

# CHE 1000: INTRODUCTORY CHEMISTRY

## 2019/2020

### ISOMERISM

#### ❖ Prior knowledge

- Know the functional groups found in organic chemistry
- know the arrangement of bonds around carbon atoms
- know what affects the boiling point of organic molecules

## Index Hydrogen Deficiency (IHD)

$$\text{IHD} = \frac{(2n+2) - (\# \text{hydrogen atoms} + \text{halogens} - \text{nitrogen atoms})}{2}$$

Where;  $n$  = number of carbon atoms in a given molecule  
halogens = F, Cl, Br and I

### Note;

If IHD = 0, it means all bonds connecting the atom are single bond

= 1, it means there is a double bond or the a cyclic (ring) chain

= 2, it means there is triple bond or a double bond an a cyclic (ring) chain  
or 3 cyclic (ring) chains

And so on and so forth.....

**Example: Calculate the IHD of a compound with the molecular formula,  $\text{C}_2\text{H}_6\text{NCl}$**

$$\text{IHD} = \frac{(2n+2) - (\# \text{hydrogen atoms} + \text{halogens} - \text{nitrogen atoms})}{2}$$

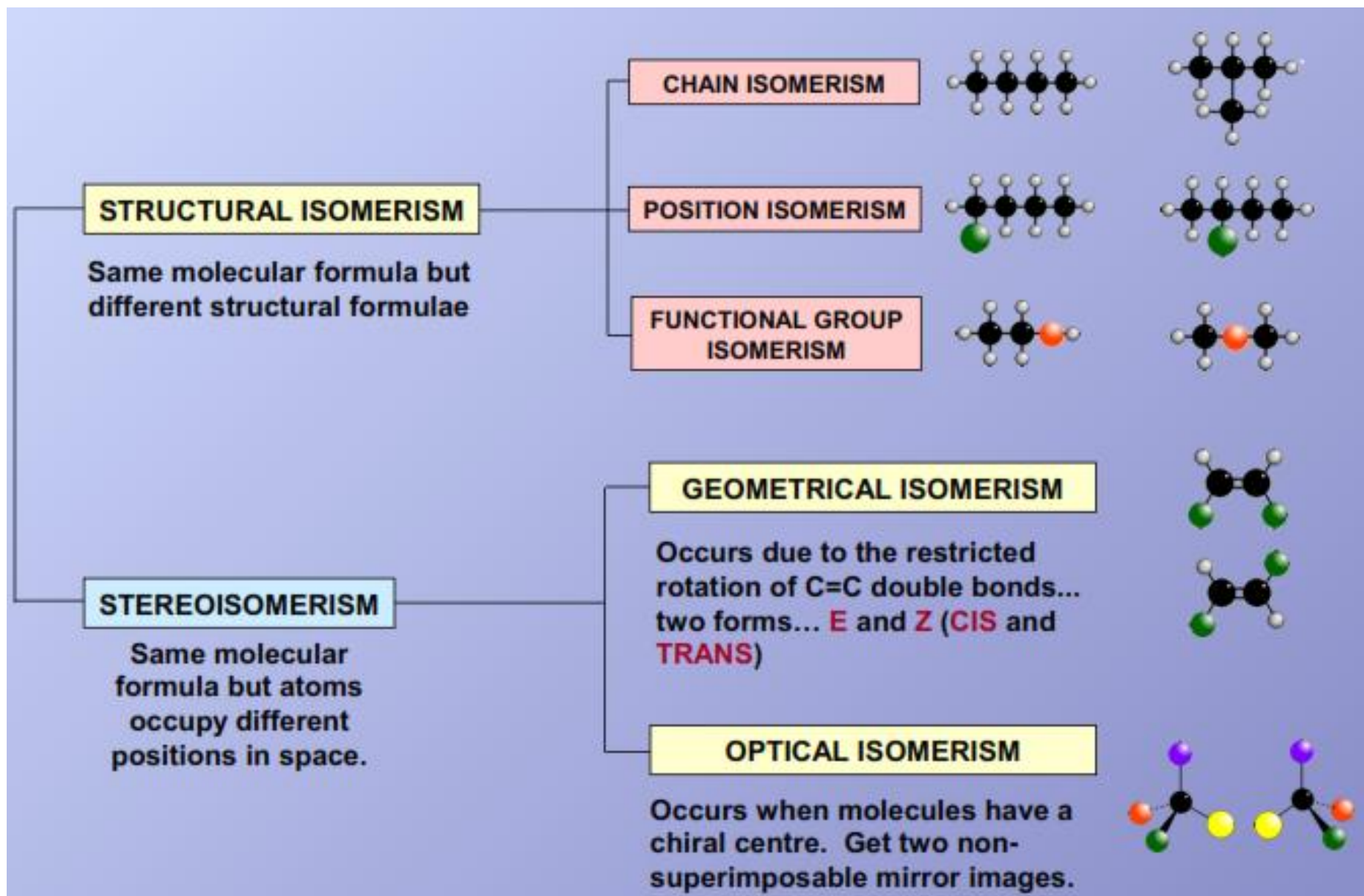
$$= \frac{(2*2+2) - (6+1-1)}{2}$$

$$= 0$$

# What is isomerism?

- ❖ Isomerism is the phenomenon in which more than one compounds have the same chemical formula but different chemical structures
- ❖ Chemical compounds that have identical chemical formulae but differ in properties and the arrangement of atoms in the molecule are called **isomers**
- ❖ Therefore, the compounds that exhibit isomerism are known as isomers

# Types of isomerism

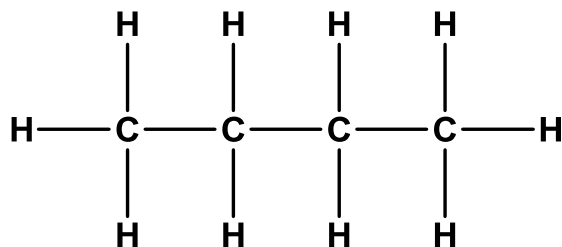


## Chain Isomerism

- ❖ This is kind of structural isomerism in which there is different arrangements of the carbon skeleton
- ❖ Usually chain isomerism exhibits similar chemical properties but slightly different physical properties

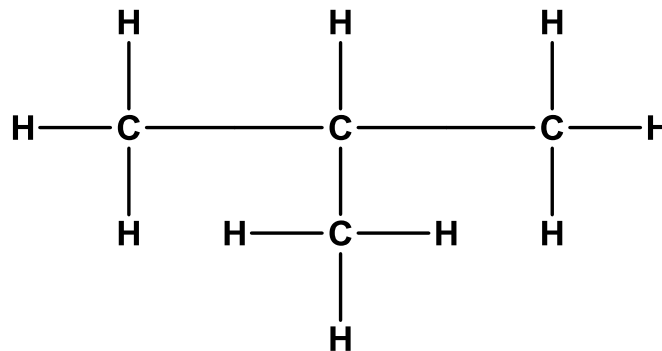
Example,  $C_4H_{10}$  (IHD = 0) and all its possible isomer(s)

straight



butane

branched



2-methylpropane

## Differences between Chain Isomers

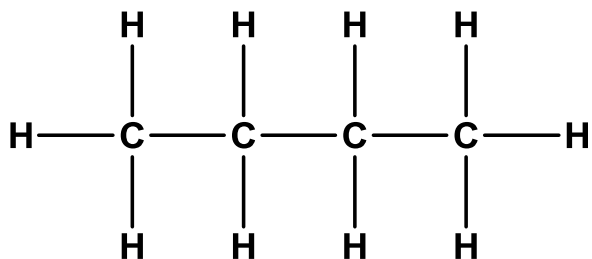
**Chemical:** Isomers show similar chemical properties because the same functional group is present

**Physical:** Properties such as density and boiling point show trends according to the degree of branching

**Boiling Point :** Straight chain isomers have higher values than branched ones the greater the degree of branching the lower the boiling point branching decreases the effectiveness of intermolecular forces less energy has to be put in to separate the molecules

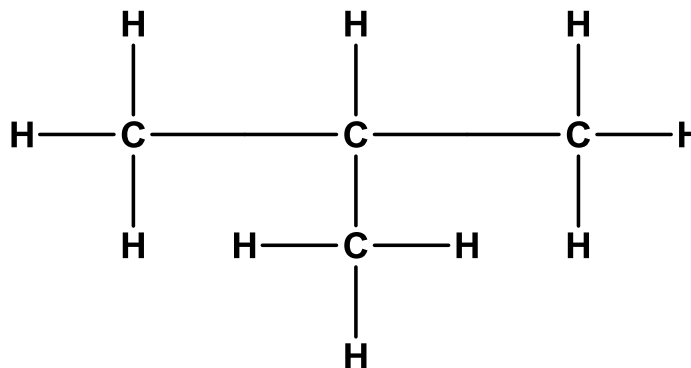
- 0.5°C

straight



- 11.7°C

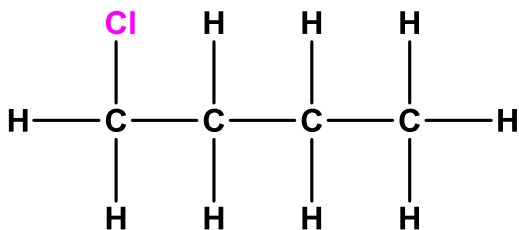
branched



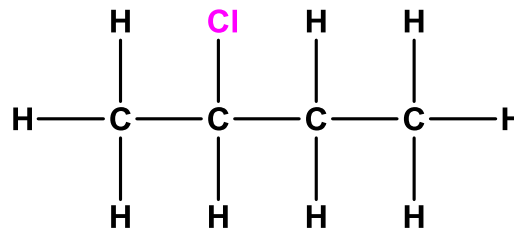
# Positional Isomerism

- ❖ This is a type of structural isomerism in which the carbon skeleton of a molecule has the same functional group
- ❖ The functional group can move in different positions around the molecule, and the resulting isomers have similar chemical properties but different physical properties

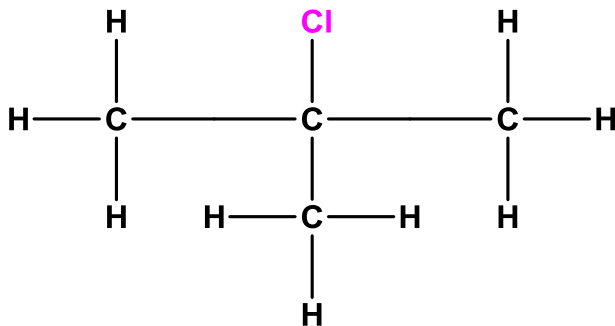
## Example 1, $C_4H_9Cl$ (IHD = 0) and all its possible isomers



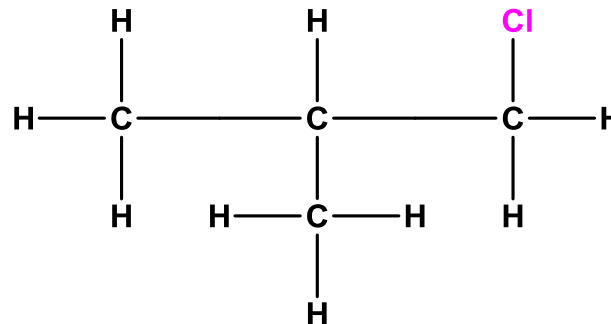
1-chlorobutane



2-chlorobutane

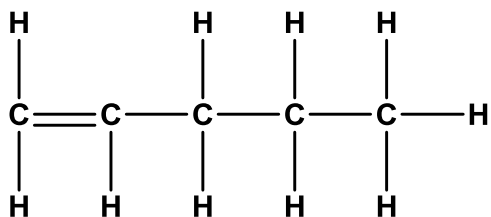


2-chloro-2-methylpropane

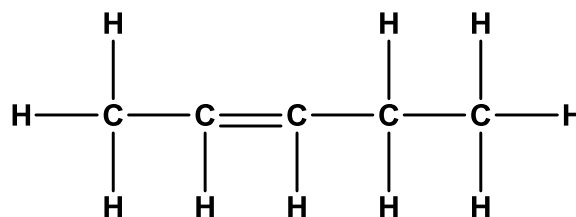


1-chloro-2-methylpropane

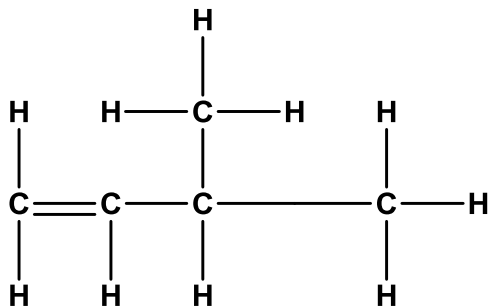
Example 2,  $C_5H_{10}$  (IHD = 1) position of double bonds in pentene and all non-cyclic possible isomers



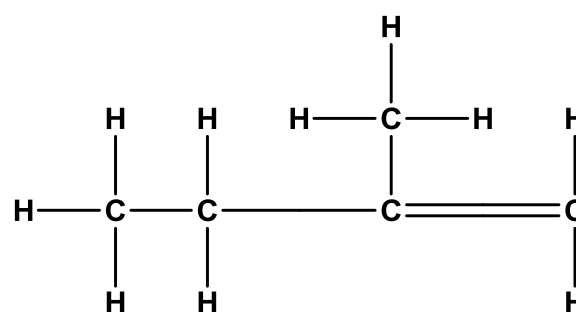
1-pentene



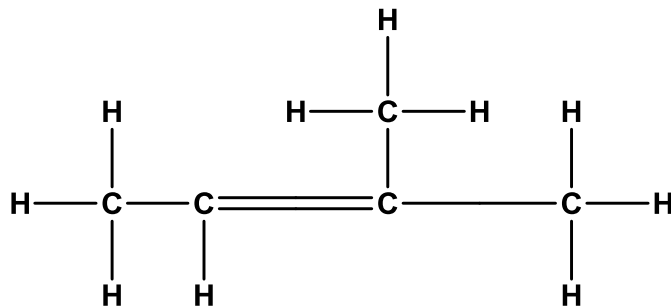
2-pentene



3-methyl-1-butene



2-methyl-1-butene



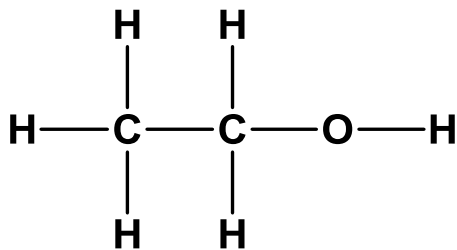
2-methyl-2-butene

## Functional Isomerism

- ❖ This is a type of structural isomerism in which molecules have the same molecular formula but different functional groups
- ❖ In functional isomerism molecules have different chemical properties and different physical properties

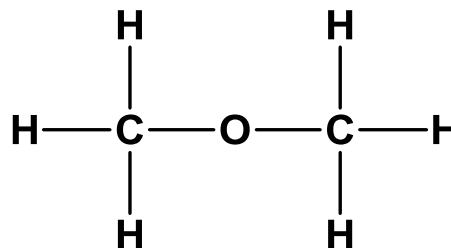
Example 1, Molecular Formula,  $C_2H_6O$  (IHD = 0) and all its possible isomers

alcohol



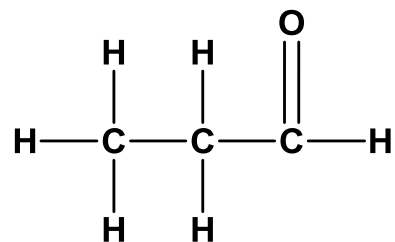
ethanol

ether

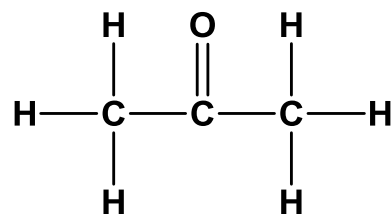


methoxymethane

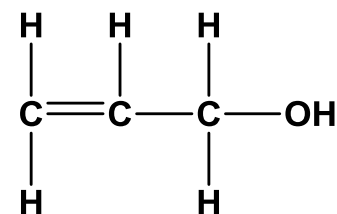
## Example 2, Molecular Formula, $C_3H_6O$ (IHD = 1) and all its non-cyclic possible isomers



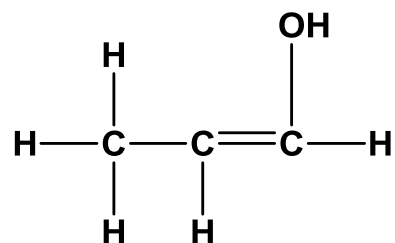
propanaldehyde



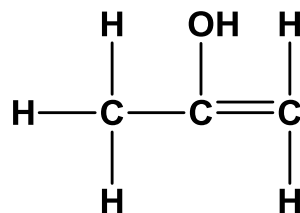
propan-2-one



prop-2-en-1-ol



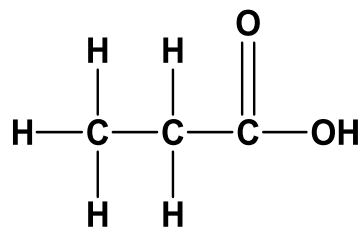
prop-1-en-1-ol



prop-1-en-2-ol

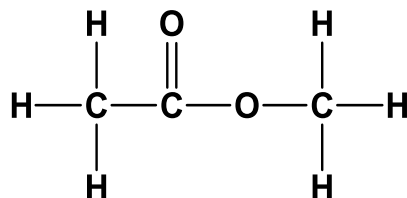
## Example 3, Molecular Formula, $C_3H_6O_2$ (IHD = 1) and all its non-cyclic possible isomers

carboxylic acid

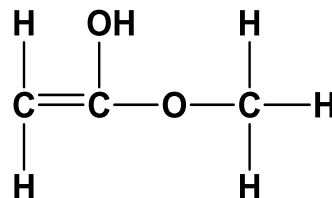


propionic acid

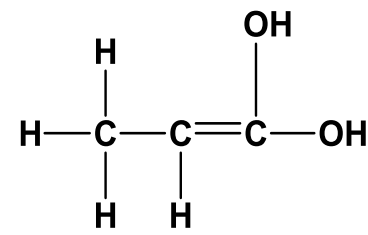
ester



methyl acetate



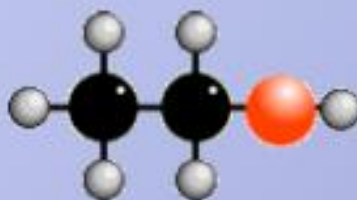
1-methoxyethen-1-ol



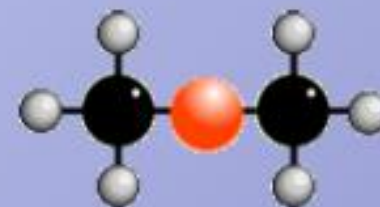
prop-1-ene-1,1-diol

# Differences in Physical and Chemical properties between Functional Isomers

## ALCOHOLS and ETHERS



ETHANOL



METHOXYMETHANE

Name

Classification

Functional Group

Physical properties

Chemical properties

ALCOHOL

R-OH

polar O-H bond gives rise to hydrogen bonding. get higher boiling point and solubility in water

Lewis base  
Wide range of reactions

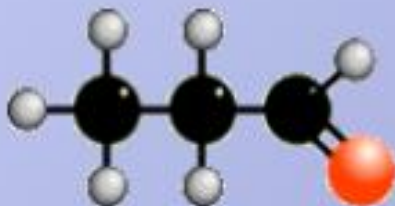
ETHER

R-O-R

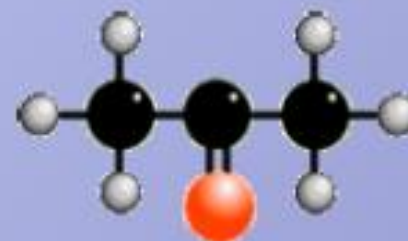
No hydrogen bonding  
low boiling point  
insoluble in water

Inert

# ALDEHYDES and KETONES



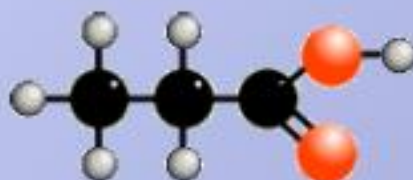
PROPANAL



PROPANONE

<b>Name</b>	PROPANAL	PROPANONE
<b>Classification</b>	ALDEHYDE	KETONE
<b>Functional Group</b>	R-CHO	R-CO-R
<b>Physical properties</b>	polar C=O bond gives dipole-dipole interaction	polar C=O bond gives dipole-dipole interaction
<b>Chemical properties</b>	easily oxidised to acids of same number of carbons  reduced to 1° alcohols	undergo oxidation under extreme conditions only  reduced to 2° alcohols

# CARBOXYLIC ACIDS and ESTERS



PROPANOIC ACID



METHYL ETHANOATE

**Name**

**Classification**

**Functional Group**

**Physical properties**

**Chemical properties**

CARBOXYLIC ACID

R-COOH

O-H bond gives rise to hydrogen bonding. get higher boiling point and solubility in water

acidic  
react with alcohols

ESTER

R-COOR

No hydrogen bonding  
insoluble in water

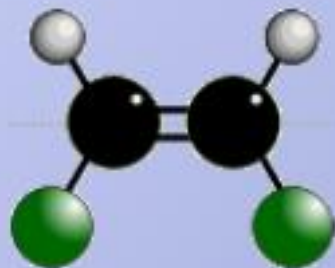
fairly unreactive  
hydrolysed to acids

# Take home problems;

1. Write down the remaining possible cyclic isomers for pentene,  $C_5H_{10}$
2. Write down all the possible cyclic and non-cyclic isomers for a compound with the molecular formula,  $C_3H_6O$
3. How many possible isomer can be drawn from Dibromobenzene

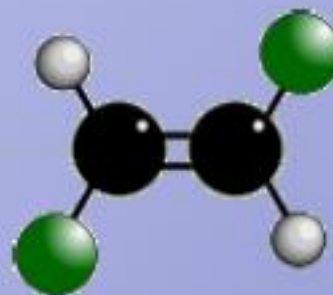
## Geometrical Isomerism

- ❖ This is a kind of stereoisomer in which molecules have the **SAME MOLECULAR FORMULA** but the atoms are joined to each other in a **DIFFERENT SPACIAL ARRANGEMENT** – they occupy a different position in 3-dimensional space
- ❖ Geometrical isomers exist in two forms...*cis (Z)* / *trans (E)* , and as a result they have different chemical and physical properties



**CIS (Z)**

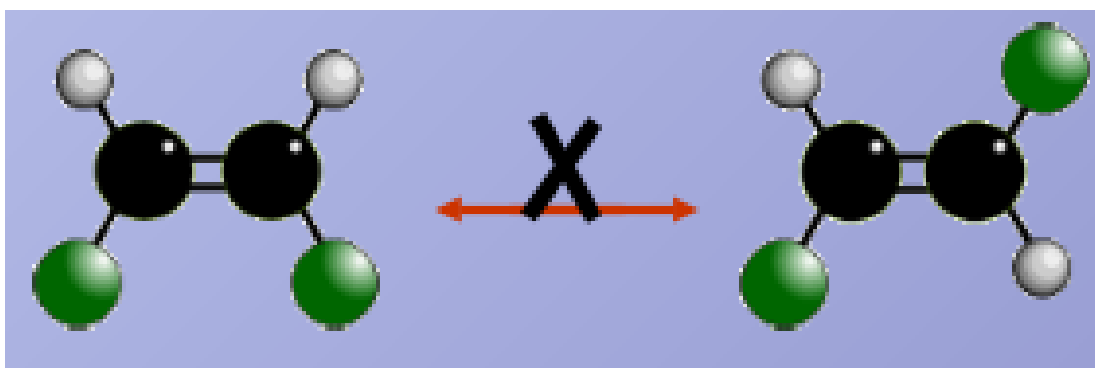
Groups/atoms are on the **SAME SIDE** of the double bond



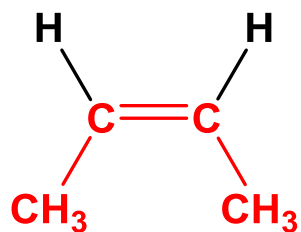
**TRANS (E)**

Groups/atoms are on **OPPOSITE SIDES** across the double bond

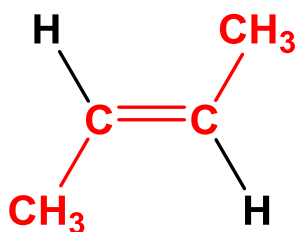
- ❖ C=C bonds have restricted rotation so the groups on either end of the bond are 'frozen' in one position
- ❖ As a result, the two structures cannot interchange or flip easily so the atoms in the two molecules occupy different positions in space



❖ Examples;

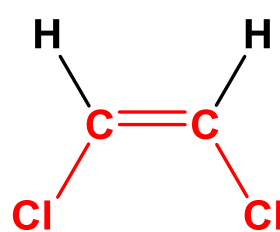


(Z)-but-2-ene

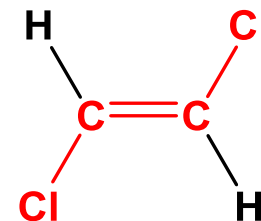


(E)-but-2-ene

or

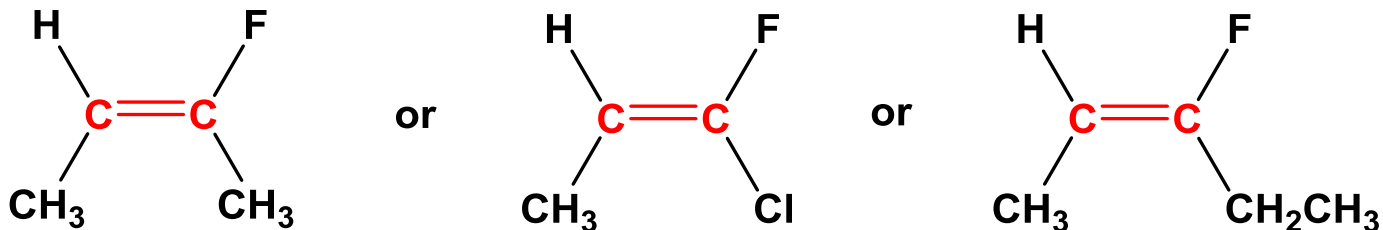


(Z)-1,2-dichloroethene

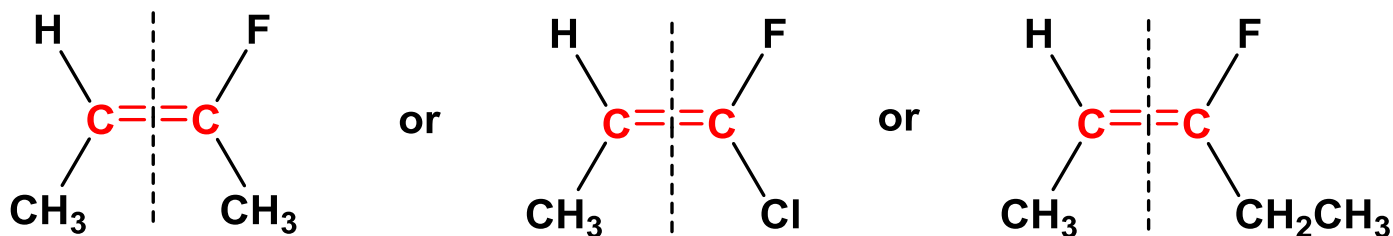


(E)-1,2-dichloroethene

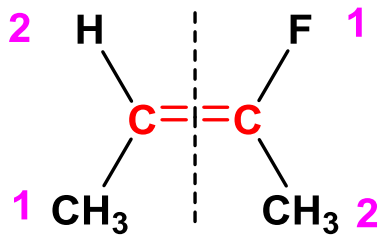
❖ If the alkene contains two or more atoms or groups of atoms which are different attached to it as shown below, How can we assign the **E** or **Z** configuration?



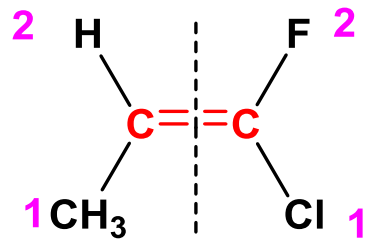
**RULE 1:** Split the double bond into half



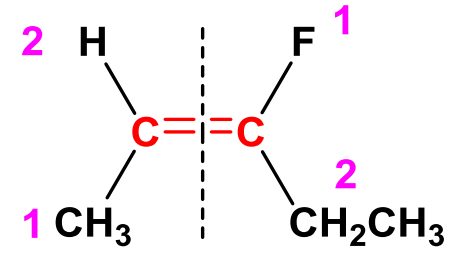
**RULE 2:** Based on the molecular weight of the atoms, assign the priority of each atom directly attached on each side of the split double bond e.g the atom with a high molecular weight is given the first priority [1] and the atom with a lower molecular weight is given the second [2] priority



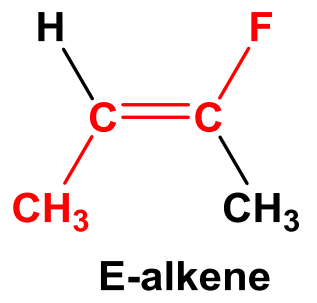
or



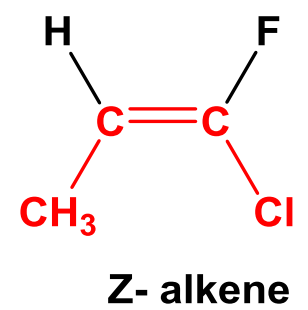
or



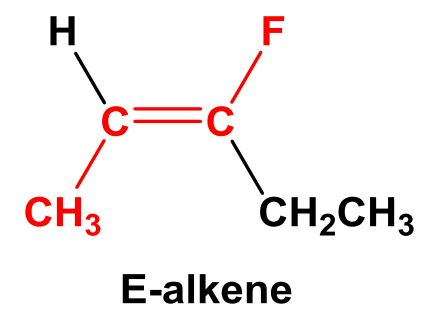
**RULE 3:** Assign E or Z based on the location of two higher group



or

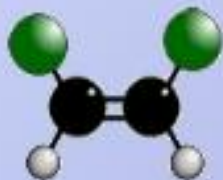


or



# How to tell if geometrical isomers exist in any given alkene

Two **different** atoms/groups attached

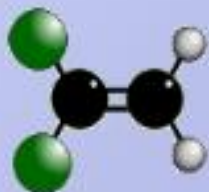


Two **different** atoms/groups attached



GEOMETRICAL ISOMERISM

Two **similar** atoms/groups attached

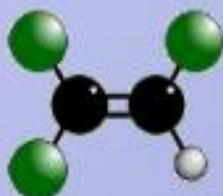


Two **similar** atoms/groups attached



Once you get two similar atoms/groups attached to one end of a C=C, you cannot have geometrical isomerism

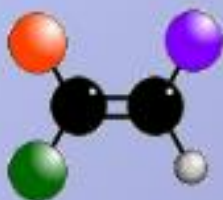
Two **similar** atoms/groups attached



Two **different** atoms/groups attached



Two **different** atoms/groups attached



Two **different** atoms/groups attached



GEOMETRICAL ISOMERISM

**END!!!!**