

Structure Of All Organic Compounds

Compound	Geometry	No of Bonds	Bond Angle	Bond Length	Hybridization
1. Alkanes (ethane)	tetrahedral	① C-H (all σ bonds)	109.5° (true angle)	① C-H (154 pm)	sp ³
↓ carbon atom bonded to four other atoms, so it uses sp ³ -hybrid orbitals to form these bonds.					
		linear overlap of sp ³ of sp ³ -s	hybridization	② C-C (109.5 pm)	
		② 1-C-C linear overlap of sp ³ -sp ³			
2. Cyclo-alkanes (cyclopropane)	carbon atoms form an equilateral triangle.	↳ all sigma bonds.	→ 60° (C-C-C) → form bent bonds → 115° approx. (H-C-H)	→ C-C (151 pm) (sp ³ -s overlap) → C-H (108 pm)	sp ³ 109.5° angle compression
↓ like alkanes, it is bonded to four other atoms, so it uses sp ³ -hybrid orbitals for bond formation.					

1) In case of cyclopropane, the sp³-sp³ overlap of C-C bond is not max. as in case of alkanes. It is bcz in cyclopropane the C-C-C bond angle is 60° and not 109.5° (tetrahedral angle) due to which the orbitals do not overlap exactly along their axes but overlap outside of the inter-nuclear axes and form bent bonds.

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2) The C-C bond of cyclopropane is therefore weaker than C-C bond of alkane, due to less effective overlap of sp^3 hybrid orbitals of cyclopropane.

3) In cyclopropane, the three carbon atoms occupy the corners of an equilateral triangle which results in the bond angles to 60° .

4) Since, the hybridization of carbon is sp^3 , these C-C bond angles should be 109.5° . This deviation from the normal tetrahedral angle of 109.5° to 60° causes a strain in the molecule which is called angle strain.

5) angle strain $\uparrow$ so bond strength $\downarrow$.

$$\rightarrow \text{angle strain} = \left[\frac{\text{original bond angle}}{\text{normal angle}} - 1 \right] \times 100\%$$

e.g. cyclobutane $\therefore 109.5^\circ - 90^\circ = 19.5^\circ$

3. Alkenes	Planar	3 sp^2 hybrid orbitals with each C-atom (coplanar)	120° approx. H-C-H and H-C-C	$\rightarrow C=C$ (134 pm) $\rightarrow C-H$ (108 pm)	sp^2
① 3 orbitals (sp^2) sp^2-sp^2 (C-C) sp^2-s (H) sp^2-s (H) sigma bonds. ↓ all sp^2 orbitals are coplanar ② unhybridized p-orbital $\rightarrow$ remain perpendicular to the plane of hybridized orbitals $\rightarrow$ overlap in sidewise manner (parallel) to form π-bond b/w two carbon atoms.					
$\rightarrow$ carbon atoms are coplanar and the rotation of one C-at w.r.t other is restricted which results in cis/trans isomerism in alkene.					

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of ethane ($1.54 \text{ \AA}$). It is due to $\uparrow$ density b/w carbon atoms.

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4. Alkynes	Linear	$\rightarrow 3$ sigma bond.	180°	$\rightarrow C \equiv C$	sp
(acetylene)		(linear overlap) i) $C-C (sp-sp)$	$(H-C-C)$	(119 pm)	
$\rightarrow$ the cloud of the π -e's is present cylindrically symmetrical abt the $C-C$ σ -bond.		ii) $C-H (sp-s)$		$\rightarrow C-H$	
		iii) $C-H (sp-s)$		$(106 \text{ pm}) \rightarrow H$ (old-K)	
		$\rightarrow 2$ π -bonds		C -atom	
		unhybridized $p-p$ overlap		$2 sp^2$ -orbitals	
				(lie on the same plane).	
geometrical isomer is not possible (both) observed in it.					
$\rightarrow$ each carbon atom has two unhybridized p -orbitals, which are perpendicular to each other and to the plane of sp^2 -hybrid orbitals. They approach each other in a side-wise manner to form two π -bonds.					
				$(p_y-p_y) \ \& \ (p_z-p_z)$	

5. Benzene	planar	(sp^2-sp^2) $\rightarrow C-C (6)$	$\rightarrow 120^\circ$	$\rightarrow C=C$	sp^2
		and $C-H (6)$		(139 pm)	
		(sp^2-s)		$\rightarrow C-H$	
		(planar sp^2 -hybrid orbitals)		(108 pm)	

$\rightarrow$ structure of benzene is best described in terms of molecular orbital hybridization model. (MOT)

$\rightarrow$ each carbon atom has 3 sp^2 and one half-filled unhybridized p -orbital which is perpendicular to the plane of sigma bonds.

$\rightarrow$ the side-wise/lateral overlap of p -orbitals produces delocalized π -molecular orbitals containing six electrons, which are associated with all six carbon atoms.

$\rightarrow$ Stability of Benzene Ring:- due to the extensive π -electron delocalization.

$\rightarrow$ the electronic cloud of these delocalized π -electrons lies half-below and half-above the ring.

(Full concept $\rightarrow$ FTB)

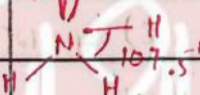
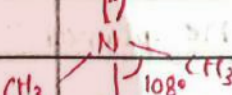
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6. Alkyl Halides (methyl chloride)	tetrahedral	→ all 'C'	→ 109.5° approx	→ C-Cl
		bonds are	H-C-H & H-C-Cl	(178 pm)
		sigma bonds.		→ C-H
		→ 4 sp^3 hybrid orbitals		(108 pm)
	sp^3-s (C-H)	sp^3-s (C-H)	sp^3-s (C-H)	sp^2 half-filled p-orbital of Cl (C-Cl)
	all are sigma bonds			

<u>7. Amines</u>	trigonal pyramidal	→ all are → close to pyramidal sigma bonds.	107-5° 	
	↓		↓	
	 (ammonia)		 (trimethyl amine)	

→ 'N' in amines is sp^3 -hybridized with a lone-pair in one of its sp^3 -hybrid orbitals.

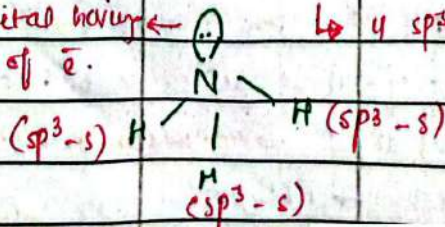
→ Amines are the derivatives of NH_3 molecule where one/more hydrogen atoms have been replaced by alkyl/aryl groups.

→ Since, NH_3 has trigonal pyramidal geometry, the resulting amines also have the same geometry.

→ FTB (amines have nearly tetrahedral structure).

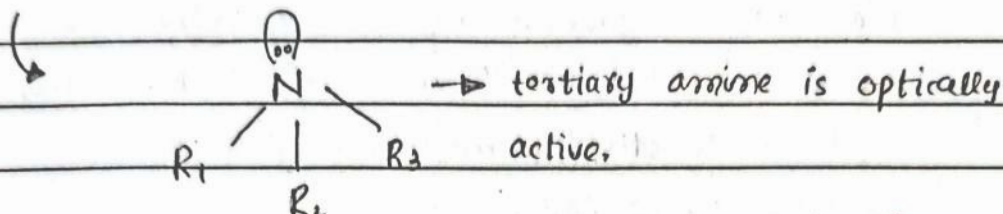
4th sp^3 -orbital having
lone pair of e^- .

↳ 4 sp³ hybrid orbitals

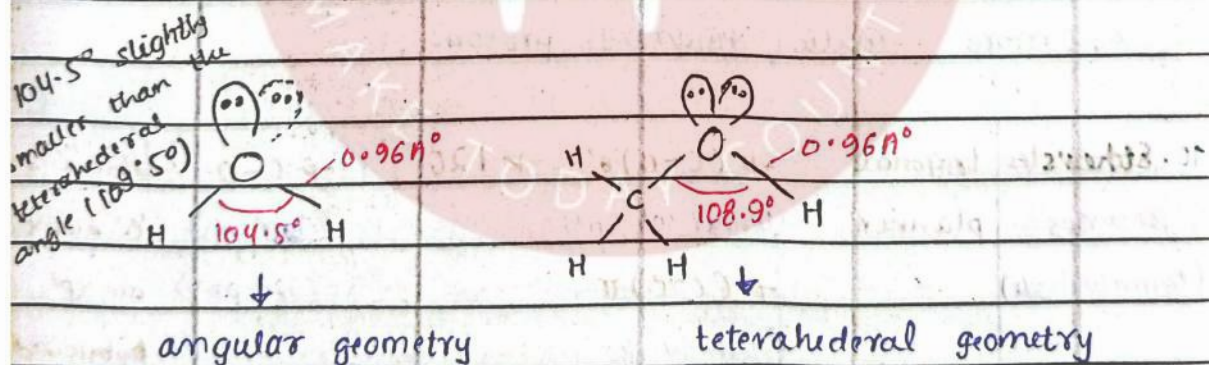


→ the non-bonding $\bar{e}$ -pair is extremely imp in explaining the chemical behaviour of amines bcz it is responsible for the basic & nucleophilic properties of these compounds.

→ An amine with 3 diff. groups is optically active.



3. Alcohols	tetrahedral	→ all are σ bonds.	108.9°	$\rightarrow C-O$ (sp^2-sp^3) (142 pm)	sp^3
alkyl derivatives of H_2O -molecule	↓	has the sp^3 hybridized tetrahedral oxygen atom.		$\rightarrow O-H$ (96 pm)	
		with non-bonding $\bar{e}$ -pairs occupying two of the four sp^3 -hybrid orbitals.			



→ Both the $C-O$ and the $O-H$ bonds are polar due to high ϵN of the O -atom.

3. Phenols	tetrahedral	$\rightarrow C-H$ (σ bond)	$\rightarrow C-O-H$ (109°)	$\rightarrow C-O$ (136 pm)	sp^2
		$\rightarrow C-C$ (σ + delocalized π bond)	$\rightarrow$ internal angles (120°)	$\rightarrow O-H$ (96 pm)	

→ the molecule of phenol is planar.
→ In phenol, six carbon atoms are sp^2 -hybridized forming a hexagonal ring with internal angles to be 120° .

→ Since, the bonds formed by sp^2 -hybridized carbon are shorter than those formed by sp^3 -hybridized carbon; therefore C-O bond length (136 pm) is slightly less than the C-O bond length in methanol (142 pm).

→ In resonance terms, shorter C-O bond in phenol is due to the partial double bond character that results from conjugation of the unshared $\bar{e}$ -pair of the 'O' with the aromatic ring.

→ Phenol differ from alcohols as;

- 1) has shorter C-O bond distance.
- 2) more basic hydroxyl Oxygen.
- 3) more acidic hydroxyl proton.

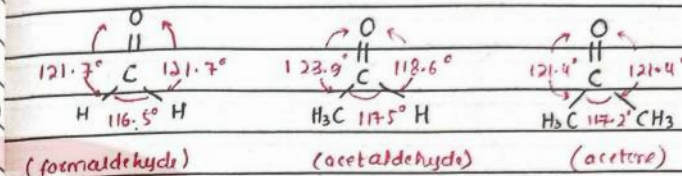
10. Aldehydes	trigonal	→ (C-O) σ	→ 120°	→ C-O
& Ketones	planar	(linear sp^2-sp^2)		(120 pm)
(formaldehyde)		→ (C=O) π		(120 pm)
		(sidewise p-orbital overlap)		
		→ C-H		
		(sp^2-s)		
		ether,		

1) C-O bond length of R-OH (142 pm) > C-O bond length of aldehydes & ketones / carbonyl group (120 pm).

< C-O bond length in ether (142 pm) same as R-OH.

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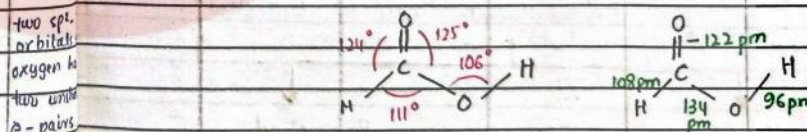
2) Slight deviation from the angle of 120° is observed depending upon the nature of atoms/groups attached to carbonyl carbon.



carboxylic acids.	planar	→ 120°	→ C=O	→ sp^2
		approx. at	(122 pm)	hybridization
		carbon.	→ G-O	both at 'C'
structural features		→ H-C=O	(134 pm)	and 'O'
most apparent in formic acid.		(124°)	→ H-C	
		→ H-C-O	(108 pm)	
		(111°)	→ O-H	
		→ O-C=O	(96 pm)	
		(125°)		

1) C=O (122 pm) < C-O (134 pm).

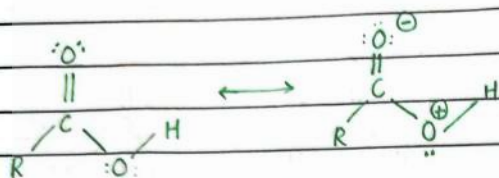
2) C=O (similar to that of aldehydes and ketones).
3) sp^2 -hybridization of hydroxyl oxygen allows one of its unshared $\bar{e}$ -pair to be delocalized by orbital overlap with the pi system of the carbonyl carbon.



→ due to sp^2 -hybridization $COOH$ carbon exhibit trigonal structure.
→ the hydroxyl 'O' allows one of its lone pair $\bar{e}$ s to conjugate with the pi system of the carbonyl carbon group.

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This makes the carboxyl group planar and can be represented with the following resonance structures.



CHAPTER: ORGANIC CHEMISTRY

1.

Classification of Organic Compounds:-

i. Classification On the basis of structure (OLD - CLASSIFICATION)

Open chain / Acyclic
Organic compounds
(Aliphatic compounds)

Closed chain / Cyclic
Organic compounds

i. Open chain / Acyclic Organic Compounds

In these compounds, carbon atoms are linked to each other in open chains which may be branched/unbranched.

Straight

Branched

Saturated

unsaturated

iso

Neo.

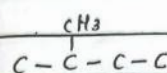
(Alkanes/
paraffins)

i, Alkenes (olefins)

ii, Alkynes (acetylenes).

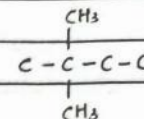
"ISO"

→ having one branch at the 2nd last carbon of a continuous chain.



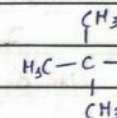
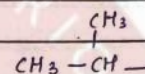
"NEO"

→ having two branches at the 2nd last carbon of the continuous chain.



Representation:- $(CH_3)_2CH-$

$(CH_3)_3C-$



ii, closed chain / Cyclic Organic Compounds

Compounds in which carbon atoms are arranged in the closed chain forms.

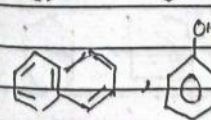
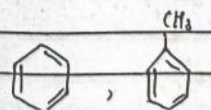
Homocyclic

Heterocyclic

(carbocyclic compounds)

→ those compounds in which cycle/ring is made up of only carbon atoms.

→ those cyclic compounds in which the ring contains at least one atom other than carbon. (N, O, S, P).



(pyridine)



(thiophene)



(Furan)



(pyrrole)

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HOMOCYCLIC

AROMATIC

NON-AROMATIC /
ALICYCLIC

→ those compounds having benzene ring or benzene-like special properties.

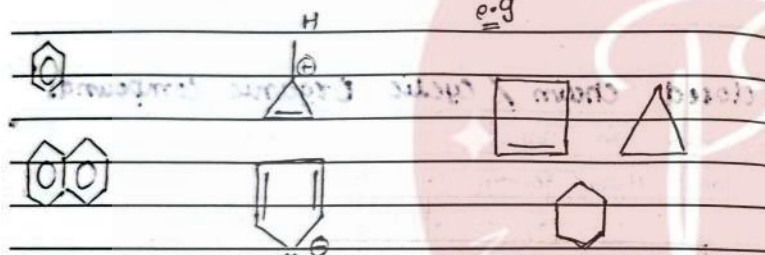
→ they are the cyclic compounds having properties similar to that of open chain alkanes.

→ further divided into

→ may be saturated or unsaturated.

Benzoid

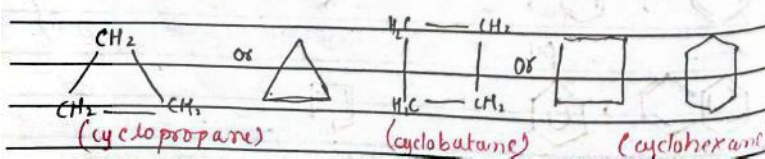
Non-Benzoid



→ Benzoid :- aromatic compounds containing rings like benzene e.g. naphthalene.

→ Non-Benzoid :- compounds are aromatic, they have conjugated systems, planar structures but they lack benzene rings in their structure.

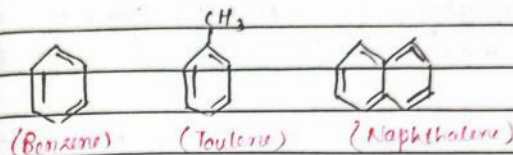
→ Alicyclic Organic compounds :-



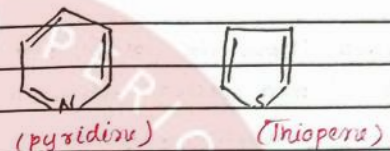
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→ Aromatic Homocyclic Organic compounds :-



→ Heterocyclic Organic compounds :-



b. Classification On the Basis of functional group (modern classification)

2.

Functional Group :-

"An atom or group of atoms that gives certain characteristic properties to an organic compound is called a functional group."

Characteristics :-

- 1) give special properties to a compound.
- 2) It is the chemically active / functional part of a molecule.
- 3) Each functional group represents a diff. class of organic compounds.
- 4) provide a base for classification.
- 5) provide a base for nomenclature.
- 6) site of rxn / active part.
- 7) face of organic compounds.

→ A functional group can also be defined as:
"the atom/group of atoms that replace the hydrogen atoms of hydrocarbons."

→ the properties of an organic molecule are predominantly determined by the properties of the functional group in that compound.

→ Polyfunctional = A molecule can contain more than one functional group. It is then called polyfunctional and the properties of each functional group may be modified by the presence of others.

3. HOMOLOGOUS SERIES :-

→ Definition :-

"a series of organic compounds in which all the members possess similar structural features & similar chemical characteristics but each member differs from the next one by a methylene ($-CH_2$) group (or by 14amu by molar mass) is called homologous series."

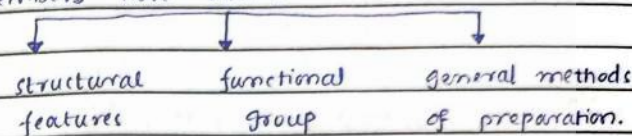
→ Homologues :- the members which differ from each other by methylene group ($-CH_2$).

→ Characteristics of Homologue series :-

- 1) each class of organic comp have its own homologous series having general formula.

② all members have similar chemical properties.

③ members have same



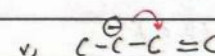
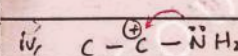
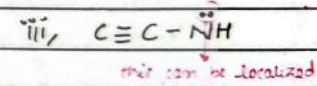
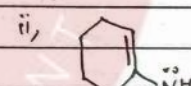
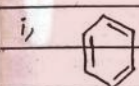
④ the physical properties like (MP, BP, densities etc) inc $\uparrow$ down the series due to inc $\uparrow$ in their molecular mass.

4. CONDITIONS FOR AROMATICITY OF ORGANIC COMPOUNDS:

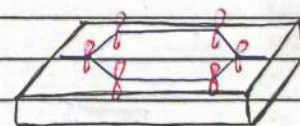
① must be cyclic

② planar (sp^2 hybridized carbon cycle)

③ conjugation (delocalization of π /non-bonded $\bar{e}$ -system)



④ parallel π -orbitals.



A parallel π -orbital refers to the arrangement of multiple π orbitals in a parallel orientation. When

they are aligned parallel to each other, they can interact and form pi-bond.

⑥ follow the Huckel Rule (most imp)

$$(4n+2)\pi = 2, 6, 10, 14, 18, 22$$

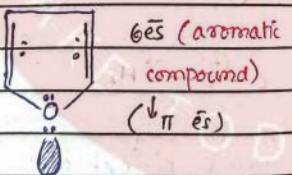
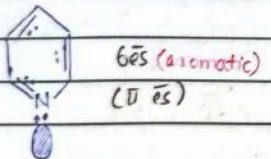
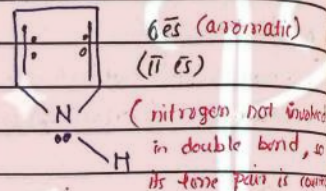
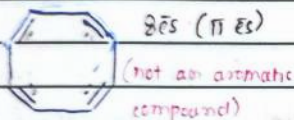
(n=1,2,3,...) (s) (p) (d) (f) (g) (h)

(Aromatic no. of electrons)

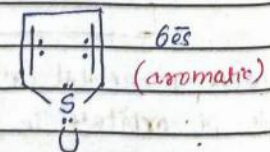
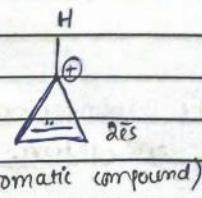
$$= 4, 8, 12, 16, 20, \dots$$

(anti-aromatic no. of electrons)

e.g



→ nitrogen is involved in double bond, so its lone pair is not counted.

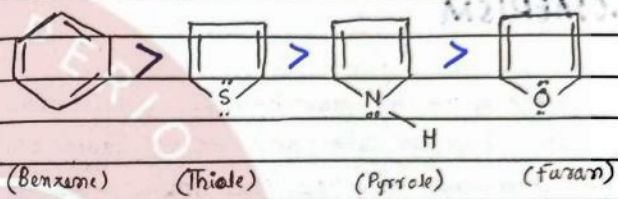


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Aromatic Character:-

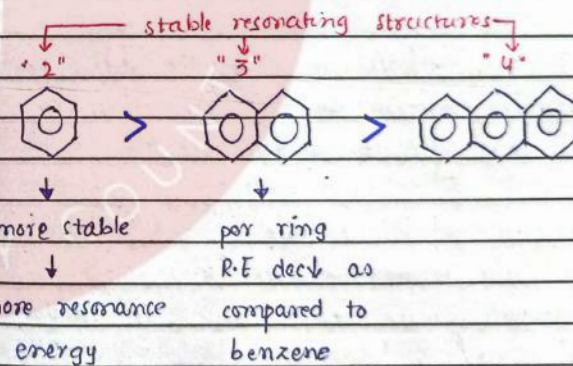
① Aromatic character $\propto \frac{1}{EN}$

- more delocalization, → more aromatic
- more electronegativity → less delocalization
- EN decides the aromaticity.



→ EN Order :- C < S < N < O

→ Resonance Energy or Stability



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Q. CO₂ is cyclic compound? :
 (A) cyclobutane (B) cyclohexane (C) Benzene (D) cyclopentane
 (E) All

Q. CO₂ is cyclic compound but not alicyclic?
 (A) cyclobutane (B) cyclohexane (C) Benzene (D) cyclopentane
 (E) all.

5. ISOMERISM

"the compounds having the same molecular formula but having diff structure and properties are called isomers and the phenomena is called isomerism."

Types :-

1. STRUCTURAL ISOMERISM :-

"the type of the isomerism in which the isomers have same molecular formula but (diff. connectivity) in structure is called structural (isomerism)."

responsible for great variety of organic comp.

- also called constitutional isomerism.
- compounds (same MF and molecular mass)
- same molecular formula means same ; i) molecular weight, ii, vapour density.

1. Chain isomerism:

"the isomerism in which there is a difference in the arrangement of the carbon atoms in the main

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→ main condition for isom.
 → same MF (✓)
 → diff. physical and chemical properties (✓)

chain of the molecule.

OR

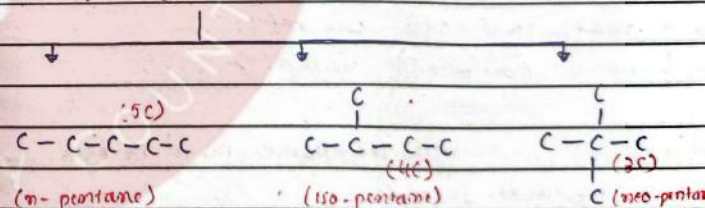
"compounds having the same molecular formula but have different parent chain." / or side chain

- skeleton / Nuclear Isomerism
- diff. in the nature of carbon atoms.
- mainly shown by "alkanes" which show chain isomer and conformational isomerism.

- same :- molecular formula means same
 - i, molecular mass
 - ii, %age composition and atoms
 - iii, functional group (due to this chemical properties are also same).
 - iv, homologue series.

- different :- i) chain and physical properties. ii, IUPAC name

→ example : (C₅H₁₂).



→ To have the chain isomerism:-

- 1) Alkanes :- 4 or greater no. of C-atoms.
- 2) Alkenes :- 4 or greater no. of C-atoms.
- 3) Alkynes :- 5 or greater no. of C-atoms.

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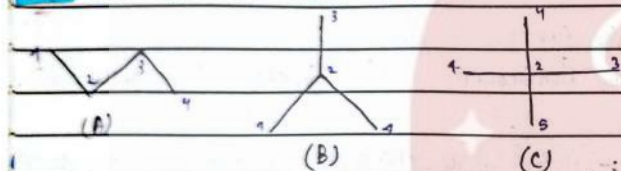
- 1) ketone :- 5 or greater no. of carbon atoms.
2) aldehyde :- 4 or greater no. of carbon atoms.

* Alkane: $[C_1 - C_n]$ $[2^{n-4} + 1]$
 C_8 $[2^{n-4} + 2]$

* Alkene: even no. carbon-atoms $[2^{n-2} + 1]$
odd no. C-atoms $[2^{n-2}]$

* Alkyne: even no. C-atoms $[2^n - (2n-1)]$
odd no. C-atoms $[2^n - 2n]$

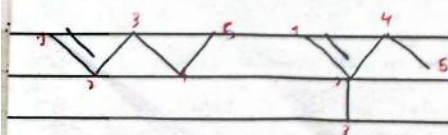
Ques 1) are the chain isomers.



- i) A and B (same MF) isomers (✓)
ii) A and C (diff. MF) isomers (x)
iii) B and C (diff. MF) isomers (x)

Note :- main condition for isomerism is to have same molecular formula.

Ques 2) are the chain isomers.



(same MF) isomers (✓)

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2. Positional Isomerism :-

"the compounds having the same molecular formula but different position of the branch or FG (double/triple bond).

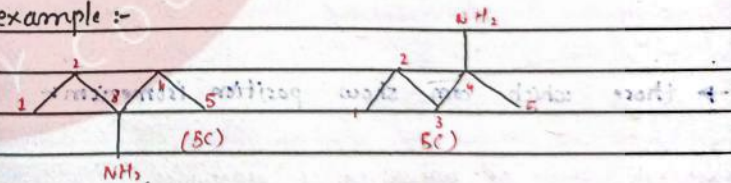
→ Branch :- not carbon containing e.g. NH_2 , OH etc.

→ same :- i, FG ii, homologous series iii, chemical properties
iv, molecular formula
v, molecular mass
vi, percentage composition.

→ different :- i, position of FG
ii, structure
iii, physical properties may or may not be same.

→ have the same parent chain.

→ example :-



→ those which can't show position isomerism.

1) terminal FG e.g. i) carboxylic acid ($R-C(=O)OH$)

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ii, nitriles ($R-C \equiv N$)

iii, 1°-amines ($R-\overset{\overset{O}{\parallel}}{C}-NH_2$)

iv, acid halides ($R-\overset{\overset{O}{\parallel}}{C}-Cl$)

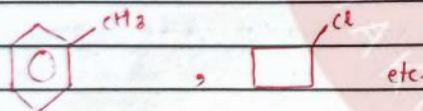
v, acid anhydrides ($R-\overset{\overset{O}{\parallel}}{C}-O-\overset{\overset{O}{\parallel}}{C}-R$)

vi, aldehydes ($R-\overset{\overset{O}{\parallel}}{C}-H$)

vii, ether ($R-O-R$)

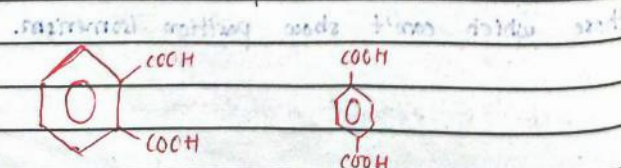
viii, carboxylic acids derivatives except 2° and 3° amides and ester ($R-\overset{\overset{O}{\parallel}}{C}-OR$)

2) monosubstituted cyclo organic compounds;



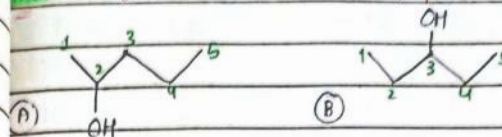
→ those which can show position isomerism

carboxylic acids or derivatives or aldehydes attached to cyclo compounds show position isomerism.

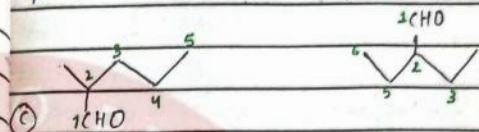


ketones can also show P.I

Q. The given isomers are chain/position isomers?



→ parent chain, molecular formula (same) P.I (✓)



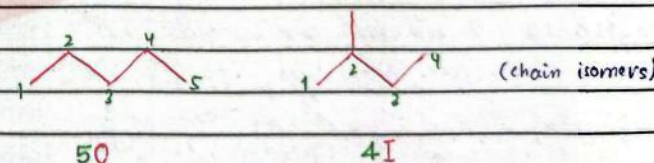
→ molecular formula, FG (same) → isomers (✓)
→ parent chain (diff.) so they are chain isomers not position isomers.

→ Secondly, terminal FG → don't show P.I

→ MAGIC TRICK NO. FOR DIFFERENTIATING CHAIN ISOMERISM & POSITION ISOMERISM:

X → No. of carbon atoms in parent chain

Y → No. of branch of carbon. (means carbon-containing branch)

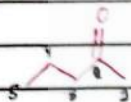


→ magic no. is different (chain isomerism)

Checked By: _____

→ magic no same (position isomerism)

→ position isomers having keto-FG



(Pentane-2-one)

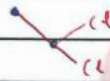


(Pentane-3-one)

in the following two isomers are position isomers / not?



(vic-dihalide)



(gem-dihalide)

applying the magic number trick

$$XY \text{ (vic-dihalide)} = 20$$

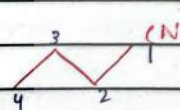
$$XY \text{ (gem-dihalide)} = 20$$

→ Position isomers (✓)

$Y = 0$ (bcz only branches having C-atom are counted).

$$Y = Cl = 0.$$

the following isomers are chain / position isomers?



40



31

chain isomers (✓)

3. Metamerism: (meta means in middle / in b/w).

"this type of isomerism is exhibited due to the unequal distribution of carbon atoms (or alkyl groups) on either side of the functional group."

OR

"the isomers having the same MF but diff. arrangement of atoms / groups on either side of the bridging FG. (polyvalent)."

metamers are those which

→ same :- i, molecular formula ii, FG iii, homologous

↳ molecular mass

↳ %age composition

→ different :- i, physical and chemical properties

ii, diff. arrangement of carbon atoms on either side of the FG.

→ compounds which can show metamerism :-

i, ether ($R-O-R$)

ii, amides (2° & 3°) ($R-\overset{\overset{O}{\parallel}}{C}-NH-R$) & ($R-\overset{\overset{O}{\parallel}}{C}-N-R$)

iii, amines (2° & 3°) ($R-NH-R$) and ($R-\overset{\overset{R}{\mid}}{N}-R$)

iv) thioether $(R-S-R)$

v) ketone $(R-\overset{\overset{O}{\parallel}}{C}-R)$

vi) thioketone $(R-\overset{\overset{S}{\parallel}}{C}-R)$

vii) anhydride $(R-\overset{\overset{O}{\parallel}}{C}-O-\overset{\overset{O}{\parallel}}{C}-R)$

viii) ester $(R-\overset{\overset{O}{\parallel}}{C}-OR)$

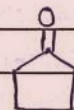
→ those which can't show metamerism :-

(terminal FG).

i) acid halide $(R-\overset{\overset{O}{\parallel}}{C}-Cl)$

vi) cyclic ethers

ii) 1°-amide $(R-\overset{\overset{O}{\parallel}}{C}-NH_2)$

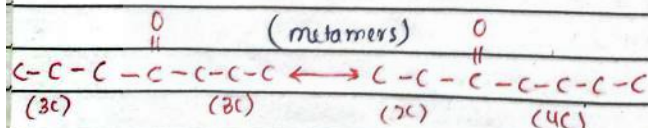


iii) 1°-amine $(R-NH_2)$

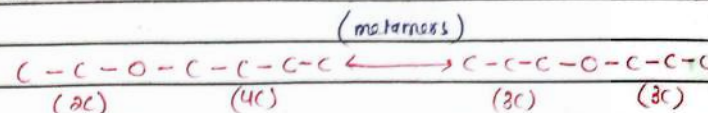
iv) COOH $(R-\overset{\overset{O}{\parallel}}{C}-OH)$

v) nitrile $(R-C\equiv N)$

→ ketone can show metamerism and position isomerism at the same time.



→ ether can show only metamerism and not the position isomerism.



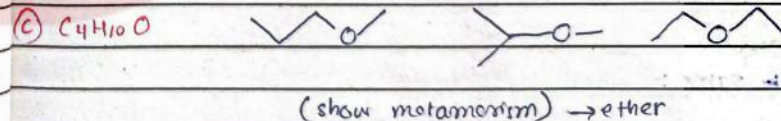
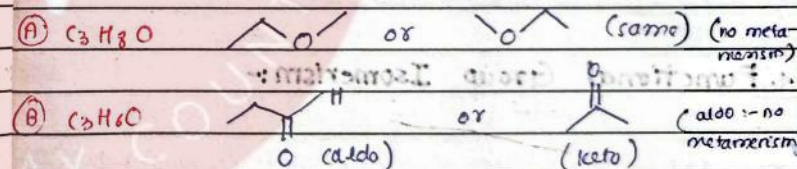
→ for metamerism 'R' must be present on both sides of FG.

MCQ :- the compound which shows metamerism is :-

(A) C_3H_8O (B) C_3H_6O (C) $C_4H_{10}O$ (D) C_5H_{12}

($C_nH_{2n+2}O$)
 ether alcohol
 show FG isomerism.

→ alcohol can't show metamerism.



Note :- the minimum no. of carbon atoms in ether to show metamerism is 4.

Checked By: _____

① C_5H_{12} (alkane) and alkanes don't show metamerism.

Note:- the minimum number of carbon atoms in ketone is 3 to show position isomerism.

③ 3 ④ 4 ⑤ 5 ⑥ 6

3-carbon atoms $R-\overset{\overset{O}{\parallel}}{C}-R$

4-carbon atoms $CH_3-\overset{\overset{O}{\parallel}}{C}-CH_2-CH_3$ or $CH_3-CH_2-\overset{\overset{O}{\parallel}}{C}-CH_3$

FG at same no. so no position isomerism possible

5-carbon atoms $CH_3-\overset{\overset{O}{\parallel}}{C}-CH_2-CH_2-CH_3$ or $CH_3-CH_2-\overset{\overset{O}{\parallel}}{C}-CH_2-CH_3$
[position isomerism (V).]

Note:- the minimum no. of carbon atoms in ketone is 3 to show position isomerism.

4. Functional Group Isomerism:-

the isomers having the same molecular formula but different functional groups.

→ same:- molecular formula.

Li, molecular mass

Lii, %age composition and atoms

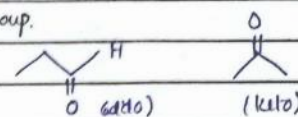
→ different:- i, FG ii, chemical properties

iii, physical properties iv, homologous series

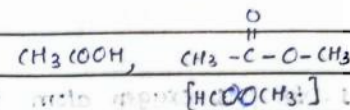
Checked By: V) structural formula

→ some examples of functional isomers:-

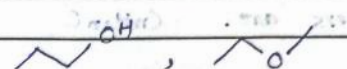
1) aldo and keto



2) acid and ester

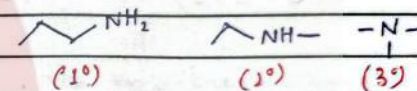


3) alcohol and ether

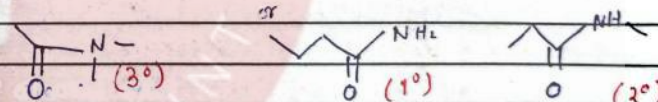
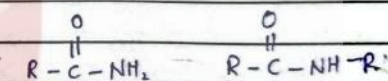


4) cyanoide & isocyanoide $(R-C\equiv N)$, $(R-N\equiv C)$
(iso)

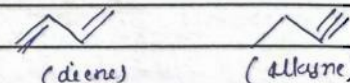
5) 1°, 2°, 3° amines



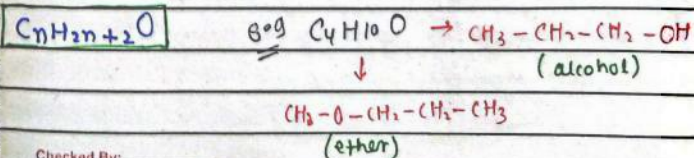
6) 1°, 2°, 3° amides



7) diene, yne



→ If no DBE (double bond), all saturated then the possible FG isomers are ether and alcohol.



Checked By:

DBE ($-H_2$ or $2H$)

- by double bond (unsaturated)
- by cyclization (saturated)

→ If 1 DBE, 1 oxygen atom then the possible FG isomers are. $C_nH_{2n}O$

1) ketone and aldehyde

2) unsaturated ether and alcohol (alkenol)
($C=C-O-C$) ($C=C-OH$)

3) cyclic alcohol and cyclic ether. (having 2-H less than n-ether and n-OH).

e.g. C_4H_8O — $CH_3-CH_2-C(=O)-CH_3$ (ketone)

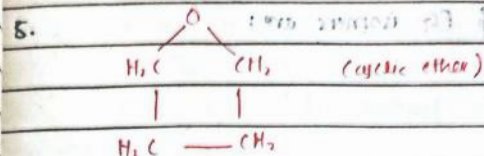
$CH_3-CH_2-CH_2-C(=O)-H$ (aldehyde)

2. $CH_2=CH-CH(OH)-CH_3$ (unsaturated alcohol)
(alkenol)

3. $CH_2=CH-O-CH=CH-CH_3$ (unsaturated ether)

4. $H_2C-CH_2-CH_2-CH_2$ (cyclic alcohol)
 $H_2C-CH_2-CH_2-CH_2-OH$

Checked By: _____



→ If 1 DBE and 2 oxygen atoms then the possible FG isomers are; $C_nH_{2n}O_2$

1. carboxylic acid and ester

e.g. $C_4H_8O_2$ → $CH_3-CH_2-CH_2-C(=O)-OH$ (COOH)
→ $CH_3-CH_2-C(=O)-O-CH_3$ (ester)

2. hydroxy aldehyde and hydroxy ketone

$CH_3-CH(OH)-C(=O)-H$
(hydroxy aldehyde)

$CH_3-CH(OH)-C(=O)-CH_3$
(hydroxy ketone)

3. unsaturated diether

4. cyclic diol and unsaturated diol.

$H_2C-CH_2-CH_2-CH_2$ (cyclic diol)
 $H_2C-CH_2-CH_2-CH_2-OH$

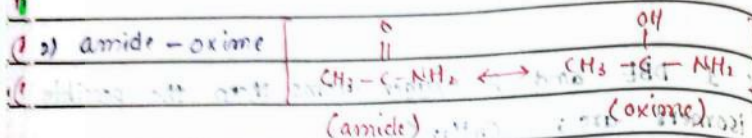
$CH_2=CH-CH(OH)-CH(OH)-CH_3$
(unsaturated diol)

Checked By: _____

→ Other examples of FG isomers are;

1) glucose (aldehyde) and fructose (keto)

2) amide - oxime

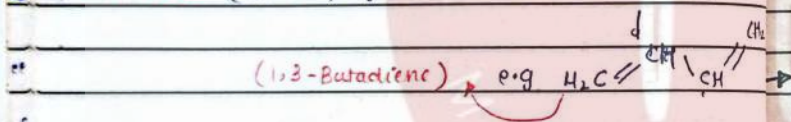


3) 1°, 2° and 3° amines shows;

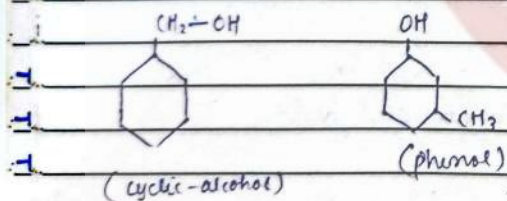
- position isomerism
- functional group isomerism
- metamerism.

4) C_nH_{2n} (alkene and cycloalkanes)

5) $\text{C}_n\text{H}_{2n-2}$ (alkene, cyclic-alkene, and alka-diene)



6) Alcohol vs Phenol



5. Ring - Chain Isomerism :-

→ difference in the mode of carbon-atom

"Molecular formula → same"

Checked By: _____

→ 1st ring and 2nd chain.

→ special type of functional group isomerism
Ring ↔ Chain

→ e.g. (cyclobutane) C_4H_8 ↔ butene

(cycloalkane) C_nH_{2n} ↔ (alkene)

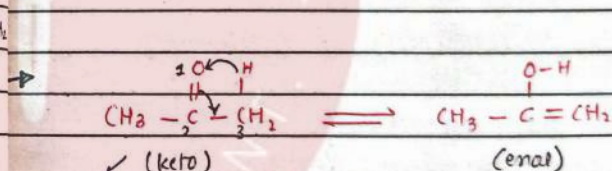


6. Tautomerism :- the comp. which are diff. in the position of π -bond or mostly H-atom.

→ dynamic

→ there is intramolecular H^+ transfer

→ has keto-enol system / 1-3 system



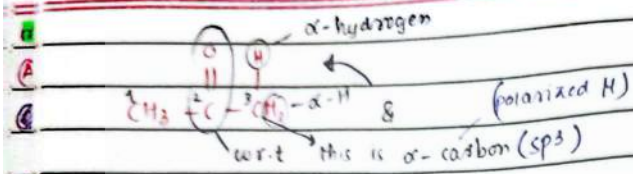
more stable than enol.

↓
'3' transfers to 1 and 1 transfers to two.
(H^+)

→ Condition for exhibition of tautomerism

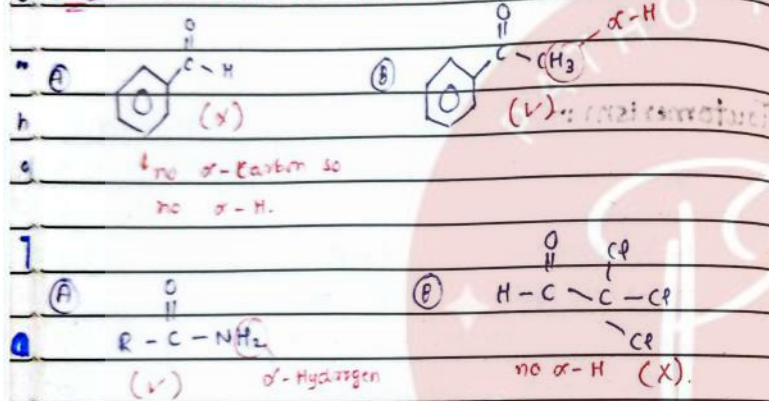
1) 3rd carbon (α -carbon) should be sp^3 -hybridized and must have a hydrogen (α -hydrogen)

Checked By: _____

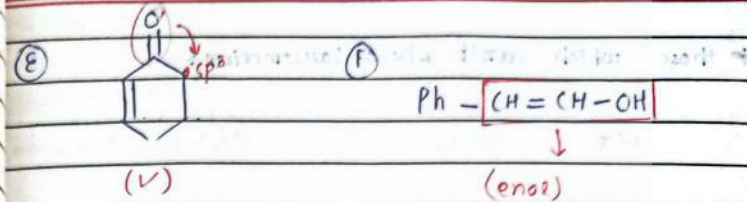
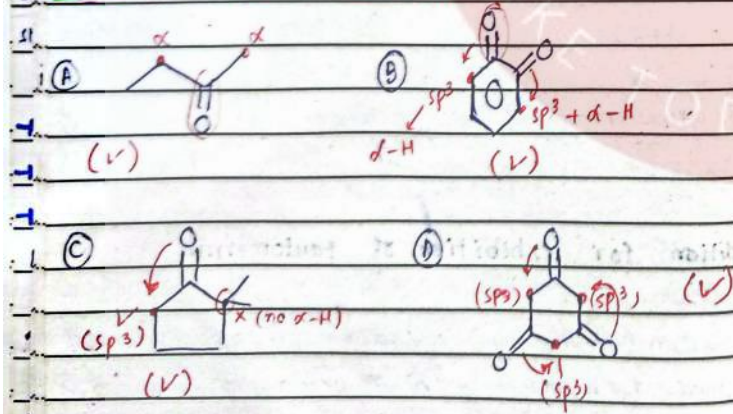


- (1) must have C=O, C=S, or C=N
- (i) (a compound having multiple heteroatoms)

5. WCF show tautomerism



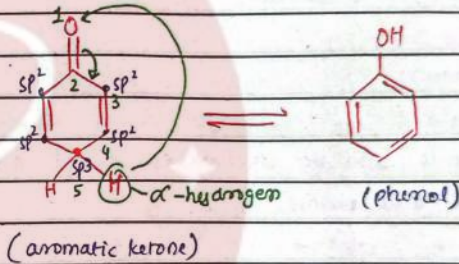
6. WCF exhibits tautomerism?



→ always remains in equilibrium with its keto form. so it will exhibit tautomerism.

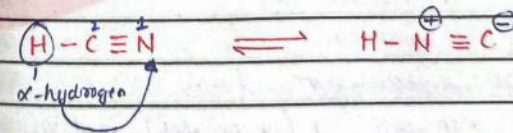
1,5 - system :-

→ (when 1,3 system fails)



→ double bond shifts to '2' and α-Hydrogen from sp³ carbon shifts to one.

1,2 - System :-



→ On the 1,5 system, phenol is more stable so the rxn mostly completes in the forward direction.

→ those which can't show tautomerism:-

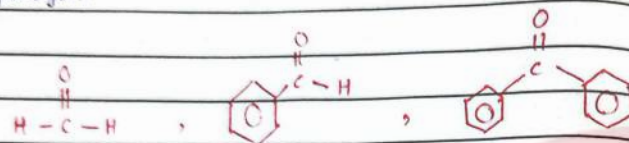
①

1) which heteroatoms (C=O, C=S, C=N etc).

② α-hydrogen.

③

e.g.

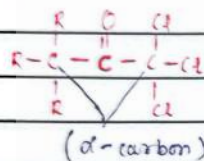


5

(formaldehyde)

h

a



1

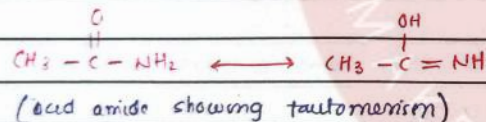
2) carboxylic acids and its derivatives except acid

anhydride and acid amides.

e.g.

s

st



(acid anhydride showing tautomerism)

→ more points about tautomerism:-

1

1) special type of FG isomerism

2) tautomers exist in equilibrium

3) two compounds with diff FG (same MF) exist in equilibrium.

4) can be catalyzed by acids/bases

5) only exist in liquid and gaseous state.

6) can't exist in solid state

7) chemical process (chemical equilibrium)

→ Same :- 1) molecular formula

↳ molecular mass

↳ %age composition and no. of atoms

→ different :- 1) functional group

ii) structural formula

iii) Physical and chemical properties.

→ Calculation of number of structural isomers:-

D.U (Degree of unsaturation) or D.B.E (Double Bond equivalent)

$$DU = \frac{(C+1) - (H+X-N)}{2}$$

where

C = no. of carbon atoms

H = no. of Hydrogen atoms

X = no. of halogen atoms

N = no. of nitrogen atoms.

→ If DBE/DU = 0 then all single bond.

→ if DU = 1 there will be either a π-bond or a ring not both.

Checked By: _____

→ If $DU = 2$ then
 2π 2 Ring 1 π + 1 Ring

Q. What are the total structural isomers of C_5H_{10} .

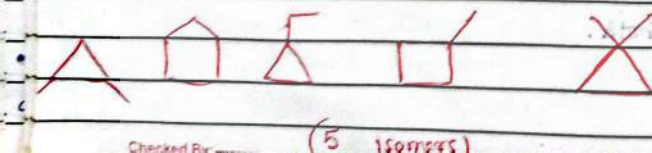
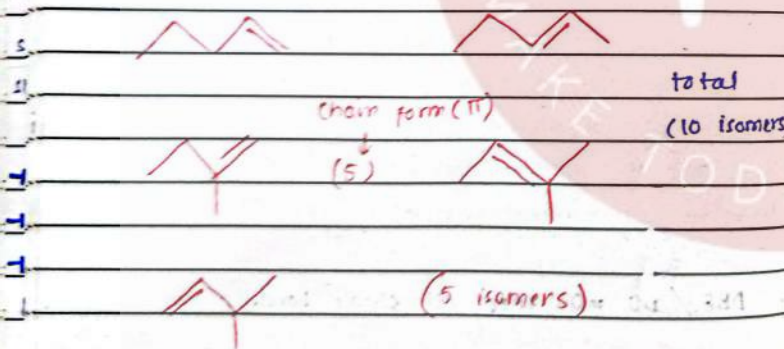
$$DU = \frac{(C+1) - (H+X-N)}{2}$$

$$= \frac{(5+1) - (10+0-0)}{2}$$

$$= \frac{6 - 10}{2} \Rightarrow 6 - 5 \text{ so } DU = 1$$

1 π or 1 ring

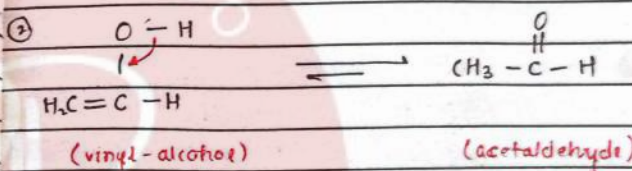
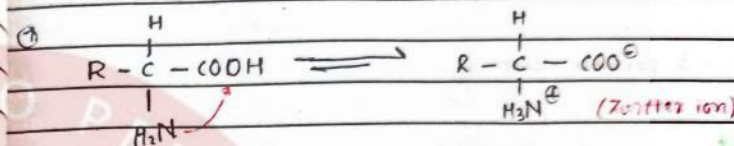
→ there are 5-carbons so 5-carbon parent chain and change the position of π bond in each.



Checked By: _____

→ points of tautomerism:-

→ shifting of proton (H^+) from one atom to another within the same molecule.



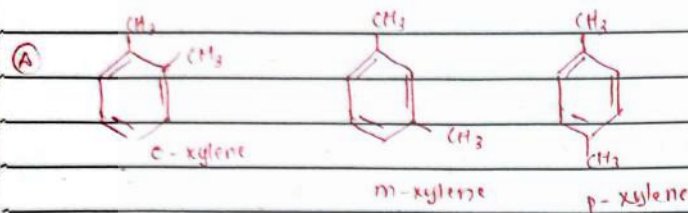
→ at equilibrium any one of the tautomer can be isolated.

→ two compounds having same general formula will show FG isomerism:-

- 1) alkene and cycloalkanes (C_nH_{2n})
- 2) alkenes, cycloalkanes and alkadienes (C_nH_{2n-2})
- 3) alcohols and ethers ($C_nH_{2n+2}O$)
- 4) aldehydes, ketones, cyclic alcohols, cyclic ethers (also called epoxides) ($C_nH_{2n}O$)
- 5) carboxylic acid, esters, hydroxy aldehydes, hydroxy-ketones. ($C_nH_{2n}O_2$)

Checked By: _____

Q. How many position isomers xylene can have?



Ans - 3 possible isomers.

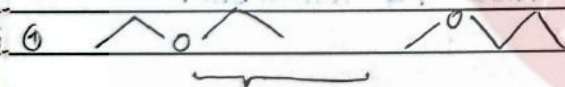
Q. Alcohols with molecular formula $C_nH_{2n+2}O$ are isomeric with :-

(A) acids (B) ethers (C) esters (D) aldehydes

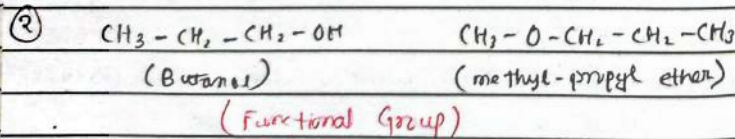
Q. the types of isomerism possible with molecular formula $C_4H_{10}O$ is/are :-

(A) FI (B) PI (C) Metamerism (D) all of these

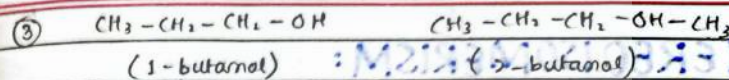
$C_4H_{10}O$ (ether) = $[C_nH_{2n+2}O]$



showing FI + metamerism.



Checked By: _____



(Position - I)

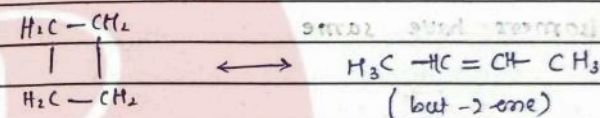
→ FI (possible bcz of R-OH and R-O-R)

→ PI (possible in -OH)

→ metamerism (shown by ethers)

Q. cyclobutane and but-2-ene are the examples of :-

(A) PI (B) Ring-chain isomerism (C) Metamerism (D) Geometrical isomerism



→ Isomers of Alkanes:

Alkanes	No. of isomers
1) Methane, Ethane, Propane	No isomers
2) Butane (C_4H_{10})	2
3) Pentane (C_5H_{12})	3
4) Hexane (C_6H_{14})	5
5) Heptane (C_7H_{16})	9
6) Octane (C_8H_{18})	18
7) Nonane (C_9H_{20})	35
8) Decane ($C_{10}H_{22}$)	75
9) Isotriacontane ($C_{30}H_{62}$)	366,319
10) squalane ($C_{30}H_{62}$)	more than 4 billions
11) Tetracontane ($C_{40}H_{82}$)	625 millions

Checked By: _____

(b)

STEREISOMERISM: (in 3D space)

1. CONFORMATIONAL ISOMERISM:-

→ a form of stereoisomerism in which the isomers can be interconverted just by rotations about formally single bonds.

→ alkanes mainly show CI and conformational isomerism.

→ stereo isomers have

i) same :-

- i) MF ii, structural formula iii, connectivity of atoms
- iv, IUPAC - Names

ii, Different :-

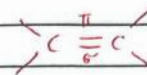
- i, 3D - arrangement of atoms (configuration)
- ii, physical properties
- iii, some chemical properties.

2. GEOMETRIC ISOMERISM

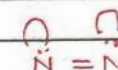
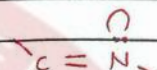
"Geometric isomers have diff. arrangement of atoms/groups when the rotation is restricted in a molecule."

→ Necessary conditions for compounds to show stereoisomerism :-

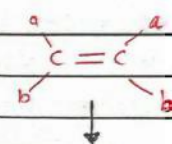
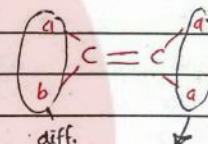
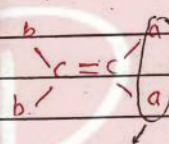
i, Restricted rotation (ensured by the presence of the double bond).



→ cyclic structural arrangement also ensures restricted rotation.



ii, Diff. groups must be attached to restricted atom.

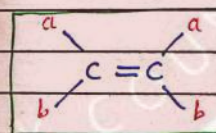


same group: but these are same. presence of π bond (✓)

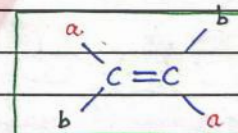
no restricted rotation

ii) diff groups (✓)

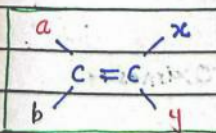
→ there will be restricted rotation.



(cis-form)



(trans-form)



(E and Z-forms)

→ when all the groups attached to the restricted atoms are diff. group then it is called E and Z form.

Ques - Geometric isomerism is usually found in:

- (A) Alkanes (B) Alkenes (C) Alkynes
(D) Esters (E) Alkynes (presence of π bond)

Ans - alk compounds will exhibit cis-trans isomerism

- (A) 2-Butene (B) 2-Butyne (C) 2-Butanol (D) Butanal
(alkene)

→ Alkynes can't show geometric isomerism;

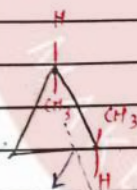
due to the linear geometry enforced by the triple bond, which doesn't allow for the spatial variation required for cis-trans isomerism.

→ Cis-trans isomerism in Cycloalkanes:-



same side, same groups

(cis-form)



same side, diff. groups

(trans-form)

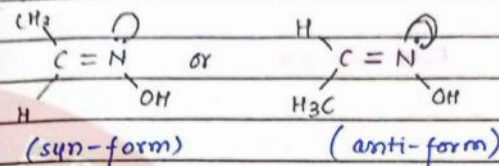
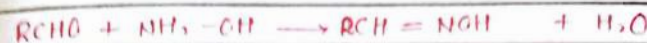
→ Anti-Syn form isomerism in Oximes:-

Oxime:-

the compounds synthesized by the condensation of b/w hydroxylamine and a carbonyl compound.

Checked By: _____

→ For an aldehyde:-



→ Syn-form:- H and OH present on same side of the π bond.

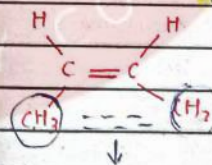
→ anti-form:- H and OH present on opposite side of the π bond.

→ Comparison of Different properties of Cis-trans form.

Cis-form

Trans-form

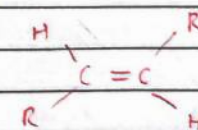
1. Reactivity



steric repulsion

→ more bulky groups on same side, steric repulsion more and it becomes unstable.

Checked By: _____



→ more bulky groups on opp. side so less steric repulsion.

Cis-form

Trans-form

→ more reactive (less stable)

→ less reactive (more stable)

2. Dipole Moment

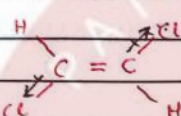
$\mu \propto$ polarity

$\mu = 0$
(polar)



$\mu = 1.90D$

$\mu \neq 0$
(non-polar)



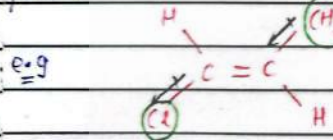
$\mu = 0.00D$

→ polar (due to unsymmetrical shape)

→ non-polar (due to symmetrical shape)

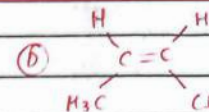
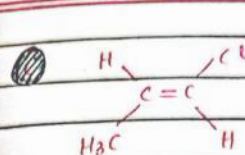
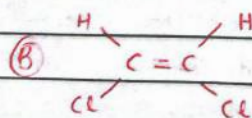
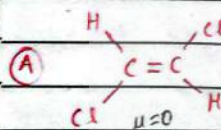
EXCEPTION:-

there are some trans-forms which are not non-polar.



→ here ' μ ' has some but still it is less than cis-form.

MCQ:- WOF has the highest dipole moment?



3. Melting Point & Boiling Point

→ Melting Point (solids) and → BP (liquids)

→ BP is concerned with the strength of intermolecular forces.

cis-form

trans-form

→ polar → strong attractive force

→ non-polar → weak attractive force

→ So, have high BP.

→ So, have Low BP.

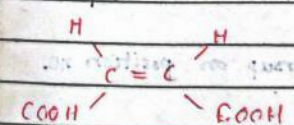
→ poor packing due to unsymmetrical arrangement.

→ good packing due to symmetrical arrangement

→ so have Low MP.

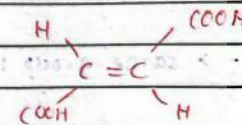
→ so have high MP.

Examples:



Maleic acid (cis-isomer)

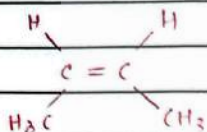
MP = 130°C



Fumaric acid (trans-isomer)

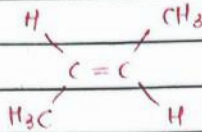
MP = 286°C

Checked By:



(cis-2-Butene)

BP = 4°C



(trans-2-Butene)

BP = 1°C

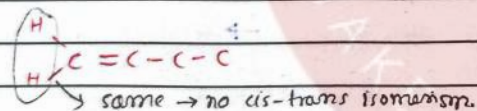
4. Solubility, Density, Refractive Index

polarity, solubility, density, refractive index

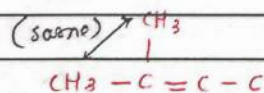
→ cis-form (has more viscosity)

→ those alkenes which can't show cis-trans isomerism :-

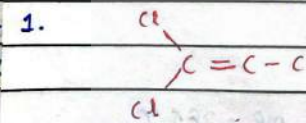
1) 1-ene:



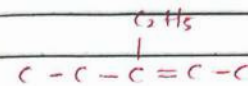
2) 2-methyl-2-ene:



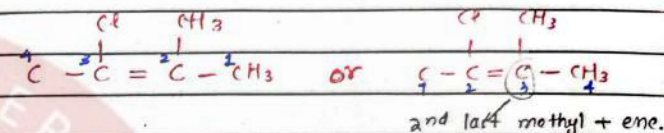
3) 1, 1 → same group i.e. same group on position no.



4) 3-ethyl-3-ene:-



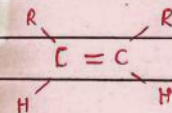
5) 2nd last methyl and 2nd last ene:-



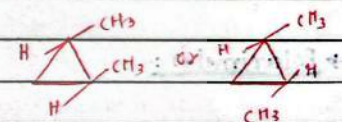
→ Compounds which can have cis-trans isomers :-

→ cis-trans isomerism (bec of frozen bond which can't rotate).

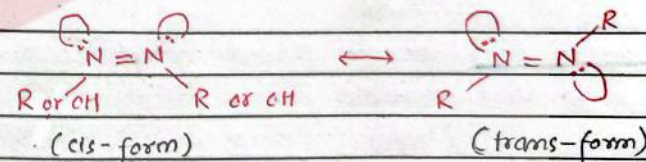
i, substituted alkene



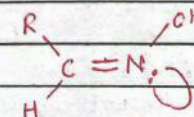
ii, substituted cycloalkane



iii, Azo-compounds



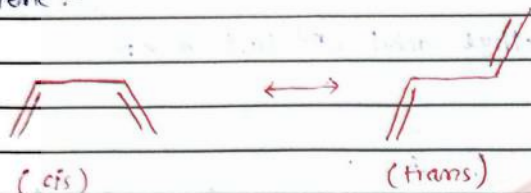
iv, Oximes (gmines):-



Checked By:

* lone-pair is also considered as a separate group substituent.

v) Diene :-



3. OPTICAL ISOMERISM:

→ Optical Active:-

the compounds which can rotate the plane of the polarized light.

→ Optical Activity:-

the property of the optically active compounds.

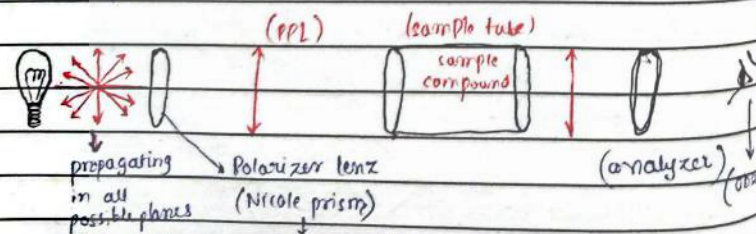
→ Polarimeter:-

identify and measure the optical rotation

identify whether a compound is optically active or not.

in (Polarimeter)

→ source of light:- produces EM-waves, that oscillate in all possible planes.



→ soln of the compound placed in the sample tube is made with a compound which is not optically active

e.g

= (H₂O, CCl₄, CHCl₃)

→ Results:-

i,

- plane
- no rotation
- compound is optically inactive

ii,

- clockwise rotation
- dextrorotatory, d (+)

iii,

- anticlockwise rotation.
- levorotatory, l (-)

→ θ (degree of rotation) depends upon:

i, length of sample tube ii, conc. of sample soln
iii, temperature iv, λ of light used.

→ Specific Rotation (α_s):-

→ a physical property just like MP, BP etc.

$$[\alpha]_{\lambda}^{25} = \frac{\alpha_{obs}}{c \times l}$$

Checked By: _____

where c = conc. of sample soln in g/ml.

λ = wavelength (usually Na-light is used so its

$\lambda = 589 \text{ nm}$)

l = length = 1 decimeter = 10 cm

→ Chirality:

→ a compound which shows optical activity must have;

i, non-superimposable mirror images

ii, stereogenic centre [chiral atom (carbon), stereo-centre, chiral centre]

iii, do not have element of symmetry.

→ (left hand, right hand); (right foot - left foot) and (left ear - right ear) are optical isomers / non-superimposable mirror images of each other. or enantiomers.

→ Optically Active Centre

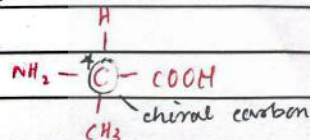
CHIRAL

A-CHIRAL

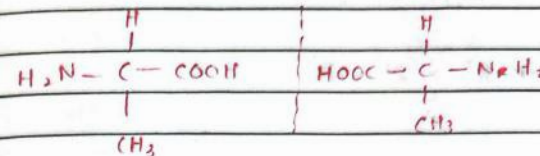
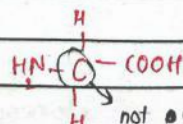
→ four diff groups are attached.

→ doesn't have four diff. attached groups.

e.g amino acid (alanine)



e.g amino acid (glycine)

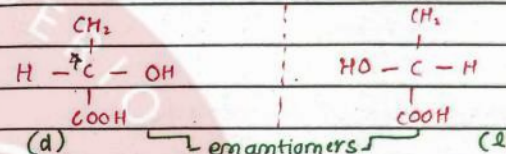


(non-superimposable mirror images)

↓

(enantiomers)

② Lactic acid (2-hydroxypropanoic acid) → has 2 enantiomers.



i, chiral carbon (✓)

ii, no plane of symmetry

→ optically active

→ same specific rotation $[\alpha] = 2.67$ at 15°C .

→ same physical properties.

↓

e.g solubility, refractive index, mp, bp etc.

→ formula to calculate the no. of enantiomers

when different groups are present at the opposite ends;

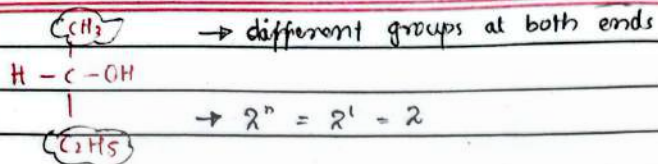
No. of enantiomers = 2^n

→ when same groups are present at the opposite ends.

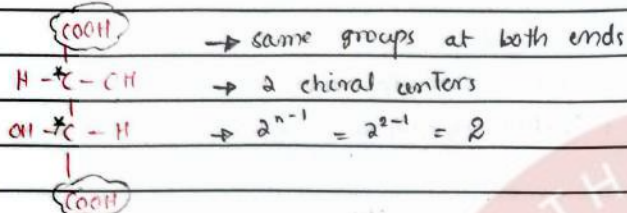
No. of enantiomers = 2^{n-1}

where n = no. of stereogenic centres

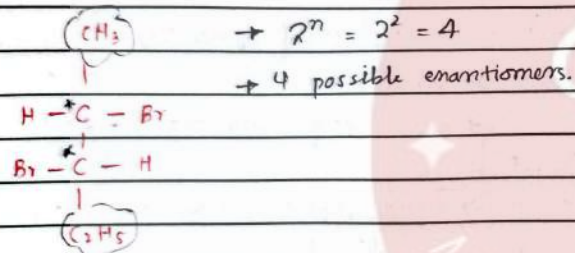
Checked By: _____



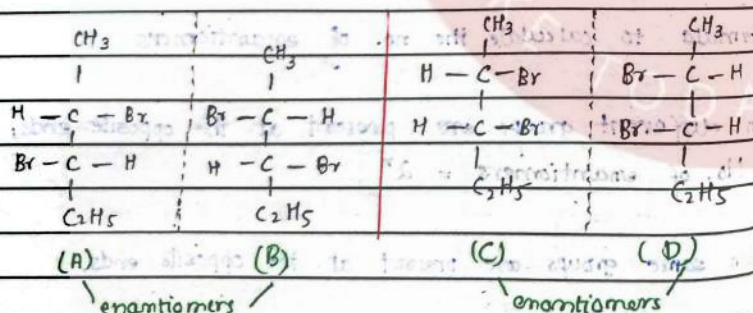
(2-Butanol)



(tartaric acid)



(2,3-dibromopentane)



But: 2,3-dibromopentane

A and C or A and D → Diastereomers.

A and C or B and D are not superimposable images of each other. (Diastereomers)

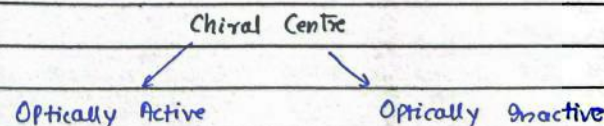
ENANTIOMERS

DIASTEREOMERS

- | | |
|--|---|
| → mirror images | → non-mirror images |
| → non-superimposable | → superimposable |
| → at least one chiral centre | → two / more than two chiral centres |
| → optically active | → may / may not be optically active |
| → same physical properties (except behaviour towards plane polarized light). | → diff. physical properties |
| → may / may not have same chemical properties. | → may / may not have the same chemical properties. |
| → 2 forms of the same molecule (exist in pairs). | → they may have more than two forms of the same molecule. |

Racemic Mixture:-

- 50% D-isomer and 50% L isomer
- mixture is optically inactive bcz both the isomers rotate ppl in diff. directions to the same degree
- have diff. physical properties than the enantiomers



Checked By: _____

Optically Active

Optically Inactive

→ 4 diff. atoms/groups of atoms attached.

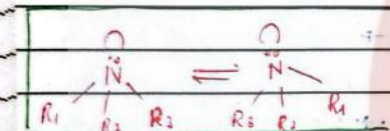
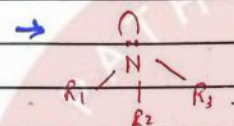
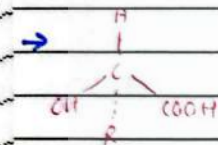
→ 3 diff. atoms/groups of atoms and 1 lone.

→ asymmetrical

→ may be symmetrical (having plane of symmetry).

→ stereogenic

→ non-stereogenic



Due to lone pair presence, group can flip at RTP, so l and d isomers.

Other Points:

→ Only glycine (having H) is optically inactive.

→ Rest of the 19^{essential} amino acids are optically active due diff. R group.

→ amino acids form proteins so proteins are also optically active.

→ enzymes are specific in action due to the optical activity.

→ D-glucose after metabolism produces energy.

→ L-glucose (present in artificial sweeteners) doesn't produce energy and is excreted through the urine out of the body.

(ISOMERISM)

[Different compounds with same molecular formula]

Structural/Constitutional Stereoisomerism

i, Chain Isomerism

ii, Conformational

ii, PI

iii, FG Isomerism

ii, Configurational

iv, Metamerism

v, Tautomerism

Geometric Isomerism

Optical Isomerism

• cis-Trans

• Enantiomerism

• E and Z

• Syn and anti

• Diastereomerism

• Exo and Endo

→ Priority Order for Structural Isomerism:

1) Position

2) Functional Group

3) Ring-chain

Checked By: