**Organic compounS** 

**Organic Compounds: Definition and Source: —**

Organic chemistry is perhaps best defined as the chemistry of containing compounds.

However, carbon is not the only element present in organic compounds. Hydrogen atoms are almost always present. In addition, organic molecules often contain atoms of

Originally the word “Organic” used for materials obtained from living source, i.e. plants and animals, but now-a-days a series of synthetic compounds are also belongs to organic compounds.

**General Introduction to Organic Compounds: —**

Carbon is common to all organic compounds. Carbons form single, double or triple bonds to other carbons. However, carbon is not the only element present in the organic compound. Hydrogen atoms are almost always present. In addition, organic molecules often contain atoms of

A variety of organic compounds has been synthesised in the laboratory. Synthesis of synthetic rubber, nylon, plastics and polymer contributes a lot to the human civilization. Similarly, discoveries of medicinal compounds, pesticides, weedicides helps us to fight ourselves from various naturals as well as air born & water born hazards. Similarly, organic dyes played a major role in the human civilization.

Thus, without organic chemistry, one can’t think about the development of modern science and technology as well as human civilization.

**Historical Developments of Organic Chemistry: —**

Developments of the theories of atomic & molecular structures as well as weights & bonding theories lead to the developments of organic chemistry. Actually, modern organic begins just after the introduction of Dalton’s atomic theory in the early of 19th century.

Lavoisier, for the first time shows that combustion takes place only in presence of oxygen, which leads to Berzelius in 1814 to determine the atomic weight. He determined the weight of the combustion products of acetic acid obtained from vinegar.

Acetic acid

So the allowed empirical formula , but determination of molecular weight of acetic acid, gives the accurate molecular formula, .

Gay-Lussac, Thenard, Liebig introduced many important improvements to the combustion technique to determine empirical formula, and finally accurate molecular formula.

Since, all organic compounds studied in the early 19th century had their origin in living materials, either animal or plant, and are complex — which leads a strong feeling that such materials possessed some special “vital force”. It was originally believed that compounds having this vital force can’t be synthesised in the laboratory from inorganic materials. But, it was Wöhler who synthesised urea by heating a mixture of and or only from .

So, ultimately the theory was rejected.

Discoveries of isomers and the concept of isomerism contribute a large in the structural organic chemistry.

To explain the tetra valency of carbon and its unique nature to form bonds with other carbon and to almost every element of periodic table leads to the synthesis of huge number of organic compounds and ultimately its importance enhanced in modern life and technology.

A major contribution from Keküle in 1895 for the discovery of the structure of benzene develops the scope of organic chemistry surprisingly.

**Berzelius Hypothesis: —**

Lavoisier suggested that is necessary for the combustion of substances, and Berzelius followed this idea to determine some of the first atomic weights. In 1884, he burns known amount of acetic acid obtained from vinegar in excess oxygen and then determining the weights of the combustion products, , he was able to determine the percents of in the acetic acid molecules.

Acetic acid

This added to the knowledge that oxygen also was present, allowed the empirical formula to be calculated. Determination of molecular formula latter on establishes the actual molecular formula to be . Thus, Berzelius hypothesis originally used to determine the empirical formulas of organic compounds and to ultimately molecular weights for accurate formula.

**Vital Theory: —**

Up to the middle of 19th century, it was believed that it was not possible to prepare organic compounds artificially in the laboratory. At that time people thought that a mysterious force known as the vital force present in the living organism i.e. plants or animals that can derived organic compounds. This concept is known as vital force theory. At that time it was proposed that the organic compounds possessed this vital force and inorganic compounds not, and this leads to differentiate organic and inorganic compounds.

**Wohler’s Experiment: —**

Since all the organic compounds studied in the early 19th century had their origin in living materials, either plant or animal, and there was a strong feeling that such materials possessed some special “vital force”, and so are can’t be synthesised in the laboratory from inorganic materials. But, in 1828, Wohler carried out an experiment that generally considered the mark the beginning of the end of the vital force theory. Wohler accidently obtained urea (the 1st synthetic organic compound) by heating a mixture of (potassium cyanate) and (ammonium sulphate) or only from (ammonium cyanate) by heating.

Urea had been isolated from urine of animals, so it was surely organic, it contained vital force. Later in 1845, Kolbe prepared acetic acid and in 1856, Berthelot synthesised methane in the laboratory. Since then millions of organic compounds have been prepared in the laboratory and ultimately the vital force theory was discarded.

**Sources of Organic Compounds: —**

Organic compounds can be obtained by **synthetic** process and also from natural sources. Natural sources are of 4 – types —

1. Plants,
2. Animals,
3. Minerals, and
4. Fungi & micro-organism.

**Plants**: Substances like carbohydrates, proteins, oils, gums, resins, alkaloids, terpenes, perfumes, etc. are directly obtained from plants. Acetic acid, acetone and methanol are obtained by the destructive distillation of wood.

**Animals**: Substances like fats, proteins, urea, uric acid, honey, vitamins, hormones, etc. are directly obtained from animals.

**Minerals**: From coal and petroleum almost 80% organic compounds are obtained. Coal-tar is the source of many aromatic hydrocarbons like phenols, heterocyclic compounds, dyes, perfumes, drugs, fuels, etc.

On fractional distillation, petroleum gives a large number of compounds, which serve as the starting materials for the synthesis of thousands of other compounds. Some important petroleum products are petrol, kerosene, lubricating oils, Vaseline and other petrochemicals.

**Fungi and Micro-organisms**: These are responsible for the fermentation process. Acetic acid, lactic acid, etc. can be prepared by fermentation.

The various sources or organic compounds can be schematically represented as:



**Isolation of Organic Compounds:—**

Isolation of an organic compound from its source (Plant, Animal, Coal tar, Petroleum, etc.) means its separation or extraction in a crude from containing many other substance.

Isolation of a pure compound from its source consist of 3 steps —

1. Isolation,
2. Purification, and
3. Test of purity.

Isolation step consist of

1. Sublimation,
2. Distillation at atmospheric pressure,
3. Distillation under reduced pressure, and
4. Steam distillation.

The substances which contaminate a desired compound are called **impurities** and the process of removal of impurities from the concerned compound is called purification. This involves:

1. Liquid – Liquid Extraction,
2. Chromatographic Separation, and
3. Recrystallization.

**Characterization of Organic Compounds:—**

In order to characterize an organic compound, first we purify it with various physical as well as chemical methods and finally by its sharp boiling and melting point.

After purification, the chemical analysis has been done in order to determine its empirical formula, and finally determination of molecular weights leads to determine the accurate molecular formula.

Now, to find the actual structure for the organic compound of known molecular formula, we take the help of **Spectroscopic** techniques such as —

1. Infra-red and visible spectroscopy,
2. NMR Spectroscopy,
3. Mass Spectroscopy,
4. ESR Spectroscopy, and finally
5. HPLC techniques.

**Organic Compounds: Classification: —**

[For alternative way of Classification, See below also]

Organic compounds are basically of 2 – types —

1. Open Chain compounds, and
2. Closed Chain compounds.

The simplest compounds of these two classes are **Hydrocarbons**; other can be shown as the derivatives of hydrocarbon. The basic classification of organic compounds can be schematically represented as shown below in the flow-chart diagram.

Depending upon this classification, we can broadly classify the organic compounds into the following 4 – categories:

1. Aliphatic compounds,
2. Alicyclic compounds,
3. Aromatic compounds, and
4. Heterocyclic compounds.



**OR**

**Organic Compounds: Classification: —**

Carbon has the unique property of catenation i.e. it can combine with one another to form rather long chains and rings of different sizes. Organic compounds are large in number though carbon atoms in these compounds are attached to only a few elements, like etc. by covalent bonds. For systematic study, they have been divided into different classes, depending on the nature of the **functional group** (i.e. the reactive part of the molecule and specific to a particular class showing similar chemical properties) present. Saturated hydrocarbons do not contain any functional group.

On the basis of structure, organic compounds are mainly classified into **two** main classes and these are —

1. **Open chain** or **Acyclic** and
2. **Closed chain** or **Cyclic** compounds.

**Open chain** or **acyclic** organic compounds are also known as **aliphatic** (Greek means fat) compounds has open chain of carbon atoms which may be a straight chain or a branched chain. For example,



**Closed chain** or **Cyclic** compounds contain a closed ring of carbon atoms (**Carbocyclic** or **homocyclic**) or carbon atoms with other atoms, like in the ring system (**heterocyclic**). When a cyclic compound contains two or more rings, they are known as **Polycyclic** compounds.

Closed ring system are further subdivided as —

1. **Carbocyclic** or **homocyclic**: These contains only one type of element i.e. carbon in the ring system. These are subdivided into two types —
   1. **Alicyclic** and
   2. **Aromatic** compounds

**Alicyclic** Compounds: These homocyclic compounds behave like aliphatic compounds and hence, known as aliphatic or alicyclic compounds. The word is used before the name of the corresponding alkane. For example,



**Aromatic** or **Benzenoids**: Benzene like compounds having aromatic properties are called the aromatic or benzenoid compounds. These may be polycyclic compounds with benzene ring systems. For example,



1. **Heterocyclic**: These compounds contain more than one kind of atoms in the ring system, hence termed as heterocyclic compounds. For example,



These heterocyclic compounds may also contain more than one ring system. For example,



Briefly, the above classification can be summarized schematically as follows:



Various functional groups attached to basic chain of above main classes give rise to separate classes. For example, group containing compounds are classified as carboxylic acid, as alcohol and phenol, etc.

**Naming Organic Compounds: *IUPAC* Nomenclature: —**

Before discussing the naming of organic compounds, it will be better to know about the **hydrocarbon groups**.

**Hydrocarbon groups**:

If one or more - atoms are taken from a hydrocarbon, the group left is known as a hydrocarbon group. These are of 3 major types as hydrocarbons are broadly of 3 types:

1. Acyclic hydrocarbon groups,
2. Alicyclic hydrocarbon groups, and
3. Aromatic benzenoid hydrocarbon groups.

**Acyclic hydrocarbon groups**: These are of 3 – types —

1. Alkyl groups (),
2. Alkenyl groups, and
3. Alkynyl groups.

**Alkyl Groups**: Alkyl groups are denoted by “” and obtained by removing one - atom from an alkane. So the alkane is and the alkyl group is . These are monovalent groups and named by adding the suffix “” for “” of the parent alkane’s name. These are of 5- types.

1. **Normal Groups**: These are the straight chain groups. To name these prefix “-” is used in common system but in IUPAC prefix - is dropped. For example,

is-Propyl, but in IUPAC it is only propyl

1. **Secondary Alkyl Groups**: It is obtained by removing one - from the parent alkane, and - is used as prefix for naming in either system. For example,



1. **Tertiary Alkyl Groups**: It is obtained by removing one - from the parent alkane, and named by using the prefix - in either system. For example,
2. **Isoalkyl Groups**: If an alkyl group contains one terminal group and group on the other end with no other branching, then it is called an Isoalkyl group or alkyl group. For example,



1. **Neoalkyl Groups**: A ***neoalkyl*** group contains one group on one end and one group on the other end with no other branching in the chain. For example, group (common name).

Hydrocarbon groups containing double and triple bonds are called **alkenyl** and **alkynyl** groups respectively. Their common names are accepted in IUPAC system in most of the cases.

**Alkylidene and Alkylene Groups**: Hydrocarbon groups obtained by removing two - atoms either from a single - atom (Alkylidene) or from a two side-by-side - atoms or from a two separate - atoms (Alkylene) are also well known. For example —



**Some Common Acyclic Hydrocarbon groups**:

|  |  |  |  |
| --- | --- | --- | --- |
| Serial  Number | Condensed Structural Formula | Common name with its  Abbreviated form | IUPAC name with its  Abbreviated form |
| 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18 |  | Methyl ()  Ethyl ()  Ethylene  Vinyl  Ethylidene  Allyl  Propylidene  Isopropylidene  Propylene  Methyne  Ethynyl  Propargyl  Propynyl | Methyl ()  Ethyl ()  Ethylene  Vinyl or Ethenyl  Ethylidene  Allyl  Propylidene  Isopropylidene  Propylene  Methyne  Ethynyl  Propargyl  Propynyl |

**Alicyclic Hydrocarbon groups**: These are obtained by removing one - atom from an alicyclic hydrocarbon. These are of 3 – types

1. Cycloalkyl groups,
2. Cycloalkenyl groups, and
3. Cycloalkynyl groups,

Following are the examples of commonly used alicyclic hydrocarbon groups with their IUPAC names.



**Aromatic Benzenoid Hydrocarbon Groups**: These groups have one or more - atoms less than the parent hydrocarbons, and are generally denoted by and called aryl groups. The simplest aryl group is phenyl group, and it is denoted by .

Some common Aryl groups are —



**Some common Benzenoid Aromatic Hydrocarbons**:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **SL**  **No.** | **Molecular**  **Formula** | **Structural Formula** | **Common Name** | **IUPAC Name** |
| 1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18 |  |  | Benzol  Phenol  Toluene  Benzaldehyde  Benzoic acid  Aniline  Nil  - Xylene  - Xylene  - Xylene  Styrene  Acetophenone  Mesitylene  Cumene  - Methylethylbenzene  Naphthalene  Biphenyl  Benzophenone | Benzene  Hydroxybenzene, Phenol  Methylbenzene, Toluene  Benzaldehyde  Benzoic acid  Aniline  Ethylbenzene  1,2- Dimethylbenzene,  - Xylene  1,3- Dimethylbenzene,  - Xylene  1,4- Dimethylbenzene,  - Xylene  Phenylethene  Acetophenone,  Phenylethanone  1,3,5- Trimethylbenzene  Isopropylbenzene  3- Methylethylbenzene  Naphthalene  Biphenyl  Benzophenone, Diphenylmethanone |

**Naming Organic Compounds: *IUPAC* Nomenclature: —**

Organic compounds are usually named by the following three systems —

1. **Trivial names** or **common names**,
2. **Derived names**, and
3. **Systematic names** (**IUC** or **IUPAC** or **Geneva** names)

**Trivial names** or **common names**:

These refer to the **source** from which the compound is obtained or to a characteristic **property** or the **name** of the **discoverer** of the compound. Thus the names —

Oxalic acid (Oxalis), malic acid (pyrusmalus, the apple), citric acid (citrus), urea (urine), hippuric acid (horse urine) and testosterone (testis) are derived from the **source** given in brackets.

Acrolein (Greek, - pungent), glucose (Greek - sweet), Pentane (Greek five) refer to the distinctive properties such as odour and taste.

Pelletierine, the alkaloid obtained from pomegranate was named after the name of its discoverer Pelletier.

However, the origin of many trivial or common names in organic chemistry is not quite clear. The names of the first four members of the homologous series ‘saturated aliphatic hydrocarbons’ viz. methane, ethane, propane and butane, are typical examples of this kind.

The IUPAC names have no doubt become very popular now-a-days, but certain common or trivial names have come to say. These common names may include the simple compounds such as acetone, glycerol, acetylene, benzene, toluene, phenol, aniline, etc. or complex compounds like quinine, penicillin, streptomycin, chloromyceteine, morphine, chlorophyll, vitamin A, etc.

For a list of some common names in organic chemistry see page 130 of Jain & Sharma.

The common or trivial names are generally short and easy to remember, but they suffer from the following disadvantages:

1. A particular compound may have a number of names. Methyl alcohol, for example, is also called **wood sprit or wood naphtha or carbinol**.
2. As the number of carbon atoms increases in the organic compound, the number of isomers also increases enormously. For example, there are 5 possible hexanes, 9 heptanes and 35 nonanes; hence, it is very difficult to give common names to them.

**Derived names**:

These names are derived from the common names of some familiar organic compounds. For example, names of alcohols are derived from the name carbinol, for the familiar member of the series.

Similarly, names derived from acetic acid and acetylene are given below:

**Systematic names** (**IUC** or **IUPAC** or **Geneva** names):

These refer to the universally accepted of naming of organic compound in a systematic way based on some principles. The most important feature of an IUPAC or IUC (International Union of Chemists) or systematic name is that a compound with a well-defined structure will have one and only one IUPAC or systematic name in terms of the principles given by the IUPAC system of nomenclature. The basic rules for this system are —

1. **The Root Words**: The root word is obtained from the longest number of - atoms of the continuous - chains. For the chains up to have the common names but from on words, Greek number roots are used as:
2. **Primary Suffix**: A primary suffix is added to the root word to indicate the saturation or unsaturation of the - chain.
3. **Secondary Suffix**: A secondary suffix which follows the primary suffix is added to indicate the functional group. For example —

|  |  |  |  |
| --- | --- | --- | --- |
| Functional Group | Suffix | Homologous Series | General Name |
|  |  | Alcohol  Aldehyde  Ketone  Carboxylic acid | Alkanol  Alkanal  Alkanone  Alkanoic acid, etc. |

1. **Numbering**: The longest chain is numbered in such a way so that the substituents have the minimum position.
2. **Naming of Substituents**: The substituents are named with the position separated by a hyphen before the root name i.e. as prefix in a single word.
3. **Similar Substituents**: For two or more similar substituents prefix are used.
4. **Different Substituents**: For two or more different substituents, substituents are named in their alphabetical order.
5. **Multiple Bonds**: For unsaturated compounds, containing multiple bond, the longest chain is numbered such that the position of the multiple bond in minimum.

**Examples**: Simple mono-functional Organic Compounds:

**Common as well as IUPAC names of some Aromatic Compounds**: **Group A**







**Group B**: **Polynuclear Hydrocarbons and Heterocyclic Compounds**:





**Question**: Write the IUPAC names for the following:





**Few more IUPAC Rules especially applicable to a particular Class of Compound**:

**ALKANES: Rules for IUPAC Nomenclature**—

1. Select the longest chain for root/ parent name,
2. Add at the end of the root name i.e. as suffix,
3. Number the longest chain so that the position of the substituent is minimum and write it as the secondary prefix with position separated by a hyphen,
4. Use for similar substituents,
5. For cycloalkanes add the prefix immediately before the parent name,
6. For dissimilar substituents, name then in their alphabetical order, irrespective of their position, and
7. Substituents in a substituent are written in parenthesis.

**For example**:



**H/W**: **Write the IUPAC name or Structure whatever applicable**:



**ALKENES& CYCLOALKENES:**

Both contains one or more double bonds — and are also called Olefins. For one double bond, general formula is respectively.

**Rules for IUPAC Nomenclature**—

1. The longest continuous sequence of - atoms containing the double bond is the basis for the parent name of an alkene.
2. The position of the double bond is indicated by numbering the parent chain from the end that will give the double bond the lowest possible number.
3. **Polyenes** are named as , , etc.

Polyenes may be conjugated, if the double bonds are separated by one single bond (i.e. alternate), for example, a conjugated diene is —



On the other hand, compounds in which a single - atom is connected to two other - atoms by double bonds are called **allenes**. Simplest allene is —



Allene is the common name of the simplest member of the series (), allenes are obtained as the derivative of allene.

1. The following three unsaturated side-chain groups may retain their common names in the IUPAC nomenclature:
2. If a side chain possesses a double bond, it is named as a substituent ends in . The side numbered from the point of attachment to the parent chain (Example 1).
3. Rest are (may require, if any) same as in alkane.

**Some typical examples are**—





**H/W (Set - A)**: **Draw the structural formula for the following**—

**H/W (Set - B)**: **Write the IUPAC name for the following**—



**ALKYNES:**

These are the unsaturated hydrocarbons which possess one or more triple bonds. For one triple bond, general formula is . The simplest member is ethyne (acetylene, ). Alkynes are often referred to as acetylenes, a non-IUPAC name.

**Rules for IUPAC Nomenclature**—

1. The longest continuous - chain containing the triple bond is the basis for the parent name of an alkyne. The ending is added to the root.
2. Rest rules are same as in alkanes and alkenes.

**Some typical examples are**—



**Compounds containing both bonds**:

These types of compounds are found in open chain series. The root name is “”, for example, , and the suffix is (). In naming **preference is given** for i.e. the chain is numbered such that the position of the double bond is the minimum. For example,



**Heteroatom Functional Groups:**

**[A] Alcohols (), Phenols () and Thiols (): —**

**Definition**: Hydroxy () and mercapto () derivatives of acyclic and alicyclic series are called alcohols and thio-alcohols or thiols respectively. The suffixes of these compounds are respectively.

On the other hand nucleus substituted hydroxy derivatives of benzene and its homologues are called phenols, and their corresponding mercapto derivatives are called thio-phenols.

**Rules for IUPAC system of Nomenclature**:

1. The longest continuous chain to which the hydroxy group is connected provides the root name for the parent name. The final ‘’ of the corresponding hydrocarbon name is dropped and the “” suffix is added.
2. Numbering begins from the end of the parent chain so that the position of is minimum, i.e. group’s position not necessarily always one. Examples are —



1. For polyols suffixes are Glycerol is the common name given to . For example,



1. For unsaturated alkanols, preference is given over to groups, not to the multiple bonds. For example,



**H/W**: **Provide the IUPAC name for the following**:



**A wide variety of hydroxy compounds have their plant or animal origin**: For example,



**Few more complex hydroxy molecules are**—



**Phenols () or Carbolic acids: —**

**Rules for IUPAC system of Nomenclature**:

1. These are named as the hydroxy derivative of benzene. For example,



1. Phenols containing substituents other than group may be named as the derivative of phenol or hydroxy compound. For example,



**Thiols () and Thiophenols (): —**

**Rules for IUPAC system of Nomenclature**:

1. These are the sulphur analogues of alcohols i.e.- atom replaces the - atom in the functional group. They are named by adding the suffix “” to the parent name. Thiols are also called/ referred to **mercaptans**.



**[B] Ethers () and Thioethers ()**:

Both ethers and thioethers are of two types —

Simple — if both the - groups are same, and

Mixed — if both the - groups i.e. alkyl groups are different.

**Rules for Nomenclature**:

1. In **common system**, the names of the ethers are given by adding the word “ether” to the names of the alkyl groups. The alkyl groups are arranged alphabetically in separate words. For example,



1. In **IUPAC system**, ethers are named as the derivatives of alkane () in a single word, where - atom the alkane is replaced by group. In the case of mixed i.e. unsymmetrical ethers, the larger alkyl group is chosen as the parent hydrocarbon. Thus, groups are named as substituents. For example,



1. **Process**: This system of nomenclature is also closest to the systematic nomenclature. Here, the - atom is counted as a - in determining the parent name and it is then named by prefix with a number to designate its position. For example,



1. **Ethers**: In IUPAC system three membered cyclic ethers are called or . These are commonly called epoxides, and are named as the oxidation products of the corresponding alkenes. For example,



**H/W: Provide IUPAC name for the following**:



1. : In IUPAC system, - analogues of ethers are named as thioethers or alkyl sulphides. For example,



**[C] Amines ()**:

Amines are the organic derivative of and are basic in nature. One, two or three alkyl groups may replace the of to give - amines respectively.

**Rules for Nomenclature**:

1. In IUPAC system for - amines, the final “” of the parent hydrocarbons name is dropped, and the suffix “”is added. The - atom is neither counted to establish the parent name nor numbered.

The groups of - amines are named as substituents on the parent and the letter “” is used to show that the substituent is bonded to the - atom

1. In common system, the suffix is added to the root name of the hydrocarbon. For example,



1. **When group is a substituent**: The prefix or is used when the amine group () is a substituent on a parent molecule. In some cases, in a parent chain, it is identified by adding the prefix analouges to the use of for ethers. For example,



1. Aromatic amines have their common names (accepted by IUPAC) and named as the derivative of **aniline**. Anilines are amines in which the group is directly attached to a atom of the benzene ring. For example,



1. When four alkyl groups are attached to the - atom, the compound is no longer basic, the analogues - atom possesses a formal charge and is the cationic portion of a type of compound known as a ***quaternary ammonium salt***. For example,



**H/W: Provide IUPAC name for the following**:



**Important**: - containing compounds are most common in organic natural products. For example, **alkaloids** are the basic nitrogenous compounds distributed in plants and have physiological activity. Similarly, **amino acids** are the components of proteins.



**[D] Organ-halogen Compounds ()**:

Substances in which one or more halogen atoms are bonded (covalently) to carbon are known as organo-halogen compounds, also referred to as organic halides.

**Rules for Nomenclature**:

1. In IUPAC system, organic halides are named as the halogen substituted hydrocarbons, since there is no suffix to represent halogen. However, in common system, these are named as alkyl halides (two words). For unsaturated halogen derivatives preference is given for multiple bonds. For example,



1. **Aromatic Halogen Compounds**: Nuclear substituted halogen compounds are known as the **aryl halides,** , and named as **halo benzene**. For example,



1. **Side chain substituted Aryl halides**: Side chain substituted aromatic halogen derivatives are known asand are obtained by the replacement of one or more- atoms in the chain by halogen atoms. For example,



**H/W: Provide IUPAC name for the following**:



**[D] Aldehydes and Ketones**:  **(IUPAC)**



**Rules for Nomenclature**:

1. In IUPAC system, suffix is added to designate a ketone and a number is used to indicate the position of the group (carbonyl group). When another functional group has nomenclature priority over ketone (such as aldehyde), the - atom of ketone carbonyl group is regarded as a substituent and is designated by the prefix (NB: for ethers and for amines). In common system, the name of the two hydrocarbon groups is followed by the word ketone (three word name). For example,



1. If the - atom of a compound is attached to a benzene ring; the compound may be named as . For example,



[**Important**: Both acetophenone and benzophenone are used as base names for their derivatives]

1. Ketones containing **Cycloalkyl, aryl and heterocyclyl** groups may be named as the derivatives of or as their derivatives. The IUPAC sanctioned names of some such groups are:

1. **Aldehydes**: Aldehydes are named by using the suffix . When acompound is named as aldehyde, the function is always at the end of the chain, so the number -1- is omitted.

The suffix (or ) is used when the group is attached to a ring. If the aldehyde group is named as a substituent the term (or ) is used to name it only as prefix. For example,



**H/W: Provide IUPAC name for the following**:



**[E] Carboxylic or Fatty acids**:  **(IUPAC)**



High molecular carboxylic acids such as Palmitic acid, steric acid, etc. are the constituents of fats, hence carboxylic acids are also known as the fatty acids.

**Rules for Nomenclature**:

1. In IUPAC system, suffix is used for “” of the parent long chain hydrocarbon to designate carboxylic acids. The group has always the position 1, so need not to be mentioned.
2. When the carboxylic acid functional group, is connected to a cyclic structure, becomes the appropriate suffix.
3. The term is employed, when the group is named as a substituent in the parent chain of compound having higher priority.
4. Aromatic carboxylic acids are named as the derivative of benzoic acid, the simplest aromatic acid. For example,



**Common Name of some Mono Carboxylic Acids**:

**Common Name of some Di Carboxylic Acids**:

**Naming of Derivatives of Carboxylic**:

There are 4- derivatives of carboxylic acids, and these are —

1. Acid or acyl halides (),
2. Carboxylic acid anhydrides (),
3. Esters or carboxylic acid esters (), and
4. Amides or acid amides ().

All these derivatives are obtained by the replacement of segment of the acid by a group to obtain the desired derivative. Thus,



**Rules for Nomenclature**:

1. : In IUPAC system, acyl halides are named by adding the suffix instead of to the parent name followed by a separate word to designate the specific halogen atom. When common acid names are used as the parent, is the suffix. Thus,



1. : In IUPAC system acid anhydrides are named from the appropriate carboxylic acid with the subsequent additional word anhydride. When both the groups connected to the common - atom is the same, the acid name is used without the prefix “-”. If two different groups are attached to the - atom, their carboxylic acid names are employed in separate words. For example,



1. : In IUPAC system, carboxylic acid esters are named by using a combination of the names of the alcohol and the carboxylic acid components of the molecule. The alcohol root name is given with an “” ending (i.e. as substituent). The second word is the parent name for the carboxylic acid with the suffix “” ending, replacing ‘’. Thus,



1. : In IUPAC system, amides are named by adding the suffix “” with the parent word, omitting ‘’ of the parent carboxylic acid. For example,



**H/W: Provide IUPAC name for the following**:



**IUPAC Nomenclature for Bicyclo Compounds**: Or

**IUPAC Nomenclature of Fused Bicyclic Compounds**:

In compounds where 2 rings or cyclic systems fused together, then are named as bicyclic compounds. These compounds have **two** structural features in common ―

1. **Two** bridgehead carbon atoms, and
2. **Three** arms connecting the two bridgehead carbon atoms.

These compounds (bicyclic compounds) are named as the derivative of alkanes corresponding to the total number of atoms in both the rings. Or

Polycyclic compounds possess two or more rings with at least two common atoms are termed as bicyclic, tricyclic compounds. Those two atoms are the bridging points in the polycyclic structure are known as the bridgehead atoms. For example,

***Norbornane*** is a bicyclo compound in which the six-membered ring must have the boat conformation. ***Camphor*** is a pleasant smelling natural product closely related to norbornane.



**IUPAC rules for the Nomenclature of Bicyclo Compounds**:

1. The prefix bicyclo followed by the name of the alkane containing the same total number of atoms.
2. The number of atoms in each of three bridges connecting the two tertiary atoms is indicated in square brackets in **decreasing order**.
3. The numbering used to assign substituents or functional groups begins from the bridgehead position, proceeds **along the longest arm** to the other bridge head, and continues along the next longest arm. The bridgehead position selected is **one** that is close to the carbon bearing functional group or substituent. For example,



 













**Question**: Write the structure of a bicyclic compound that is an isomer of bicyclo[2.2.1]heptane.

**Solution**: Bicyclo [2.2.1] heptane is



Hence, one of the possible isomer of bicyclo [2.2.1] heptane will be bicyclo [3.2.0] heptane,



**Question**: Write the structure/ IUPAC name for the following bicyclic compounds —





**IUPAC Nomenclature for Spiro Compounds**:

An unusual class of polycyclic compounds possesses the structural characteristic in which one - atom is a member of two different rings, and these are called spiro compounds.

In IUPAC system, spiro compounds are named by prefixing the word “spiro” to the name of the parent hydrocarbon obtained by counting the total number of atoms of both the rings. The numbers in the square brackets show the number of atoms on each side of the common atom i.e. fused point, also called the “spiro atom”. The numbering begins from the ring atom next to spiro atom, and proceeded through the **smaller ring** (reverse of bicyclic compound) then to the spiro atom and finally round the large ring. The numbers within the square bracket are written in increasing order (reverse of bicyclic compound). When numbering is required to designate a substituent, it begins at the adjacent to the common - atom and proceeds the smaller ring and then the larger ring. For example ―



Similarly,



**H/W: Provide the IUPAC name for**—



**Geometric Isomerism of the Compounds containing Hetero-atoms**:

**& Isomerism**:

**Geometric Isomerism involving ,** :

The , i.e. the compounds containing double bonds exhibit geometrical isomerism owing to the restricted rotation about the double bond (- bond).

Oximes are of two types —

1. **Aldoximes**, and
2. **Ketoximes**.



The configuration of stereo-isomeric oximes is usually denoted by the prefixes “- and -” instead of “- &-” respectively.

In an aldoxime, the - isomer is the one in which the group of the oxime is in the side of the - of the aldehyde carbon, otherwise it is -. Thus,



**Typical examples are**—



In ketoxime, it is necessary to specify the group with respect to which the oxime group is - or -. Thus,



**Beckmann Rearrangement: —**

The acid catalysed conversion of **ketoximes** to **- substituted amides** is usually called the Beckmann rearrangement. The acid catalysts used are may be , , , polyphosphoric acid, etc.

In this rearrangement reaction, the migration of the alkyl or aryl group, from the - atom to - atom takes place and the migration is always - with respect to the leaving group in the oxime. Thus, the reaction is an example of - rearrangement. In some cases - atom of an aldoxime migrates, especially in presence of polyphosphoric acid. Thus,



For example,



In the case of cycloalkane oximes, ring expansion takes place. For example,



**Mechanism**: The reaction probably involves an intramolecular anion-tropic 1,2- shift mechanism involving the following steps:

**Step I**: Formation of a better leaving group:



**Step II**: Elimination of the leaving group and migration of the group - to the leaving group:



**Step III**: Addition of water to the carbonium ion to form an of the amide which rapidly isomerises to yield a - substituted amide:

//

**General Properties of Organic Compounds:**

**Chemical Bonds: —**

Regrouping and rearrangement of outer electrons, called valence electrons of the constituting atoms resulting in the formation of the molecule, and the process required energy/ forces. The forces that hold the atoms or molecules or ions together may be called chemical bonds. Depending upon the mechanism of formation of bonds and properties possessed by several types of chemical substances these may be:

1. Electrovalent bond,
2. Covalent and dative bond,
3. Metallic bond,
4. Hydrogen bond and
5. Van der Waal’s force.

**Nature of Covalent Bond:**

A covalent bond is formed by the sharing of electrons, and by this process both the atoms completes their octet, i.e. nearest inert gas configuration to attain stability. Thus, a covalent bond is the force that holds the atoms together by sharing of electrons. For example, formation of F2 – molecule:



Compounds containing covalent bonds are called covalent compounds. Usually a covalent bond is represented by a pair of dots (due to Lewis GN) or by a dash (due to Couper).

When a pair of electrons is shared between 2 – atoms a **single bond** is formed, as in the case of H2, Cl2, F2, etc. On the other hand, when 2 – pairs are shared a **double bond** (as in O2) and **triple bond** (as in N2) when 3 – pairs of electrons are shared.

**Modern Concept of Covalent Bonding: —**

To explain the stability and shapes of covalently bonded molecules (Lewis theory fails to explain this) two modern theories are parallelly applied viz.

1. Valence bond theory — by Hitler & London and latter extended by Pauling & Slater
2. Molecular orbital theory — by Hund & Mullikan

**VBT:**

VBT is based on wave – particle duality nature of electrons. As particle electron possesses spin motion and as waves they have orbital diagrams. Following are the basic assumptions and silent features of valence bond theory (VBT): —

1. A covalent bond between two atoms results from the maximum overlap of two pure or hybrid AO’s each containing one electron of anti-parallel spins, thus a larger common orbital of two atoms, called bond orbital is formed having a pair of electrons of opposite spins. The probability of finding the electron pair is the maximum between the two nuclei of the bonded atoms.
2. Each electron of the shared pair has an equal probability of being found in its own atom as well as in the other atom and each nucleus may be associated with equally with both of the electrons, i.e. exchange of electrons between bonding atoms is a condition to form a covalent bond.

**Shape and Orientation of Bond Orbitals:**

Bond orbitals may be sigma (σ), pi (π), delta (δ), banana, etc. but organic chemistry basically involved σ &π - orbitals and in some extent banana or bent bonds.

**Sigma (σ –) Bonds**:

A sigma bond orbital is formed when two AO’s pure or hybrid, overlap around their axes, i.e. head – to – head. An axis is the imaginary line which joins two nuclei and is known as bond axis. Sigma orbital is bigger in size than that of the overlapping AO’s. It has cylindrical charge density around the bond axis and hence symmetrical in nature. The charge density is the maximum between the nuclei. The bond formed by head – to – head overlap is called sigma (σ) bond.

Because of the symmetrical charge density of the σ – bond orbital, σ – bonds are strong, single bonds are σ – bonds. These may result in the overlap of several types of AO’s. Some of them are:



Actually, head – to – head overlap of lobes of like sign () give rise to sigma bond orbital. Some of the σ – bond formation is shown below:



**Pi – (π –) Bonds**:

The bond orbital formed by the side – to – side overlap of two parallel AO’s is known as pi – bond orbital. It has a maximum charge density in its cross – sectional plane. The perpendicular to it has no charge density and is called nodal plane, i.e. a plane of no charge density. The bond formed by side – to – side overlap is known as π - bond. As in π - bonds, bond axis lies in the plane of no electron charge density, hence π - bonds are weaker in nature and easy to break. A double bond is considered to consist of one σ – bond and one π - bonds, triple bonds may be supposed to have one σ – bond and two π - bonds. π - Bonds are formed by  and  overlap.



**Banana Bond Orbital**:

Oblique overlap of two AO’s produces bent bond or banana bond. Obviously, this type of overlap is neither head – to – head nor side – to – side and may be taken as an intermediate between the two types. Normally the charge density along the bond axis is very minimum and hence is weak. overlap can form such type of orbitals.

**MOT: Molecular Orbital Theory**: —

MOT starts with the consideration that after the covalent bond formation the concerned electrons do not belong to their individual atoms. Instead associated themselves with the molecules as a whole embracing all the nuclei; the nuclei in their turn, remain in equilibrium positions. Following are the important features of MOT:

1. A covalent bond is formed by the overlap of two AO’s – one from each atom.
2. The interaction of two AO’s forms two new MO’s — sum of the energies of 2 MO’s is equal to the sum of two interacting AO’s. The MO having lower energy is called Bonding Molecular Orbital (BMO) and that has higher energy is called Anti-bonding Molecular Orbital (ABMO).
3. MO’s are of different types viz. σ, π, δ, tec. In fact, bond orbitals in VBT are the MO’s in MOT.
4. The outer AO’s of similar energy only overlap, inner AO’s remaining undisturbed. Outer AO’s of each atom may mix up before forming MO’s. This is not actually equal to the hybridization of AO’s but for convenience it may be taken as such.
5. The energy order of MO’s in a molecule are:



Where ‘\*’ denotes the anti-bonding MO’s and the process of filling in of MO’s is identical to that of AO’s i.e. follows Aufbau principle, Pauli’s exclusion principle and Hund’s rule of maximum spin multiplicity.

1. A covalent bond will form only if number of bonded electrons are greater than to that of anti-bonding electrons, such that,

Bond order  //

**Formation of Nitrogen molecule by VBT**:

Ground state electronic configuration of N (7) → 

In the excited state, each of the N – atoms forms two linear  hybrid orbitals;  orbitals are oriented mutually perpendicular to each other of thehybrid orbitals.



Two  hybrid AO’s one from each N – atom, overlap head – to – head to form an σ – bond. The other  AO of each N – atom contains lone pair of electrons. Now  orbitals of each N – atom being parallel to each other, they overlap side – by – side and thus a π - bond is formed. Similarly,  orbitals of two N – atoms overlap side – by – side to form another π - bond. Owing to the formation of two π - bonds and greater s – character of the σ – bond (for involvement of – AO’s) the internuclear distance between two N – atoms is very small and they are, therefore, hold together very strongly by the Coulomb’s force of attraction between the nuclei and electrons; hence the N2 – molecule will be inert in nature. The formation of three covalent bonds release much of energy and the molecule is, therefore, exceptionally stable. The bonding between two N – atoms are given in the figure given below:



Figure: Formation of Nitrogen molecule by MOT:

**Orbital Representation: Quantum Numbers**: —

The numbers that are used to designate the actual state of an atom completely are called quantum numbers. These are of 4 – types —

1. **Principal Quantum Number** (): → designated by  and it indicates the principal energy level of the orbital of the electron.



Thus, the permitted values of 

And the total number of electrons that can be present in a principal shell 

1. **Azimuthal or Angular Momentum Quantum Number** (): → designated by  and it indicated the shape of the orbital.

Values of, depends on the value of 

For any value of,  i.e. total - values



1. **Magnetic Quantum Number** (): → designated by  and it indicates the orientation of the angular momentum of the orbital in an applied magnetic field.

Values of, depends on the value of, and

For any values of, i.e. total values

1. **Spin Quantum Number** (): → designated by  and it indicates the spin momentum of the electron. For any value of,  - values are 

Thus,

for = 2,  = 0 and 1

Implies  and  atomic orbitals.

**[Question**: Why “*2d*” orbital does not exist?]

**Shape, Size and Orientation of AO’s**:

**-Orbital**:

For - orbital,  = 0

 = 0, i.e. no direction

Hence, - orbitals are spherical; the charge density is symmetrically oriented about the nucleus but decreases with increasing distance from the nucleus. Spherical symmetry of the orbital gives rise to two important properties:

1. It is a non – directional orbital and
2. Electrons of this orbital are very strongly bound to the nucleus.

The size of the - orbitals of different elements is different. The decreasing order of - orbital is





**-Orbital**:

For - orbitals,  = 1

 = –1, 0, +1 i.e. are oriented in three directions .

Hence there are three degenerate sub-orbitals for a - AO, viz..

The shape of a 2p – orbitals resembles a dumb – bell, and in such orbitals, there is no chance of finding an electron at the nucleus. The nucleus therefore is called a node point, and the plane through it is called nodal plane, in which probability of finding the electron is zero. 

**Note:**

To describe carbon compounds —

We generally need - pure atomic orbitals. However, to describe the molecular structure of - compounds we need to consider mixed orbitals, called **hybrid orbitals** instead of pure AO’s. It should be remembered that all the AO’s; pure or AO’s are the results of wave equation. Finally, the AO’s of ground state atom do not mix up.

**Hybridization**:

The phenomenon of intermixing of the pure atomic orbitals of comparable energy and the formation of completely new orbitals of equal energy (degenerate orbitals) is known as **hybridization** and the new orbitals are called **hybrid orbitals**. The bonds formed by such orbitals are called **hybrid bonds**. The compounds which are formed from these bonds are known as hybrids.

**Conditions for Hybridization**:

Following are the rules for hybridization —

**Rule I**: Only orbitals of similar energies belonging to the same atom or ion can undergo hybridization.

**Rule II**: Number of hybrid orbitals produced is equal to the number of orbitals mixed. Hybrid bonds are stronger than the single non – hybrid bonds of comparable energy.

**Rule III**: Most of the hybrid orbitals are similar but they are not necessarily identical in shape. They differ from one another in orientation in space.

**Rule IV**: For equivalent hybrids, the orientation in space is determined by (a) the number of orbital mixed and consequently the number of hybrid obtained and (b) which of X, Y & Z directions are preferred by the pure atomic orbitals.

**Rule V**: Once the orbital has been used to build a hybrid it is then no longer available to hold electrons in its pure form.

**Rule VI**: The type of hybridization indicates the geometry of molecules. From the type of hybridization, one can tell about the bond angles and structure. Some of these are shown below in tabular form:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Serial No | Shape of the molecule | Hybrid type | Bond angles (in degree) | Examples |
| 1.  2.  3.  4.  5.  6. | Linear  Planar  Tetrahedral  Square planar  Trigonal pyramidal  Octahedral | *sp2*  *sp3*  *dsp2*  *dsp3*  *sp3d2* | 180  120  109.5  90  90, 120  90 | BeCl2, HgCl2, C2H2  BF3, BCl3, CO32-, NO3-, C2H4  CH4, NH4+, BH4-, SO42-  [Ni(CN)4]2-, [PtCl4]2-  PF5, PCl5  [CrF6]3-, SF6, [Co(NH3)6]3+ |

**- Hybridization**:

**- Hybridization**:

**- Hybridization**:

**Bond Length**:

Bond length is a 1D’al parameter and it is measured by the distance between the atomic nuclei joined by single or multiple bonds. Actually, the average distance between atoms in molecules which are actually vibrating is called bond length. The length of a chemical bond is the result of a balance of attractive and repulsive forces between the atoms which are bonded. Bond lengths are experimentally determined by various diffraction and spectral techniques, and are measured in angstrom unit (Å, 1Å = 10 –8 cm = 10 –10 m = 0.1 nm) or in nanometres (1 nm = 10 –7 cm = 10 –9m = 10Å).

[**Important**: The single bond lengths between two particular atoms A & B, are found to be almost constant in their different types of compounds. For example, C — C bond length in diamond as well as in propane is found to be same and it is 1.54Å. This is also true for double and triple bonds]

If two atoms are capable of forming single, double and triple bonds between them, then it is found that



**Bond length basically depends on** —

1. **Nature of the overlapping orbitals**: ***s –*** orbitals being symmetrical in nature, greater is the***s –*** character in the overlapping AO, shorter is the bond length.
2. **Resonance**: Ionic structures involved in resonance hybrid of a molecule make the ions come closer to each other and hence bond distance decreases.



Some of the typical bond lengths in Å are given below:

**Note:** Atoms below the second row of the periodic table form relatively larger bonds in order to accommodate their larger sizes — *cf*. C — F < C — Cl< C — Br < C — I

**Correlation between the Structure and Bond Length**:

Smaller the internuclear distance, i.e. bond length, the stronger the bond. For example —

**Bond** **Bond length (Å)** **Bond Energy (– 1)**

C — C 1.54 83

C = C 1.34 146

C ≡ C 1.20 200

**Question:** Why the C — C bond length in ethene (1.34 Å) is larger than that in tetrafluoroethene (F2C = CF2, 1.31 Å)?

**Solution**: Hints:

**Bond** **Bond length (Å)** **Bond Energy (– 1)**

C — H 1.1 99

C — F 1.39 116

**Bond Energies and Bond Strength**:

Bond energies are specified in 2 – ways viz.

1. The average bond energy and
2. Bond dissociation energy.

Both are represented in –1 or –1

In CH4, there are 4 C — H bonds, each required 413.35–1 to break but 1653.4 –1 is needed to break all the bonds. So, the average bond dissociation energy for CH4 is 1653.4/ 4 = 413.35–1. This average bond dissociation energy is called **bond energy**.

Bond dissociation energy and bond formation energy are exactly same, i.e. the amount of energy required to break a chemical bond to form two atoms, exactly same amount of energy is released when they combine to form the molecule.

Bond energy is a measure of bond strength. Greater is the bond dissociation energy; greater is the stability of the bond.

**Dependence of Bond Energies**:

1. If ***s*** – character of the involved AO’s in the bond formation increases, the bond strength, i.e. the bond energy increases. For example,

C — H Bond energy in CH4 (*sp3, s* = 25 %) = 413.3 –1

C2H4 (*sp2, s* = 33.3 %) = 506.4 –1

C2H2 (*, s* = 50 %) = 836.0 –1, etc.

1. Normally, greater is the overlap of orbitals to form the bond, greater is its stability and higher its bond dissociation energy. For example,

σ – Bonds are stronger than π - bonds

1. With the decreasing electronegativity or increasing size, bond energy decreases. For example,

C — F C — Cl C — Br C — I

439.6 330.75 276.3 238.6 k J mol–1

**Bond Angle ()**:

Bond angle is a 2D’al molecular parameter and is measured by the angle subtended by two atoms covalently linked to a 3rd atom. For example, in the covalent molecule ACB, with ‘C’ as central atom, bond angle is represented as:



Dihedral angle (θ), is a 3D’al parameter and it is the angle between the two planes containing x ― C1― C2 and C1 ― C2 ― y, respectively, in a molecule x ― C1― C2 ― y, for example,



**\*Correlation between Bond length (l), Bond angle (α) and Hybrid state:**

Both the Bond length (l) and Bond angle (α) of hybridized C – compounds depend on the nature of the hybridised state of the C – atom.

As the s – character increases in the hybrid orbitals from , the efficiency of the overlap of orbitals by the head-on approach increases. This results in a bond shortening. This is the reason why the C ― H bond length in alkynes is the shortest one and in alkanes it is the largest one.

In the case of 2D’al molecular parameter, that is, the bond angle in C – compounds, the **percentage of s – character in the hybridized state of the central atom is important to determine the bond angle of the compound**. For example, if the s – character in the hybridized state of the C – atom is 25%, then the interorbital angle (α) will be given by the relation ―



That is why in a purely - hybridized state of the C – atom, the bond angle of its compound remains equal to.

The % contribution of the orbital in the C – atom toward its hybridized state is governed by the criterion of a favourable orientation of the orbitals for the best overlap. In general, as the **electronegativity** difference () between the C – atom and the other atom bonded to it increases, the % of s – character in the hybrid AOs used by the C – atom in forming such bonds decreases. This **results in shrinking of the bond angle**. For example,

In the - hybridized molecule(dichloro methane), the hybrid AOs used by the central - atom to form two and two bonds are not equivalent.

The hybrid AOs used to form bonds has lesser, and those used in bonds have higher -contribution. This is due to the fact that the electronegativity difference of atoms is greater than that of the atoms. Experimentally, it has been found that all the bond angles of the - atom in are not equal. The bond angle is  and the bond angle is. Thus, though is - hybridized and tetrahedral in shape, bond angles are not.

In a similar way, it can be explained why bond angle in water molecule is . The electronegativity difference between – atoms causes 20% s – contributions to the hybrid orbitals used by O – atom to form an  molecule. This means that the inter orbital angle in the  molecule is ―





**Heats of reaction**:

The energy associated with breaking or making of bonds during a chemical transformation is known as heat of reaction and is measured in terms of a change of enthalpy (ΔH), which is defined as



For example, for the reaction: 





**Dipole Moments:**(): ― **Polarity of Bonds & Electronegativity**

Dipole Moments () is a vector quantity, and can be defined as the product of the electric charge () and the distance () between the charges (positive & negative charges). Thus,

Since, electric charge, is of the order of; and distance between the charges, is of the order of , thereforeis of the order of , and this unit is known as the Debye () unit. The value of dipole moments gives an indication of relative polarities of bonds in different molecules.

The dipole moment values of some molecules in Debye are listed below:

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Molecule | - Value (D) | Molecule | - Value (D) | Molecule | - Value (D) |
|  | 0 |  | 1.75 |  | 0 |
|  | 0 |  | 1.84 |  | 1.86 |
|  | 0 |  | 1.46 |  | 0 |
|  | 0 |  | 0.24 |  | 0 |
|  | 0 |  | 0 |  | etc. |

**Discussions from the µ values of the molecules from the table:**

Molecules like , , ,  and  have zero dipole moments (), that are non-polar. The two identical atoms of each of these molecules have, of course, the same electronegativity and share electrons equally. Thus, in the equation and hence, .

A molecule like has the large dipole moment of . Although, hydrogen fluoride is a small molecule, the very high electronegative fluorine pulls the electrons strongly; although  is small,  is large in the equation and hence  is large, too.



Polarity of a molecule depends not only upon the polarity of its individual bonds but also upon the way the bonds are directed, that is, upon the shape of the molecule (structure).

For example,  and ― the symmetric top molecules have zero dipole moments, though their individual bonds are polar. Because of the very symmetrical tetrahedral arrangement, the individual bonds bond moments cancel each other out, and as a result the resultant dipole moment is zero for such molecules.

But, in the case of methyl chloride,, the polarity of the C ―Cl bond is not cancelled, and  has a dipole moment of 1.86 D.



Ammonia has a dipole moment of 1.46D. This could be accounted for as a net dipole moment (a vector sum) resulting from the three individual bond moments, and would be in the direction shown in the diagram. In a similar way, we could account for water’s dipole moment of 1.84D.



**Dipole moments incompared with**:

Nitrogen trifluoride,like ammonia is a pyramidal molecule. Fluorine is the most electronegative element of all and should certainly pull electrons strongly from nitrogen: Thebonds should be highly polar, and their vector sum should be large ― far larger than for ammonia with its modestly polar bonds.



Nitrogen trifluoride has a dipole moment of only 0.24D, and that for ammonia is 1.46, i.e. rather much smaller dipole moment value for nitrogen trifluoride compared with ammonia. This can be accounted by considering the effect of lone pair (unshared) electron on the central atom as ―

In(as in) the unshared electron pair occupies an  hybrid orbital and this must contribute a dipole moment in the direction opposite to that of the net moment of the bonds as shown below. These opposing moments are evidently of about the same size, and as a result is a small moment, in which direction we cannot say. Inthe observed moment is probably due to chiefly to the unshared pair, augmented by the sum of the bond moments.

In a similar way, unshared pairs of electrons must contribute to the dipole moment of water and, indeed, of any molecules in which they appear.



**Correlation between the Dipole moment value and Structure of the Molecule:**

Dipole moments can give valuable information about the structure of molecules. For example, any structure for that would result in a polar molecule can be ruled out on the basis of dipole moment alone. The evidence of dipole moment thus supports the tetrahedral structure for carbon tetrachloride. Similarly, zero value of dipole moment for carbon dioxide molecule suggests a linear structure for the molecule.