02 Isomerism

Isomerism :

Two or more than two compounds having the same molecular formula but different physical/chemical properties or both properties are different are called isomers and this phenomenon is known as isomerism.

- **Isomerism**
  - **Structural isomerism**
    - Chain
    - Position
    - Functional
    - Metamerism
    - Tautomerism
  - **Stereoisomerism**
    - Configurational
      - Geometrical
      - Optical
    - Conformational

Structural Isomerism :

Compounds which have same molecular formula, but have different structures are called structural isomers.

Chain Isomerism (C.I.) :

The compounds which have same molecular formula, same functional group but length of carbon chain is different, show chain isomerism.

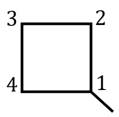
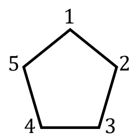
Illustration 1

(I) $\overset{1}{C}H_3—\overset{2}{C}H_2—\overset{3}{C}H_2—\overset{4}{C}H_3$ and $\overset{1}{C}H_3—\overset{2}{C}H(CH_3)—\overset{3}{C}H_3$

Butane (4C) — 2–Methyl propane (3C)

(II) $\overset{4}{C}H_3—\overset{3}{C}H_2—\overset{2}{C}H_2—\overset{1}{C}H_2—OH$ and $\overset{3}{C}H_3—\overset{2}{C}H(CH_3)—\overset{1}{C}H_2—OH$

1–Butanol (4C) — 2–Methyl–1–propanol (3C)

(III)  and 

Methylcyclobutane (4C) — Cyclopentane (5C)

Position Isomerism (P.I.) :

The compounds which have same molecular formula, same functional group, same parent carbon chain but different position of functional group or multiple bond or substituents, shows position isomerism.

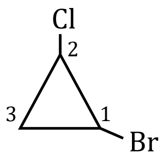
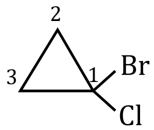
Illustration 2

(I) $\overset{1}{C}H_2=\overset{2}{C}H-\overset{3}{C}H_2-\overset{4}{C}H_3$ and $\overset{1}{C}H_3-\overset{2}{C}H=\overset{3}{C}H-\overset{4}{C}H_3$

But–1–ene — But–2–ene

(II) $\overset{4}{C}H_3-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}H_2-OH$ and $\overset{4}{C}H_3-\overset{3}{C}H_2-\underset{\underset{OH}{|}}{\overset{2}{C}H}-\overset{1}{C}H_3$

1–Butanol — 2–Butanol

(III)  and 

1-Bromo-2-chlorocyclopropane — 1-Bromo-1-chlorocyclopropane

Degree of Unsaturation/Double Bond Equivalent/Index of Hydrogen Deficiency :

D.U/D.B.E./I.H.D. = No. of π bond + No. of rings

If D.U. = 0 (No π bond/ring)

D.U. = 1 (1 π bond/1 ring)

D.U. = 2 (2 π bonds/2 rings/1 π bond + 1 ring/1 triple bond)

Formula

$$\mathbf{D.U.=(C+1)-\frac{(H+X-N)}{2}}$$

C ⇒ Number of carbon atoms **H ⇒ Number of hydrogen atoms**

X ⇒ Number of halogen atoms **N ⇒ Number of nitrogen atoms**

Illustration 3

(I) CH_3-CH_3 has D.U. =

(II) $CH_2=CH_2$ has D.U. =

(III) $CH\equiv CH$ has D.U. =

Solution:

(I) CH_3-CH_3 has D.U. = 0

(II) $CH_2=CH_2$ has D.U. = 1

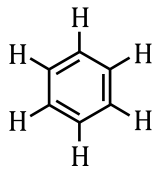
(III) $CH\equiv CH$ has D.U. = 2

Illustration 4

Find degree of unsaturation (D.U.) in-

(i) C_4H_8

(ii) Benzene



Benzene = C_6H_6

(iii) C_2H_5Cl

$CH_3—CH_2—Cl$

Solution:

(i) $D.U. = (4+1) - \frac{(8+0-0)}{2}$

D.U. = 5 – 4 = 1

(ii) $D.U. = (6+1) - \frac{(6+0-0)}{2}$

D.U. = 7 – 3 = 4

(iii) $D.U. = (2+1) - \frac{(5+1-0)}{2}$

D.U. = 3 – 3 = 0

BEGINNER'S BOX-1

1. Structures $CH_3–CH_2–CH=CH_2$ and $CH_3–\underset{\displaystyle CH_3}{\underset{|}{C}}=CH_2$ are :–

(1) Chain isomers (2) Position isomers

(3) Both chain & position isomers (4) Not isomers

CIS046

2. How many minimum carbons are required for Chain isomerism and Position isomerism in alkanes ?

(1) 4, 5 (2) 3, 5 (3) 4, 6 (4) 4, 4

CIS047

3. How many minimum carbons are required for Chain isomerism and Position isomerism in alkenes ?

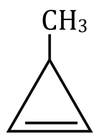
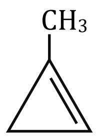
(1) 4, 5 (2) 3, 4 (3) 4, 4 (4) 5, 5

CIS048

4. How many minimum carbons are required for Chain isomerism and Position isomerism in alkynes ?

(1) 5, 4 (2) 5, 3 (3) 4, 6 (4) 4, 4

CIS049

5.  and  are

(1) Chain isomers (2) Position isomers (3) Hologues (4) Identical

CIS050

Functional Isomerism :

Compounds which have same molecular formula but different functional group, are functional group isomers.

Following compounds show Functional isomerism, as they have same molecular formula and different functional group.

(i) Alcohol and Ether $\longrightarrow CH_3-CH_2-OH$ and CH_3-O-CH_3

(ii) Aldehydes and Ketones $\longrightarrow CH_3-CH_2-\underset{\underset{O}{\|}}{C}-H$ and $CH_3-\underset{\underset{O}{\|}}{C}-CH_3$

(iii) Acids and Ester $\longrightarrow CH_3-\underset{\underset{O}{\|}}{C}-OH$ and $H-\underset{\underset{O}{\|}}{C}-O-CH_3$

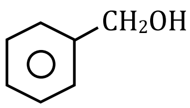
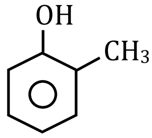
(iv) Cyanide and Isocyanide $\longrightarrow CH_3-CH_2-CH_2-CN$ and $CH_3-CH_2-CH_2-NC$

(v) Nitro and Nitrite $\longrightarrow CH_3-CH_2-N\genfrac{}{}{0pt}{}{\nearrow O}{\searrow O}$ and $CH_3-CH_2-O-N=O$

(vi) 1°, 2°, 3° Amines

(i) $CH_3-CH_2-CH_2-NH_2$ (ii) $CH_3-NH-CH_2-CH_3$ (iii) $CH_3-\underset{}{\overset{\overset{CH_3}{|}}{N}}-CH_3$

(vii) Alcoholic and Phenolic compounds (different chemical properties)

 and 

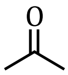
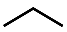
(viii) Alkyl halides do not show Functional isomerism due to different molecular formula.

BEGINNER'S BOX-2

1. Which of the following isomerism is not related to structural isomerism :-

(1) Position (2) Functional (3) Geometrical (4) Chain

CIS051

2.  and  CHO exhibit the isomerism :-

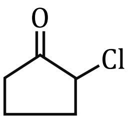
(1) Functional (2) Chain (3) Position (4) Tautomerism

CIS052

3. Which molecular formula does not exhibit position isomerism :-

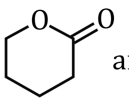
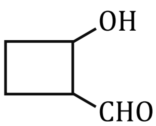
(1) C_5H_{12} (2) C_4H_8 (3) C_6H_{14} (4) C_5H_{10}

CIS053

4. DU for  is

(1) 2 (2) 3 (3) 4 (4) 5

CIS054

5.  and  are

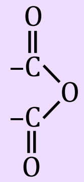
(1) Functional isomers (2) Position isomers
(3) Chain isomers (4) Not isomers

CIS055

Metamerism :

Compounds which have same molecular formula, same functional group but different alkyl groups attached to polyvalent functional group.

Polyvalent functional group [Which have more than one valency] are :

$-O-$, $-S-$, $-\underset{\underset{O}{\|}}{C}-$, $-\underset{\underset{O}{\|}}{C}-O-$, $-\underset{\underset{O}{\|}}{C}-NH-$, $-\underset{\underset{O}{\|}}{C}-\underset{|}{N}-$ $-NH-$, $-\underset{|}{N}-$, 

ester, 2° amide, 3° amide, 2° amine, 3° amine

Illustration 5

(I) $CH_3—O—CH_2—CH_2—CH_3$ and $CH_3—CH_2—O—CH_2—CH_3$ are metamers

(II) $CH_3—CH_2—NH—CH_2—CH_3$ and $CH_3—NH—CH_2—CH_2—CH_3$ are metamers

(III) $CH_3—NH—CH_2—CH_2—CH_2—CH_3$ and $CH_3-CH_2-NH-CH_2-CH_2-CH_3$ are metamers

(IV) $CH_3-\underset{\underset{O}{\|}}{C}-CH_2-CH_2-CH_2-CH_3$ and $CH_3-CH_2-\underset{\underset{O}{\|}}{C}-CH_2-CH_2-CH_3$ are metamers

Number of Structural Isomers :

(I) C_5H_{12} has three structural isomers:

$CH_3-CH_2-CH_2-CH_2-CH_3$ — **Pentane**

$CH_3-CH_2-\underset{\underset{CH_3}{|}}{CH}-CH_3$ — **2–Methylbutane**

$CH_3-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-CH_3$ — **2,2–Dimethylpropane**

(II) C_6H_{14} has 5 structural isomers:

(a) $CH_3CH_2CH_2CH_2CH_2CH_3$ — **Hexane**

(b) $CH_3-CH_2-CH_2-\underset{\underset{CH_3}{|}}{CH}-CH_3$ — **2–Methylpentane**

(c) $CH_3-CH_2-\underset{\underset{CH_3}{|}}{CH}-CH_2-CH_3$ — **3–Methylpentane**

(d) $CH_3-\underset{\underset{CH_3}{|}}{CH}-\underset{\underset{CH_3}{|}}{CH}-CH_3$ — **2,3–Dimethylbutane**

(e) $H_3C-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-CH_2-CH_3$ — **2,2–Dimethylbutane**

- (a–b), (a–c), (a–d), (a–e) (b–d), (b–e), (c–d), (c–e) ⟶ **Chain isomers**
- b–c, d–e ⟶ **Position isomers**

(III) $C_3H_6Cl_2$ has 4 isomers:

(a) $H_3C-CH_2-\overset{\overset{Cl}{|}}{CH}-Cl$

(b) $H_2\overset{\overset{Cl}{|}}{C}-CH_2-CH_2-Cl$

(c) $H_3C-\overset{\overset{Cl}{|}}{\underset{\underset{Cl}{|}}{C}}-CH_3$

(d) $H_2\overset{\overset{Cl}{|}}{C}-\underset{\underset{Cl}{|}}{CH}-CH_3$

(IV) Structural isomers of C_7H_{16} are 9.

1. → $CH_3-CH_2-CH_2-CH_2-CH_2-CH_2-CH_3$ **Heptane**

2. → $CH_3-CH_2-CH_2-CH_2-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_3$ **2-Methylhexane**

3. → $CH_3-CH_2-CH_2-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-CH_3$ **3-Methylhexane**

4. → $CH_3-CH_2-CH_2-\overset{\displaystyle CH_3}{\overset{|}{\underset{\displaystyle CH_3}{\underset{|}{C}}}}-CH_3$ **2,2-Dimethylpentane**

5. → $CH_3-CH_2-\overset{\displaystyle CH_3}{\overset{|}{\underset{\displaystyle CH_3}{\underset{|}{C}}}}-CH_2-CH_3$ **3,3-Dimethylpentane**

6. → $CH_3-\overset{\displaystyle CH_3}{\overset{|}{CH}}-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-CH_3$ **2,3-Dimethylpentane**

7. → $CH_3-\overset{\displaystyle CH_3}{\overset{|}{CH}}-CH_2-\overset{\displaystyle CH_3}{\overset{|}{CH}}-CH_3$ **2,4-Dimethylpentane**

8. → $CH_3-CH_2-\overset{\displaystyle CH_2-CH_3}{\overset{|}{CH}}-CH_2-CH_3$ **3-Ethylpentane**

9. → $CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-\overset{\displaystyle CH_3}{\overset{|}{\underset{\displaystyle CH_3}{\underset{|}{C}}}}-CH_3$ **2,2,3-Trimethylbutane (Triptane)**

(V) Number of structural isomers possible for the $C_4H_{10}O$ are 7.

$C_4H_{10}O \rightarrow$ D.U = 0 (no π bond), so only alcohols and ethers are formed.

Alcohol : $CH_3-CH_2-CH_2-CH_2-OH$ $\quad CH_3-CH_2-\underset{\displaystyle OH}{\underset{|}{CH}}-CH_3$

$CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_2-OH$ $\quad CH_3-\overset{\displaystyle CH_3}{\overset{|}{\underset{\displaystyle CH_3}{\underset{|}{C}}}}-OH$

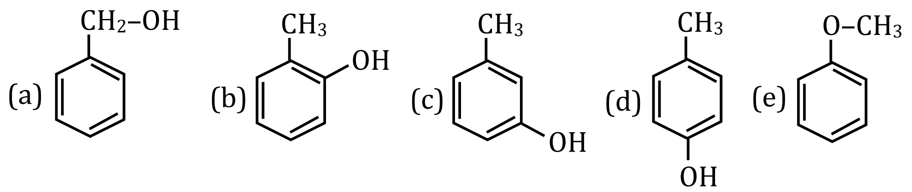
Ethers : $CH_3-O—CH_2—CH_2—CH_3$, $\quad C_2H_5-O-C_2H_5$, $CH_3-O-\underset{\displaystyle CH_3}{\underset{|}{CH}}-CH_3$

(VI) Determine number of Benzenoid isomers possible for the C_7H_8O

Solution:

Benzenoid isomers of C_7H_8O = 5

D.U. for C_7H_8O = 4 (1 ring + 3π bonds).



- **a-b, a-e – Functional isomers**
- **b,c,d – Position isomers**

Note : Alcoholic and phenolic groups are Functional isomers.

BEGINNER'S BOX-3

1. $CH_3–CH=CH–CH_3$ and $CH_3–\underset{\underset{CH_3}{|}}{C}=CH_2$ are :–

(1) Metamers (2) Chain Isomers
(3) Functional Isomers (4) Position Isomers

CIS056

2. $CH_3—CH_2—CH_2—\overset{\overset{O}{||}}{C}—OH$ and $CH_3—CH_2—\underset{\underset{OH}{|}}{CH}—\overset{\overset{O}{||}}{C}—H$ are

(1) Position isomers (2) Functional isomers
(3) Identical (4) Chain isomers

CIS057

3. $CH_3—S—CH_2—CH_3$ and $CH_3—CH_2—S—CH_3$ are –

(1) Ring-chain Isomers (2) Chain Isomers
(3) Functional Isomers (4) Identical

CIS058

4. $CH_3—CH_2—\overset{\overset{O}{||}}{C}—O—\overset{\overset{O}{||}}{C}—C_6H_5$ and $CH_3—\overset{\overset{O}{||}}{C}—O—\overset{\overset{O}{||}}{C}—CH_2—C_6H_5$ are –

(1) Metamers (2) Chain Isomers (3) Identical (4) Position Isomers

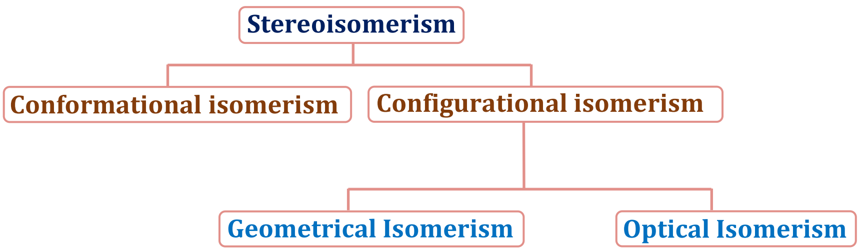
CIS059

5. Minimum number of C-atoms to show metamerism in ketone, is

(1) 4 (2) 3 (3) 5 (4) 6

CIS060

Stereoisomerism :



Compounds having same molecular formula, same structural formula but have different arrangement / configuration of atoms or groups in space are known as stereoisomers.

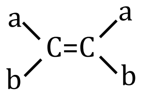
(A) Geometrical Isomerism (G.I.): Different configuration due to restricted rotation.

(i) Alkenes (>C=C<), oximes (>C=N—) and azo compounds [—N=N—] etc., show G.I. due to restricted rotation about double bond.

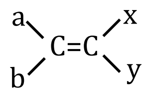
(ii) Cycloalkanes show G.I. due to restricted rotation about single bond in ring.

(1) Geometrical isomerism in acyclic molecules (around π bond)

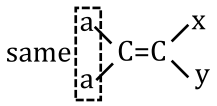
(a) Only those alkenes show G. I. in which "Each sp^2 carbon have different atoms or groups"



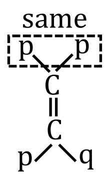
Geometrical isomerism possible



Geometrical isomerism possible

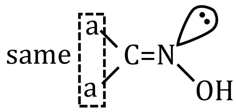


Geometrical isomerism not possible

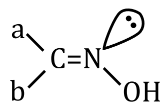


Geometrical isomerism not possible

(b) Oximes (>C=N̈–)

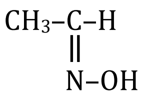


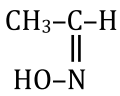
Geometrical isomerism not possible



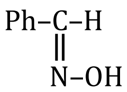
Geometrical isomerism possible

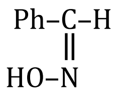
Example : Acetaldoximes has two Geometrical isomers –



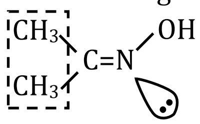


Example : Benzaldoxime (formed from Benzaldehyde)

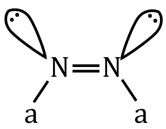




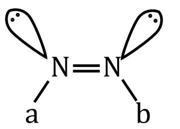
- Acetoneoxime does not show geometrical isomerism.

Example : same 

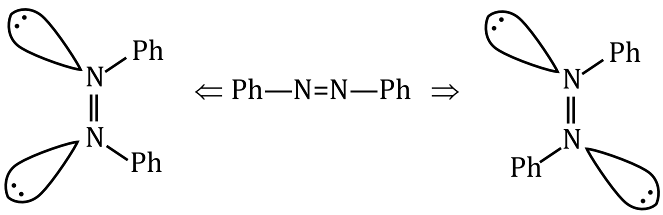
(c) Azo compounds (–N̈=N̈–)



Geometrical isomerism possible



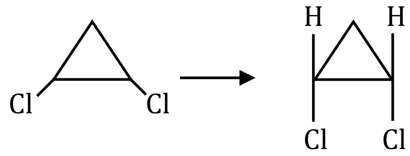
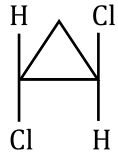
Geometrical isomerism possible



(2) Geometrical Isomerism in Cycloalkane

(a) Restricted rotation about single bond

(b) In cycloalkane system; atleast two sp^3 hybrid atom of ring individually must have different atoms / groups attached to it.

BEGINNER'S BOX-4

1. Which of the following shows Geometrical isomerism –

(a) $CH_3—CH_2—CH=N—OH$ (b) $H_2C=N—OH$

(c) $CH_3—\underset{\underset{N–OH}{||}}{C}—CH_3$ (d) $CH_3—\underset{\underset{N—OH}{||}}{C}—CH_2CH_3$

(1) a, c (2) c, d (3) a, d (4) b, c

CIS061

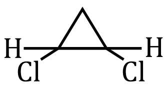
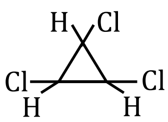
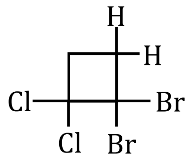
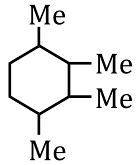
2. Which of the following show Geometrical isomerism –

(1) 1,1–Diphenyl–1–butene (2) 1,1–Diphenyl–2–butene

(3) 2,3–Dimethyl–2–butene (4) 3-Phenyl–1–butene

CIS062

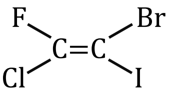
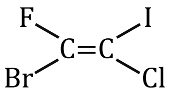
3. Which of the following show Geometrical isomerism –

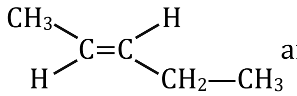
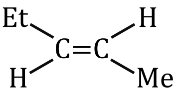
(a)  (b)  (c)  (d) 

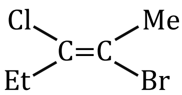
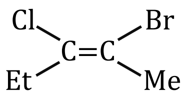
(1) a, b, d (2) a, c, d (3) a, b, c (4) b, c, d

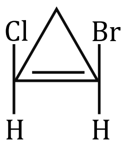
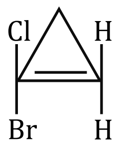
CIS063

4. Which are geometrical isomers?

(1)  and 

(2)  and 

(3)  and 

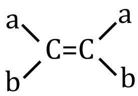
(4)  and 

CIS064

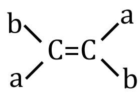
Nomenclature Systems of Geometrical Isomers with Configuration :

Cis–Trans configuration

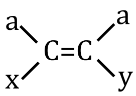
If same groups are at same side then cis and if same groups are at different side then trans.



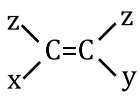
[Same groups, same side]
cis



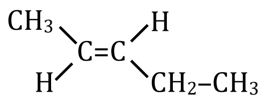
[Same groups different side]
trans

Ex. 

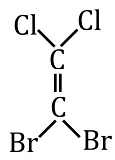
cis



cis

Ex. 

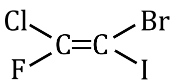
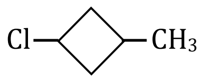
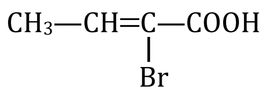
trans-2–Pentene



It does not show Geometrical isomerism
So no cis–trans

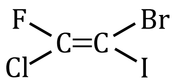
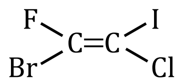
BEGINNER'S BOX-5

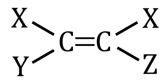
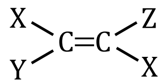
1. Which compound shows cis. trans isomerism ?

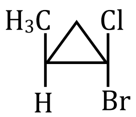
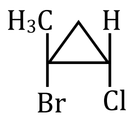
(1)  (2) $CH_3—CH=C(CH_3)_2$ (3)  (4) 

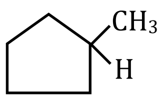
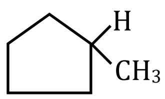
CIS065

2. Which are G.I. ?

(1)  and 

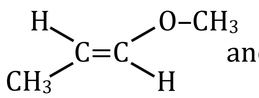
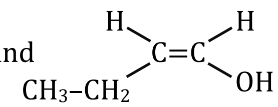
(2)  and 

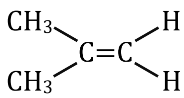
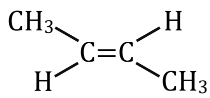
(3)  and 

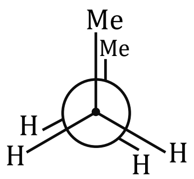
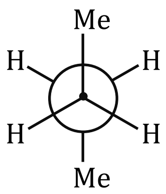
(4)  and 

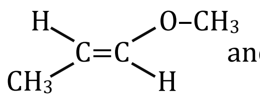
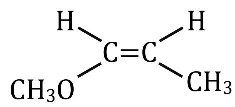
CIS066

3. Which are geometrical isomers?

(1)  and 

(2)  and 

(3)  and 

(4)  and 

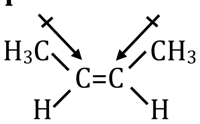
CIS067

1. Physical Properties of cis and Trans Alkenes :

(i) Dipole moment (μ):

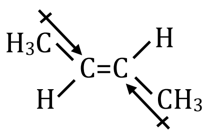
Dipole moment arises due to difference in EN and shape of the molecule.

Example : But-2-ene



cis-But-2-ene

($\mu \neq 0$)



trans-But-2-ene

($\mu = 0$)

Therefore, cis > trans (Dipole moment)

(ii) Polarity $\propto \mu$ (Dipole moment)

Generally, cis > trans

(iii) Boiling Point (B.P.) :

Boiling point depends on dipole-dipole interaction

Generally, cis molecule has higher boiling point than trans molecule due to more polarity.

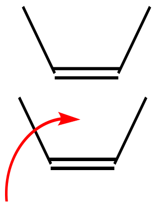
Boiling Point $\propto$ polarity $\propto$ dipole moment (μ)

(iv) Melting point :

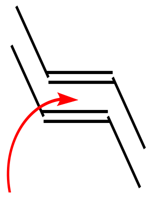
Melting point depends on packing efficiency.

Trans molecule has higher melting point than cis molecule as trans molecule is more symmetrical and shows high packing efficiency compared to cis form which has low packing efficiency.

Example :



More voids
(less packing efficiency)

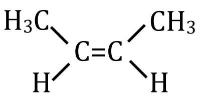


less voids
(more packing efficiency)

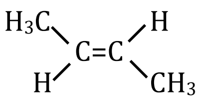
Melting point order: trans > cis

Note : Generally trans alkene is more stable than cis alkene because there is more repulsion between the group present on same side in cis alkene.

Example :



more repulsion



less repulsion

2. Calculation of Total Number of Geometrical Isomerism :

When compound is unsymmetrical $\Rightarrow$ No. of G.I. = 2^n

When compound is symmetrical $\Rightarrow$ No. of G.I. = $2^{n-1} + 2^{p-1}$

where $p = \dfrac{n}{2}$ (when n is even) and $p = \dfrac{n+1}{2}$ (when n is odd)

where n = no. of restricted rotatory system (double bond) about which G.I. is possible

Illustration 6

$CH_3-CH=CH-CH=CH-C_2H_5$

Solution:

n = 2

No. of geometrical isomers = $2^n = 2^2 = 4$

Illustration 7

$CH_3-CH=CH-CH=CH-CH_3$

Solution:

n = 2 (even)

$p = \dfrac{n}{2} = \dfrac{2}{2} = 1$

No. of geometrical isomers (symmetrical compound) = $2^{n-1} + 2^{p-1} = 2^{2-1} + 2^{1-1} = 3$

BEGINNER'S BOX-6

1. Calculate total number of geometrical isomers in the following compound

$CH_3-CH=CH-CH=CH-CH=CH-C_6H_5$

(1) 2 (2) 4 (3) 6 (4) 8

CIS068

2. The number of geometrical isomers in case of a compound with the structure $CH_3-CH=CH-CH=CH-C_2H_5$ is

(1) 4 (2) 3 (3) 2 (4) 5

CIS069

3. The number of geometrical Isomers possible for the compound Cl–CH=CH–CH=CH–CH=CH–Cl

(1) 8 (2) 10 (3) 6 (4) 4

CIS070

4. Choose the correct option for dipole moment order

(a) cis-1,2-dichloroethene (b) trans–1,2-dichloroethene

(1) a > b (2) b > a (3) a = b (4) None of these

CIS071

(B) Conformational Isomerism / Rotational Isomerism / Conformations :

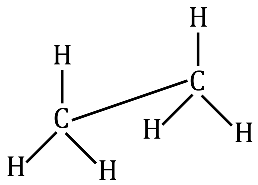
- The different arrangement of atoms in space that result from the rotation around single bond are called conformations. The phenomenon is called conformational isomerism.
- They cannot be isolated at room temperature from each other as they are interconvertible at room temperature.
- Bond length, bond angle are same in all the conformers.
- These are interconvertible forms of a same compound so there is no change in boiling point, melting point, dipole moment.
- There are infinite conformations of a compound
- If there are three continuous single bond present in a compound then it shows conformation.

Representations of tetrahedral carbon

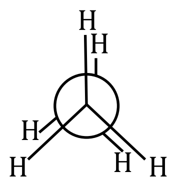
1. Sawhorse projection **2. Newman projection**

3. Wedge-dash projection **4. Fischer projection**

Saw horse projection

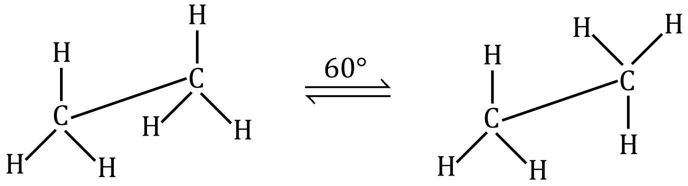


Newman projection



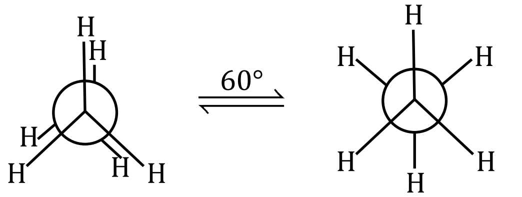
Conformations of Ethane [CH_3—CH_3] :

Saw horse projection



Eclipsed **Staggered**

Newman projection



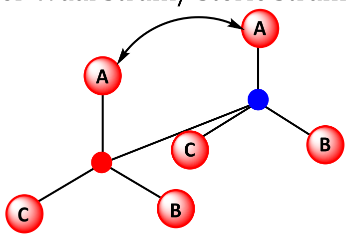
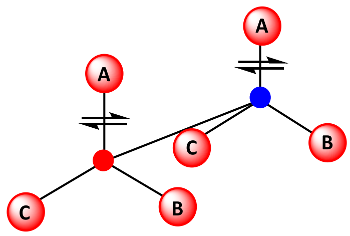
Eclipsed **Staggered**

Stability order : Staggered > Eclipsed

In ethane, staggered form is more stable than eclipsed form by 12.5 kJ/ mol

Some important terms:

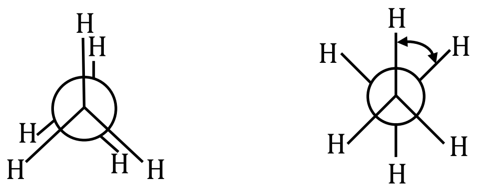
1. Types of Strain:

Van der Waal Strain / Steric strain	Torsional Strain
• When 2 non-bonded atoms or groups are brought close together then they repel each other. This type of repulsion is called van der Waal strain/ steric strain. 	• Repulsion between bond pair-bond pair electrons. 

2. Dihedral Angle/ Torsional Angle (θ):

Angle between two bonds of adjacent atoms.

Angle of rotation or angle of tortion or Dihedral angle



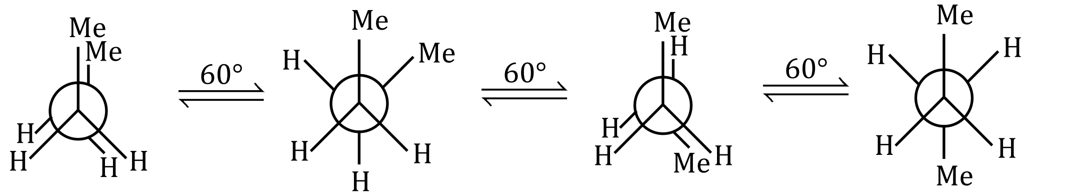
Newman's projections of ethane

Skew Form: There are infinite conformations between eclipsed and staggered forms known as skew form.

Dihedral Angle : Dihedral angle in eclipsed form of ethane is 0°.
Dihedral angle in staggered form of ethane is 60°.

Conformations of Butane :

$CH_3—CH_2—CH_2—CH_3$



Fully eclipsed (I) **Gauche (II)** **Partially eclipsed (III)** **Anti / Staggered (IV)**

I (Fully eclipsed form): In this form distance between two methyl groups is minimum so maximum repulsion or minimum stable.

IV (Anti or staggered): In this form distance between two methyl groups is maximum so minimum repulsion or maximum stable.

III (Gauche form): In this form the angle between two methyl groups is 60°

Stability order : IV > II > III > I

Energy order : I > III > II > IV

Note :

If staggered form is at 60° (in ethane) then it is not gauche form.

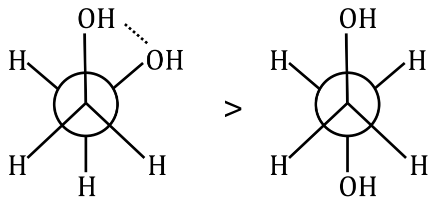
Special Cases:

It is not necessary that anti conformation is always more stable than gauche conformation.

$$\underset{OH}{CH_2}—\underset{Z}{CH_2}$$

Here Z= (–F, –COOH, –NH₂, –OH, –NO₂, –OCH₃ etc.)

Example : **Ethylene glycol** $\underset{OH}{CH_2}—\underset{OH}{CH_2}$



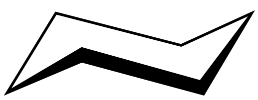
(Stability Order)

Gauche (Intra molecular H-bonding) **Anti**

More stable **Less stable**

Conformations of cyclohexane:

Boat

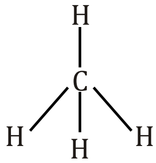


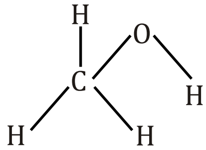
Chair

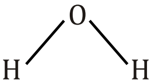
- Chair form is most stable conformation of cyclohexane.
- Stability Order: Chair > Boat

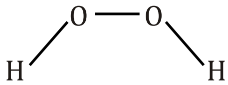
BEGINNER'S BOX-7

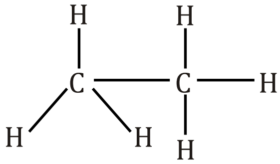
1. Which of the following shows conformational isomerism.

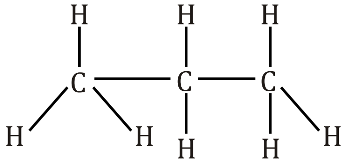
(a) 

(b) 

(c) 

(d) 

(e) 

(f) 

(1) b, c, e, f (2) a, b, c, f (3) b, c, d, e (4) b, d, e, f

CIS072

2. Most stable conformation of butane is :-

(1) Partial eclipsed (2) Eclipsed (3) Staggered (4) Gauche

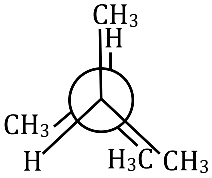
CIS073

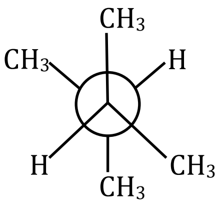
3. What is dihedral angle in staggered form of ethane :-

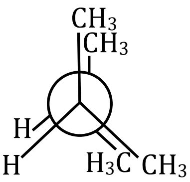
(1) 30° (2) 45° (3) 75° (4) 60°

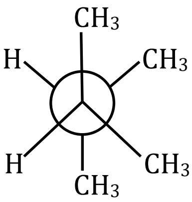
CIS074

4. In the given four conformational isomers which of the following has minimum torsional strain and minimum steric strain.

(1) 

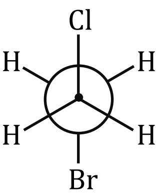
(2) 

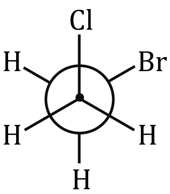
(3) 

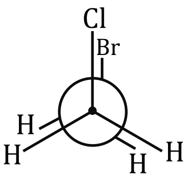
(4) 

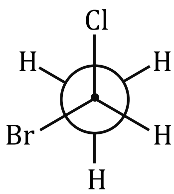
CIS075

5. Following are conformations of each other, except

(1) 

(2) 

(3) 

(4) 

CIS076

BEGINNER'S BOX — ANSWERS KEY

BEGINNER'S BOX-1	Que.	1	2	3	4	5
	Ans.	1	3	3	1	2

BEGINNER'S BOX-2	Que.	1	2	3	4	5
	Ans.	3	1	1	1	1

BEGINNER'S BOX-3	Que.	1	2	3	4	5
	Ans.	2	2	4	1	3

BEGINNER'S BOX-4	Que.	1	2	3	4
	Ans.	3	2	1	3

BEGINNER'S BOX-5	Que.	1	2	3
	Ans.	3	2	4

BEGINNER'S BOX-6	Que.	1	2	3	4
	Ans.	4	1	3	1

BEGINNER'S BOX-7	Que.	1	2	3	4	5
	Ans.	4	3	4	2	4