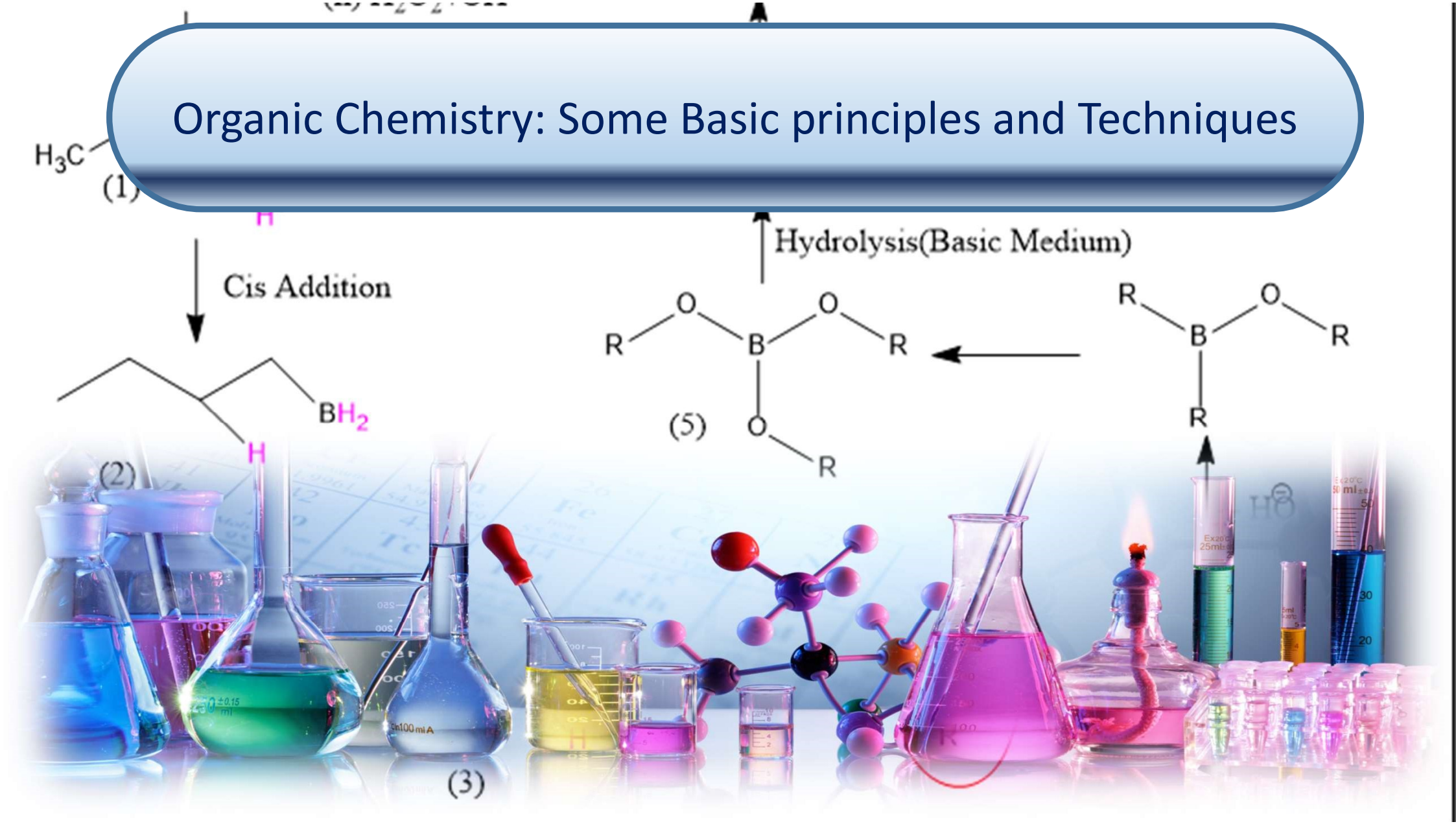
Organic Chemistry: Some Basic principles and Techniques



Important Topics

- Classification
- IUPAC Nomenclature – Rules and Practices
- Isomerism
- Fundamental concepts of Organic reaction Mechanisms
- Electron movement in Organic Reactions & compounds. (Effects)
- Methods of Purification of Organic Compounds
- Types of Organic reactions
- Qualitative and Quantitative analysis of Organic Compounds (Numericals)

Organic Chemistry: The 'Vital force' theory

- Carbon has the unique property called catenation due to which it forms covalent bonds with other carbon atoms.
- Carbon has ability to bond with four other atoms.
- It also forms covalent bonds with atoms of other elements like hydrogen, oxygen, nitrogen, sulphur, phosphorus and halogens.

Organic compounds are produced only under the influence of living force within living organisms called vital force- Berzilius(1815)

This notion is rejected when F Wohler and others synthesized many organic compounds synthetically

Synthesis of Organic compounds

1. F.Wohler(1828) -synthesised an organic compound, urea from an inorganic compound, ammonium cyanate.

$$NH_4Cl + KCN \rightarrow NH_4CNO \rightarrow NH_2 - CO - NH_2$$

[O] Δ (Rearrangement)

2. Herman Kolbe (1845) – synthesized Acetic acid using Carbon

$$2C + H_2 \xrightarrow{\text{Electric Discharge}} C_2H_2 \xrightarrow{\text{dil } H_2SO_4 + HgSO_4} CH_3CHO \xrightarrow{[O]} CH_3COOH$$

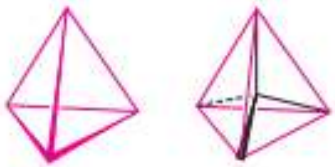
3. Berthelot(1856) – Synthesised methane etc

Organic Chemistry- Chemistry of hydrocarbons and their derivatives.

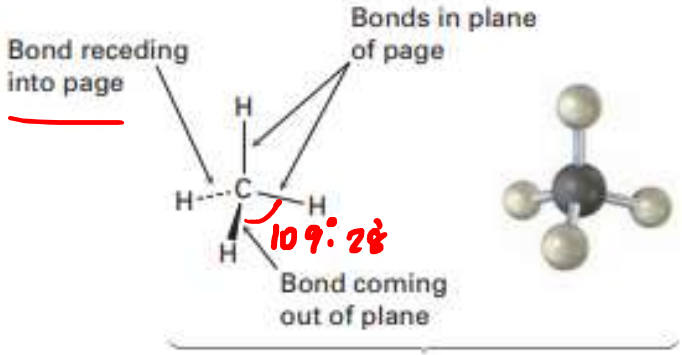
Organic compounds- Compounds containing Carbon and hydrogen and traces of O,N,S,halogen etc

Structure of Organic Molecules

Tetravalence of carbon and the formation of covalent bonds by it are explained in terms of its electronic configuration and the hybridisation of *s* and *p* orbitals.

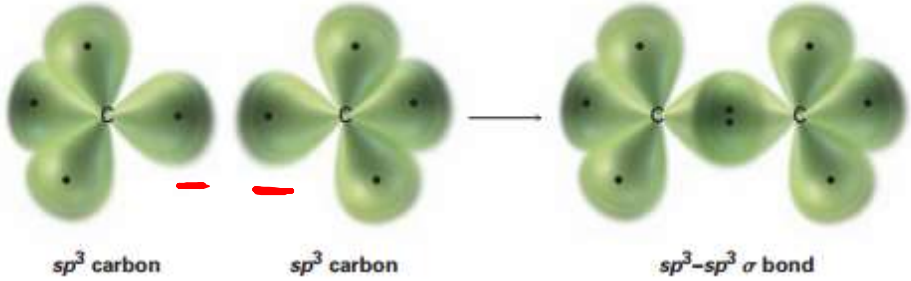


A regular tetrahedron

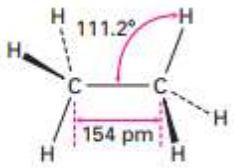


A tetrahedral carbon atom

4σ Bonds

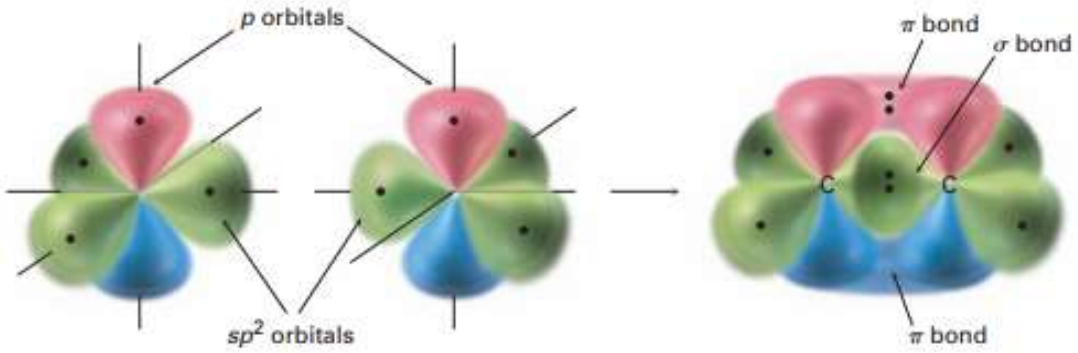


sp^3 carbon sp^3 carbon sp^3–sp^3 σ bond

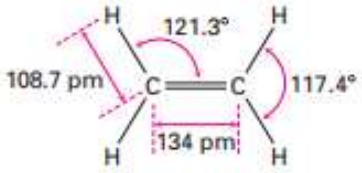


Ethane

Structure of Organic Molecules



sp^2 carbon sp^2 carbon Carbon–carbon double bond

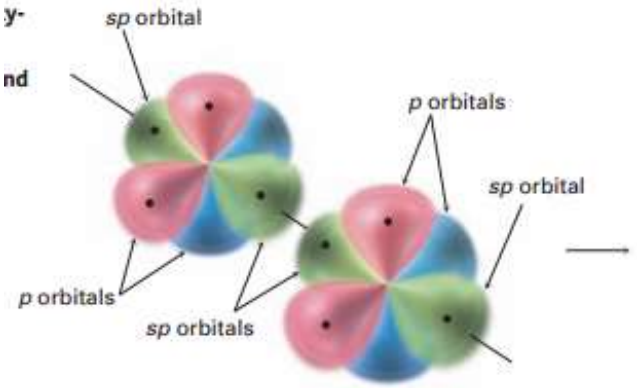


5 σ-Bonds

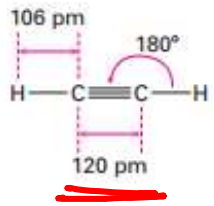
1 π-Bond

y-

nd

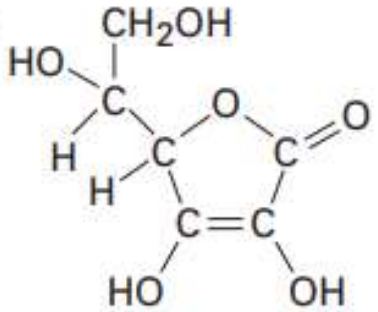


Carbon–carbon triple bond



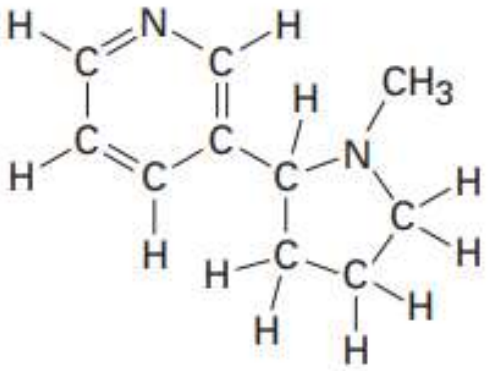
Structure of Organic Molecules

(a)



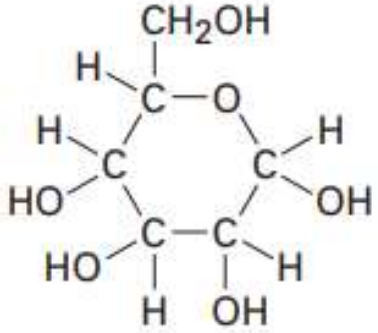
Vitamin C
(ascorbic acid)

(b)



Nicotine

(c)



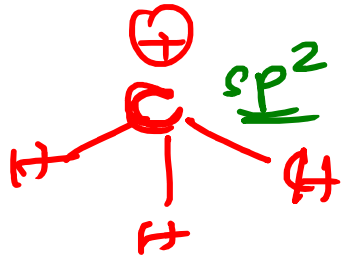
Glucose

for carbon compounds,

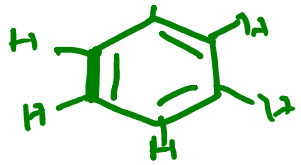
4 σ bonds — sp^3 hybrid

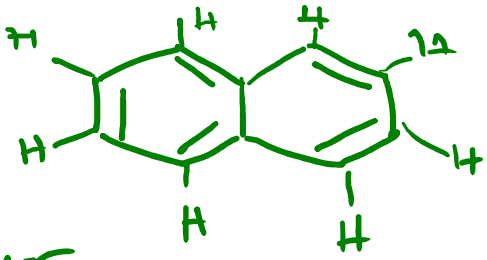
3σ + 1π → sp^2 "

2σ + 2π → sp "



Example

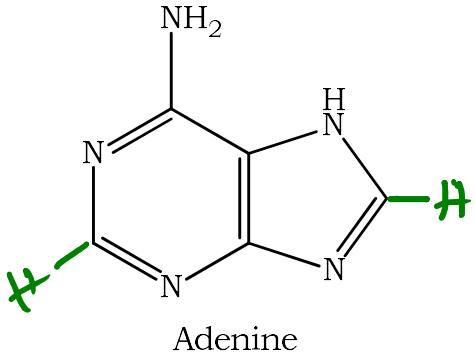




1. How many sigma bond and pi bonds are present in (a) C_6H_6 (b) Napthalene

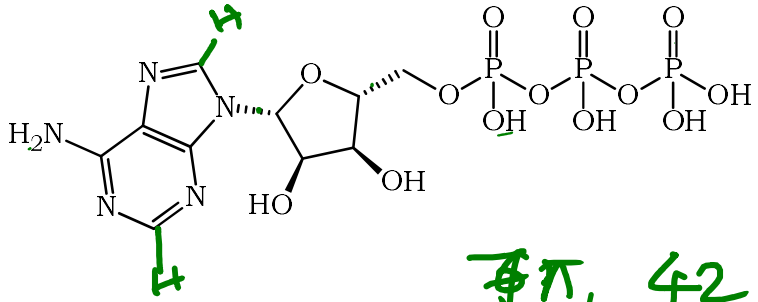
3π, 12σ

5π, 19σ



Adenine

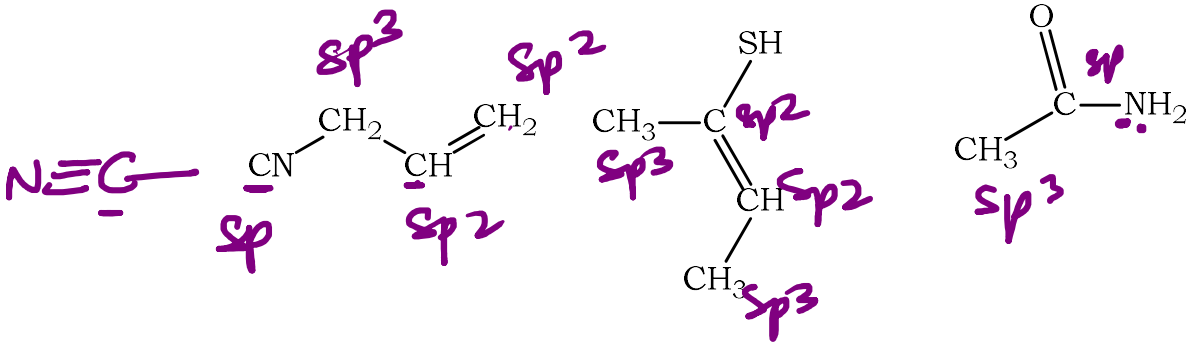
4π, 16σ



ATP

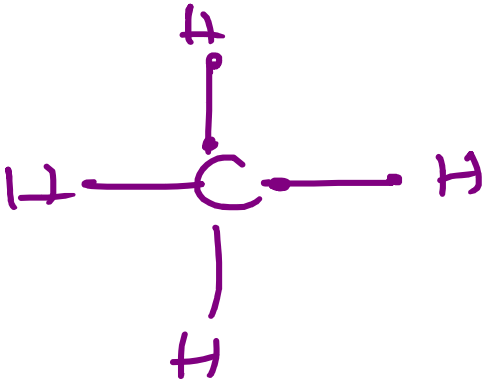
13π, 42σ

2. Identify hybridization of each carbon atom in the following



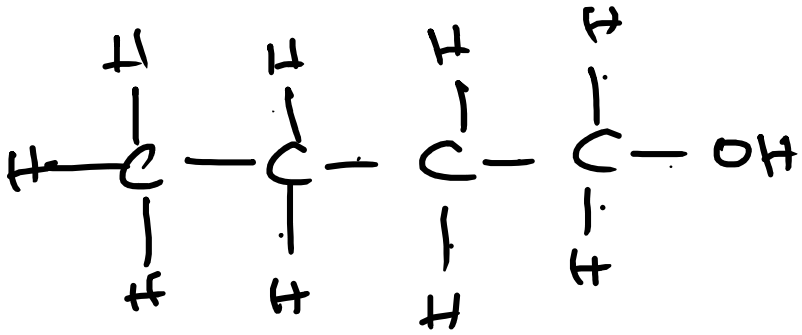
Structural Representation of Organic Molecules

1. **Complete Structural formula**-Such a structural formula focuses on the electrons involved in bond formation. (Open structures)



Methane

Butanol

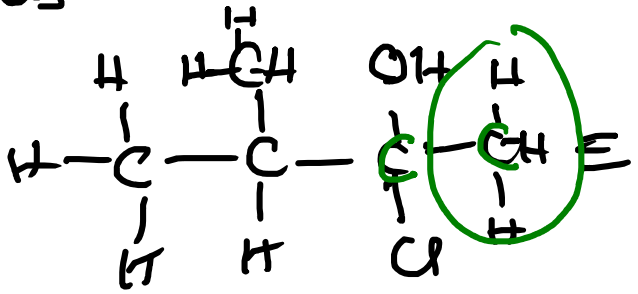


2. **Condensed structural formula**

C–C single bond & C–H bonds are not shown.

Butanol – $CH_3CH_2CH_2CH_2OH$

Methane – CH_4

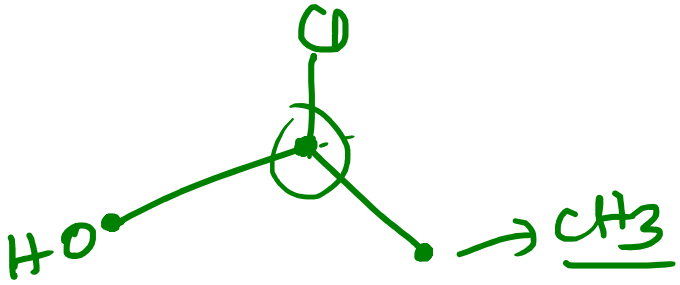


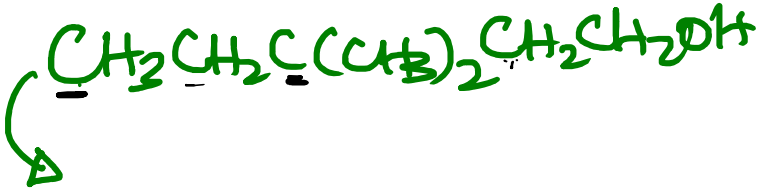
$CH_3CH(CH_3)CCl(OH)CH_3$

Structural Representation of Organic Molecules

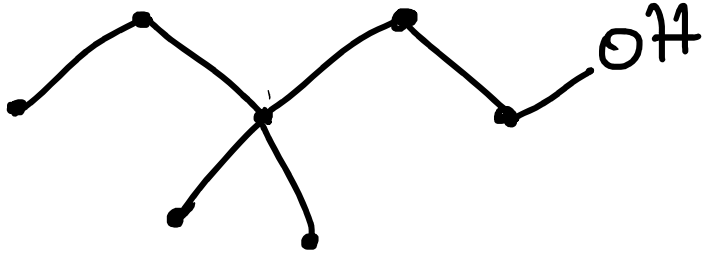
3. **Bond line Structural representation-carbon and hydrogen atoms are not shown and the lines representing carbon-carbon bonds are drawn.**

   The terminals denote methyl (–CH3) groups (unless indicated otherwise by a functional group), while the line junctions denote carbon atoms bonded to appropriate number of hydrogens required to satisfy the valency of the carbon atoms

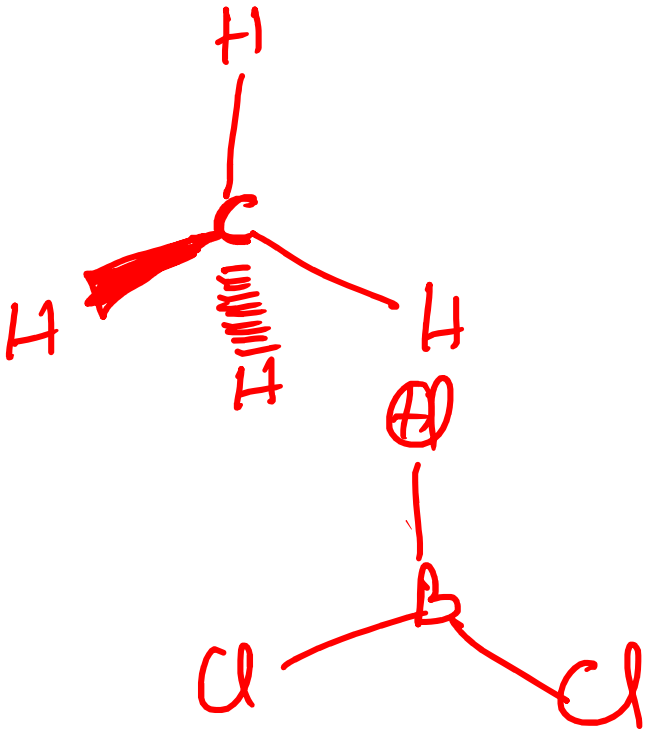




Butanol →

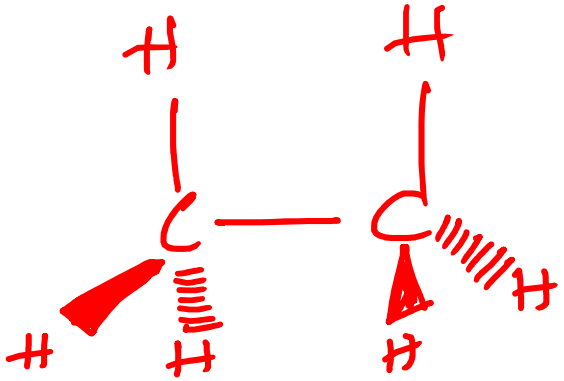


4. **3-D representation (Dash-wedge formula)-In these formulas the solid-wedge is used to indicate a bond projecting out of the plane of paper, towards the observer. The dashed-wedge is used to depict the bond projecting out of the plane of the paper and away from the observer**



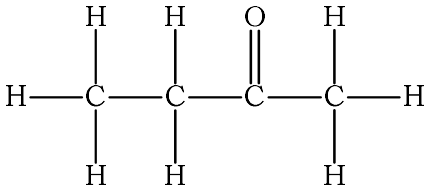
– Useful in discussing mechanism and orientation of groups.

C_2H_6

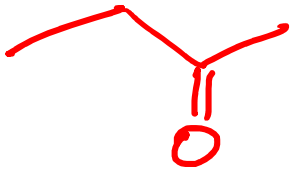


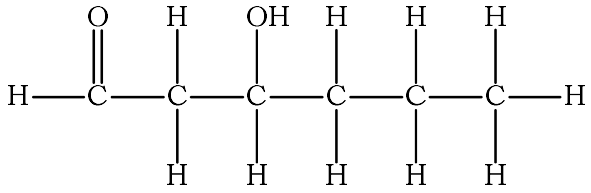
Example

1. Write following in condensed form



$CH_3CH_2COCH_3$

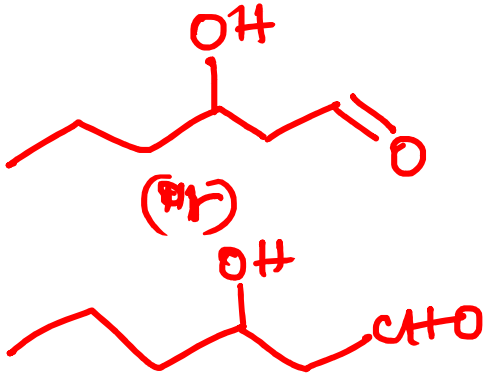


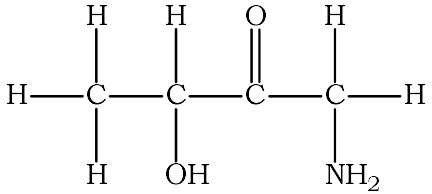


$CH_3CH_2CH_2CHOHCH_2CHO$

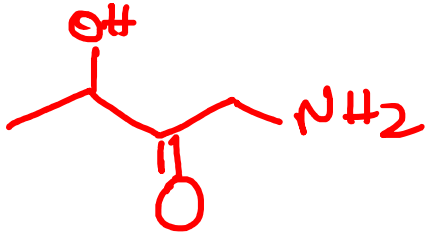
(or)

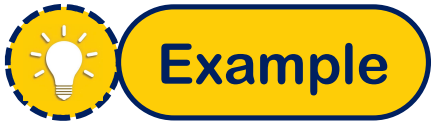
$OHCCH_2CHOHCH_2CH_2CH_3$





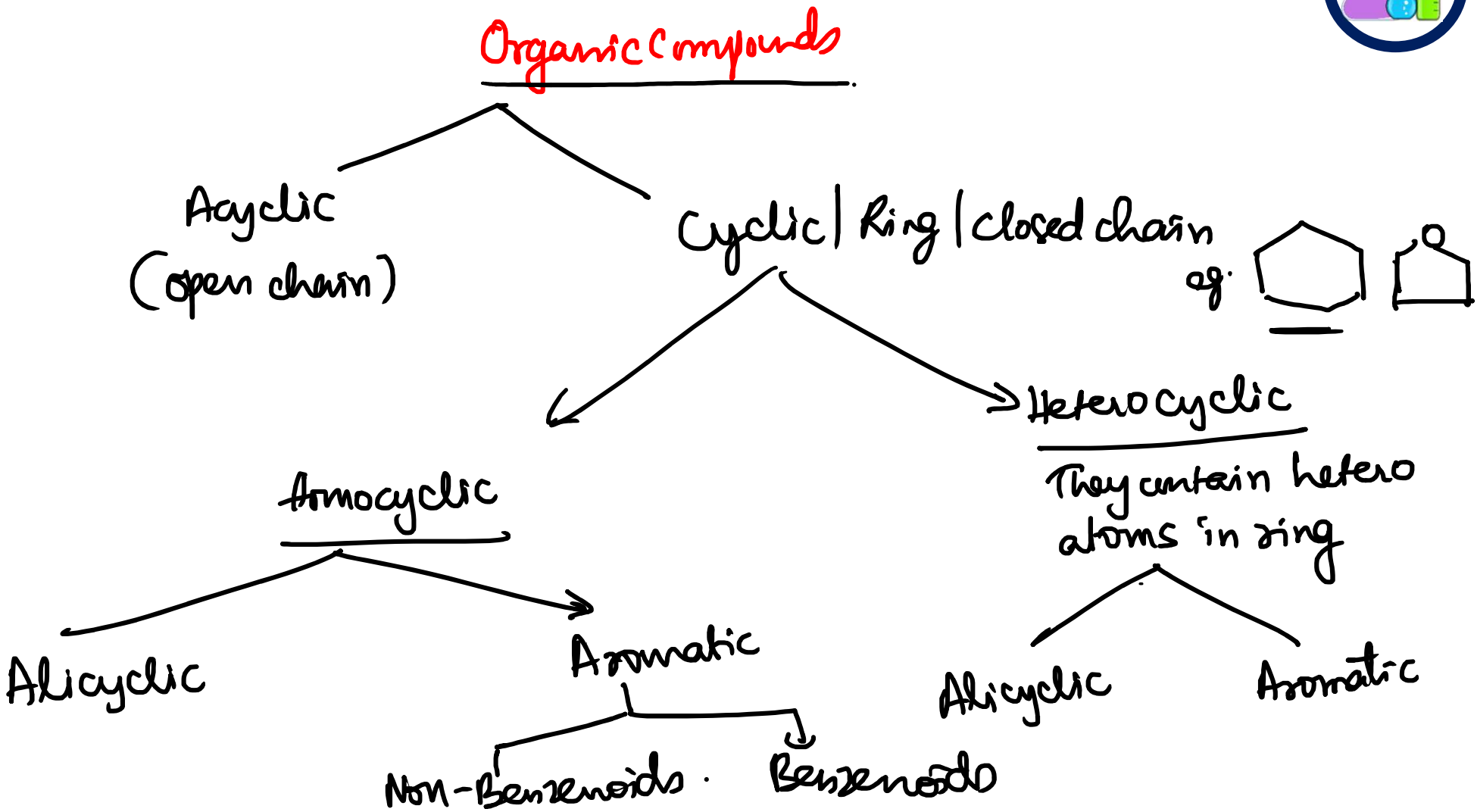
$CH_2CHOHCOCH_2NH_2$





1. Write following in Open structure and bond line structure

Classification of organic compounds

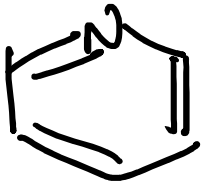


Classification of organic compounds

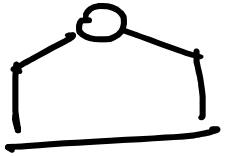
Open chain / Acyclic — $CH_3CH_2CH_3$

Cyclic Compounds → (Heteroatomic) —

(Pyrole - aromatic)



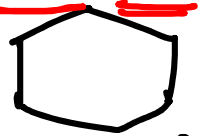
Pyridine - aromatic



- Tetrahydrofuran (Alicyclic)

Homoatomic

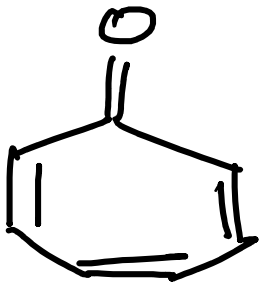
Cyclohexane



Alicyclic

Benzene

(Aromatic)



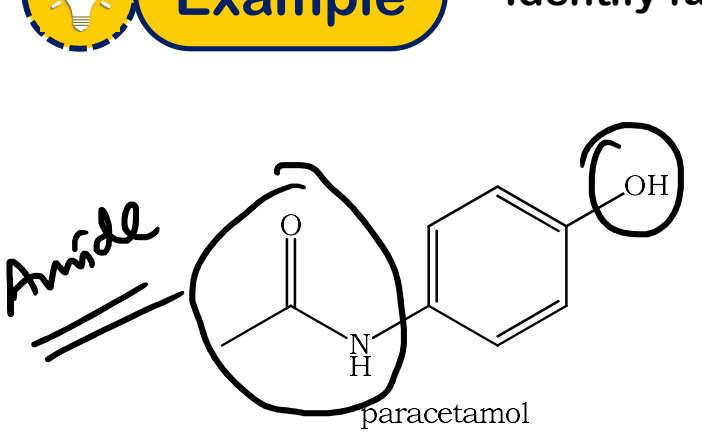
Tropolone (Non-benzenoid)

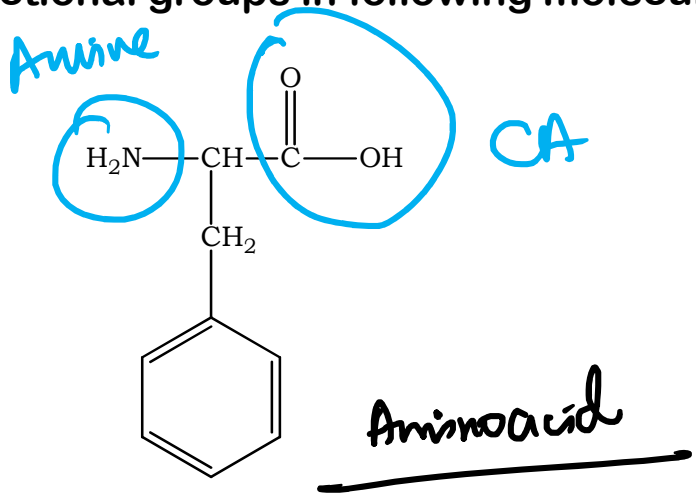
Functional group

The functional group is an atom or a group of atoms joined to the carbon chain which is responsible for the characteristic chemical and physical properties of the organic compounds.

The examples are hydroxyl group (–OH), aldehyde group (–CHO) and carboxylic acid group (–COOH) etc

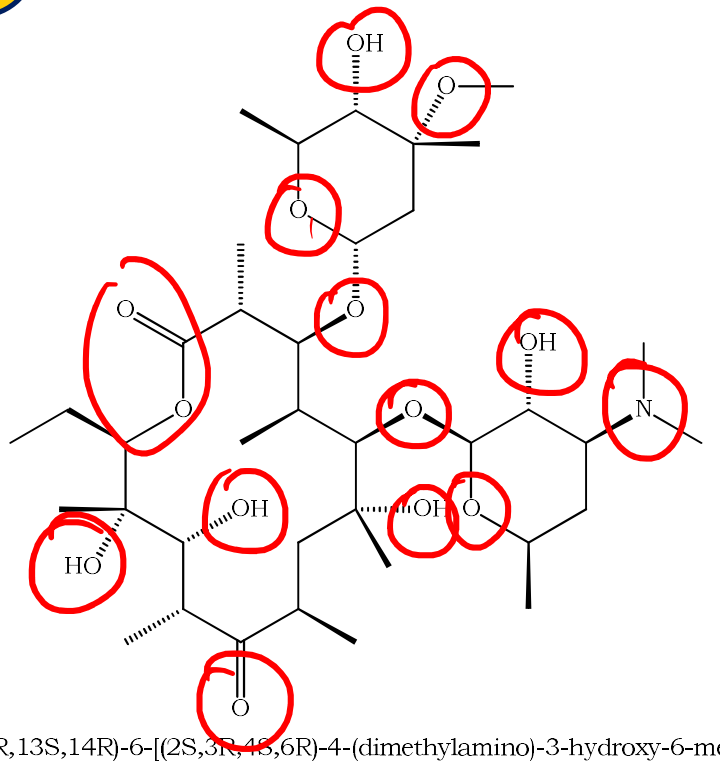
Example Identify functional groups in following molecule





Example

Identify functional groups in following molecule



No. of FG = 13

(3R,4S,5S,6R,7R,9R,11R,12R,13S,14R)-6-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy-14-ethyl-7,12,13-trihydroxy-4-[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy-3,5,7,9,11,13-hexamethyl-oxacyclotetradecane-2,10-dione

Erythromicine

Homologous series

A group or a series of organic compounds each containing a characteristic functional group forms a homologous series and the members of the series are called homologues.

The members of a homologous series can be represented by general molecular formula and the successive members differ from each other in molecular formula by a $-CH_2$ unit.

- They show similarity and gradation in physical & chemical properties.

Alkanes – C_nH_{2n+2}

Alkenes – C_nH_{2n}

Alkynes – C_nH_{2n-2}

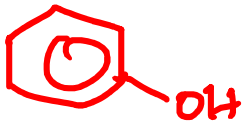
Alcohols – $C_nH_{2n+2}O$

Aldehydes – $C_nH_{2n}O$

IUPAC Naming

Before the IUPAC system of nomenclature, however, organic compounds were assigned names based on their origin or certain properties

Compound	Common name
CH_4	Methane
$H_3CCH_2CH_2CH_3$	*n*-Butane
$(H_3C)_2CHCH_3$	Isobutane
$(H_3C)_4C$	Neopentane
$H_3CCH_2CH_2OH$	*n*-Propyl alcohol
HCHO	Formaldehyde
$(H_3C)_2CO$	Acetone
$CHCl_3$	Chloroform
CH_3COOH	Acetic acid
C_6H_6	Benzene
$C_6H_5OCH_3$	Anisole
$C_6H_5NH_2$	Aniline
$C_6H_5COCH_3$	Acetophenone
$CH_3OCH_2CH_3$	Ethyl methyl ether



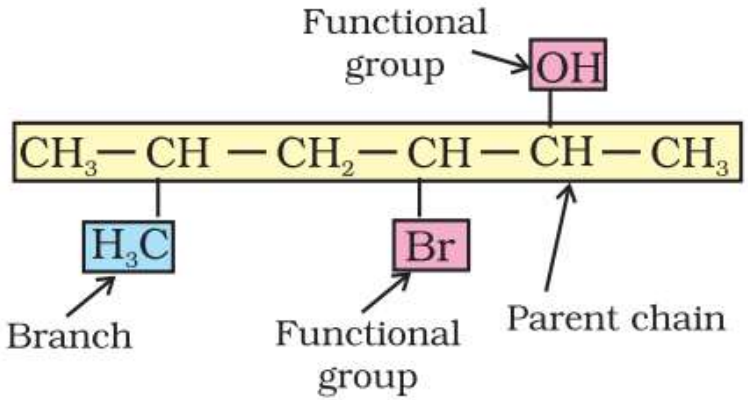
– Phenol (carbolic acid)

Why we need IUPAC Name?

IUPAC Naming

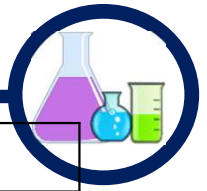
A systematic name of an organic compound is generally derived by identifying the parent hydrocarbon and the functional group(s) attached to it.

Secondary prefix	Primary Prefix	Word root	Primary suffix	Secondary suffix
Substituents	Cyclo- cyclic/acyclic	Parent chain containing FG and MB	Multiple bond if any	Principal functional group



IUPAC Naming

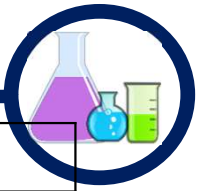
Secondary Prefixes



FG (in order of priority)	Suffix	Prefix	Exanple
$-NR_3X$	-Amine salts		
-COOH	-oic acid	carboxy	CH_3COOH- Ethanoic acid
$-SO_3H$	-sulphonic acid	Sulphonyl/sulpho	CH_3SO_3H- Methane sulphonic acid
-COOCO-	-oic anhydride		$CH_3COOCOCH_3$-Ethanoic anhydride
-COOR	-oate	Alkoxycarbonyl	CH_3COOCH_3- Methyl ethanoate
-COX (X=Cl,F,Br,I)	-oyl halide	Halocarbonyl	CH_3COCl- Ethanoyl chloride
$-CONH_2$	-amide	-carbamoyl	CH_3CONH_2- Ethanamide
-CN	-nitrile	Cyano	CH_3CN- Ethanenitrile
-CHO	-al	Formyl/oxo	CH_3CHO- Ethanal
-CO-	-one	Oxo/keto	CH_3COCH_3 -Acetone
-OH	-ol	Hydroxy	CH_3CH_2OH- Ethanol
-SH	-thiol	Mercapto/sulphanyl	CH_3SH- Methane thiol
$-NH_2$	-amine	Amino	CH_3NH_2 - Methanamine

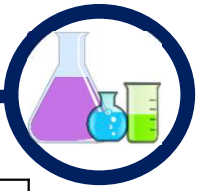
IUPAC Naming

Secondary Prefixes



FG (in order of priority)	Suffix	Prefix	Exanple
$-NR_3X$	-Amine salts		
-COOH	-oic acid	carboxy	CH_3COOH- Ethanoic acid
$-SO_3H$	-sulphonic acid	Sulphonyl/sulpho	CH_3SO_3H- Methane sulphonic acid
-COOCO-	-oic anhydride		$CH_3COOCOCH_3$-Ethanoic anhydride
-COOR	-oate	Alkoxycarbonyl	CH_3COOCH_3- Methyl ethanoate
-COX (X=Cl,F,Br,I)	-oyl halide	Halocarbonyl	CH_3COCl- Ethanoyl chloride
$-CONH_2$	-amide	-carbamoyl	CH_3CONH_2- Ethanamide
-CN	-nitrile	Cyano	CH_3CN- Ethanenitrile
-CHO	-al	Formyl/oxo	CH_3CHO- Ethanal
-CO- >C=O	-one	Oxo/keto	CH_3COCH_3 -Acetone
-OH	-ol	Hydroxy	CH_3CH_2OH- Ethanol
-SH	-thiol	Mercapto/sulphanyl	CH_3SH- Methane thiol
$-NH_2$	-amine	Amino	CH_3NH_2 - Methanamine

IUPAC Naming



-C=C	-ene	Enyl	CH_2CH_2- Ethene
-C≡C	-yne	Ynyl	C_2H_2- Ethyne
–C–C	- ane	yl	Cthy - Methane.

Groups which are always substituents (Secondary prefix)

Nitro	$-NO_2$
Fluoro	-F
Chloro	-Cl
Bromo	-Br
Nitroso	-NO
Iodo	-I

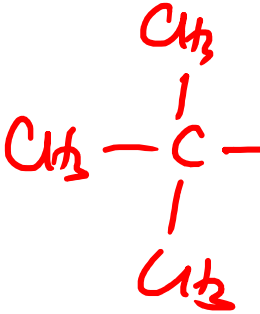
Diazo	$-N_2$
Alkoxy	-OR
Phenyl	$-C_6H_5$
Alkyl	-R

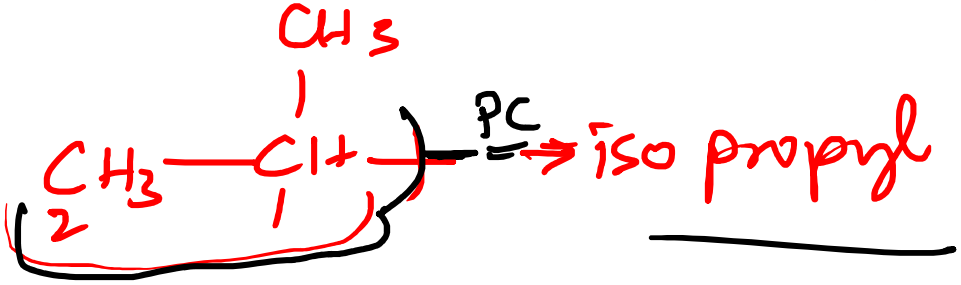
→ CH_3 - Methyl

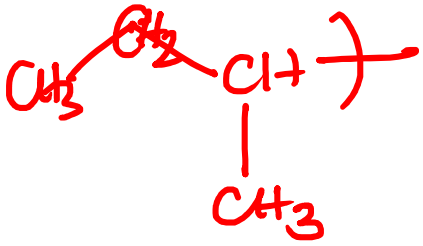
CH_3CH_2 – Ethyl.

Some alkyl groups

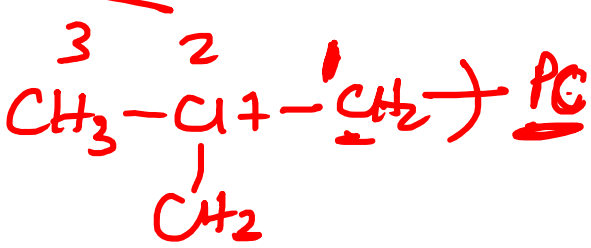
$CH_3-CH_2-CH_2-CH_2-$ (PC) — n-Butyl (butyl.)







→ Sec-Butyl. (1-methylpropyl)



IUPAC Naming

Primary suffix → Cyclo (if compound is cyclic else it is absent)

Word Root → No of carbons in Parent chain

Addresses

C_1 → Meth

C_2 – Eth

C_3 – Prop

C_4 – But

C_5 – Pent

C_6 – Hex

C_7 – hept

C_8 – Oct

C_9 – Non

C_{10} → dec

C_{11} → undec

C_{12} → dodec.

IUPAC Naming

Primary suffix

$-C\equiv C-$ -yn-

$-C-C-$ -an-

Secondary suffix

$-C=C-$ -en-

It addresses functional group (PFG). If 2 FG's are present then PFG is decided based on priority order discussed before.

Alkanes

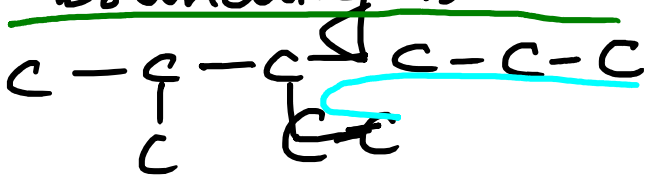
(i) Identify longest chain and number them (locants).

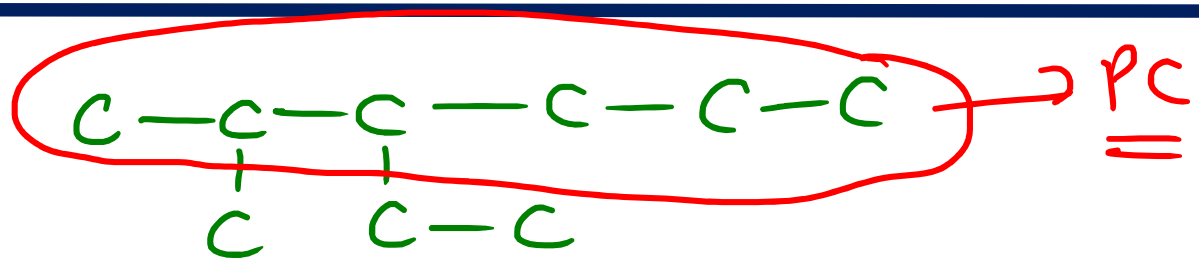
$$\overset{4}{C}-\overset{3}{C}-\overset{2}{C}-\overset{1}{C} \Rightarrow \underline{\text{Butane}}$$

Numbering should be done such that FG / mb gets smallest possible no.

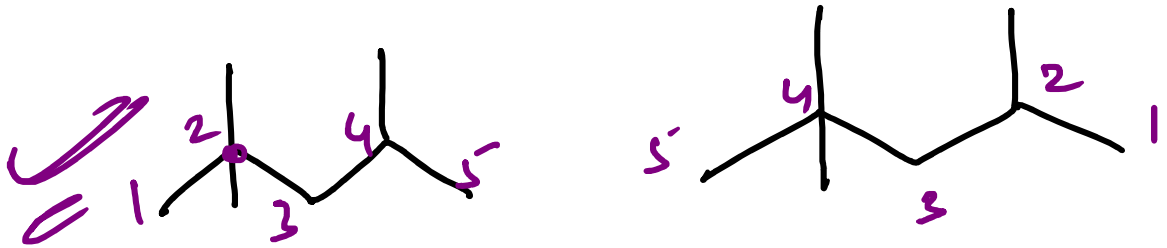
(ii) If 2 chains are possible with same length (No. of carbons) then choose the one with more branching as Parent chain

Preferred





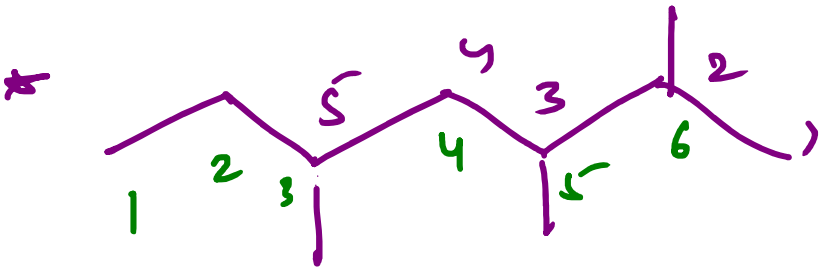
(VII) locants have to be assigned such that the sum of locants for the carbon containing branches/substituents gives lowest value. (lowest locant sum rule)



(2,3,4)

(4,4,2)

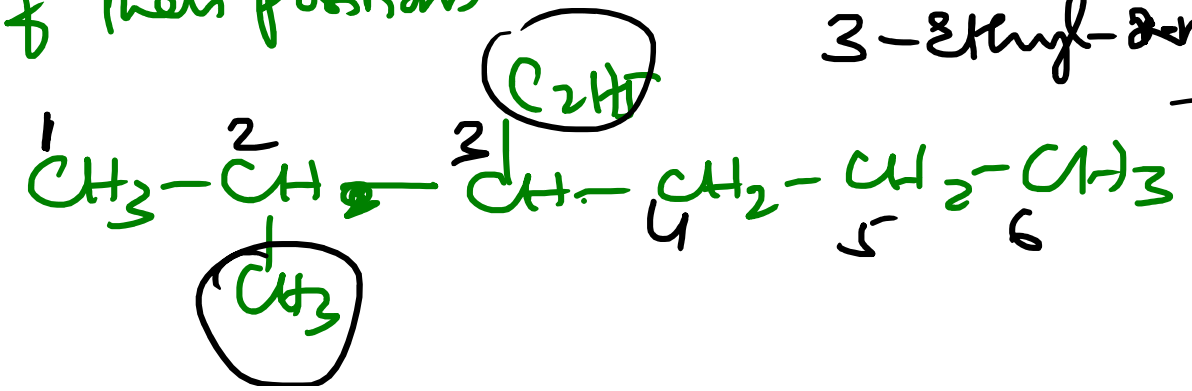
If 2 sets are possible with same sum, then lowest first point of diff is chosen



2, 3, 5 ~

3, 5, 6 X

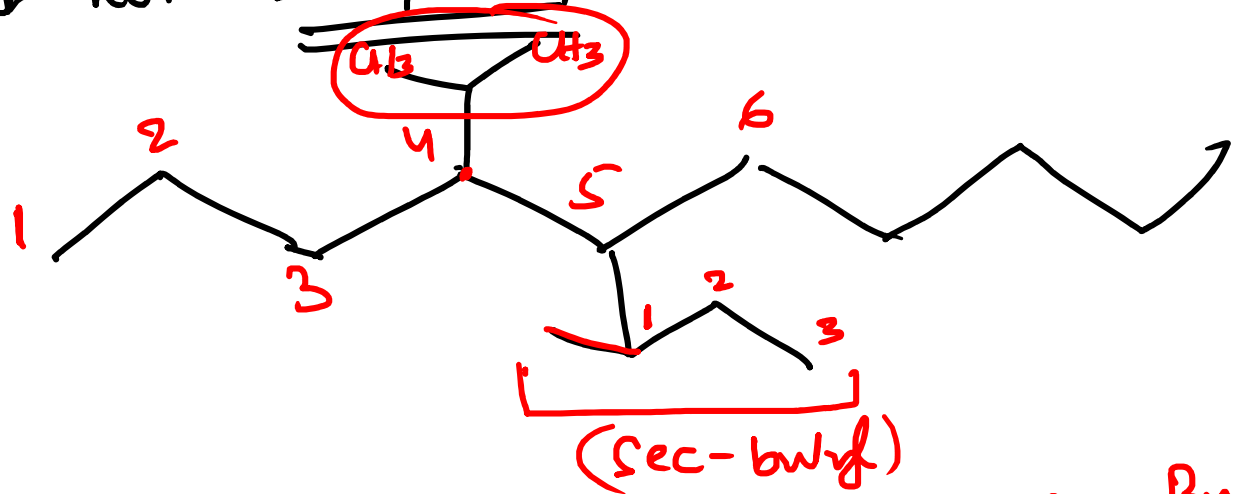
(14) When 2- or more alkyl groups are present as substituents then they have to be named in alphabetical order. irrespective of their positions.



3-Ethyl-2-methylhexane

(v) In case of iso, neo these words are considered as part of fundamental names and considered for alphabetical order.

But not sec, tert



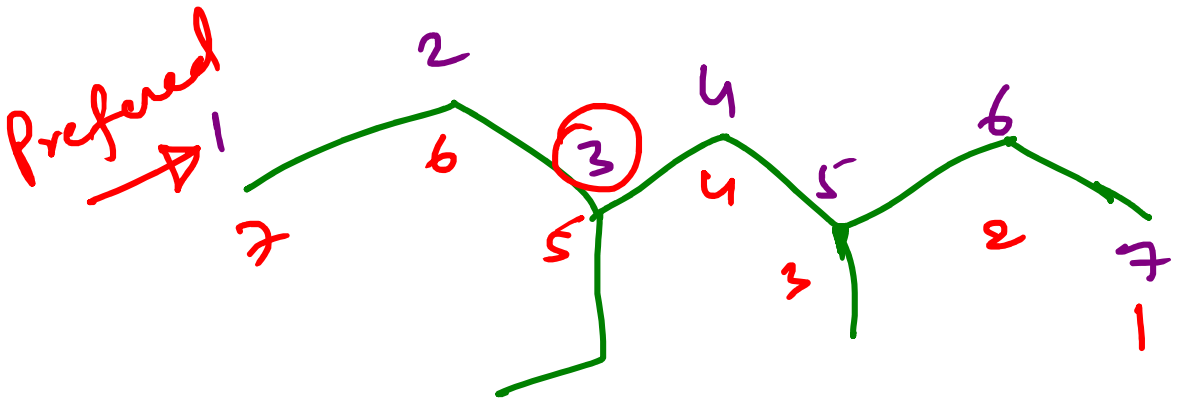
(sec-butyl)

4-(1-methylpentyl)-5-(1-methylpropyl) decane

5-sec-Butyl-4-isopropyldecane

(Substituent)

(VI) If 2 alkyl groups are present at equivalent positions Lowest no. is given to alphabetically prior group.



3,5

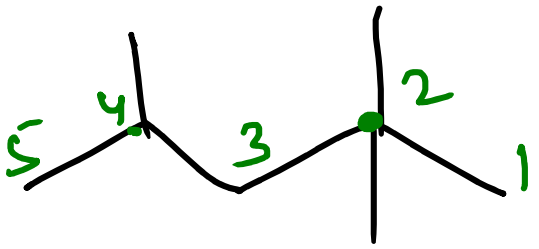
3-Ethyl-5-methylheptane

~~3-Methyl~~

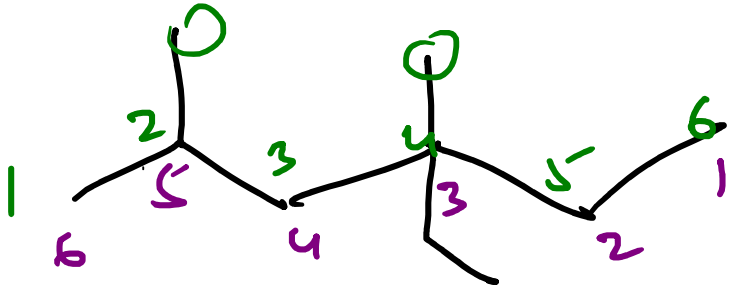
5-Ethyl-3-methyl

(VII) When same alkyl group occurs more than once at different positions, prefixes like di, tri, tetra are used.

(They are not considered for alphabetical order)



2,2,4-Trimethylpentane.

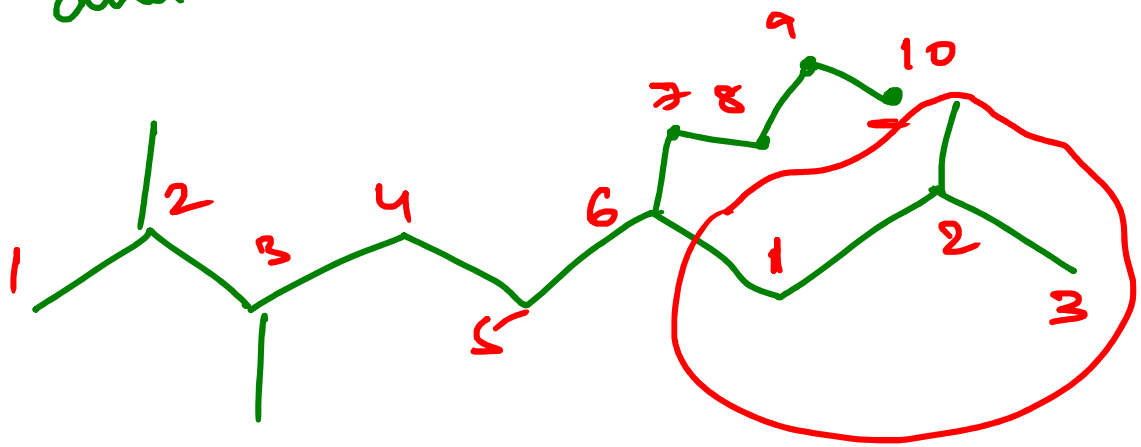


2,4,4

3,3,5

4-Ethyl-2,4-dimethyl hexane

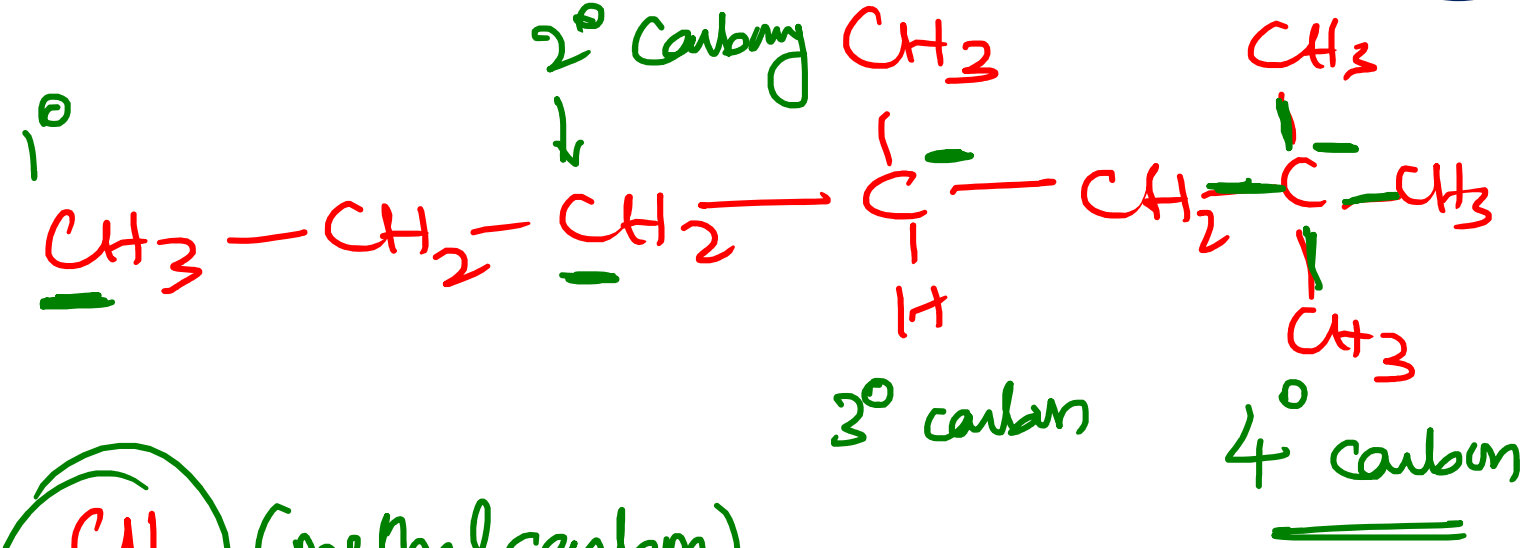
(VIII) While naming compound with complex substituent- (Branch with branch or FG), substituent is also numbered and its name is enclosed in paranthesis.



-complex-substituent

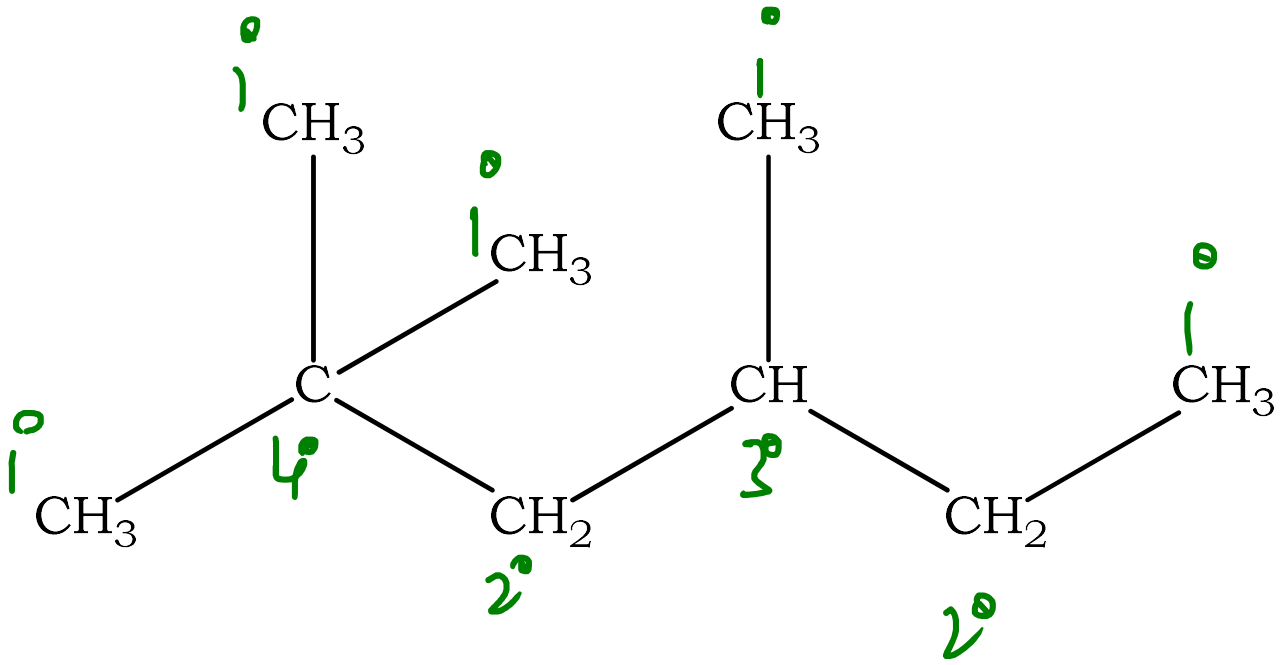
2,3-Dimethyl-6-(2-methylpropyl) decane

Nature of carbon



CH_4 (methyl carbon)

IUPAC Naming- Nature of Carbon



1° → 5

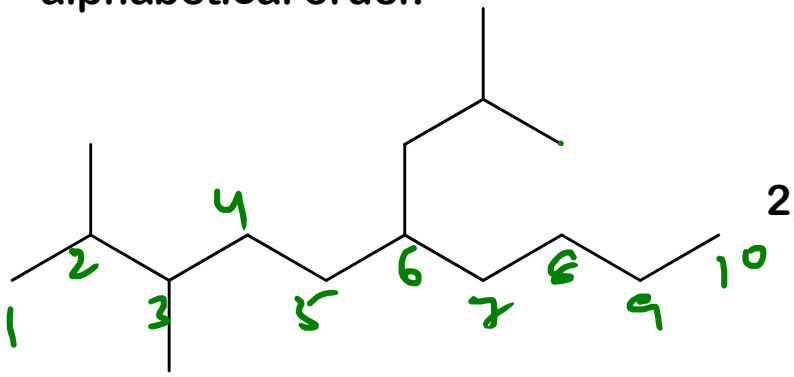
2° — 2

3° — 1

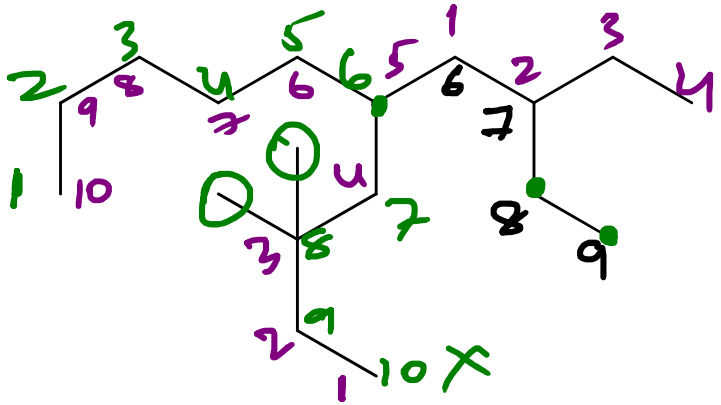
4° — 1

IUPAC Naming

9. If substituent itself is branched or has functional group, it has to be numbered starting from the carbon attached to parent chain. Name of such a substituent has to be enclosed in parenthesis . The first letter of the part enclosed in parenthesis is considered for alphabetical order.



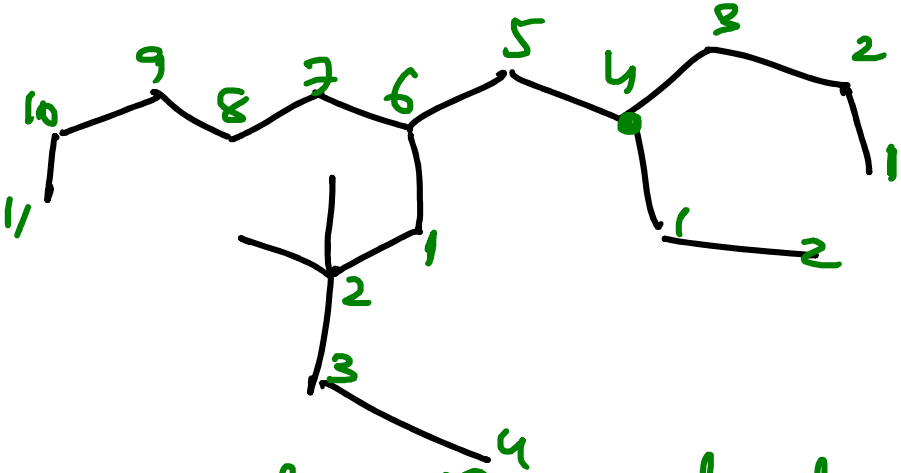
2,3-Dimethyl-6-(2-methylpropyl)decane



5-(2-ethylbutyl)-3,3-dimethyldecane

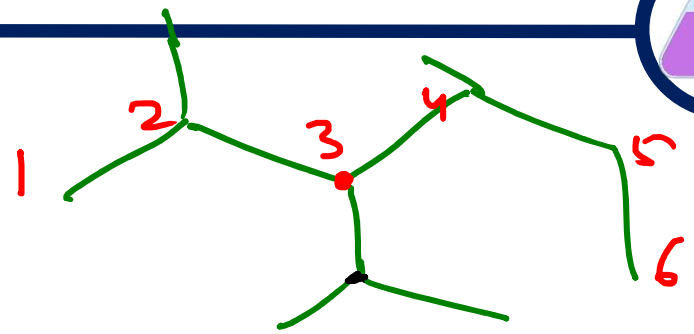
6, 8, 8

5, 3, 5

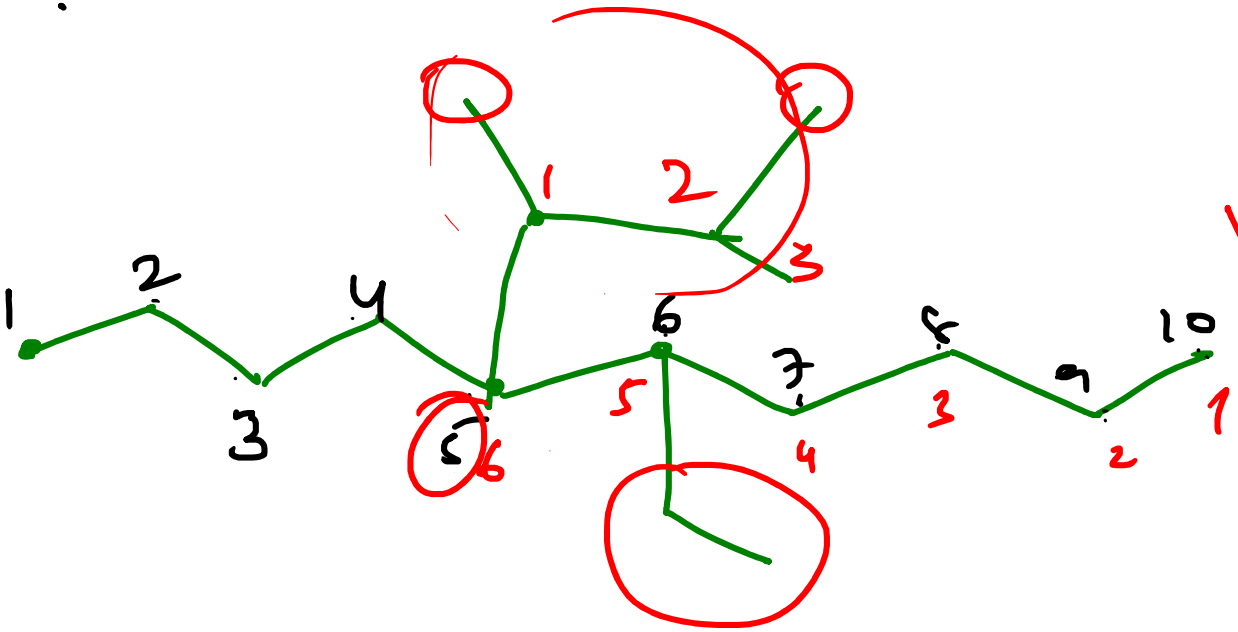


6-(2,2-dimethylbutyl)-4-ethylundecane

IUPAC Naming



2,4-Dimethyl-3-(1-methyl ethyl) hexane

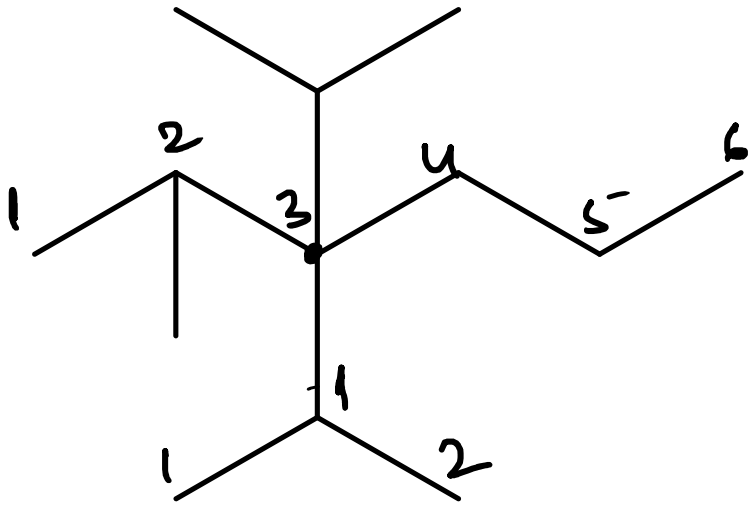


5-(1,2-Dimethylpropyl)-6-ethyldecane

3-isopropyl-2,4-dimethylhexane

10. If same complex substituent occurs more than once, prefixes like bis, tris,tetrakis,pentakis are used.

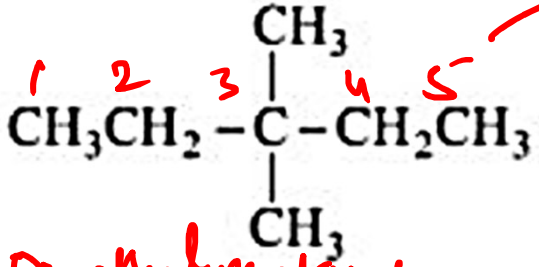
(bis / tris are not considered for alphabetical order.)



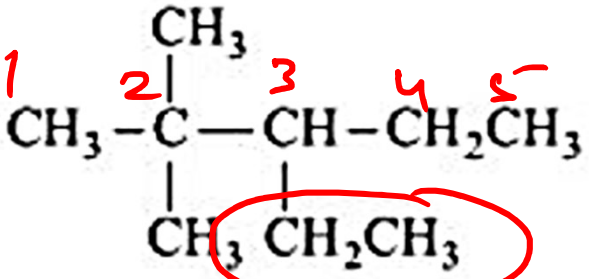
2-Methyl-3,3-bis(1-methylethyl)hexane

(3,3-diisopropyl-2-methylhexane)

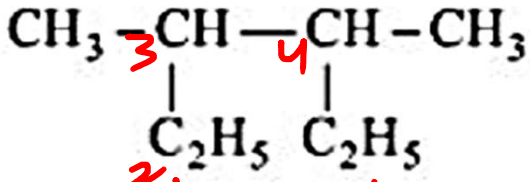
Example Write IUPAC Name for following

(1) 

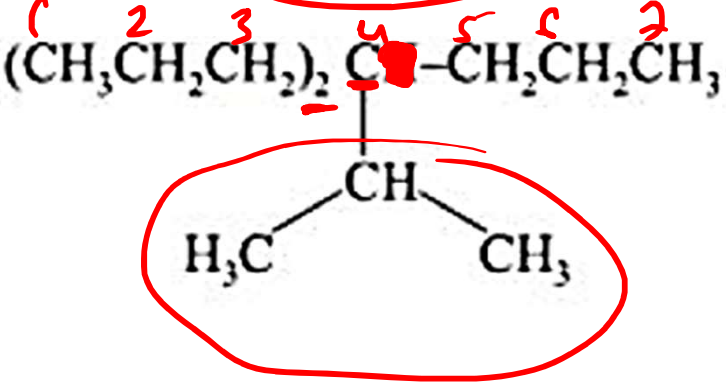
3-3-Dimethylpentane

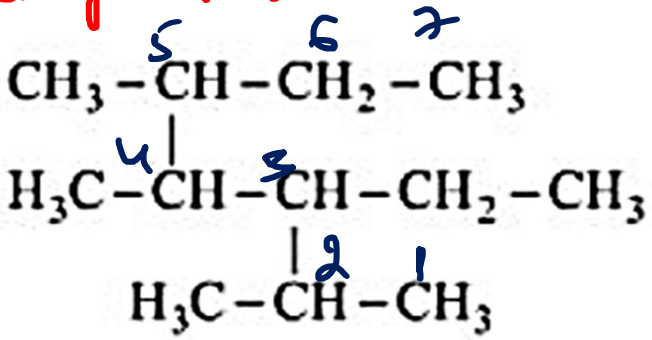
(2) 

3-Ethyl-2,2-dimethylpentane

(3) 

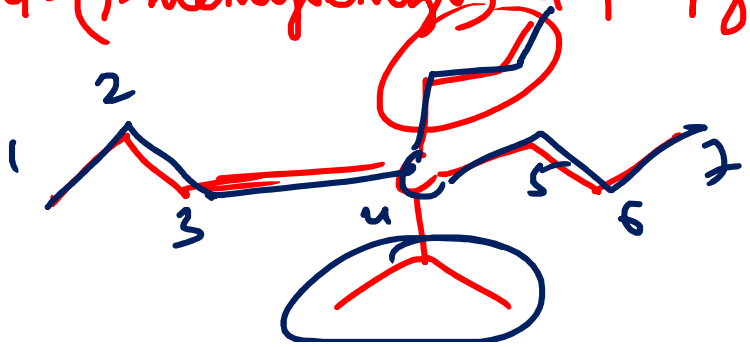
3,4-Dimethylhexane.

(4) 

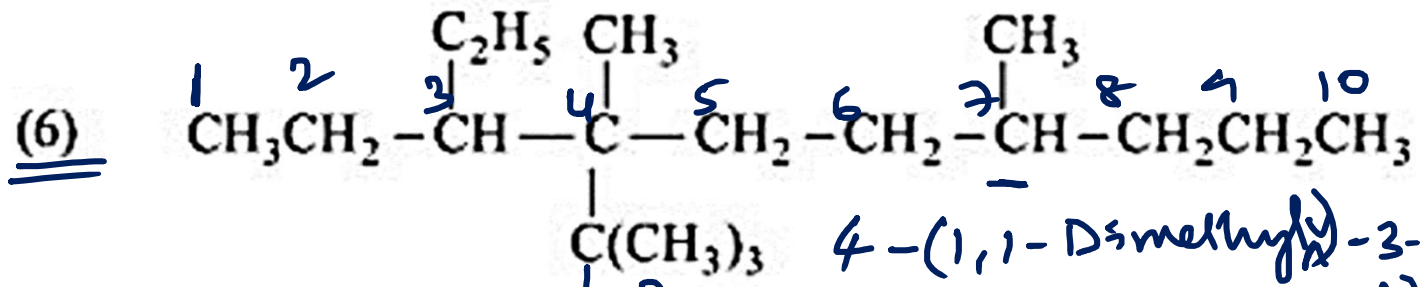
(5) 

3-Ethyl-2,4,5-trimethylheptane.

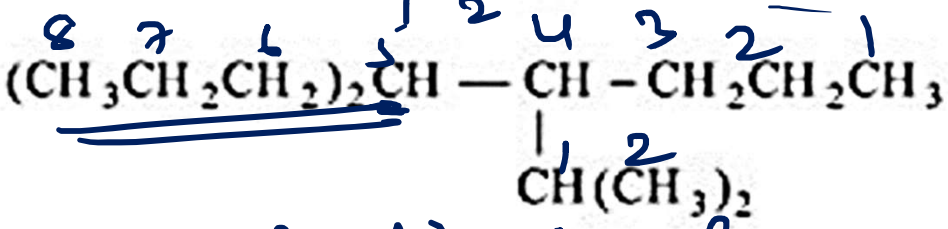
4-(1-methylethyl)-4-propylheptane



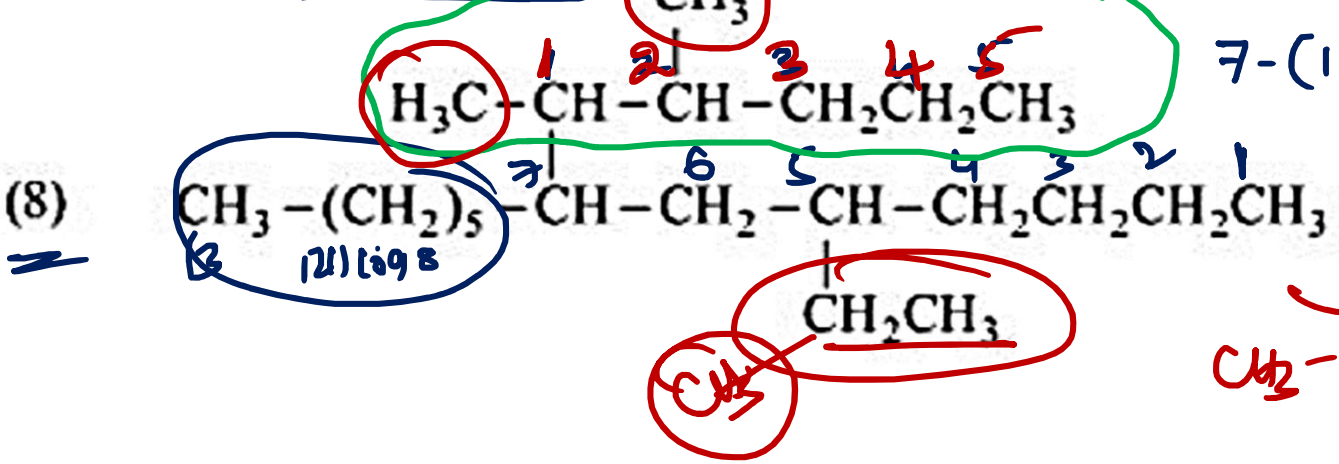
Example

(6) 

4-(1,1-Dimethyl)-3-ethyl-4,7-dimethyl decane

(7) 

4-(1-methylethyl)-5-propyloctane

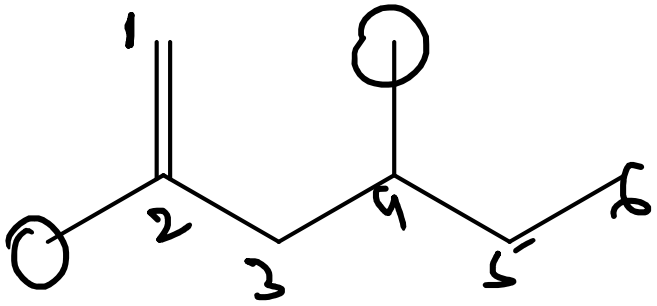
(8) 

7-(1,2-dimethylpentyl)-5-ethyl undecane

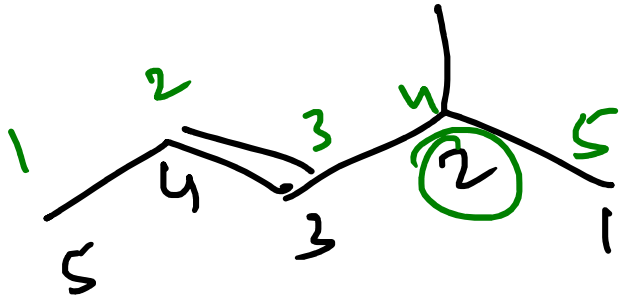
IUPAC Naming of Unsaturated Hydrocarbons

C c=c / c≡c / Δ

1.Parent chain must contain multiple bond and lowest locants must be assigned for multiple bonds according to lowest set of locants rule.



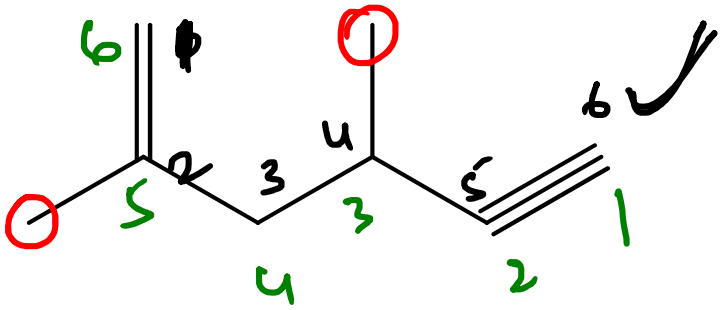
2, 4 - Dimethylhex-1-ene



4-methylpent-2-ene

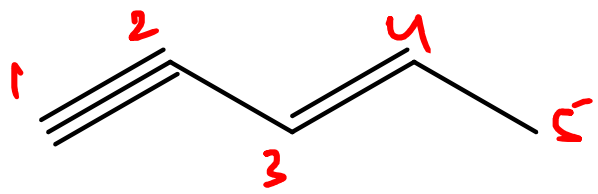
IUPAC Naming of Unsaturated Hydrocarbons

2.In case both double bond and triple bond is present in a molecule at same position(terminals), double bond is given preference and allotted lower locant.



2,4- Dimethylhex-1-en-5-yne

3. If triple bond is at one terminal and double bond is at any other position than the other terminal, numbering is done from triple bond.



Pent-3-en-1-yne.

IUPAC Naming of Unsaturated Hydrocarbons

* $\overset{1}{CH_2}=\overset{2}{CH}-\overset{3}{CH}=\overset{4}{CH_2}$

* Buta-1,3-diene

* $\overset{1}{CH_2}=\overset{2}{CH}-\overset{3}{C}(=\overset{CH_2}{\overset{|}{}})-\overset{4}{CH}=\overset{5}{CH_2}$

3-Methylenepenta-1,4-diene

* $\overset{1}{CH_2}=\overset{2}{CH}-\overset{3}{CH}=\overset{4}{CH}-\overset{5}{CH}(-\overset{6}{C}\equiv\overset{7}{CH})-\overset{6}{CH}=\overset{7}{CH_2}$

5-Ethynyl hepta-1,3,6-triene

$CH_3-CH=$ (PC) ethylidene

$CH_2=$ – methylene

$CH_2=CH-$ (PC)

ethenyl

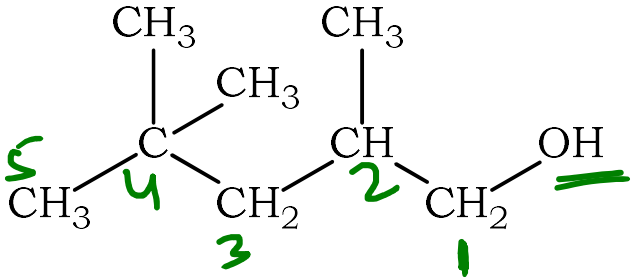
$CH\equiv C-$ (PC)

ethynyl.

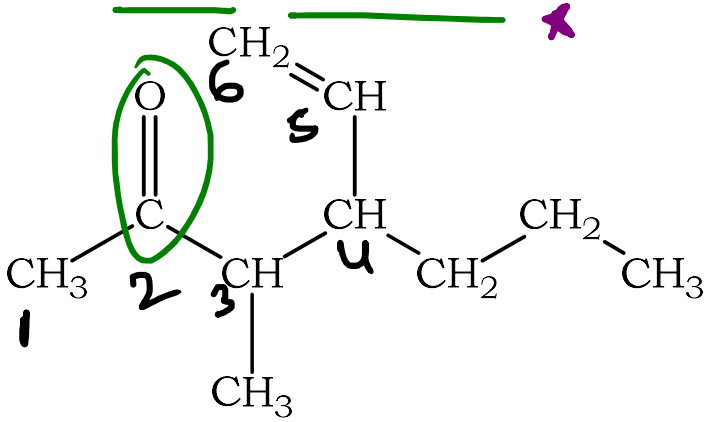
IUPAC Naming compounds with functional group

1. If functional group is present, that along with multiple bonds should be contained in parent chain. It is ensured that FG has lowest locant.

2, 4, 4 – Trimethylpentan–1–ol.



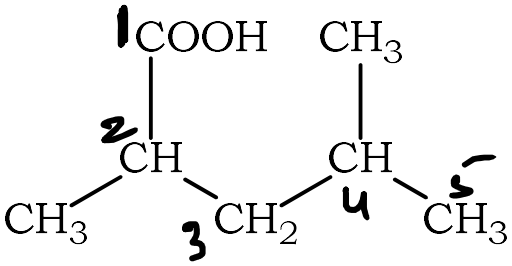
2. Once FG gets lowest locant, next lowest locant should be assigned to DB/TB whichever is closer to FG.



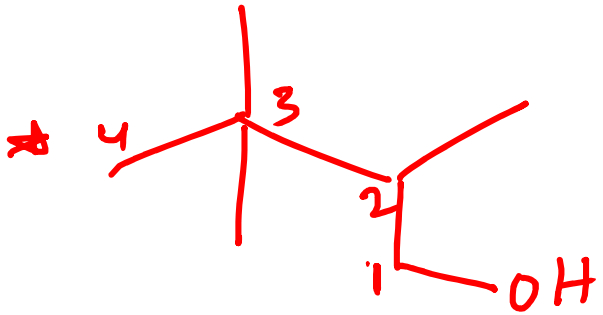
3-Methyl-4-propylhex-5-en-2-one

IUPAC Naming compounds with functional group

3. When functional group is chain terminating FG like –COOH, CHO, -COOR, -$CONH_2$ CN etc, the locant 1 has to be assigned to carbon of FG.

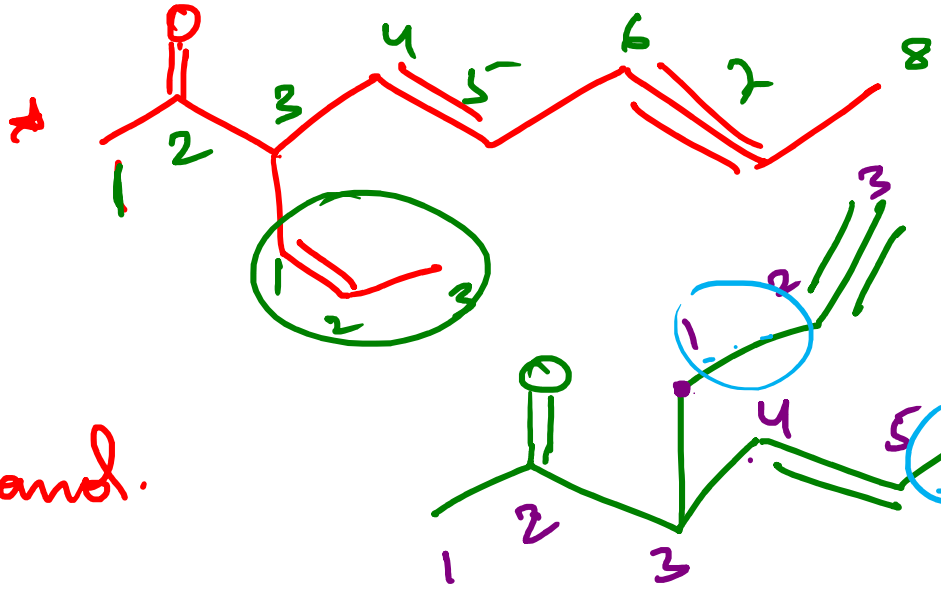


2,4-dimethylpentan-1-oic acid



2,3,3-Trimethylbutanol.

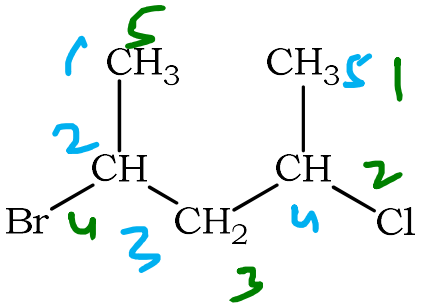
3-(Prop-1-enyl)oct-4-en-6-yn-2-one

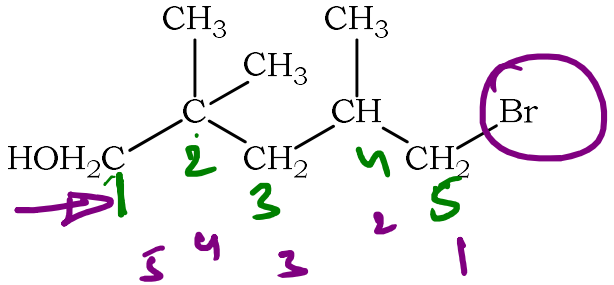


3-(Prop-2-ynyl)hex-4-en-2-one

IUPAC Naming compounds with functional group

4. If many functional group's are present, then select parent chain such that maximum functional groups and multiple bonds are present and while numbering , give priority to FG>C=C> C≡C >Substituent (Alphabetical order has to be followed as usual for substituents)





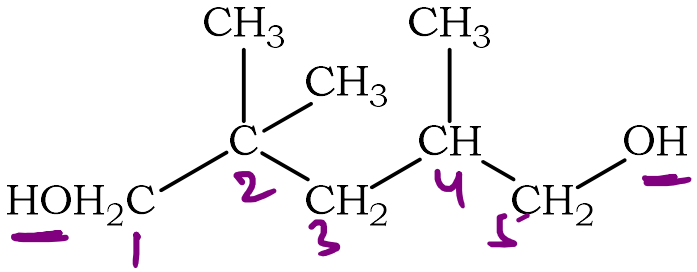
Substituent

2-Bromo-4-chloropentane.

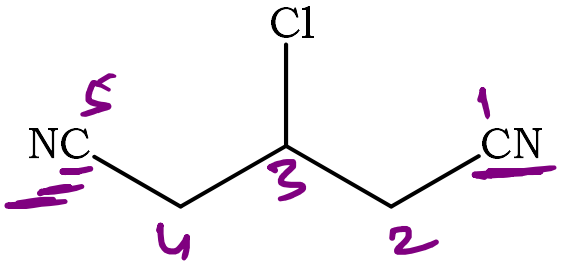
5-Bromo-2,2,4-trimethylpentan-1-ol

IUPAC Naming compounds with functional group

5. When two identical functional group that has highest priority is present in a molecule, both are addressed in suffix and locants are assigned to get lowest set.



2, 2, 4 – Trimethylpentane-1, 5–diol.



3-Chloro pentane-1,5-dinitrile.

COOH
COOH
Ethane-1,2-dioic acid

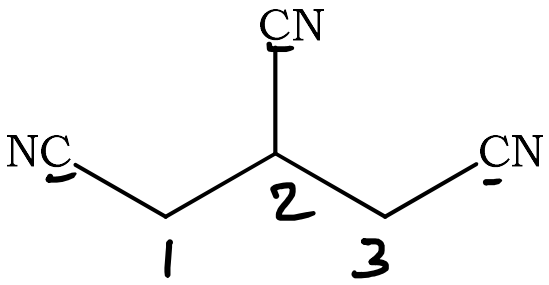
CH_2OH
CH_2OH
Ethane-1,2-diol

* CH_2 – $COOC_2H_5$
CH_2 – $COOC_2H_5$
Diethyl butane-1,4-dioate

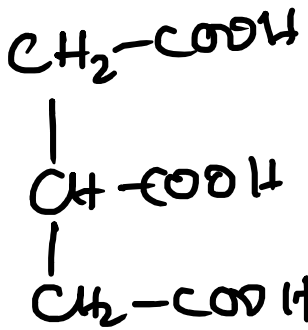
IUPAC Naming compounds with functional group

COOH, CHO, CONH$_2$, COX, COBR, CN

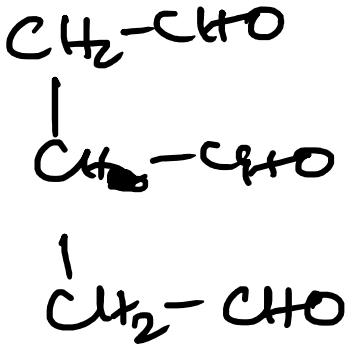
6. If more than two identical carbon containing FG are present on a same parent chain, the compound is named as derivative of parent hydrocarbon without counting the carbon of FG for parent chain.



Propane-1,2,3-tricarbonitrile

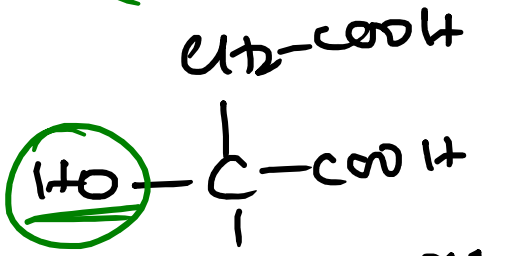


Propane-1,2,3-tricarboxylic acid



Propane-1,2,-3 tricarbaldehyde

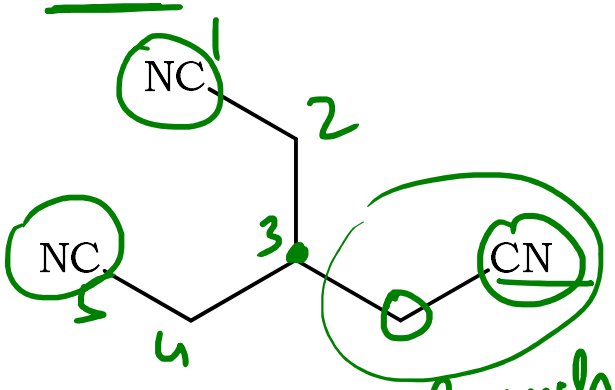
(citric acid)



2-Hydroxy Propane-1,2,3-tricarboxylic acid.

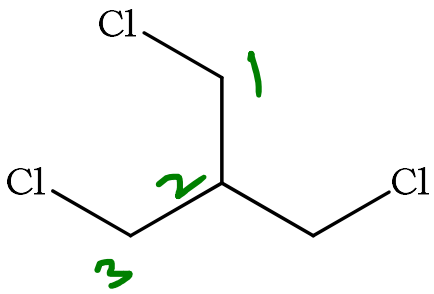
IUPAC Naming compounds with functional group

- **Note: If all FG are not directly connected to unbranched parent chain, the one at branch is made substituent.**

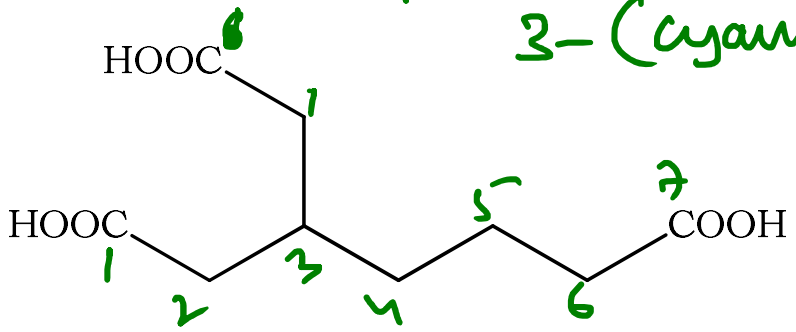


Branch

3-(cyanomethyl)pentane-1,5-dinitrile.



1,3-Dichloro-2-(chloromethyl propane



3-(Carboxymethyl)heptane-1,7-dioic acid

Example

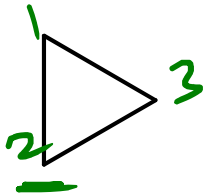
Write IUPAC Name for the following

Example

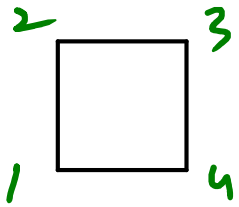
Write IUPAC Name for the following

IUPAC Naming- Alicyclic Compounds

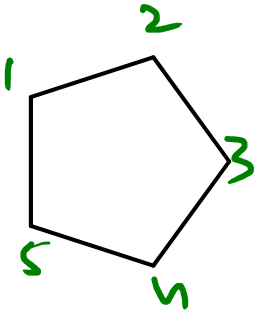
1. Name contains primary prefix 'cyclo' followed by regular word root. Lowest set of locant rule and alphabetical order is followed when substituents are present.



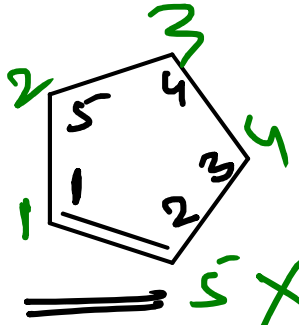
Cyclopropane



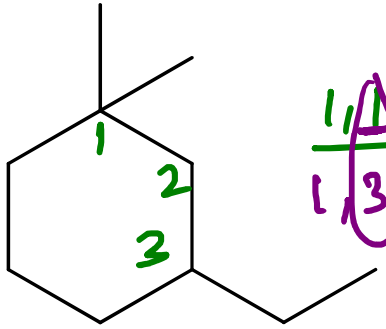
Cyclo butane



Cyclopentane



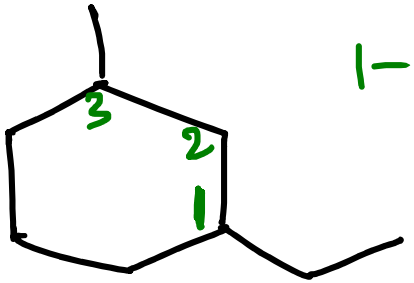
Cyclopent-1-ene



1,1,3 ✓

1,3,2

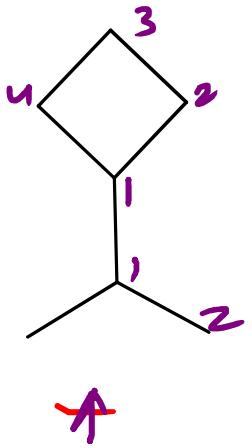
3-Ethyl-1,1-dimethylcyclohexane.

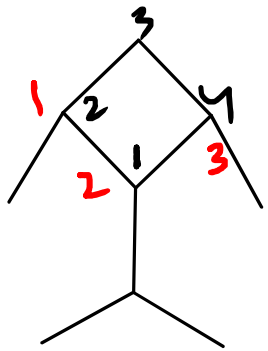


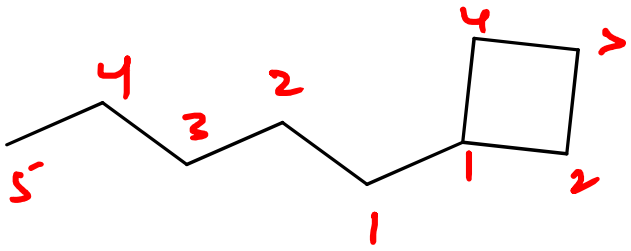
1-Ethyl-3-methylcyclo hexane

IUPAC Naming- Alicyclic Compounds

2. If side chain attached to ring has more carbon than the carbon in the ring, then the compound is named as derivative of straight chain hydrocarbon.

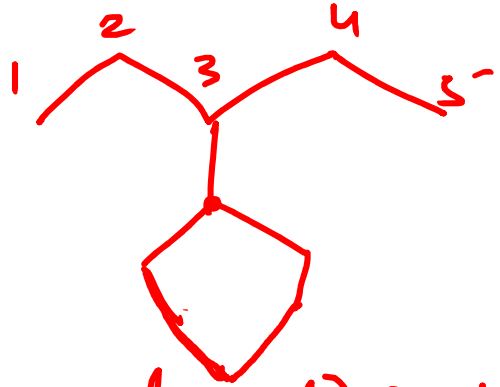






1-Cyclobutylpentane

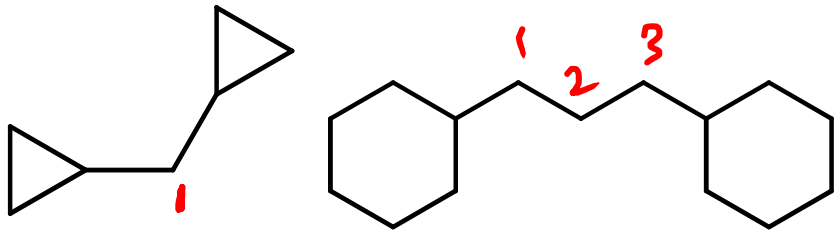
1-(1-methylethyl) cyclobutane



3-Cyclobutyl pentane

1,3-Dimethyl-2-(1-methylethyl) cyclobutane

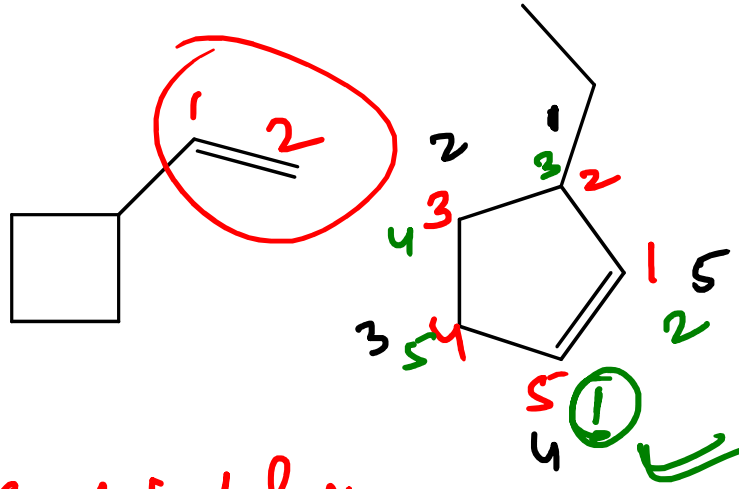
3. If more than one alicyclic rings are attached to single chain then its derivative of straight chain.



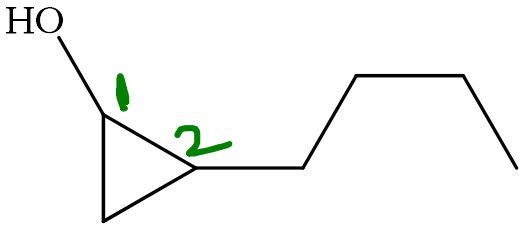
1,1 – Dicyclopropylmethane

1,3 – Dicyclohexylpropane

4. Among ring and side chain, whichever contains FG or MB becomes parent chain.



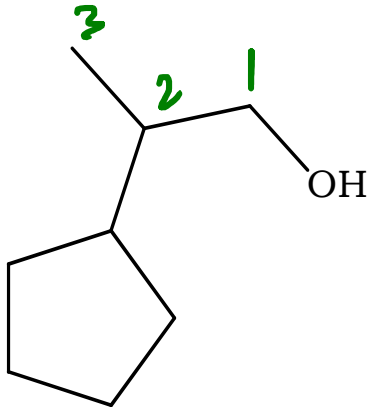
1- Cyclobutylethene



2- Butylcyclopropanol

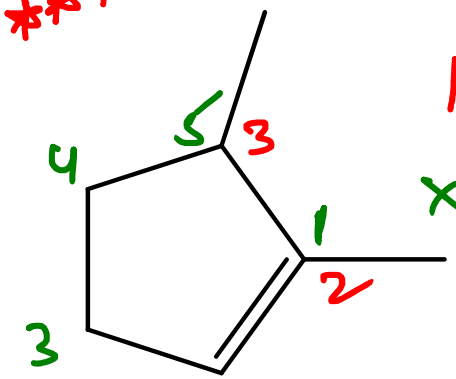
3- Ethylcyclopent-1-ene

5.Lowest set of locants rule is still applicable for multiple bond and substituents



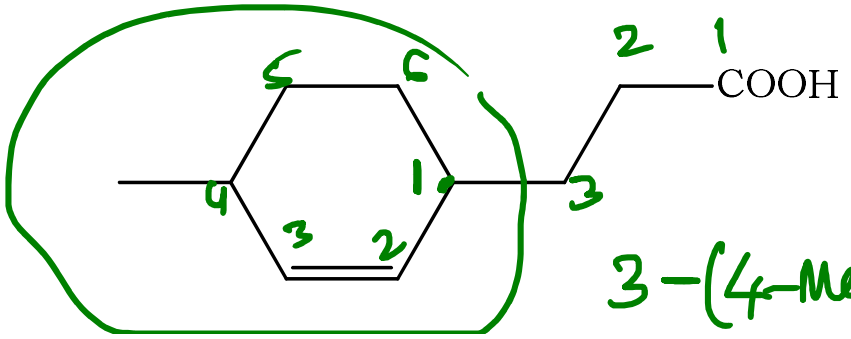
2-Cyclopentylpropan-1-ol

***



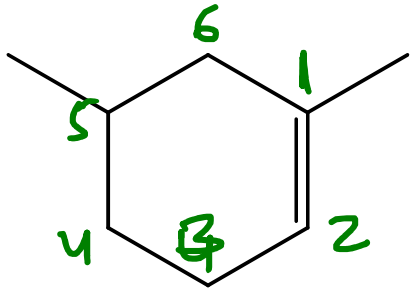
1,5-Dimethylcyclopent-1-ene

~~2,3-Dimethyl cyclopentene~~

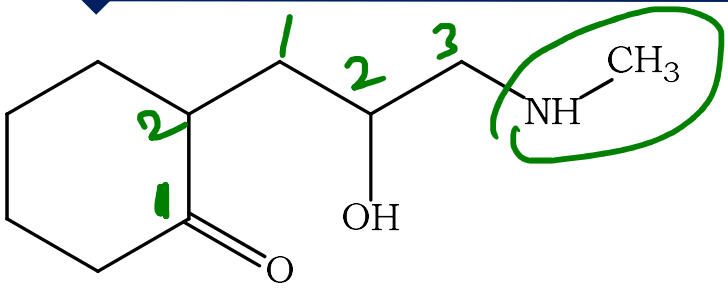


3-(4-Methylcyclohex-2-en-1-yl) propanoic acid.

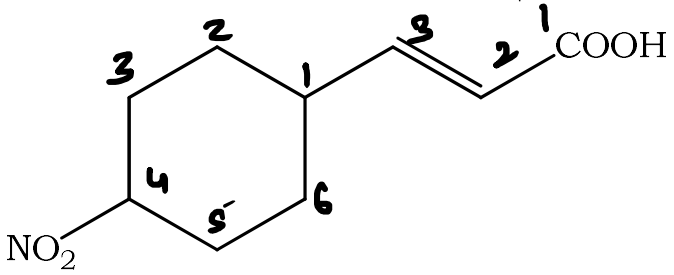
1,5-Dimethyl cyclohexene



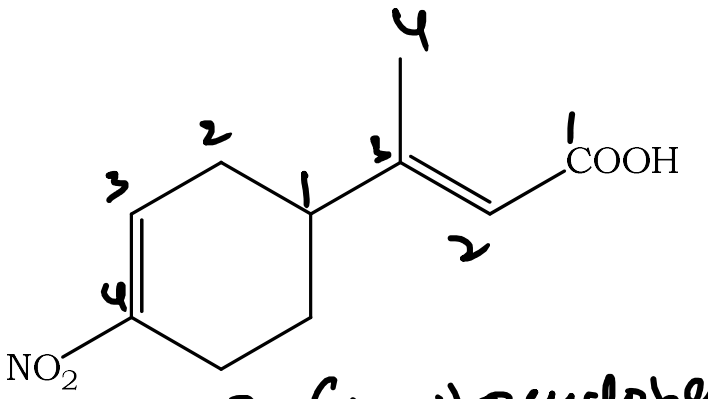
IUPAC Naming



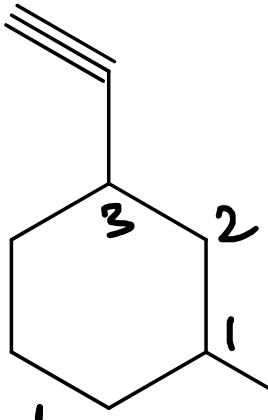
2-(3-Aminomethyl-2-hydroxypropyl) cyclohexanone



3-(4-Nitrocyclohexyl) prop-2-en -1-oic acid.



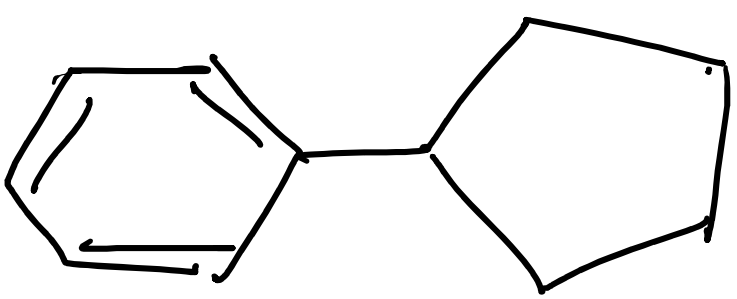
3-(4-nitrocyclohex-3-enyl) but-2-en-1-oic acid



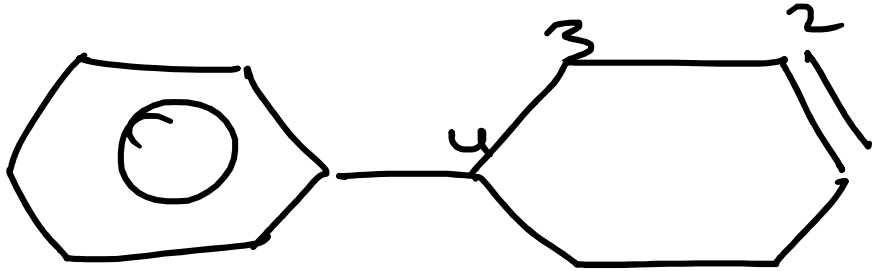
3-Ethynylcyclohexan-1-ol

6. If Benzene ring is directly attached to alicyclic ring, then the compound is derivative of benzene ring . Among the many substituents on ring, the PFG must get lowest locant.

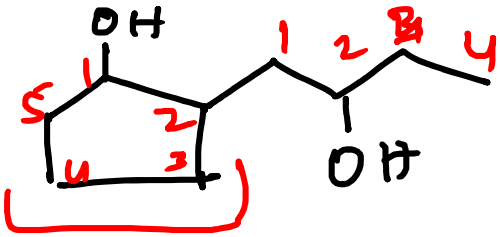
(Aromatic ring)



Cyclopentyl benzene



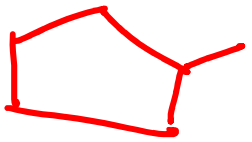
4-Phenylcyclohexene



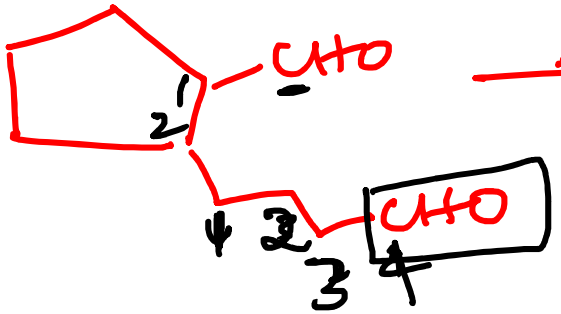
2-(2-Hydroxy butyl) cyclo pentanol.

* **7. If Alicyclic ring is directly attached to PFG containing carbon, their naming is done as follows.**

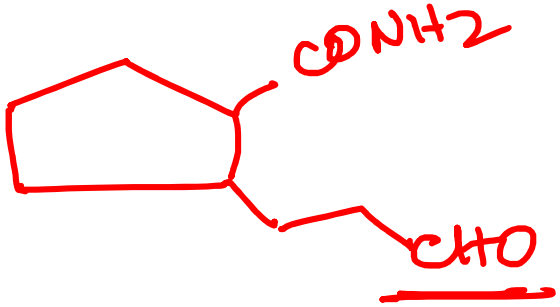
-CHO- carbaldehyde
-COOH- carboxylic acid
-COX- carbonyl halide
COOR- alkyl---carboxylate
-CN- Carbon nitrile
-$CONH_2$ - Carboxamide



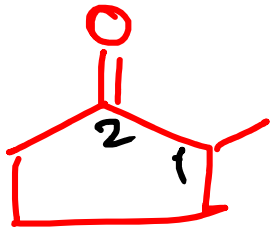
→ Cyclopentanecarbaldehyde



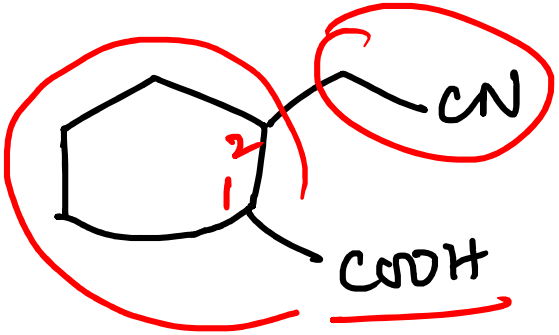
→ 2-(4-oxobutyl) cyclopentanecarbaldehyde



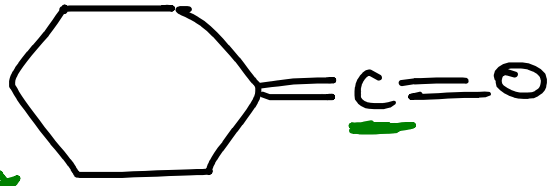
2-(3-oxopropyl)cyclopentane carboxamide



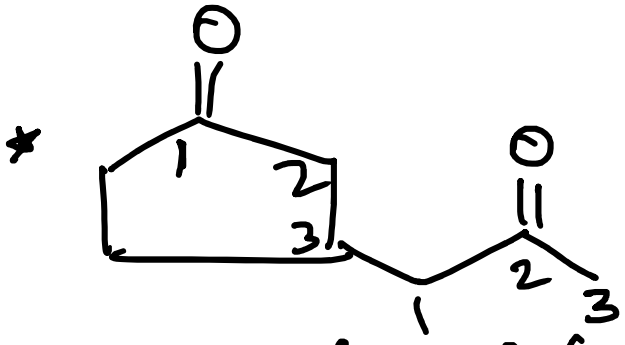
Ethyl-(2-oxocyclohexane)-1-carboxylate



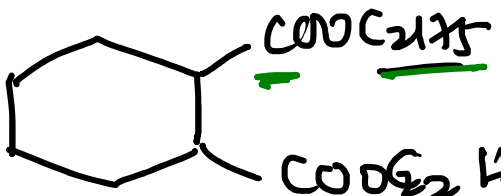
(2-Cyanomethyl) cyclohexane carboxylic acid.



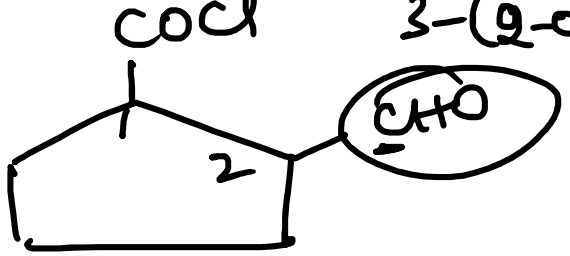
* ⊕ Cyclohexylidene methanone



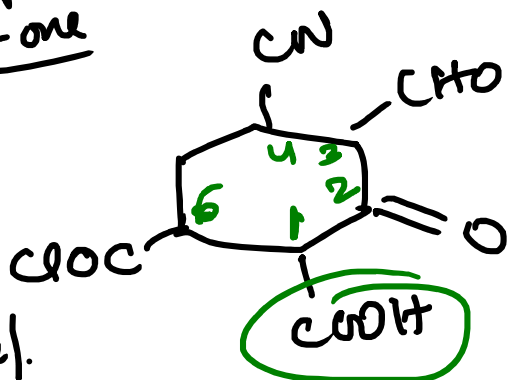
3-(2-oxopropyl) cyclopentan-1-one



Diethyl cyclo hexane -1,2-dicarbo xylate

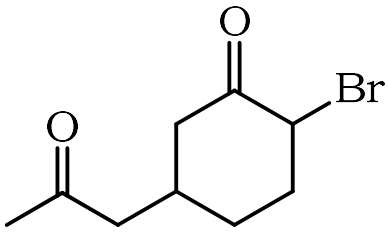


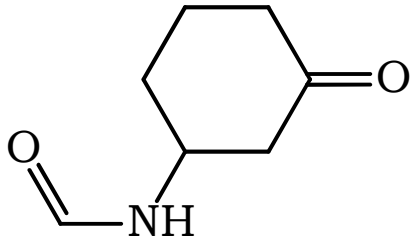
2-formyl cyclopentane carbonyl chloride.

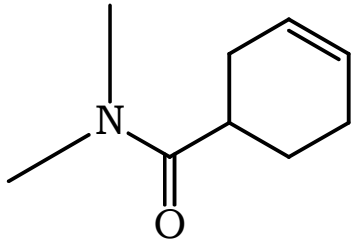


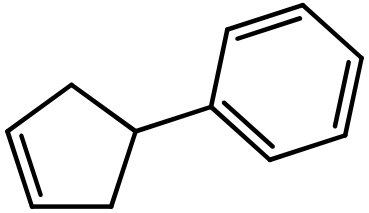
6-Chlorocarbonyl 4-cyano-3-formyl 2-oxocyclohexane carboxylic acid

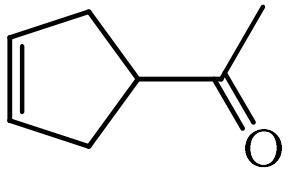
IUPAC Naming

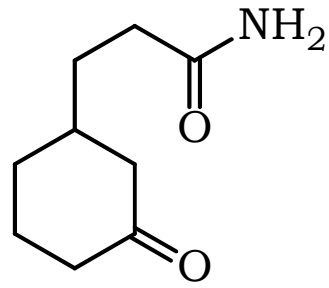








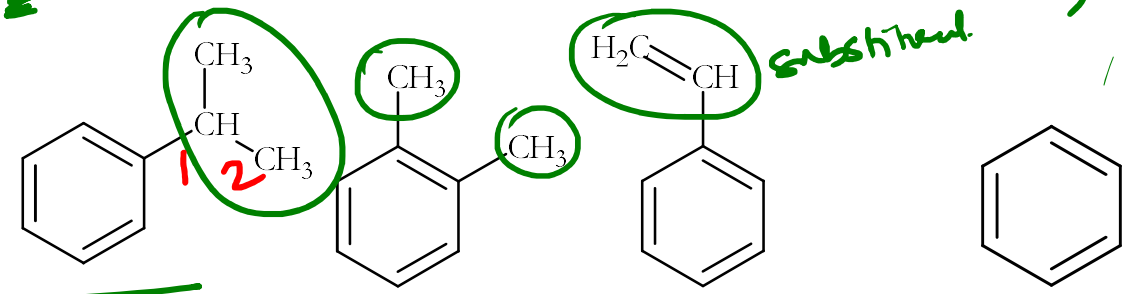




IUPAC Naming- Aromatic compounds

Compound consists of generally nucleus(benzene) and sidechain. If FG is directly attached to benzene ring, then it is named as benzene derivative. If FG is attached to sidechain, then it is named as phenyl derivative.

1. Arenes(contain both aliphatic and aromatic units)



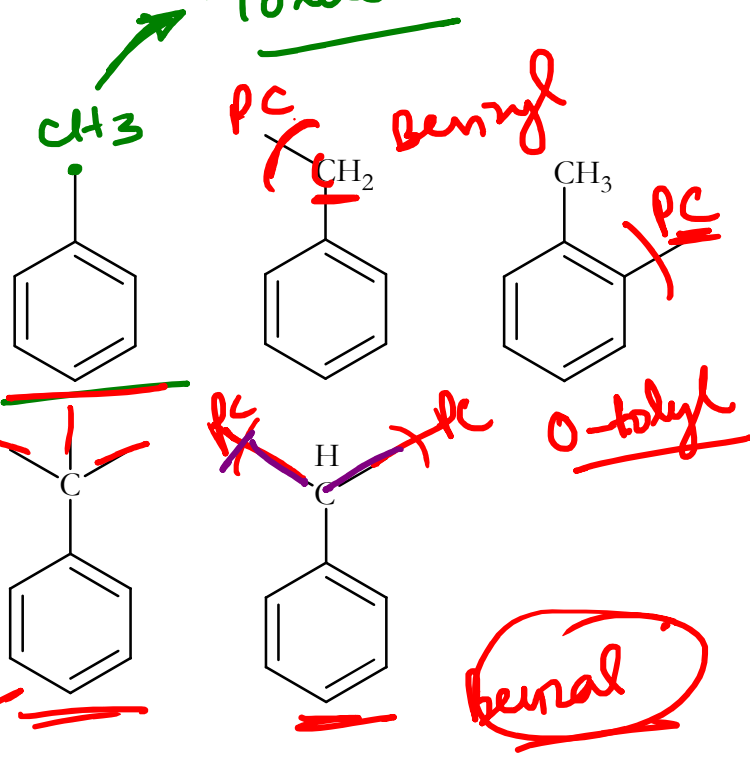
Isopropyl benzene or 1-methylethyl benzene

Dimethylbenzene 1,2-methyl toluene

Ethenyl benzene

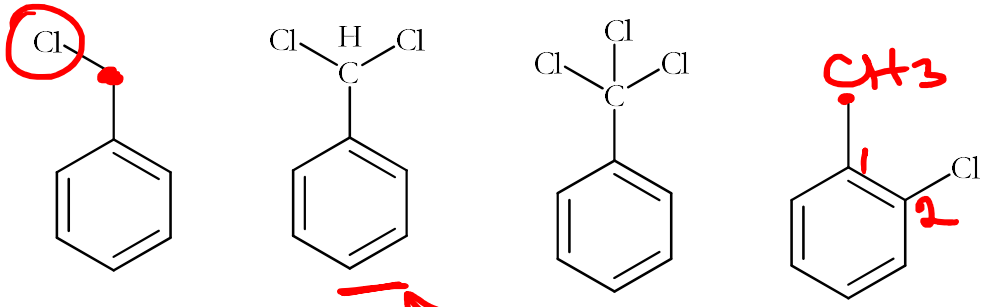
Benzene

Hydrocarbons



IUPAC Naming- Aromatic compounds

2.Halogen derivatives



2-Chlorotoluene

(Benzyl chloride)

1,1,1-Trichlorophenylmethane

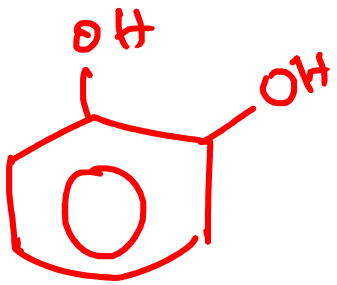
1,1-Dichlorophenylmethane

Chlorophenylmethane

IUPAC Naming- Aromatic compounds

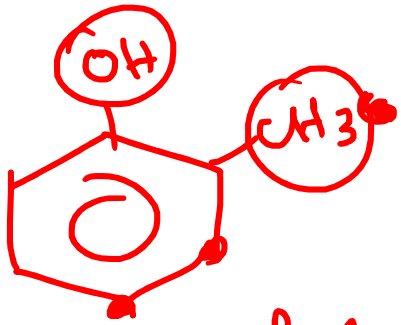
(3) Hydroxy derivatives

Phenol



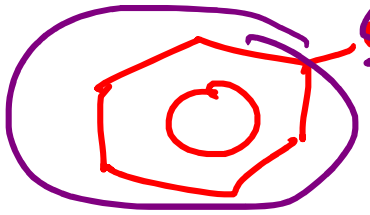
Benzene-1,2-diol

(catechol)



2-Methyl phenol

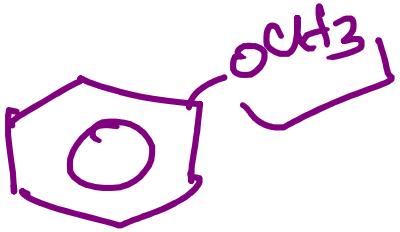
(O-Cresol)



(Benzyl alcohol)

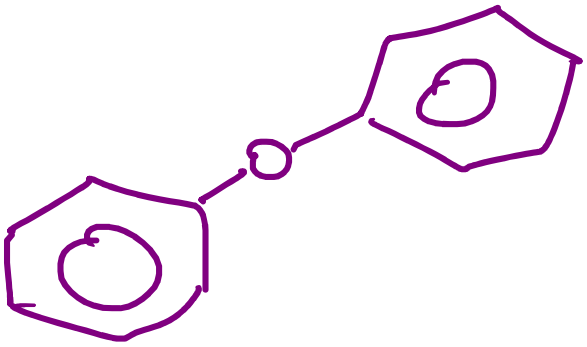
1-Phenyl methanol.

④ Ethers (R–O–R)

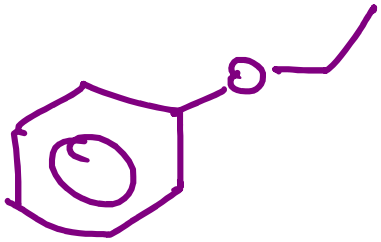


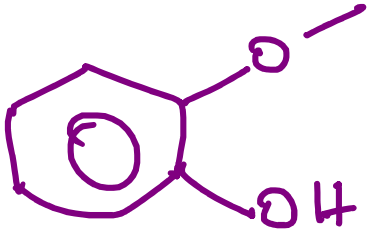
Methoxy benzene

Anisole *

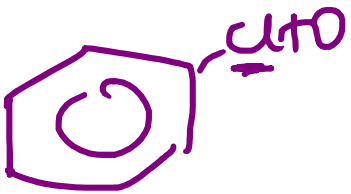


Phenoxy benzene (diphenyl ether)



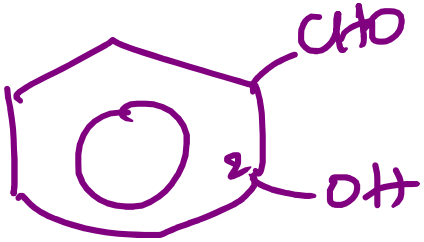


(5) Aldehyde & ketones



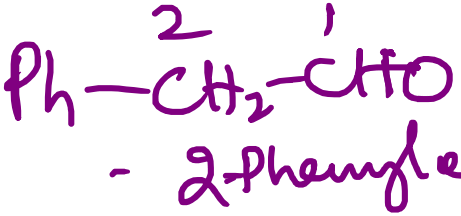
Benzenecarbaldehyde

Benzaldehyde *



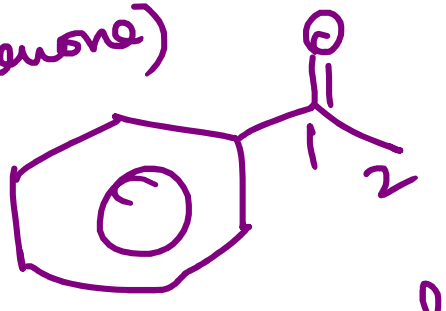
2-Hydroxy benzaldehyde

(Salicaldehyde)

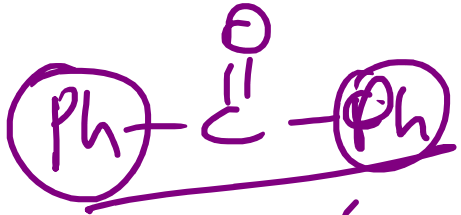


- 2-Phenylethanal

(Acetophenone)



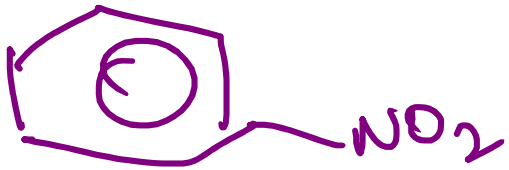
1-Phenylethanone



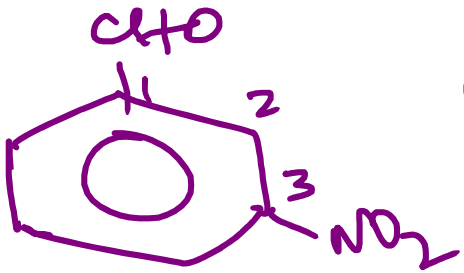
(Benzophenone)

* Diphenylmethanone

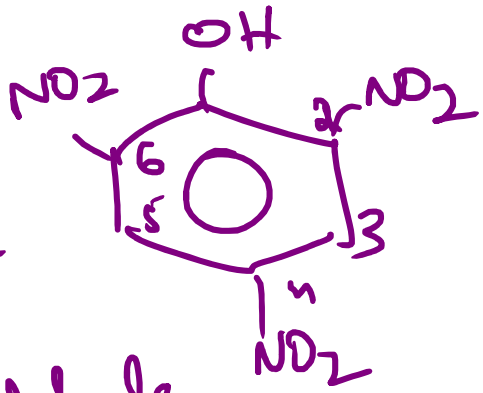
(6) Nitro compounds



Nitrobenzene



3-Nitro benzaldehyde



2,4,6,-Trinitro phenol

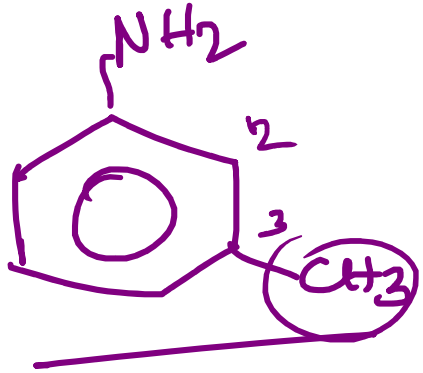
(picric acid)

Phenyl (phenol)

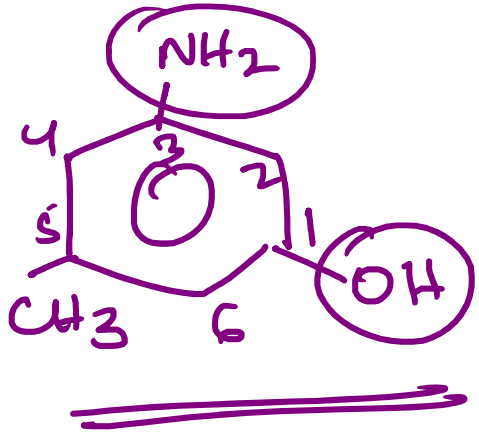
(7) Amines

Benzenamine

Aniline



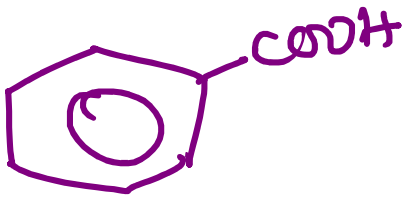
3-Methylaniline



3-Amino-5-methyl phenol

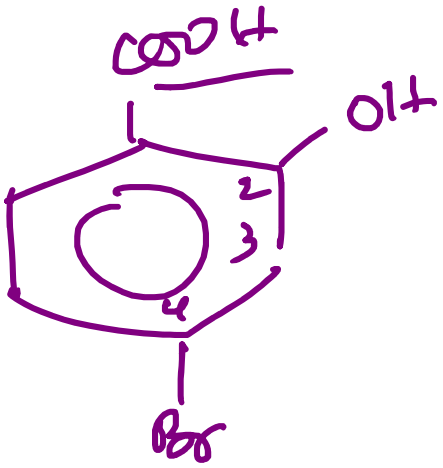
→ 1-Phenylmethanamine

⑧ Carboxylic acids :



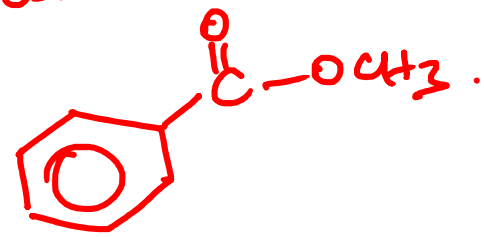
* Benzene carboxylic acid

(Benzoic acid)

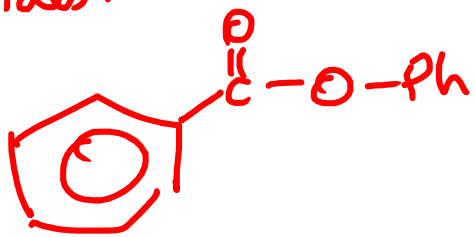


→ 4-Bromo-2-hydroxybenzoic acid

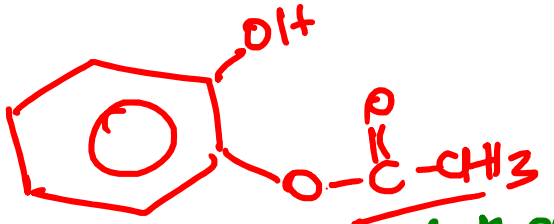
(9) Esters and acid anhydrides.



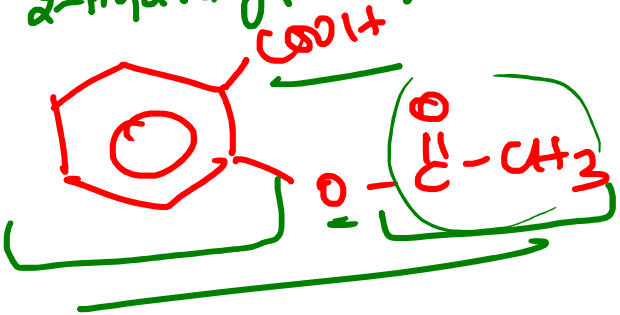
Methyl benzoate



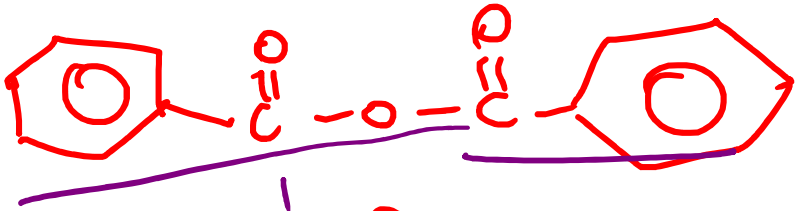
Phenyl benzoate

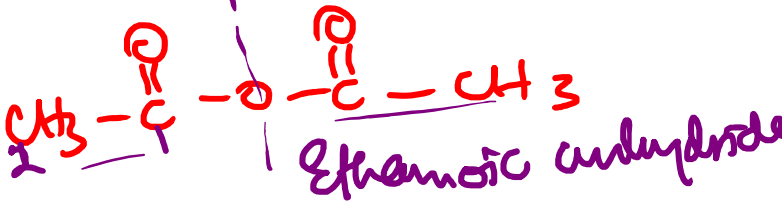


2-Hydroxy phenyl ethanoate

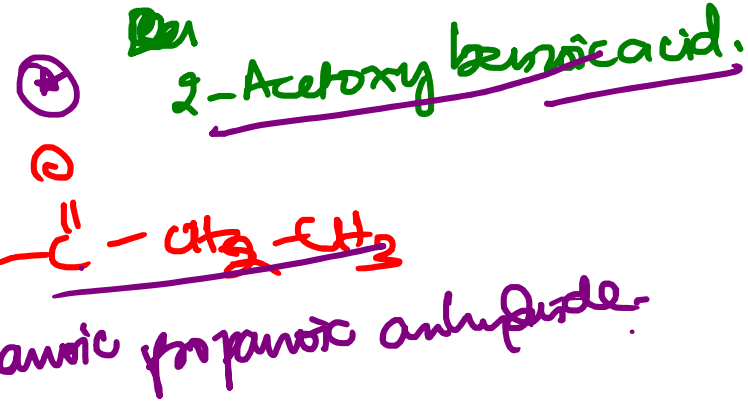


Benzoic anhydride.



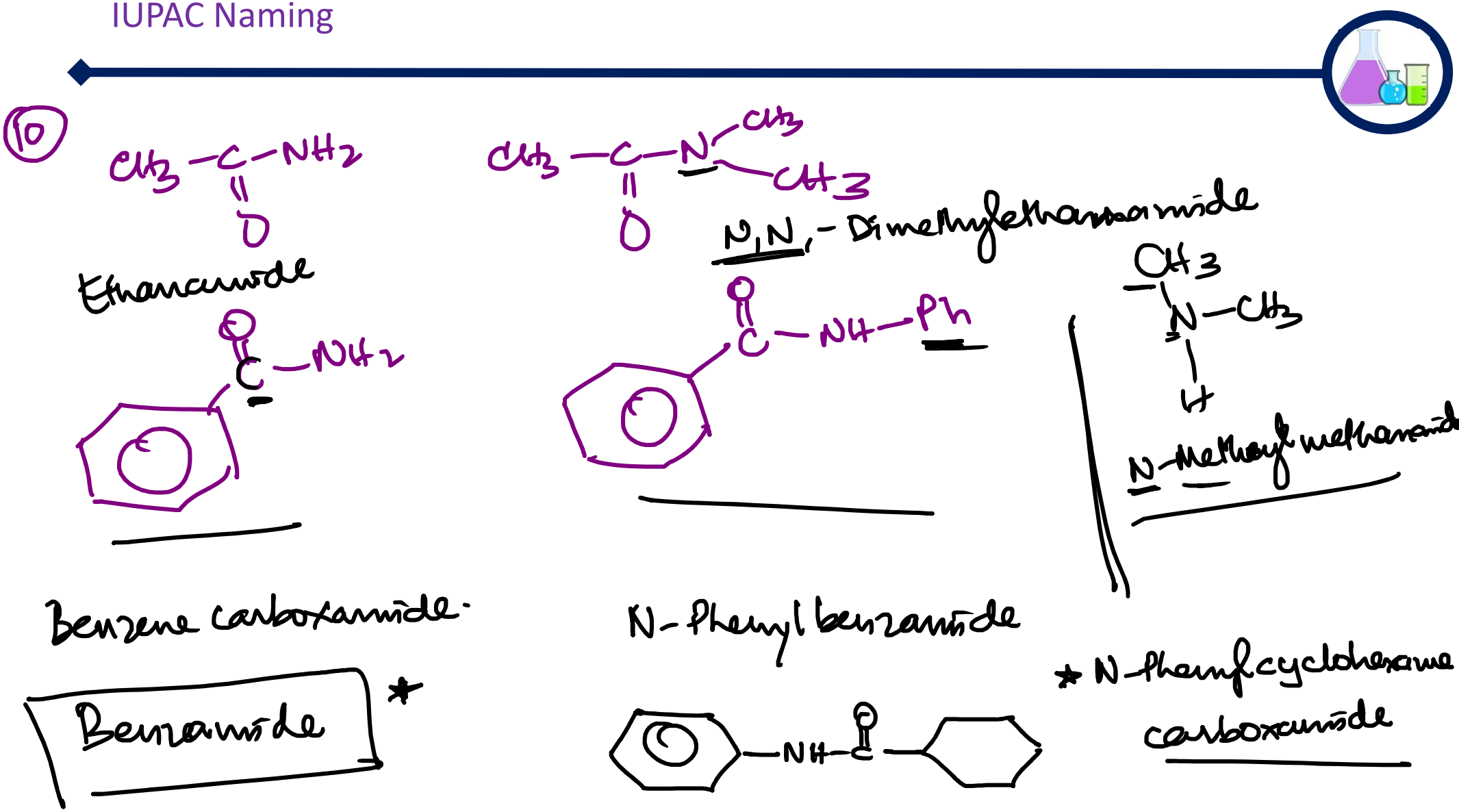


Ethanoic anhydride



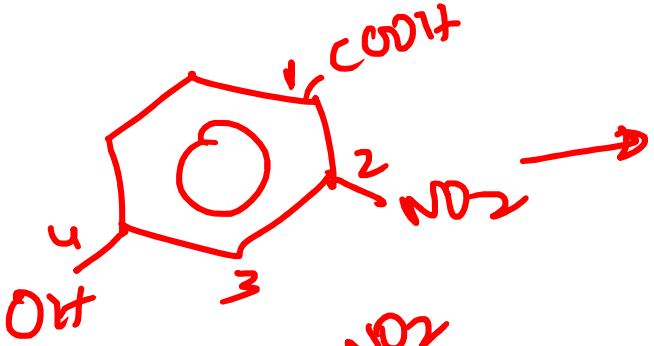
2-Acetoxy benzoic acid.

Ethanoic propanoic anhydride.

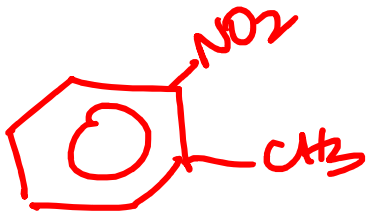

(10)
Ethanamide
N,N,-Dimethylethanamide
N-Methylmethanamide
Benzene carboxamide.
Benzamide *
N-Phenyl benzamide
* N-Phenylcyclohexane carboxamide

* When Phy functional groups are present on benzene ring we consider PFG & Number accordingly.

If Substituent on benzene ring results in special compound, then the molecule is named as derivative of special compound.

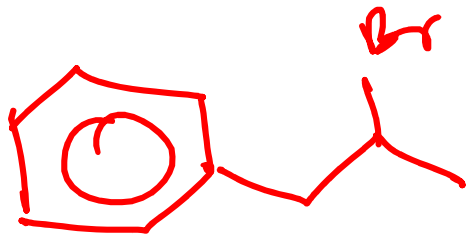


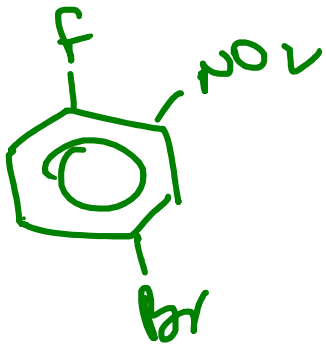
→ 4-Hydroxy-2-nitro benzoic acid.



→ 2-Nitrotoluene

IUPAC Naming

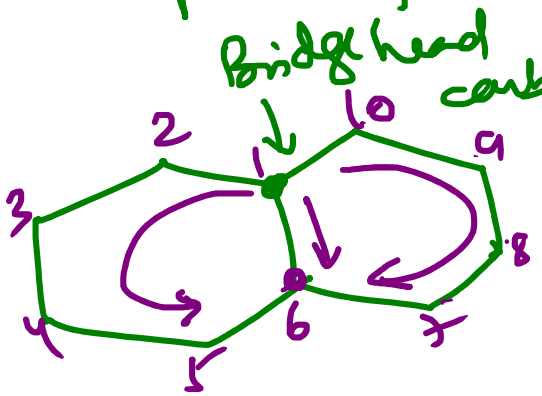




– Bicyclic compounds

* If 2 rings are fused at 2 common carbon.

The compound formed is bicyclic compound. (2 bonds are to be broken to make it st. chain)

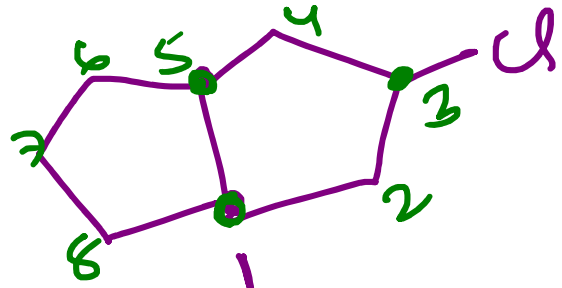


Bicyclo [4.4.0] decane.

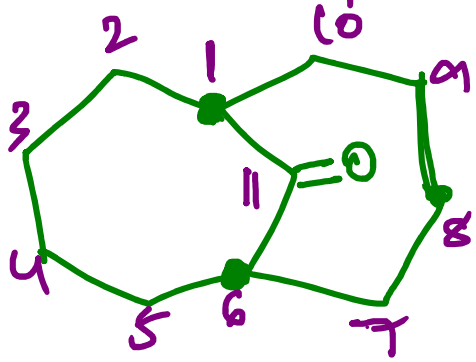
Bicyclo + [ ] + Suffix.

no. of carbon atoms in each bridge in decreasing order

* Substituted bicyclic compounds are numbered starting from a bridgehead carbon towards longest bridge then smaller, then smallest.



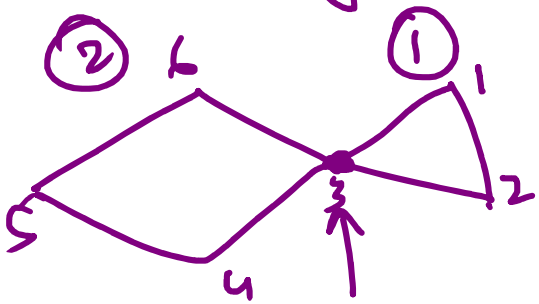
3-Chloro bicyclo[3.3.0] octane.



Bicyclo[4.4.1]undecan-11-one

– Spiro Compounds

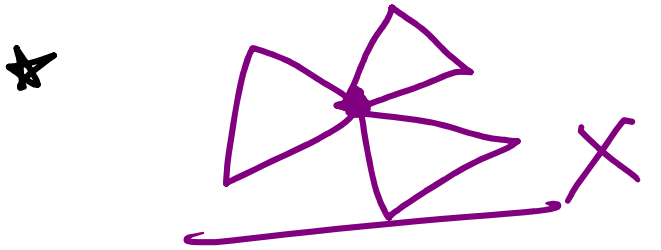
⊛ Two cyclic rings are fused at one carbon.

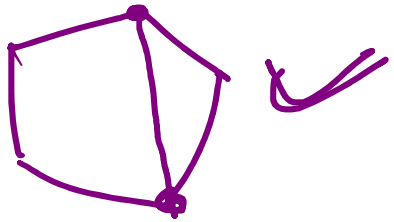


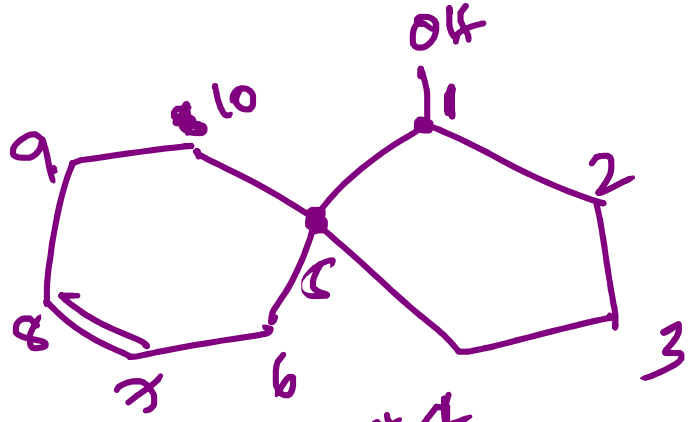
Prefix + no. of carbon in rings in increasing order (Not count spiro carbon) + Suffix.

Spiro [2.3] hexane

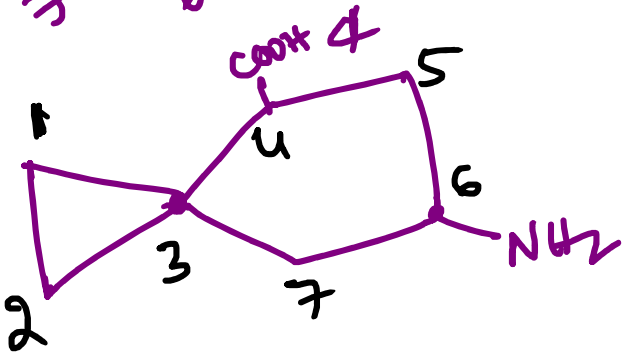
* In spiro compounds numbering starts from carbon next to spiro carbon. and proceeds towards other atoms of small ring then larger ring via spiro carbon







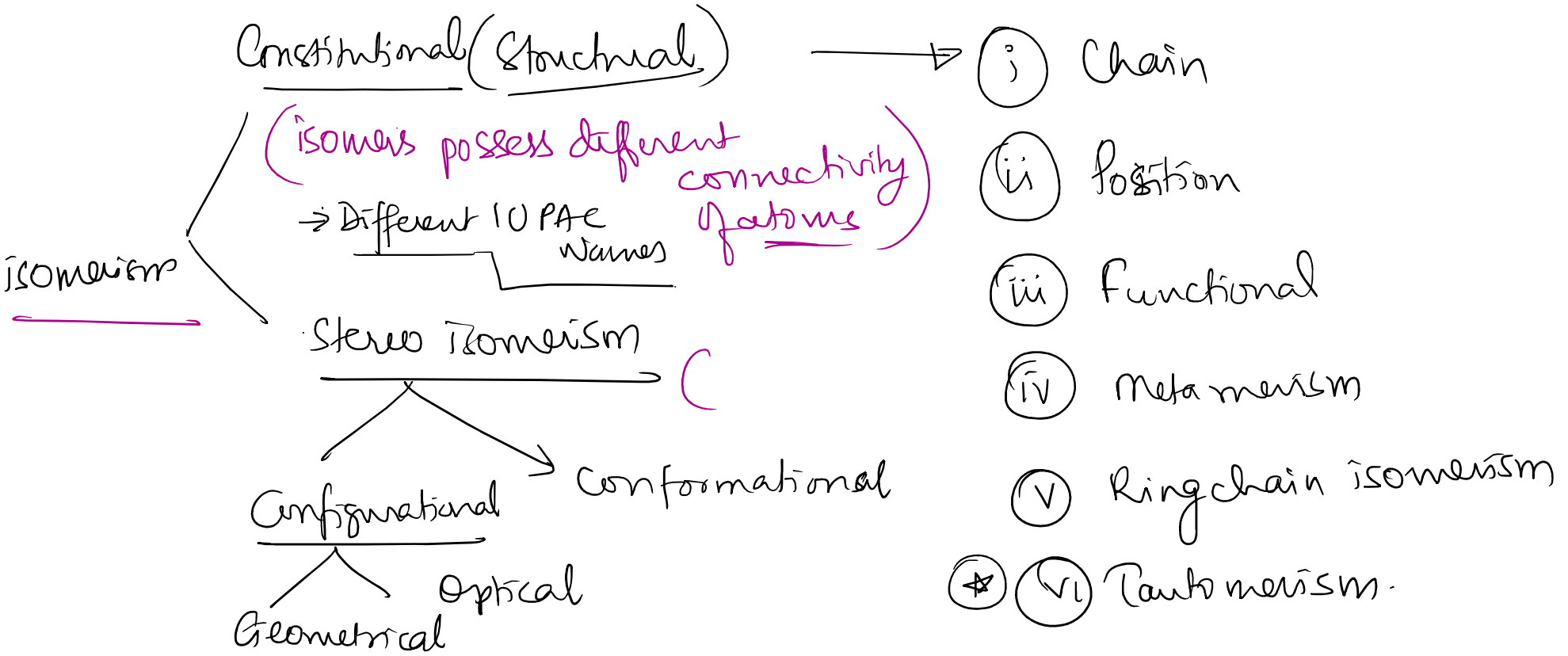
→ Spiro[4.5]dec-7-en-1-ol.



6-Aminospiro[2.4]heptane-4-carboxylic acid.

ISOMERISM

2 or more compounds having same molecular formula but different physical chemical properties are called isomers. Phenomena is called as isomerism.



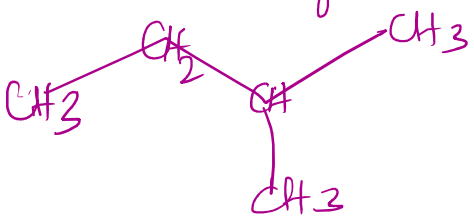
ISOMERISM – Chain Isomerism.

Isomerism arising due to different arrangement of atoms into carbon skeleton (different parent chains).

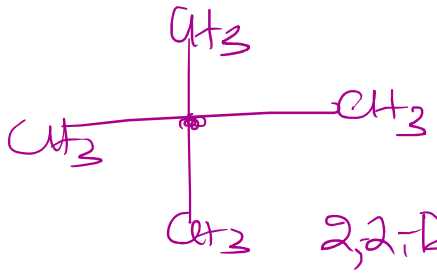
Pentane

and

2-Methylbutane



and

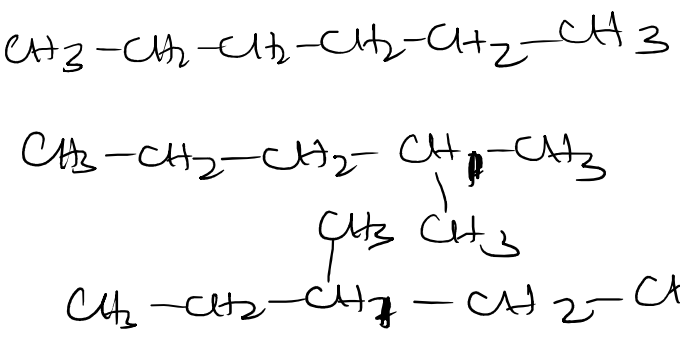


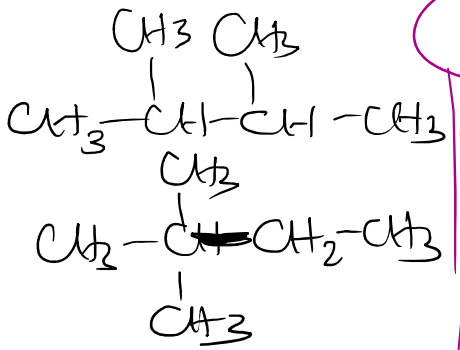
2,2-Dimethyl propane

C_5H_{12}

* same formula but different carbon skeletons.

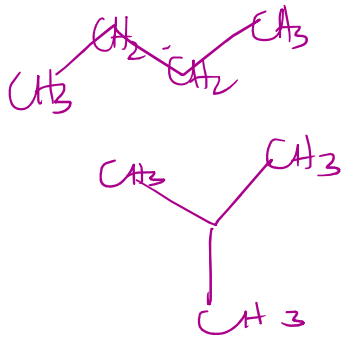
* C_6H_{14}





5

N-Butane



ISOMERISM

* C_4H_9OH :

$CH_3-CH_2-CH_2-CH_2-OH$

and

$CH_3-CH(CH_3)-CH_2-OH$

Position isomerism : 2 or more compounds having same molecular formula but different positions of substituent atom / groups. (FG) / MB on the carbon skeleton.

$CH_3-CH_2-CH_2-OH$

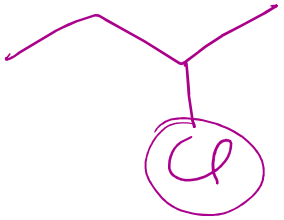
Propan-1-ol

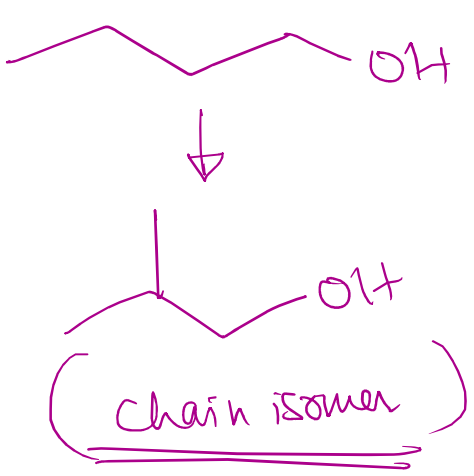
$CH_3-CH(OH)-CH_3$

Propan-2-ol.

ISOMERISM

Conditions: MF is same, same length of carbon chain, same functional group.





(iv) Functional isomerism

Compounds with same MF but different functional groups.

(i) Alcohols and ethers
($C_nH_{2n+2}O$)

CH_3CH_2OH & CH_3-O-CH_3

Ethanol ⊛ Methoxy methane

ISOMERISM

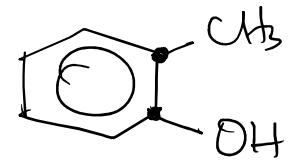
(ii) Aldehydes, ketones, unsaturated alcohols $(C_nH_{2n}O)$

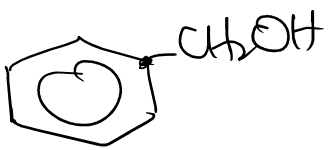
$CH_3-CH_2-\underset{\underset{O}{\|}}{C}-H$ $\quad$ $CH_3-\underset{\underset{O}{\|}}{C}-CH_3$ $\quad$ $CH_2=CH-CH_2-OH$

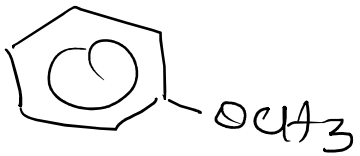
(iii) CA & esters, $C_nH_{2n}O_2$

CH_3COOH $\quad$ $H-\underset{\underset{O}{\|}}{C}-O-CH_3$ (methyl methanoate)

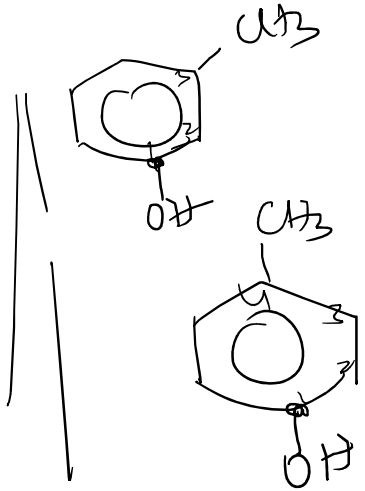
(iv) Aromatic alcohols, Phenols, aromatic ethers.





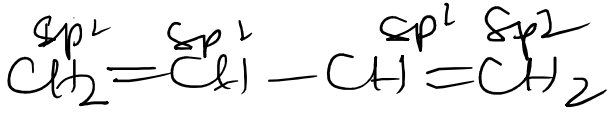


Anisole

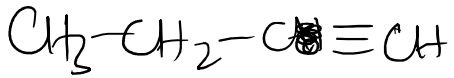


ISOMERISM

(V) Dienes, alkynes, allenes (compounds with consecutive DB)



Buta-1,3-diene



Butyne

(allene)

Buta-1,2-diene

(VI) Cyanides and Isocyanides

CH_3CN and CH_3NC → $(C_{n+1}H_{2n+1}N)$

CH_3CH_2CN and CH_3CH_2NC

(VII) Amides and oximes $(C_nH_{2n+1}NO)$

CH_3CONH_2 and 

(VIII) Amines

$C_nH_{2n+3}N$

$CH_3CH_2NH_2$ and $CH_3-NH-CH_3$

(I) **Metamerism** : Isomerism arising due to difference in alkyl groups attached to either side of divalent functional groups.

eg.

–O–

–S–

–NH–

–C(=O)–

–C(=S)–

–C(=O)–O–

–C(=O)–O–C(=O)–

–C(=O)–NH–

eg. Ethyl formate $H–C(=O)–O–C_2H_5$ and

$CH_3–C(=O)–O–CH_3$ Methyl ethanoate

eg.

Q. Write all possible isomers of C_3H_7OH (3)

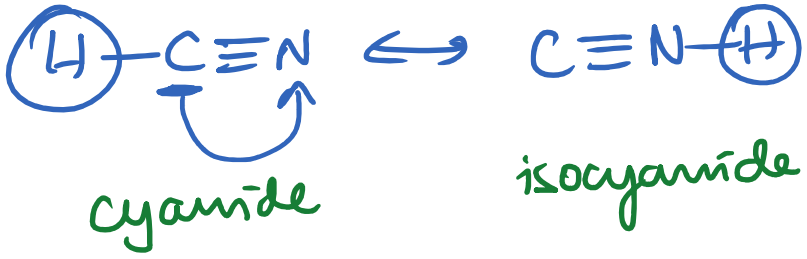
$CH_3–CH_2–CH_2–OH$

$CH_3–CH(OH)–CH_3$

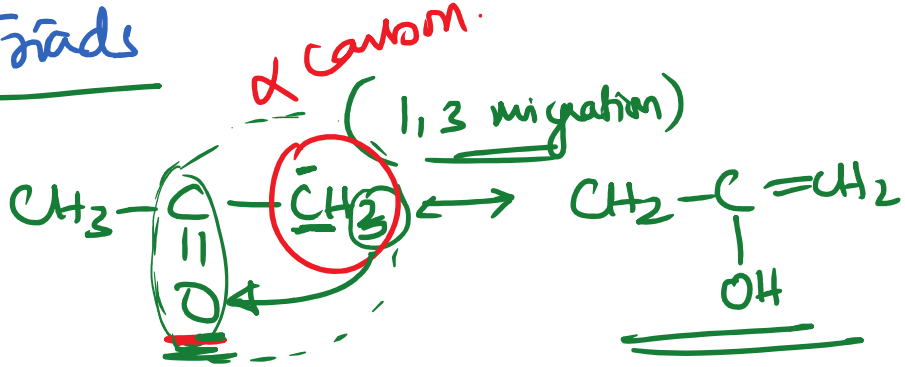
$CH_3–O–C_2H_5$

(i) Tautomerism : Isomerism arising due to migration of H atom from one polyvalent atom to another.

(ii) diad



(iii) Triads



(*) along with α H,

$>C=O$, $>C=N-$, $>C=S$, $-N=O$

$CH_3-\underset{\underset{O}{\|}}{C}-CH_3 \rightleftharpoons CH_2=\underset{\underset{OH}{|}}{C}-CH_3$

* high BE } $-C=O$ conjugated to $-C=C-$ (OH)

99.9% keto form

0.01% enol

Factors influencing enol content → (i) Stability } enol / keto form.

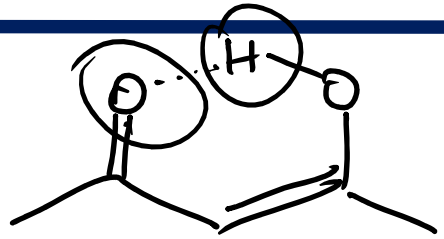
→ Conjugation

→ Aromaticity

→ Intra molecular H bonding

→ Steric hinderance.

⇒ Solvent polarity. (Polar solvents favour keto form).



$\xrightarrow[\text{or } CH_3OH \text{ etc.}]{H_2O}$ keto form

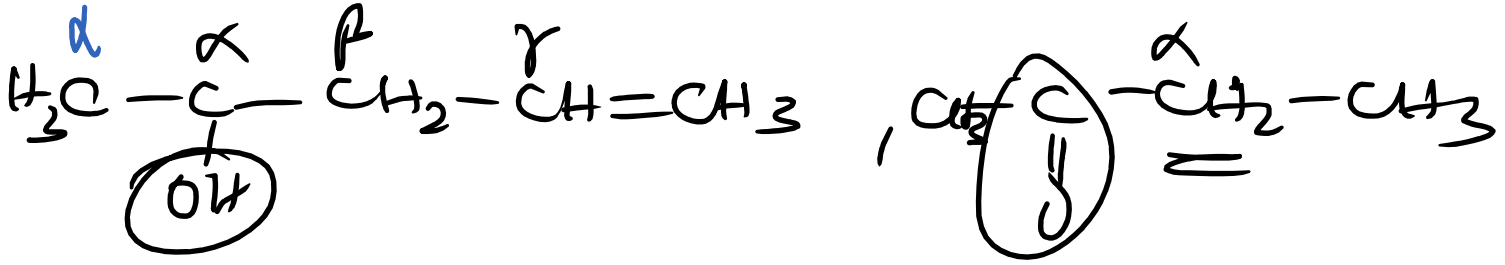
enol

Hexane > toluene > Methanol > H_2O

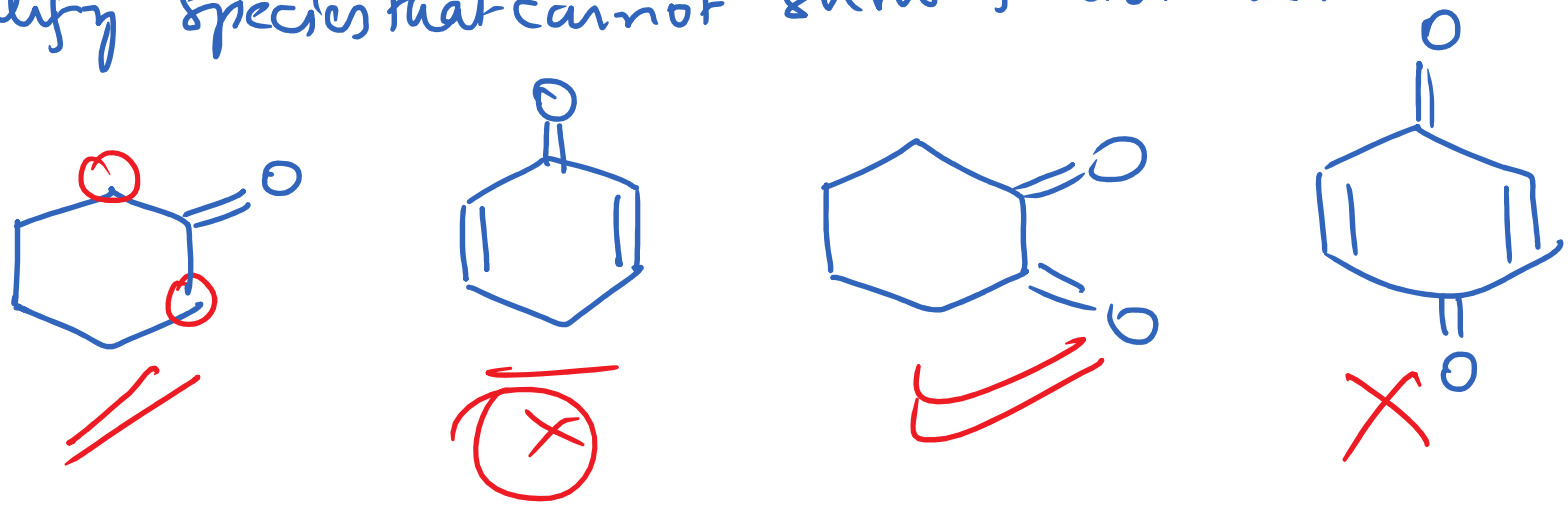
Heptane etc Benzene

Essential conditions for Tautomerism :→ EN element with multiple bond

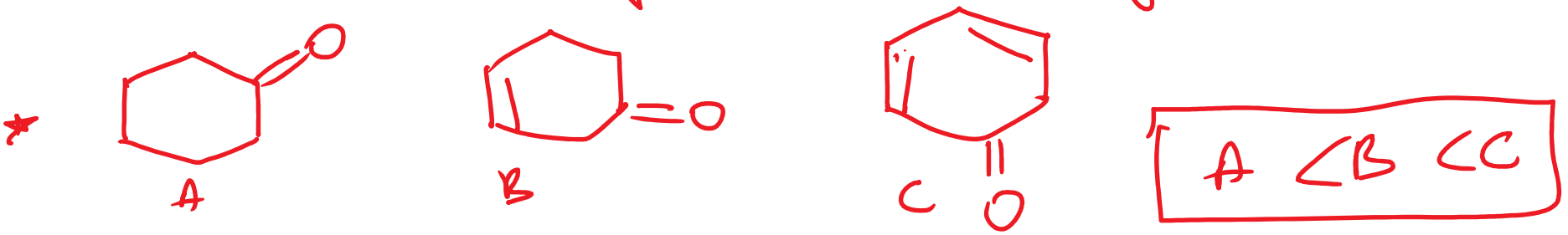
→ acidic 'α' 'H' atom



* Identify species that cannot show tautomerism



* Arrange the following in the increasing order of enol content



A < B < C

(VI) Ring chain isomerism : Isomerism arising due to existance compound in both straight chain and cyclic form.

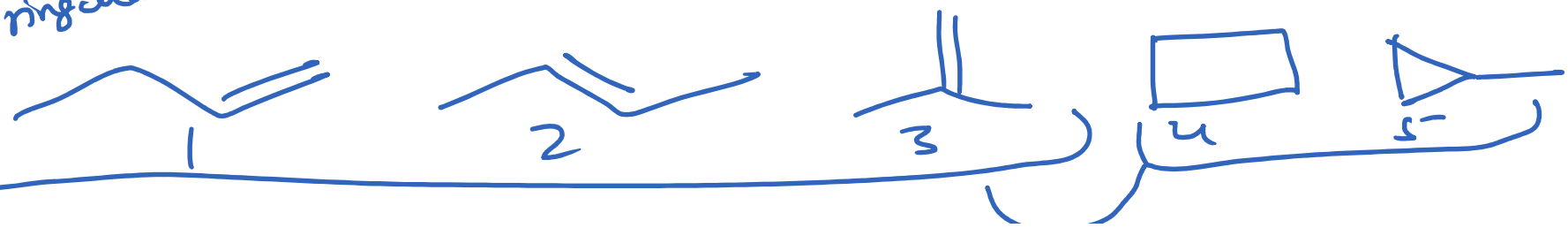
$$\text{Degree of Unsaturation} = \frac{2C+2-X-H+N}{2}$$

Eg C_4H_8

$$DU = \frac{2(4)+2-0-8+0}{2} = 1 \quad (\text{Double bond / Ring})$$

(5) ring chain

3-4 →
3-2-
↓ chain



(*) C_4H_6 (NSO) → $DU = \frac{4(x2) + 2 - 6 = 0 + 0}{2}$

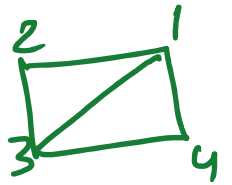
$= 2 - (2DB/1TB/2ring/1ring+1DB)$

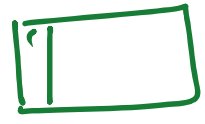
$= 3$

$= 4 \rightarrow$ (Aromatic ring) | Bicyclo[1.1.0] butane







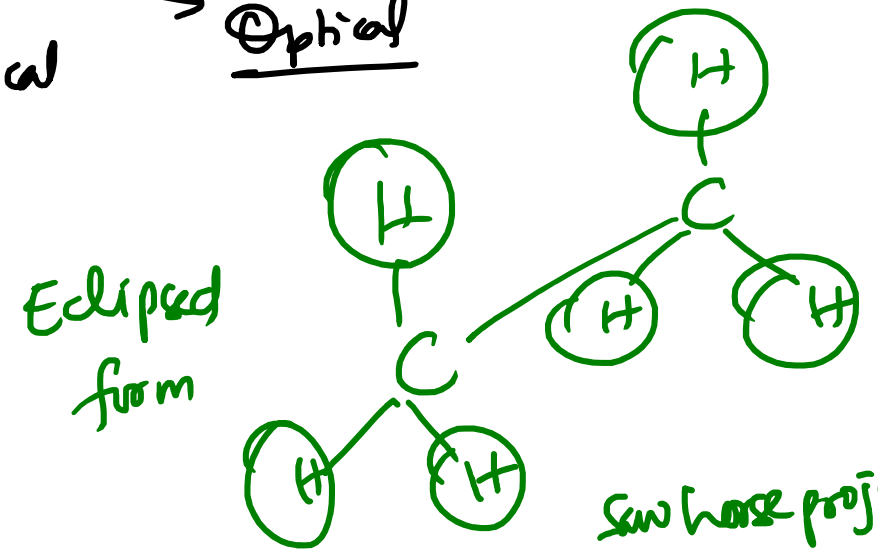


(9)



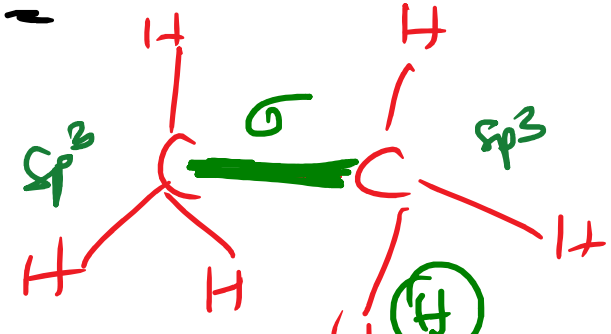
Stereo isomerism (Isomerism arising due to different orientations in 3D space of groups attached in a molecule)

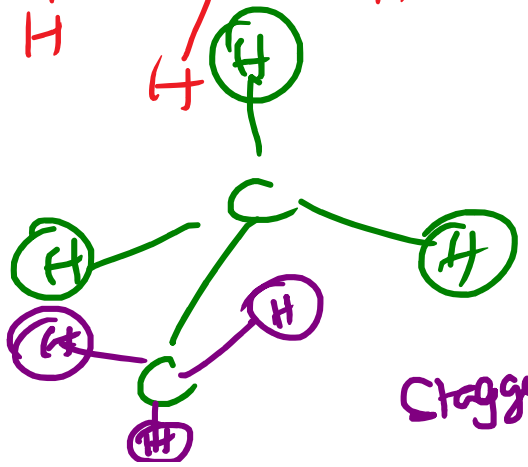
- Conformational — arises due to free rotation about 'C–C' bond.
- Configurational
  - Geometrical
  - Optical



Eclipsed form

Sawhorse projection

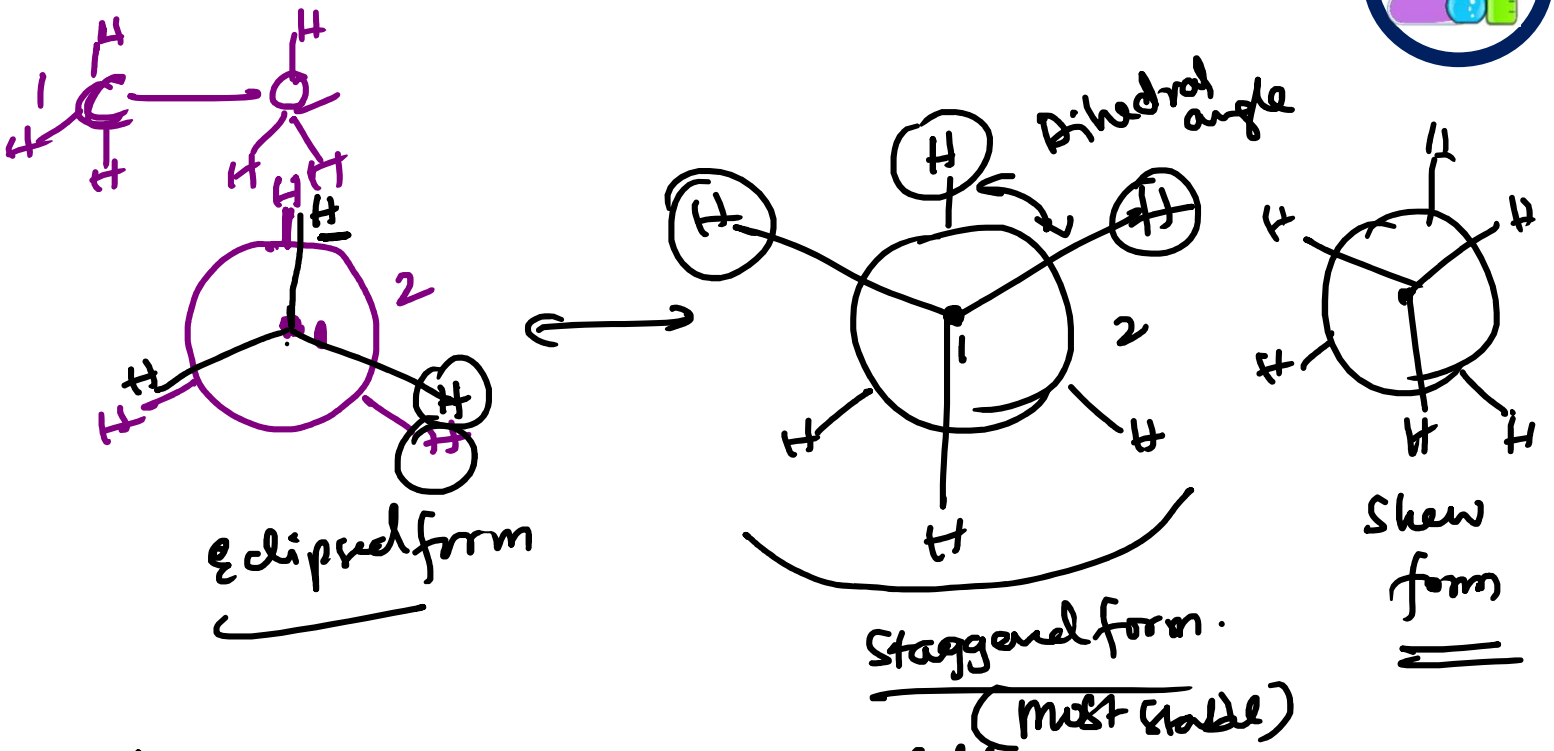




Staggered form.

Newmann Projection

View →



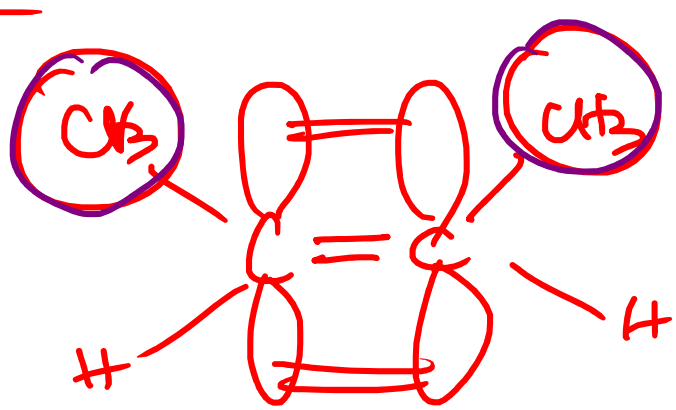
→ Conformers are not isolable. due to very small energy difference.

→ staggered form is most stable due to min repultions.

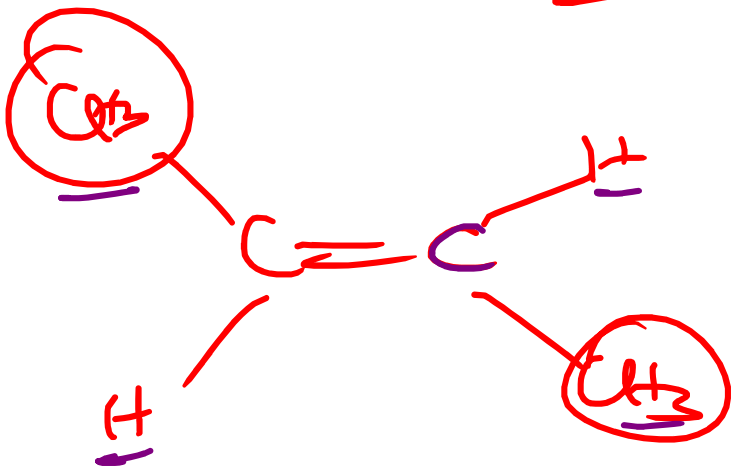
→ Propane, butane, cyclohexane. ☆

Geometrical Isomerism

Arises due to restricted rotation about C=C / ring / C=N etc.



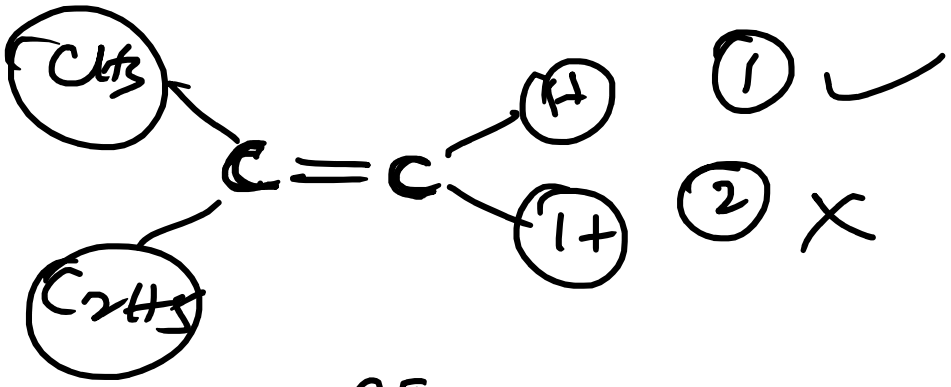
cis isomer



trans isomer

★ Existance of C=C

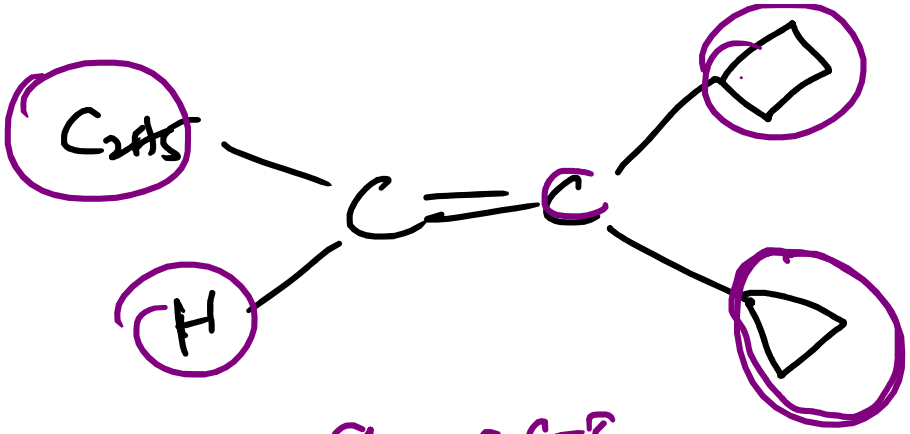
★ Both double bonded carbons must have 2 different groups attached.



(1) ✓

(2) ✗

No GI



Shows GI

⊛ Optical isomerism :

Plane Polarised light

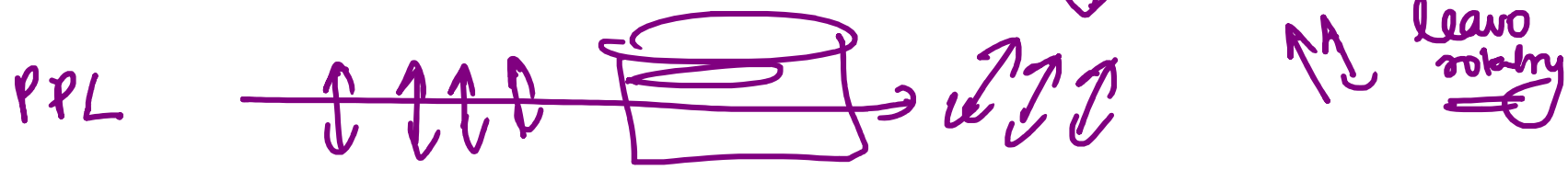
White light

Nicol Prism

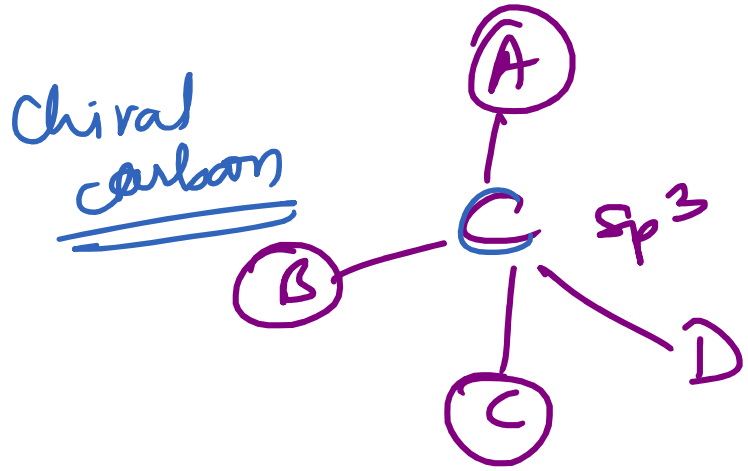
Polarimeter

(+) dextrorotatory — CW

(−) — CCW

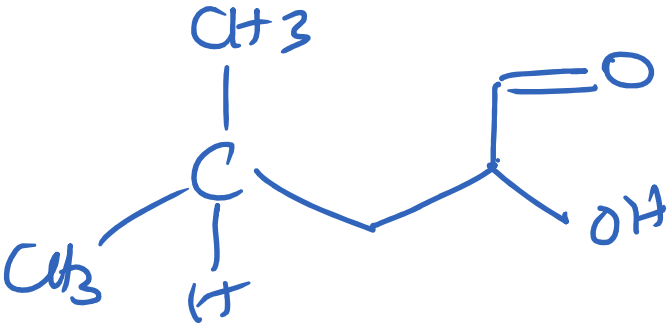


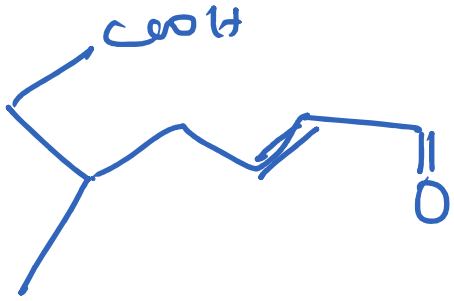
Chiral carbon



★ Compounds that contain sp3 carbon that has 4 different groups attached.

Q. Identify chiral carbon

① 

② 

③