

Tutorial Letter 203/1/2018

General Chemistry 1B

CHE1502

Semester 1

Department of Chemistry

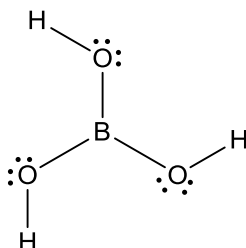
This tutorial letter contains the key to assignment 05.

BARCODE

FIRST SEMESTER

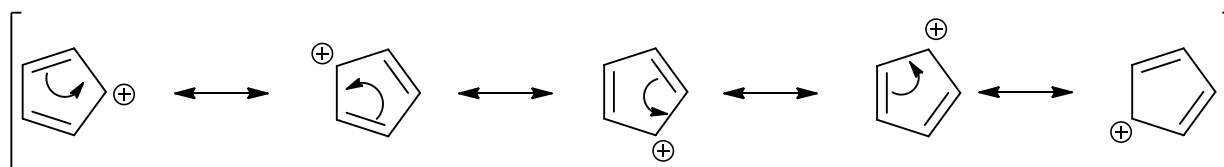
KEY TO ASSIGNMENT 5

1. The Lewis structure for boric acid, $B(OH)_3$:



B has 3 valence electrons; O has 6 valence electrons and H has 1 valence electron.

2. The resonance delocalization takes place as follows:



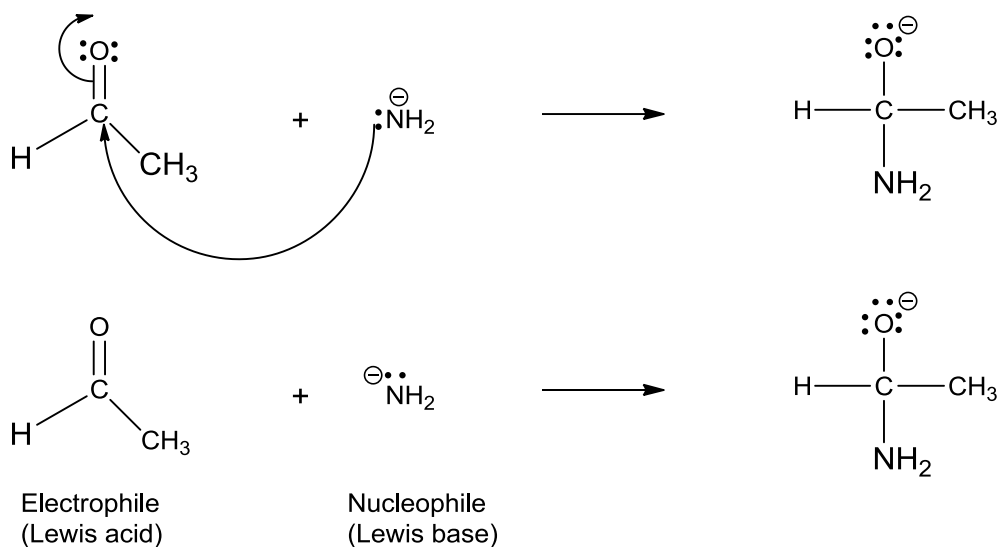
Note that electrons move from the electron rich pi bond to the electron deficient carbocation.

Guidelines for Drawing Resonance Structures:

- 1) Do not change the connection of atoms - leave the atoms in the structure exactly where they are located.
- 2) Draw complete Lewis structures to start with – i.e. draw in all hydrogens and lone pairs of electrons
- 3) ONLY the position of electrons change when drawing resonance structures
- 4) The electrons in π bonds or non-bonding (unshared) pairs can freely participate in resonance. Therefore, anions and lone pairs of electrons on for example, nitrogen, oxygen, halogens, etc. can participate in resonance.
- 5) The total number of electrons does not change.
- 6) Obey the octet rule on any atom - do not exceed the octet rule.

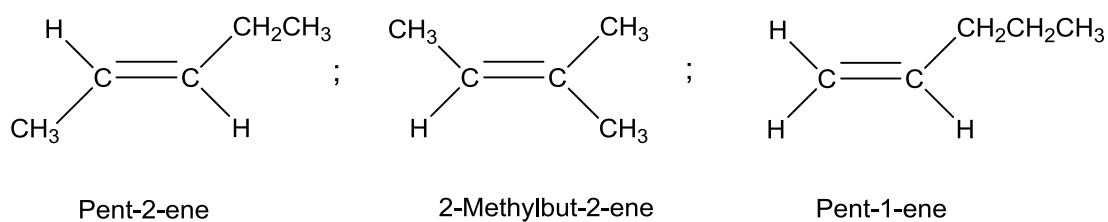
Electrons can only move if the π bonds are conjugated and/ or if a charge (positive or negative) is conjugated to π bond(s).

3. The movement of electron pairs in the reaction:

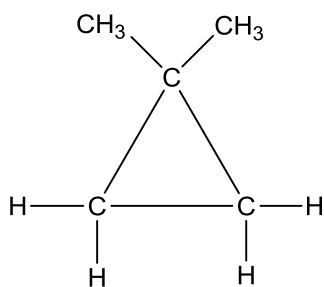


A Lewis base is a species that have a pair of electrons that can be donated to form a new bond. A Lewis acid is a species that can accept a pair of electrons. Species having a positive charge or an empty orbital are examples of Lewis acids. In the above example, the Lewis base is the compound having the negatively charged N with lone pairs of electrons, which can be donated to the Lewis acid (created when the C=O bond breaks). The curved arrow always starts at the center/ atom that donates electrons and ends at the atom that accepts the electrons.

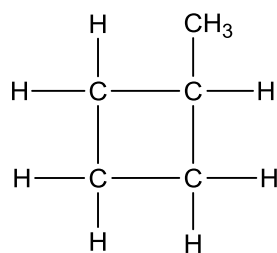
4. The structural formulas of the four structural (constitutional) isomers must all have a molecular formula of C_5H_{10} but the atoms must be connected differently. Possible structural isomers with carbon-carbon double bonds:



Possible isomers with cyclic structures:



IUPAC Name
1,1-Dimethylcyclopropane



Methylcyclobutane

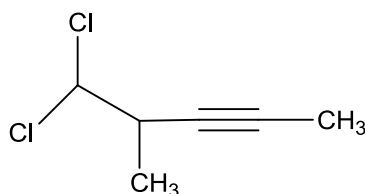


Cyclopentane

Try to draw the other isomers not shown.

5. (a) Consider the compound with the proposed name:

The structure consistent with the proposed name, 2-methyl-1,1, dichloropent-3-yne is:



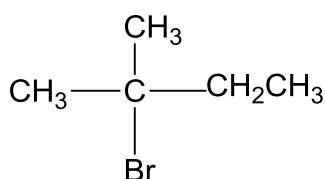
(b) The numbering is from the wrong side of the molecule. This is an alkyne and the numbering should start at the end that would give the $C\equiv C$ the lowest possible number. Therefore, the parent name should be pent-2-yne and not pent-3-yne. The change in numbering will change the location of the other substituents.

The substituents in the given name are not listed in alphabetical order. The dichloro atoms should be named before the methyl group. The 1,1,-dichloro is incorrect since there should be commas between two numbers i.e. 1,1 and there is a comma between the 1 and 'di' it should have been 1,1-dichloro. The methyl group is on C-4 and not on C-2 and should be 4-methyl.

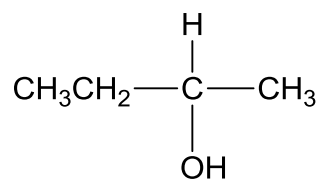
The correct IUPAC name for the compound is thus: **5,5-dichloro-4-methylpent-2-yne**

6. The structures for MAJOR product of each reaction/ reaction sequence is shown below:

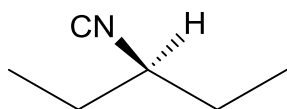
(a)



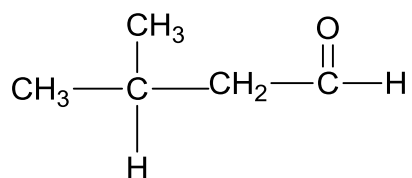
(b)



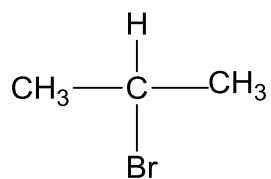
(c)



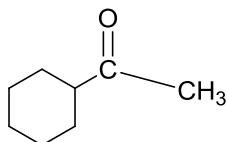
(d)



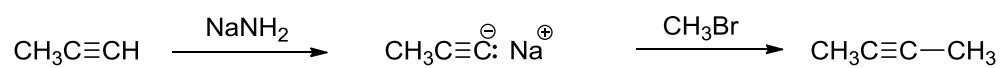
(e)



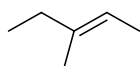
(f)



(g)

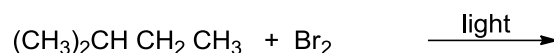


(h)



7. The detailed reaction mechanism for the reactions shown in:

(i) Question 6(a)

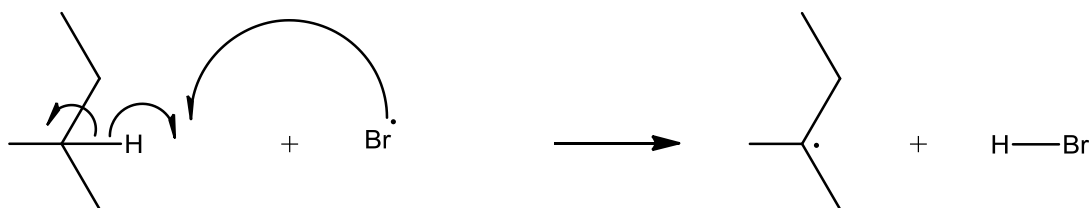


Initiation:

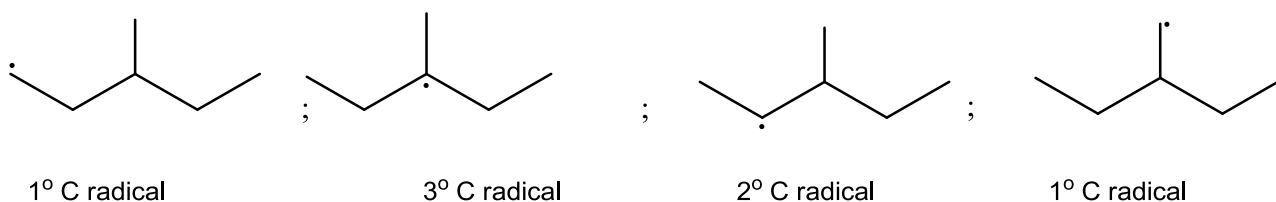


Propagation:

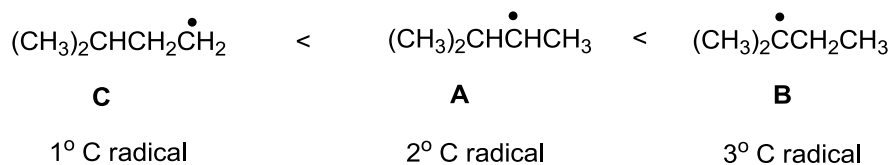
First step:



The halogenation reaction of alkanes proceeds via a radical intermediate. The propagation step shown above gives a radical intermediate. There are different possible radicals that can form in the reaction which are shown below:



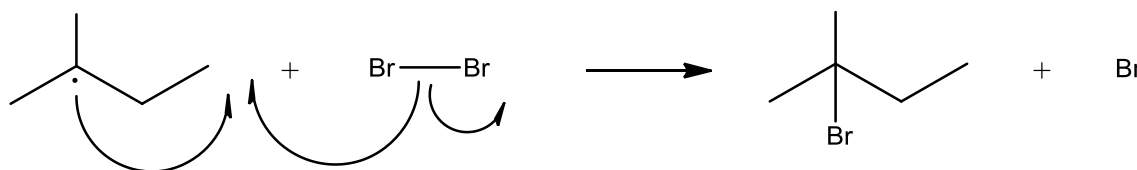
The halogenation reaction of alkanes proceeds via a radical intermediate. Some reaction with different types of carbon atoms in the alkane molecule, can form more than one radical. Below is the ranking of the radicals in order of INCREASING stability i.e. from the least stable to the most stable.



The tertiary carbon radical is the most stable radical and the primary radical is the least stable.

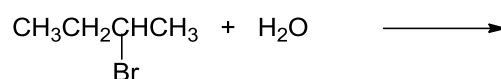
The tertiary carbon radical is the most stable radical (has the lowest energy) and will produce the major product in the second propagation step.

Second step:



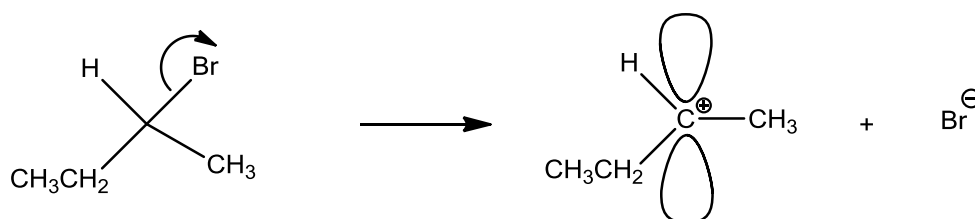
There are also termination reactions in a halogenation reaction. Please consult the textbook on how these steps are drawn.

(ii) Question 6(b)



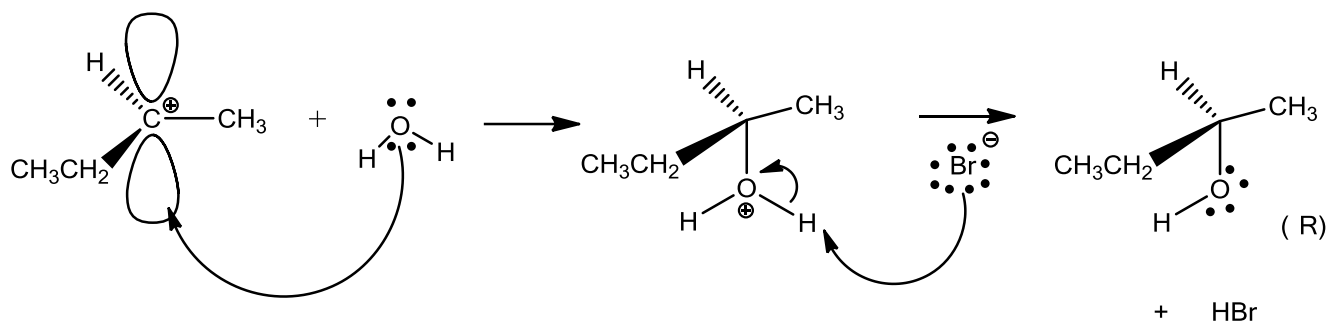
Water (H_2O) is a poor nucleophile, which promotes nucleophilic substitution via an $\text{S}_{\text{N}}1$ reaction mechanism. This mechanism involves more than one step. The mechanism for the reaction of 2-bromobutane with water:

Firstly, carbocation formation:



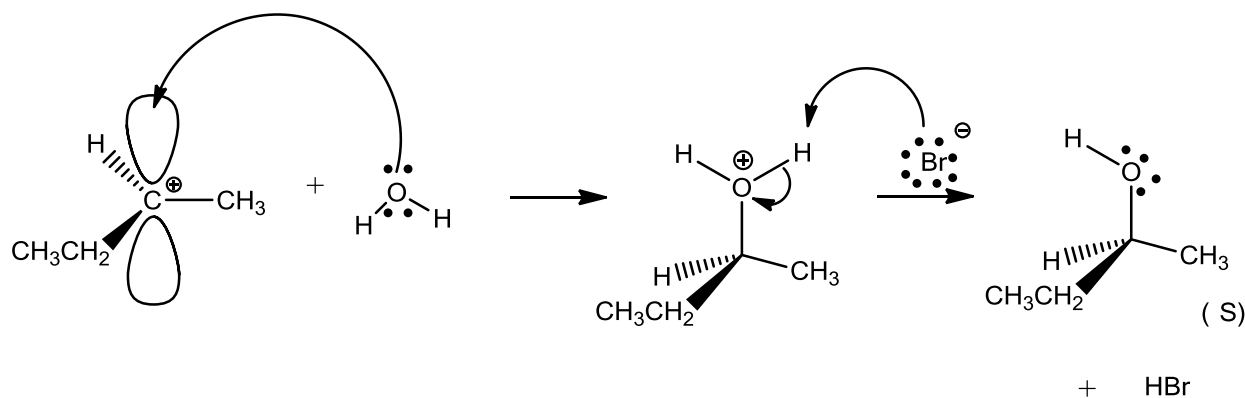
The carbocation is planar and the nucleophile can attack from either side of the carbocation.

Secondly, we redraw the carbocation (in 3-D format) and show the nucleophile attacking from the bottom:



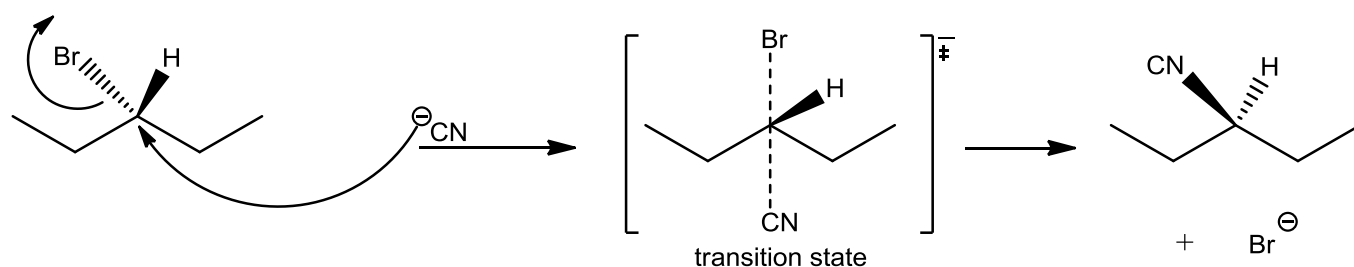
The nucleophilic attack is followed by removal a proton from the oxonium ion by the bromide ion to give the corresponding ether molecule, which has a (R)-configuration.

Similarly, the nucleophile attacking from the top is shown below. The above nucleophilic attack from the top gives the (S)-isomer. [See question 9 below for an explanation on how to determine the (R)- and (S)- configurations.



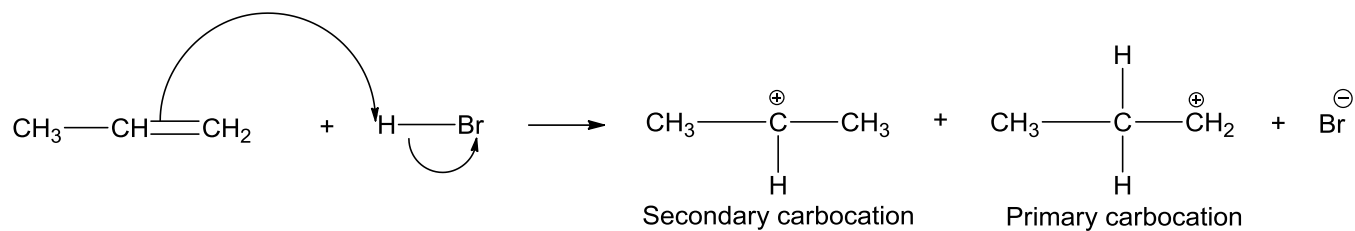
Methanol, CH_3OH , reacts similar to water.

(iii) Question 6(c)

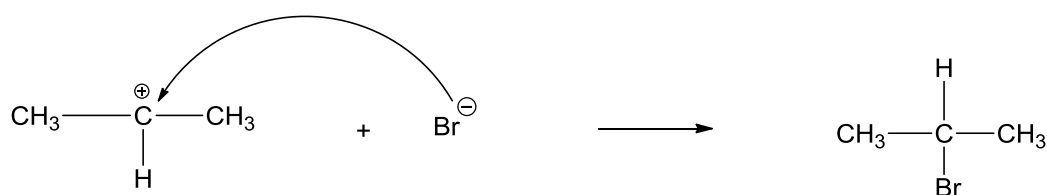


(iv) Question 6(e)

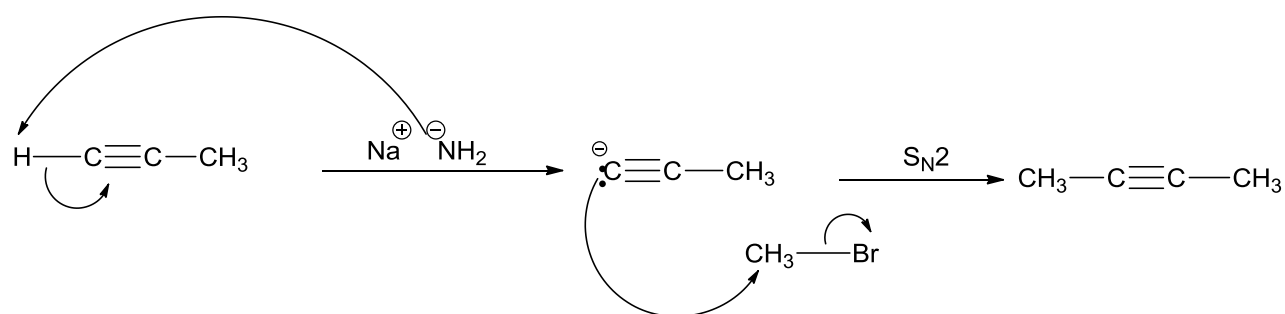
The reaction mechanism of the reaction of HBr with $\text{CH}_3\text{CH}=\text{CH}_2$ is:



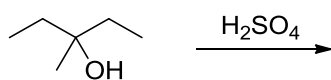
The secondary carbocation is more stable and lower in energy than the primary carbocation and the secondary carbocation will mostly form in the reaction.



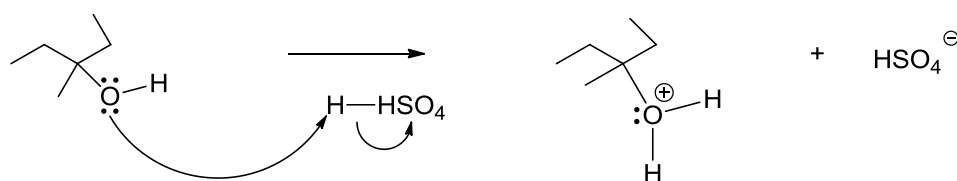
(v) Question 6(g)

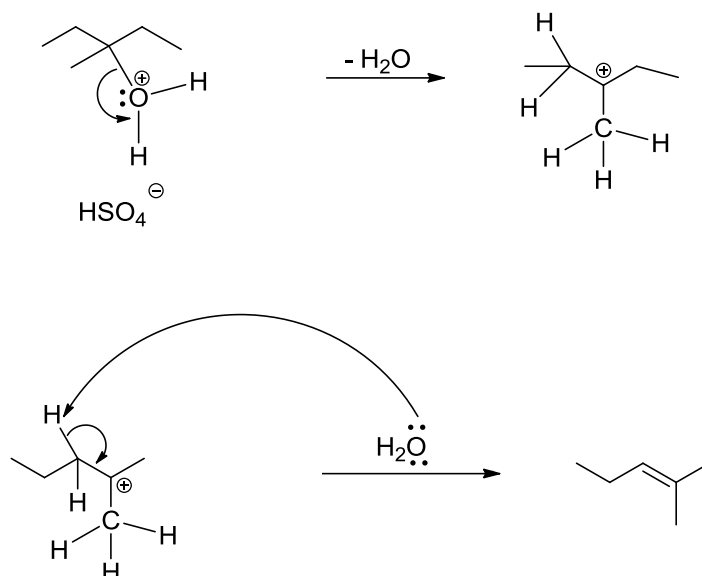


(vi) Question 6(h)

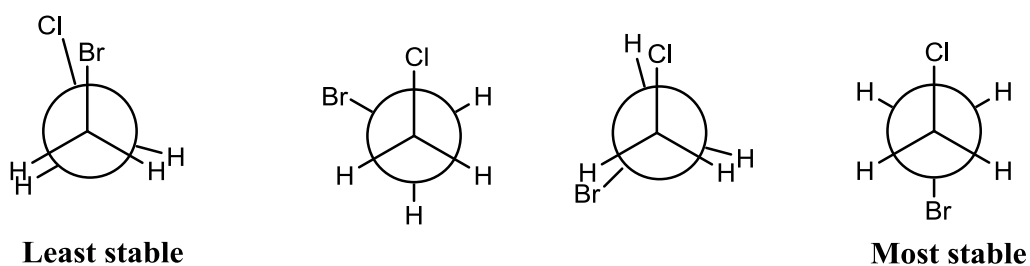


The complete mechanism of the reaction above is:

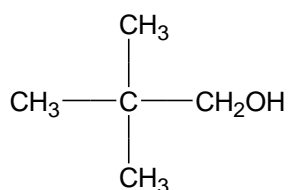




8. The different Newman projections for the molecule, $\text{CH}_2\text{ClCH}_2\text{Br}$ are:

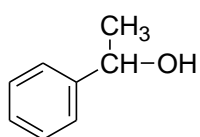


9. (a) When the OH group is attached to a primary carbon i.e the carbon is attached to ONE other carbon. The alcohol below is therefore a primary alcohol.



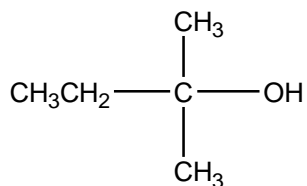
IUPAC name: 2,2-Dimethylpropan-1-ol

When the OH group is attached to a secondary carbon i.e the carbon is attached to TWO other carbon atoms. The alcohol below is therefore a secondary alcohol.



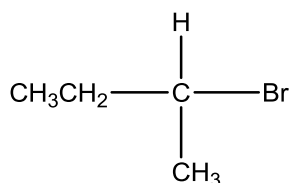
IUPAC name: 1-Phenylethanol

When the OH group is attached to a tertiary carbon i.e the carbon is attached to THREE other carbon atoms. The alcohol below is therefore a tertiary alcohol.



IUPAC name: 2-Methylbutan-2-ol

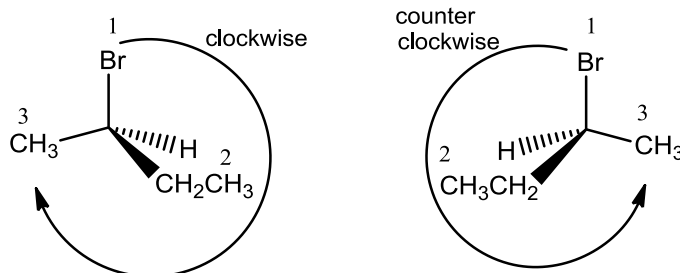
(b) A chiral molecule must have a chiral center, i.e. a carbon containing four different groups or atoms.



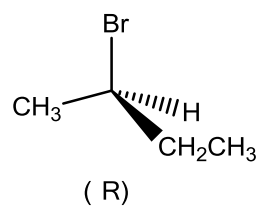
According to the Cahn-Ingold-Prelog rule, assigning priorities to the groups/atoms around the chiral center:

Group	Priority
Br	1
CH ₂ CH ₃	2
CH ₃	3
H	4

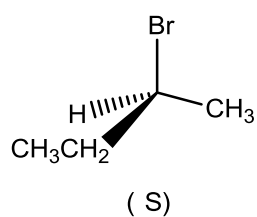
The 3-dimensional structures of the enantiomers of the above compound:



The enantiomers are:



(R)-2-bromobutane



(S)-2-bromobutane
