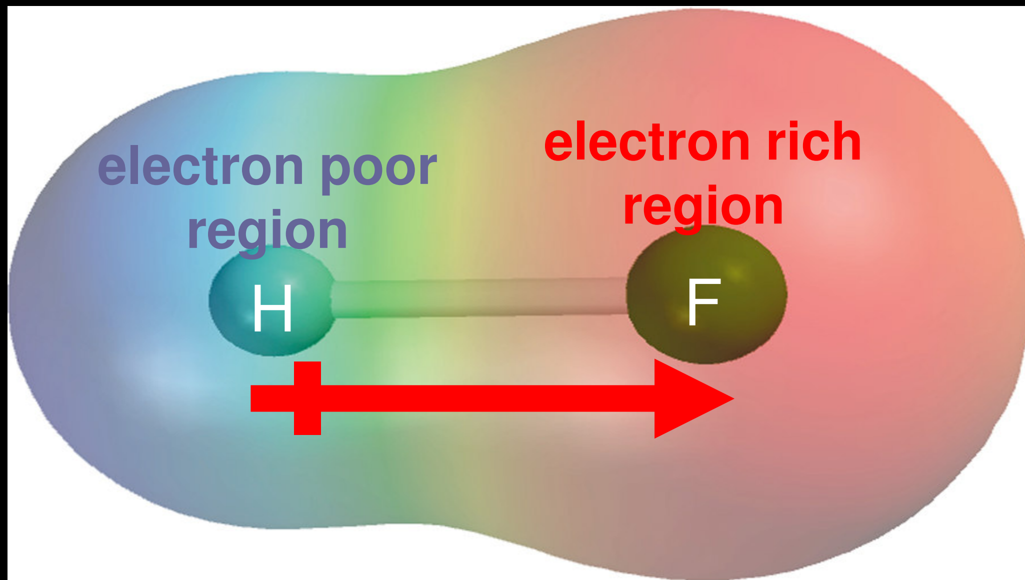
1A	2A	3B	4B	5B	6B	7B	8B	8B	8B	1B	2B	3A	4A	5A	6A	7A	8A
H 2.1																	
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.9	Ni 1.9	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	
Cs 0.7	Ba 0.9	La-Lu 1.0-1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.9	Bi 1.9	Po 2.0	At 2.2	
Fr 0.7	Ra 0.9																

Examples:

- the molecule HCl
  - The more electronegative chlorine draws electron density away from the hydrogen
    - Chlorine develops a partial negative charge





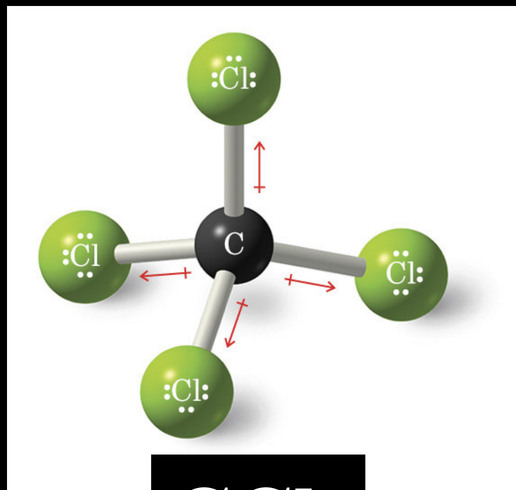


e^- poor e^- rich

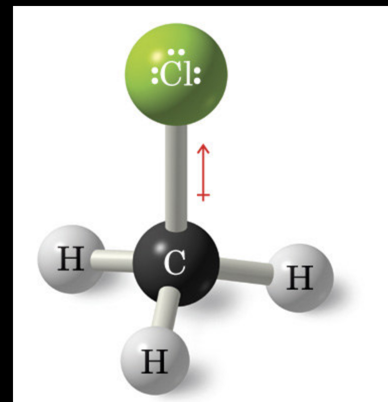
H—F:

δ^+ δ^-

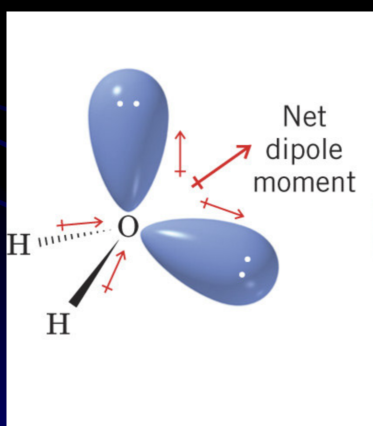
Dipole Moment



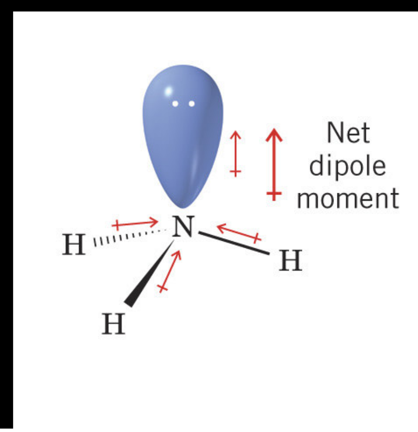
CCl_4



CH_3Cl



H_2O



NH_3

Water

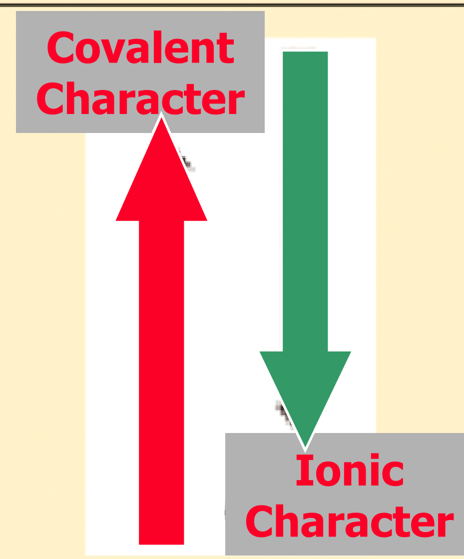
Ammonia

Covalent or Ionic?

- Covalent and ionic are simply extreme cases.
- Most molecules share electrons but **"Unequally"** due to the difference in electronegativity and electron affinity.
- This will give rise to a **dipole moment** and the molecule becomes polar.

The Relationship Between Electronegativity and Bond Type

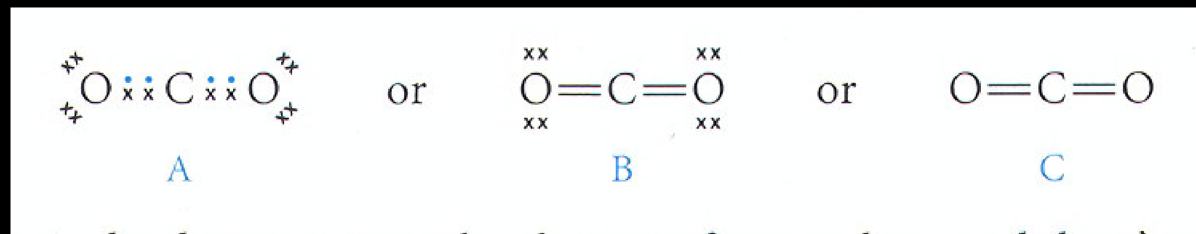
Electronegativity Difference in the Bonding Atoms	Bond Type
Zero	Covalent
Intermediate	Polar covalent
Large	Ionic

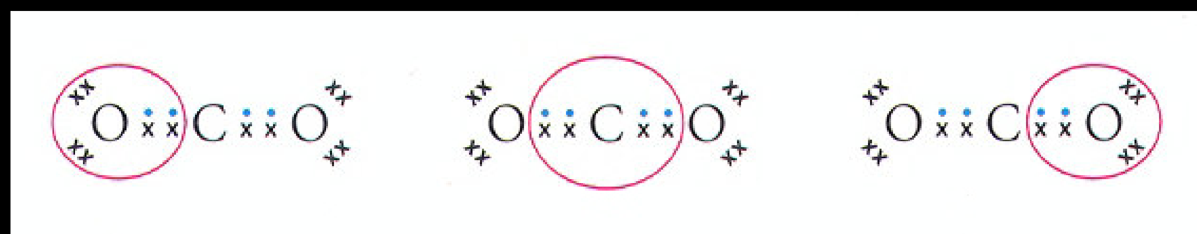


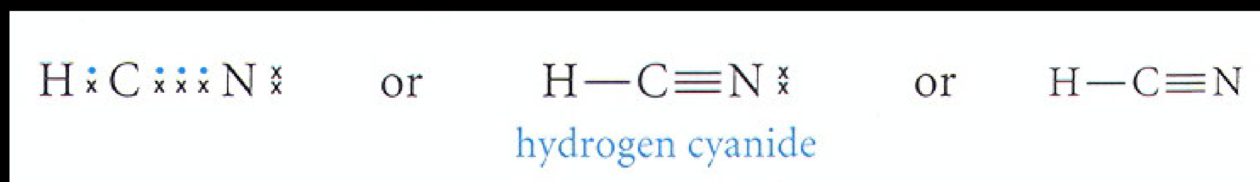
1.6 Multiple Covalent Bonds

- Occur when atoms share more than one electron pair.

Examples:





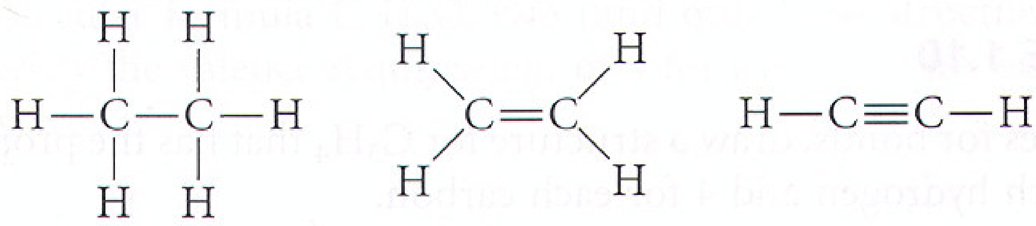


EXAMPLE 1.8

Determine what, if anything, is wrong with the following electron arrangement for carbon dioxide:

$$:O:::C::\ddot{O}:$$

Carbon-carbon multiple bonds



ethane — ethene (ethylene) — ethyne (acetylene)

EXAMPLE 1.9

Draw the structure for C_3H_6 having one carbon–carbon double bond.

SOLUTION First, draw the three carbons with one double bond.

Then add the hydrogens in such a way that each carbon has eight electrons around it (or in such a way that each carbon has four bonds).

PROBLEM 1.17 Draw three different structures that have the formula C_4H_8 and have one carbon–carbon double bond.

1.7 Valence

- Valence of an element is the number of bonds that an atom of the element can form.
- Usually it is the number of electrons needed to fill the valence shell.
- Notice the difference between the number of valence electrons and the valence.

Table 1.5 Valences of common elements

Element	H	C	N	O	F	Cl
Valence	1	4	3	2	1	1

EXAMPLE 1.10

Using dashes for bonds, draw a structure for C_3H_4 that has the proper valence of 1 for each hydrogen and 4 for each carbon.

SOLUTION There are three possibilities:

A compound that corresponds to each of these three different arrangements of the atoms is known.

PROBLEM 1.18 Use dashes for bonds and use the valences given in Table 1.5 to write a structure for each of the following:

a. CH_5N b. CH_4O

PROBLEM 1.19 Does C_2H_5 represent a stable molecule?

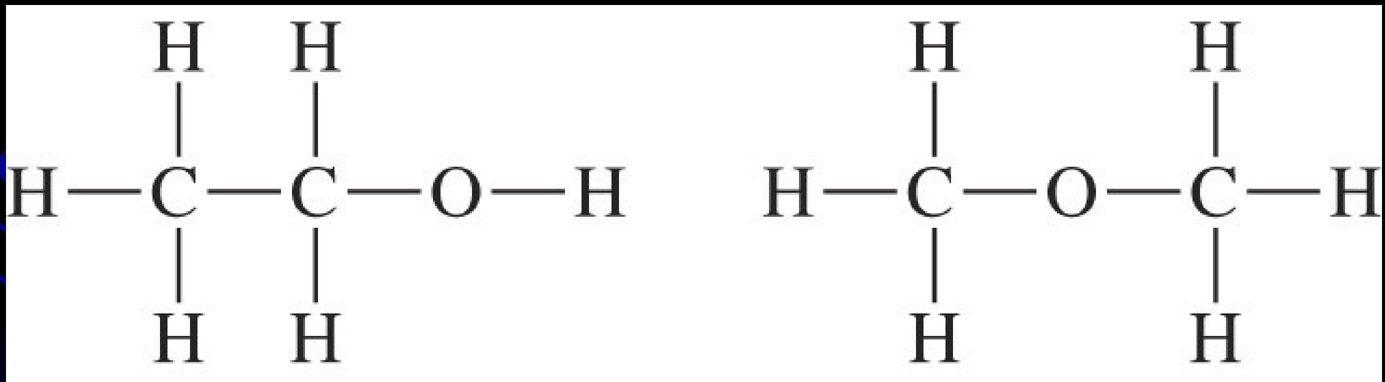
1.8 Isomerism

- The molecular formula of a substance: gives the number of different atoms present.
- The structural formula: indicates how those atoms are arranged.
- Isomers: are molecules with the same number and kinds of atoms but different arrangements of the atoms.
- Structural (or constitutional) isomers have the same molecular formula but different structural formulas.

- Constitutional Isomers
  - Constitutional isomers are one type of isomer
  - They are different compounds that have the same molecular formula but different connectivity of atoms
  - They often differ in physical properties (e.g. boiling point, melting point, density) and chemical properties

	Ethyl Alcohol C_2H_6O	Dimethyl Ether C_2H_6O
Boiling point (°C)	78.5	−24.9
Melting point (°C)	−117.3	−138

- Example
  - Consider two compounds with molecular formula C_2H_6O
  - These compounds cannot be distinguished based on molecular formula; however they have different structures
  - The two compounds differ in the *connectivity* of their atoms



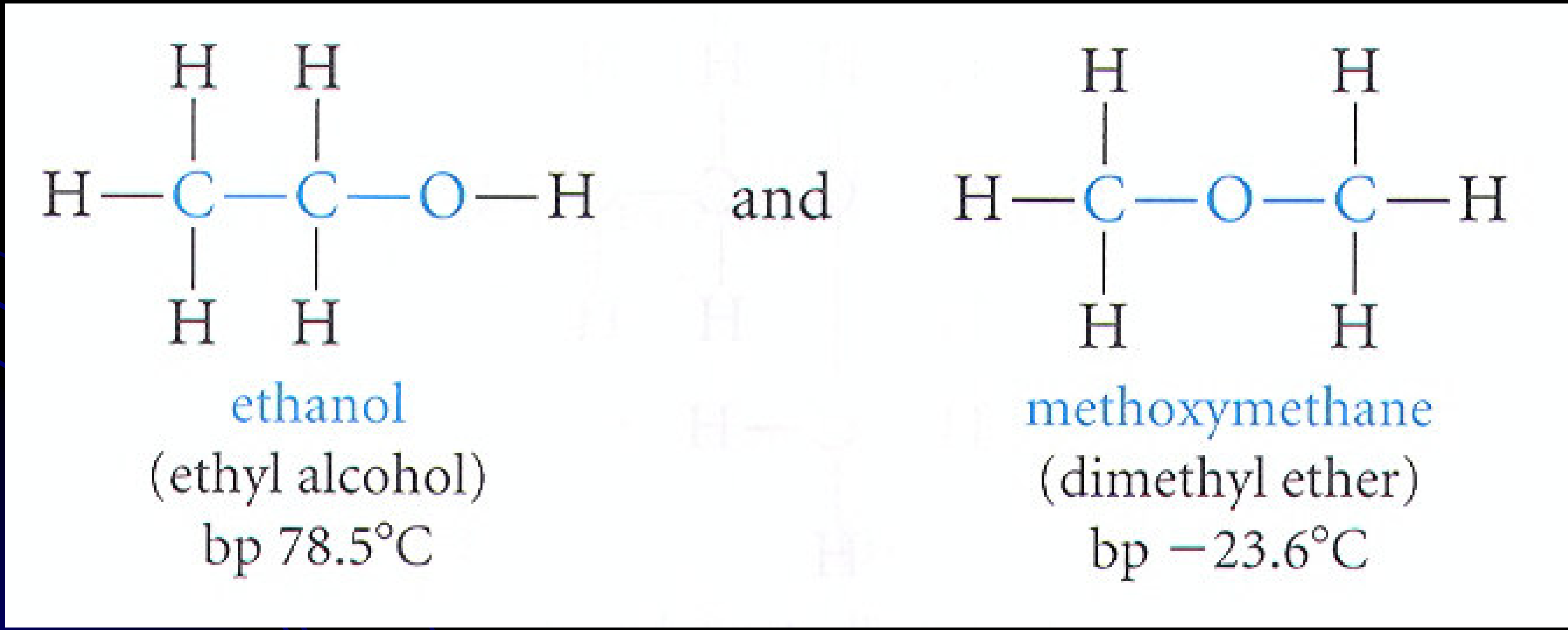
Ethyl alcohol

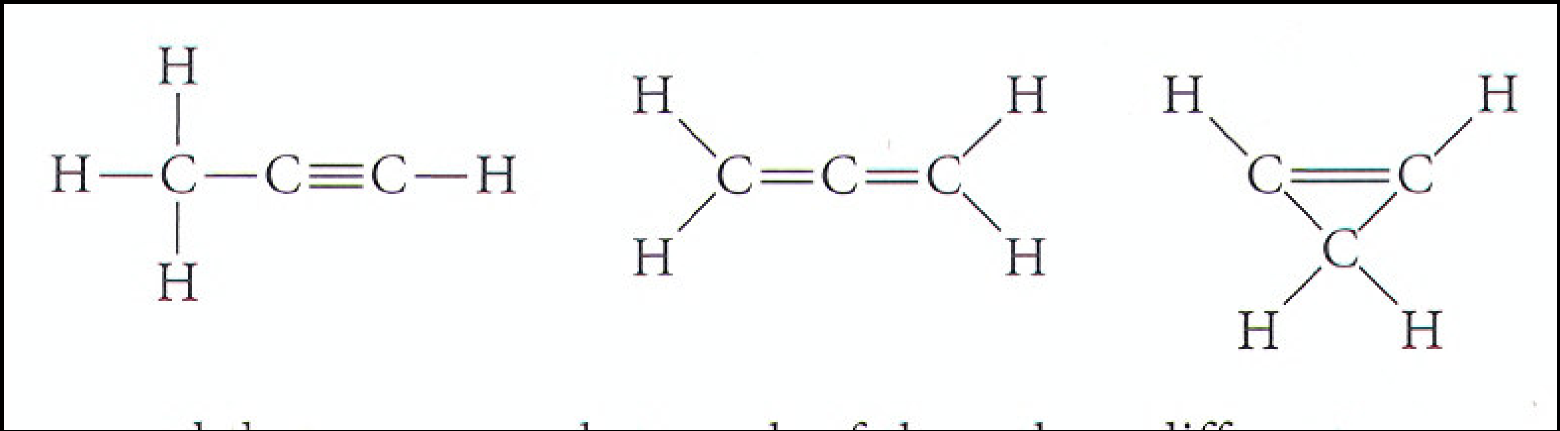
Dimethyl ether

examples

For the formula C_2H_6O

Two (and only two) structural formulas are possible that satisfy the valence requirements of C, H, and O





C_3H_4