Lecture 3 Organic Chemistry (2)

Test situation analysis

Testing points	Number of examinations in 2010-2021
Structural Isomer	17
Cis-trans isomer and E&Z isomer	2
Optical isomer	25
Conformation isomer	15

Intensive Teaching and Practicing

Point 1：Hybridization

Hybridization: It is a mathematical procedure in which the standard atomic orbitals are combined to form new atomic orbitals called hybrid orbit als.

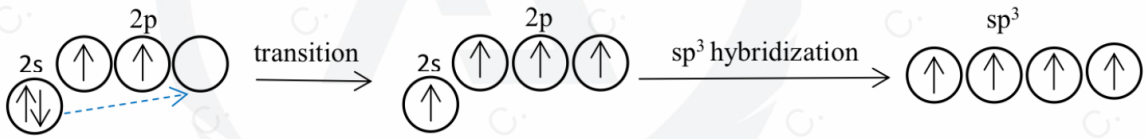
1) Greater Strength of Bond: Greater the overlap, stronger the bond and the lower the energy. In hybrid orbitals, the electron probability density is more concentrated in a single directional lobe, allowing greater overlap with the orbitals of other atoms.

2) Greater Number of Bonds: Often more number of bonds are formed after promotion and hybridization.

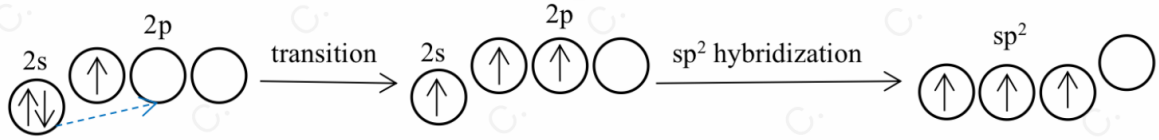
1.1 Type of hybrid track

1.1.1 sp hybrid

✓ **sp^3 hybrid**: **sp^3 hybrid** orbit is composed of **1 s** orbit and **3 p** orbits. For example, CH_4 central atom C is bonded to the coordination atom by **sp^3** hybridization.

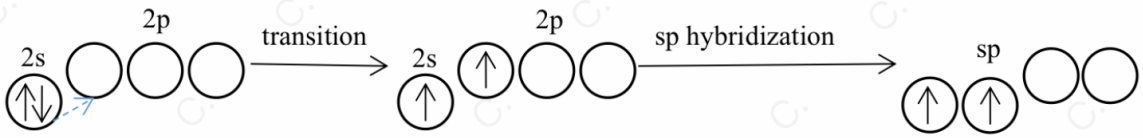


✓ **sp^2** hybrid: **sp^2** hybrid orbit is composed of 1 **s** orbit and 2 **p** orbits. For example, BF_3 central atom B is bonded to the coordination atom by **sp^2** hybridization.



✓ **sp** hybrid: **sp** hybrid orbit is composed of 1 **s** orbit and 1 **p** orbit. For example, $BeCl_2$ molecular center atom be is bonded to Cl atom by sp hybridization.

✓



1.2 A shortcut to determine the hybridization

1.Look at the atom.

2.Count the number of atoms connected to it ***(atoms** – not bonds!)*

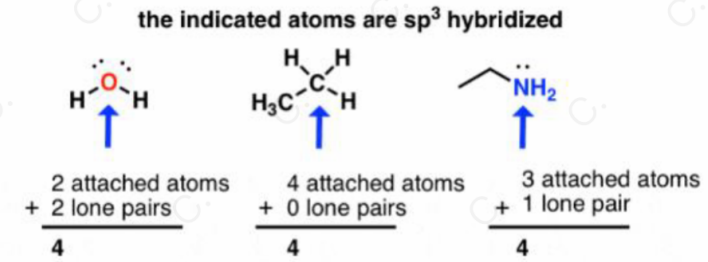
3.Count the number of lone pairs attached to it.

4.Add these two numbers together.

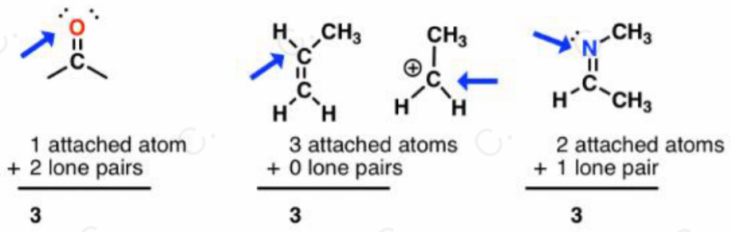
- If it's 4, your atom is sp^3.
- If it's 3, your atom is sp^2.
- If it's 2, your atom is sp.

Some examples:

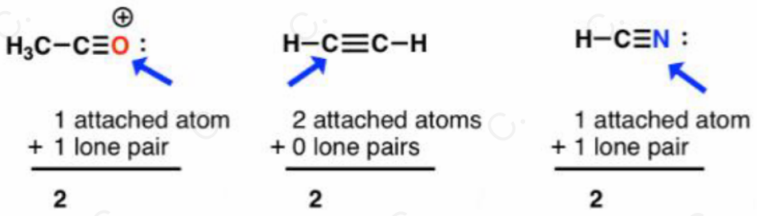
sp^3 hybridization: sum of attached atoms + lone pairs = 4



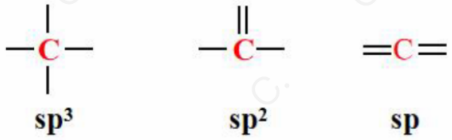
sp^2 hybridization: sum of attached atoms + lone pairs = 3



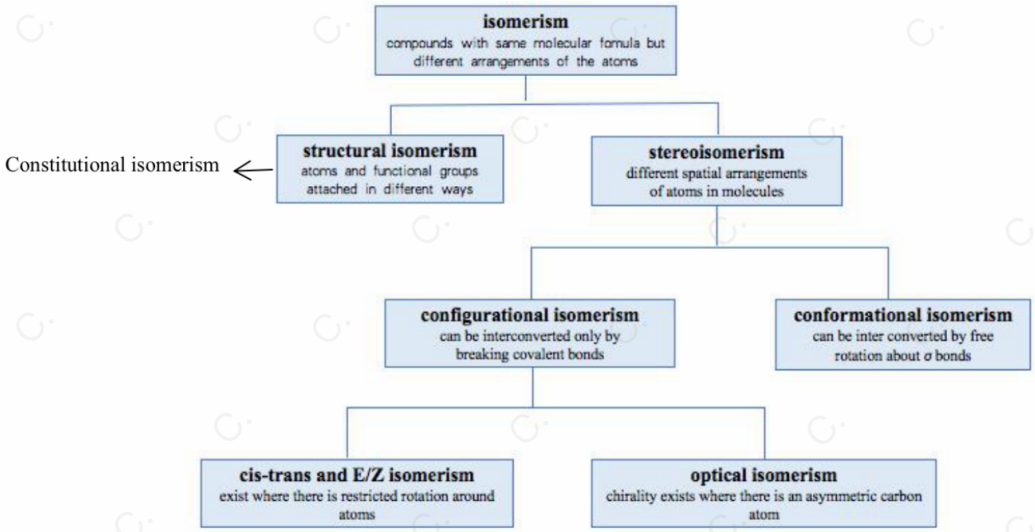
sp hybridization: sum of attached atoms + lone pairs = 2



Tips: To the carbon atom in organic compounds:



Point 2： Structural Isomer



There are various forms of isomerism – the simplest is structural isomerism.

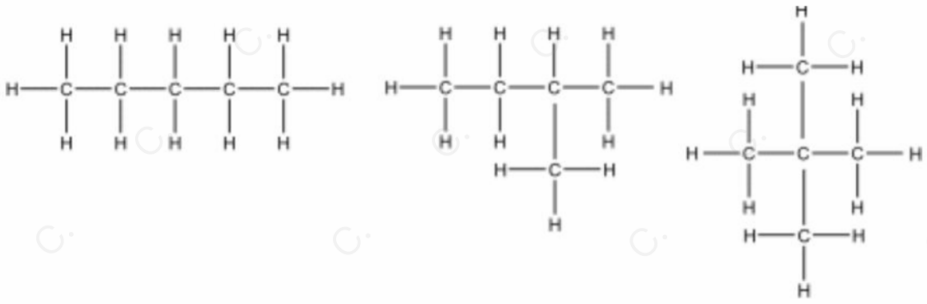
2.1 Structural isomerism (constitutional isomerism)

Definition: two or more compounds that have the same molecular formula but different arrangements of the atoms

Three types of structural isomers

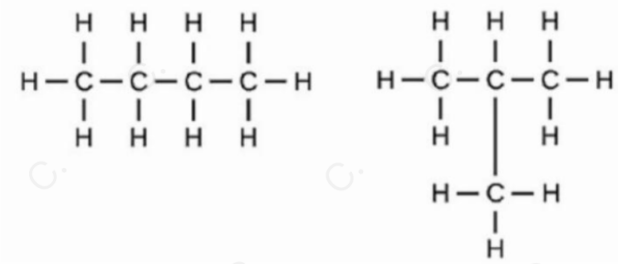
1. Chain isomer: compounds with the same molecular formula but different structures of the carbon skeleton.

For example: the structural isomers of C_5H_{12} are:



Pentane 2-methylbutane 2,2-dimethylpropane

The structural isomer for C_4H_{10} are:

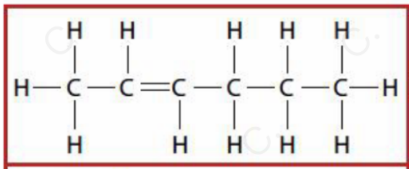
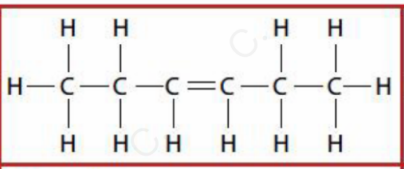
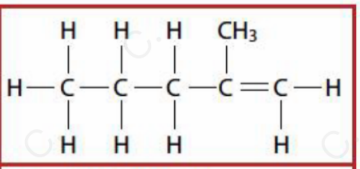
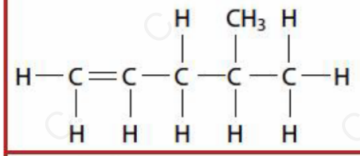
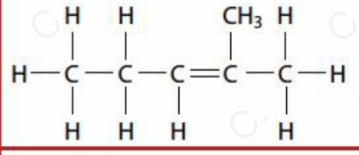
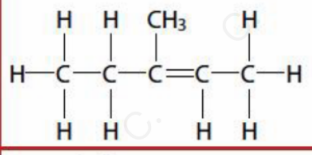


Butane 2-methylpropane

(from https://www.quora.com/How-many-isomers-are-there-for-butane)

2.Position isomer: compounds with the same molecular formula but different structures due to different positions of the same functional group on the same carbon skeleton.

For example, structural isomers for alkene C_6H_{12}

		
hex-2-ene	hex-3-ene	2-methylpent-1-ene
		
4-methylpent-1-ene	2-methylpent-2-ene	3-methylpent-2-ene

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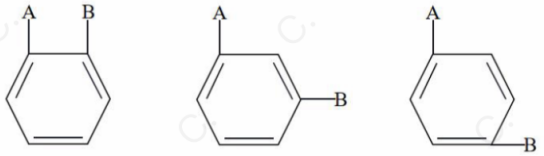
✯Positional isomerism on benzene ring

If there are two different substituents on the benzene ring, the relative positions of the two substituents can be ortho, meta and para.

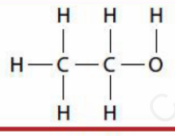
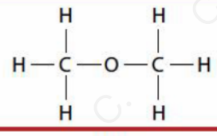
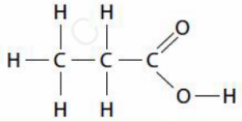
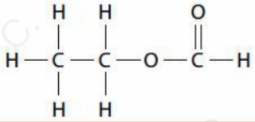
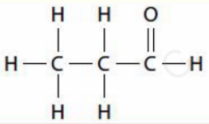
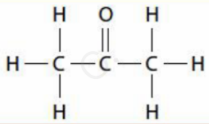


You can also remember other groups of benzene rings by the way:

six positional isomers ten positional isomers

3.Functional group isomer: compounds with the same molecular formula but with atoms arranged to give different functional groups.

Some pairs of functional group isomers are shown in the following tables.

	
alcohol	ether
	
carboxylic acid	ester
	
aldehyde	ketone

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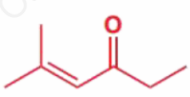
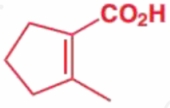
2.2 DBE(Double bond equivalent)

Double bonds (of all kinds) and rings are called **double bond equivalents** (DBEs). You can work out how many DBEs there are in a given atomic composition just by making a drawing of one possible structure for the formula (all possible structures for the same formula have the same number of DBEs).

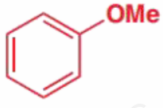
For example:



$C_7H_{12}O$
= two DBE



$C_7H_{10}O_2$
= three DBE



C_7H_8O
= four DBE

For the compounds with molecular formula $C_aH_bO_c$, the calculation formula of DBEs is

$$\text{DBEs} = a + 1 - \frac{1}{2}b$$

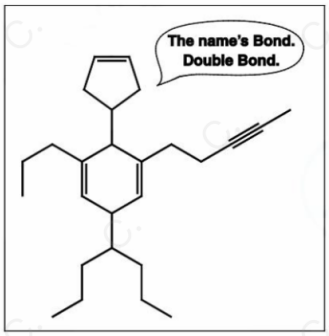
For the compounds with molecular formula $C_aH_bO_cN_d$, the calculation formula of DBEs is

$$\text{DBEs} = a + 1 - \frac{1}{2}(b - 1)$$

Example 1.*(source,UKChO,2016,3a)*

The idea of Double Bond Equivalents, DBE, the number of double bonds and / or rings that a compound contains, can be extremely useful when working out possible structures from formulae.

Mr Bond, shown on the right, has 007 DBE.



(a) The general formula for a non-cyclic alkane is C_nH_{2n+2}. Give the general formulae for the following:

(i) an alkene or cycloalkane

(ii) an alkyne (a hydrocarbon containing a C≡C triple bond)

(iii) a cycloalkene **(iv)** a di-alkyne.

(source,UKChO,2016,3b)

(b) The table below shows the possible combinations of rings, double bonds and triple bonds for DBE = 1 and DBE = 2. In your answer booklet, extend the table to show the possible combinations for DBE = 3 and DBE = 4.

DBE	Ring	Double bond	Triple bond
1	1	0	0
	0	1	0
2	2	0	0
	0	2	0
	1	1	0
	0	0	1

(source,UKChO,2016,3c)

The number of DBE in a hydrocarbon may be calculated by comparing the actual number of hydrogens (X) in a given hydrocarbon of formula C_nH_X with the number of hydrogens (A) in the non-cyclic alkane with the same number of carbon atoms (C_nH_A):

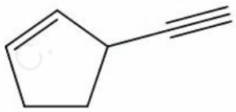
$$\mathbf{DBE = ½ \times (A - X)}$$

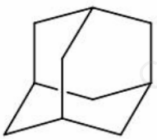
As an example, to work out the DBE for cyclohexene, C_6H_{10}, since the number of hydrogens in hexane (the alkane with 6 carbons) is 14, DBE(cyclohexene) = ½ × (14 – 10) = 2.

(c) Determine the number of double bond equivalents in:

(i) C_5H_4 **(ii)** $C_{18}H_{20}$ **(iii)** C_{60}

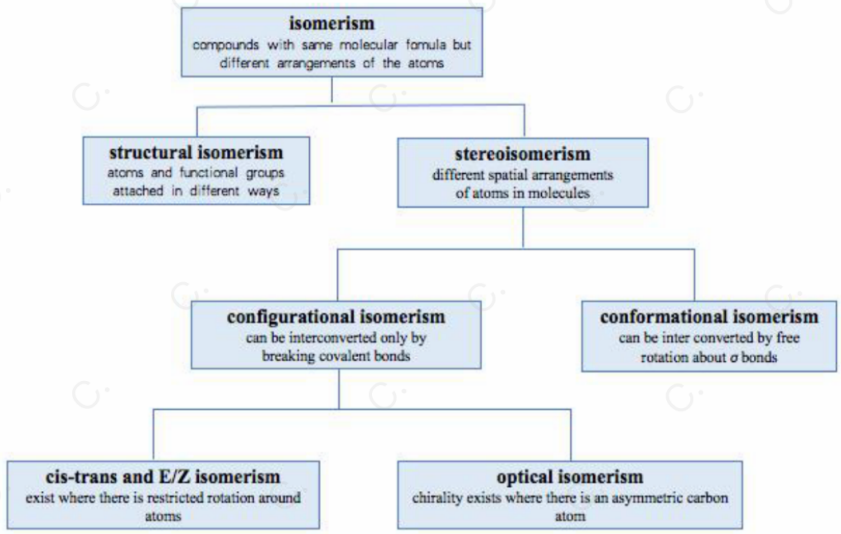
(iv) 

(v) 

(vi) 

Point 3：Stereoisomerism

Another type of isomerism known as stereoisomerism has molecules with atoms attached in the same order but which differ from each other in their spatial or three-dimensional arrangement . Where as structural isomers can represented relatively easily in two dimensions on paper. the study of stereoisomerism requires three-dimensional representation Stereoisomerism can be further broken down into different types , as shown below.



Stereoisomerism has two categories:

3.1 Configurational isomers—can only be interconverted by the breaking of bonds

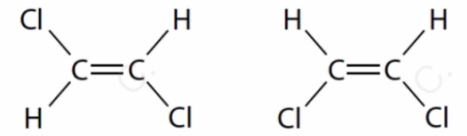
Two classifications: Cis-trans and E/Z; Optical isomerism

3.1.1 Cis-trans isomers:

Isomers that differ in their arrangement about restricted bond rotation. Also, there must be two different groups on both sides of double bonds.

cis: two functional group are in the same side

trans: two functional group are in the different side



trans -1,2-dichloroethene *cis* -1,2-dichloroethene

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★Cis-trans isomerism in cycloalkanes

The condition for a cycloalkane to exhibit cis-trans isomerism is that at least two carbon atoms must have two different groups attached.

cis isomer *trans* isomer

(from organic chemistry HL.pdf)

For example:

Cis(-1,3-dichlorocyclobutane)

Trans(-1,3-dichlorocyclobutane)

★ **Properties of cis/trans isomers**

- Cis/trans isomers have different physical properties.
- The cis isomer is polar and the trans isomer is non-polar.
- The trans form is non-polar because the orientation of the chlorine atoms around the double bond means that the dipoles cancel.
- So, there are permanent dipole-dipole interactions for the cis form but not for the trans form.
- Thus, cis has higher boiling point because cis is more polar.

- Trans has high melting point because there is strong intermolecular force in trans but strong intramolecular force in cis, so attraction between molecules in cis is less hence lower melting point

3.1.2 E/Z isomer

The cis and trans nomenclature only works when there are two different functional groups around C=C bonds.When there are four different groups around the C=C bond, it should be called E/Z isomer.

E/Z isomer based on the Cahn-Ingold-Prelog (CIP) rules which assign priority around a double bond based on the atomic numbers of attached atoms.

The priority rules:

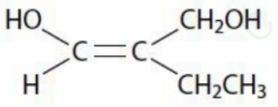
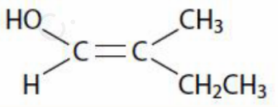
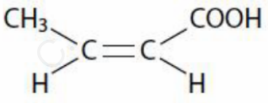
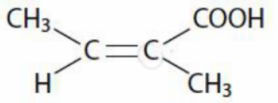
Rule 1: the atom with the higher atomic number has higher priority.

Rule 2: the longer hydrocarbon chains have higher priority

Compare the positions of the highest priority:

Two highest priority groups are on the same side of double bond, the isomer is 'Z'.

Two highest priority groups are on the opposite side of the double bond, they are 'E'.

	
Z	*E*
	
Z	*Z*

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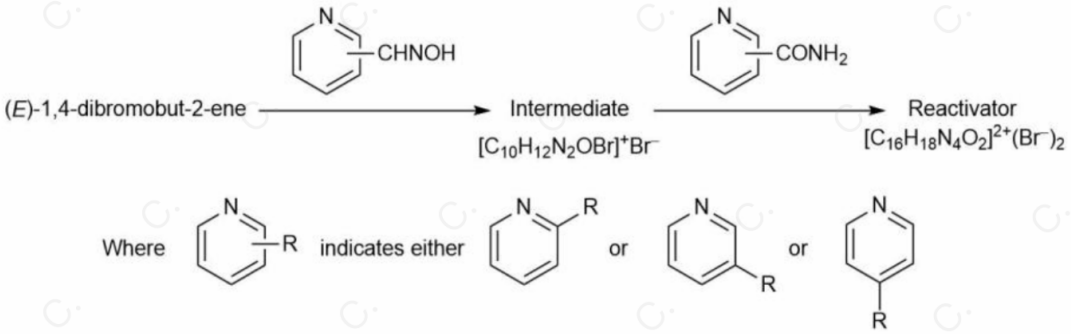
Example 2.(source,UKChO,2019,3e)

Another important research area is developing more effective AChE reactivators fortreating nerve agent poisoning. One new group of reactivators was developed using

(*E*)-1,4-dibromobut-2-ene as a starting material.

(e) Draw the structure of (*E*)-1,4-dibromobut-2-ene.

This group of reactivators was synthesised via a 2-step pathway, using a series of related reagents:

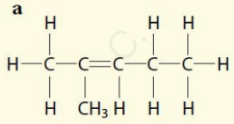


(f) How many different reactivators could be made with the above set of reagents?

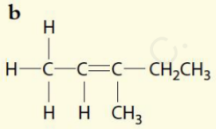
Exercise 2:

42 Which of the following will exhibit *cis–trans* isomerism? If the molecule exhibits *cis–trans* isomerism, draw the *cis* and *trans* forms.

a



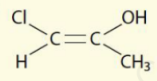
b



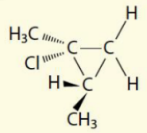
c 2,3-dimethylpent-2-ene
d 3,4-dimethylpent-2-ene
e 1,2,3-trimethylcyclopropane
f 1,3-dimethylcyclobutane

43 Classify each of the following isomers as *E* isomers or *Z* isomers.

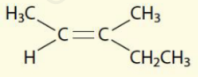
a



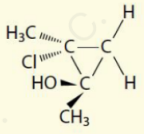
c



b



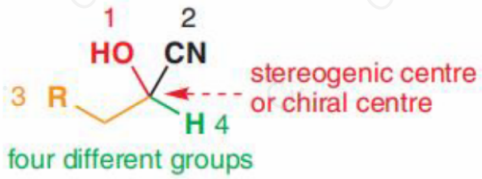
d



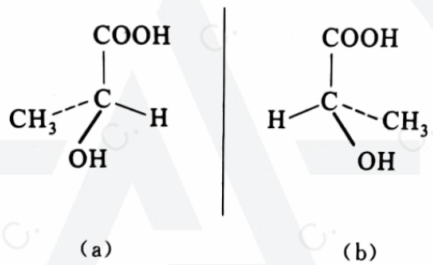
3.2 Optical isomers

3.2.1 Chair centre

If a molecule contains one carbon atom carrying four different groups it will not have a plane of symmetry and must therefore be chiral. A carbon atom carrying four different groups is a stereogenic or chiral centre.

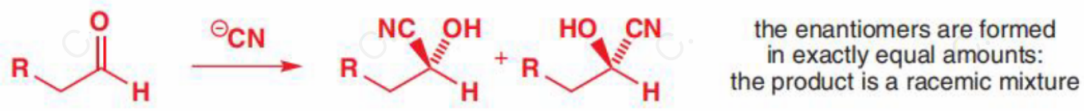


Compounds containing one chiral centre can have two configurations, for example:



No matter how **(a)** and **(b)** are flipped, they cannot completely overlap. They are the relationship between real object and mirror image.**Therefore, such isomers are called enantiomers.**

We saw how the two enantiomers of the aldehyde cyanohydrin arose by attack of cyanide on the two faces of the carbonyl group of the aldehyde. We said that there was nothing to favour one face over the other, so the enantiomers must be formed in equal quantities. A mixture of equal quantities of a pair of enantiomers is called a **racemic mixture**.



Isomers of each other are non-superimposable.

A solid wedge indicates a bond coming out the plane of the paper; a dashed wedge goes into the paper.

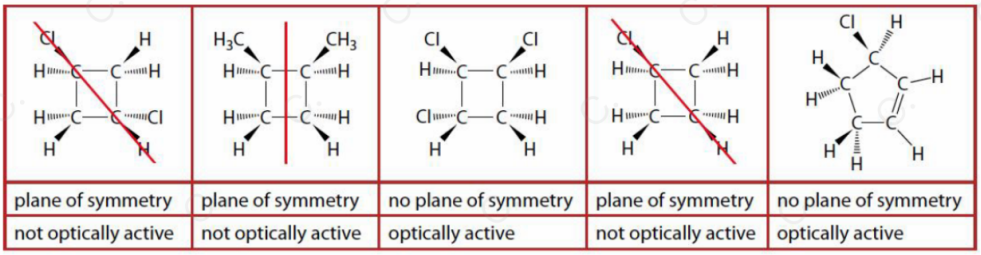
Enantiomers have identical physical and chemical properties but may have different physiological effects.For example:The artificial sweetener Aspartame is an optical isomer, one of its enantiomers tastes sweet, the other bitter.

- Optical isomerism and ring compounds

  Optical isomerism can also occur with ring compounds.

  To determine if a ring compound has optical isomers, it is necessary to look at whether or not the molecule has a plane of symmetry.

  If a ring compound does have a plane of symmetry, then it will not have optical isomers.

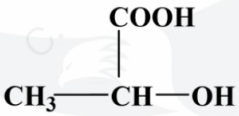


plane of symmetry	plane of symmetry	no plane of symmetry	plane of symmetry	no plane of symmetry
not optically active	not optically active	optically active	not optically active	optically active

(Page 497 Chemistry for IB Diploma Coursebook 2nd editions)

3.2.2 R and S can be used to describe the configuration of a chiral centre

We can use the following set of rules to assign a letter, *R* or *S*, to describe the configuration of groups at a chiral centre in the molecule.For example:



1. Assign a priority number (1–4) to each substituent at the chiral centre. Atoms with higher atomic numbers get higher priority.

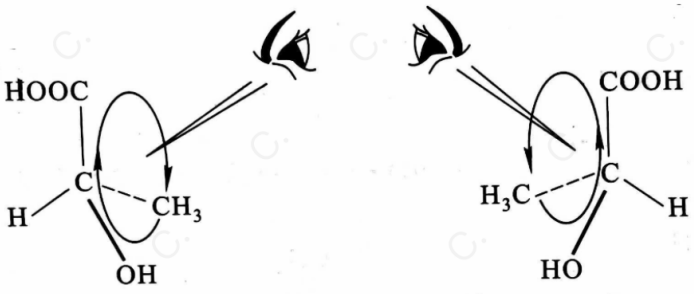
If two (or more) of the atoms attached to the chiral centre are identical, then we assign priorities to these two by assessing the atoms attached to those atoms. In this case, one of the carbon atoms carries oxygen atoms (atomic number 8) and one carries only hydrogen atoms (atomic number 1). So —COOH is higher priority that —CH_3;

So: —OH＞—COOH＞—CH_3＞H

2. **Arrange the molecule so that the lowest priority substituent is pointing away from you.**

In our example, naturally extracted alanine, H is priority 4, so we need to look at the molecule with the H atom pointing into the paper.

3.Mentally move from substituent priority 1 to 2 to 3. If you are moving in a clockwise manner, assign the label *R* to the chiral centre; if you are moving in an anticlockwise manner, assign the label *S* to the chiral centre.



顺时针方向 反时针方向

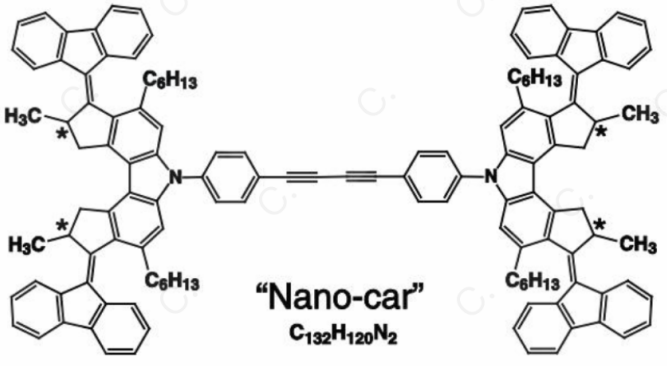
（*R*）−乳酸 （S）−乳酸

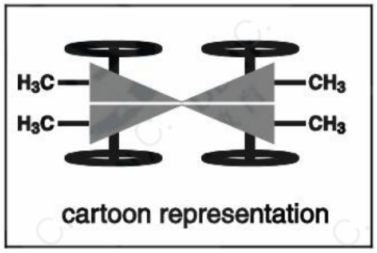
A pair of enantiomers are both chiral molecules with mirror symmetry , one compound is (S),the other compound is(R)

Example 3.*(source,UKChO,2012,5a)*

This question is about the world's smallest powered car

In November of 2011, the premier scientific journal Nature published an article titled "Electrically driven directional motion of a four-wheeled molecule on a metal surface". Essentially, this paper reported the synthesis and observations of the world's smallest powered car – the "Nano-car".





On completion of the synthesis, the sample was analysed using NMR and mass spectrometry. Not surprisingly, the group did not submit their precious material for combustion analysis!

(a) i) Give an equation for the complete combustion of nano-car.

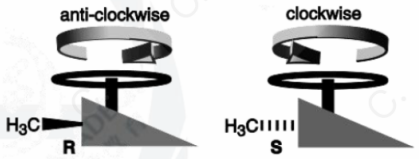
ii) Calculate the percentage by mass of carbon, hydrogen and nitrogen that would be predicted were the analysis to be performed. Give your answers to two decimal places.

(source,UKChO,2012,5b)

Crucial in the design of the molecule are the hexyl and methyl groups shown explicitly in the structure above. It is because of these that the aromatic "wheels" of the car are actually arranged at an angle, straining the double bond that attaches them to the rest of the structure. This double bond can break, rotate and reform when sufficient electronic energy is provided using the tip of a scanning tunnelling microscope.

The carbon atoms to which the methyl groups are attached are chiral centres – each has four different groups attached to it. These are marked with an asterisk in the structure above.

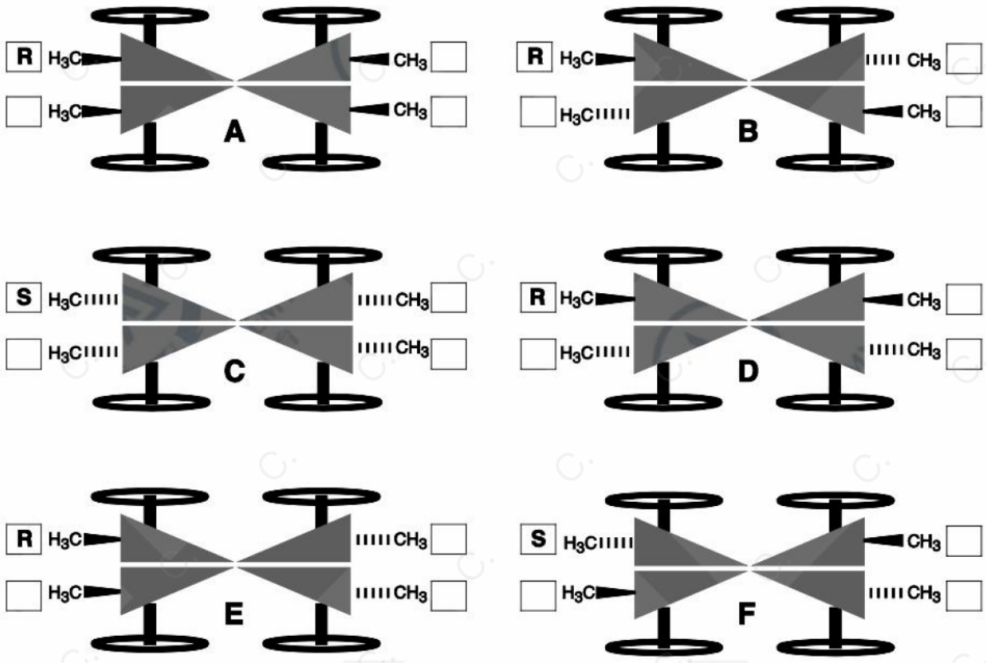
The car is made up of four rotor units. A separate rotor unit exists as optical isomers – non-superimposable mirror images called enantiomers. Chemists distinguish between them with the labels "R" and "S" as shown on the right.



The bold wedge comes out of the paper; the hashed bond goes into the plane.

The "wheels" on each enantiomer turn in opposite directions as shown (as viewed as if standing next to the car facing the wheel).

In the synthesis of the car, a number of different stereoisomers were formed. These are shown in cartoon form below, in the arrangements the chemists detected on a surface of copper atoms (as viewed from above).



(b) In your answer booklet, assign the label "R" or "S" to each rotor unit in the cars **A-F** in the boxes provided. The top left rotor in each car has already been assigned.

(source,UKChO,2012,5c)

(c) Which of the cars **A-F** are optical isomers?

(source,UKChO,2012,5d)

(d) Before being deposited on the copper surface, rotation is possible about the triple bonds linking the two halves of the car. Taking this into account, which of the cars **A-F** are the same molecule when free from the surface?

(source,UKChO,2012,5e)

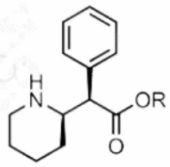
(e) By considering the directions of rotation for the four rotor units in each car, and assuming that all four rotors are active simultaneously, complete the table in the answer booklet, indicating whether each car will :

- spin round on the copper surface clockwise
- spin round on the copper surface anti-clockwise
- remain stationary on the copper surface
- move forwards over the copper surface.

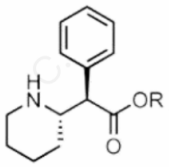
Exercise 3. ***(source,UKChO,2015,3g)***

Stereoisomers of a molecule are isomers that have the same connectivity between the atoms but a different three-dimensional arrangement in space. The effectiveness of a drug depends on its three-dimensional shape.

This synthesis leads to the production of a mixture of four stereoisomers of Ritalin, shown below. Some of these isomers are more effective than others.



1



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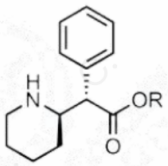

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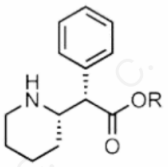


4

(g) Indicate which of these isomers are enantiomers (non-superimposable mirror images).

Point 4： Conformation

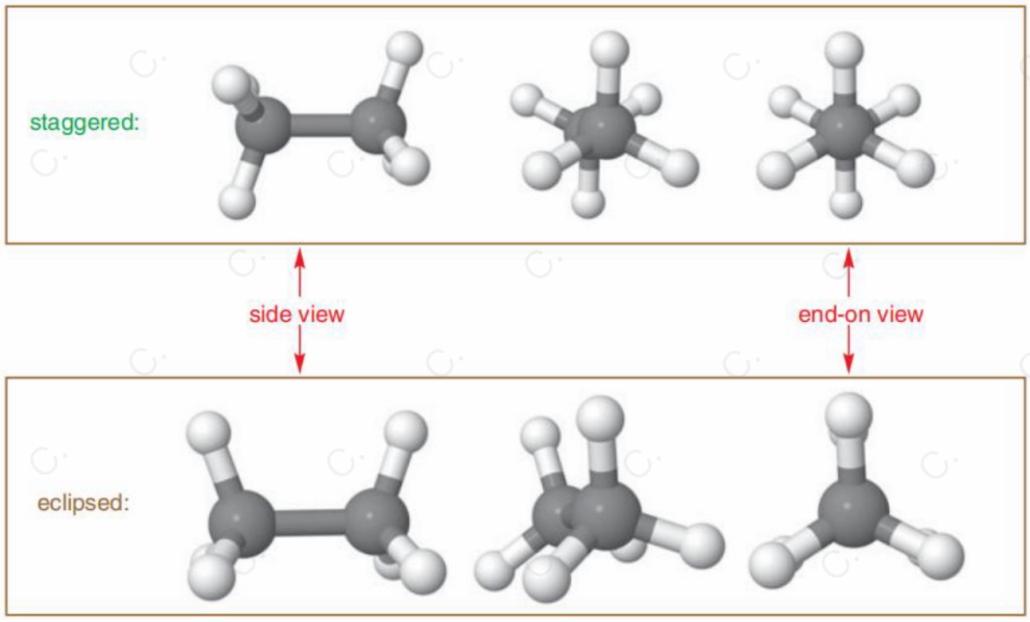
Conformational isomerism interconvert by rotation about a σ bond, which belongs to stereoisomerism.

4.1 Conformations of ethane

Due to the free rotation of the C-C bond, ethane can have a wireless number of conformations.But only one conformation has the lowest thermodynamic energy, may be more stable than others, and so are favoured.Ethane has two extreme conformations called the staggered and eclipsed conformations.

Three different views of these are shown below.

the two extreme conformations of ethane, staggered and eclipsed, each shown from three different viewpoints



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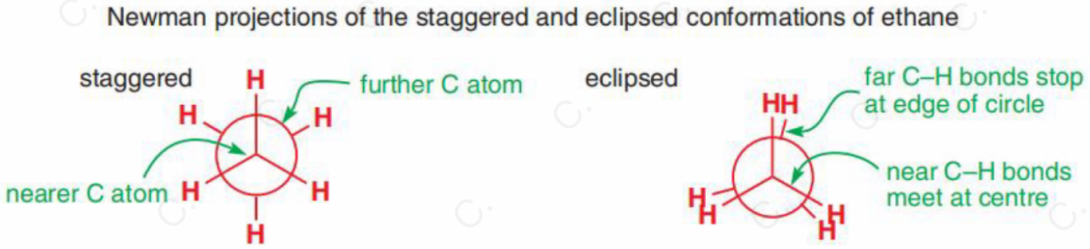
The conformation can be expressed by **Newman projection formula.**



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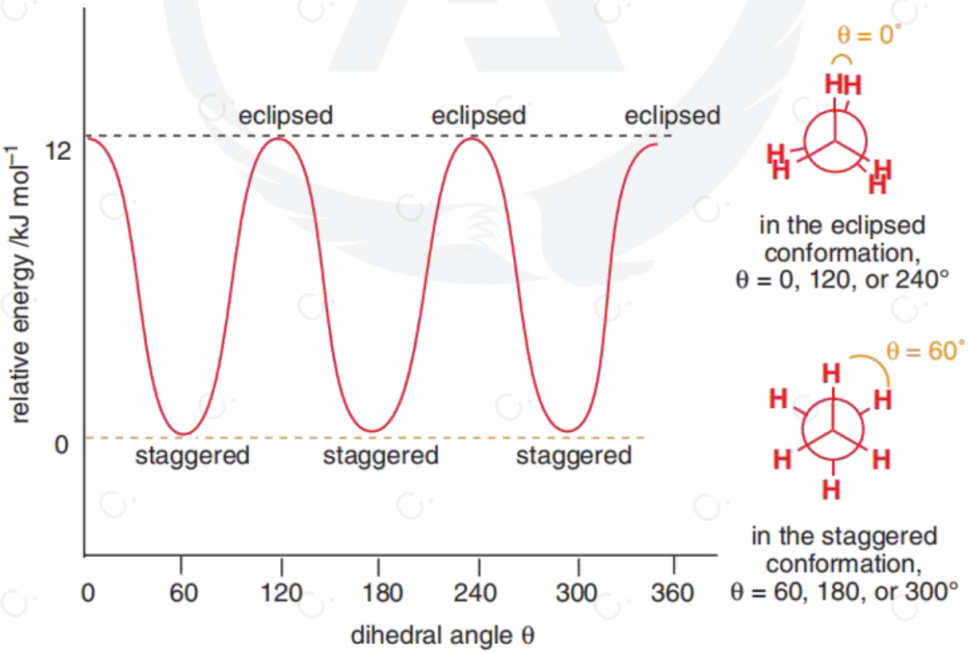
The staggered and eclipsed conformations of ethane are not identical in energy: the staggered conformation is lower in energy than the eclipsed by 12 kJ mol^{-1}.The energy level diagram shows the staggered conformation as a potential energy minimum whilst the eclipsed conformation represents an energy maximum. This means that the eclipsed conformation is not a stable conformation since any slight rotation will lead to a conformation lower in energy. The molecule will actually spend the vast majority of its time in a staggered or nearly staggered conformation and only briefly pass through the eclipsed conformation *en route* to another staggered conformation.



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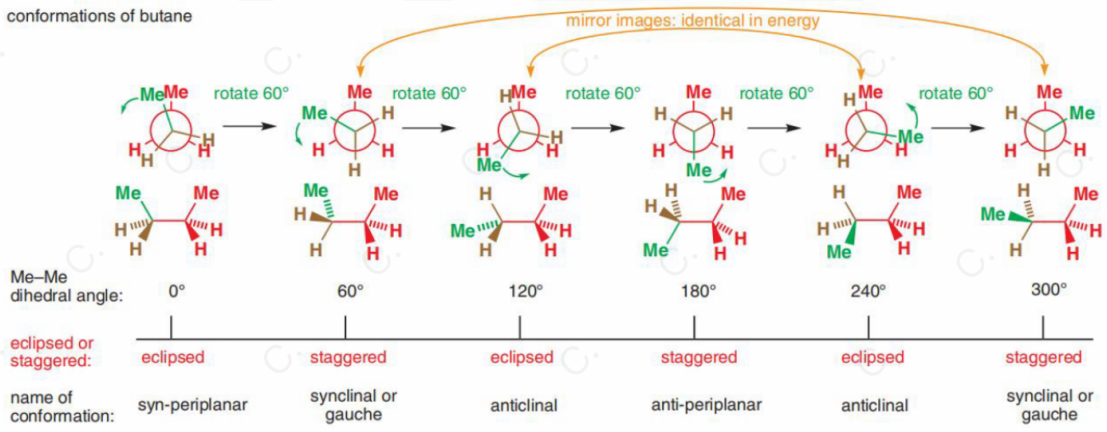
Why is the eclipsed conformation higher in energy than the staggered conformation?

In the staggered conformation, the distance between the hydrogen atoms on the two carbon atoms is the farthest and the repulsive force between them is the smallest, so the molecular thermodynamic energy is the lowest.

4.2 Conformations of butane

Now we have effectively replaced two hydrogen atoms in ethane by larger methyl groups. These are large enough to get in the way of each other, and steric repulsion becomes a significant contribution to the rotational energy barriers. However, the main complication is that, as we rotate about the central C–C bond, not all the staggered conformations are the same, and neither are all the eclipsed conformations. The six conformations that butane can adopt as the central C–C bond is rotated in 60° intervals are shown below. The green Me group and the brown hydrogens are rotating while the substituents on the other carbon atom remain still.



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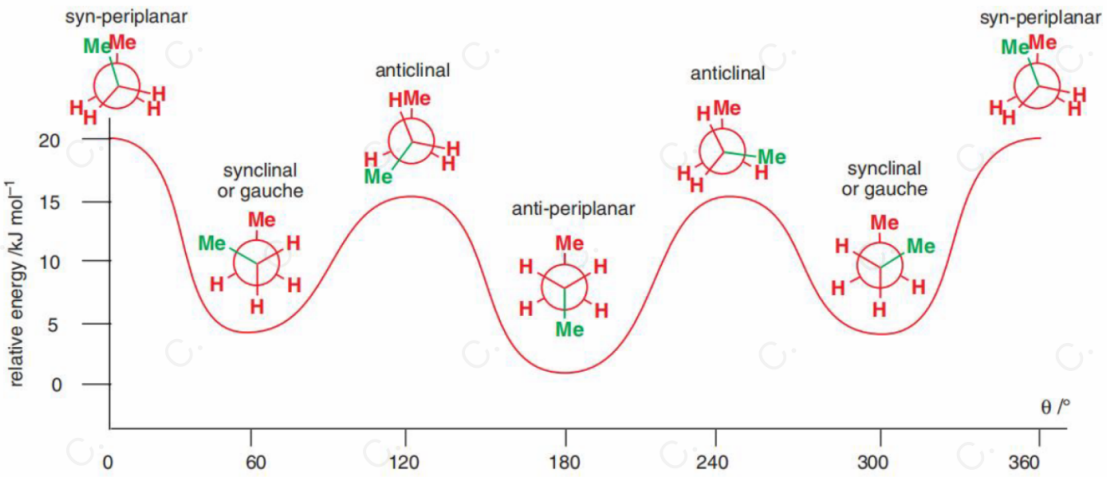
Look closely at these different conformations. The conformations with dihedral angles 60° and 300° are actually mirror images of each other, as are the conformations with angles 120° and 240°. This means that we really only have four different maxima or minima in energy as we rotate about the central C–C bond: two types of eclipsed

conformation, which will represent maxima in the energy–rotation graph, and two types of staggered conformation, which will represent minima. These four different conformations have names, shown in the bottom row of the diagram.



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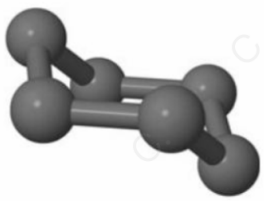
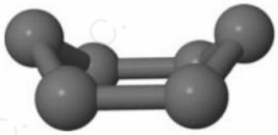
4.3 Conformations of cyclohexane

If you were to join six tetrahedral carbon atoms together, you would probably find that you ended up with a shape like this—the **chair conformation.**All the carbon atoms are certainly not in the same plane, and all the bond angles are 109.5°.



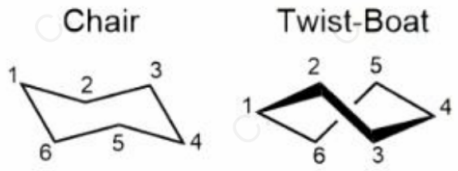
There is another conformation of cyclohexane that you might have made that looks like this.This conformation is known as the **boat conformation**.However, this is not a stable conformation of cyclohexane, even though there is no bond angle strain (all the angles are 109.5°).



Example 4.*(source,UKChO,2017,4a)*

This question is about the molecule twistane

Although the skeletal structure of cyclohexane (C_6H_{12}) is often represented as a regular hexagon, it is actually a flexible molecule that exists in a variety of different shapes referred to as *conformations*. Two of these conformations, the *chair* and the *twist-boat*, are shown below. The carbon atoms in the six-membered rings have been numbered 1-6 to show their connectivity.

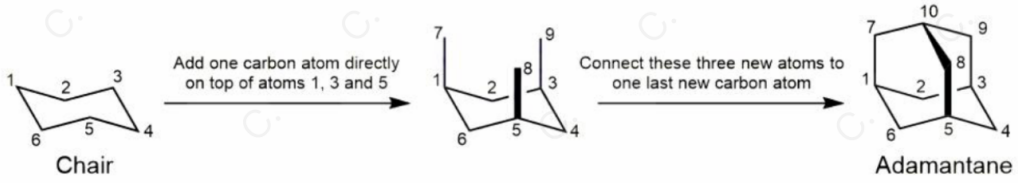


The chair is the lowest energy conformation of cyclohexane with all the bond angles almost equal to the ideal angle for a tetrahedral carbon atom. The twist-boat is higher in energy.

(a) By how many degrees does the ideal C–C–C angle in the chair form of cyclohexane differ from that in a regular hexagon?

(source,UKChO,2017,4b)

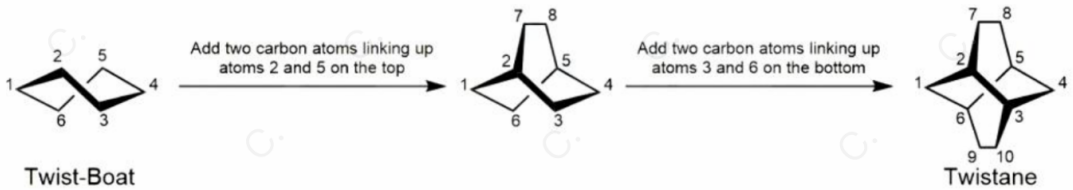
The molecule *adamantane* can be visualised by the addition of a further four carbon atoms onto the chair conformation of cyclohexane as shown below. In doing this, other six-membered rings are created. In adamantane all the six-membered rings are locked in the chair conformation.



(b) For each unique six-membered ring in adamantane, write down the numbers of the six carbon atoms in that ring in the order they are connected, beginning with the lowest number (e.g. -1-2-3-4-5-6-).

(source,UKChO,2017,4d、f)

The molecule *twistane* can be visualised by the addition of a further four carbon atoms onto the twist-boat conformation of cyclohexane as shown below. In doing this other six-membered rings are created. In twistane all the six-membered rings are locked in the twist-boat conformation, which gives the molecule its name.



(d) For each unique six-membered ring in twistane, write down the numbers of the six carbon atoms in that ring in the order they are connected, beginning with the lowest number (e.g. -1-2-3-4-5-6-).

(f) Adamantane and twistane are isomers of each other. What is their molecular formula?

Point 5: Reaction—Alkane/ Alkene/ Alcohol /Halogen alkane Reaction

Alkane / alkene / alcohol / halogen alkane conversion requires addition, elimination and substitution.

5.1 Substitution reaction

$$R\text{-}X + R'\text{-}Y \rightarrow \quad R\text{-}Y + R'\text{-}X$$

5.1.1 Substitution reactions of alkanes: such as the reaction of methane with chlorine.

$$\underset{\text{methane}}{CH_4} + Cl_2 \xrightarrow{\text{sunlight}} \underset{\text{chloromethane}}{CH_3Cl} + HCl$$

5.1.2 Nucleophilic substitution reaction

Nucleophile: a nucleophile is an electron-rich species containing a lone pair that it donates to an electron-deficient carbon.

- Nucleophilic substitution with aqueous hydroxide ions.

$$CH_3CH_2CH_2Br + NaOH \rightarrow CH_3CH_2CH_2OH + NaBr$$

- Alcohol is replaced by a halogen atom to produce a halogenoalkane

$$\underset{\text{ethanol}}{CH_3CH_2OH} + HCl \longrightarrow \underset{\text{chloroethane}}{CH_3CH_2Cl} + 3H_2O$$

Sulfur dichloride oxide, $SOCl_2$, can also be used to substitute a chlorine atom into an alcohol molecule, as shown below:

$$C_2H_5OH + SOCl_2 \longrightarrow C_2H_5Cl + HCl + SO_2$$

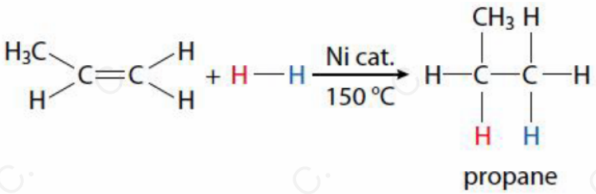
Note that in this reaction the two byproducts of the reaction (HCl and SO_2) are both gases. These escape from the reaction mixture, leaving the halogenoalkane.

5.2 Addition reaction

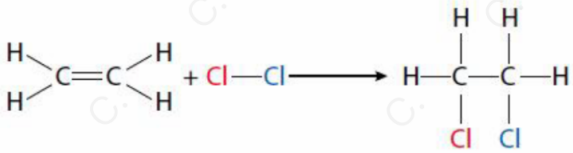
Addition involves the formation of a single product from two reactant molecules.

Addition of alkenes, for example:

Addition of alkenes with hydrogen (hydrogenation)

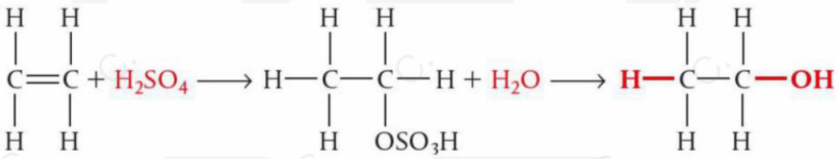


Addition of alkenes with halogens



Addition of alkenes with hydrogen halides:

Addition of alkenes with water:



5.3 Elimination

5.3.1 Halogenoalkanes also undergo elimination reactions.

An elimination reaction involves the loss of a small molecules from the original organic molecules.

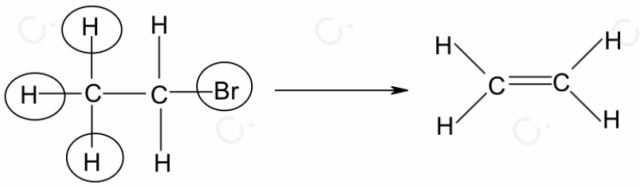
For example:

$$C_2H_5Br + C_2H_5ONa \rightarrow C_2H_4 + NaBr + C_2H_5OH /$$
$$C_2H_5Br + NaOH \rightarrow C_2H_4 + NaBr + H_2O ;$$

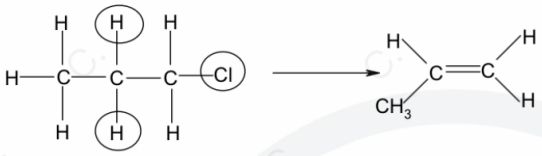
Reagent: sodium hydroxide

Condition: in ethanol, heat

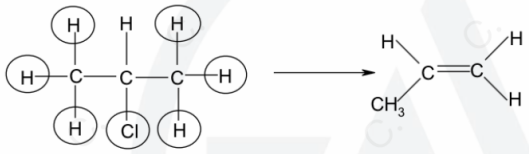
The hydrogen is always lost from a carbon atom adjacent to the carbon atom attached to the halogen (all the hydrogen atoms which could be removed have been circled). Sometimes this can result in more than one possible product:



bromoethane ethene

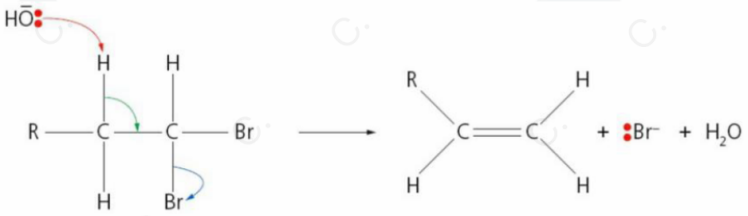


1-chloropropane propene



2-chloropropane propene

Mechanism:



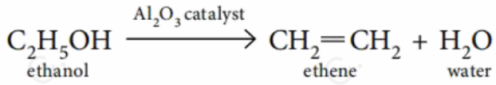
(page 552 aqa chemistry for year 1 and AS)

5.3.2 Dehydration

Alcohols can also undergo elimination reactions in which water is lost and alkenes are formed. As the small molecule removed from the alcohol molecule is H_2O, this reaction is also known as **dehydration**.

The reaction takes place when alcohol vapour is passed over a hot catalyst of aluminium oxide powder. Pieces of porous pot or pumice also catalyse the reaction.

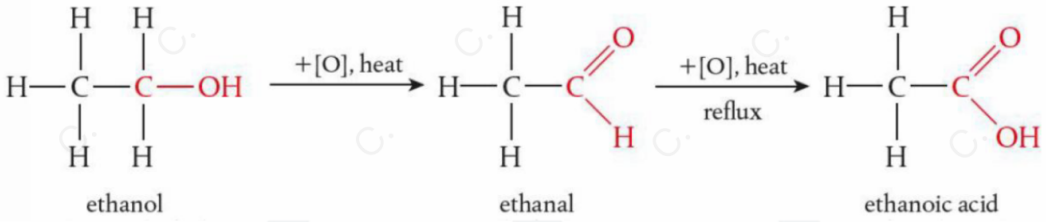
For example:



5.4 Oxidation

- Oxidation of alcohols:

Primary alcohols are oxidised to aldehyde first (partial oxidation), and then aldehyde is oxidised further to a carboxylic acid (complete oxidation).



(from notes – fundamentals of organic chemistry SL ppt)

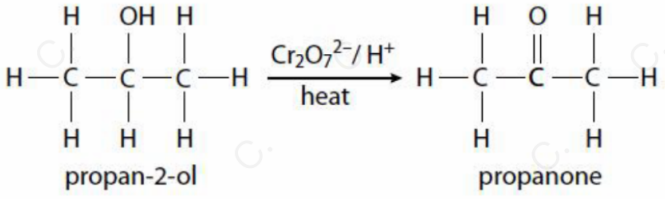
Also, each reaction can be shown as a balanced equation using [O] to represent oxygen from the oxidising agent.

$$CH_3CH_2OH + [O] \rightarrow CH_3CHO + H_2O$$

$$CH_3CHO + [O] \rightarrow CH_3COOH$$

- Secondary alcohol

Secondary alcohol will be oxidised to ketone by using heat under reflux, which cannot be oxidised any further.



(Page 461 Chemistry for IB Diploma Coursebook 2nd editions)

The balanced equation for the reaction is:

$$CH_3CH(OH)CH_3 + [O] \rightarrow (CH_3)_2CO + H_2O$$

5.5 Reduction reactions

5.5.1 Reduction of aldehydes, ketones and carboxylic acid

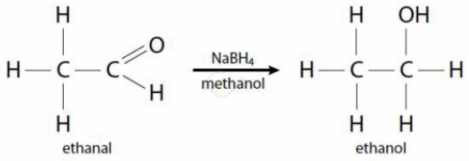
Common reducing agents are lithium aluminium hydride ($LiAlH_4$) and sodium borohydride ($NaBH_4$).

$LiAlH_4$ is the stronger reducing agent and can be used to reduce carboxylic acids, aldehydes and ketones. Conditions should be in dry ether.

$NaBH_4$ is only strong enough to reduce aldehydes and ketones. Conditions should be in alkaline or alcohol solution.

(1) Reduction of aldehydes

Aldehyde could be reduced to primary alcohol.



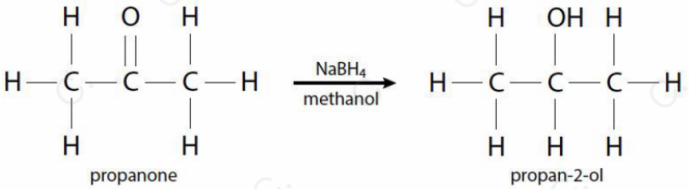
(Page 481 Chemistry for IB Diploma Coursebook 2nd editions)

A balanced equation for the reaction can be written using [H] to represent hydrogen from the reducing agent:

$$CH_3CHO + 2[H] \rightarrow CH_3CH_2OH$$

(2) Reduction of ketones

Ketones could be reduced to secondary alcohol.



(Page 481 Chemistry for IB Diploma Coursebook 2nd editions)

(3) Reduction of carboxylic acids

Carboxylic acid could be reduced to primary alcohols.

A stronger reducing agent $LiAlH_4$ must be used for the reduction of carboxylic acids.

Exercise 4.*(source,UKChO,2015,4a)*

This question is about hangovers

After the consumption of too much alcoholic beverage, people sometimes experience a hangover the following day. There are a variety of causes of a hangover, one of these is the accumulation of the toxic metabolites of ethanol in the body.

In the body, ethanol is first converted into acetaldehyde by the enzyme alcohol dehydrogenase and then into acetic acid by the enzyme acetaldehyde dehydrogenase.

$$\text{Ethanol} + NAD^+ \xrightarrow{\text{Alcohol Dehydrogenase}} \text{Acetaldehyde} + NADH + H^+$$

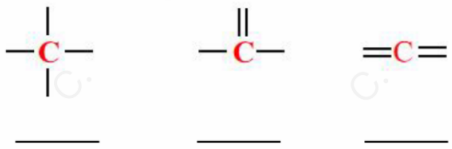
(a) What happens to the NAD^+ in this reaction? Circle the correct answer.

it is oxidised	it is reduced	it is hydrolysed	it is isomerised	it remains chemically unchanged

Summary

Point 1:Hybridization

Hybridization of carbon atoms in organic compounds:



_____ _____ _____

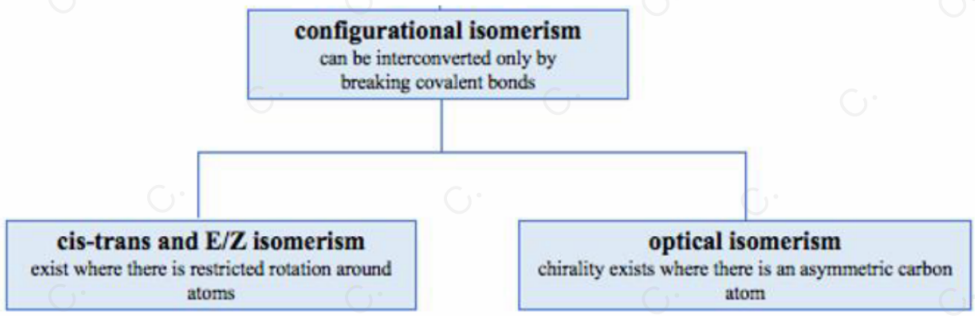
Point 2:Structural isomer

Same molecular formula , different arrangements of the atoms

There are three types of structural isomer:

1. _____ isomer
2. _____ isomer
3. _____ isomer

Point 3: Stereoisomerism



1.Cis-trans＆E/Z isomerism

Isomers that differ in their arrangement about restricted bond rotation. Also, there must be two different groups on both sides of double bonds.

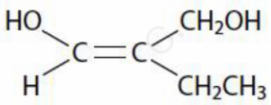
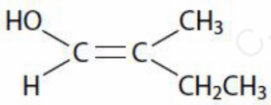
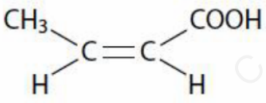
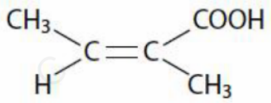
cis: two functional group are in the _____ side

trans: two functional group are in the _____ side

The cis and trans nomenclature only works when there are two different functional groups around C=C bonds.When there are four different groups around the C=C bond, it should be called E/Z isomer.

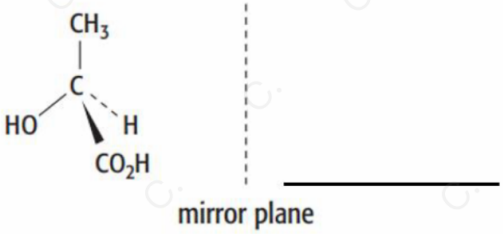
Two highest priority groups are on the _____ side of double bond, the isomer is 'Z'.

Two highest priority groups are on the _____ side of the double bond, they are 'E'.

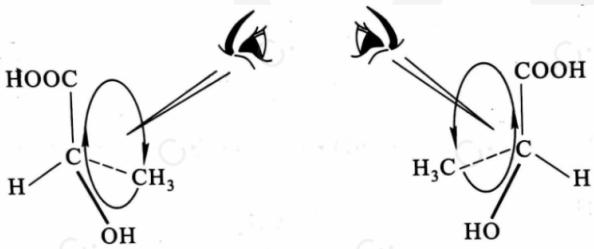
	
Z	*E*
	
Z	*Z*

2.Optical isomerism

Compounds containing one _____ centre can have two configurations:

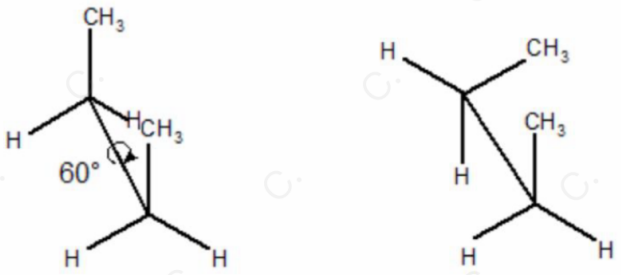


R&S

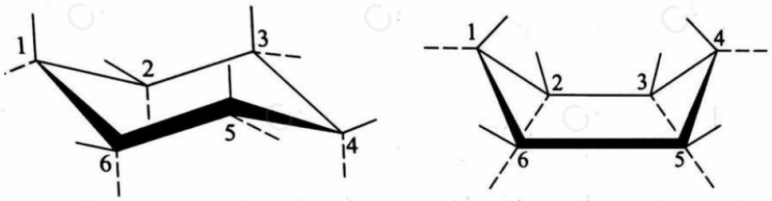


Point 4:Conformation

Conformational isomerism interconvert by rotation about a ____ bond. so in most cases cannot be isolated separately. Some conformers of a compound though , may be more stable than others, and so are favoured.



Conformations of cyclohexane



Point 5: Reaction—Alkane/Alkene/Alcohol /Halogen alkane Reaction