

Constitution, Configuration &
Conformation

Isomerism - Two or more compounds having the same molecular formula but different structural arrangements

↓
This phenomenon is called isomerism - The molecules which exhibit this phenomenon are called isomers

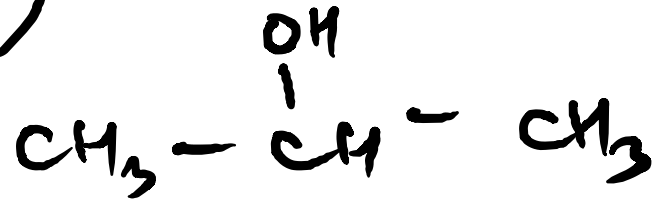
Structural Isomerism

Constitutional isomerism -

Constitutional isomers have the same molecular formula but different connectivity.

Eg. Isopropyl alcohol (2 Propanol)

are
constitutional
isomers



(n-Propanol)

Configuration refers to the spatial arrangement of atoms that can only be changed by breaking bonds. The most common configurations are R/S, D/L . . . etc.

Conformation refers to the spatial arrangement of atoms in a molecule that can be determined through

single-bond rotation -

Wikipedia: Cis and trans descriptors are not used for cases of conformational isomers where the two geometric forms easily interconvert such as most open-chain single bonded structures.



Syn - anti.
Conformational isomers.

Isomerism

2d problem

Structural isomerism

Stereoisomerism

Isomers that have the same structure and bond sequence but different orientation in space.

Isomers with different structures.

1. Chain isomerism

2. Position isomerism

3. Functional group isomerism

4. Metamerism

owing to arrangement of carbon skeleton.

owing to position of functional group arises due to different functional group.

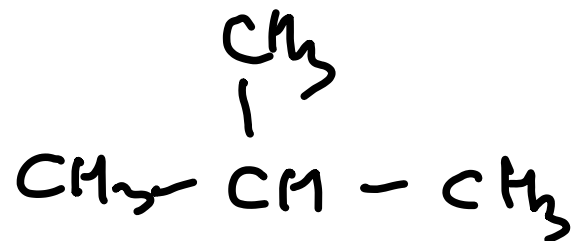
owing to different alkyl chains on either side of functional group

Structural isomers

1. Chain isomerism; Example:



Butane



Isobutane



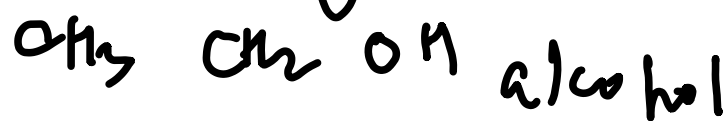
2. Position isomer: Eg:



position of -OH groups are different

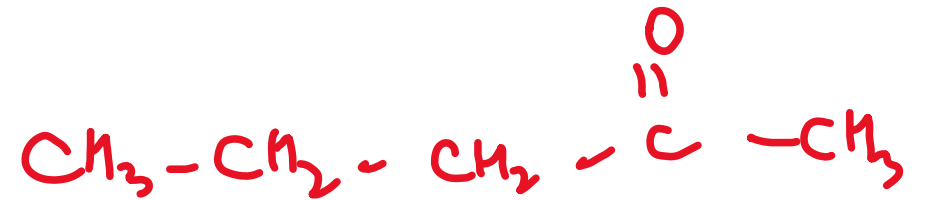
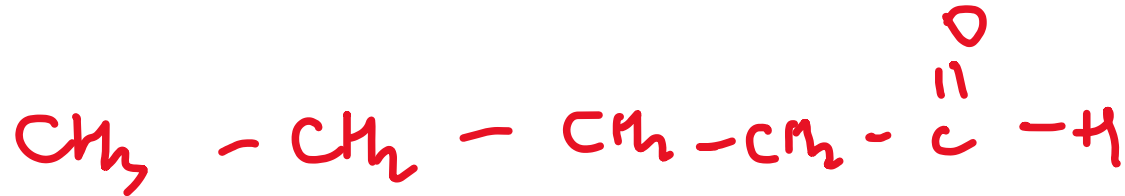


3. Functional group isomerism -



dimethyl ether

Metamerism :-

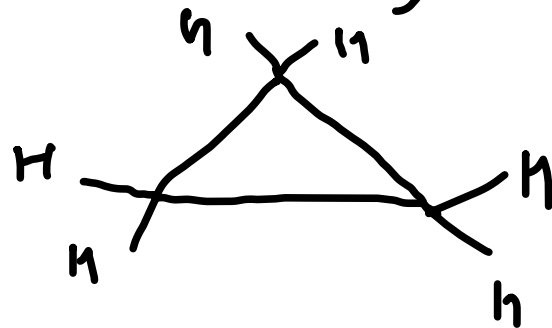


Ring chain isomers:

Compounds that have the same molecular formula but possess open chain or cyclic structure are called ring chain isomers.

Propene: $\text{CH}_2 = \text{CH} - \text{CH}_3$

Cyclopropane:



Alkynes and Cycloalkenes .

Propyne - cyclopropane



Tautomerism: A single compound that can exist in two readily interconvertible structures

that differ in the relative position of at least one atom (generally hydrogen).



Essential condition for an aldehyde or ketone to exhibit keto-enol tautomerism is the presence of at least one α -hydrogen atom.

Imine - enamine tautomerism

Stereoisomerism

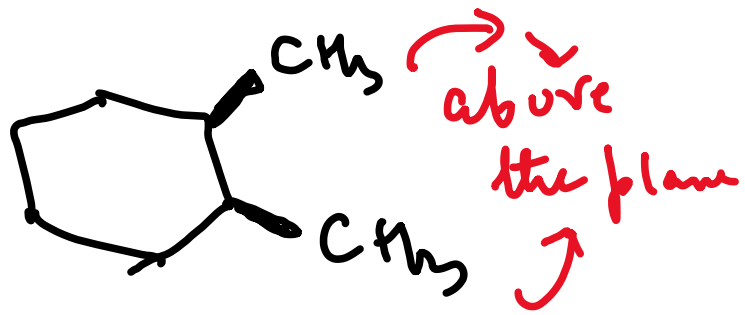
Say A & B are 2 stereoisomers

Like / common properties:

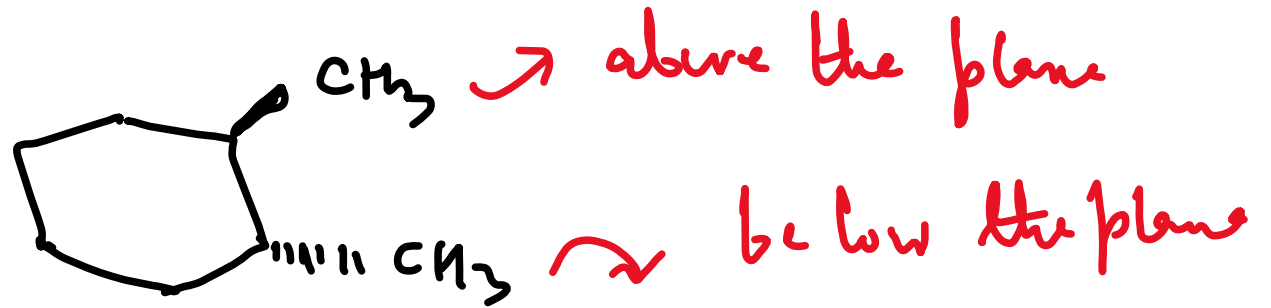
1. Same molecular formula
2. Same connectivity of atoms in their molecules

Unlike / difference: -

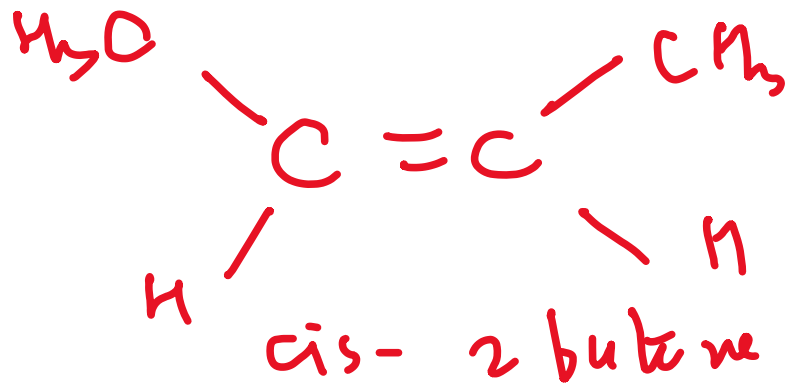
Different three dimensional orientations of their atoms in space.



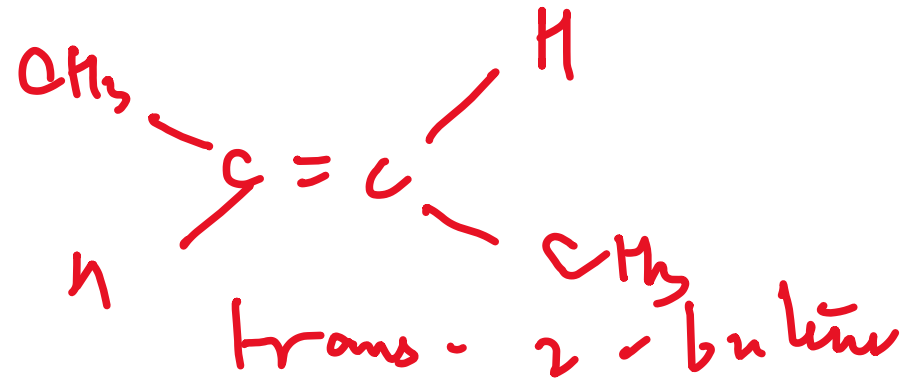
cis-1,2
dimethyl cyclohexane



trans-1,2 dimethyl
cyclohexane

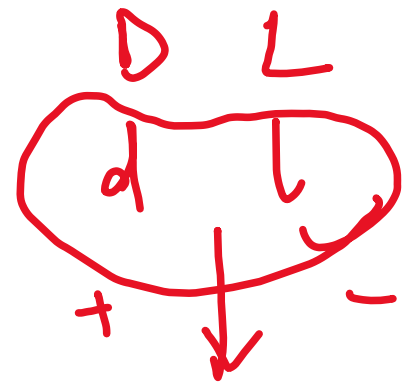
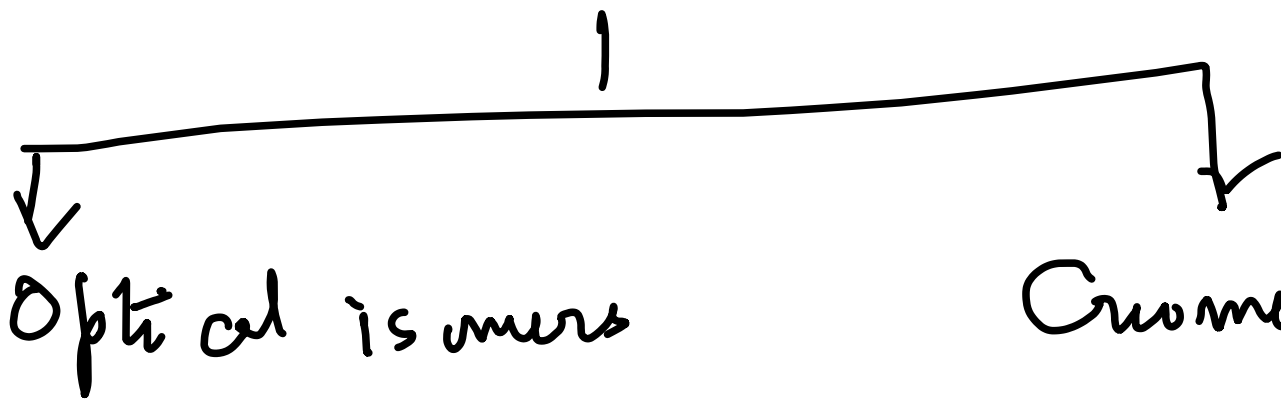


Same
structural
formula



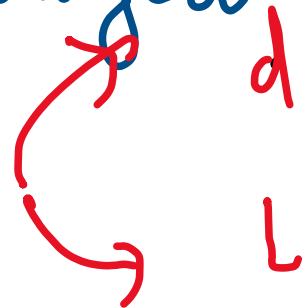
but orientation in space is different.

Stereoisomers



Stereoisomers that include substances that can rotate the plane of polarized light

Enantiomer



Geometrical isomers

Molecules that have identical atomic organization but different geometries

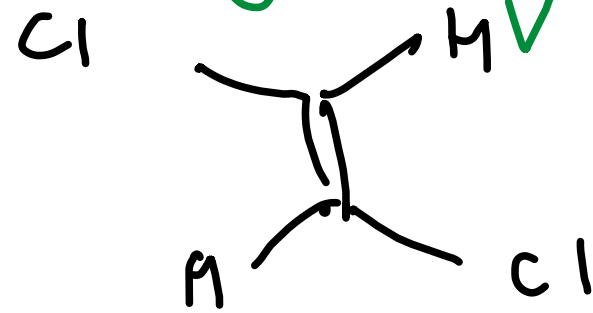
cis - trans isomers

Enantiomers are stereoisomers whose molecules are non superimposable mirror images of each other.

Diastereomers are stereoisomers whose molecules are not mirror images of each other.



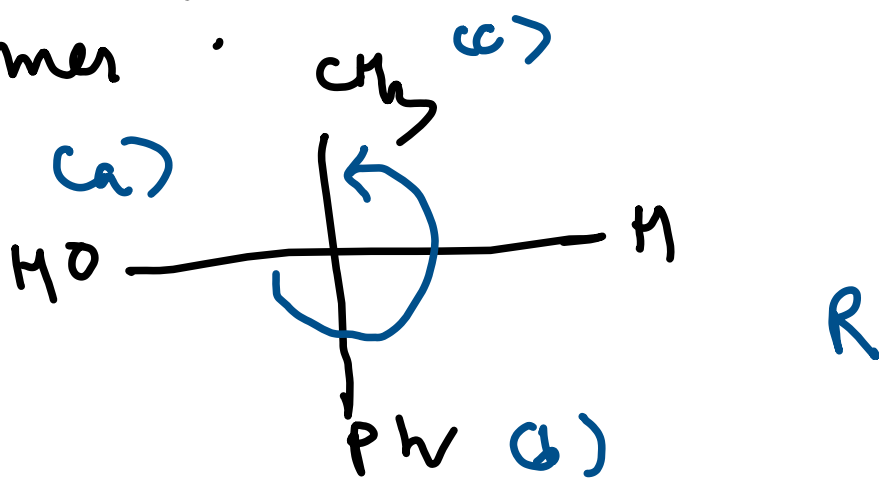
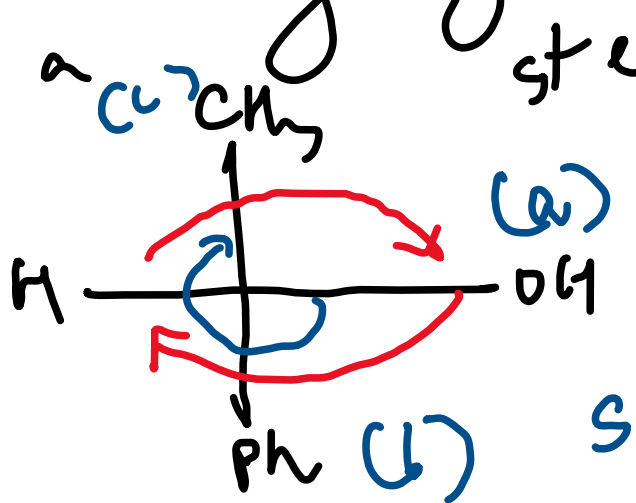
All stereoisomers other than enantiomers are diastereomers.



cis- and trans isomers are diastereomers

Enantiomers must have a stereogenic center

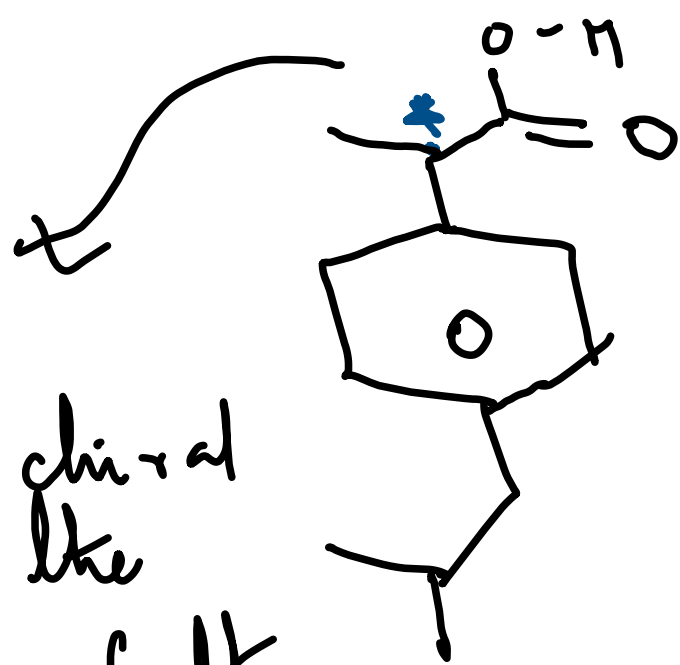
Stereogenic center - A stereocenter or stereogenic center in any point in a molecule, though not necessarily an atom, bearing different substituents, such that interchanging any two substituents lead to a stereoisomer.



Two compounds that are enantiomers of each other have the same physical properties, except for the direction in which they rotate the plane-polarized light and how they interact with different optical isomers of other compounds.

Therefore, enantiomers have certain biological effects.

Ibuprofen contains a chiral carbon in the \pm position of the propionate moiety



2 enantiomers
derivatives

Ibuprofen.

NSAID

non-steroidal
anti-inflammatory
drug

There are two possible isomers

(enantiomers) of ibuprofen

with the potential for different biological

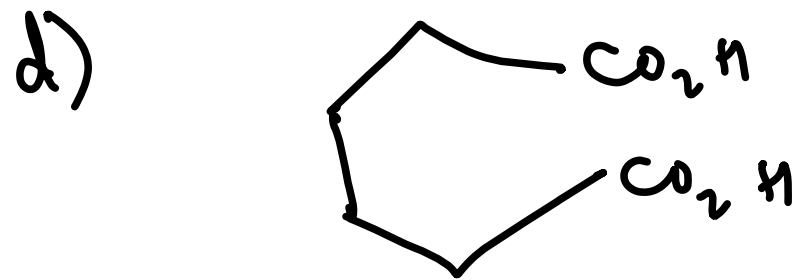
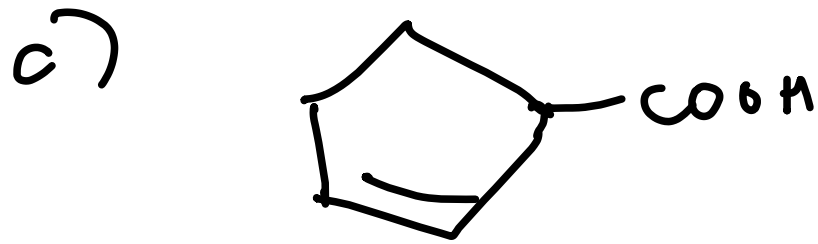
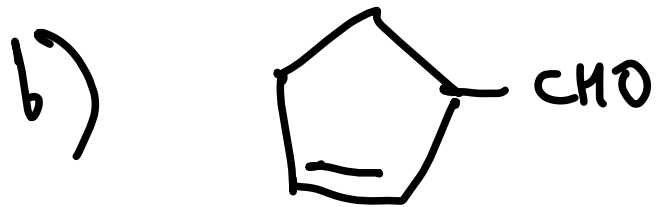
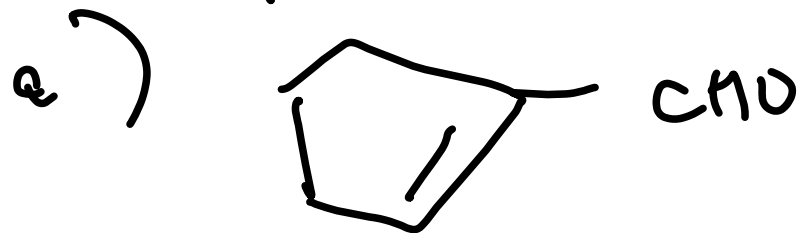
(ketoprofen, flurbiprofen, naproxen etc.)

effects and metabolism for each enantiomer.

Interestingly, it has been found that (S)-(+)-ibuprofen (dexibuprofen) was the active form both in vitro and in vivo.

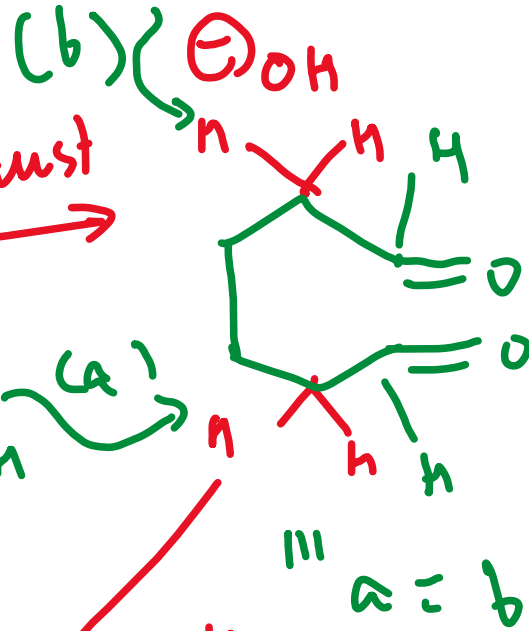
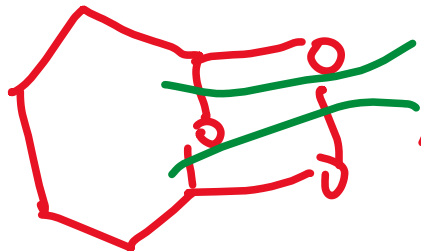
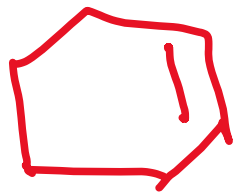
So, there was the potential for improving the selectivity and potency of ibuprofen formulation by marketing product as a single enantiomer. This occurs in neoprofen

18.) Cyclohexane on ozonolysis followed by reaction with zinc dust and water gives compound E. Compound E on further treatment with aqueous KOH yields compound F. Compound F is

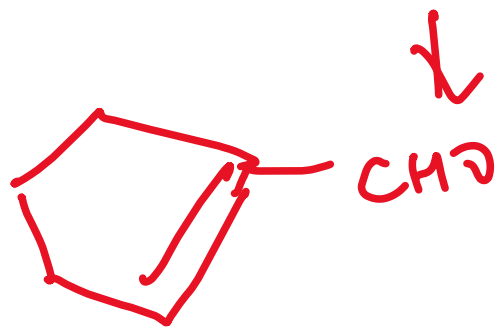
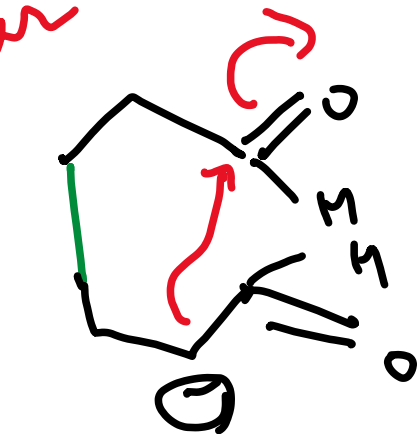


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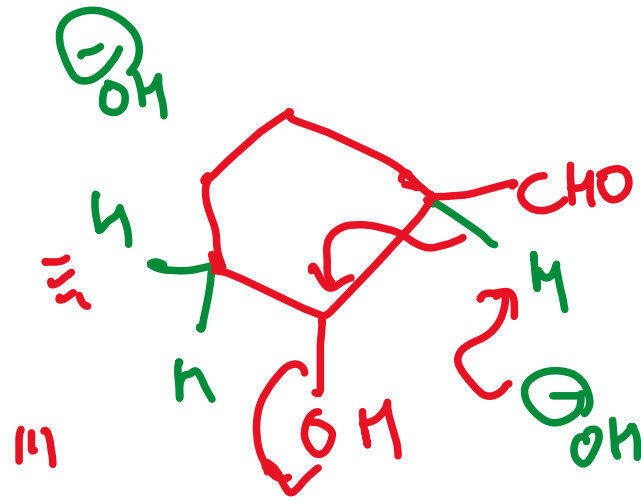
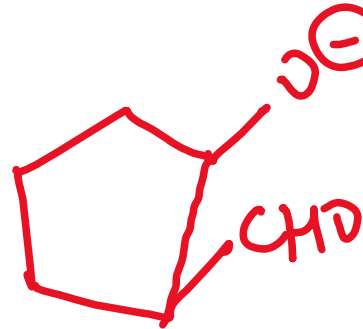


Intramolecular
aldol
Condensation



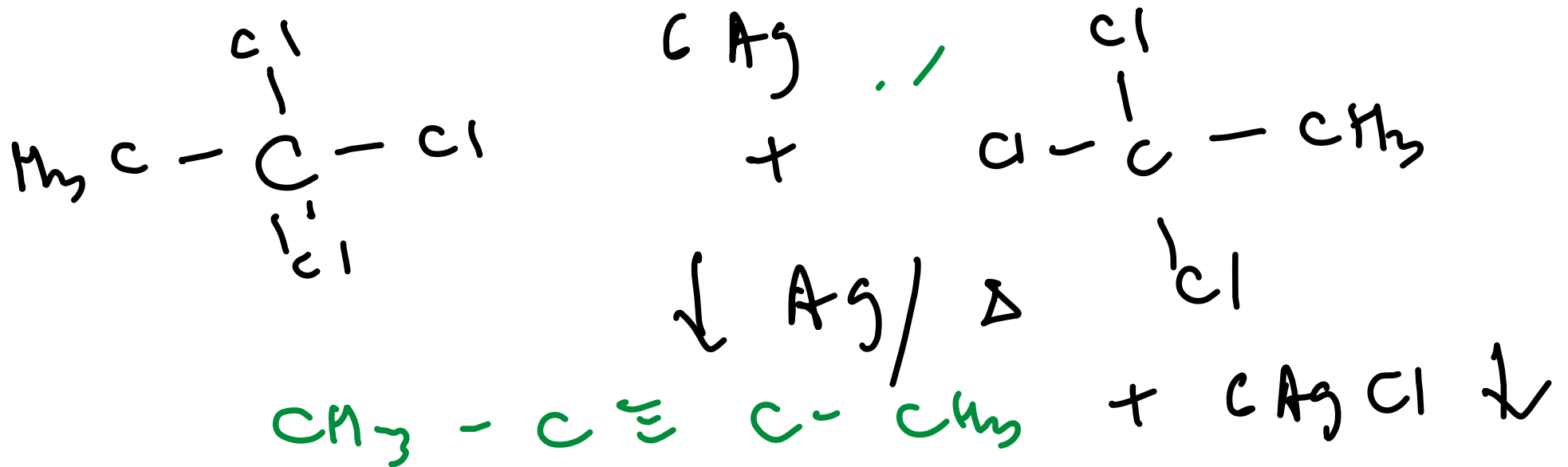
aq.

KOH



Q/ The major organic compound formed by the reaction of 1-trichloroethane with silver powder is -

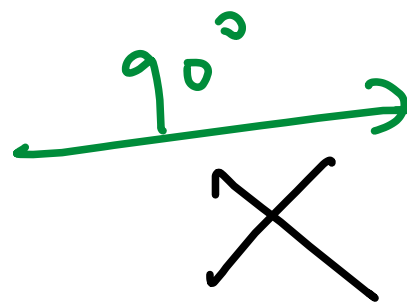
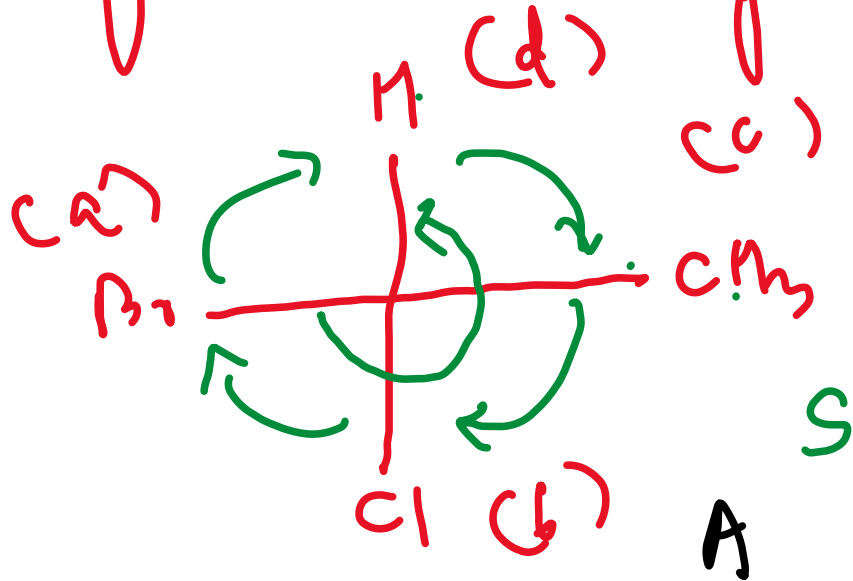
- a) 2-butene, b) acetylene c) ethene d) 2-butyne.



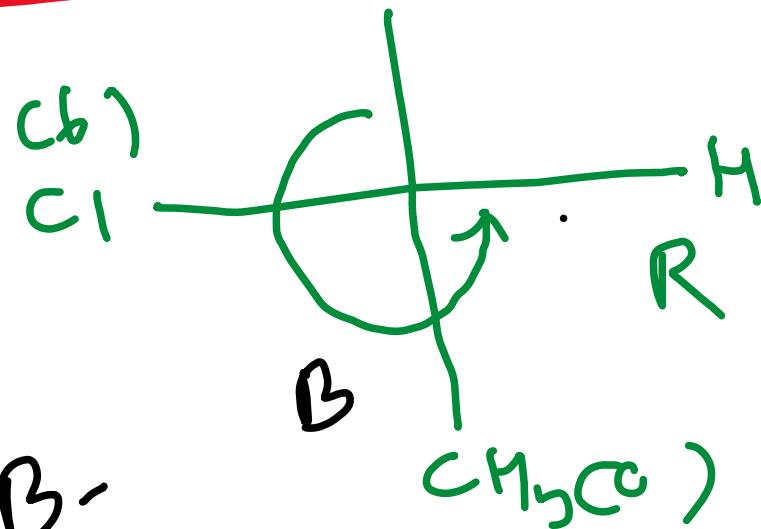
Fischer Projection:

Equivalent operation.

1.

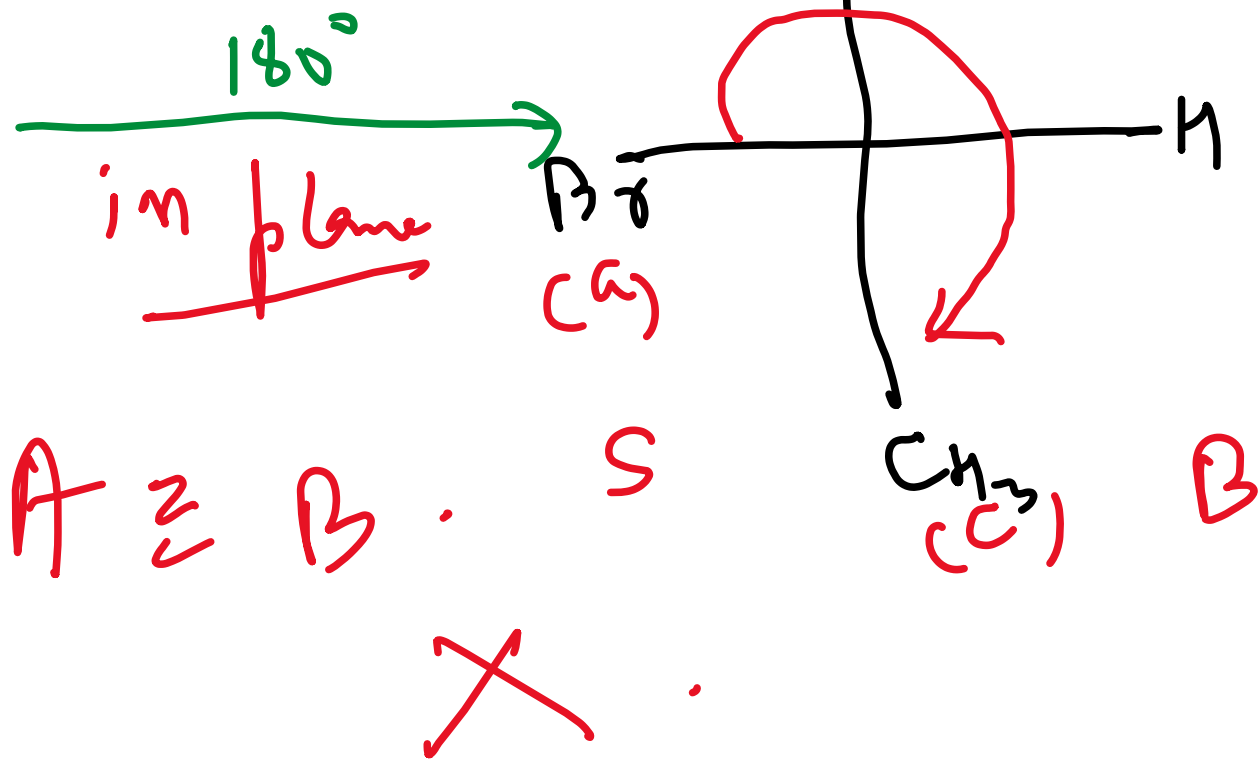
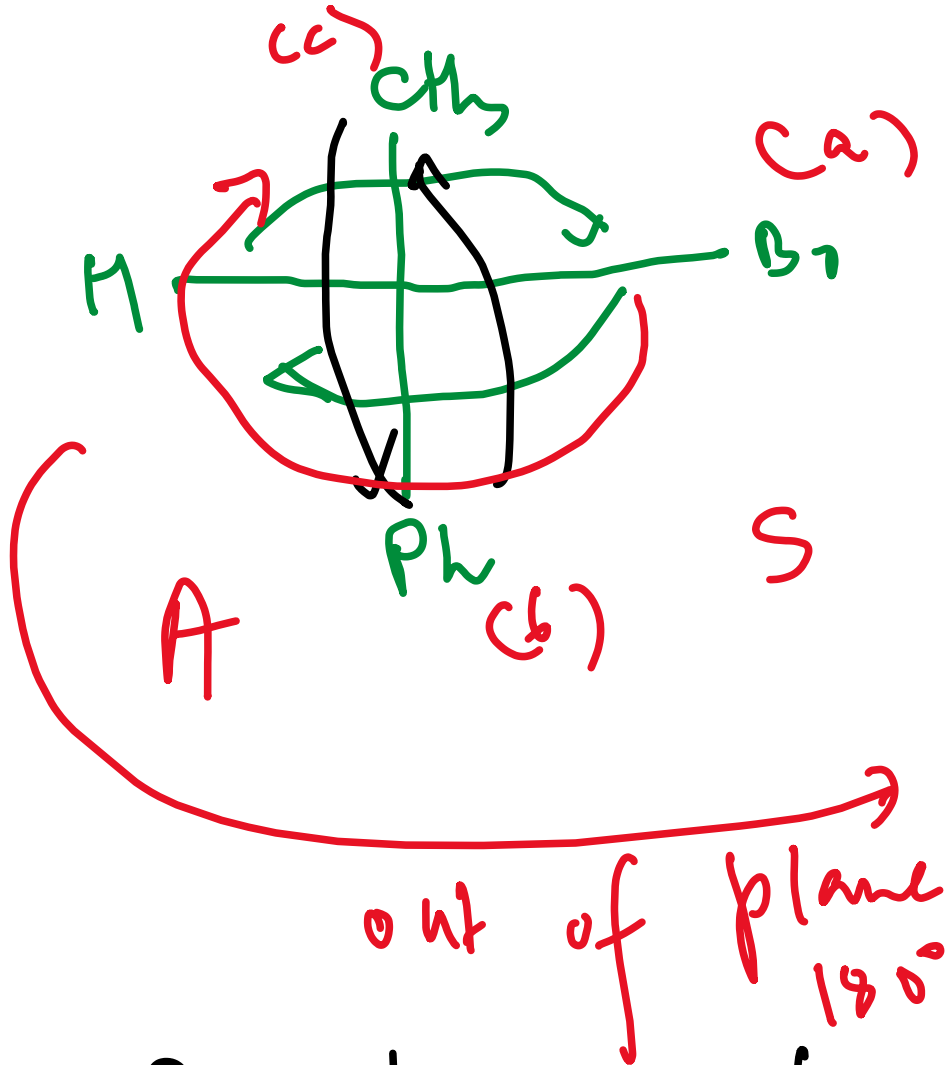


enantiomer B+

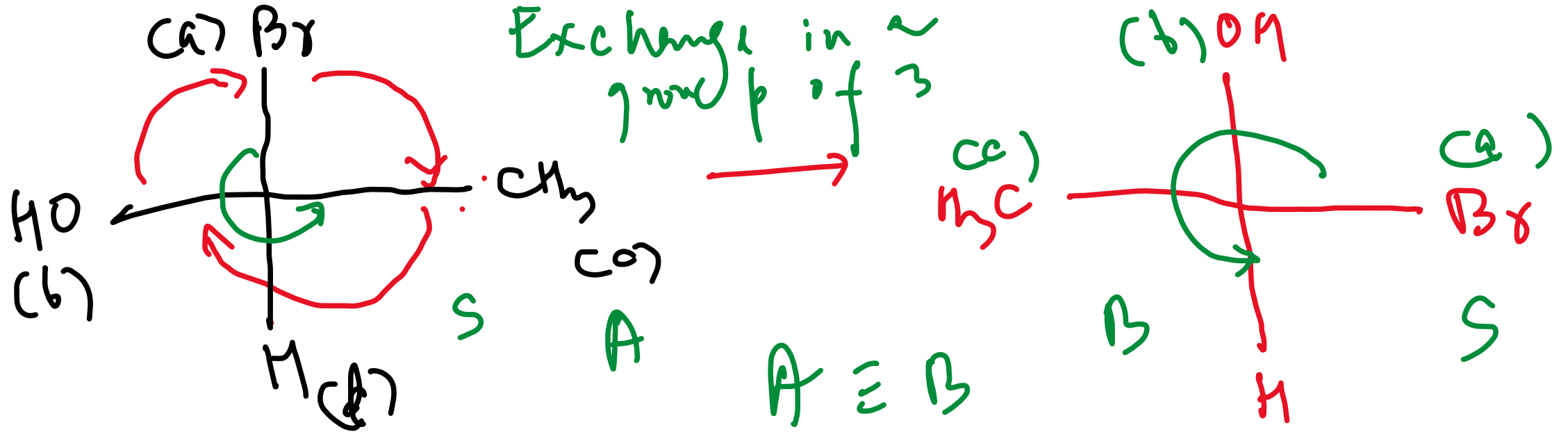


90° rotation along the chiral C is not allowed because it results in different stereoisomers. A ≠ B-

2.



3. Position of ligands / Ligand exchange



We keep the position of any one atom constant and interchange the position of rest 3 substituents.

Result is Same / Equivalent molecule.

Summary

Allowed

1. 180° in plane
2. Keep position of one atom constant and rotate/exchange the rest

Same \downarrow Equivalent molecule

Not allowed

1. 180° out of plane
2. 90° rotation

Exchange in group is allowed

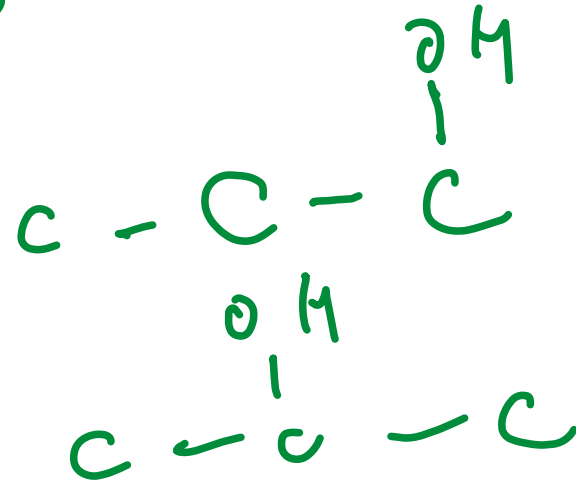
One exchange is disallowed

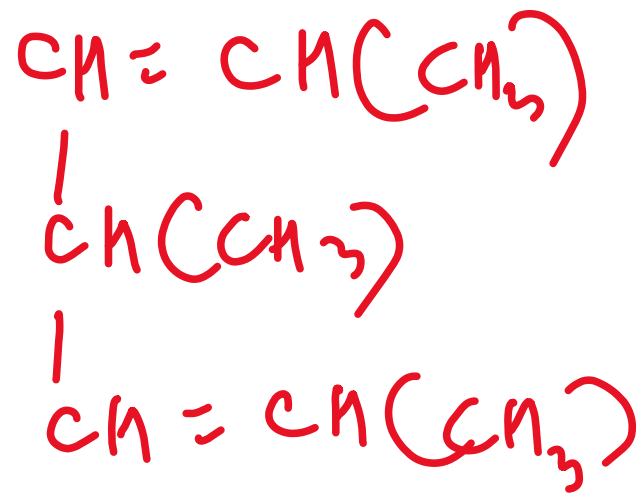
Q.12

Compounds with the same molecular formula but different bond connectivities are called

- a) Geometrical isomers
- b) Diastereomers
- c) Configurational isomers
- d) Constitutional isomers

↓ definition of





How many stereoisomers are possible for this structure?

a) 1

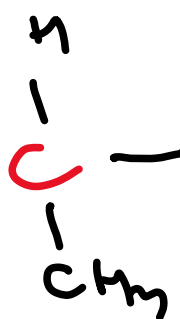
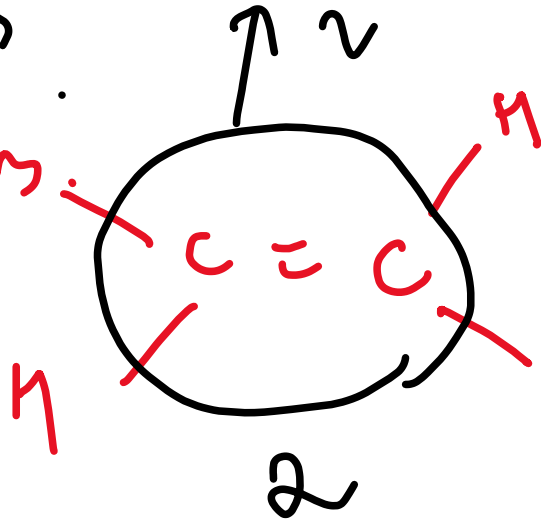
b) 2

c) 3

d) 4

cis-trans

CH₃



cis-trans

2



The London Dispersion Force

It is the weakest intermolecular force.

This is a temporary attractive force that results when the electrons in two adjacent atoms occupy positions that make the atoms form temporary dipoles. This force is sometimes called as induced dipole-dipole attraction.

London dispersion forces are often found in the halogens (e.g. F_2 and I_2), the noble gases (e.g. Ne & Ar) and in other non-polar molecules, such as carbon dioxide and methane.

London dispersion forces are part of the van der Waals forces or weak intermolecular attractions.

