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ISOMERISM

Education

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KEYWORDS

Hydrocarbons show isomerism in succession with the addition of the carbon in the linear chain.The organic compounds with similar molecular formulae but different structural formulae are known as isomers and the phenomenon is known as Isomerism.The simpler hydrocarbons such as Methane,Ethane,and Propane show linear structure and they have normal structural formula. In these cases, the original substance acts as the isomer of itself.The self mirror image is the property.The physical properties of these compounds are relatively stable and they show conformation properties. When there are more than three carbon atoms in the chain the structural isomers are created for example, normal butane and iso-butane.

$CH_3-CH_2-CH_2-CH_3$

n-Butane

$_3HC-CH-CH_3-CH_3$

Iso Butane

Isomerism: The phenomena of existence of two or more compounds possessing the same molecular formula but different properties is known as Isomerism. Such compounds are called Isomers. The compounds having molecular formula, structure and shape as mirror image but having different properties are showing Isomerism.

Isomerism is the existence of chemical compounds (isomers) that have the same molecular formulae but different molecular structures or different arrangements of atoms in space. There are different types of Isomerism in Organic Chemistry. They are:

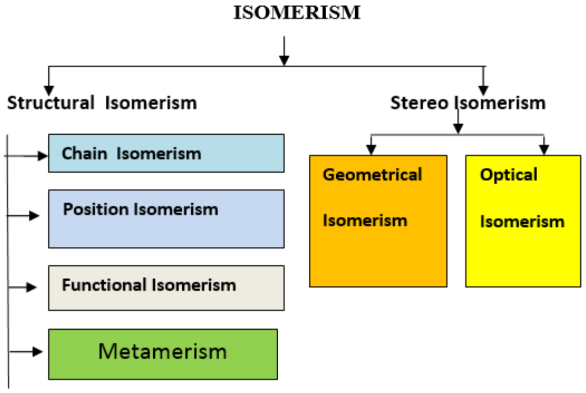


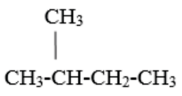
Figure No. 1 Flow chart showing types of Isomerism

Structural Isomerism: Compounds having the same molecular formula but different structures (showing different linkages) are classified as structural isomers. In structural isomerism the molecules have different types of molecular structures i.e. they may be of different types or they may simply differ in the position of the functional group in the molecule. Structural isomers generally have different physical and chemical properties. Cotton and Wilkinson have remarked that isomers are the true representation of chemical species and demonstrate different properties. The different types of structural isomerism are shown below:

I. Chain Isomerism: When two are more compounds have similar molecular formula but different carbon skeletons is termed as chain isomerism for example, C_5H_{12}

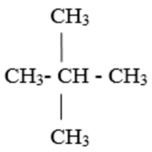
$CH_3-CH_2-CH_2-CH_2-CH_3$

Pentane


$CH_3-\overset{\overset{CH_3}{|}}{CH}-CH_2-CH_3$

Isopentane

(2- Methyl butane)


$CH_3-\underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{CH}}-CH_3$

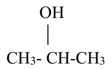
Neopentane

(2,2-Dimethyl Propane)

ii. Position Isomerism: When two or more compounds differ in the position of substituent atom or functional group on the carbon skeleton,they are called as position isomers and this phenomenon is termed as Position Isomerism for example, the molecular formula C_3H_8O represents two alcohols:

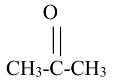
$CH_3\ CH_2\ CH_2OH$

Propan-1ol

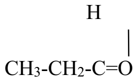

$CH_3-\overset{\overset{OH}{|}}{CH}-CH_3$

Propan-2-ol

iii. Functional group Isomerism: two or more compounds having the same molecular formula but different functional group are called functional isomers and this phenomenon is called as functional group isomerism for example, the molecular formula C_3H_6O represents an aldehyde and a ketone.


$CH_3-\overset{\overset{O}{||}}{C}-CH_3$

Propanone

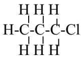

$CH_3-CH_2-\overset{\overset{H}{|}}{C}=O$

Proponal

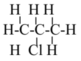
iv. Metamerism: It arises due to different alkyl chains on either side of the functional group in the molecule for example,
($CH_3OC_3H_7$) and ethoxyethane [$C_2H_5O\ C_2H_5$].

Stereo Isomerism: The compounds that have the same constitution and sequence of covalent bonds but differ in relative positions of their atoms or groups in space are called Stereo isomerism and it is further classified as geometrical isomerism and optical isomerism.

The optical isomerism requires that one of the carbon in the chain is asymmetrical. On passing the unipolar light over the substance, when the light is deflected to the left it is called as Levos rotation represented by (-) and when the light is deflected to the right is called as dexterous rotation represented by (+). Most of the known optical isomers are dexterous rotation showing substances exhibiting a tilt in the positioning of the molecules. This is also called as 'Cis-trans' isomerism in which the isomers have different positions of groups with respect to a double bond or central atom. Octahedral complexes can display Cis-trans isomerism if they have formulae of the type MX_2Y_4. Octahedral complexes with formulae of the type MX_2Y3 can display a different type of isomerism. If the three X legands are in a plane that includes the metal atom and the three Y legands are in a different plane at right angles, then the structure is a mer-isomer(meridional). If the three X ligands are all on one face of the octahedron and the three Y ligands are on an opposite face, then it is a fac-isomer(facial).

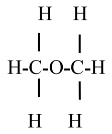

$H-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-Cl$

-Chloropropane


$H-\underset{H}{\overset{H}{C}}-\underset{Cl}{\overset{H}{C}}-\underset{H}{\overset{H}{C}}-H$

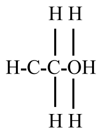
2-Chloropropane

These are the examples of structural isomers in which the functional group has different positions.



$\mathrm{H}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\mathrm{O}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\mathrm{H}$

Methoxymethane

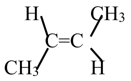


$\mathrm{H}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\mathrm{OH}$

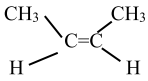
Ethanol

These are structural isomers in which the functional groups are different.

Cis-Trans isomers:

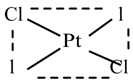


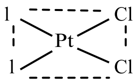
Trans-but 2-ene

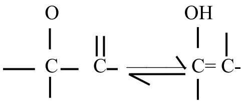


Cis-but-2 ene

Cis-trans isomers in which the groups are distributed on a double bond. The following example shows the cis-trans isomers in a square –planar complex.

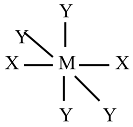




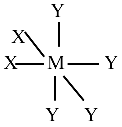


Keto form Enol form

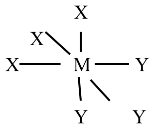
Keto-enol tautomerism



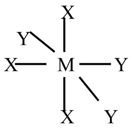
Trans Isomer



Cis Isomer



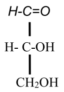
Fac Isomer



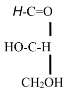
Mer Isomer

Figure No. 2 Showing Different Types of Isomers

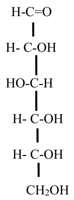
Stereo isomerism is an important characteristic to identify the mono saccharides. Stereo isomers are compounds that are optically active. Stereo isomers are the compounds that have the same structural formulae but differ in their special configuration. In this, the carbon is asymmetric when it is attaché to four different atoms or groups. The number of asymmetric carbon atoms (n) determines the possible isomers of a given compound which is equal to 2^n . Glucose contains 4 asymmetric carbons and thus has 16 isomers. It could be observed that more the isomers more are the optical activity. For this reason preserving the optical substance such as Glucose for longer time is difficult.



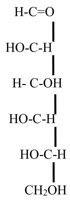
D-Glyceraldehyde



L-Glyceraldehyde



D-Glucose

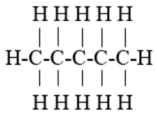


L-Glucose

Figure No. 3 Showing *D and L –isomers –Optical activity of Sugars*

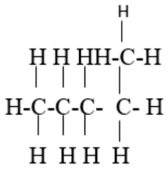
Isomerism in Hydrocarbons: These hydrocarbons (Methane, Ethane, and Propane) are considered as the saturated hydrocarbons for all the valences of the carbon in the chain are satisfied. The stretch in the IR spectra is relatively stable. The physical properties are relatively stable. All of them are naturally in the gaseous state.

Under relatively more pressure in an enclosed place or in an air tight container, these gases could transform into liquid state.Their ignition temperature is relatively low. The compounds of Ethane such as Ethyl alcohol, n-butane in the gaseous state are used as fuels in automobiles. In the case of comparison of physical properties of n-butane with that of the iso-butane it is clear that they exhibit different physical properties. In unbranched chain structure not more than two carbon atoms are connected with each other but in branched chain structure at least one carbon atom is connected with other three carbon atoms. Pentane shows three isomers. They are: n-pentane, iso-pentane and neo-pentane.



$\mathrm{H}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\underset{\mathrm{H}}{\overset{\mathrm{H}}{\mathrm{C}}}-\mathrm{H}$

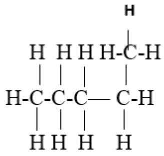
n-Pentane



Iso Pentane

Figure No. 4.1 Pentane in different forms

The increase in the carbon atom in the alkane increases the likelihood of increase of the isomer. The successive alkane has shown more isomers in the increasing order. The number of isomers increasing closely corresponds to the structural isomers up to Heptane .



Neo Pentane

Figure No. 4.2 Pentane in different forms

The later alkanes show more isomers with varied physical properties. The important characteristic of alkanes is that they are more saturated than the alkenes and alkynes. The higher the alkane, it is more likely that it is found in combined state with the other lower alkanes. The combustion of these gases results in very low order alkane such as Methane. The disintegration also shows similar results for example, petroleum cracking process. The alkanes show relatively stable structure and physical properties. The number of compounds formed in the increasing order of the alkanes shows that the compounds are more in almost all the alkanes. The modern process in chemistry has helped in the increased use of the alkanes such as Methane, Ethane for the preparation of many organic compounds in the laboratory as well as in the industries. This is possible to chemists for in the modern days to separate the gases and identify with the help of gas chromatographic techniques(GC/MS Spectrophotometer has helped in the separation better in the recent period in the laboratory).Table No.1 shows the number of isomers of Alkanes. It may be observed that the number of isomers are less up to Heptane and later alkanes have many isomers. This makes the task of isolating the isomers more difficult as one moves from the lower alkanes to the higher alkanes. The transformations are rather uniform. It results in a thinking of that the hydrocarbons have the same properties.

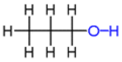
Table No.1 showing number of isomers of Alkanes

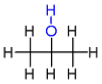
Name of Alkane	Number of Carbon	Number of Isomers
Methane	1	1

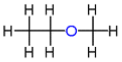
Ethane	2	1
Propane	3	1
Butane	4	2
Pentane	5	3
Hexane	6	5
Heptane	7	9
Octane	8	18
Nonane	9	35
Decane	10	75
Undecane	11	159
Dodecane	12	355
Tridecane	13	802
Tetradecane	14	1858
Pentadecane	15	4347
Hexadecane	16	10359
Heptadecane	17	24894
Octadecane	18	60523

The homologous structures have lead to homologous properties. However, the alkane being more saturated than the alkenes and alkynes shows more stability and uniformity. Alkanes show conformation reaction and other hydrocarbons such as alkenes and alkynes do not show conformation reaction. Table No.1 shows the number of isomers of Alkanes. The alkanes are stable under standard temperature and pressure. However, when a chance is available for the mixing of different alkanes, alkanes mix with each other. However, it becomes easier to separate them for they do not react easily with each other. They readily react with alcohol to produce Methyl alcohol, Ethyl alcohol etc.

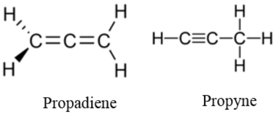
In **skeletal isomers** the main carbon chain is different between the two isomers. This type of isomerism is most identifiable in secondary and tertiary alcohol isomers.Tautomers are structural isomers of the same chemical substance that spontaneously interconvert with each other, even when pure. They have different chemical properties and, as a consequence, distinct reactions characteristic to each form are observed. If the interconversion reaction is fast enough, tautomers cannot be isolated from each other.An example is when they differ by the position of a proton, such as in keto/enol tautomerism, where the proton is alternately on the carbon or oxygen for example: propanols and methoxyethane. A simple example of isomerism is given by propanol: It has the formula C_3H_8O (or C_3H_7OH) and occurs as two isomers: propan-1-ol (n-propyl alcohol; **I**) and propan-2-ol (isopropyl alcohol;**II**).


I


II

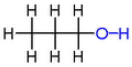

III

Note that the position of the oxygen atom differs between the two: It is attached to an end carbon in the first isomer, and to the center carbon in the second.There is, however, another isomer of C_3H_8O that has significantly different properties: methoxyethane (methyl-ethyl-ether; **III**). Unlike the isomers of propanol, methoxyethane has an oxygen connected to two carbons rather than to one carbon and one hydrogen. Methoxyethane is an ether, not an alcohol, because it lacks a hydroxyl group, and it has chemical properties more similar to other ethers than to either of the above alcohol isomers for example: propadiene and propyne.Propadiene (or *allene*) and propyne (or *methylacetylene*) are examples of isomers containing different bond types. Propadiene contains two double bonds, whereas propyne contains one triple bond.



Example: propanols and methoxyethane

A simple example of isomerism is given by propanol: It has the formula C_3H_8O (or C_3H_7OH) and occurs as two isomers: propan-1-ol (n-propyl alcohol; **I**) and propan-2-ol (isopropyl alcohol; **II**)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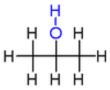
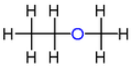
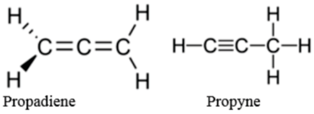

II


III



A covalent bond can get cleaved either by (i) heterolytic cleavage or by (ii) hemolytic cleavage.

Inductive effect: A highly electronegative element such as Fluorine, Chlorine, Bromine or Iodine tries to draw the electrons towards itself. This shows orientation. This is called as inductive effect. This effect is observed clearly in the Friedel Craft reaction. This is a common aspect in the halogenation of compounds.

Nomenclature and Isomerism: In Benzene, the six hydrogen atoms resonate with each other with cyclic arrangement of the six carbon chain. It shows two forms as follows (it is an artificial representation of the alternate forms):

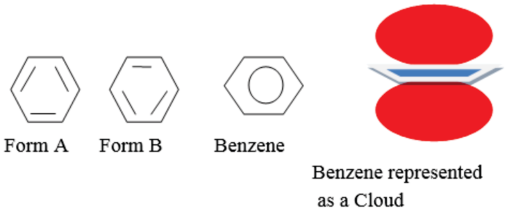


Figure No.5 Showing the isomeric representation of the benzene and its compounds.

The Kekule (1865)gave the structure of benzene as in two forms A and B. However, the resonating structures were having equalizing effect due to resonating single and double bonds.The recent understanding of the Benzene as given by Linus Pauling is that the benzene is in a cloud of alternate bonds shared equally with sharing electrons. The examples for the isomeric substances are : 1, 2 dibromobenzenes(o-xylene).Benzene has around 108 compounds formed (one of the more interactive element) however, Benzene shows reluctance in addition reactions.

In 1825, Michael Faraday gave the molecular formula of Benzene as C_6H_6. Benzene was found to be a stable molecule and form a triozonide which indicates the presence of three double bonds. Benzene was further found to produce one monosubstituted derivative which indicated that all the six carbon and six hydrogen atoms of benzene are identical.

Isomers in Nano forms as coordination compounds-the example being reviewed is the Iron and its iso mers: Melnik ,M and Kohutova,M(2010) states that the systematic studies in the field stereoselectivity of coordination compounds over the last 50 years of increasing interest. Stereo selectivity of biological systems, catalysis and stereochemical effects in technical processes. Isomers can be categorized into two major categories , Structural and Stereoisomers. The structural isomerism is sub divided into ionization, hydrate, coordination, linkage, and polymerization. The Geometric isomers are further classified as Cis, -trans, fac, -mer , optical and distortion isomers.(Please see the types of isomers in graphic forms- on page No.2).Melnik,M and Kohutova,M (2010) have surveyed covering the crystallographic and structural data of almost one thousand and three hundred coordination complexes. About 6.7% of these complexes exist as isomers. It includes distortion(96.6%) and cis- trans (3.4%) isomers. The coordination of the iron atom depends on the oxidation number, bond length, and inter bond angles.

Distortion isomers, differing in degree of distortion in Fe-L, Fe-L-Fe and L-Fe-L parameters, are the most common. Iron is found in the oxidation states of Zero, +2 and +3 of which +3 is most common. The stereochemistry around iron centers are tetrahedral, five-coordinated(mostly trigonal-bipyramid) and six –coordinated. The most common legends have O and N donor sites.

Iron exists in a wide range of oxidation states from -2 to +4 and +6 including mixed oxidation states [average Fe(II),Fe(III) or Fe(III) Fe (IV)].Of these oxidation states of +2 and +3 are most common. In the Iron co- ordination chemistry almost one hundred twenty isomeric examples are identified and noted. Iron has alpha(α) and gamma (γ) allotropes are observed in Iron. This provides for more orientation to Iron than other substances. Further, Iron shows paramagnetic properties after it is heated in a closed container up to 700 Kelvin. (Please refer Micro solid –Steel).

Monomeric complexes –Isomeric forms: There are three examples which exist in two isomeric forms.It exhibits the characteristic properties in the nano forms also. The two isomeric forms are: Dark red (Fe II{η 6-(pp)2H}PF6·2 H_2O which exists in two crystal classes orthorhombic[4] and monoclinic[4] consists in well separated [FeII {η 6-(pp) 2H}$^+$ cations, PF_6 – anions and water molecules. The hexadentate (pp)2H ligand forms low spin derivatives with a FeN_6 core with the mean Fe-N bond distances of 1.95 Ă and the mean five-membered metallocyclic rings of 82.0 and 81.2°,respectively.

Two isomeric forms of black [FeIII{η 2-(CH_2) 4NCS^3] are homo clinic.In both three homo-bidentate-S,S$'$ ligands created around each iron (III) atom a pseudo-octahedral arrangement (FeS_6). The mean Fe-S bond distances are 2.456Ă and 2.41 Ă.The mean four-membered metallocyclic rings are 72.6 and 74.4° respectively.

CONCLUSION:

There are many applications of the isomers in industry , home and society. A comparative study of the isomers will help the student in properly understanding the structure, transformations and functional basis of the chemical transformations.

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