STEREOCHEMISTRY

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Semester I
Lecture 8

Outline

- An introduction to stereochemistry
- Isomers
- Classification of isomers
- Structural isomers
- Stereoisomers
- Conformational isomers
- Visualization of conformers
- Configurational isomers
- Chirality

Objectives

- Our main aim is to understand different classes of isomers, various methods to visualize them, and concept of chirality

An introduction to Stereochemistry

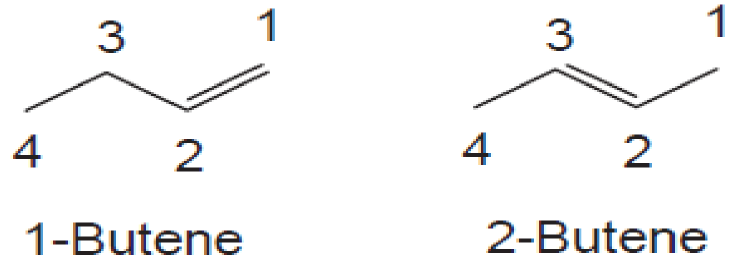
- ❖Stereochemistry is the study of three-dimensional arrangements of atoms and molecules and the effect of this on chemical properties.
- ❖It is the three-dimensional chemistry of the molecules.
- ❖Stereoisomers are compounds that have the same structural formula in terms of order of attachment but differ in arrangements of the atoms in space.

Isomerism

❖Compounds with the same molecular formula but different structures are called isomers.

❖For example, 1-butene and 2-butene have the same molecular formula, C_4H_8, but structurally they are different because of the different positions of the double bond.

❖There are two types of isomers: constitutional isomers and stereoisomers.



Classification of isomers

1 . **Structural Isomers or Constitutional isomers**

- Positional isomers
- Chain Isomers
- Metamerism
- Functional Isomers

2 . **Stereoisomers**

- Conformational Isomers
- Configurational Isomers
  - *a. Optical isomers*
  - *b. Geometrical Isomers (cis-trans & E-Z nomenclature)*

Structural Isomers

- Structural Isomers are isomers which have the same molecular formula but differ in their structures.
- Structural isomers show a difference in their physical properties like melting points, boiling points etc.

Position Isomers: Position Isomers are isomers which show difference in the point of attachment of the functional group to the main carbon chain, for example 1-butanol, $CH_3CH_2CH_2CH_2OH$ and 2-butanol, $CH_3CH(OH)CH_2CH_3$

Chain Isomers: Chain Isomers differ in the structure of their chain for example:

n-butane, $CH_3CH_2CH_2CH_3$

Isobutane, $CH_3CH(CH_3)_2$

Metamerism: Metamers are isomers especially found in the class of ethers. Metamers have different alkyl groups attached on either side of oxygen in the ether molecule for example

Methyl propyl ether, $CH_3OCH_2CH_2CH_3$ and Diethyl ether, $CH_3CH_2OCH_2CH_3$

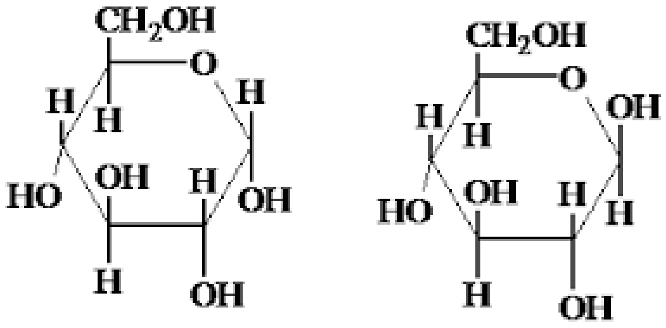
Functional Isomers: Functional Isomers are isomers that differ in the functional groups attached to the main carbon chain for example:

Ethylalcohol, CH_3CH_2OH

Dimethyl ether, CH_3OCH_3.

Stereoisomers

- Stereoisomers are compounds where the atoms are connected in the same order but with different geometries.
- They differ in the three-dimensional arrangements of groups or atoms in space.
- Example: α-glucose and β-glucose
- In α-glucose and β-glucose, the atoms are connected in the same order but three dimensional presentation of the hydroxyl group at C-1 is different, so these are stereoisomers .



alpha-glucose beta-glucose

Conformational isomers

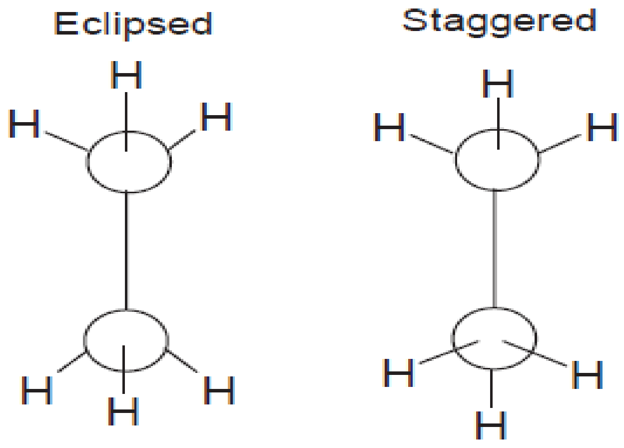
- Atoms with in a molecule move relative one another by rotation around single bonds. Such rotation of covalent bond gives rise to different conformations of a compound.
- Each structure is called a conformer or conformational isomer.

◦ ***Example 1***:

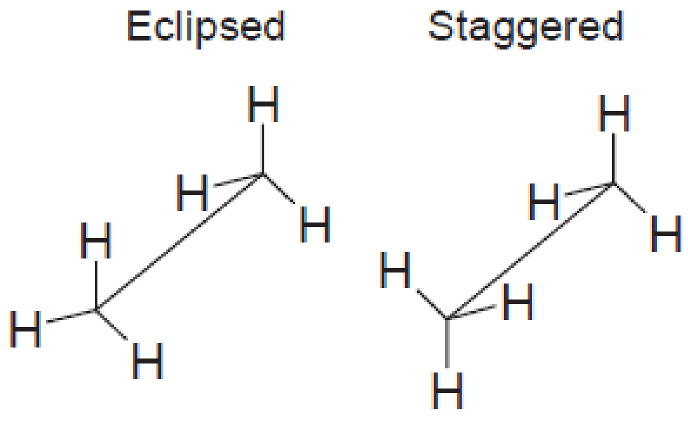
- Conformational isomerism can be presented by simple example of ethane (C_2H_6) .
- Ethane can exist as an infinite number of conformers by the rotation of the C-C bond. Ethane has two Sp^3–hybridized carbon atoms and tetrahedral angle of 109.5°.

Visualization of conformers

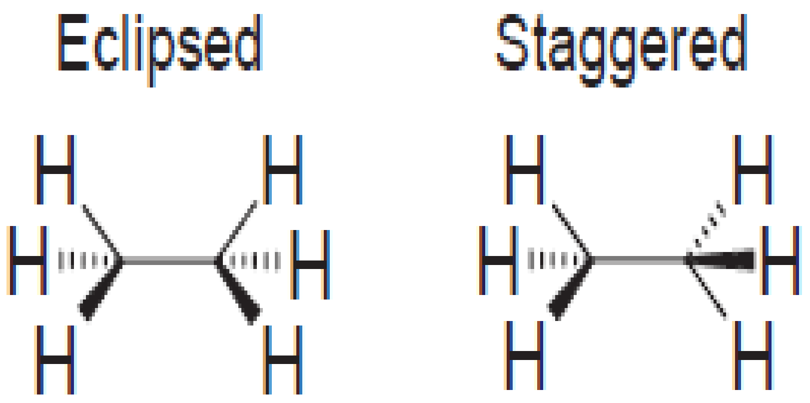
- There are four conventional methods for visualization of three-dimensional structures on paper.
- These are the ball and stick method, the sawhorse method, the wedge and broken line method and the Newman projection method.
- Using these methods, the staggered and eclipsed conformers of ethane can be drawn as follows.



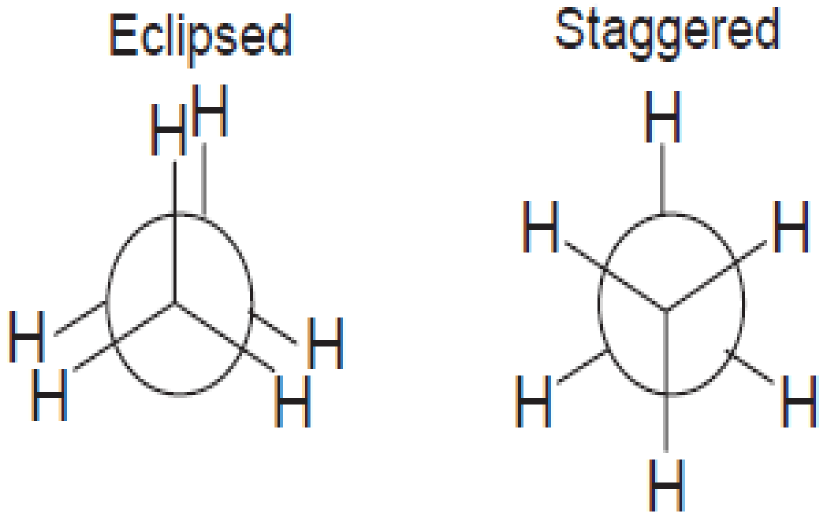
Ball and stick method



Sawhorse method



Wedge and broken line method



Newman projection method

➢ Staggered and eclipsed conformers

- In the staggered conformation, the H atoms are as far apart as possible. This reduces repulsive forces between them.
- This is why staggered conformers are stable. In the eclipsed conformation, H atoms are closest together.
- This gives higher repulsive forces between them. As a result, eclipsed conformers are unstable.
- At any moment, more molecules will be in staggered form than any other conformation.

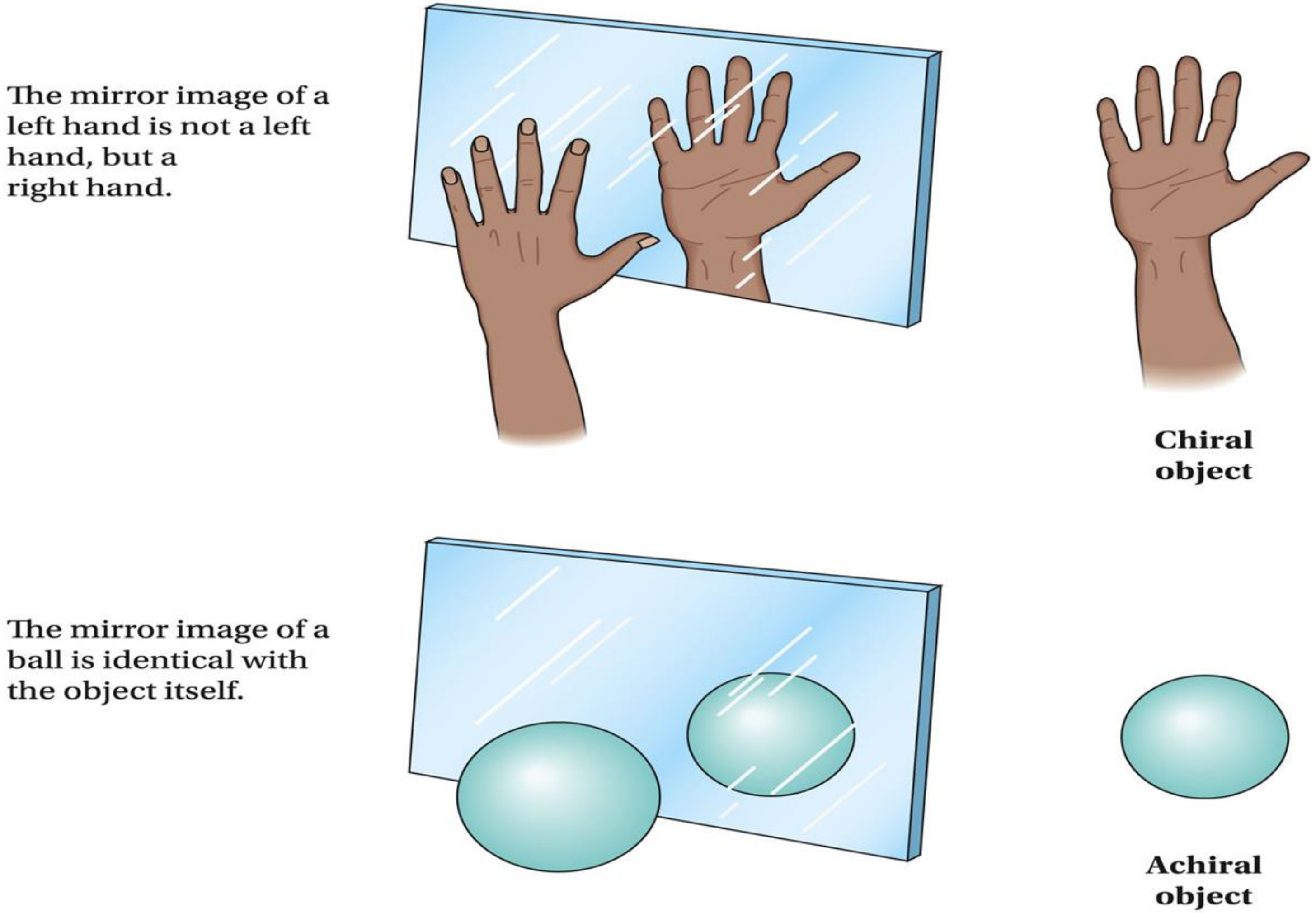
Configurational isomers

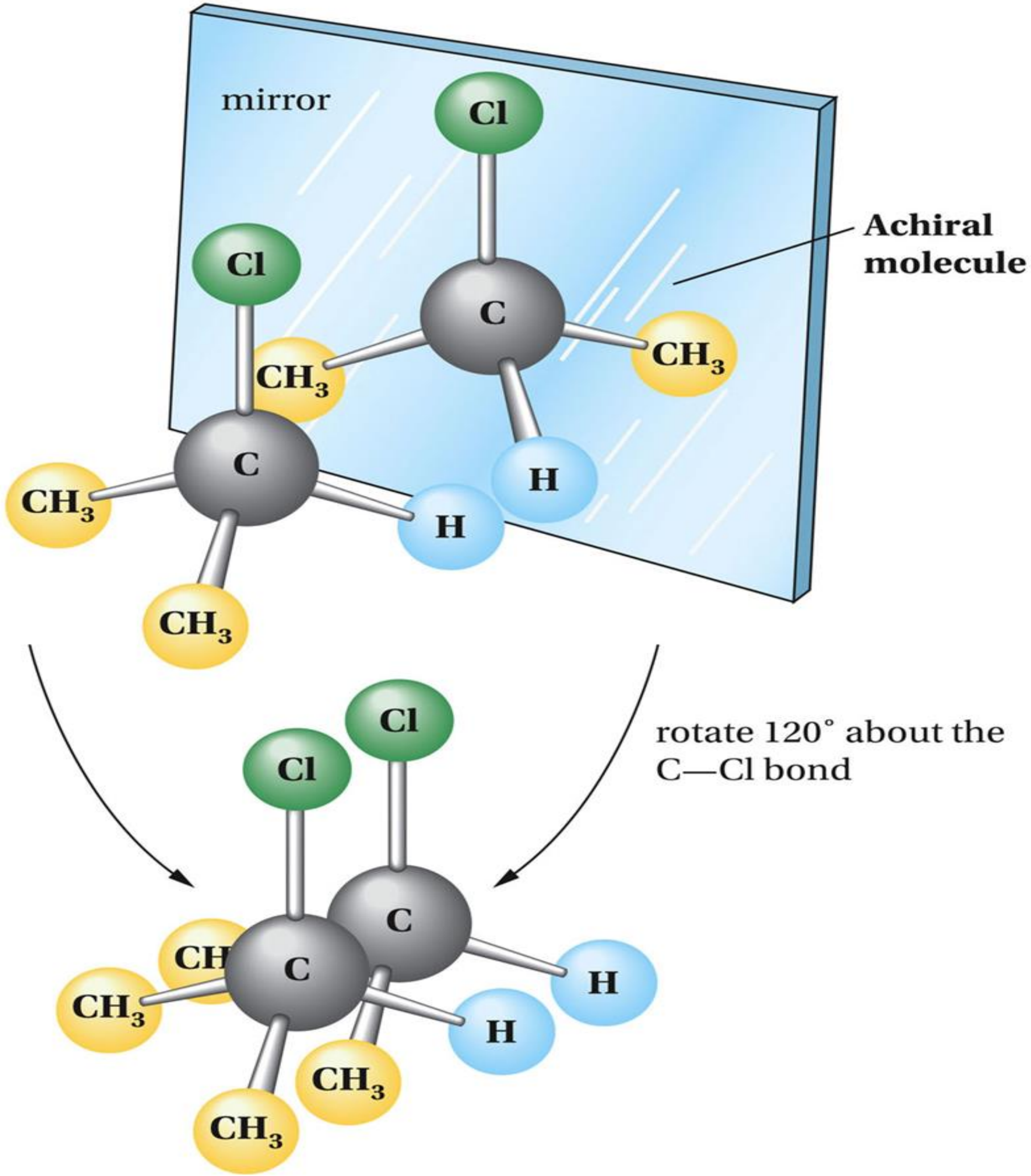
- Configurational isomers differ from each other only in the arrangement of their atoms in space and cannot be converted from one into another by rotations about single bonds within the molecules.
- Here carbon atoms are bound to four different substituents.

Chirality

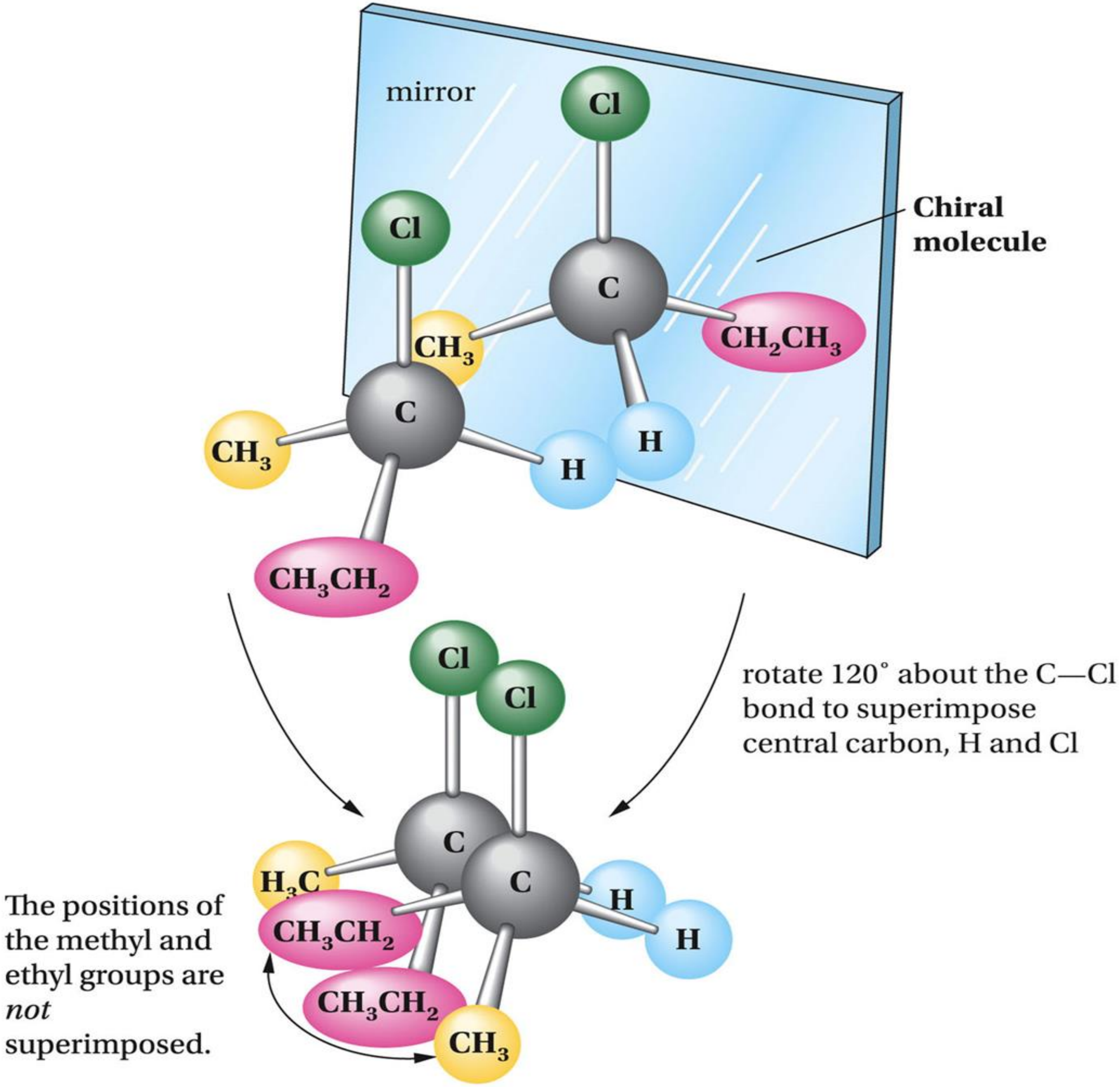
- A molecule is considered chiral if there exist another molecule that is of identical composition of atoms, but which is arranged in a non-superimposable mirror image.
- The presence of an asymmetric carbon atom is often the feature that causes chirality in molecules.

Mirror-image relationship of chiral and achiral objects





mirror
Cl
Cl
C
C
CH_3
CH_3
CH_3
CH_3
H
H
Achiral molecule
rotate 120° about the C—Cl bond
Cl
Cl
C
C
CH_3
CH_3
CH_3
H
H


mirror
Chiral
molecule
Cl
C
CH_3
H
CH_3CH_2
CH_2CH_3
rotate 120° about the C—Cl
bond to superimpose
central carbon, H and Cl
H_3C
The positions of
the methyl and
ethyl groups are
not
superimposed.

- Many compounds that occur in living organisms are chiral.
  - **Examples**: Carbohydrates and Proteins

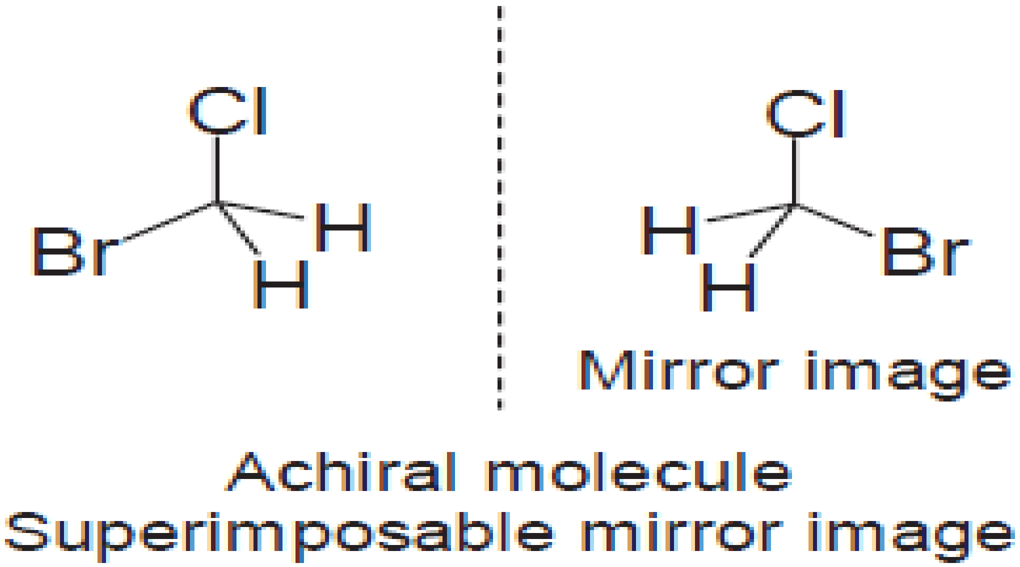
Chiral carbon
Four different groups/atoms present

Achiral carbon
At least two same groups/atoms (**Z**) present

❖When two or more atoms or functional groups are same, the carbon is called achiral.

❖In achiral molecules the compound and its mirror image are the same means they can be superimposed.

Example:



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Thank you