Symmetry Operations:

In order to study the symmetry of a molecule, certain operations such as rotation and reflection are performed and if by so doing, an arrangement is obtained which is indistinguishable from the original one, the operation is called a symmetry operation and the molecule is said to possess an element of symmetry defined by the operation performed.

The symmetry operation and symmetry element are thus inseparably linked* and often represented by the same symbols.

There are two types of symmetry operations─ (i) rotation and (ii) reflection (and a combination thereof).

1. Symmetry of First Kind:

Symmetry based solely on simple rotation is often called symmetry of the first kind

2. Symmetry of Second Kind:

The symmetry based on reflection or combination of rotation and reflection is known as symmetry of the second kind.

Element of Symmetry:

There are **four types** of element of symmetry ─

(i) Simple axis of symmetry or proper axis of symmetry or rotational axis of symmetry (C_n)

(ii) Plane of symmetry (σ)

(iii) Centre of symmetry or inversion centre (i)

(iv) Improper axis of symmetry or alternating axis of symmetry or rotation-reflection axis of symmetry. (S_n)

Simple axis of symmetry or proper axis of symmetry or rotational axis of symmetry (C_n)

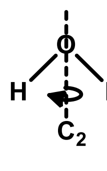
Definition: If a molecule is rotated around an appropriate imaginary axis by an angle of 360°/n and arrives at an arrangement which is indistinguishable from the original, the axis is called an n-fold simple or proper axis of symmetry or a simple axis of order 'n'.

The axis is designated C_n, and the operation is called a C_n operation.

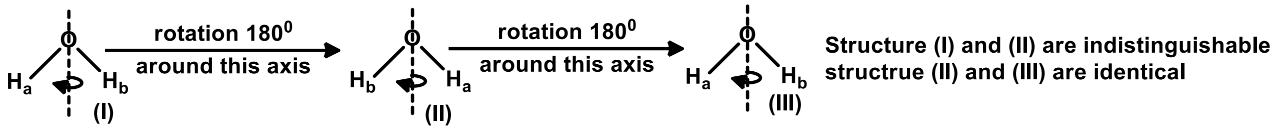
The operation if repeated 'n' times leads to an orientation identical with the original.

The order 'n' = 360/θ (θ=angle of rotation)

Example (i): Water molecule has one two-fold simple axis of symmetry ($1C_2$) bisecting the H—O—H angle



NB: The terms indistinguishable refers to any equivalent arrangement arrived at by exchanging similar atoms or groups while the term identical refers strictly to the original.



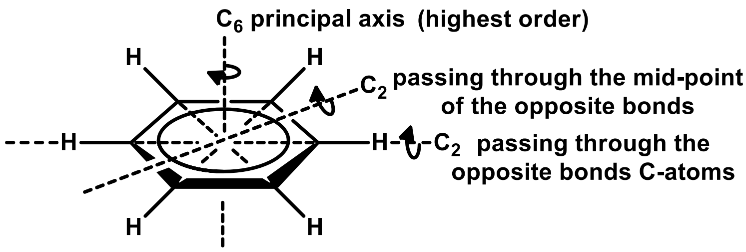
(ii) Chloroform ($CHCl_3$) has one C_3 axis of symmetry along H─C bond.

<u>Trivial Axis</u> (C_1) : A C_1─axis does not represent a rotational axis in true sense of definition, because rotation of any molecule (or object) around any axis by 360^0 leads to the original arrangement (identical structure). Therefore C_1─axis is known as trivial axis.

<u>Principal axis</u>: Simple axis of symmetry of the highest order is known as the principal axis. In the case where a molecule has several symmetry axes of the same order, the one passing through the greatest number of atoms is taken as the principal axis.

The principal axis is placed vertically, i.e., along the z-axis and it provides a good reference for describing other axes and planes.

Example: (i) Benzene has one C_6 axis of symmetry and $6C_2$ axis of symmetry among them C_6 axis is considered as principal axis as the order is highest 6.



(ii) Ethylene contains three C_2 axes (C_2─axes having same order) but the C_2─axis shown vertically passes through two C-atoms is considered as principal axis.

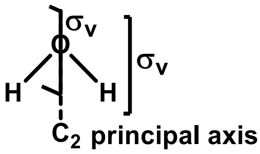
<u>Plane of symmetry</u> (σ):

Definition: A plane of symmetry is a plane which divides the molecule (or an object) into two halves which are mirror images of each other. The plane is called a σ–plane and the operation a σ–operation.

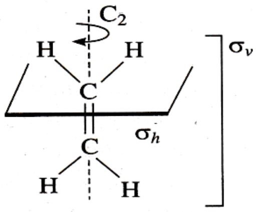
In other words, reflection of the two halves of the molecule across the plane (a reflection plane) gives a structure indistinguishable from the original.

Vertical plane of symmetry (σ_v): The σ-plane containing the principal axis is designated as σ_v.

Example: (i)

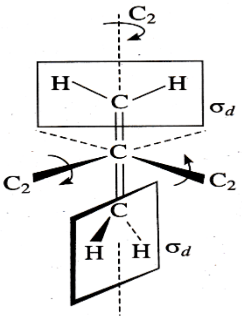


Horizontal plane of symmetry (σ_h): The σ-plane perpendicular to the principal axis designated as σ_h.



Diagonal plane of symmetry (σ_d): The σ-plane bisecting the angle between two C_2-axis of symmetry is known as diagonal plane of symmetry (σ_d)

Allene has two mutually perpendicular C_2 axis of symmetry passing through the central carbon atom and perpendicular to the C─C─C bond axis. The two H─C─H planes bisect the two C_2 axis so they are diagonal plane of symmetry (**σ_d**)



Two σ–operations are equivalent to an identity operation since they turn the molecule into the original.

<u>Centre of symmetry or inversion centre</u> (i):

Definition: A centre of symmetry or an inversion centre (i) is a point within a molecule such that if an atom (or point) is joined to it and the line extrapolated to an equal distance beyond, it encounters an equivalent atom (or point).

In other words, inversion of all atoms (or points) in the molecule through the point gives an arrangement indistinguishable from the original.

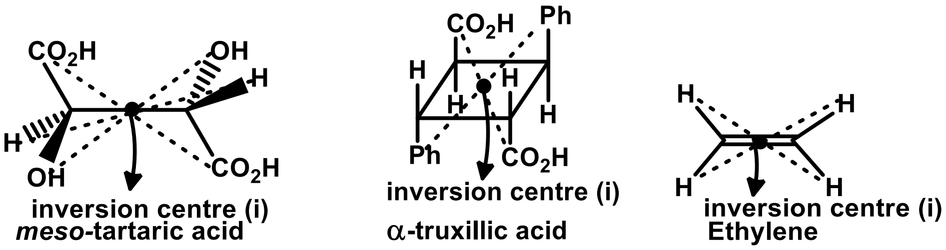
There can be only one inversion centre in a molecule.

Mathematically, for every atom with coordinates x, y, z there must be a similar atom with coordinates —x, —y, —z, the inversion centre being the origin of the coordinates.

Example:1. *meso*-tertaric acid has an inversion centre at the mid-point of the C─C bond.

2. α-truxillic acid has an inversion centre at the centre of the four membered ring.

3. Ethane has an inversion centre at the midpoint of the C=C



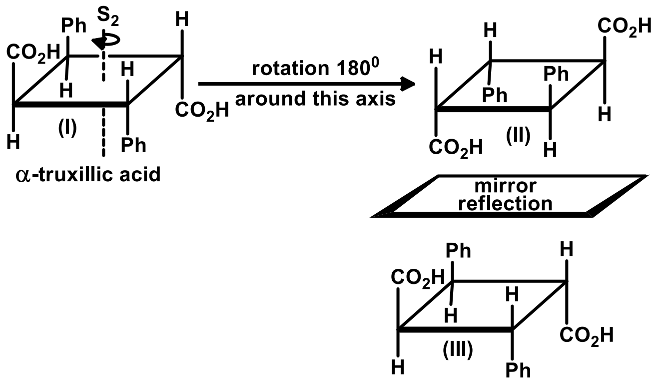
Improper axis of symmetry or alternating axis of symmetry or rotation-reflection axis of symmetry. (S_n)

Definition: An improper or an alternating or a rotation-reflection axis of symmetry of order ‘n’ (S_n) is an (n-fold) axis such that a rotation of 360°/n around it followed by reflection in a plane perpendicular to the axis generates a structure indistinguishable from the original.

The order of the two operations may be reversed without change in the result.

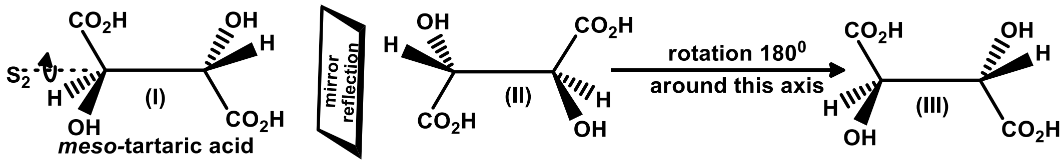
Q2.14. Define, with and example, the term ‘alternating axis of symmetry’ 1 **C.U. 2003**
2. 4. Define with an example each of the following terms:─ (iii) Alternating axis of symmetry **2 C.U. 1994**

Example 1.



The vertical axis in α-truxillic acid (I) is an S_2 axis since a rotation of 180° around it leads to the structure (II) which on being reflected across the plane of the ring, gives a structure (III) which is indistinguishable on the original (I).

Example 2. Conformation (I) of *meso*-tartaric acid on being similarly reflected in a plane placed at the centre of the C—C axis and at right angles to it gives an orientation (II) which on being rotated around the axis by 180° becomes indistinguishable (superposable) with the original (I). The conformation (I), therefore, contains an S_2 axis.



Q2. 2. Explain what is meant by simple axis of symmetry, plane of symmetry, centre of symmetry and alternating axis of symmetry. Give an example of each. 4 **C.U. 1991**

Show that S_1 is equivalent to σ and S_2 is equivalent to i.

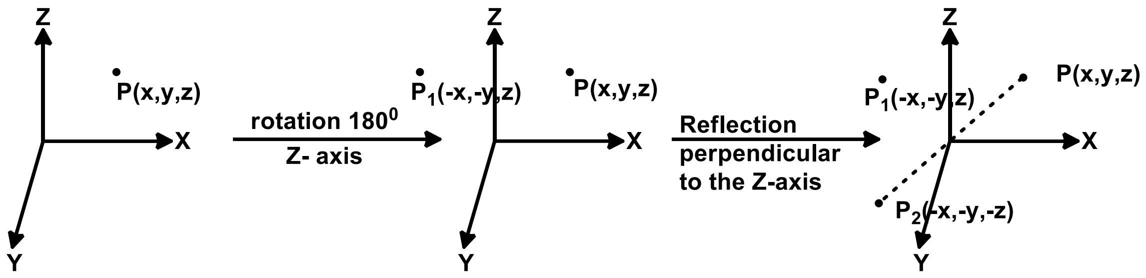
Q2.15. Justify the statement – ‘S_2’ and ‘ i ’ are equivalent operations. 2 **C.U. 2004**
Q2. 3. Indicate with reason whether each of the following statement is true or false: 2 **C.U. 1992**

(ii) One fold alternating axis of symmetry is equivalent to a plane of symmetry.

S_1 is the combination of C_1 and perpendicular σ-plane; $S_1 \equiv C_1.\sigma$

As the C_1 is an identity operation and rotation of any molecule or object by an angle of 360^0 gives identical arrangement, so S_1 is equivalent to σ-plane.

S_2 is a combination of the rotation of the molecule by 180^0 around an axis and then reflection in a plane perpendicular to the axis.



Let us consider a point P(x,y,z), now rotation around Z-axis by an angle of 180^0 gives the point P_1(-x,-y,z). Then reflection in a plane perpendicular to this axis, gives the point P_2(-x,-y,-z).

Thus S_2 operation brings about the exchange of like pairs of atoms or groups which are equidistant but in opposite directions from a centre (origin). i.e., their coordinates change from x, y, z to —x, —y, —z with respect to the centre (origin). This is precisely what an inversion operation (i) does. Thus an S_2 axis is equivalent to an inversion centre (i).

In fact, any axis passing through an inversion centre present in a molecule is an S_2 axis.

α-truxillic acid and *meso*-tartaric acid have S_2 axis of symmetry as well as an inversion centre.

Equivalent symmetry operations:

Different manipulations of elements of symmetry that transform molecules into indistinguishable and identical structures are called symmetry operations and operation of identity respectively. The element of identity is designated as **E or I.**

When a molecule is rotated n-times about a Cn axis we get identical molecule. i.e.

$$C_n^n \equiv E$$

$\sigma^2 \equiv E$, because reflection of a molecule in a plane, followed by reflection back again, returns all points of the molecule to the position from which they started, i.e., to the identical position.

$i^2 \equiv E$, because inversion of a molecule followed by second inversion results retention of the original orientation.

$S_n^n \equiv E$ (n=even), because one S_n, operation is equal to 1/n of a turn of a whole circle followed by reflection in a plane perpendicular to the S_n axis. Therefore, when 'n' times of S_n

rotation are carried out followed by reflection in a plane perpendicular to the axis, we get identical structure.

Again, $S_n^{2n} \equiv E$ (n = odd), because S_n^n operation amounts to reflection in a plane (σ) and so

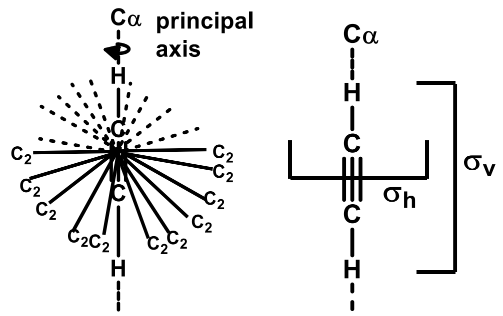
$$S_n^{2n} \equiv \sigma^2 \equiv E$$

<u>Symmetry elements of some molecules</u>:

1. Linear molecule : Acetylene (H─C≡C─H) has─

(i) One C_∞ axis along the H─C≡C─H bond (**principal axis**), and **(ii) infinite number of C_2** axis passing through the midpoint of the C≡C and perpendicular to the principal axis.

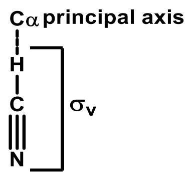
(iii) one σ_h passing through the midpoint of the C≡C and perpendicular to the principal axis**. (iv) Infinite number of σ_v** containing the principal axis.



Q2.9. Indicate symmetry elements present in (ii) acetylene.	1 **C.U. 2001**

2. Other linear molecule: H─C≡N or H─Cl has ─

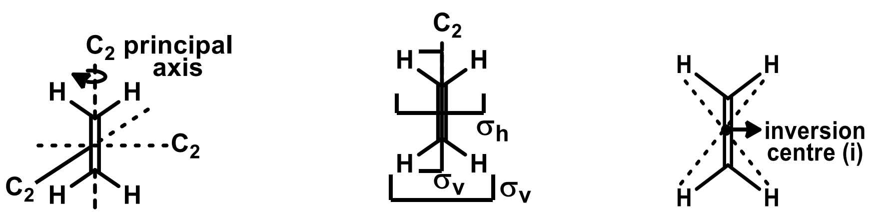
(i) One C_∞ axis along the H─C≡N bond (**principal axis**), and **(ii) Infinite number of σ_v** containing the principal axis.



3. Ethylene molecule (planar molecule): has ─ **(i) Three C_2 axis ─** one along the C=C bond (**principal axis**). One passing through the midpoint of the C=C and lying on the molecular plane and other perpendicular to the molecular plane.

(ii) Two σ_v. One **σ_v** lying on the molecular plane **other σ_v** passing through the C=C and perpendicular to the molecular plane. **One σ_h** passing through the midpoint of the C=C and perpendicular to the molecular plane.

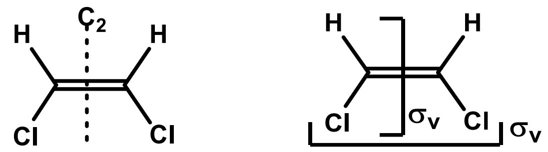
(iii) an inversion centre (i) at the midpoint of the C=C.



4. *cis*-1,2-Dichloroethylene molecule (planar molecule): has ─

(i) One C_2 axis of symmetry passing through the midpoint of the C=C and lying on the molecular plane.

(ii) Two σ_v. One σ_v lying on the molecular plane **other σ_v** passing through midpoint of the C=C and perpendicular to the molecular plane.



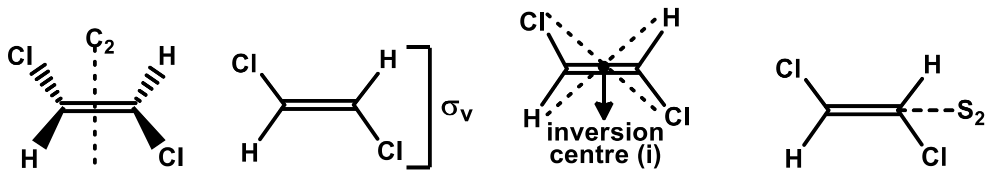
5. *trans*-1,2-Dichloroethylene molecule (planar molecule): has ─

(i) One C_2 axis of symmetry passing through the midpoint of the C=C and perpendicular to the molecular plane.

(ii) One σ_h passing through the molecular plane.

(iii) An inversion centre at the midpoint of the C=C

(iv) One S_2 axis of symmetry along the C=C and.



Q2.7., 2.13., Depict the symmetry elements of the following molecule in terms of σ and C_n

(ii) *trans*-1,2-dichloroethene 2 **C.U. 2000, 2003,**

Q2.11., 2.20, 2.21., Locate σ, i, Sn, if any in (*E*)-1,2-dichloroethene. 2 **C.U. 2002, 2010, 2012**

Ans: mentioned above.

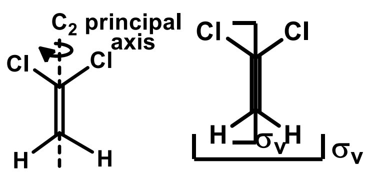
Q2.17. Indicate the symmetry elements present in (ii) 1,2-dibromoethene 1 **C.U. 2007**

Ans: The symmetry element should be indicated for both *cis*─ and *trans*─1,2-dibromoethene similar to *cis*- and *trans*-1,2-dichloroethene.

6. 1,1-Dichloroethylene molecule (planar molecule): has ─

(i) One C_2 axis of symmetry along the C=C bond and lying on the molecular plane.

(ii) Two σ_v. One σ_v lying on the molecular plane **other σ_v** passing through the C=C and perpendicular to the molecular plane.

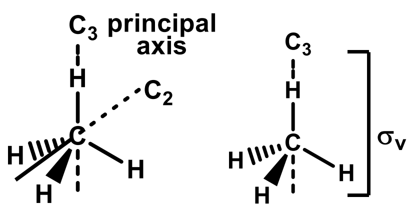


7. Methane molecule (CH_4) has─

(i) Four C_3 axes of symmetry along four H─C bond and **three C_2 axes of symmetry** passing through the carbon atom and bisecting H─C─H bond angle.

(ii) Three σ_v passing through three H─C─H planes

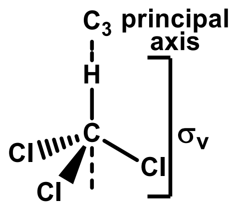
NB: Similar symmetry elements present in CCl_4.



7. Chloroform molecule ($CHCl_3$) has─

(i) One C_3 axis of symmetry along four H─C bond.

(ii) Three σ_v passing through three H─C─Cl planes

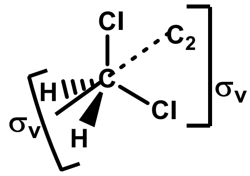


<u>NB</u>: Similarly, bromoform ($CHBr_3$), Iodoform(CHI_3), methyl chloride(CH_3Cl), NH_3(pyramidal), NR_3 and CH_3^- (pyramidal) have same element of symmetry.

Q2.9., 17., 22., Indicate symmetry elements present in (i) chloroform	1 **C.U. 2001, 2007, 2013**
Q2.16. Indicate the symmetry elements present in (i) bromoform,	1 **C.U. 2005**

8. Dichloromethane or methylenechloride (CH_2Cl_2): has─

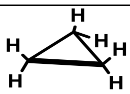
(i) One C_2 axis of symmetry passing through the C-atom and bisecting the H─C─H bond angle.



(i) Two σ_v passing through Cl─C─Cl planes and H─C─H planes.

Q2.20. Indicate the symmetry elements present, in each of (iv) dibromomethane. 2

<u>Ans:</u> Same as dichloromethane.

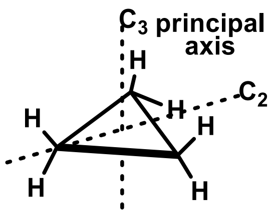
9. Cyclopropane  **(trigonal): has─**

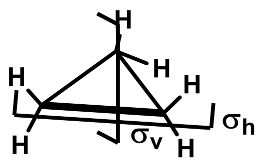
(i) One C_3 axis of symmetry passing through the centre of the ring and perpendicular to the ring.

And **three C_2 axis of symmetry** passing through an apex of the ring and midpoint of the opposite bonds

(ii) Three σ_v passing through an apex of the ring and bisecting the opposite bond.

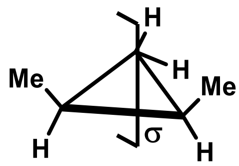
And **one σ_h** passing through the plane of the ring.





10. *Cis*-1,2-dimethyl cyclopropane: has─

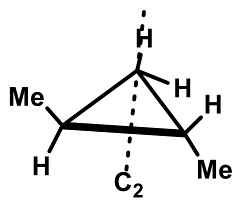
One σ-plane only no C_n axis of symmetry except C_1.



11. *Trans*-1,2-dimethyl cyclopropane: has─

Only one C_2 axis of symmetry passing through the methylene (CH_2) carbon and bisecting the opposite bond.

<u>NB</u>: It is chiral dissymmetric molecule.



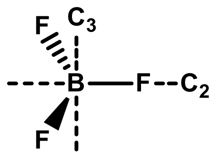
12. Planar trigonal molecules ─ BF_3, BCl_3, BBr_3, $^+CH_3$ etc.: have─

(i) One C_3 axis of symmetry passing through the B-atom and perpendicular to the molecular plane.

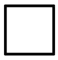
Three C_2 axis of symmetry along the three B─F bonds

(ii) Three σ_v passing through three B─F bonds and perpendicular to the molecular plane.

One σ_h passing the molecular plane.



NB: Similar symmetry elements are observed in 1,3,5-trichlorobenzene.

12. Cyclobutane (for planar structure):  has─

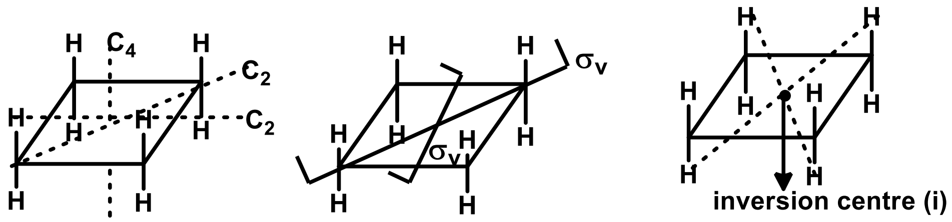
(i) One C_4 axis of symmetry passing through the centre of the ring and perpendicular to the ring. **Four C_2 axis of symmetry;** two C_2 passing through the opposite carbon atoms and two C_2 passing through the midpoint of the opposite bonds.

(ii) Two σ_d passing through the opposite carbon atoms and

Two σ_v passing through the midpoint of the opposite bonds.

One σ_h passing the plane of the ring.

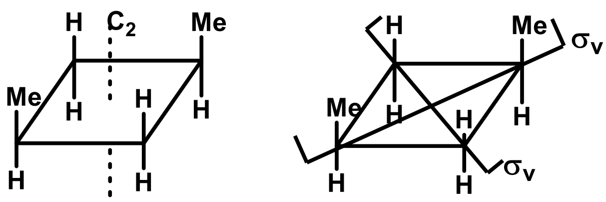
(iii) an inversion centre (i) at the centre of the ring.



13. *Cis*-1,3-dimethylcyclobutane: has─

(i) One C_2 axis of symmetry passing through the centre of the ring and perpendicular to the ring.

(ii) Two σ_v; one σ_v passing through the opposite methyl bearing carbon atoms and perpendicular to the ring. Other σ_v passing through the methylene (CH_2) carbon atoms and perpendicular to the ring.



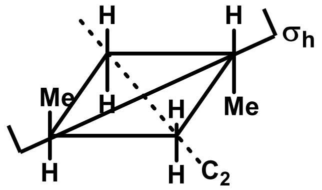
Q2.7. Depict the symmetry elements of the following molecules in terms of σ and C_n (i) cis-1,3-dimethylcyclobutane 1 **C.U. 2000**

14. *Trans*-1,3-dimethylcyclobutane: has─

(i) One C_2 axis of symmetry passing through the methylene (CH_2) carbon atoms.

(ii) One σ_h passing through the opposite methyl bearing carbon atoms and perpendicular to the ring.

(iii) an inversion centre (i) at the centre of the ring.



15. Benzene: has─

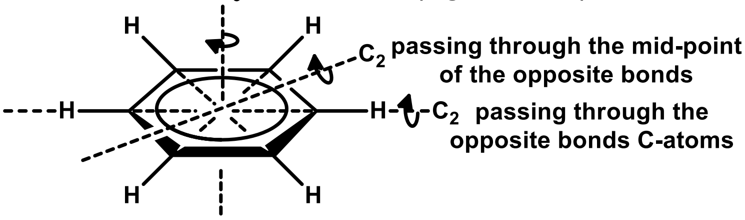
(i) one C_6 axis of symmetry passing through the centre of the ring and perpendicular to the ring.

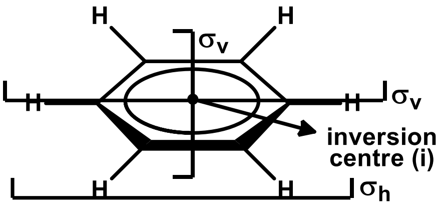
And $6C_2$ axis of symmetry lying on the molecular plane; three passing through the opposite carbon atoms and three passing through the midpoint of the opposite bonds.

(ii) One σ_h passing through the molecular plane.

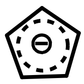
Six σ_v; three σ_v passing through the opposite carbon atoms and three passing through the midpoint of the opposite bonds they are perpendicular to the molecular plane.

(iii) an inversion centre (i) at the centre of the ring.





Q2. 3. Indicate with reason whether each of the following statement is true or false: 4 **C.U. 1992**
(i) Benzene has six C_2 and one C_6 simple axis of the symmetry.

16. Cyclopentadienyl anion:  **has-**

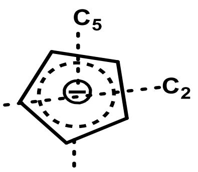
(i) one C_5 axis of symmetry passing through the centre of the ring and perpendicular to the ring.

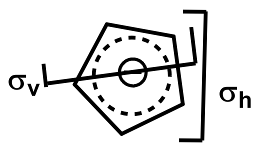
And $5C_2$ axis of symmetry lying on the molecular plane passing through each carbon atom and midpoint of the opposite bonds.

(ii) One σ_h passing through the molecular plane.

Five σ_v passing through each carbon atom and midpoint of the opposite bonds perpendicular to the molecular plane.

(iii) an inversion centre (i) at the centre of the ring.

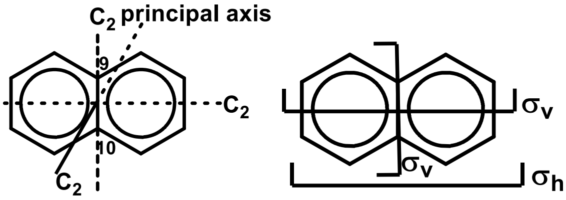




16. Naphthalene: has─

(i) Three C_2 axis of symmetry; one C_2 axis of symmetry passing through the C_9─C_{10} carbon atoms. **One C_2 axis of symmetry** perpendicular to the principal axis and lying on the molecular plane. **One C_2 axis of symmetry** passing through the midpoint of the C_9─C_{10} bond and perpendicular to the molecular plane.

(ii) One σ_h and **two σ_v; One σ_h** passing through the molecular plane. **One σ_v** passing through the midpoint of the C_9─C_{10} bond and perpendicular to the molecular plane. **One σ_v** passing through the C_9─C_{10} bond and perpendicular to the molecular plane.



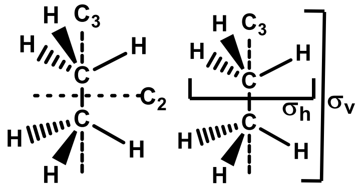
17. Ethane molecule: in (a) Eclipsed conformation: has-

(i) One C_3 axis of symmetry along the C-C bond

Three C_2 axis of symmetry passing through the midpoint of the C-C bond and perpendicular to the principal axis.

(ii) One σ_h passing through the midpoint of the C-C bond and perpendicular to the principal axis.

Three σ_v passing through the three H-C-C-H planes.



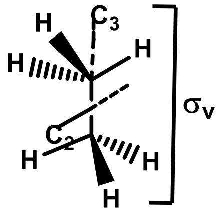
18. Ethane molecule: in (b) Staggered conformation: has-

(i) One C_3 axis of symmetry along the C-C bond

Three C_2 axis of symmetry passing through the midpoint of the C-C bond and perpendicular to the principal axis.

(ii) Three σ_v (or σ_d) passing through three H-C-C planes. Each of the planes bisects the angle between the two C_2-axis so they are also designated as **σ_d.**

(iii) an inversion centre (i) at the midpoint of C-C bond



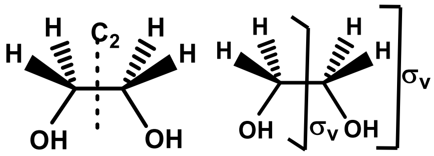
Q**2.20. Indicate the symmetry elements present, in each of the following molecules.**

(i) Staggered ethane, 2**C.U. 2010**

19. Ethylene glycol: in (a) *syn*-conformation: has-

(i) One C_2 axis of symmetry passing through the midpoint of the C-C bond and lying on O-C-C-O plane

(ii) Two σ_v; one passing through the midpoint of the O-C-C-O plane and other bisecting the C-C bond.

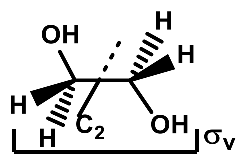


20. Ethylene glycol: in (a) *anti*-conformation: has-

(i) One C_2 axis of symmetry passing through the midpoint of the C-C bond and perpendicular to the O-C-C-O plane

(ii) One σ_h passing through the O-C-C-O plane

(iii) an inversion centre (i) at the midpoint of C-C bond



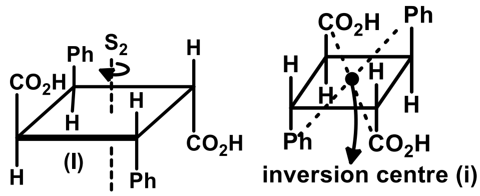
Q2.16. Indicate the symmetry elements present in (ii) anti-conformation of ethylene glycol.

2 **C.U. 2005**

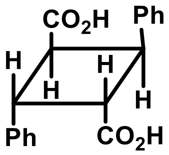
21. α-Truxillic acid: has─

(i) an inversion centre at the centre of the ring.

(ii) S_2 axis of symmetry passing through the centre of the ring and perpendicular to the ring.



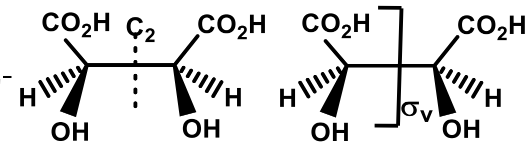
Q2.5. Indicate whether the following compounds possess any element of symmetry designates the element of symmetry present. 4 **C.U. 1996**

(i) 

22. *meso*-Tartaric acid (in eclipsed conformation): has─

(i) One C_2 axis of symmetry passing through the midpoint of the C-C bond and lying on the C-C-C-C plane

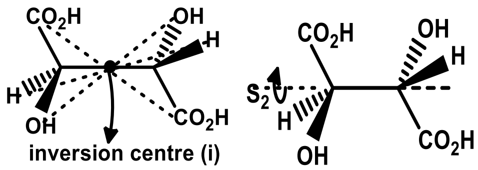
(ii) One σ_v passing through the midpoint of the C-C bond and perpendicular to C─C bond.



23. *meso*-Tartaric acid (in staggered conformation): has─

(i) an inversion centre at the midpoint of C─C bond

(ii) S_2 axis of symmetry along the C─C bond



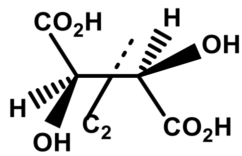
Q2.13. What are the symmetry elements present in (ii) meso-tartaric acid (in staggered conformation)? 1 **C.U. 2003**

Q2.22. Indicate the symmetry elements present in (ii) *meso*-tartaric acid (in staggered conformation). 2 **C.U. 2013**

24. *active*-Tartaric acid (in staggered conformation): has─

(i) Only one C_2 axis of symmetry along the C─C bond

<u>**NB**</u>**: It is chiral dissymmetric molecule**.

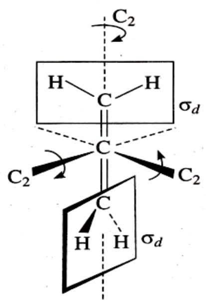


25. Allene ($H_2C{=}C{=}CH_2$): has─

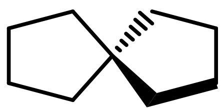
(i) Three C_2 axis of symmetry; one C_2 axis (principal axis) along the C=C=C bond. Other two mutually perpendicular C_2-axis passing through the central C-atom and perpendicular to principal axis.

(ii) Two σ_d containing two mutually perpendicular H─C─H planes.

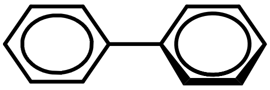
(iii) S_4 axis of symmetry collinear (along C=C=C bond) **with C_2 axis (principal axis).**



NB: Spiro[4,4]nonane, Biphenyl have the same elements of symmetry like allene



Spiro[4,4]nonane

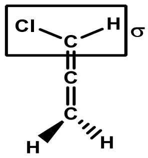


Biphenyl

Q2.21. Indicate the symmetry elements (C_n,σ) present in (i) Allene 1 **C.U. 2012**

26. 1-chloroallene ($ClCH=C=CH_2$): has─

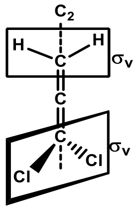
(i) One σ-plane containing H─C─Cl plane.



27. 1,1-dichloroallene ($Cl_2C=C=CH_2$): has─

(i) One C_2 axis of symmetry (principal axis) along the C=C=C bond.

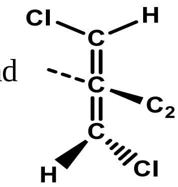
(ii) Two $σ_v$ containing two mutually perpendicular H─C─H and Cl─C─Cl planes.



28. 1,3-dichloroallene (ClCH=C=CHCl): has─

(i) One C_2 axis of symmetry passing through the central C-atom and perpendicular to C=C=C bond.

NB: Similar elements of symmetry is observed in 1,3-dimethyl allene

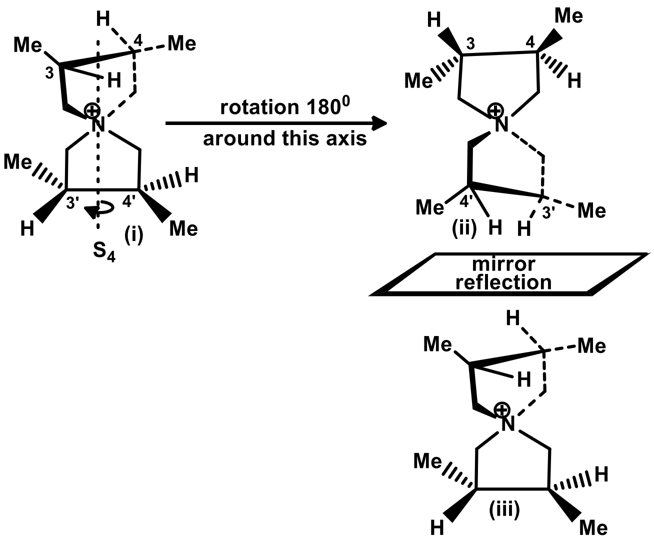


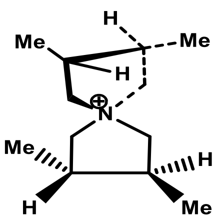
29. 3,4,3´,4´,-tetramethyl-spiro-(1,1´)-dipyrrolinidium cation: has─

(i) One C_2-axis of symmetry passing through the N-atom and containing the two five-membered ring.

(ii)S_4-alternating axis of symmetry collinear with C_2

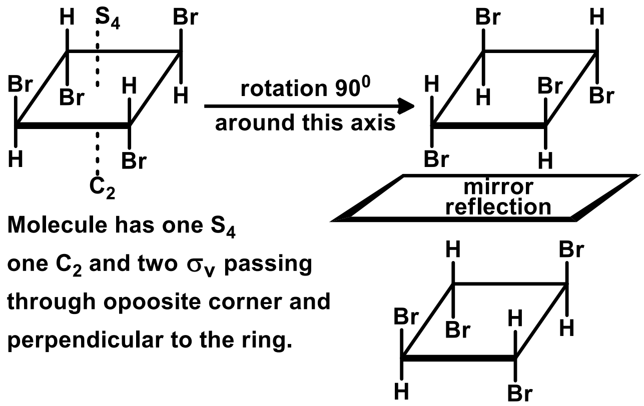
NB: This is optically inactive molecule.



Q 2.5. Indicate whether the following compounds possess any element of symmetry designates the element of symmetry present. 1 **C.U. 1996**    (ii)   **Q 2.18. Give an example of a molecule possessing four-fold alternating axis of symmetry and**

explain. 2 **C.U. 2007**

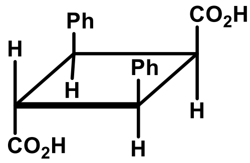
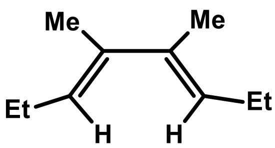
<u>Ans</u>: Example: 29 Or



Q2.24. Give examples which corroborate the following facts: (iii)A molecule having only S_4 as element of symmetry. 1 **C.U. 2015**

<u>Ans</u>: Example 29 only.

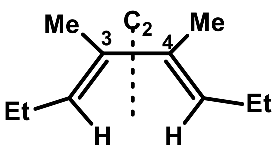
Q 2.5. Indicate whether the following compounds possess any element of symmetry designates the element of symmetry present. 1+1 **C.U. 1996**

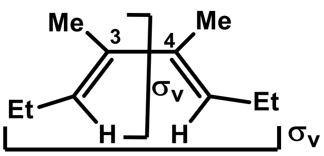
(iii)  (iv) 

Ans: (iii) It has **one σ-plane** passing through the –CO_2H bearing carbon atoms and perpendicular to the ring.

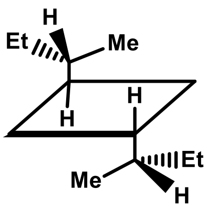
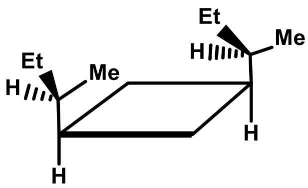
(iv) It has— **one C_2—axis of symmetry** passing through the midpoint of C_4—C_5 bond and lying on the molecular plane.

It has **two σ_v;** one passing through the molecular plane and other passing through the midpoint of C_4—C_5 bond and perpendicular to the molecular plane.





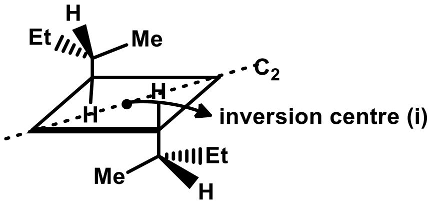
Q2.6. Indicate the elements of symmetry, if any, present in the following molecules.

(i)  (ii)  2 **C.U. 1998**

<u>Ans</u>: The two chiral groups are constitutionally and configurationally alike.

The compound (i) has **one C_2—axis of symmetry** passing through the methylene (CH_2) carbon atoms and a σ_h passing through the chiral groups and perpendicular to the ring.

It has **an inversion centre (i)** at the centre of the ring.



Compound (ii) has **one C_2—axis of symmetry** passing through the centre of the ring and perpendicular to the ring.

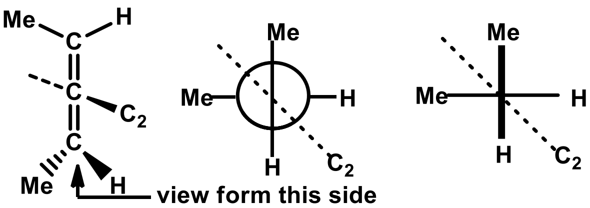
It has **two σ_v;** one passing through the methylene (CH_2) carbon atoms and perpendicular to the ring and other passing through the chiral groups and perpendicular to the ring.

It has **an inversion centre (i)** at the centre of the ring.

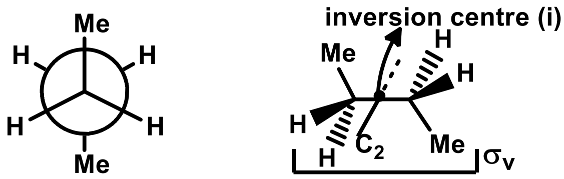
Q2.12. Give an example of an optically active compound possessing a C_2- axis. Indicate the axis. 1 **C.U. 2002**

Q2.23. Find out the Symmetry elements present in the following: (i) penta-2,3-diene (ii) most stable conformer of n-butane. 2 **C.U. 2014**

<u>**Ans**</u>: (i) it has **One C_2 axis of symmetry** passing through the central C-atom and perpendicular to C=C=C bond.



(ii) The most stable conformer of n-butane is anti-conformation.



It has (a) One C_2 axis of symmetry passing through the midpoint of the C-C bond and perpendicular to the C-C-C-C plane

(b) One σ_h passing through the O-C-C-O plane

(c) an inversion centre (i) at the midpoint of C-C bond

<u>Symmetry Number</u> (σ): It is defined as the number of equivalent or indistinguishable but non-identical orientations into which a molecule can be turned by simple rigid rotation i.e. rotation of the molecule as a whole around an axis or axes.

Q2.10. What is meant by symmetry number?	1 **C.U. 2001**

This is another symmetry parameter. The symmetry number is important since it is related to the entropy of a molecule. **The entropy contribution due to symmetry = ─R.lnσ**

The number of indistinguishable arrangement of first C_n axis of symmetry = n; for other C_n axis it is (n-1) (for this we have to subtract the identity (E).

So the symmetry number of first C_n axis of symmetry (σ) = n

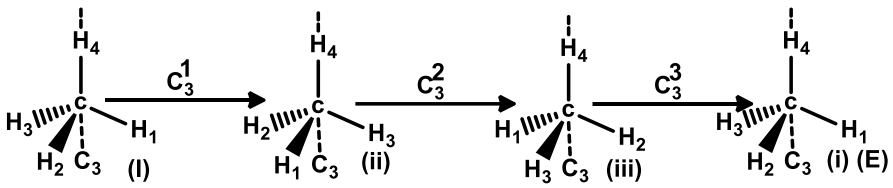
For other C_n axis σ = (n-1)

1. Symmetry Number of Methane:

Methane or any symmetrical molecule has **symmetry number σ=12**

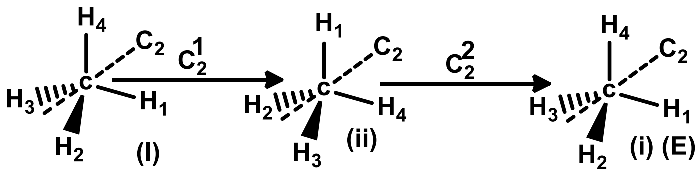
Methane has $4C_3$ axis and $3C_2$ axis of symmetry.

For 1st C_3 axis of symmetry the number of indistinguishable arrangement or symmetry number = $C_3^1, C_3^2, C_3^3 \equiv E$ = 3



For other three C_3 axes , symmetry number (σ) = [C_3^1, C_3^2, ~~$C_3^3 \equiv E$~~] X 3= 2X 3= 6

For other three C_2 axes , symmetry number (σ) = [C_2^1, ~~$C_2^2 \equiv E$~~] X 3= 1X 3= 3



So the Symmetry number of methane (σ)= 3+6+3=12

2. Symmetry number of benzene:

Benzene has one C_6 axis (principal axis) and six C_2 axes of symmetry

For one C_6 axes , symmetry number (σ) = [$C_6^1, C_6^2, C_6^3, C_6^4, C_6^5, C_6^6 \equiv E$] X 1= 6X 1= 6

For other six C_2 axes , symmetry number (σ) = [C_2^1, ~~$C_2^2 \equiv E$~~] X 6= 1X 6= 6

So the Symmetry number of methane (σ)= 6+6=12

Q2.10. Find out the symmetry number of benzene.	1 **C.U. 2001**