AN INTRODUCTION TO ORGANIC CHEMISTRY

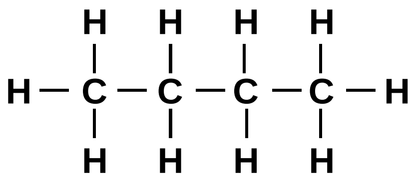
Taylor's College Subang Jaya

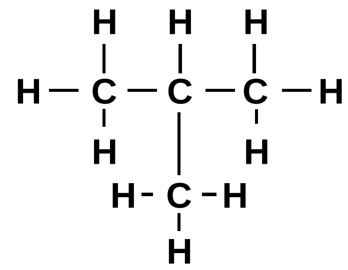
Empirical, molecular, structural & displayed formulae

- **Molecular formula**
  The ………………………………… of atoms of each element present in the molecule
  actual number
  eg: C_4H_{10}
- **Empirical formula**
  The ……………………………………………………………… of atoms in the molecule
  simplest ratio number
  eg: C_2H_5
- **Structural formula**
  The minimal detail using conventional groups
  eg: $\mathbf{CH_3CH_2CH_2CH_3}$ $\mathbf{CH_3CH(CH_3)CH_3}$

- **Displayed formula**

eg:





Skeletal formula : does not show the carbon and hydrogen only

Nomenclature

- Number of carbons

  eg: meth-, eth-
- Linking or bonding in the chain

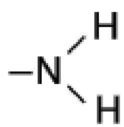
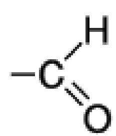
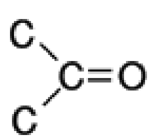
  eg: -an-, -en-, -yn-
- Functional group

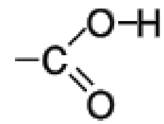
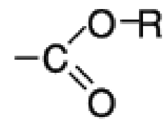
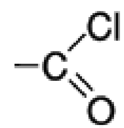
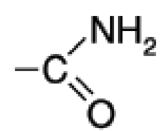
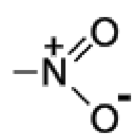
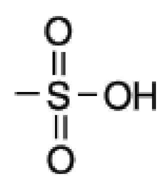
  eg: -e, -ol, -amine
- Lowest number for functional group.
- Same substituent occur more than once: di, tri, tetra
- 2 or more different substituent – alphabetical order.

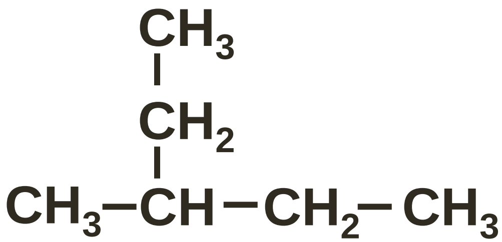
COMMON FUNCTIONAL GROUPS

GROUP	ENDING	GENERAL FORMULA	EXAMPLE	
ALKANE	- ane	RH	C_2H_6	ethane
ALKENE	- ene		C_2H_4	ethene
ALKYNE	- yne		C_2H_2	ethyne
HALOALKANE	halo -	RX	C_2H_5Cl	chloroethane
ALCOHOL	- ol	ROH	C_2H_5OH	ethanol
ALDEHYDE	-al	RCHO	CH_3CHO	ethanal
KETONE	- one	RCOR	CH_3COCH_3	propanone
CARBOXYLIC ACID	- oic acid	RCOOH	CH_3COOH	ethanoic acid
ACYL CHLORIDE	- oyl chloride	RCOCl	CH_3COCl	ethanoyl chloride
AMIDE	- amide	$RCONH_2$	CH_3CONH_2	ethanamide
ESTER	- yl - oate	RCOOR	CH_3COOCH_3	methyl ethanoate
NITRILE	- nitrile	RCN	CH_3CN	ethanenitrile
AMINE	- amine	RNH_2	CH_3NH_2	methylamine
NITRO	nitro-	RNO_2	CH_3NO_2	nitromethane
SULPHONIC ACID	- sulphonic acid	RSO_3H	$C_6H_5SO_3H$	benzene sulphonic acid
ETHER	- oxy - ane	ROR	$C_2H_5OC_2H_5$	ethoxyethane

COMMON FUNCTIONAL GROUPS

ALKANE	C–C
ALKENE	C=C
ALKYNE	C≡C
HALOALKANE	C–X
AMINE	
NITRILE	–C≡N
ALCOHOL	–O–H
ETHER	C–O–C
ALDEHYDE	
KETONE	

	CARBOXYLIC ACID
	ESTER
	ACYL CHLORIDE
	AMIDE
	NITRO
	SULPHONIC ACID



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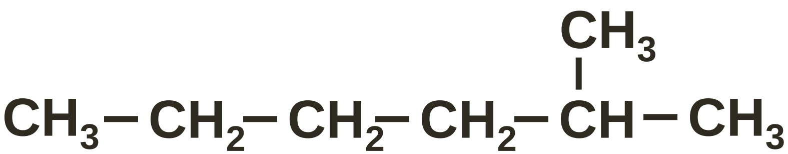

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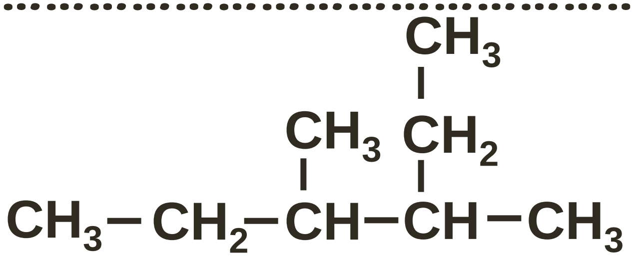

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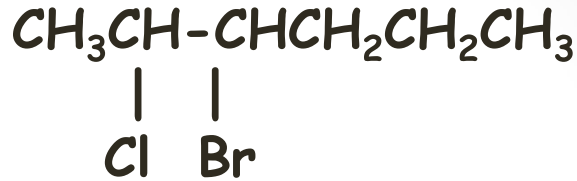

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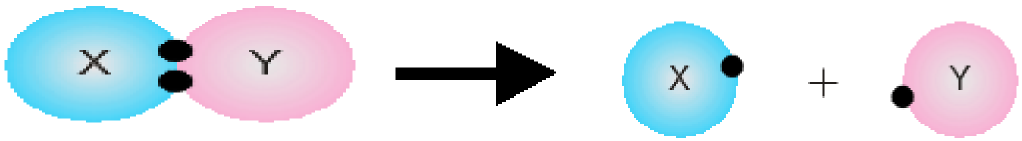
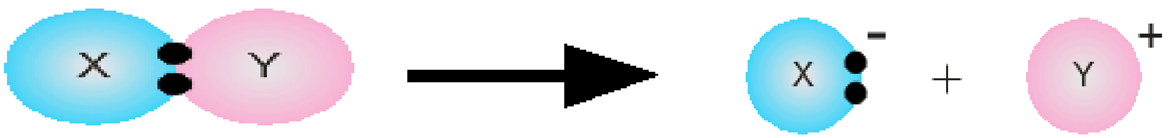
Homolytic & heterolytic



Homolytic fission: the breaking of a covalent bond in such that **one electron goes to each of the atom**, forming **free-radicals**.

Free radical is an atom or group with an unpaired e^- formed from the homolytic fission of a covalent bond & are very reactive

Homolytic & heterolytic



- **Heterolytic fission:** breaking of a covalent bond such that **both** the **electrons** go to the **same atom**, forming **positive and negative ions**.

Nucleophile & electrophile

- **Nucleophile: Contains a lone pair of e^- & are attracted to electron deficient sites (δ+)**

  eg: CN^- ,Br^- ,H_2O

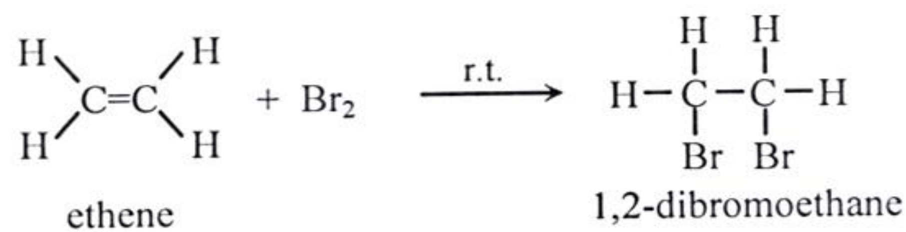
- **Electrophile: Electron-deficient species** which can accept electrons and **attracted** to regions of negative charge or **electron rich sites** (δ-) in a molecule.

  eg: H^+, Cl^+, R^+

Organic Reactions

- **Addition** – involves two molecules joining together to form a single new molecule. Usually involve reactions with unsaturated organic compounds.

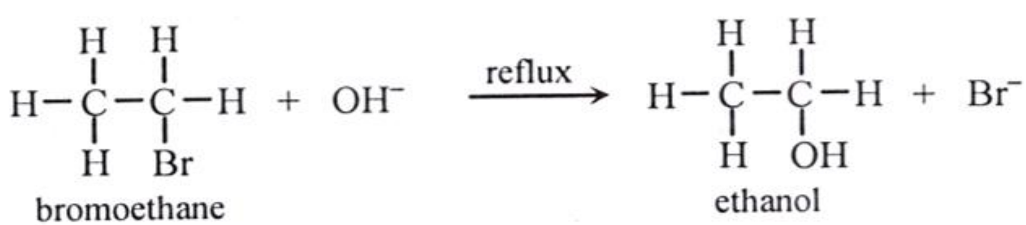
e.g.



i.e. Br_2 *adds* to ethene to form 1,2-dibromoethane.

- **Substitution** – involves replacing an atom (or group of atoms) by another atom (or group of atoms).

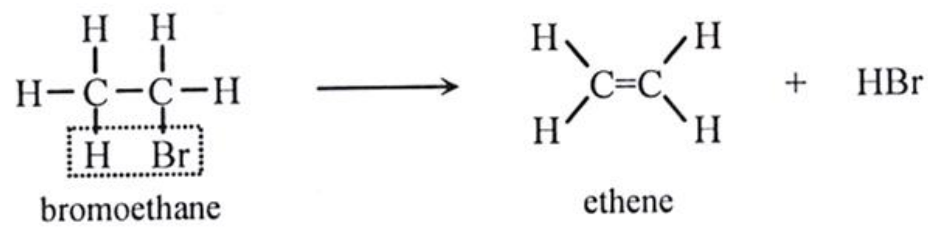
e.g.



i.e. The Br atom is *substituted* (or *replaced*) by the OH group.

- **Elimination** – involves the removal of a molecule from a larger molecule.

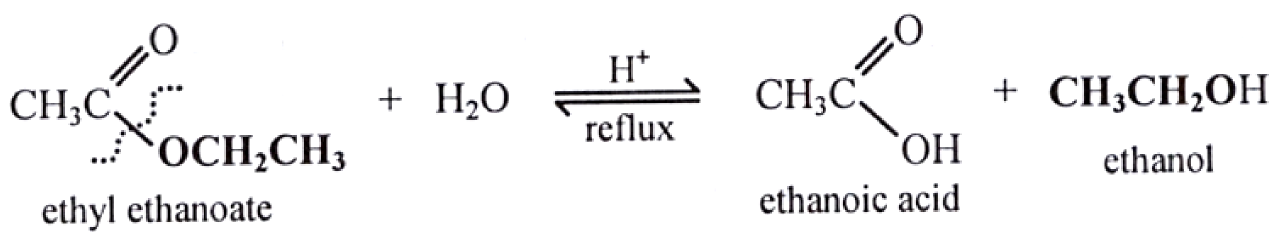
e.g.



i.e. HBr is *eliminated* (or *removed*) from bromoethane to form ethene.

- **Hydrolysis** – involves breaking covalent bonds by reaction with water.

e.g.



i.e. Ethyl ethanoate (an ester) is *hydrolysed* (or *split up by water*) to give ethanoic acid and ethanol.

$CH_3CH_2Br(l) + H_2O(l) \rightarrow CH_3CH_2OH(aq) + HBr(aq)$

- **Free radical substitution** – the mechanism consist of 3 steps : initiation, propagation and termination.

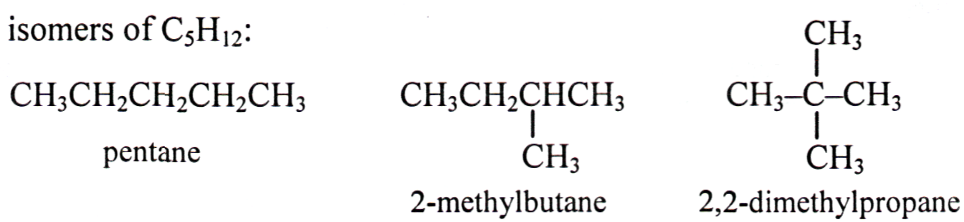
Isomerism

- **Isomerism**
  (compounds have **same molecular formula** but **different arrangement** of the atom in the molecule)
  - **Structural isomerism**
    - different structural formula.
    - Different spatial arrangement of atoms.
    - Chain isomerism
    - Position isomerism
    - Functional isomerism
  - **Stereoisomerism**
    -same structural formula.
    - Different spatial arrangement of atoms.
    - Geometrical isomerism
    - Optical isomerism

Chain Isomerism

- Due to **different arrangements of carbon atoms** in a chain.
- Chain isomers **have different carbon chains**, **straight** chain or **branched** chain.
- Chain isomers have different physical properties but similar chemical properties.
- Why?

e.g. isomers of C_5H_{12}:



Position Isomerism

- Due to **different position of functional groups** in the carbon chain.
- Position isomers have similar chemical properties (same functional group) but different physical properties.

$CH_3CH_2CH_2CH_2OH$

butan-1-ol

$$\begin{array}{l} CH_3CH_2\underset{\displaystyle\overset{|}{OH}}{C}HCH_3 \end{array}$$

butan-2-ol

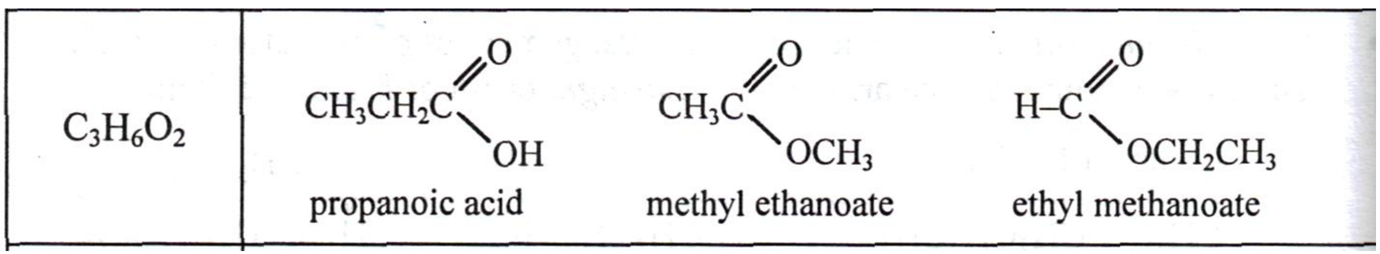
Functional Group Isomerism

- Due to **different functional group**.
- Functional group isomers have same molecular formula but different functional groups.
- The isomers have different homologous series.
- The isomers have different chemical and physical properties.

$C_4H_{10}O$	$CH_3CH_2CH_2CH_2OH$ butan-1-ol	$CH_3\underset{\underset{OH}{\vert}}{C}HCH_2CH_3$ butan-2-ol	$CH_3-\overset{\overset{CH_3}{\vert}}{\underset{\underset{OH}{\vert}}{C}}-CH_3$ 2-methylpropan-2-ol
	$CH_3\underset{\underset{CH_3}{\vert}}{C}HCH_2OH$ 2-methylpropan-1-ol	$CH_3CH_2-O-CH_2CH_3$ ethoxyethane	$CH_3-O-\underset{\underset{CH_3}{\vert}}{C}HCH_3$ 2-methoxypropane
		$CH_3-O-CH_2CH_2CH_3$ 1-methoxypropane	

Exercise

- Write the structural formula of isomers of $C_3H_6O_2$ to illustrate functional group isomerism.



Geometrical isomerisation in alkenes

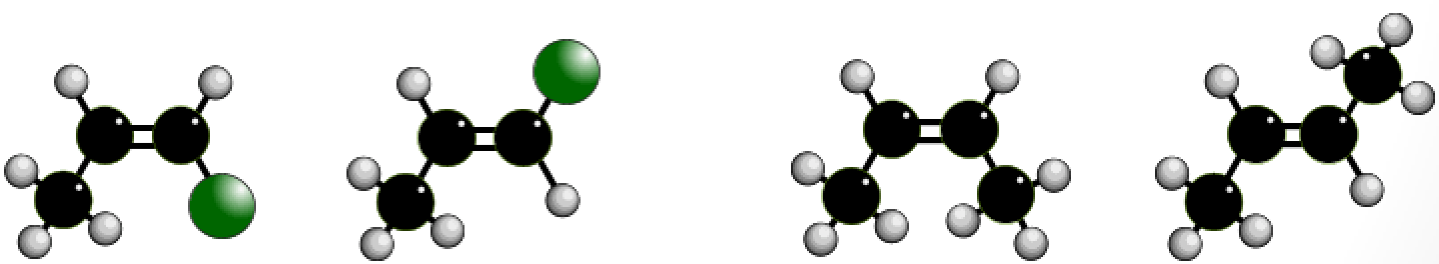
- **Arises when rotation about a bond is restricted**
- **Cis-isomer:** 2 groups on the same side of the double bond.
- **Trans-isomer:** 2 groups on the opposite side of the double bond.
- **eg: $BrCH{=}CHBr$ & $CH_3CH{=}CClBr$**

GEOMETRICAL ISOMERISM IN ALKENES

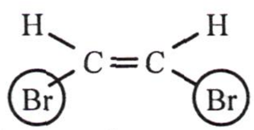
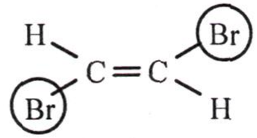
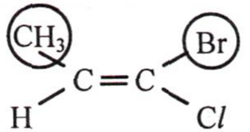
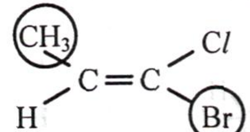
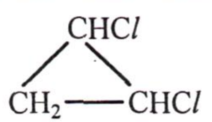
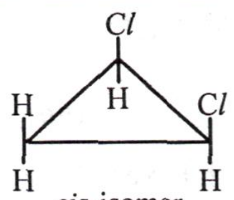
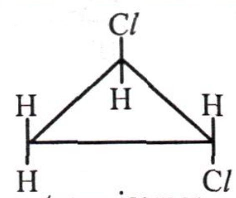
CIS-TRANS

Should only be used when there are two H's and two non-hydrogen groups attached to each carbon.

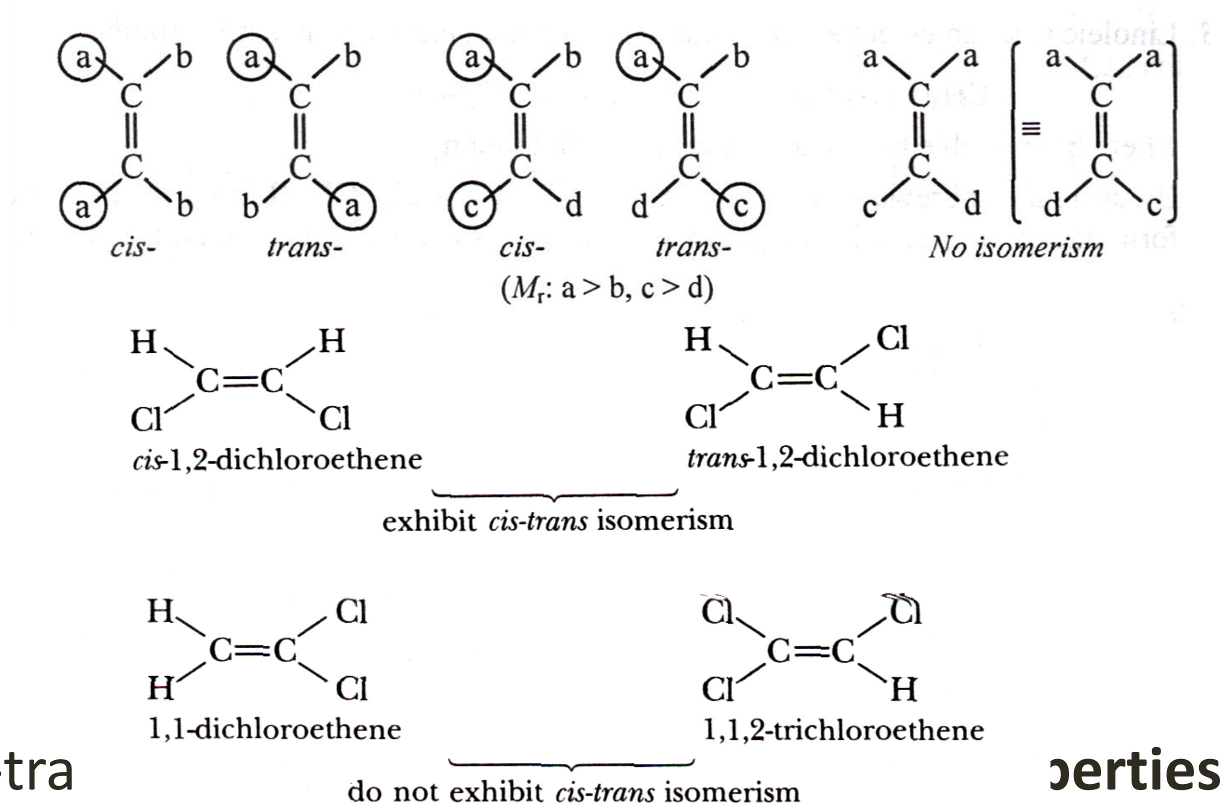
cis	non-hydrogen groups / atoms on the SAME side of C=C bond
trans	non-hydrogen groups / atoms on OPPOSITE sides of C=C bond



Geometrical isomerisation

Compound	*Geometrical (cis-trans) isomers*		*Remarks*
BrCH=CHBr	 *cis*-isomer	 *trans*-isomer	–
$CH_3CH{=}CC\mathit{l}Br$	 *cis*-isomer	 *trans*-isomer	In the *cis*-isomer, the group of ***higher priority*** (higher M_r) on each C are on the same side of C=C bond.
 1,2-dichloro cyclopropane	 *cis*-isomer	 *trans*-isomer	–

- Cis-trans isomerism cannot exist if either carbon carries 2 identical groups.



- Cis-tra **perties** (same functional group) – they react with the same reagents but at different rates.

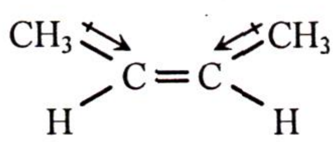
- Cis-trans isomers have **different physical properties** – due to different spatial arrangements of groups.
- **Cis**-isomers usually has **lower melting point** – structure of cis-isomer is **less symmetrical**

→hence cannot be closely packed in the crystal lattice.

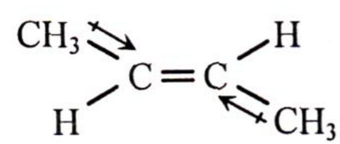
→less contact between neighbouring molecules.

→Strength of intermolecular forces reduced.

- But cis-isomers generally have **higher boiling point** – have **higher polarity**.



cis- isomer:
bond moments do ***not*** cancel out;
molecule has a net dipole moment
and so, is *polar*.



trans- isomer:
bond moments cancel each other;
molecule has no net dipole
moment and so, is *non-polar*.

Exercise

- Which of the organic compounds shown below exhibit geometric (cis-trans) isomerism?

  (a) $CH_3CH{=}CHCH_2CH_3$

  (b) $FCH{=}CHF$

  (c) $CH_2{=}C(CH_3)_2$

  (d) $FClC{=}CClF$

Optical Isomerism

- An organic molecule can only exhibit optical isomerism if it contains one **chiral carbon** atom, shown as C* (a carbon atom attached to **4 different** atoms or group).
- Optical isomers are optically active, where it is able to rotate the plane of plane-polarised light.
- They posses same structural formula but differ in effect on plane-polarised light.
- Optical isomers (**enantiomers**) are:

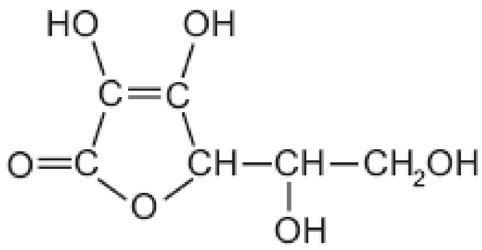
  (a) **mirror image** of each other

  (b) and **cannot be superimposed** on each other no matter how the molecule is rotated.
- http://www.youtube.com/watch?v=3WZZXPOsPNI&feature=related
- http://www.youtube.com/watch?v=uD9j3nbaHsE

Identify chiral carbons(if any)

- pentan-3-ol
- 3-chlorobutan-2-ol
- 3-chlorobut-1-ene
- 1,3-dimethylbenzene

19 The diagram shows the structure of vitamin C.



How many chiral centres are there in one molecule?

A 1 **B** 2 **C** 3 **D** 4

Optical Isomerism

- Enantiomers have same:

  a) **chemical** properties except towards optically active reagents.

  b) **physical** properties except for the **direction** of **rotation** of the plane of polarised light – rotate the plane of polarised light in different directions.

- **Racemic mixture** → A mixture containing **equal quantities** of each isomer and is optically inactive