

## 1. BONDS

1.1 Introduction to Organic Chemistry

1.2 Atoms, Electrons and Orbitals

1.3 Bonds

1.3.1 Ionic Bond

1.3.2 Covalent Bond

1.3.3 Polar Covalent Bond

1.4 Formal Charges

1.5 Lewis Structures of Organic Molecules

1.6 Resonance

1.7 Classification of Organic Compounds

1.7.1 Acyclic compounds

1.7.2 Cyclic compounds

1.7.3 Aromatic compounds

1.7.4 Heterocyclic Aromatic Compounds

1.8 Representation of the Organic Molecules

1.9 Isomers

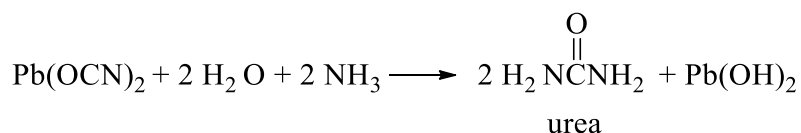
1.9.1 Structural Isomers

1.9.2 Stereoisomers

1.10. Naming of the Organic Compounds

### 1.1 Introduction to Organic Chemistry

Before 1828, it was thought to be organic compounds were very complex and only obtained from living sources like animal urine. In **1828**, Friedrich Wohler synthesized an organic compound (urea) from inorganic compounds (lead cyanate and ammonium hydroxide).



Organic Chemistry is chemistry of carbon compounds. 95% of all known compounds composed of carbon. Carbon forms a variety of strong covalent bonds to itself and other atoms. Carbon can bond to itself and other atoms: in a straight chain or a branched or cyclic manner.

Importance of Carbon:

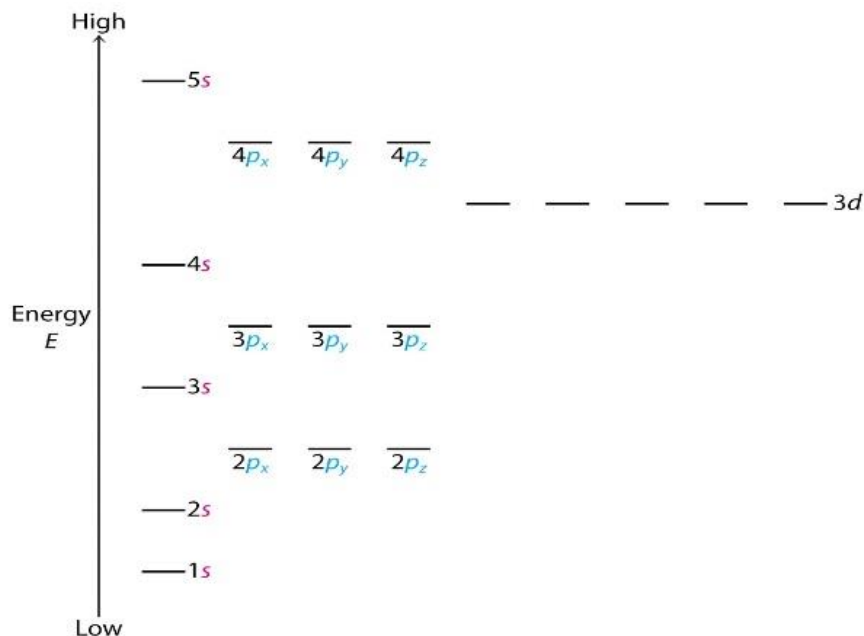
- It has **4 valence** electrons.  $\cdot\overset{\cdot}{\underset{\cdot}{\text{C}}}\cdot + 4\text{H}\cdot \longrightarrow \text{CH}_4$
- It makes **4 covalent** bonds.
- It can bond with any element, but priorities to bond with other carbon atoms and make long chains.

To understand organic chemistry, first the structure of the molecules needs to be understood. For this, some basic principles of chemical bonding and molecular structure in organic chemistry will be examined.

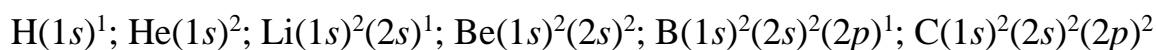
## 1.2 Atoms, Electrons and Orbitals

The atomic theory of electrons began in the early 1900s and gained acceptance around 1926 after Heisenberg and Schrodinger found mathematical solutions to the electronic energy levels found in atoms, the field is now called quantum mechanics. In a neutral atom, the number of protons and electrons are always equal to each other and the charge is 0. 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 energy of these levels increases as they get farther from the nucleus.



Electronic configurations of first 6 atoms:



The below Table indicates the basic sequence of the atomic configuration of the known elements.

*Electronegativity* is a measure of the tendency of an atom to attract a bonding pair of electrons. If atoms bonded together have the same electronegativity, the shared electrons will be equally shared. *The Pauling scale* is the most commonly used.

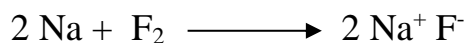
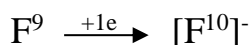
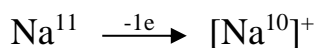
If the electrons of a bond are more attracted to one of the atoms (because it is more electronegative), the electrons will be unequally shared. If the difference in electronegativity is large enough, the electrons will not be shared at all; the more electronegative atom will "take" them resulting in two ions and an ionic bond.

Element	Atomic Number	Electron Configuration
Hydrogen (H)	1	1s <sup>1</sup> (First shell, one electron)
Helium (He)	2	1s <sup>2</sup>
Lithium (Li)	3	1s <sup>2</sup> , 2s <sup>1</sup>
Beryllium (Be)	4	1s <sup>2</sup> , 2s <sup>2</sup>
Boron (B)	5	1s <sup>2</sup> , 2s <sup>2</sup> , 2p <sup>1</sup>
Carbon (C)	6	1s <sup>2</sup> , 2s <sup>2</sup> , 2p <sup>2</sup>
Nitrogen (N)	7	1s <sup>2</sup> , 2s <sup>2</sup> , 2p <sup>3</sup>
Oxygen (O)	8	1s <sup>2</sup> , 2s <sup>2</sup> , 2p <sup>4</sup>
Fluorine (F)	9	1s <sup>2</sup> , 2s <sup>2</sup> , 2p <sup>5</sup>
Neon	10	1s <sup>2</sup> , 2s <sup>2</sup> , 2p <sup>6</sup> (Inert, completely filled)

## 1.3 Bonds

### 1.3.1 Ionic Bond

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 noble gas configuration.



### 1.3.2 Covalent Bond

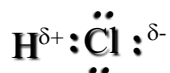
A covalent bond is formed by a sharing of two electrons by two atoms. A hydrogen atom possessing the 1s<sup>1</sup> electron joins with another hydrogen atom with its 1s<sup>1</sup>

configuration. The two atoms form a covalent bond with two electrons by sharing their electron. In a covalent bond, negative charge is between two atoms

Hydrogen molecule:  $\text{H} \cdot \cdot \text{H}$ ,  $\text{H}-\text{H}$ ,  $\text{H}_2$

### 1.3.3 Polar Covalent Bond

Polar covalent bonds are a particular type of covalent bond. Perfectly-ionic and perfectly-covalent bonds are the two extremes of bonding. In reality, most bonds fall somewhere in the middle. A polar covalent bond is an unequal sharing of electrons between two atoms with different



You should note this molecule is not an ion because there is no excess of proton or electrons, but there is a simple charge separation in this electrically neutral molecule.

### 1.4 Formal Charges

Formal charge is a measure of the extent to which an atom has gained or lost an electron in the process of forming a covalent bond. To assign formal charge, use the formula below

**Formal charge = Group number - (electrons in lone pairs + the number of bonds)**

**Group number = # of valence electrons**

For example,  $\text{CH}_4$

The number of valence electrons' carbon is 4.

The number of non-bonded electrons is zero.

The number of bonds around carbon is 4.

So formal charge =  $4 - (0 + 4) = 4 - 4 = 0$

The formal charge of C in CH<sub>4</sub> is 0

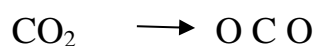
What about the hydrogens:

Formal charge =  $1 - (0 + 1) = 1 - 1 = 0$

## 1.5 Lewis Structures of Organic Molecules

Writing Lewis structures:

(i) Draw molecular skeleton

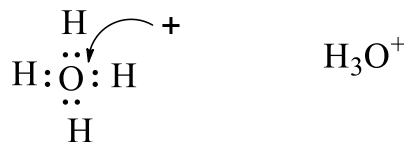


(ii) Count total number of valence electrons. If there is a negative ion, add the absolute value of total charge to count of valence electrons; if a positive ion, subtract.

(iii) Octet (Duet) Rule: Provide octets (duets for H) around all atoms. Assign 2 bonding electrons to each bond.



(iv) Take care of charges, if any. Charges occur when the formal “effective” electron count around the nucleus differs from valence electron count.



Example:  $\text{NH}_3$

1. Atom arrangement: H N H

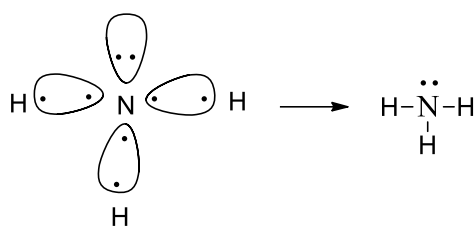
H

2. Valence electrons: H 1e, N 5e  $\longrightarrow$  8e total

3. Bonding electrons:  $3 \times 2 = 6$  e

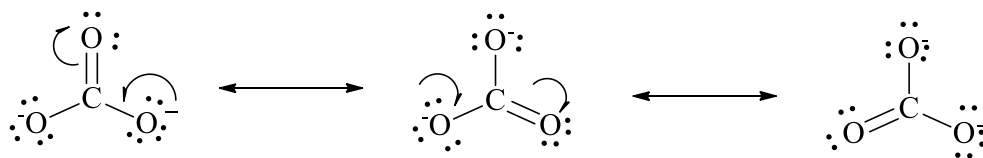
4. Remaining electrons = 2e, lone pairs

5. Octet rule



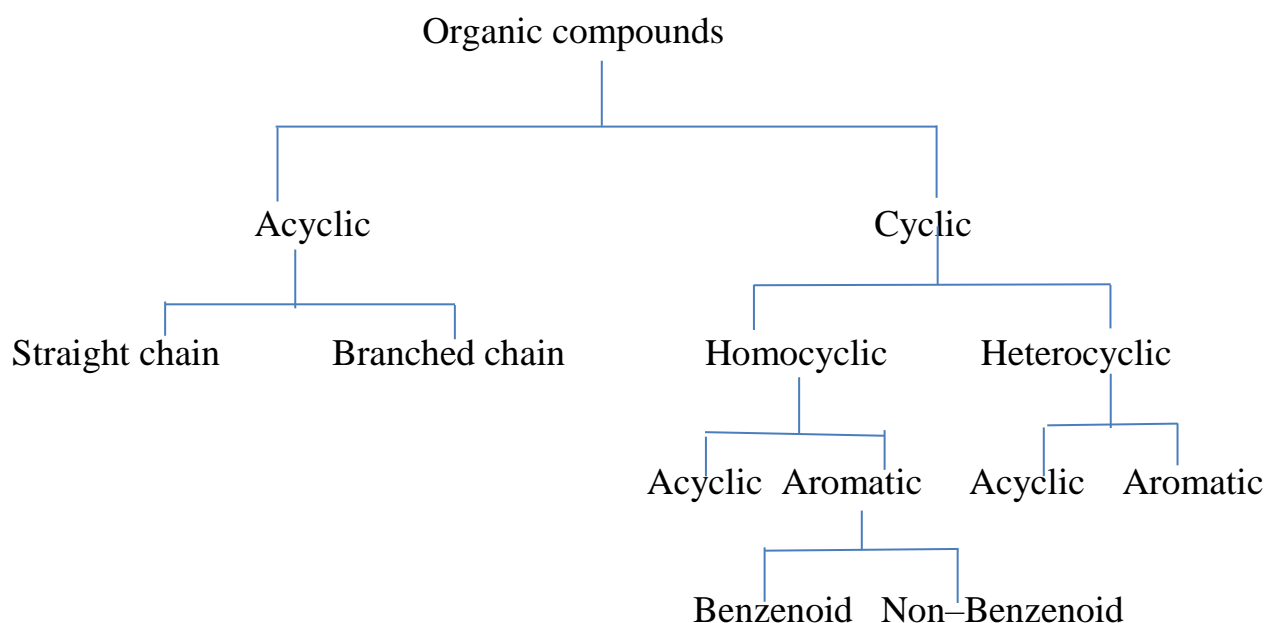
## 1.6 Resonance

Chemical reactions generally involve the movement of electrons between two or more molecules, but electrons also move within a molecule. The reactivity of a molecule is not always explained by one Lewis structure. Molecules can be thought of as hybrids or weighted averages of two or more Lewis structures, each with a different placement of electrons. These structures, called resonance structures, are not real or detectable, but they are a useful conceptual tool for understanding the reactivity of molecules.



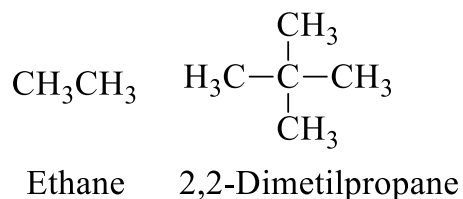
Carbonate,  $\text{CO}_3^{2-}$ . All forms are equivalent

## 1.7 Classification of Organic Compounds



### 1.7.1 Acyclic compounds

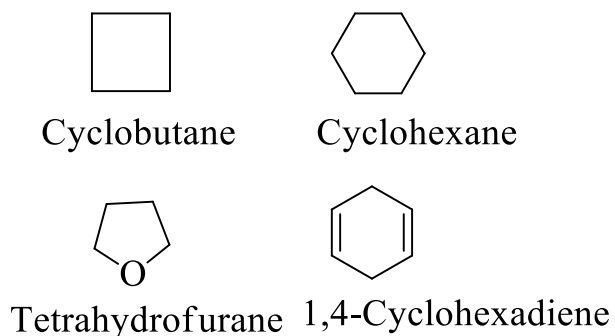
These compounds are also called as **aliphatic** compounds and consist of straight or branched chain compounds, for example:



### 1.7.2 Cyclic compounds

Alicyclic (aliphatic cyclic) compounds contain carbon atoms joined in the form of a ring (homocyclic). Sometimes atoms other than carbon are also present in the ring (heterocyclic).

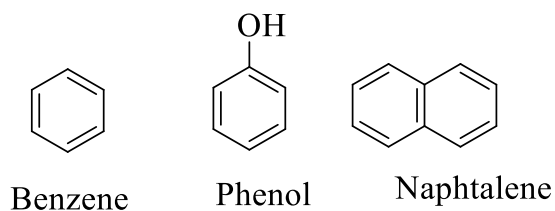




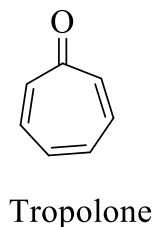
### 1.7.3 Aromatic compounds

Aromatic compounds are special types of compounds. These include benzene and other related ring compounds (benzenoid).

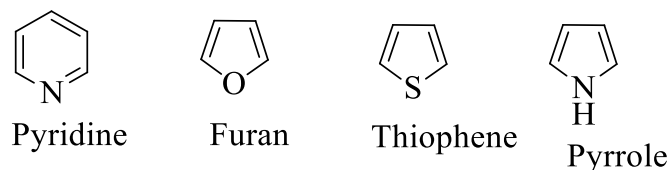
#### Benzenoid Aromatic Compounds



#### Non-Benzenoid Compounds



### 1.7.4 Heterocyclic Aromatic Compounds



Since there are many organic compounds, they must be explored in a particular order. The simplest organic compounds are taken as main structure and others is

considered the derivatives of it. Hydrocarbons are the simplest organic compounds consisting of only carbon and hydrogen. They can be divided into 3 groups.

1. **Saturated Hydrocarbons:** Alkanes (alkanes and cycloalkanes) do not contain any functional group. C-C, C-H,  $C_nH_{2n+2}$

2. **Unsaturated Hydrocarbons:** Alkenes, alkynes and aromatic hydrocarbons with multiple bonds

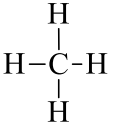
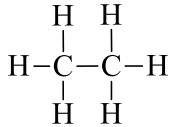
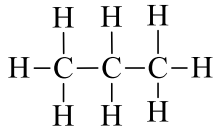


a. Alkenes have double bonds.  $C=C$ ,  $C_nH_{2n}$

b. Alkynes contain triple bonds.  $C\equiv C$ ,  $C_nH_{2n-2}$

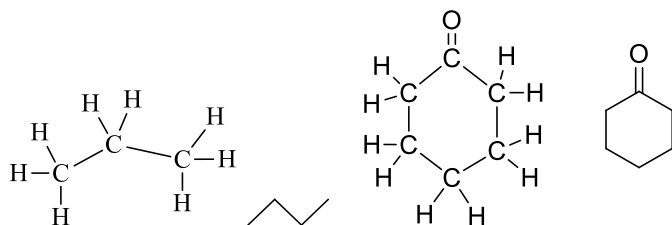
3. **Aromatic hydrocarbons (arenes):** contain conjugated double bond in a cyclic structure.

## 1.8 Representation of the Organic Molecules

The structural formulas of the organic molecules can be shown in different ways.

<b>Chemical Formula</b>	$CH_4$	$C_2H_6$	$C_3H_8$
<b>Condensed</b>	$CH_4$	$CH_3CH_3$	$CH_3CH_2CH_3$
<b>Structural Formula</b>			
<b>Lewis Structural Formula</b>			
<b>Line-Angle Formula</b>			

Simplify the drawing of complex molecular structures

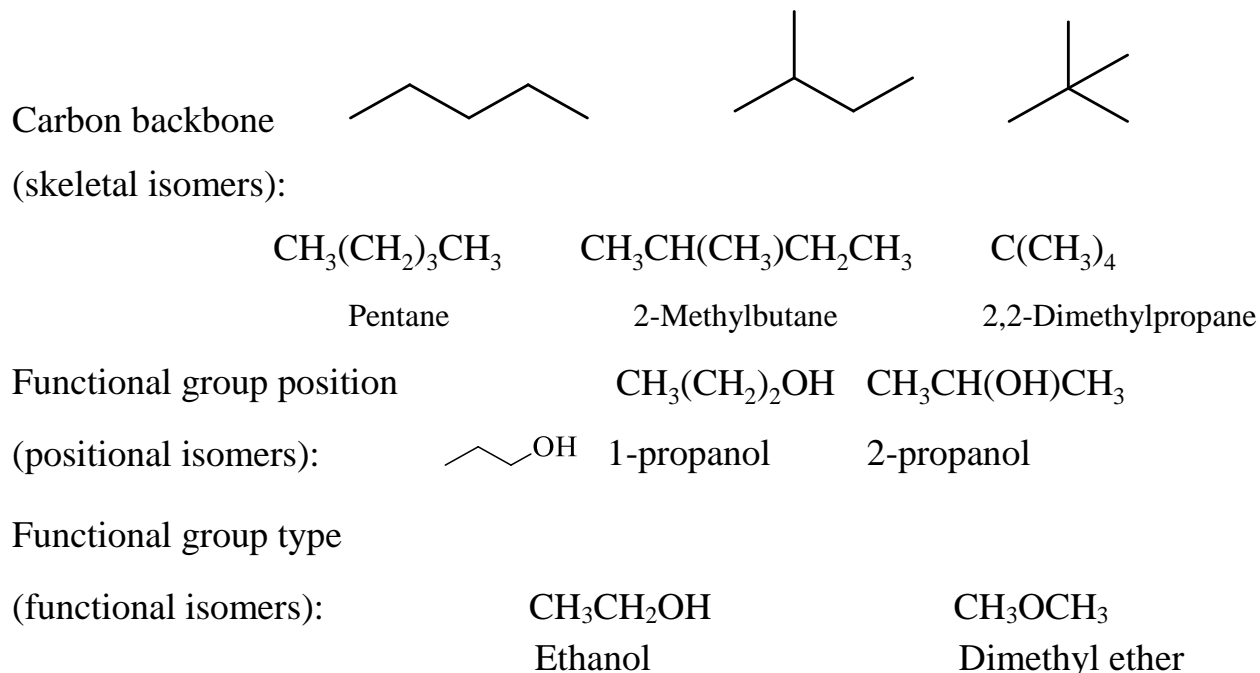


## 1.9. Isomers

Isomers: compounds with the same molecular formula, but different structures

### 1.9.1 Structural Isomers

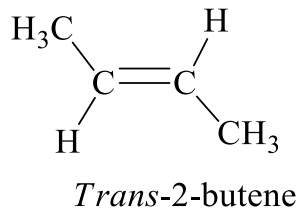
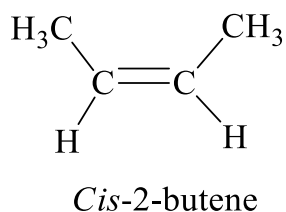
Isomers that differ in the bonding arrangement and connectivity of atoms. Such isomers can differ in terms of :



### 1.9.2 Stereoisomers

Isomers that have the same connectivity, but differ in the spatial arrangement of atoms. There are two classes:

- Geometric isomers: stereoisomers that differ in the relative orientation of substituents e.g. cis- and trans-alkenes




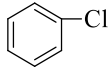
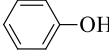
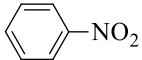
Enantiomers (or optical isomers): stereoisomers that is chiral, non-superimposable on a mirror image.

### **1.10. Naming of the Organic Compounds**

10 million organic compounds exist. Memorizing the structure, properties, and reactivity of each molecule will severely limit our abilities. In order to clearly identify compound, a systematic method of naming has been developed and is known as the IUPAC (International Union of Pure and Applied Chemistry) system of nomenclature. We can name them systematically (IUPAC).

- The most important rule of the systematic naming is 'each different item has own single name'
- The most simple organic compounds are taken as main structure and others is considered the derivatives of it
- Classification is made on the basis of functional groups contained in the compound.
- In general, the base part of the name reflects the number of carbons in what you have assigned to be the parent chain.
- The suffix of the name reflects the type(s) of functional group(s) present on (or within) the parent chain.
- Other groups which are attached to the parent chain are called substituents.

## Organic Functional Group List and IUPAC Names

Functional Group	Compound	Prefix/Suffix	Example	IUPAC Name (Common Name)
<b>Hydrocarbons</b>				
R-H	Alkane	-ane	CH <sub>3</sub> CH <sub>3</sub>	ethane
C=C	Alkene	-ene	H <sub>2</sub> C=CH <sub>2</sub>	ethene (ethylene)
C≡C	Alkyne	-yne	HC≡CH	ethyne (acetylene)
Ar-H	Arenes	-ene		benzene
<b>Halogen-Containing Compounds</b>				
R-X	Haloalkane	halo-	CH <sub>3</sub> Cl	chloromethane
Ar-X	Aryl halides	halo-		chlorobenzene
<b>Oxygen-Containing Compounds</b>				
R-OH	Alcohol	-ol (hydroxy-)	CH <sub>3</sub> OH	methanol
ArOH	Phenols	-ol		phenol
R-O-R	Ether	ether (alkoxy-)	CH <sub>3</sub> OCH <sub>3</sub>	dimethyl ether
RCOH	Aldehyde	-al	CH <sub>3</sub> CHO	ethanal (acetaldehyde)
RCOR	Ketone	-one	CH <sub>3</sub> COCH <sub>3</sub>	propanone (acetone)
RCOOH	Carboxylic acid	-oic acid	CH <sub>3</sub> COOH	ethanoic acid (acetic acid)
<b>Carboxylic Acid Derivatives</b>				
RCOOR	Ester	-oate	CH <sub>3</sub> COOCH <sub>3</sub>	methyl ethanoate (methyl acetate)
RCOOX	Acyl halides	-acyl	CH <sub>3</sub> COOCl	Acetyl chloride
RCONH <sub>2</sub>	Amide	-amide	CH <sub>3</sub> CONH <sub>2</sub>	ethanamide (acetamide)
RCOOCOR	Anhydride	-anhydride	CH <sub>3</sub> COOCH <sub>3</sub>	Acetic anhydride
<b>Nitrogen-Containing Acid Derivatives</b>				
R-NH <sub>2</sub>	Amine	-amine (amino-)	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>	ethylamine aminoethane
RC≡N	Nitriles	-nitrile (cyano)	CH <sub>3</sub> C≡N	acetonitril
ArNO <sub>2</sub>	Nitro compounds	-nitro		nitrobenzene

R = alkyl group, an unfunctionalized saturated chain; Ar= an aryl group; X = halogen