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Goc and isomerism-1

Organic chemistry

JEE/NEET-2020

Degree of Unsaturation or Double Bond Index or Hydrogen Deficiency Index

$$C_a H_b X_b N_c P_c O_d S_d$$

$$D.U. = a + 1 - \frac{(b - c)}{2}$$

Atoms like – X (Halogen) univalent add with –H

Atoms like – S – Bivalent add with –O–

Atoms like – P – Trivalent add with –N–

| |

D.U. Meaning

1 1π or 1 ring

2 2π, 2 ring or 1π and 1 ring

e.g.:

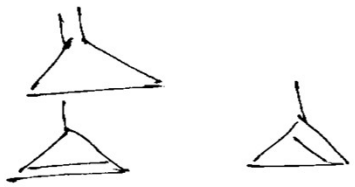
1. C_4H_6 D.U = 2

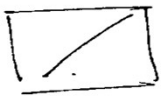
$CH_2=CH-CH=CH_2$

$CH_2=C=CH-CH_3$

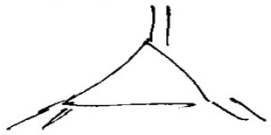
$CH_3-CH_2-C\equiv CH$

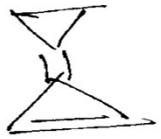
$CH_3-C\equiv C-CH_3$





2. C_6H_6 D.U = 4





$H : C = 1 : 1$

$C_n \geq 6$

D.U ≥ 4

99% benzene ring

Unsaturation
π bonds
bet^n C–C only

Isomerism

Two compounds

- **Same molecular formula**
  - **Identical**
  - **Isomers**
- **Different molecular formula**
  - **Homologs**
    - **-Same D.U.**
    - **-Same FG**
    - **- Same General formula**
    - **- $-CH_2-$ difference in successive unit**
    - **-Same chemical properties but different physical properties**
  - **No relation**

Isomers

Compounds having same molecular formula but different physical or chemical or both properties are known as isomers & the phenomenon is known as isomerism.

E.g.:

	CH_3-CH_2-OH	CH_3-O-CH_3
M.F.	C_2H_6O	C_2H_6O
B.P.	High (H-Bond)	Low (No H-Bond)
Na	Acidic H H_2	H_2 ×

Isomerism is of two types

(i) Structural or Constitutional

(ii) Stereoisomerism

Isomerism

Structural or Constitutional

- Same M.F. but different structural formula (Different connectivity of atoms or groups)
- Same molecular formula but different IUPAC name

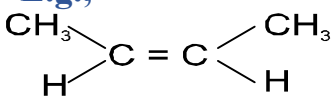
$CH_3–CH_2–OH–$ Ethanol

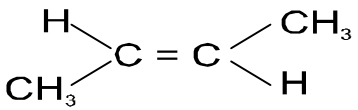
$CH_3–O–CH_3$ Methomymethan

Stereoisomerism

- Same molecular formula. (connectivity of atoms or groups). But orientation of groups or atoms in 3D space is different.
- Same IUPAC if not written with stereochemical descriptor

E.g.,



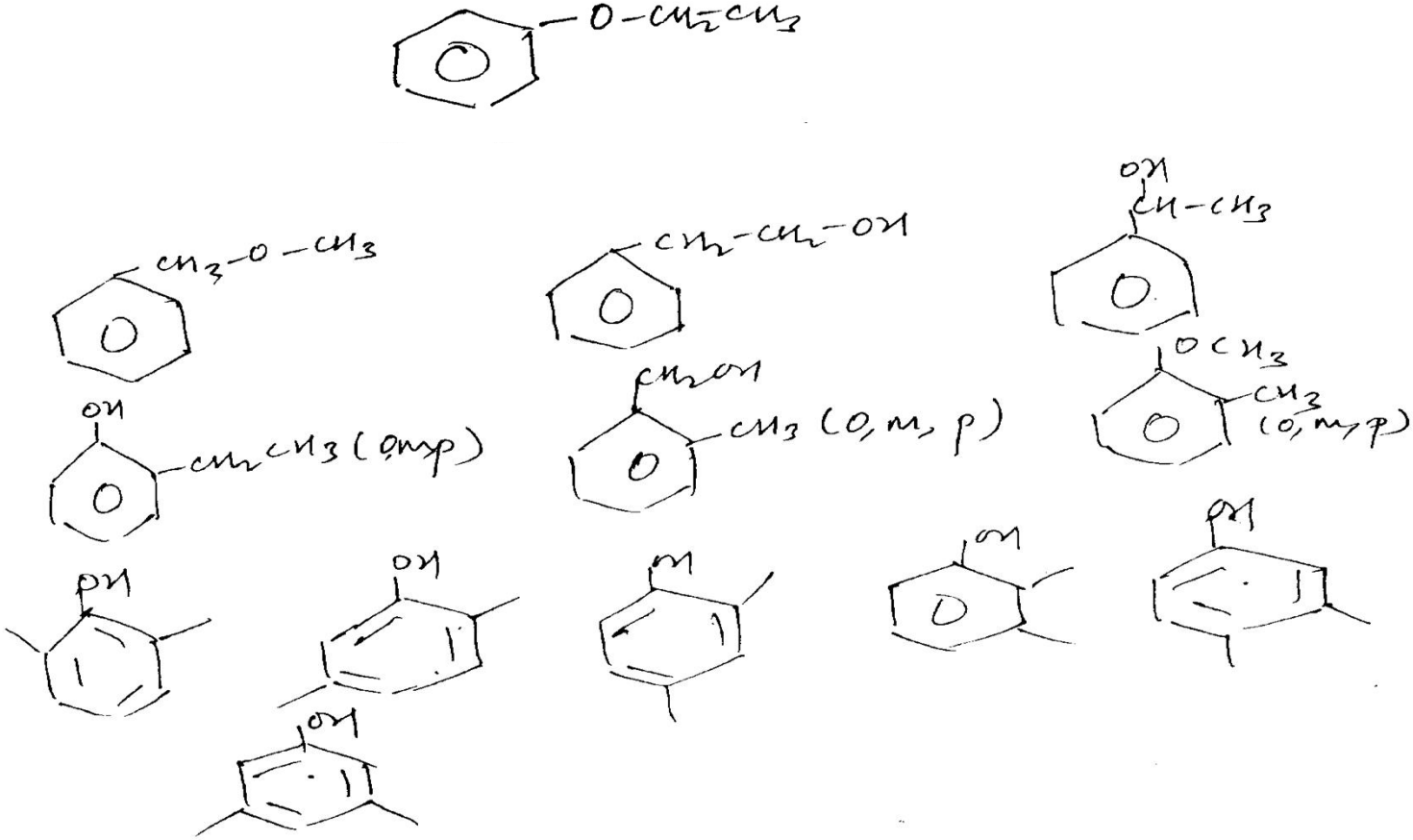


MF Same

SF Same

IUPAC Cis But–2–ene Trans But–2–ene

Q. Write all possible structural isomers (aromatic) for :



Types of structural Isomerism

Functional group different
- Functional isomers

Functional group same

- **Metamerism**
- **Chain**
- **Postion**
- **Tautomerism**

Functional Isomerism

Isomers with different functional groups are known as functional isomers.

C_nH_{2n+2} Alkane (Chain isomerism)

C_nH_{2n}

C_4H_8

D.U → 1

Alkene — cycloalkane

$CH_3-CH_2-CH=CH_2$ □

ring chain isomers

C_nH_{2n-2}

C_5H_8

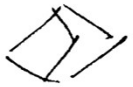
D.U → 2

Alkyne

$CH_3-CH_2-C\equiv C-CH_3$

Cycloalkane

Bicyclo



Spiro

Alkadiene

$CH_2=CH-\underset{\underset{CH_2}{\|}}{C}-CH_3$

$C_nH_{2n+2}O$

C_2H_6O

D.U = 0

Alcohol

CH_3-CH_2OH

Ether

CH_3-O-CH_3

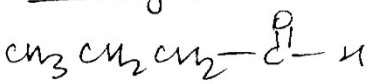
General Formula

4. $C_nH_{2n}O$

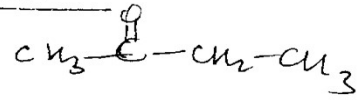
C_4H_8O

D.U → 1

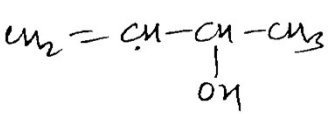
Aldehyde



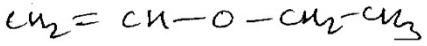
Ketone



Unsaturated alcohol



Unsaturated Ether



Cyclic alcohol

Cyclic ether

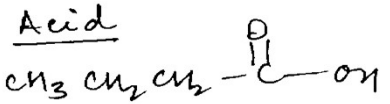
Ether aldehyde

5. $C_nH_{2n}O_2$

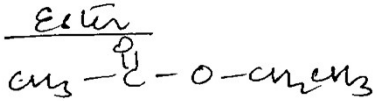
$C_4H_8O_2$

D.U → 1.

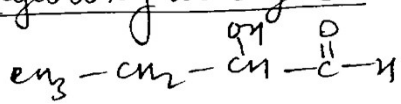
Acid



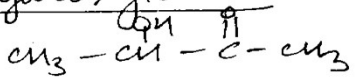
Ester



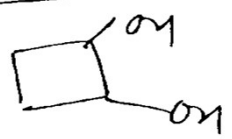
Hydroxy aldehyde



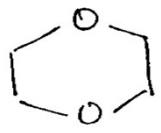
Hydroxyketone



cyclic alcohol



cyclic diether



ether aldehyde

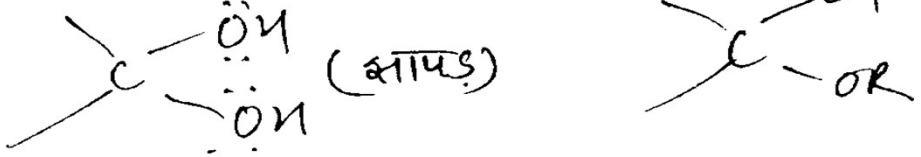
Unsaturated dialcohol

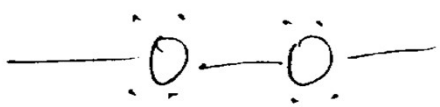
$CH_2=CH-\underset{OH}{CH}-\underset{OH}{CH_2}$

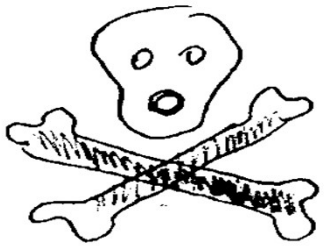
Unsaturated diether

$CH_2=CH-O-CH_2-O-CH_3$

Don't make following structure







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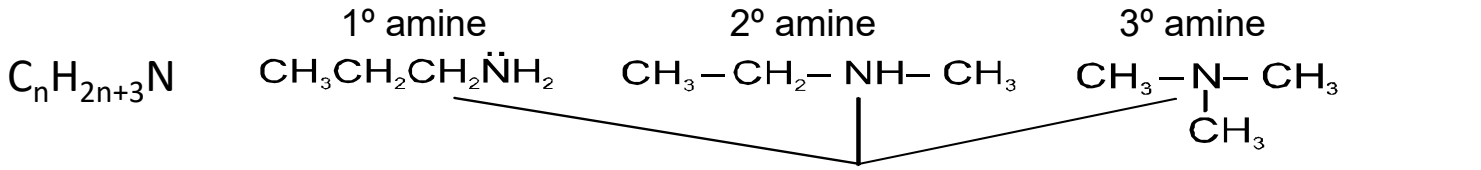
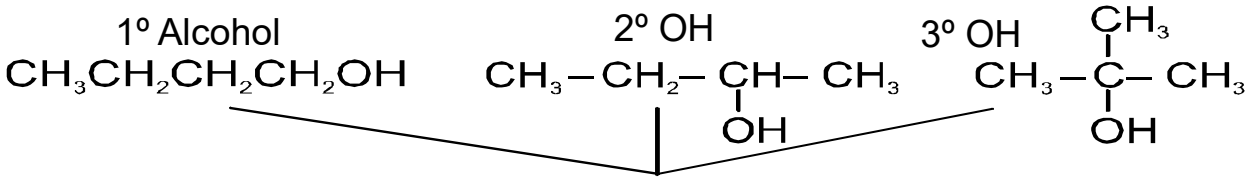
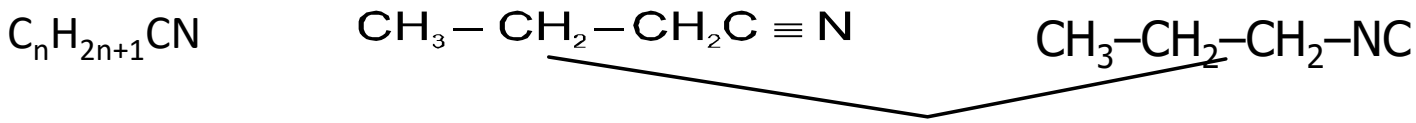


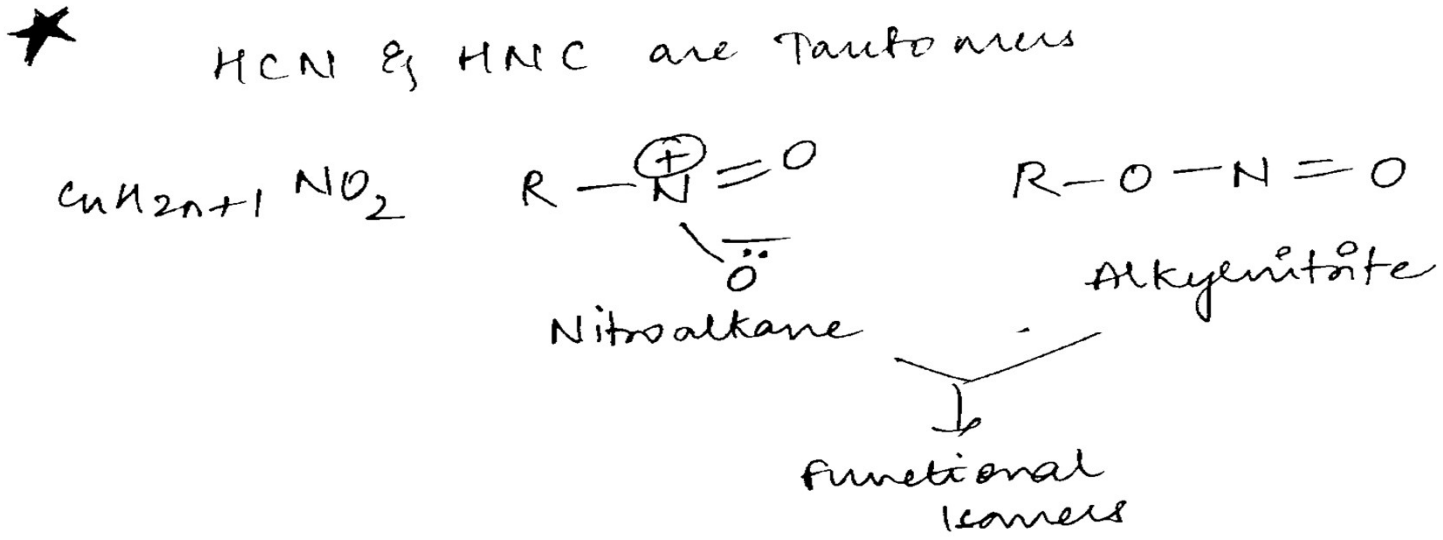
Functional Isomers



Not Functional Isomers



Functional Isomers



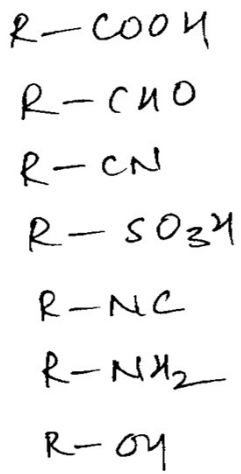
* Always remember that amines – (1º, 2º, 3º) are functional isomers but it isn't applicable for other groups like alchol etc.

Ring chain isomers are functional isomers

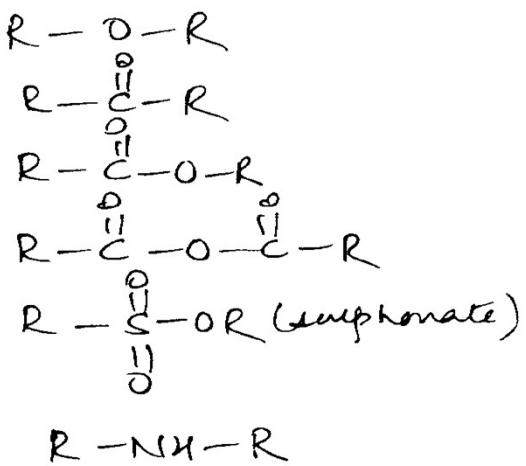
Metamerism

This isomerism arises due to difference in nature of alkyl group on either side of functional group.

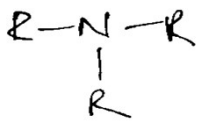
Univalent



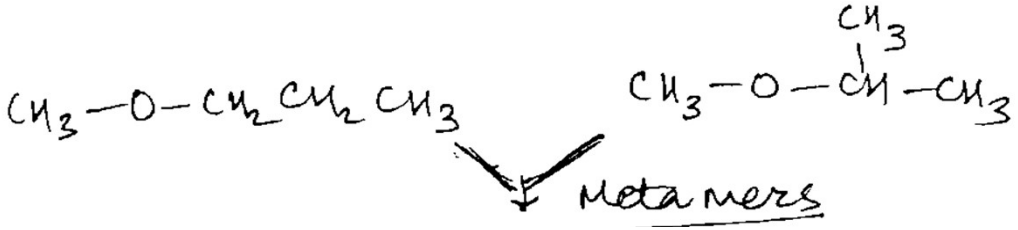
Bivalent

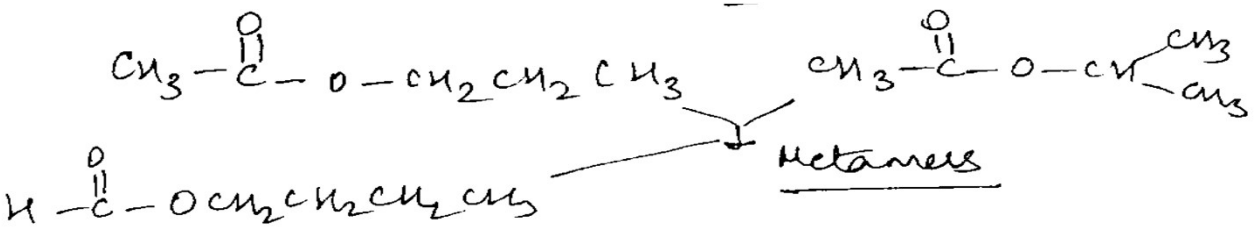


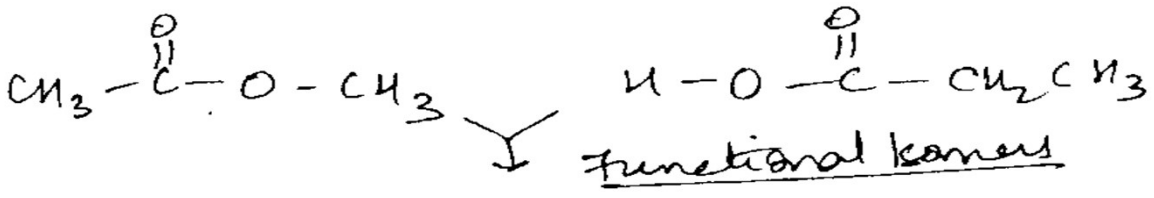
Trivalent

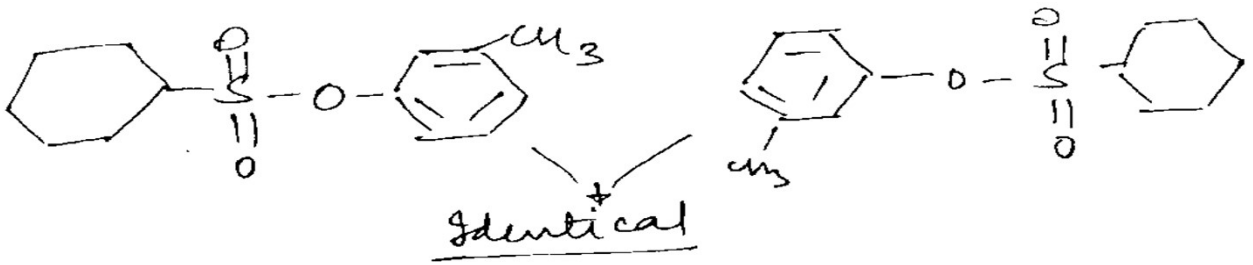


*** Functional groups which show metamerism do not show chain or position Isomerism.

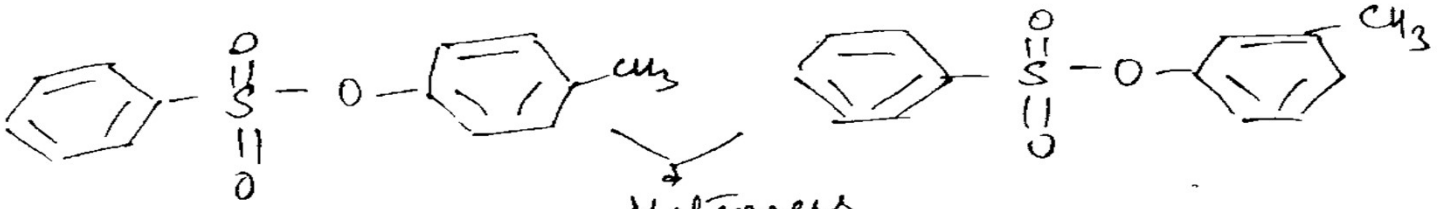
1. 







Identical

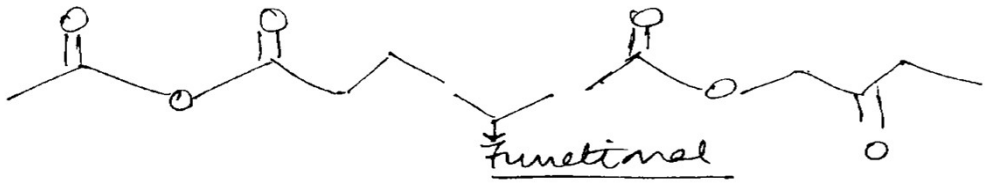


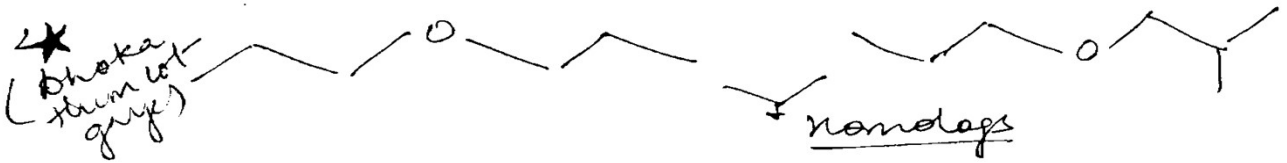
Metamers

Isomers – Structural – Functional Group

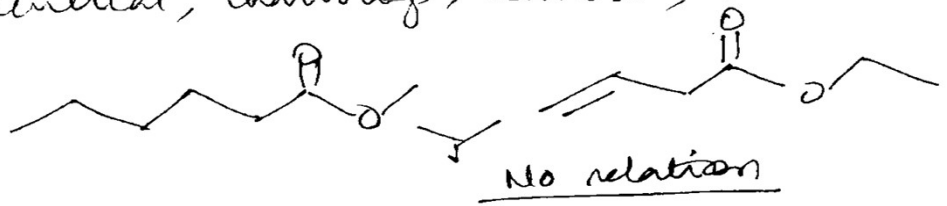
Functional isomerism (F.G. different)

Metamerism (F.G. same)





For identical, homologs, isomers, ΔU is same

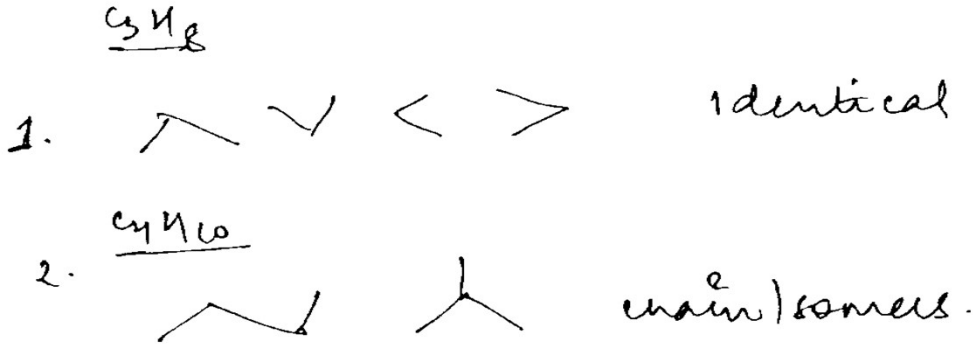


Chain isomerism/skeletal isomerism

- Isomers which have different arrangement of carbon atom (different skeleton of carbon)
- Generally length of carbon chain changes but not always.
- Alkanes show chain isomerism only.

Position isomerism

-Isomers which have different position of functional group or atom on given carbon skeleton.
- Carbon skeleton should not change in position isomerism.



C_5H_{12}

3.  Chain Isomers

C_6H_{14}

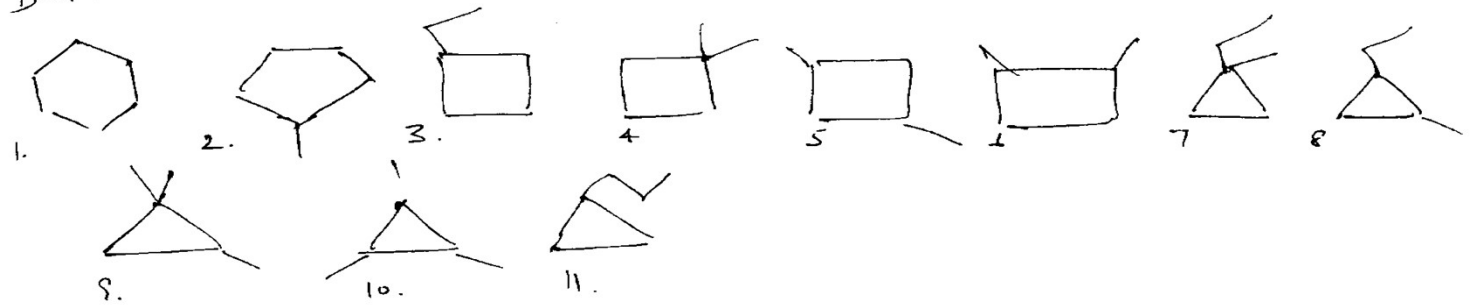
4. 

Chain Isomers

C_6H_{14} has 5 chain isomers

C_6H_{12} (Sat)

D.U. 1



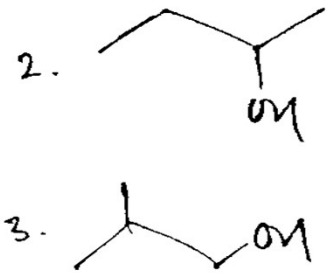
Q.1 Draw all possible alcohol isomers of $C_4H_{10}O$ and give relation between them.

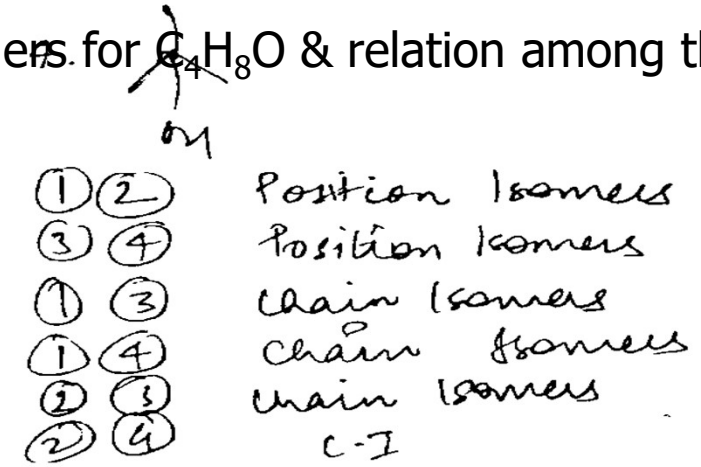
Q.2 Draw all tertiary amine possible for $C_6H_{15}N$

Q.3 Draw all aromatic ether for $PhOCH_2CH_3$ and give relation between them.

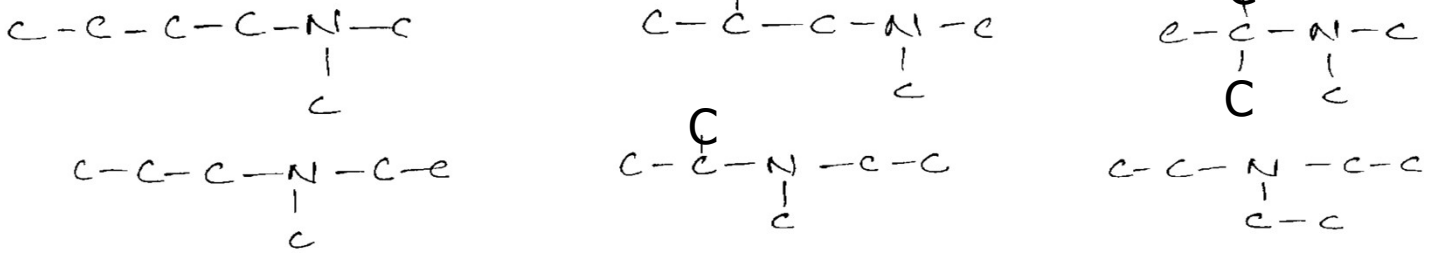
Q.4 Draw all possible benzoic aromatic isomers for $C_7H_6O_2$ & relation among them.

Q.5 Draw all possible aromatic isomers for C_4H_8O & relation among them.



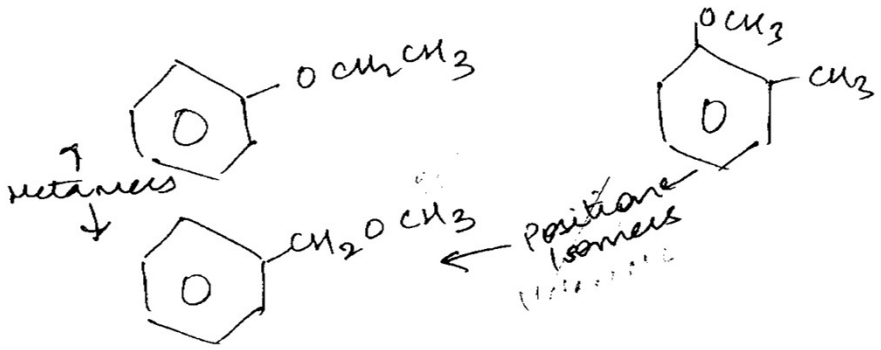


2



Total 4 metamers.

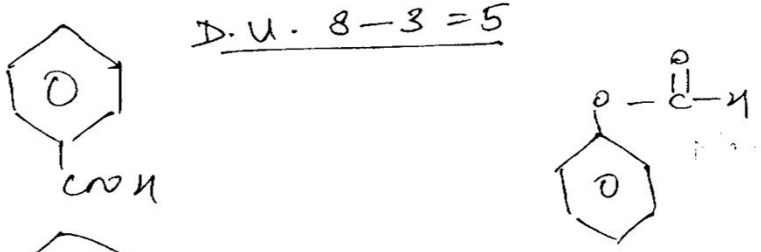
3



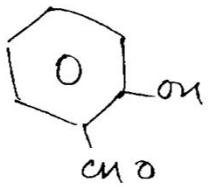
D.U. 9−5
= 4

(o, m, p)

4 D.U. $8-3=5$



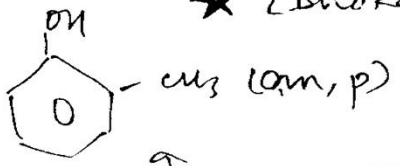
Otherwise everybody has a relⁿ of functional isomers.

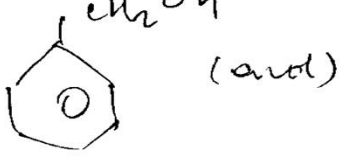


(o, m, p) within this PG. Position Isomers

5

★ (Dhoka)





(aldehyde)

Functional isomers

★ We get confused between enol & alcohol

6. $CH_3-\underset{2}{CH}(COOH)-CH_3$ $\quad$ $CH_3\overset{1}{CH_2}\overset{2}{CH_2}\overset{3}{CH_2}\overset{4}{COOH}$

Not PI ✱ (Dhoka)

7. $CH_3CH_2-NH-CH_2CH_3$ 1.

$CH_3-NH-CH_2CH_2CH_3$ 2.

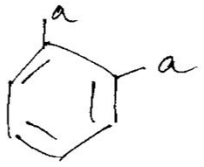
$CH_3-N(CH_3)-\underset{3}{CH}-CH_3$

$CH_3-\underset{4}{N}(CH_3)-CH_2CH_3$

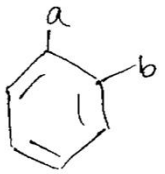
1, 2, 3 Metamers

4 is F.G. Isomer w.r.t. others

Positional isomers (DRC concept)



3



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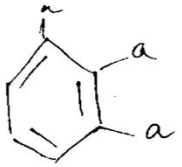

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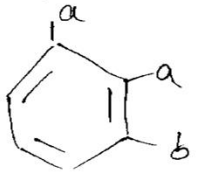

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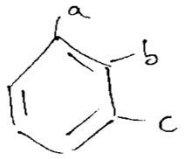
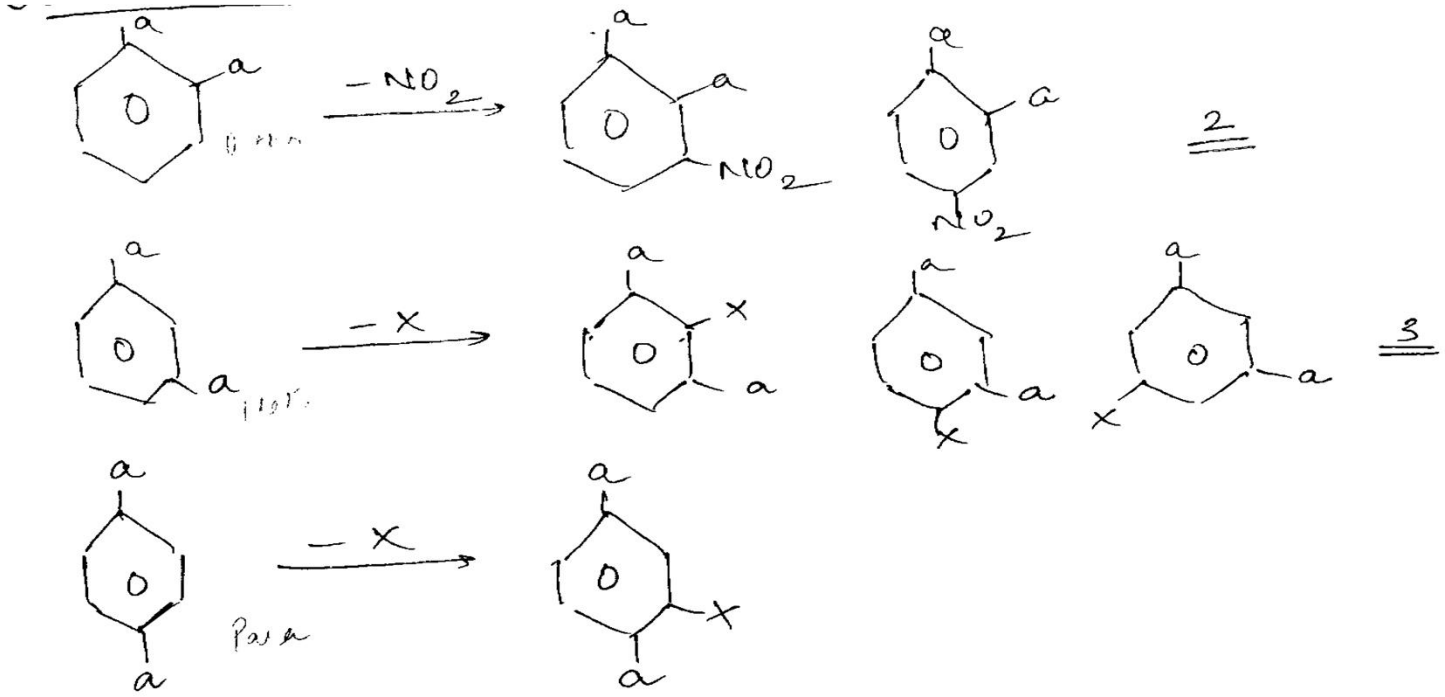


10

Korner Absolute Method (Disubstituted Benzene)



Brahmastra

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