ORGANIC CHEMISTRY

Lecture one

Introduction

What is organic chemistry and why should you study it?

Organic chemistry, is the study of carbon compounds. Because of carbon's electronic structure and its consequent position in the periodic table. Every living organism is made of organic chemicals: the proteins that make up your hair, skin, muscles, the DNA that controls your genetic heritage, Food, Medicines.

Group 1A	2A											3A	4A	5A	6A	7A	8A
H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															

Table 1: Periodic table of chemical elements

Carbon can share four valence electrons and form four strong covalent bonds. Furthermore, carbon atoms can bond to one another, forming long chains and rings. Carbon, alone of all elements, is able to form an immense diversity of compounds, from the simple methane, with one carbon atom, to the staggeringly complex DNA, which can have more than 100 million carbons.

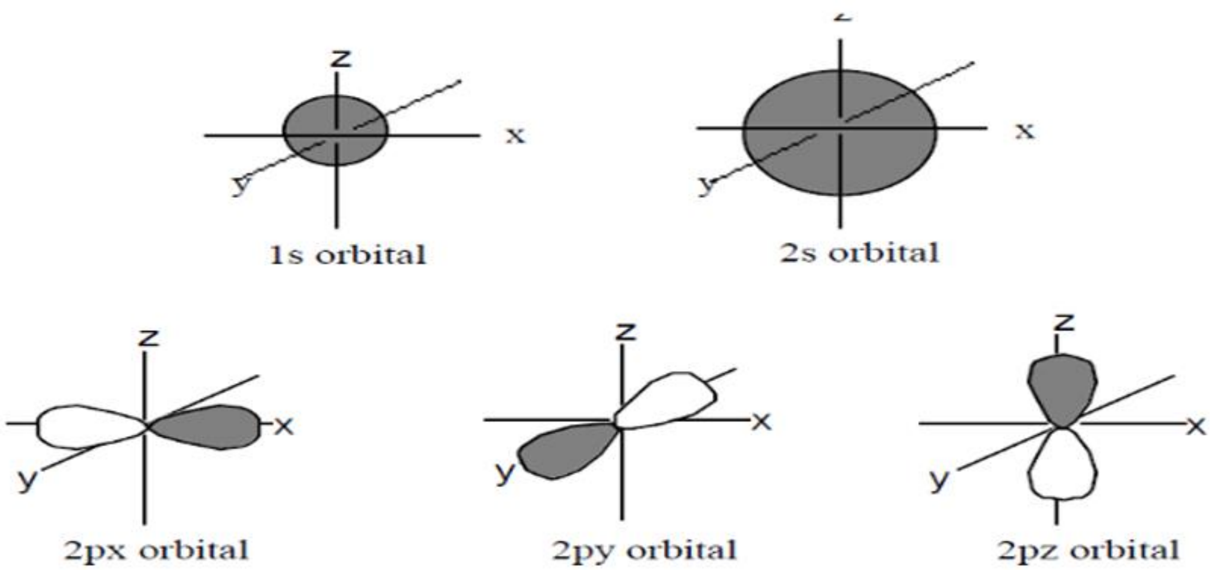
The Chemical Bonds

Electrons exist in energy levels that surround the nucleus of the atom. The energy of these levels increases as they get farther from the nucleus. The energy levels are called shells, and within these shells are other energy levels, called subshells or orbitals., that contain up to two electrons. The calculations from atomic theory give the following results for electron energy and orbitals. The results for the first two energy levels (shells 1 and 2) are the most important for bonding in organic chemistry.

		Orbitals			
Shell	s	p	d	f	Total Electrons Possible
1	1				2
2	2	3			8
3	3	3	5		18
4	1	3	5	7	32

- energy level 1 contains up to two electrons in a spherical orbital called a 1s orbital.
- energy level 2 contains up to eight electrons; two in an 2s orbital and two in each of three orbitals designated as 2p orbitals.

The p-orbitals have a barbell type shape and are aligned along the x, y, and z axes. They are thus called the px, py, and pz orbitals.



1s orbital

2s orbital

2px orbital

2py orbital

2pz orbital

- Energy level 3 contains up to eighteen electrons, two electrons in a 3sorbital, six electrons in the three 3p orbitals, and ten electrons in the five 3d orbitals.

- Energy level 4 contains up to thirty-two electrons, two electrons in a4s orbital, six electrons in the three 4p-orbitals, ten electrons in the five4d orbitals, and fourteen electrons in the seven 4f-orbitals. Electrons fill the lower energy levels first until all of the electrons are used (Aufbau Principle). An element contains the number of electrons equal to its atomic number. For the first and second row elements the electron configurations are relatively simple.

Element (atomic number)	Electron Configuration
H (1)	1s1 (1st shell, s orbital, one electron)
He (2)	1s2
Li (3)	1s2, 2s1
Be (4)	1s2, 2s2
B (5)	1s2, 2s2, 2p1
C (6)	1s2, 2s2, 2p2
N (7)	1s2, 2s2, 2p3
O (8)	1s2, 2s2, 2p4
F (9)	1s2, 2s2, 2p5
Ne (10)	1s2, 2s2, 2p6 (inert, completely filled)

Electronegativity

- Electronegativity is the ability of an atom to attract electrons to itself, and generally increases as one moves from left to the right across the periodic table.
- least most electronegative Li < Be < B < C < N < O < F
- Electronegative Electronegativity also increases as we go from the bottom to the top of a column in the periodic table.
- Least most electronegative I < Br < Cl < F electronegative Elements that easily lose electrons and attain a positive charge are called electropositive elements.

- Alkali metals are electropositive elements

Chemical bonds

Chemical bond is the attractive force holding atoms together.

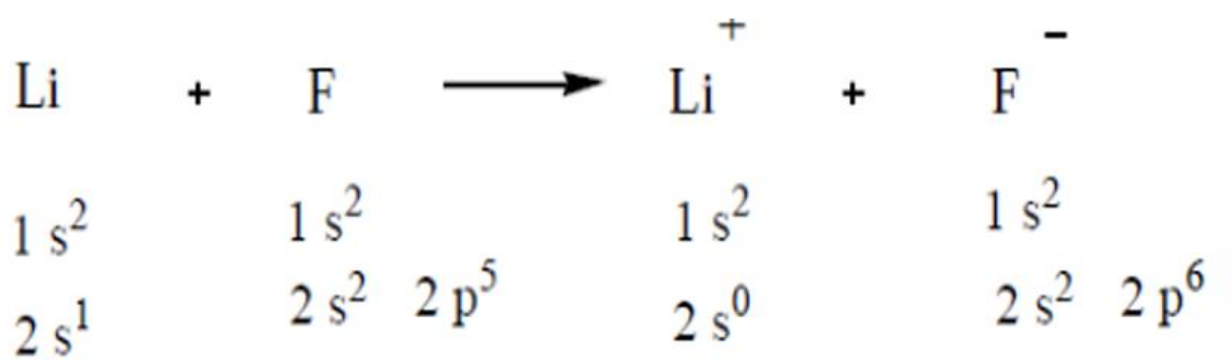
There are three categories of bonds:

- Single bond: involves an electron, e.g. H_2
- Double bond: involves two electrons, e.g. O_2
- Triple bond: involves three electrons, e.g. N_2

Atoms can become bonded with each other, and their electronic structure governs the type of bond formed. The main two types of bonds that are formed are called ionic and covalent.

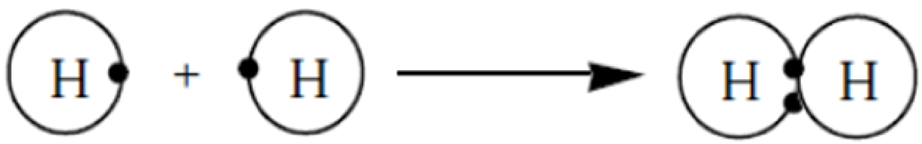
1) Ionic bonds

Ionic bonding is important between atoms of vastly different electronegativity. The bond results from one atom giving up an electron while another atom accepts the electron. Both atoms attain a stable Nobel gas configuration. For example : In the compound lithium fluoride, the 2s1electron of lithium is transferred to the 2p5orbital of fluorine. The lithium atom gives up an electron to form the positively charged lithium cation with 1s2, 2s0configuration, and the fluorine atom receives an electron to form a fluoride anion with 1s2, 2s2, 2p6configuration.Thus the outer energy levels of both ions are completely filled. The ions are held together by the electrostatic attraction of the positive and negative ions.

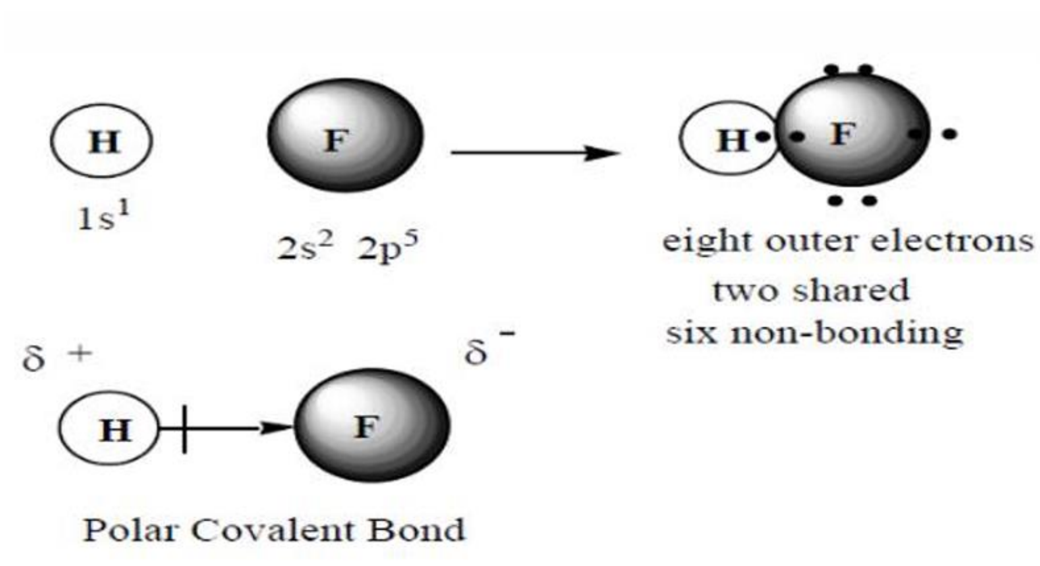


2) Covalent Bond

A covalent bond is formed by a sharing of two electrons by two atoms. A hydrogen atom possessing the 1s1electron joins with another hydrogen atom with its 1s1configuration. The two atoms form a covalent bond with two electrons by sharing their electrons.



For example : In hydrogen fluoride, HF, the hydrogen 1s electron is shared with a 2p5electron in fluorine (1s2, 2s2, 2p5), and the molecule is now held together by a covalent bond. In this case, the fluorine atom is much more electronegative than the hydrogen atom and the electrons in the bond tend to stay closer to the fluorine atom. This is called a polar covalent bond, and the atoms possess a small partial charge denoted by the Greek (δ)symbol.

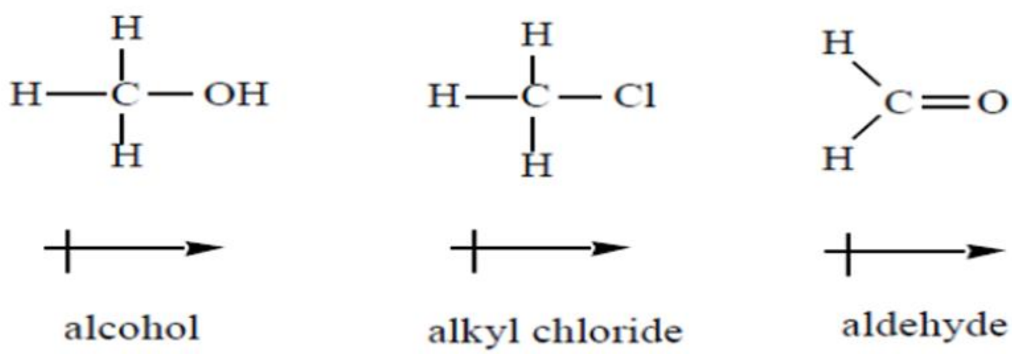


Bonding in Carbon Compounds

The property of carbon that makes it unique is its ability to form bonds with itself and therefore allows a large number of organic chemicals with many diverse properties. Carbon has the property of forming single, double and triple bonds with itself and with other atoms. This multiple bond ability allows carbon compounds to have a variety of shapes. In all carbon compounds, carbon forms four bonds. The types of bonds used by the carbon atom are known as sigma (σ) and pi (π) bonds. Different combinations of these bonds lead to carbon single bonds, double bonds and triple bonds.

Polar Covalent Bonds in Carbon

Carbon forms single, double and triple bonds with elements other than carbon. The atoms involved in the bonding are usually oxygen, nitrogen, sulfur and the halogens. These elements are more electronegative than carbon and thus attract the electrons to themselves. The bonds are therefore polar covalent bonds. Bonds that contain a separation of charge possess a dipole moment, a property that contributes to the overall polarity of the molecule.

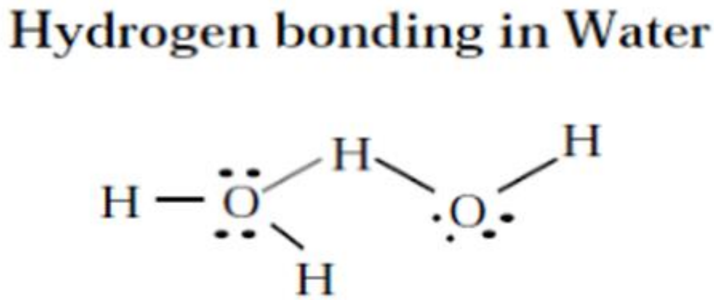


Hydrogen Bonds and Bond Polarity

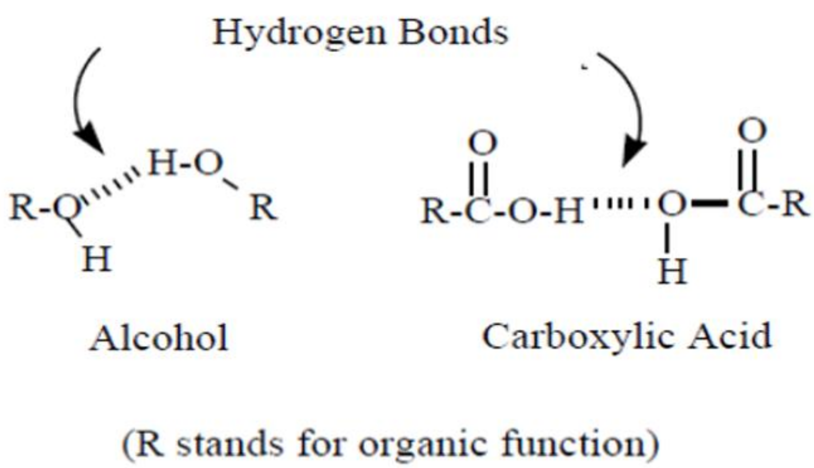
The bonds O-H, N-H and F-H are highly polar covalent bonds because the electronegative draws electrons away from the hydrogen atom. In every case the hydrogen atom has a partial positive charge.

$$O^{\delta -}\text{-}H^{\delta +} \qquad N^{\delta -}\text{-}H^{\delta +} \qquad F^{\delta -}\text{-}H^{\delta +}$$

A result of molecules having these highly polarized bonds with the hydrogen atom partly positive in nature, the hydrogen atom is attracted to the basic site in other molecules, such as the non-bonding electrons on oxygen and nitrogen (non-bonding electrons are electrons belong to an element that complete the octet but do not participate in bonding). This attraction is called hydrogen bonding and is useful for explaining high boiling points and high melting points of fairly low mass molecules. Thus hydrogen bonding in water explains why the compound with only three atoms boils relatively high when compared with other molecules of similar mass. Extra energy is required to break the hydrogen bonds during the boiling process.



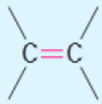
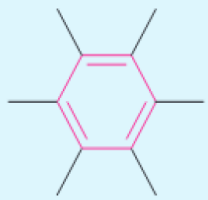
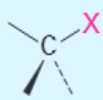
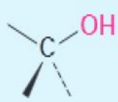
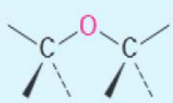
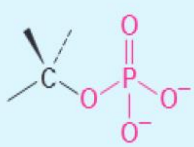
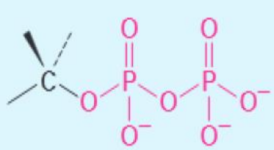
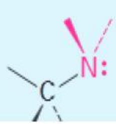
In organic compounds hydrogen bonding is very important for describing the boiling and solubility characteristics of alcohols and acids, and the concept will be given in more detail in chapters dealing with those types of molecules.



Functional Groups

- Since there are 50 millions organic compounds nowadays, a system of classification for these compounds is absolutely necessary to simplify the study of their chemistry.
- Fortunately, these compounds can be classified into a limited number of families. Each of which contains one or more functional groups.

- Functional group is an atom or group of atoms (other than hydrogen) that determines the chemical properties of the molecule. The functional group is a part of a given molecule.

Name	Structure*	Name ending	Example
Alkene (double bond)		*-ene*	$H_2C{=}CH_2$ Ethene
Alkyne (triple bond)	—C≡C—	*-yne*	$HC{\equiv}CH$ Ethyne
Arene (aromatic ring)		None	 Benzene
Halide	 (X = F, Cl, Br, I)	None	CH_3Cl Chloromethane
Alcohol		*-ol*	CH_3OH Methanol
Ether		*ether*	CH_3OCH_3 Dimethyl ether
Monophosphate		*phosphate*	$CH_3OPO_3^{2-}$ Methyl phosphate
Diphosphate		*diphosphate*	$CH_3OP_2O_6^{3-}$ Methyl diphosphate
Amine		*-amine*	CH_3NH_2 Methylamine