

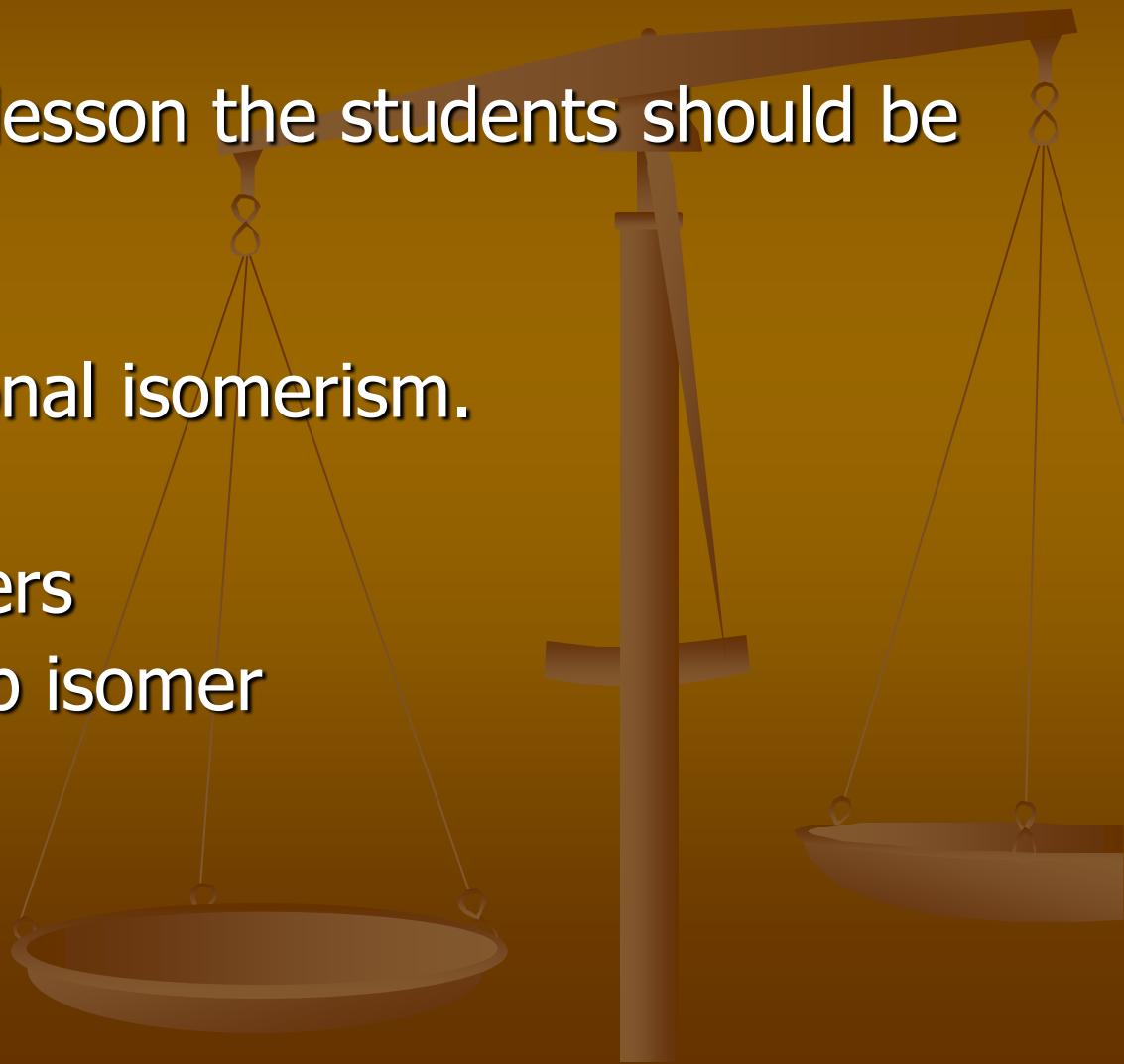
Lecture 4:

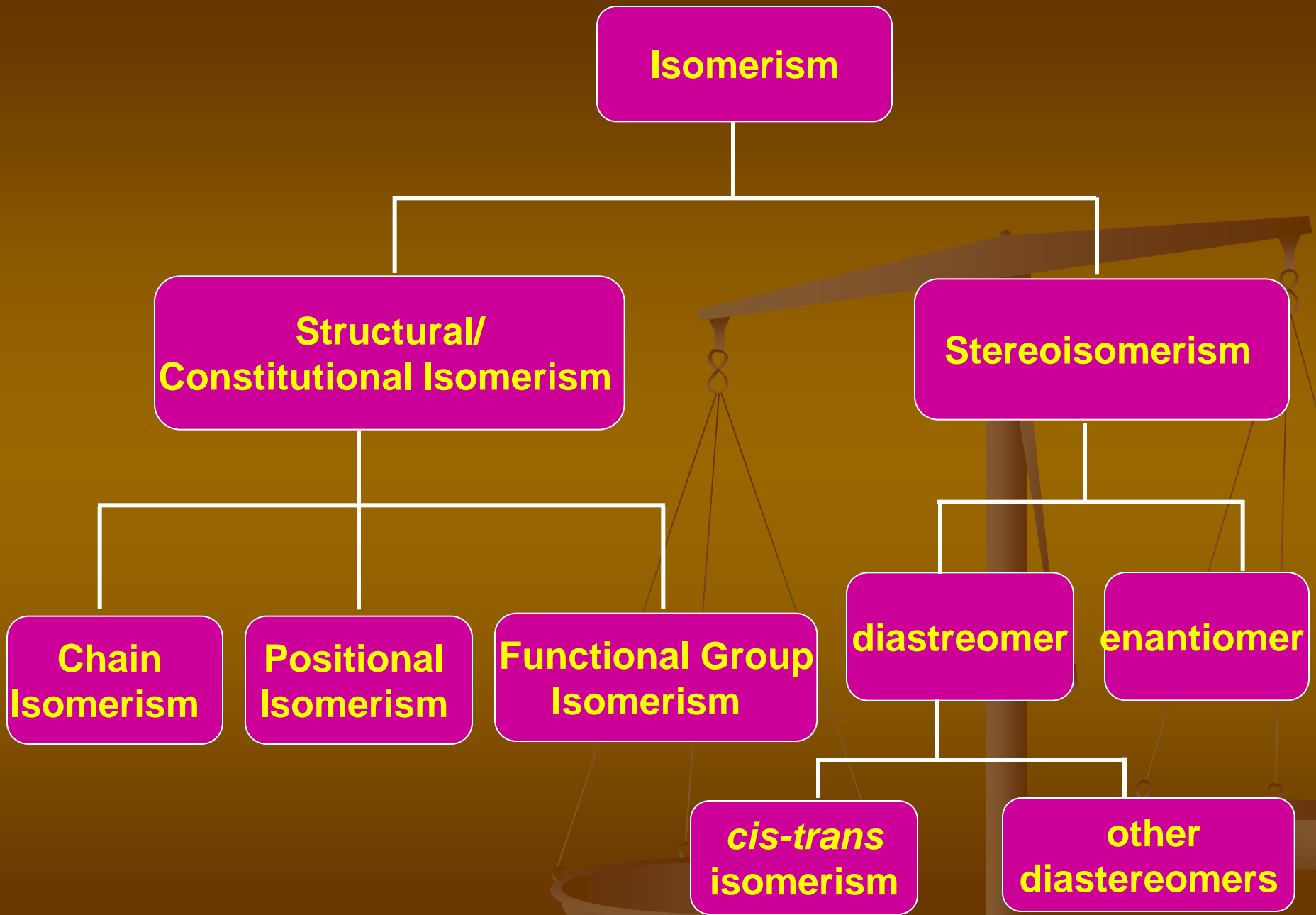
12.4 Isomerism

Learning Outcomes:

At the end of the lesson the students should be able to :

- Define isomerism.
- Explain constitutional isomerism.
 - chain isomers
 - positional isomers
 - functional group isomer

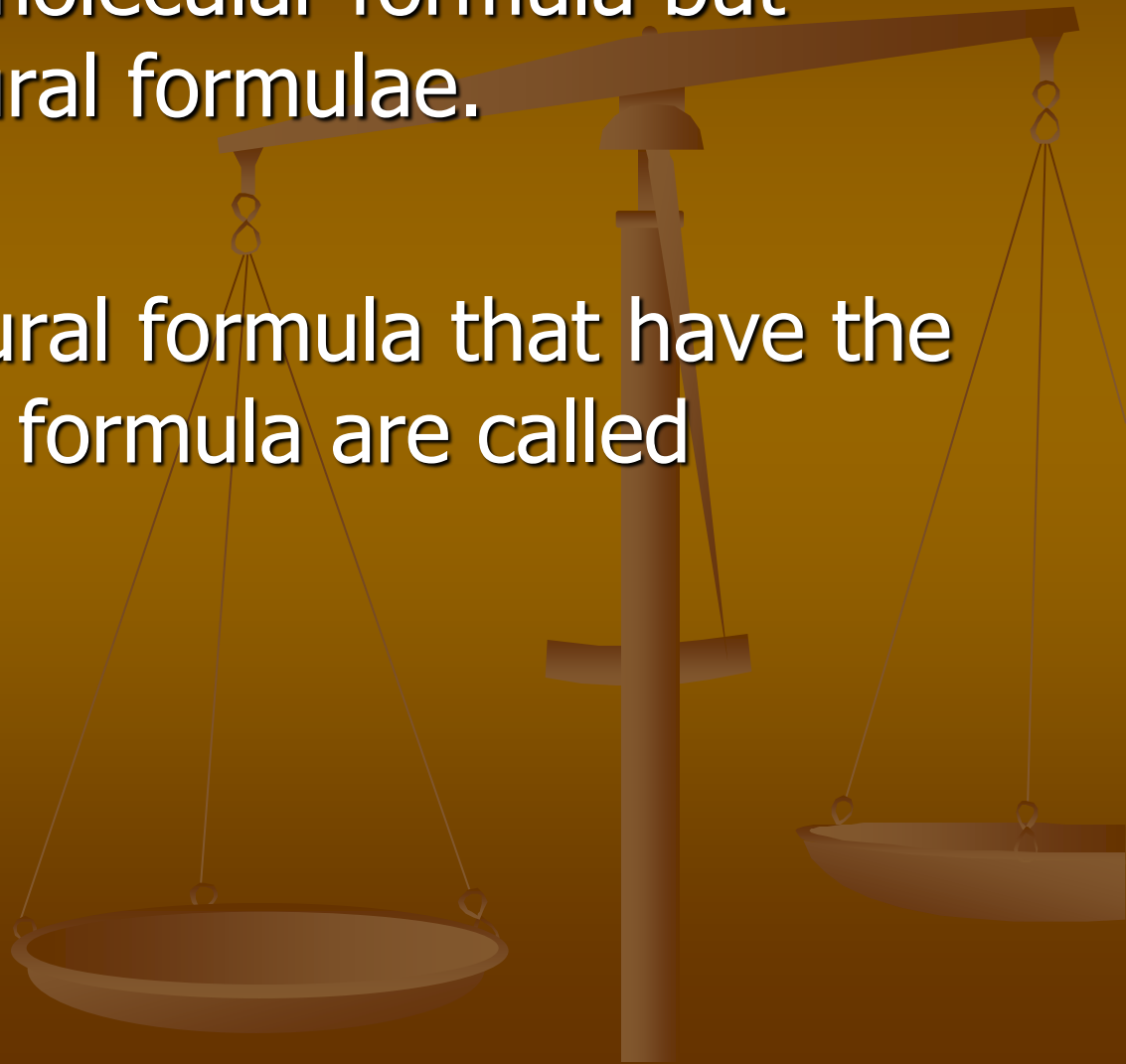




■ ***Isomerism***

is the existence of different compounds with the same molecular formula but different structural formulae.

- Different structural formula that have the same molecular formula are called ***isomers***.

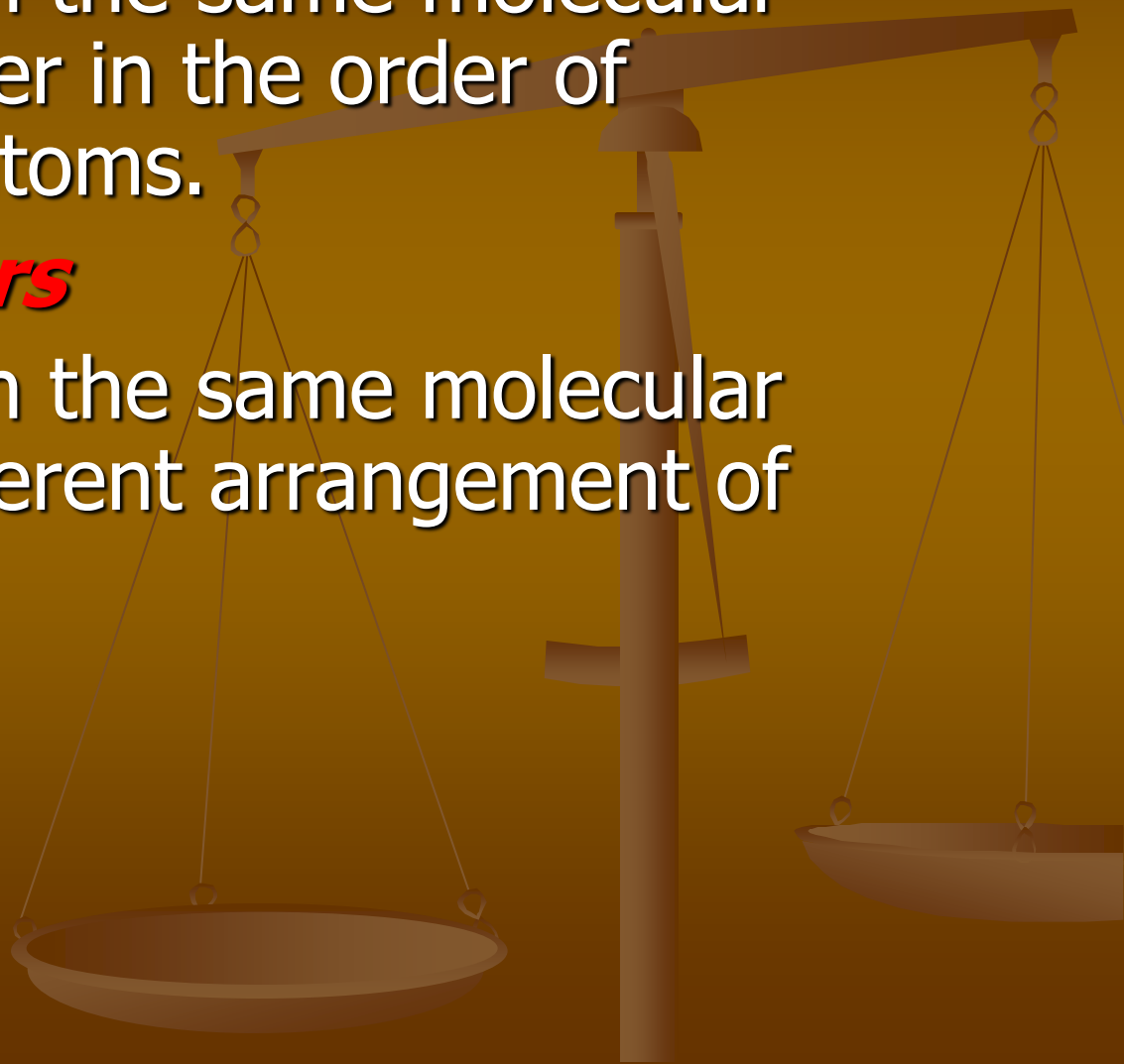


1) Constitutional isomers (Structural isomers)

- are isomers with the same molecular formula but differ in the order of attachment of atoms.

2) Stereoisomers

- are isomers with the same molecular formula but different arrangement of atoms in space



Constitutional isomerism

Isomerism resulting from different order of attachment of atoms.

■ Three types

a) Chain/skeletal isomerism

b) Positional isomerism

c) Functional group isomerism

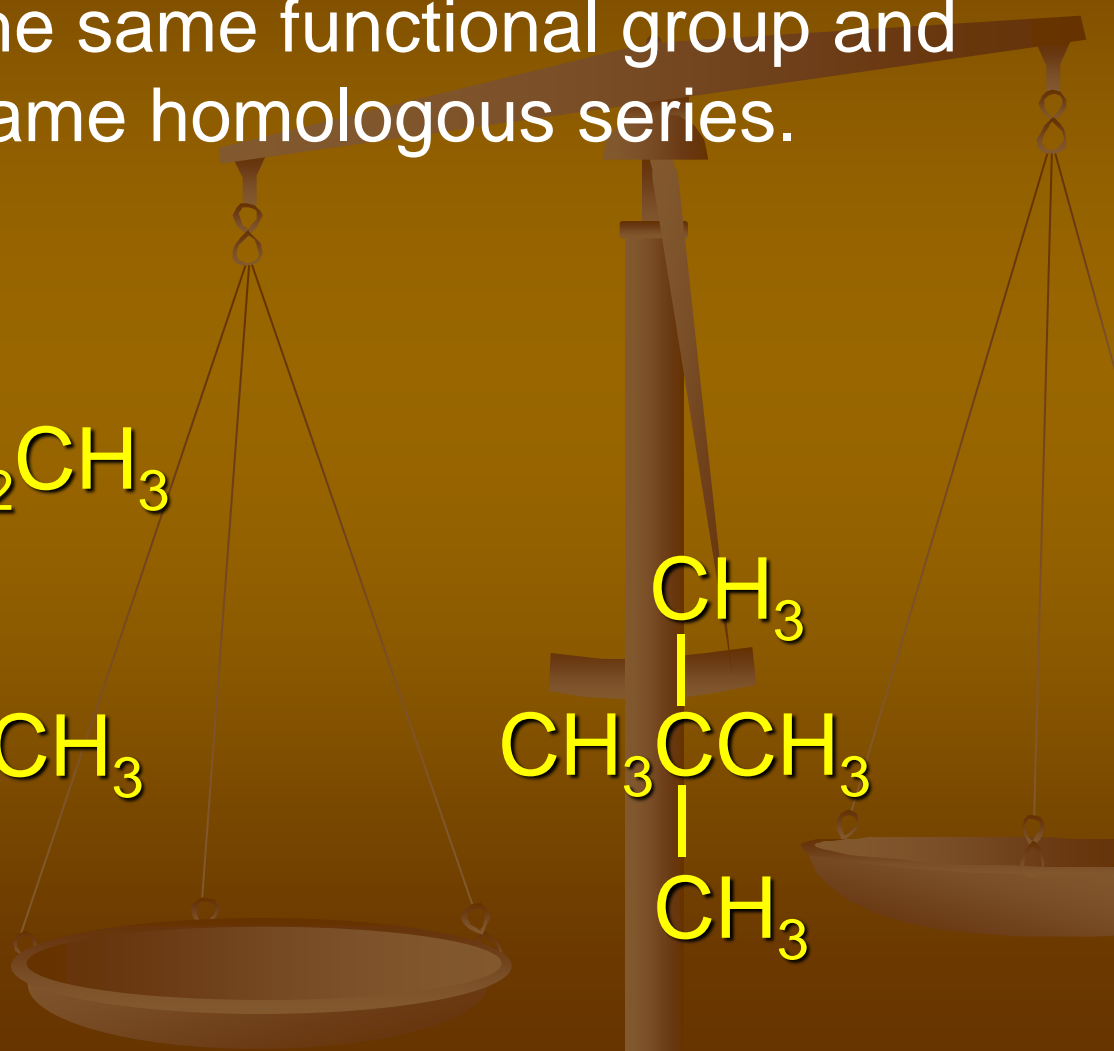
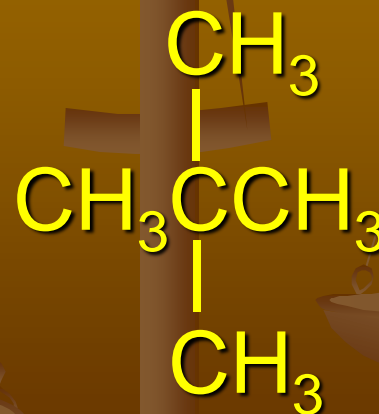
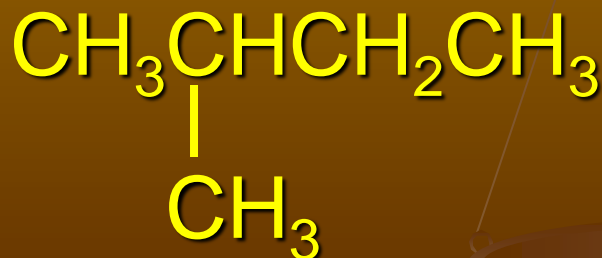


a) Chain/skeletal isomerism

The isomers differ in the carbon skeleton (different carbon chain).

They possess the same functional group and belong to the same homologous series.

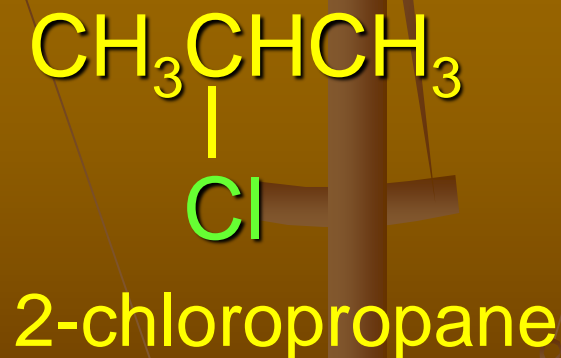
Example:



2) Positional isomerism

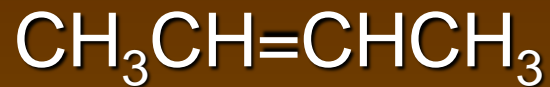
These isomers have a substituent group/
functional group in different positions.

Examples

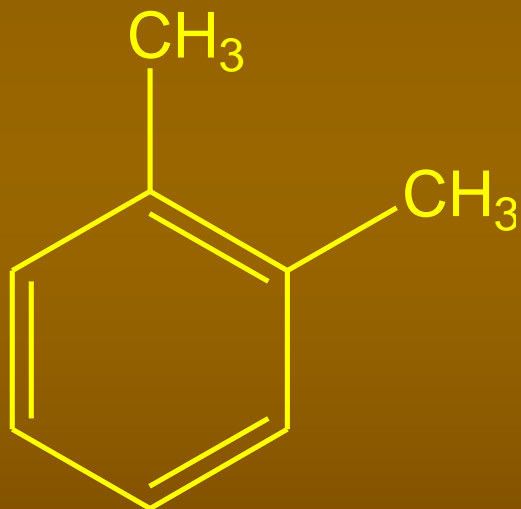




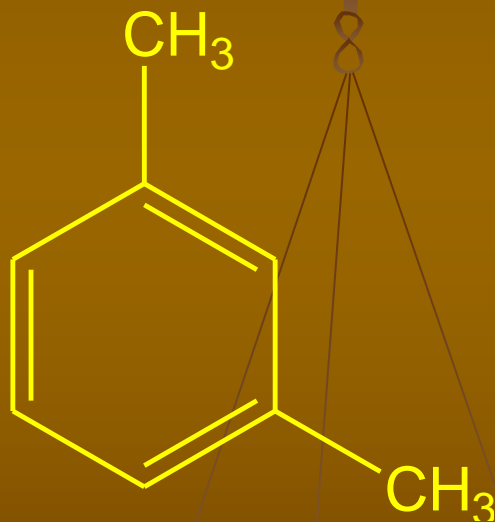
1-butene



2-butene



1,2-dimethylbenzene

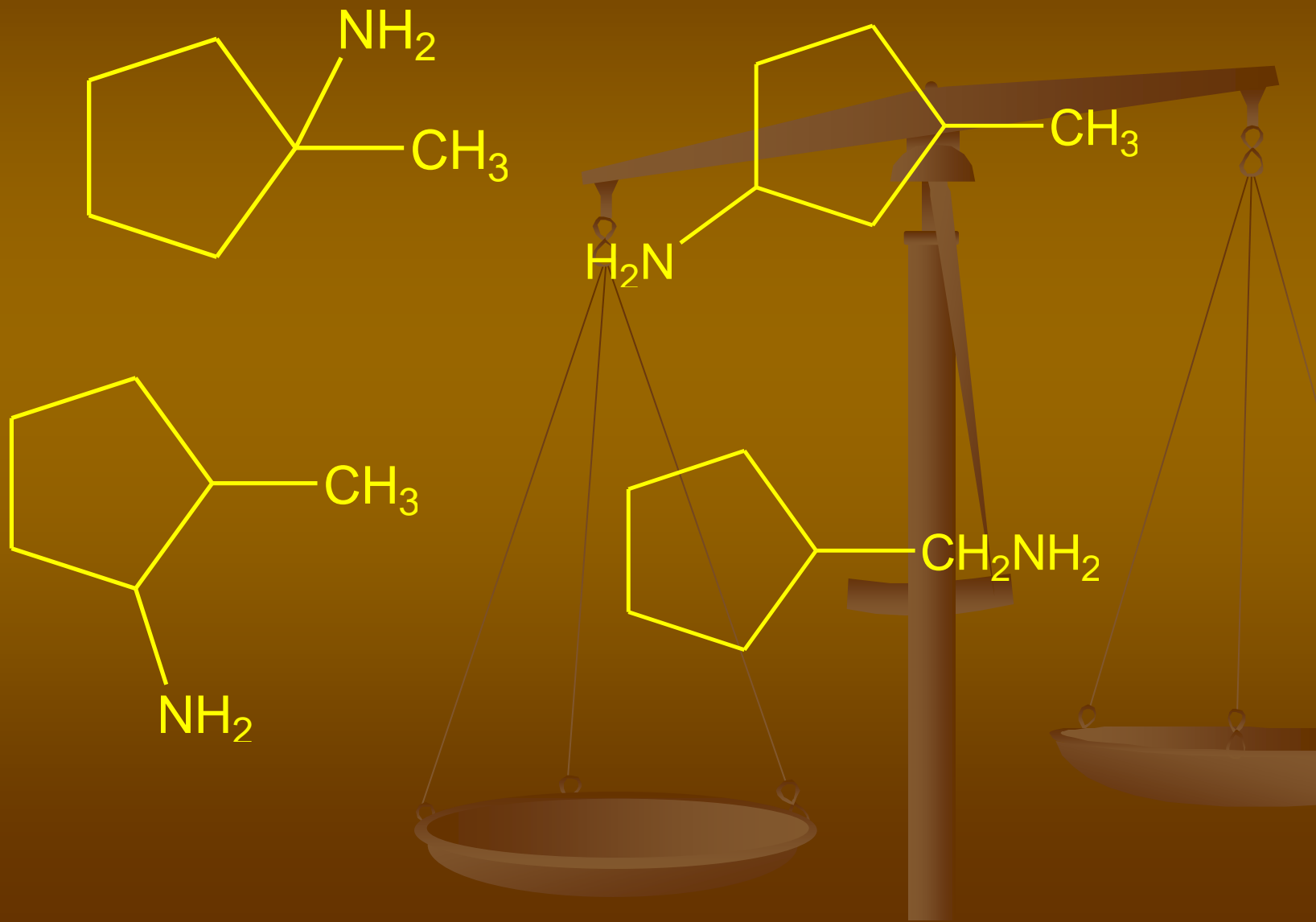


1,3-dimethylbenzene



1,4-dimethylbenzene

■ $C_6H_{13}N$



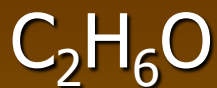
3) *Functional group isomerism*

These isomers have different functional groups and belong to different homologous series with the same general formula.

Different classes of compounds that exhibit functional group isomerism :-

General formula	Classes of compounds
$C_nH_{2n+2}O ; n > 1$	alcohol and ether
$C_nH_{2n}O ; n \geq 3$	aldehyde and ketone
$C_nH_{2n}O_2 ; n \geq 2$	carboxylic acid and ester
$C_nH_{2n} ; n \geq 3$	alkene and cycloalkane

■ Examples



ethanol



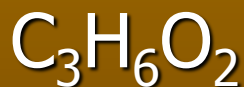
dimethyl ether



propanone



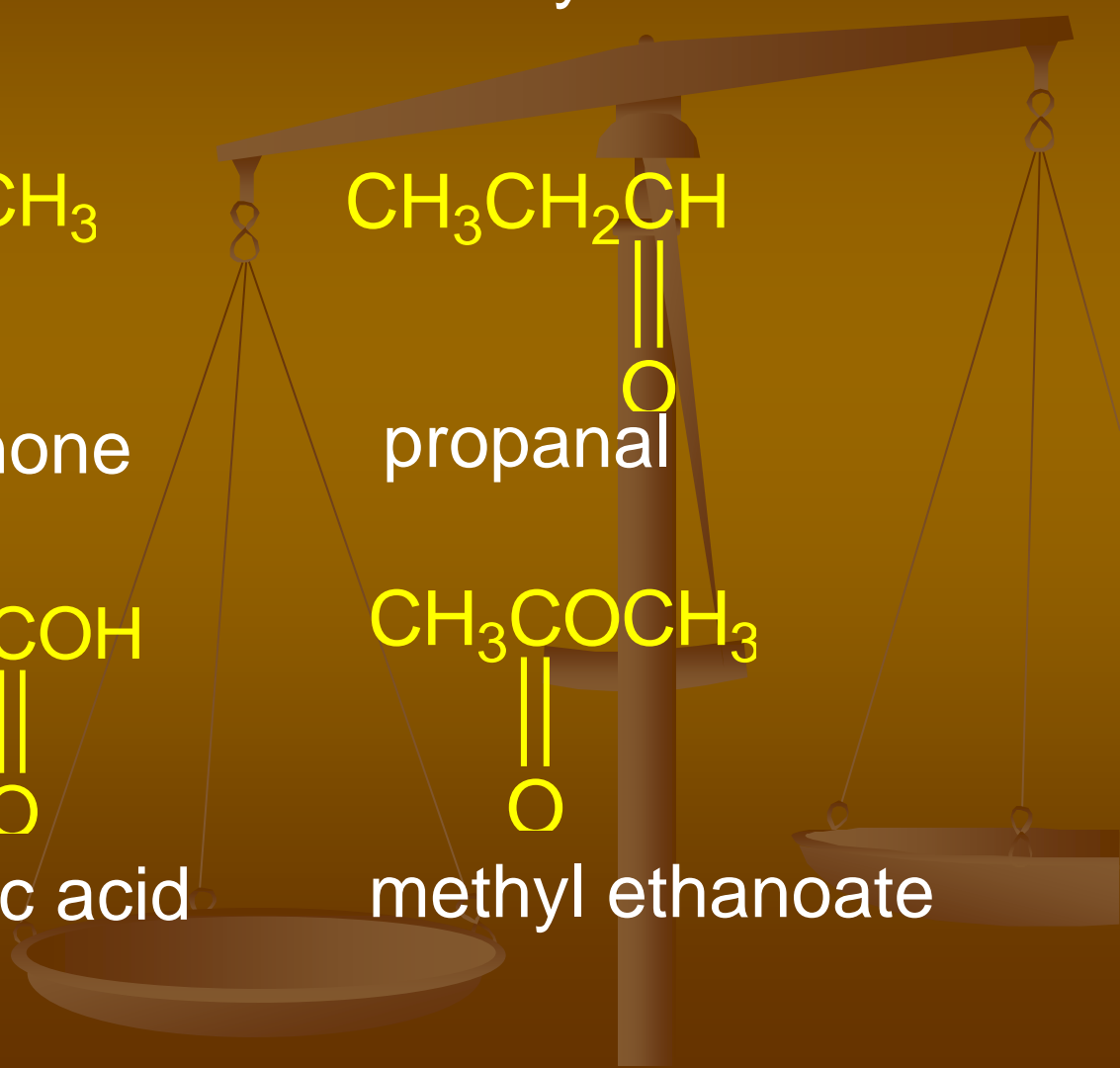
propanal



propanoic acid

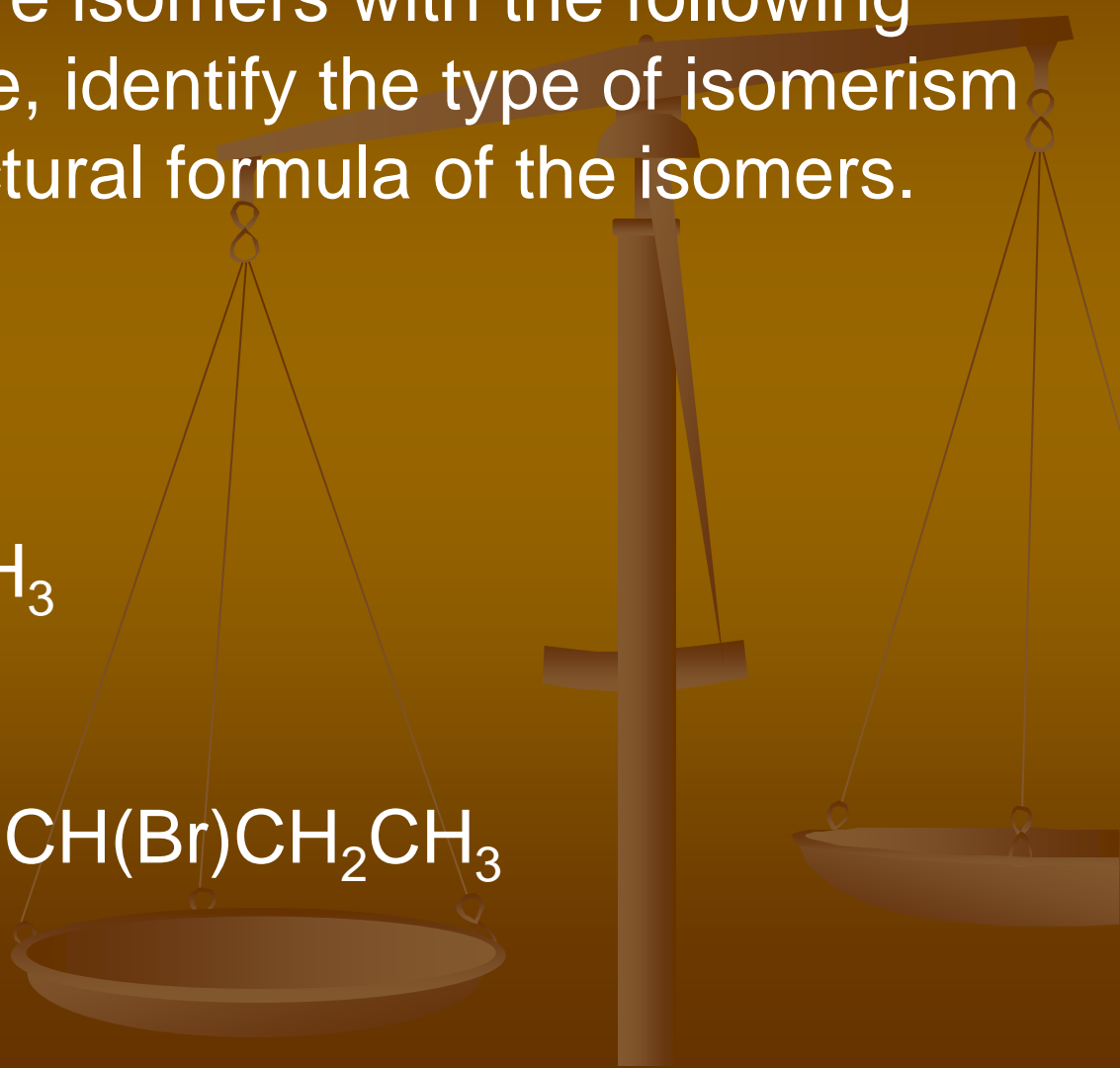
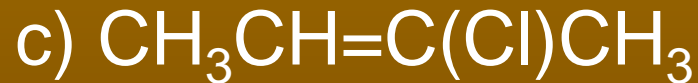


methyl ethanoate



Exercise:

1. State how many are isomers with the following molecular formulae, identify the type of isomerism and draw the structural formula of the isomers.



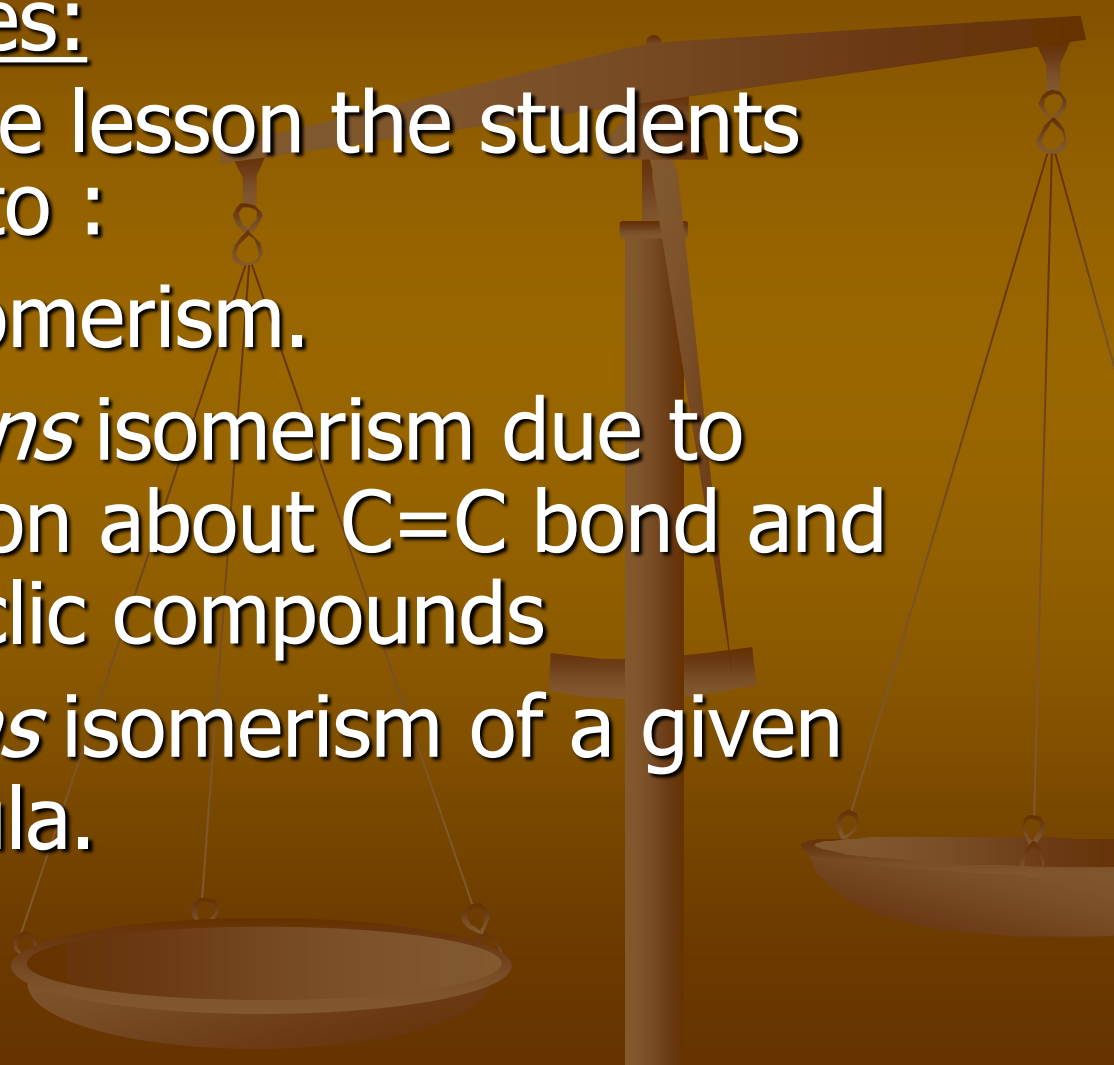
Lecture 5

12.4 Isomerism

Learning Outcomes:

At the end of the lesson the students should be able to :

- Define stereoisomerism.
- Describe *cis-trans* isomerism due to restricted rotation about C=C bond and C–C bond in cyclic compounds
- Identify *cis-trans* isomerism of a given structural formula.

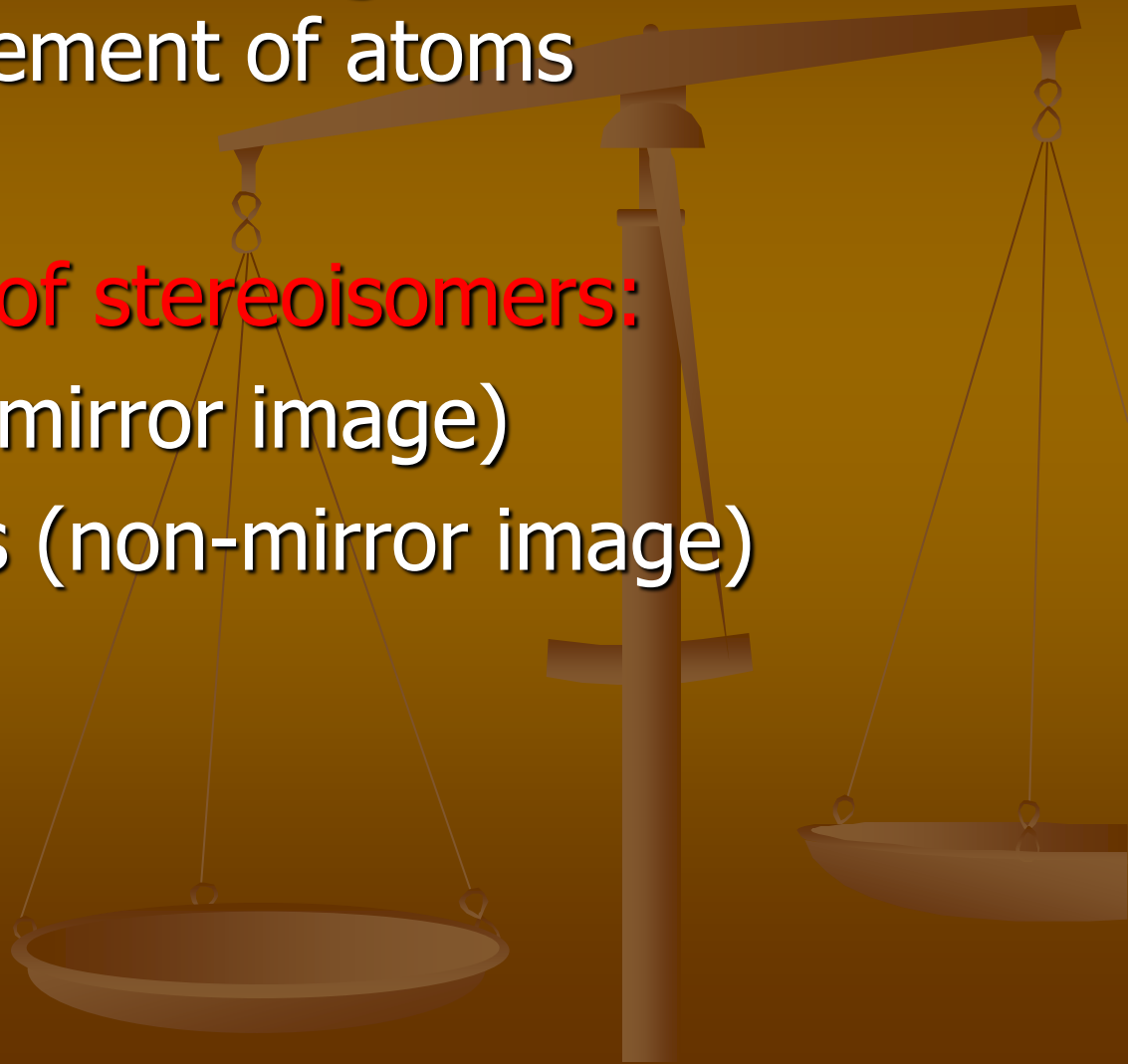


Stereoisomerism / optical isomerism :

Isomerism that resulting from different spatial arrangement of atoms in molecules.

Two subdivisions of stereoisomers:

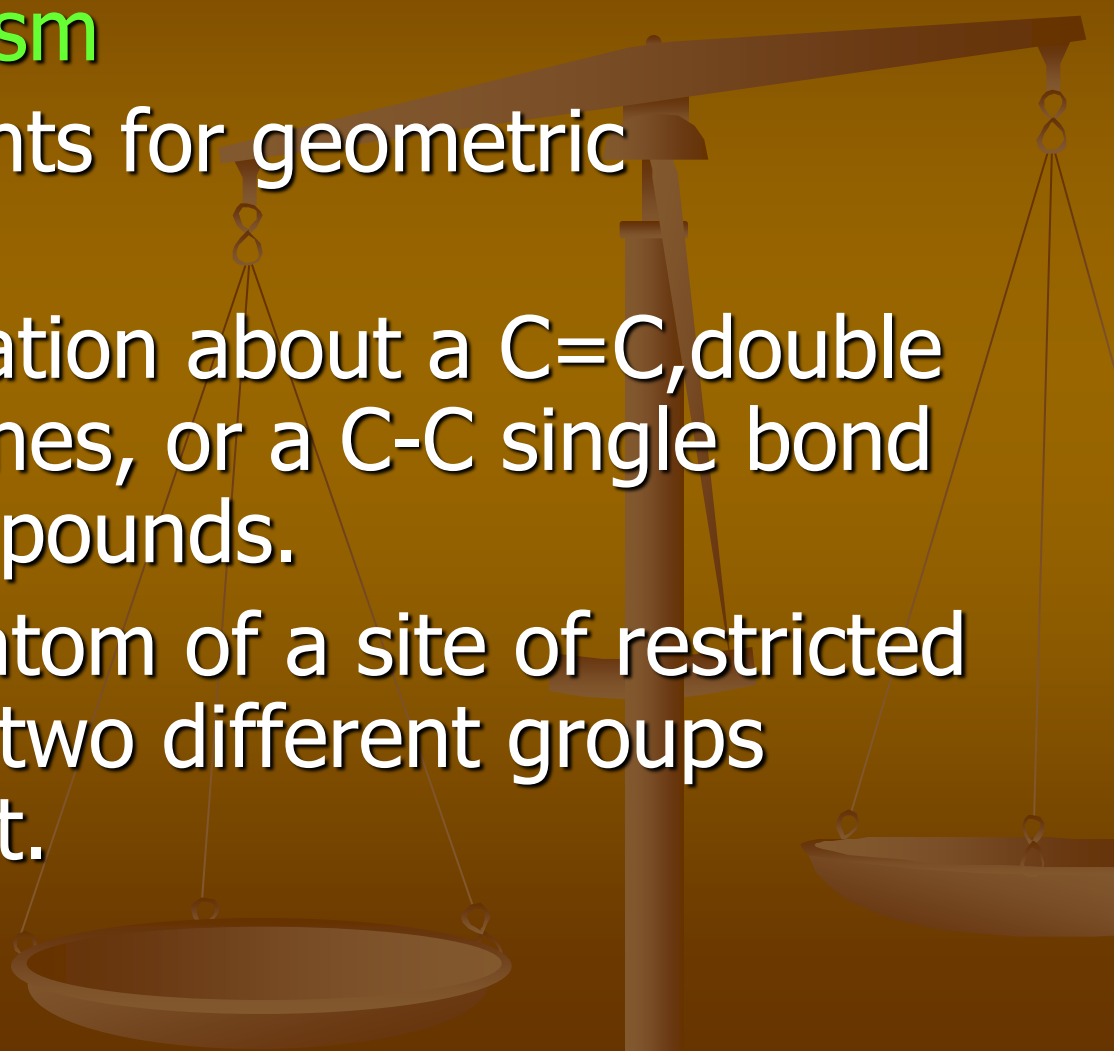
- i) Enantiomers (mirror image)
- ii) Diastereomers (non-mirror image)



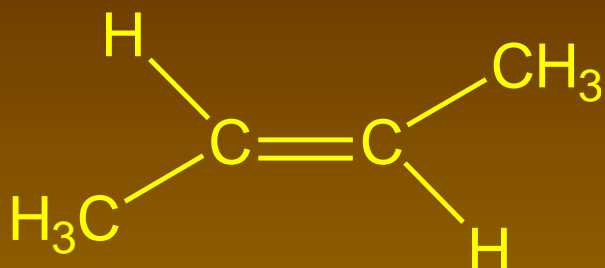
Diastereomer

Cis-Trans Isomerism

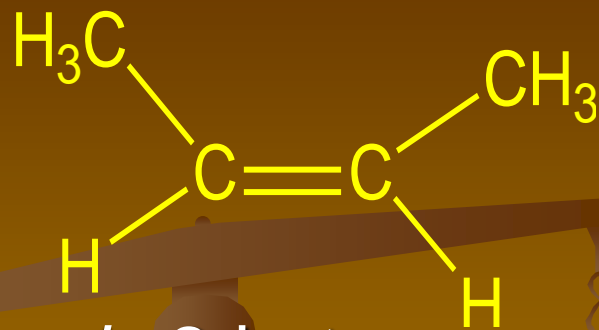
- ◆ The requirements for geometric isomerism :
 - i) restricted rotation about a C=C, double bond in alkenes, or a C-C single bond in cyclic compounds.
 - ii) each carbon atom of a site of restricted rotation has two different groups attached to it.



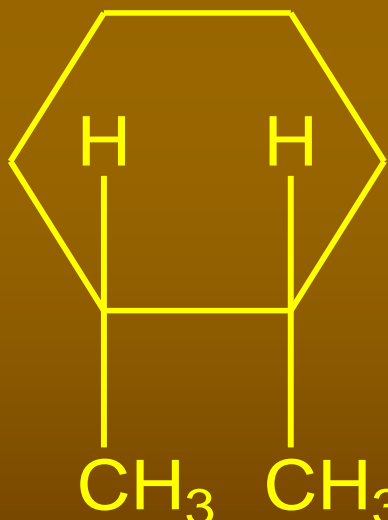
■ Examples



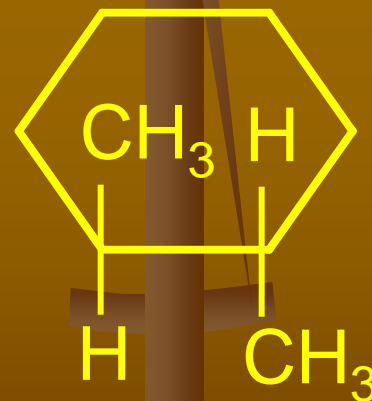
trans-2-butene



cis-2-butene

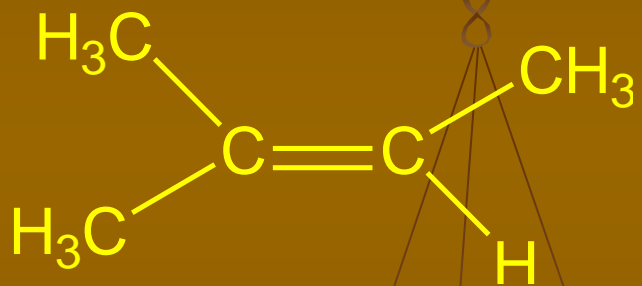


cis-1,2-dimethylcyclohexane

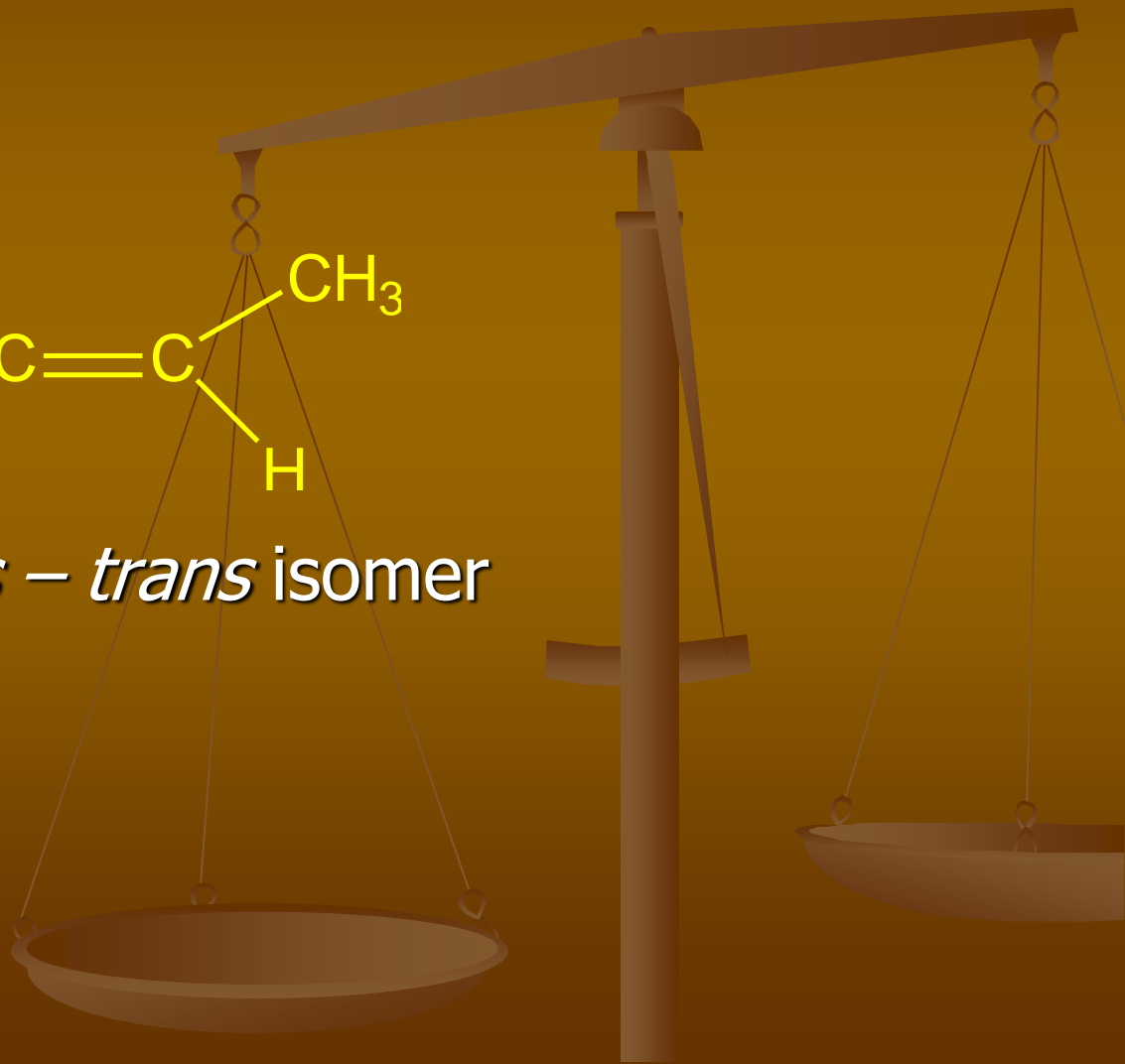


trans-1,2-dimethylcyclohexane

- If one of the doubly bonded carbons has 2 identical groups, geometric isomerism is not possible.
- Example



■ No *cis* – *trans* isomer

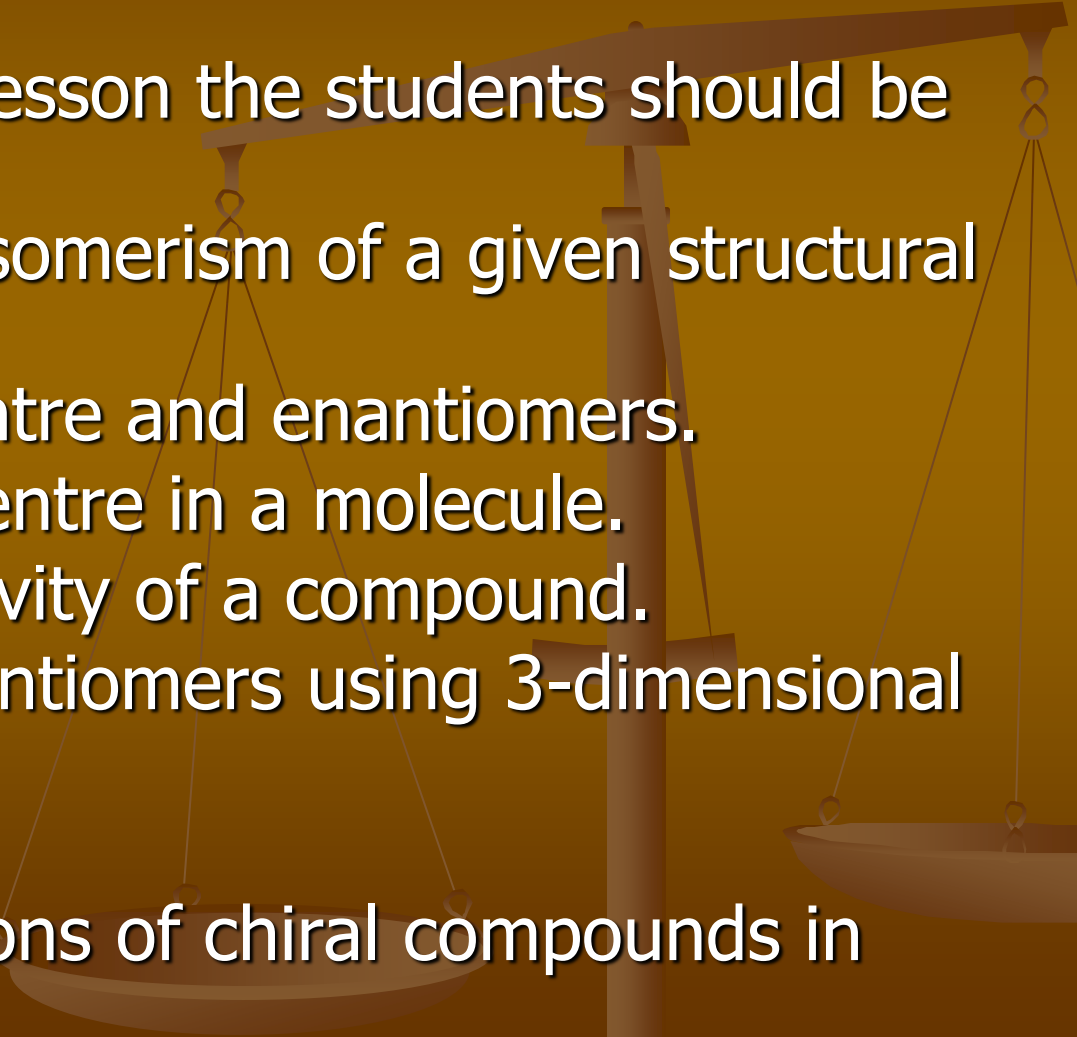


Lecture 6

12.4 Isomerism

Learning Outcomes:

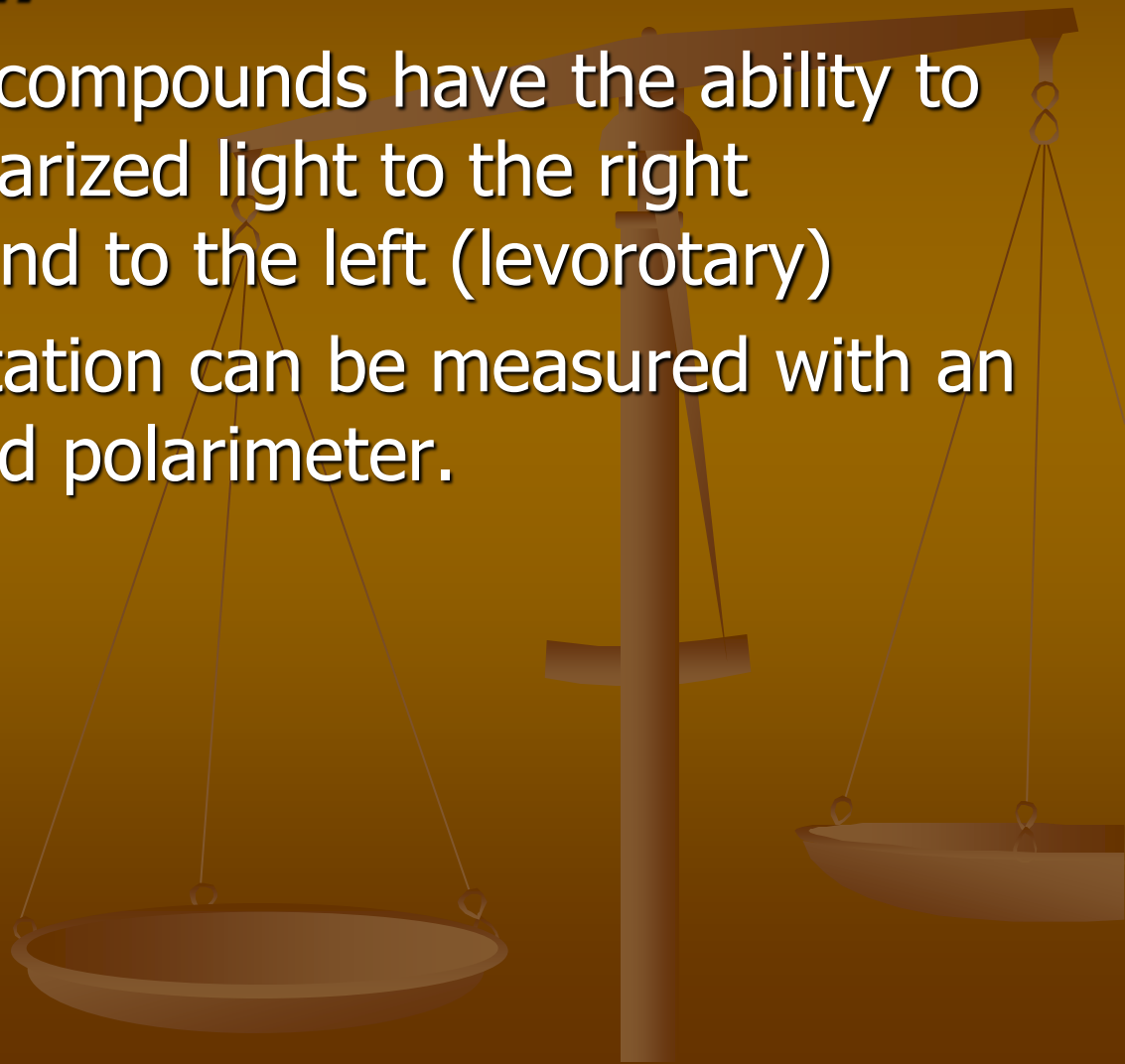
At the end of the lesson the students should be able to :

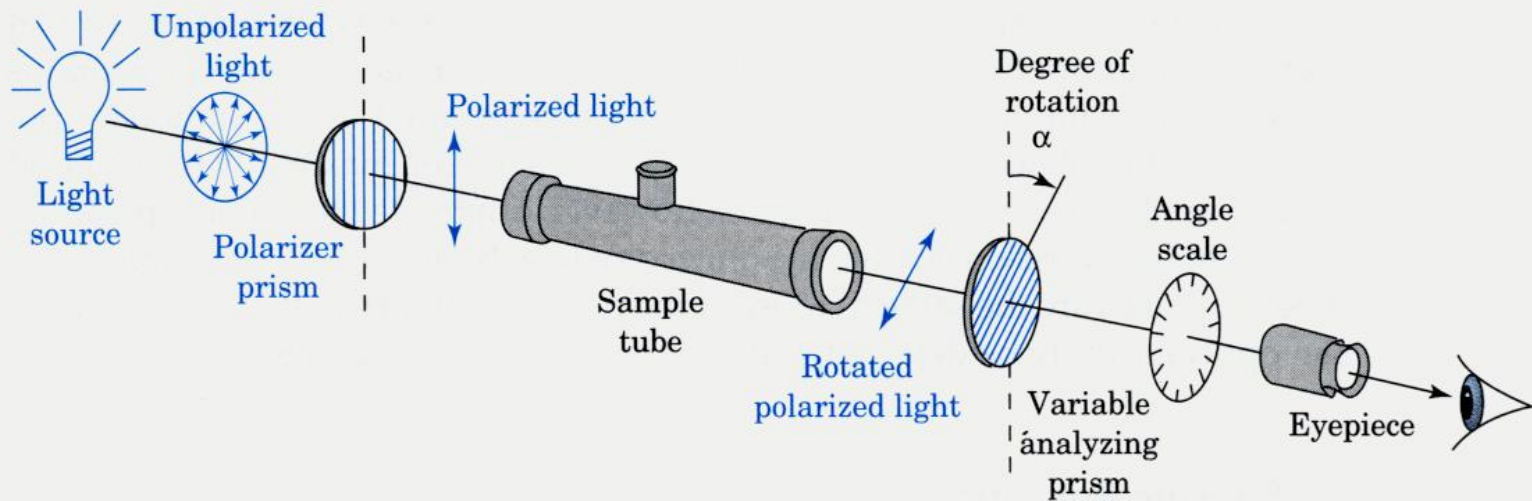
- Identify *cis-trans* isomerism of a given structural formula.
 - Define chirality centre and enantiomers.
 - Identify chirality centre in a molecule.
 - Explain optical activity of a compound.
 - Draw a pair of enantiomers using 3-dimensional formula.
 - Define racemate.
 - State the applications of chiral compounds in daily life.
- 

Enantiomer

Optical Isomerism

- Optically active compounds have the ability to rotate plane-polarized light to the right (dextrorotary) and to the left (levorotary)
- The angle of rotation can be measured with an instrument called polarimeter.

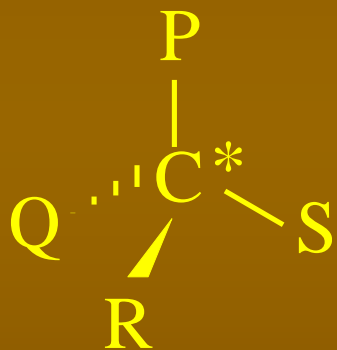




Polarimeter

The requirements for optical isomerism :-

- i) molecule contains a chiral carbon or chirality centre or stereogenic centre (a sp^3 -hybridized carbon atom with 4 different groups attached to it)



$P \neq Q \neq R \neq S$
*designates chiral centre

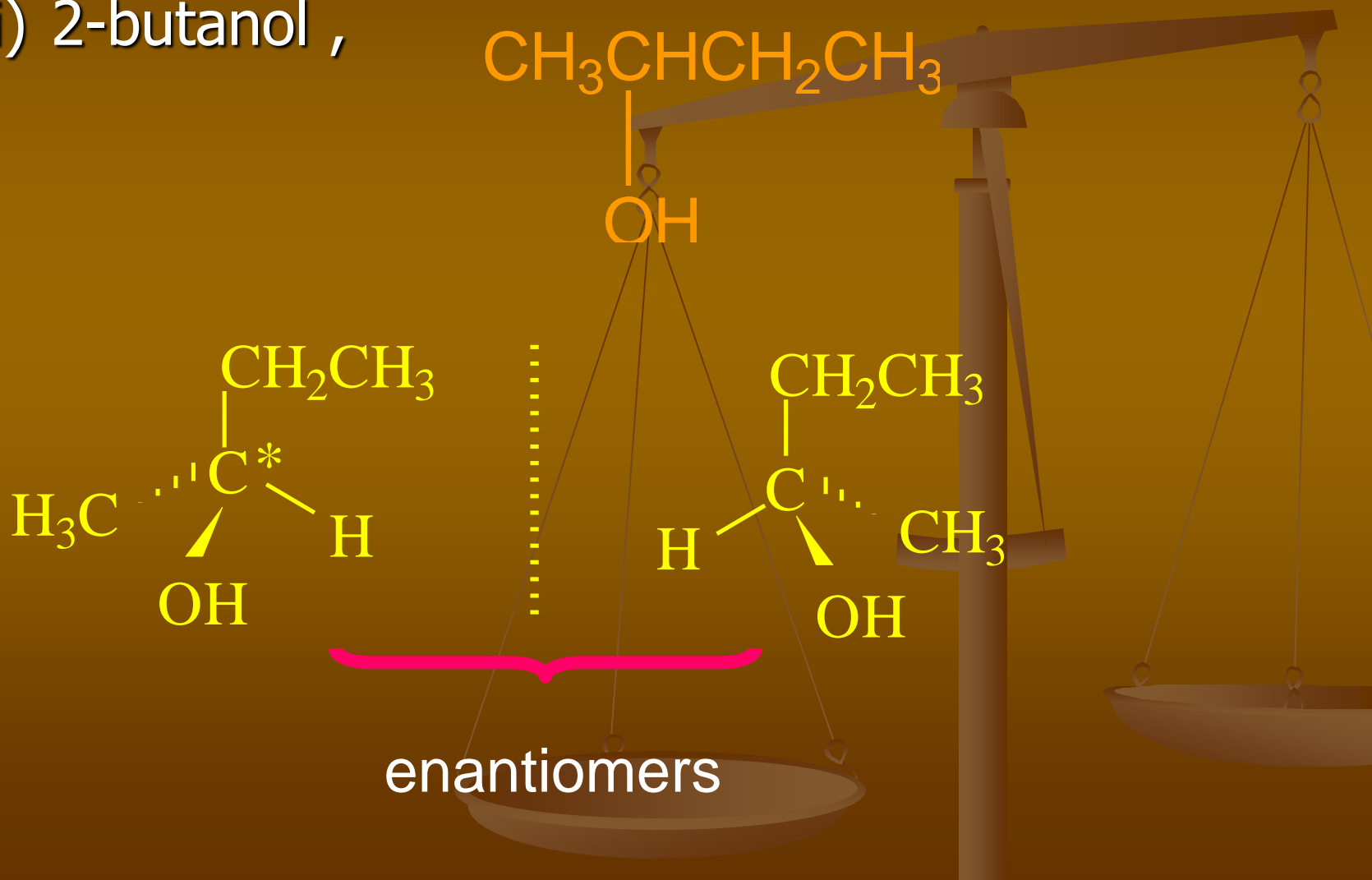
- ii) molecule is not superimposable with its mirror image.

■ *Enantiomers*

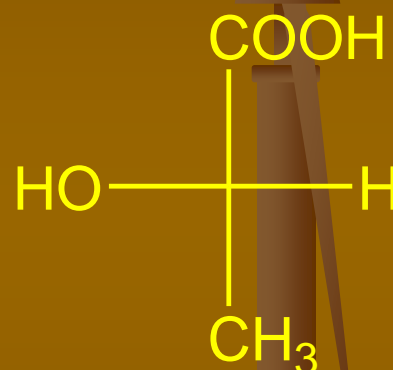
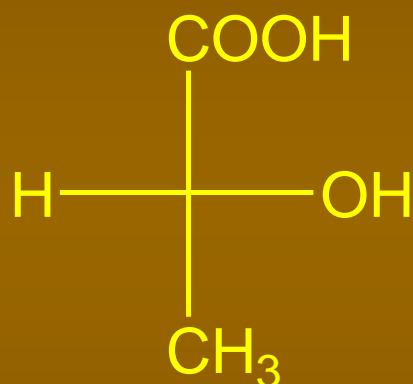
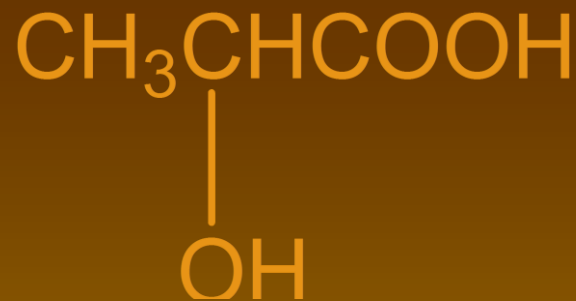
✓ a pair of mirror-image that are not superimposable.

Example:-

i) 2-butanol ,



ii) 2-hydroxypropanoic acid,

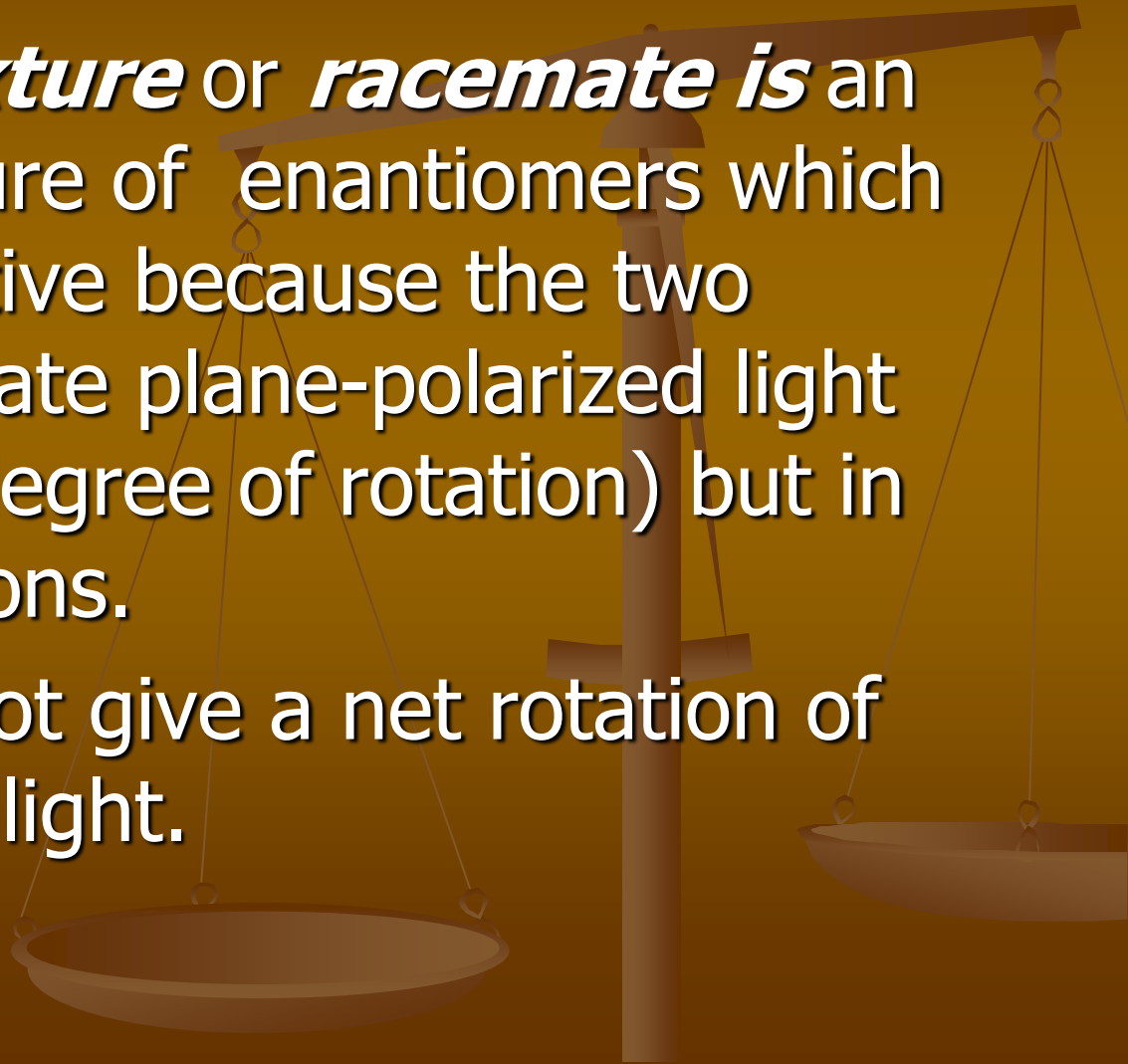


enantiomers



12.4.9 Racemate

- A ***racemic mixture*** or ***racemate*** is an equimolar mixture of enantiomers which is optically inactive because the two components rotate plane-polarized light equally (same degree of rotation) but in opposite directions.
- Hence it does not give a net rotation of plane-polarized light.



Applications of chiral compounds in daily life.

e.g.:

- (–) Dopa is used for treatment of Parkinson's disease but (+) dopa is toxic to human.
- (*S*)-Ibuprofen the popular analgesic (the active ingredient in motrin, advil, and many other nonaspirin analgesics)

