

If two or more organic compound which have same molecular formula but having different structural formula these structures are called isomers of each other and this phenomena is called isomerism.

## (1) Molecular formula of butane $C_4H_{10}$

- (a) C-C-C-C
- butane
- C-C-C(b)
- 2-methyl propane

Number of isomer = 2

## (2) Pentane C<sub>5</sub>H<sub>12</sub>

- (a) C-C-C-C
  - C-C-C-C
- (c)  $C \dot{C} C$

Number of isomer  $\pm 3$ 

### (3) Hexane $C_6H_{14}$

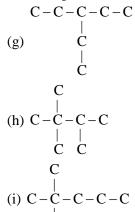
- (a) C-C-C-C-C
  - C-C-C-C-C

Number of isomer = 5

### (4) Heptane C<sub>7</sub>H<sub>16</sub>

- (a) C-C-C-C-C-C
- $\dot{C} C C C$

- (f) C-C-C-C



Number of isomer

Butane  $\rightarrow 2$ 

Pentane  $\rightarrow 3$ 

Hexane  $\rightarrow 5$ 

Heptane  $\rightarrow$  9

Octane  $\rightarrow$  18

Nonane  $\rightarrow$  35

Decane  $\rightarrow$  75

#### **Classification of Isomerism**



Isomerism

Isomerism

- 1. Chain
- 2. Position
- 3. Functional
- 4. Metamerism
- 5. Tautomerism
- (b) Optical

1. Configurational

2. Conformational

(a) Geometrical

## **Priority Order: RTFMCP**

 $R \rightarrow ring$ 

 $T \rightarrow tautomer$ 

 $F \rightarrow functional$ 

 $M \rightarrow Metamer$ 

 $C \rightarrow Chain$ 

 $P \rightarrow Position$ 

#### 1) Chain Isomerism:

Compound having same molecular formula but different arrangement of carbon within the molecule are called chain isomer of each other and this phenomena is called chain isomerism.

(i) Butane  $C_4H_{10}$ :

(a) 
$$CH_3 - CH_2 - CH_3 - CH_3 \rightarrow 4$$
 but an e
$$C - C - C \rightarrow 3$$
 2 - methyl propane
$$C$$

a and b are chain isomer of each other.



(a) 
$$\overline{C-C-C-C-C} \rightarrow 5$$

(b) 
$$|$$
  $C-C-C-C| \rightarrow 4$ 

$$\begin{array}{c|c}
 & | \\
 & | \\
 & | \\
 & | \\
 & C
\end{array}$$

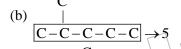
a and b

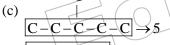
b and c are chain isomer

d and d

## (iii) C<sub>6</sub>H<sub>14</sub>:

(a) 
$$C-C-C-C-C-C \rightarrow 6$$





$$(d) \begin{array}{c|c} C - C - C - C \\ \hline & | & | \\ C & C \\ \hline & C \end{array}$$

(c) 
$$C - C - C \rightarrow 4$$

a and b

a and d

a and e

b and d > are chain isomer

b and e

c and d

c and e

 $\begin{array}{c} b \text{ and } c \\ d \text{ and } e \end{array}$  not chain isomer

## (iv) $C_2H_6$ , $C_3H_8$ :

Do not shown chain isomer.

#### (2) Position Isomer:

Compound having same structure of each carbon chain but differ only in the position of multiple bond, brand (double bond or triple bond) or functional group then these isomer are called position isomer and these phenomeno is called position isomerism. (Condition  $\rightarrow$  number of carbon in chain should be same)

(i)  $CH_3$ – $CH_2$ – $CH=CH_2$ 

but-1-ene

CH<sub>3</sub>-CH=CH-CH<sub>3</sub>

but-2-ene

Chain length is same and position of double bond change so it is called as chain isomer.

#### (ii) $C_5H_{10}$

(a)  $CH_2 = CH - CH_2 - CH_2 - CH_3$ 

pent-1-ene

(b)  $CH_3$ –CH = CH– $CH_2$ – $CH_3$ 

pent-2-ene

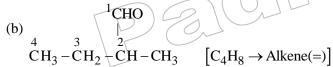
a and b are position isomer (chain length is same)

## (iii) C<sub>4</sub>H<sub>10</sub>O:

- (a) C-C-C-C-OH but tan-1-ol
- $\begin{array}{ccc} C-C-\overset{2}{C-C} & & \text{bu tan-} \ 2-\text{ol} \\ \text{(b)} & & \\ \hline \text{OH} & & \end{array}$

Position of alcohol group change from 1 to 2 carbon. a and b are position isomer.

- (iv) (a)  $\overset{4}{\text{CH}_3} \overset{3}{\text{CH}_2} \overset{2}{\text{CH}_2} \overset{1}{\text{CHO}}$
- $C_4H_8O$



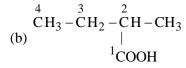
a and b not position isomer because group present only at I-position.

### (v) $C_6H_{14}O$ :

- (a) C-C-C-C-C-C-OH
- hex -1-ol
- C-C-C-C-C-C
- hexan 2 ol
- C-C-C-C-C
- hexan 3 ol

(c) OH

- a, b, c are contain 6 carbon in chain and OH is present OH different position.
- a and b
- a and c Position isomer
- b and c
- (vi) (a)  $\overset{4}{\text{CH}_3} \overset{3}{\text{CH}_2} \overset{2}{\text{CH}_2} \overset{1}{\text{COOH}}$



a, b, c are not position isomer because functional group is present at same position (1).

## **MIX Examples:**

## 1. $C_4H_8$ :

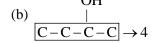
- (a) C = C C C
- (b) C-C=C-C
  - C-C=C
- (c) | C

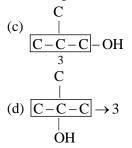
a and b position

- a and c chain
- b and c chain

#### 2. $C_4H_{10}O$ :

(a) C-C-C-C - OH

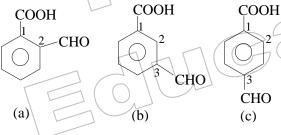




a and b	Position
a and $c$	Chain
a and $d$	Chain, position
b and c	Chain, position
b and d	Chain
c and d	Position

	96

**3.** 

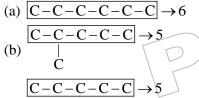


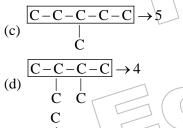
a, b and c are position isomer.

CHO
4. (a) 
$$\begin{vmatrix} C+C - 2C - COOH \\ C - C - C - COOH \end{vmatrix}$$
(b)  $\begin{vmatrix} C - C - C - COOH \\ C - C - C - COOH \end{vmatrix}$ 

a, b and c are position isomer.

5. C<sub>6</sub>H<sub>14</sub>:





(d) $C-C-C-C \rightarrow 4$ C $CC(e) C-C-C-C \rightarrow 4$	(0)	C	2	
(e) $C-C-C-C \rightarrow 4$				
	(e)		$C-C \rightarrow 4$	

_			
	$\frac{a}{a}$ and $\frac{b}{c}$		)
	a and $d$ $a$ and $e$	_	
	b and d	Chain	7//
-	b and e c and d	> 6	50
	c and e b and c		
	d and e	Position	

## **Function Isomer:**

Compound having same molecular formula but different functional group are called functional isomer and is phenomena is called functional isomer.

## (i) C<sub>4</sub>H<sub>8</sub>O:

DBE = 
$$C - \frac{H}{2} + \frac{N}{2} + 1$$

$$= 4 - \frac{8}{2} + \frac{0}{2} + 1$$

$$= 1$$
 $C \rightarrow Carbon$ 
 $H \rightarrow Hydrogen$ 
 $N \rightarrow Nitrogen$ 

DBE → double bond equivalent

- (a)  $CH_3 CH_2 CH_2 CHO$
- aldehyde



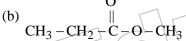


Ketone

a and b are functional isomer.

## (ii) $C_4H_8O_2$ (DBE = 1):

- (a)  $CH_3 CH_2 CH_2 COOH$
- carboxylic acid



ester

a and b are functional isomer.

## (iii) $C_4H_{10}O$ (DBE = 0):

- (a)  $CH_3 + CH_2 CH_2 CH_2 OH$
- alcohol
- (b)  $CH_3 CH_2 O CH_2 CH_3$
- ether

a and b are functional isomer.

## (iv) $C_2H_3N$ (DBE = $2 - \frac{3}{2} + \frac{1}{2} + 1 = 2$ ):

- (a)  $CH_3 CN$
- cyanide
- (b)  $CH_3 NC$
- isocyanide

a and b are functional isomer.

### (v) $C_4H_6$ :

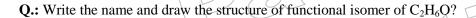
$$DBE = 4 - 3 + 1 = 2$$

2-double bond

1-triple bond

- (a)  $CH_2 = CH CH = CH_2$
- (b)  $CH_3 C \equiv C CH_3$

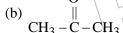
a and b are functional isomer.



## (vi) C<sub>3</sub>H<sub>6</sub>O:

DBE = 
$$3 - \frac{6}{2} + 1 = 1$$

- (a) CH<sub>3</sub> CH<sub>2</sub> CHO
- (Aldehyde)



Ketone

a and b are functional isomer.

#### **\*** Metamerism:

Compound having same molecular formula but different arrangement of alkyl group on either side of same functional group are called metamers and phenomena is called metamerism.

### (i) $C_4H_{10}O$ :

$$DBE = 4 - \frac{10}{2} + 1 = 0$$

(a) 
$$C-C-C-C-OH$$

$$(d) \qquad | \qquad \qquad \downarrow$$

(e) 
$$C-O-C-C-C$$
 1-methoxy propane

(f) 
$$C-\Theta-C-C$$

2 – methoxy propane

(g) 
$$C-C-O-C-C$$
 2—ethoxy ethane

Aldehyde, alcohol, carboxylic acid, 1 amine do not show metamerism.

a and e	
a and $f$	
a and $g$	
b and e	
b and f	
b and g	Functional
c and e	Isomer
c and $f$	
c and g	
d and e	
d and $f$	
	ı

d and g

e and g	Metamers
f and $g$	
e and f	Position isomer
a and b	Position isomer
a and c	Chain & position isomer
b and c	Chain isomer
a and d	Chain isomer
b and d	Chain & position isomer
c and d	Position isomer \

**Q.**: Write IUPAC name and draw all structure of all the metamers of  $C_5H_{12}O$ ?

**Q.**: Draw all possible structure of  $C_5H_{12}O$ ?

## Tautomerism (Keto-enol isomerism):

This is phenomena in which a single compound exist in two readily inconvertible structure which differ in the relative position of at least one atom which is generally hydrogen.

(1) 
$$O$$
  $H$   $CH_3 - C - CH_3$   $\rightleftharpoons$   $CH_2 = C - CH_3$ 

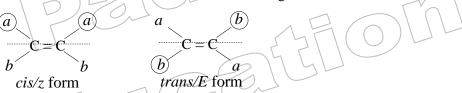
Ketone Enol

$$(2) \begin{array}{c} OH \\ | \\ CH_2 = C - CH_3 \end{array} \rightleftharpoons \begin{array}{c} O \\ | \\ CH_3 - C - CH_3 \end{array}$$

$$Enol \qquad Keto$$

## **\*** Geometrical Isomer:

Geometrical isomer one's due to different arrangement of atom or group of atom around carbon carbon double bond in alkene the isomer are called geometrical isomer.

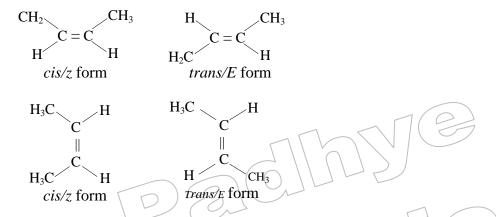


### 1) Cis isomer:

The isomer in which two identical atom or group of atoms lie on the same side of double bond are called cis-isomer.

### 2) Trans isomer:

The isomer in which two identical atoms or group of atoms lies on the opposite side of the double bond is called trans isomer.

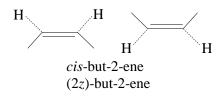


- It is not necessary that every double bond compound has geometrical isomer.
- To show geometrical isomers each double bonded carbon atom should be connected with different group.

All are show Geometrical Isomer

These not show Geometrical isomers

(1) but-2-ene



(2) hex-3-ene : C - C = C - C - C

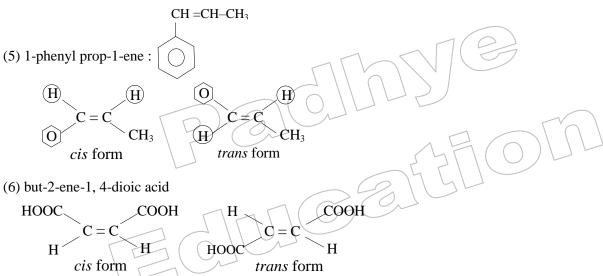
$$C_2H_5$$
  $C_2H_5$   $C$ 

(3) Pent-2-ene: C - C = C - C - C

(4) 2-methyl prop-1-ene:

$$H_2C = C - CH_3$$
 $CH_3$ 
 $CH_3$ 
 $H$ 
 $C = C$ 
 $CH_3$ 

- Here same atom or group is connected to double bonded carbon atom.
- These are not show geometrical isomer.



**Q.**: Identify the molecule which show geometrical isomerism.

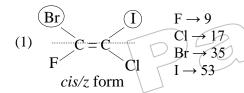


## **E/Z** system of nomenclature:

 $E \rightarrow opposite$ 

 $Z \rightarrow same$ 

- Identify the group which are connected to same double bonded carbon atom.
- Give the priority to connected group priority is decided by atomic number.
- The atom which has high atomic number has more priority.
- If the higher priority group present at same side then it is *cis* or *Z* form.
- If higher priority group present at opposite side then it is *trans*/or *E* form.



Z-2-bromo-2-chloro-1-floro-2-iodo ethene

Trans or E-1-bromo-2-chloro-1-floro-2-iodo-ethene

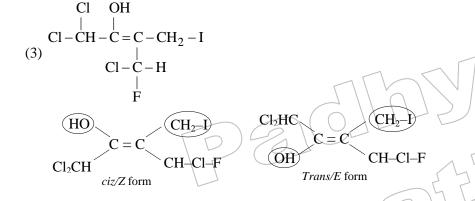
$$CH_{3}-CH=CH-CH_{3} \qquad \text{but-2-ene}$$

$$CH_{3} \qquad CH_{3} \qquad H \qquad CH_{3}$$

$$C=C \qquad H \qquad H \qquad CH_{3}$$

$$Z-\text{but-2-ene} \qquad E-\text{but-2-ene}$$

$$cis-\text{but-2-ene} \qquad trans-\text{but-2-ene}$$



**Active double bond and inactive double bond.** 

(1) 
$$CH_2 = CH$$
  $-CH = CH$   $-CH = CH_2$ 

inactive double bond (not stereo centre) inactive double bond (not stereo centre)





## Calculation of number of geometrical isomer:

#### Case 1:

When molecule has different end and it contains n number of double bond.

 $\therefore$  number of geometrical isomer =  $2^n$ 

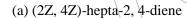
n = number of active double bond.

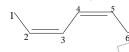
(1) 
$$CH_3 - CH = CH - CH = CH - CH_2 - CH_3$$
  
hepta-2,4-diene

Number of active double bond n = 2

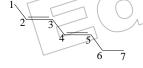
Number of geometrical isomer  $= 2^n = 2^2 = 4$ 

- (a) 2Z, 4Z (b) 2E, 2E
- (c) 2Z, 4E
- (d) 2E, 4Z

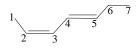




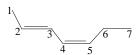
(b) (2E, 4E)-hepta-2, 4-diene



(c) (2Z, 4E)-hepta-2,4-diene



(d) (2E, 4Z)-hepta-2, 4-diene



(2) 
$$CH_3 - CH = CH - CH = CH - CH = CH - CH_2 - CH_3$$

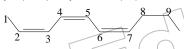
Number of active double bond n = 3

Number of geometrical isomer =  $2^3 = 8$ 

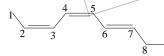
- (a) 2Z, 4Z, 6Z

- (b) 2Z, 4Z, 6E (c) 2Z, 4E, 6Z (d) 2E, 4Z, 6Z (e) 2E, 4E, 6E
- (f) 2E, 4E, 6Z
- (g) 2E, 4Z, 6E (h) 2Z, 4E, 6E.

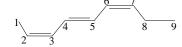
(a) (2Z, 4Z, 6Z)-nona-2, 4, 6-triene



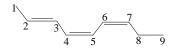
(b) (2Z, 4Z, 6E)-nona-2, 4, 6-triene



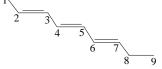
(c) (2Z, 4E, 6Z)-nona-2, 4, 6-triene



(d) (2E, 4Z, 6Z)-nona-2, 4, 6-triene



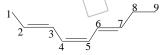
(e) (2E, 4E, 6E)-nona-2, 4, 6-triene



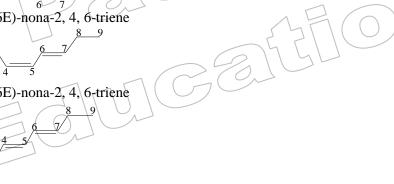
(f) (2E, 4E, 6Z)-nona-2, 4, 6-triene



(g) (2E, 4Z, 6E)-nona-2, 4, 6-triene



(h) (2Z, 4E, 6E)-nona-2, 4, 6-triene



### Case II:

When the molecule contain n number of even active double bond with same end.

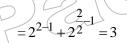
Number of geometrical isomer =  $2^{n-1} + 2^{\frac{n}{2}-1}$ 

n = number of even active double bond.

e.g.  $n = 2, 4, 6, 8, \dots$ 

(1) 
$$CH_3 - CH = CH - CH = CH$$
  $CH_3 - CH_3$   $CH = CH - CH = CH$ 

Number of geometrical isomer =  $2^{n-1}$  +

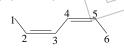


- (a) 2Z, 4Z or 2E, 4Z
- (b) 2E, 4E
- (c) 2Z, 4E or 2E, 4Z

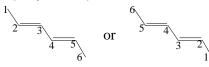
(a) (2Z, 4E)-hexa-2, 4-diene



(b) (2Z, 4Z)-hexa-2, 4-diene



(c) (2E, 4E)-hexa-2, 4-diene



Case III:

When the molecule contain n number of active odd double bond with same end.

Number of geometrical isomer =  $2^{n-1} + 2^{\frac{n-1}{2}}$ 

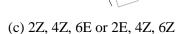
n = number of active odd double bond.

- (a) 2Z, 4Z, 6Z
- (b) 2E, 4E, 6E
- (c) 2Z, 4Z, 6E or 2E, 4Z, 6Z

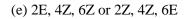
- (d) 2Z, 4E, 6Z
- (e) 2E, 4Z, 6Z or 2Z, 4Z, 6E
- (f) 2E, 4Z, 6E

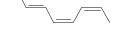
(a) 2Z, 4Z, 6Z











 $\mathbf{Q}_{\bullet}$ : Calculate the number of geometrical isomer for the following molecule ?

(i) 
$$Cl - CH = CH - CH = CH - Br$$

(ii) 
$$CH_3 - CH = CH - CH = CH - CH = CH - CH = CH - CH_2 - CH_3$$

(iv) 
$$CH_2 = CH - CH = CH - CH = CH - CH_3$$

(vi) 
$$Cl - CH = CH - CH = CH - CH = CH - Br$$

### **❖** Optical Isomerism:

- Same molecular formula
- Same structural formula
- Same physical chemical properties
- They differ in behavior of light.

## **❖** Nature of Light:

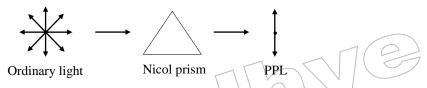
## **Ordinary light:**

• -> direction of propagation



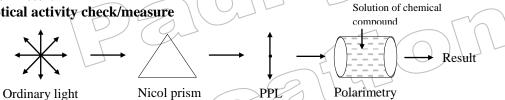
 $\vec{E} \rightarrow$  electric vector

E Vibrate in all plane perpendicular to the direction of propagation.



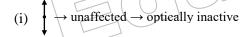
#### **Polarimeter:**

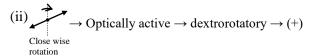
Optical activity check/measure

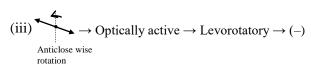


tube

#### Result







## (1) Dextrorotatory (d):

It is a property of a compound to rotate plane polarized light towards clockwise direction such molecule are called dextrorotatory molecule.

### (2) Levorotatory (l):

It is a property of a compound to rotate plane polarized light towards anticlockwise direction. Such molecule are called levorotatory molecule.

## Condition to show optical isomerism:

Molecule should have one chiral carbon.

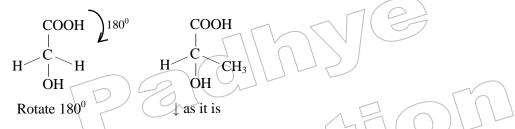


- The carbon atom which is connected to four different group is called chiral carbon bond.
- Carbon atom should connected with four single ( $\sigma$ ) bond.



- Q.: Check Optical Activity:
  - (i) 2-hydroxy propanoic acid (lactic acid)

 $\rightarrow$  1-chiral carbon molecule is optically active.



- Now we can say that both compound are non-super imposable mirror image.
- Enantiomer: Pair of optical isomer which are non-super imposable mirror image.
- (d) lactic acid and (l)-lactic acid are optical isomer of each other.
- Q.: Identify molecule which show optical isomerism.
  - (i) Pentan-3-ol:

 $\rightarrow$  No chiral carbon optically inactive.

$$\begin{array}{c} \text{OH} \\ | \\ \text{(ii)} \ \text{H}_5\text{C}_2 - \text{C} - \text{C}_2\text{H}_5 \\ | \\ \text{OH} \end{array}$$

- → No chiral carbon optically inactive.
- (iii) butan-2-ol:

$$\begin{array}{c} \text{OH} \\ | \\ \text{CH}_{3} - \text{CH}_{2} - \begin{array}{c} \text{CH} - \text{CH}_{3} \end{array}$$

→ One chiral carbon optically active.

→ Four chiral carbon optically active.

→ Three chiral carbon optically active.

→ One chiral carbon optically active.

#### **\*** Conformational isomer:

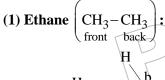
The different arrangement of atom in space that result from the tree rotation about (C–C) bond axis are called conformational isomer.

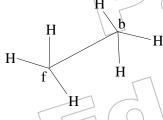
- Number of conformational isomer =  $\infty$
- Two extremes are

(a) eclipsed ( $\theta = 0^{\circ}$ )

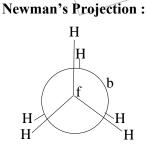
(b) staggered ( $\theta = 60^{\circ}$ )

Any other arrangement between these two extremes positions is known as  $\theta$  Gauche or skew form.  $(\theta = 0 \text{ to } 60^{\circ})$ 

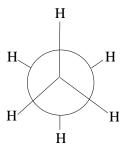




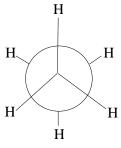
## Saw horse form



$$\theta = 0^0$$
 eclipsed

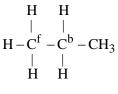


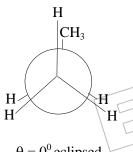
$$\theta = 0 - 60^{\circ}$$
 Gauche/skew



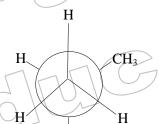
$$\theta = 60^{0} \text{ staggered}$$

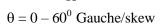
## (2) $H_3C - CH_3 - CH_3$ :

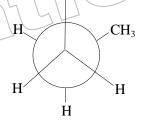








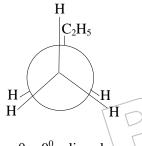




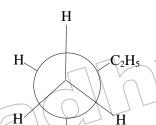
 $\theta = 60^{\circ}$  staggered

(3)  $H_3C - CH_2 - CH_2 - CH_3$ :

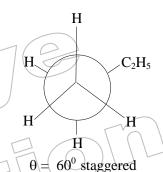
$$\begin{array}{cccc} H & H \\ | & | \\ H - C^f - C^b - C_2 H_5 \\ | & | \\ H & H \end{array}$$



 $\theta = 0^0 \, eclipsed$ 



H  $\theta = 0 - 60^{\circ}$  Gauche/skew



Q.: What isomerism exhibited by the following pairs of compound.

 $\rightarrow$  Functional isomer.

(ii) 
$$H_3C_2 - O - C_2H_5$$
 and  $H_3C - O - C_3H_7$ 

→ Metamers isomer.

(iii) 
$$H_3C-NH-C_3H_7$$
 and  $H_3C_2-NH-C_2H_5$ 

→ Metamerism isomer.

(iv) 
$$H_3C - CH_2 - CH = CH_2$$
 and  $H_3C - CH = CH - CH_3$ 

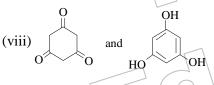
→ Position isomer.

→ Tautomerism isomer.

(vi) 
$$(CH_3)_3 CH$$
 and  $H_3C - CH_2 - CH_2 - CH_3$ 

 $\rightarrow$  Chain isomer.

→ Position isomer.



→ Tautomerism isomer.

**Q.**: Find out chiral centre in compound.

→ Four chiral carbon

Q.: Write down the name and structure of one isomer of each of the following compound.

(i) 
$$CH_2 = CH - CH_2 - CH_3$$

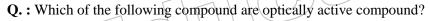
$$\rightarrow$$
 CH<sub>3</sub> - CH = CH - CH<sub>3</sub> (Position isomer)  
but-2-ene

(ii) 
$$CH_3 - CO - CH_3$$

$$\rightarrow$$
 CH<sub>3</sub> - CH<sub>2</sub> = CHO(Functional isomer)

(iv) 
$$CH_3 - O - CH_2 - CH_2 - CH_3$$

$$\rightarrow$$
 CH<sub>3</sub> -CH<sub>2</sub> -O -CH<sub>2</sub> -CH<sub>3</sub> (metamers isomer)  
1-ethoxy ethane



$$\sqrt{}$$

$$\sqrt{}$$

$$\rightarrow \qquad \text{(i)} \ \ \overset{\times}{\text{H}_{3}}\text{C-CH}_{2}\text{-CH}_{2}\text{-CH}_{2}\text{-CH}_{3}$$

(iv) 
$$\begin{vmatrix} & & & \\ & C - C - CH - C - C \\ \times & \times & \times & \times \end{vmatrix}$$



$$C - C - C - C$$

Br