

hello everyone i am dr ramesh ramapanikar an associate professor in the chemistry department at indian institute of technology kanpur ah i was talking to you in the previous classes about the chemistry of halo alkenes and haloalkanes

so we would continue to do that today

so in the previous two lectures that i have given i have talked to you about the classification of organo halogen compounds ah about their physical properties a little bit then also about how the nature of these bonds are and how to classify them and give them names the proper nomenclature according to iupac

so it can i would ah slightly discuss something that we discussed towards the end of the last lecture that is the reaction of halo alkenes and how they undergo nucleophilic substitution reactions

so we have seen that nucleophilic substitution reactions of haloalkanes are probably the most discussed and the most useful reactions of them and they are generally of two types and we started off by saying that the first type is something that can be called as nucleophilic substitution ah reaction which are bimolecular or in other words substitution nucleophilic bimolecular reactions which has to be represented as $\text{S}_{\text{N}}2$ where s stands for substitution and 2 stands for nucleophilic and two stand for the bimolecular nature of the reaction

so here you would see that in the screen i have a representation which we have already seen

so this is just to tell you that this reaction happens when a nucleophile approaches an alkyl halide from a side opposite to where the carbon halogen bond is and then the carbon halogen bond starts to weaken and carbon nucleophile bond starts to form

so in the example that i have on the screen the nucleophile is a hydroxide anion

so it reacts through the oxygen atom

so we would see that we have a transition state in which there is an oxygen carbon bond slightly being formed and the carbon chlorine bond getting weakened

so methyl chloride is the halo alkene that is being discussed in this example and this transition state i also said that in this transition state we have a planar structure of the carbon atom which is attached to three different hydrogen atoms and then you would see that through one of the sides we have the chlorine atom leaving and through the other side a hydroxide anion starting to form a bond and this transition state then collapses to give us the product in this case an alcohol plus a halide anion the mechanism as it is shown here was first proposed by huxley and in cold and the main feature salient features of the reaction can be summarized in a few points which says that this is a second order reaction that means the reaction has the rate of the reaction is affected by the concentration of the nucleophile as well as the concentration of the haloalkane it is a single step reaction

so therefore no intermediates are formed we only have a transition state which is represented here the transition state of course is a penta coordinate carbon atom ah and the reaction happens with an inversion of configuration

so this is a result of the nucleophile approaching the carbon atom from a side opposite to where the carbon halogen bond is and when the halogen leaves it looks as if we started with an umbrella and have kind of inverted it and

so therefore this is we say that the $\text{S}_{\text{N}}2$ reaction substitution nucleophilic reaction follows an inversion of configuration when the reaction actually happens

so then we went ahead and said how exactly this reaction can be viewed for a practical purpose and here i had examples where a methyl halide an ethyl halide

an isopropyl halide and a tertiary butyl halide undergoes reaction and we saw that the reactivity pattern in general is more for methyl than for other primary halides secondary and tertiary follows and tertiary alkyl halides being extremely sluggish when it comes to nucleophilic substitution reactions through the bimolecular pathway and this was explained through these pictures where you see that a nucleophile is trying to approach this carbon atom but if there are only hydrogen atoms present on the carbon to which the nucleophile has to bond to then the approach is rather hindrance free

so there are no steric crowding offered by the hydrogen atoms which are extremely small

so therefore this reaction happens and if you put a relative rate of 30 for a methyl halide then we would find that the corresponding ideal halide reacts with the rate of 1

so there is a difference of 1 to 30 when an ethyl or methyl reacts and this hindrance comes of course because in this case we have an R group that is a CH₃ in this case

so this R group offers some hindrance to the nucleophile and if you replace two of those hydrogen atoms and put two methyl groups then of course the hindrance is more

so therefore the rate falls even from one and it becomes zero point zero two and a distributed alkyl halide as shown in this case has three R groups for four distributed three methyl groups

so when the nucleophile finds it extremely difficult to reach the carbon atom to start making the bond that is required for an S_N2 reaction

so therefore rate of this reaction is practically zero

so this is what we discussed and we said that S_N2 follows the order primary greater than secondary and tertiary that is how the rate of the reaction would be ok

so now what we would do is we would go and look at the second mechanism by which is nucleophilic substitution reaction can happen and this is called substitution nucleophilic unimolecular or S_N1

so the previous one was S_N2 and this is called S_N1 the one of course stands for unimolecular reaction that means the this particular reaction would depend only on the concentration of one of the substrates

so in this case the halo alkane

so we would have a look at this particular reaction you can see

so what I have here is an example on the screen and in this particular example I have two bromo two methyl propane

so this is a carbon atom that is attached to bromine and three CH₃ groups now it is being reacted with an alkoxide anion and what you would find is that the reaction proceeds to give you two methyl propanol propanol which is tertiary butanol and a bromide anion now here I have a representation of the same molecule

so you can see that there is a carbon atom attached to a bromine and three CH₃ groups now how exactly this reaction happens is that it does not go how the S_N2 reaction did happen that means the nucleophile does not start to approach the molecule and it is clear in this case that because it is a tertiary halide it is bulky

so the nucleophile finds itself difficult to approach the carbon atom

so therefore what happens is when this particular substrate this particular halide is taken in a solvent over a period of time in an extremely slower process the bromine carbon bond can cleave a carbon halogen bond is already polarized with a considerable amount of negative charge on the bromine atom and a positive charge on the carbon atom now with time what would happen is the

carbon bromine bond would break and then we get what is called as a carbocation
so it is a cation centered on carbon
so we call it as carbocation a more appropriate time for this is carbonium ion
but it can also be called as a carbocation
so in this carbocation the structure of the carbocation is such that the carbon
in this case is sp^2 hybridized that is we have a carbon that has three bonds
which are sp^2 bonds which are in a plane
so if i hold the carbon like this you would find that it has three hydrogens
which are attached and all of them can be condensed in a particular plane now
what else does the carbon have is a p orbital
so the p orbital would be perpendicular to the plane in which the carbon and
hydrogens lie and the p orbital would have both of its lobe on either side of
this particular plane and the p orbital is empty
so this does not have an electron that is why carbon has a positive charge
so that is how a carbocation would look and now this carbocation then stays in
the solution in which the reaction is being done and it then reacts with the
nucleophile that it is being treated with
so now the carbocation can react through its empty p orbital and during the
process the hybridization of the molecule changes to sp^3 and finally we
get an sp^3 hybridized tertiary butyl alcohol as the product
so you would find in the two reactions that i have written here it has a first
step where the carbocation is being formed it is rather reversible because the
 Br^- can come back and react with this cation and give us the starting
material back
so it is a reversible reaction
so it would be appropriate to write it in an equilibrium and once the
carbocation formed which is a slower process the carbocation now has two options
either react with Br^- go back to where it started from or it could react
with the nucleophile giving us a product
so the nucleophilic unimolecular substitution are therefore SN_1 for half for
they therefore follow first order kinetics that means their rate is dependent
only on the concentration of the haloalkane because the slower step of the
reaction which determines the rate of the reaction is SN_1 only dependent on how
much of halo alkane is present because the reaction yields a carbocation
so the concentration of the carbocation is the one that determines the future
reactions ok
so this is the simplest of representation
so now let us go forward and summarize what are the main points here
so the reaction of course follows first order kinetics now it is a two step
reaction unlike SN_2 reaction which was a single step having a transition state
this is a two step reaction
so therefore the reaction has an intermediate
so there is an intermediate it is not necessary that we will be able to isolate
the intermediate but there is an intermediate formed and that is a carbocation
an unstable intermediate which would then react with the nucleophile
so now this compound
so therefore of course what kind of haloalkanes can give this reaction
effectively if that is a question that is being asked the answer is pretty clear
any compound that can give stable carbocations relatively stable carbocations
would be able to push the equilibrium of the first step towards formation of
more amount of carbocations and therefore make the SN_1 reaction faster
so therefore we could summarize that the general reactivity order of halo
alkanes towards the SN_1 reaction is tertiary greater than secondary
greater than primary

so this is exactly opposite to that of what an $\text{S}_{\text{N}}2$ reaction followed
so in this case the tertiary reacts faster secondary reacts lower than tertiary
and primary reacts the slowest and methyl halomethane generally do not follow
this mechanism because it is extremely difficult to make a methyl carbocation
so this is something probably already learnt now ah
so when we talk about the stability of carbocations there are two molecules two
kinds of species that those are worth ah listening to
so one of them is allylic and the other is benzylic halides because when these
molecules undergo an $\text{S}_{\text{N}}1$ reaction they form the corresponding allylic cation and
benzyl cations
so i have the simplest unsubstituted allyl and benzyl cations written on the
screen here
so you can see that an allyl cation has a positive charge and the positive
charge is immediately adjacent to a double bond
so now the electrons in the double bond would be able to have a resonance
relations with the carbon bearing the positive charge and have these two
resonant structures
so this particular cation is stabilized by two resonant structures and
therefore it makes the carbocation more stable
so it is unlike having a simple primary carbocation here the carbocation is the
positive charge is shared between two primary carbocations
so it becomes more stable than a single simple primary carbocation similarly in
the case of benzyl cations the positive charge on the CH_2 is shared through
resonance with three other carbon atoms that are present in the benzene ring or
in other words the benzene ring using its electron cloud supports the formation
of this positive charge because the positive charge once it is formed on the
carbon adjacent to a phenyl ring there is large amount of elect aromatic
electron cloud those are present in that is present in the benzene ring
so which would be able to support the carbocation or for its formation and the
resonance structures can be drawn as i have shown here
so therefore both benzyl and allylic cation remains to be stable carbocations
and as we have seen in one of the points here stable carbocation support
assignment reactions
so you would find that when you try to do a nucleophilic substitution reaction
on allyl or benzyl compounds they are relatively faster
so those are the main points here that one should look
so with these points you would also be able to distinguish between an $\text{S}_{\text{N}}2$ and
 $\text{S}_{\text{N}}1$ primary difference is their kinetics where $\text{S}_{\text{N}}2$ is second order follows
second order kinetics as on one reactions follow ah first order kinetics then
the order of reactivity also varies for an $\text{S}_{\text{N}}2$ it is primary greater than
secondary greater than tertiary here in $\text{S}_{\text{N}}1$ reactions it is exactly the opposite
ok now to understand these reactions better
so we have said that for example in the case of an $\text{S}_{\text{N}}2$ reaction there is an
inversion of configuration
so it it would become important that at this stage we start looking at carbon
as a tetrahedral species and understand what exactly an inversion mean to
something like a tetrahedral structure
so in order to understand that we should start talking about molecular
asymmetry that means molecule the symmetry of a molecule and or the lack of it
so if a molecule does not have symmetry we call it as an asymmetric molecule if
a molecule has symmetry we call it as a symmetric molecule
so a temp that is often discussed with in this context is chirality or a
chirality or chiral compounds or chiral materials and accurate materials
so i have some examples that would probably get you used with this particular

concept

so what we can say that if you take an object

so let us start with an object as simple as a funnel that i have shown here

so so this is the funnel that you see here right

so and then the plane that i have drawn

so i put a dotted line

so i assume that it is a mirror and what you see on the other side is the mirror image of the funnel

so now if you look at these two images they are exactly identical

so you would probably be very easily able to take one of the structures that is either the mirror image or the original one and you can get confused between the two or in other words these two would look exactly the same

so if i have to take one of the structures and put on top of the other that would be an easy job

so therefore we can say that um the mirror image of a funnel actually super imposes on its on its actual structure that means you take a funnel take its mirror image they are super impossible that means i can take one and put on top of the other and it would match exactly

so if that happens then those kind of molecules are symmetric

so they are symmetric molecules their mirror imagines original molecules are the same now for certain molecules it will not be possible that you can take the mirror image and put it on top of the other because when you take the mirror image and try to keep it on top of the original image you would find that they do not fit well

so or in other words they are not super impossible

so such substances are called chiral compounds

so chiral compounds are those compounds for which the actual object and its mirror image are not super impossible cannot be put together now if a molecule has this property of having a mirror image which is not super impossible on itself then we say that property as chirality

so chirality is a property by which a molecule distinguishes itself from its mirror image that the mirror image cannot be superimposed on its actual structure now

so as we have seen symmetric objects which are super impossible on their mirror images are said to be achiral

so that means they are not chiral they are accurate

so now here i have an example of an accurate object

so i will try to show that structure to you

so you can look at your screen and you would see that there i have an object where from a point you would start to see that there is a red object there is a blue object and there is a green object attached to a particular point

so this is exactly what i mean

so let me have the structure for you ah

so what you see here is a carbon atom that is attack means let us call this as an atom that is attached to three different units here one of them is red another is blue and i have a green on the green on the third place now if i take a mirror image of this this is how the mirror image would look

so if i keep a mirror on this side you would see that this is the mirror image now if i turn the molecules towards you you can see that one has the red sphere on the right hand side the other one has it on the left hand side

so now these two are mirror images but now if i try to take the mirror image and try to superimpose it on on the actual image you would find that i cannot do that

so when i try to put the green on green the blue is on red and the red is on

blue

so there is no way that i can rotate this and actually see if i do it like that then of course the structures are not really correct these again are mirror images

so i will not be able to superimpose this structure on this because this unit that i have shown here is asymmetric remember that the whole structure is not planar if it is planar then i would be able to do that here i have an angle between these two bonds which is not hundred and twenty

so this is kind of a pyramidal structure and this pyramidal structure leads to with three different substituents on it actually leads to a chiral object and this chiral object is not super impossible on its mirror image now coming back to molecules

so what we can say is that if an organic molecule the same way if it is not super impossible on its mirror image then we can say that that particular molecule is asymmetric or we call such molecules as asymmetric molecules

so let me take an example of such a molecule

so here now i have made the earlier structure into a carbon

so now what you see is a carbon atom which is black in color attached to four different functional groups

so one can be a chloride one can be a bromide iodide and hydrogen

so let us imagine a compound with four different substituents now this particular structure this particular carbon atom which is the central carbon atom is now asymmetric the reason is it does not have a plane of symmetry you cannot use a plane of symmetry to cut this if i cut this molecule you would see that the two sides have different substitutions

so it lacks symmetry units and now if i try to make its mirror image you would also find that these two mirror images are not super impossible on each other

so this is one of the structures this is its mirror image now i will not be able to superimpose it these two structures because i have the red and the white coinciding together but you see that the blue and blue and green atoms are mismatched

so so this tells you that this kind of a carbon atom that is attached to four different groups here

so that leads to a symmetry in the molecule

so such a carbon atom that is attached to four different units are normally called as an asymmetric carbon or such a center is called as a stereocenter because these two molecules now the actual molecule and its mirror image are not super impossible they are different molecules and these are isomers such isomers are called stereoisomers and because they are stereoisomers the carbon that is responsible for the formation of these stereoisomers are normally called as a stereocenter or they are also called as an asymmetry carbon in simple words if you find an organic molecule that has only one carbon atom that has at least one carbon atom that has one carbon atom that attached to four different functional groups then you can immediately say that that particular molecule is asymmetric

so the condition is this if a molecule has one carbon atom attached to four different units then it is asymmetric if there are two or three then there could be cases where the symmetry is retained

so normally we would only say that if a molecule has one carbon atom attached to four different functional groups then the molecule is asymmetric

so let us go forward and see how this becomes important and why how can we distinguish between such molecules

so to discuss with that we also need to understand another important point which is about plane polarized light or which is related with plane polarized

light and the property of the molecules of organic molecules related to optical activity

so i have already told you that these two molecules which are mirror images that cannot be distinguished that can be distinguished from each other that cannot be superimposed or stereoisomers

so now stereoisomerism is also associated with optical activity

so i will try to tell you what exactly is optical activity

so you can see a drawing here

so in this drawing what i have shown i have represented normal light with the number of arrows in all directions

so what do we actually mean by that is when whenever we take normal light you would find that it has its electromagnetic vectors going in all directions

so if the light starts to travel from one side to the other it would have its electromagnetic vectors going in all directions which are perpendicular to the direction of propagation of light

so if light goes this way it has its vectors going in all the directions now there are certain kind of compounds which are called as polarizers an example is a nikol prism which i have shown here

so if now this kind of a light that has its electromagnetic vectors going in all the directions

so if it starts to pass through such a prism what happens is after passing through polarizer what comes out is light that has these electromagnetic components only in one direction or only in one plane

so all the other things are cut off

so this is a property of the material from which the polarizer is made

so now the polarizer is a material that is able to cut the electromagnetic components of light in all direction except for in one plane

so one results is a plane polarized light

so now we can say that now this light is polarized because it only has this electromagnetic components in one particular plane

so which is normally represented by this double headed arrows that i have shown here indicating that we have this magnetic vectors which are moving only in only through one plane okay

so we can convert a normal light into a plane polarized light now what next if the plane polarized light is allowed to pass through a solution of an organic compound which is asymmetric

so that is the important point here

so if you have a solution of an organic compound in some solvent and if the organic compound is asymmetric what happens is the plane of the plane polarized light

so let us assume that my hand represents the plane of the plane polarized light

so now if the plane of the light is like this once it passes through the solution it just tilts either towards the right side or towards the left side

so when i am looking at it if it rotates to my right side it is in the clockwise direction and if it rotates in the left to the left side it is in the anticlockwise direction

so now again the main point is a plane polarized light passing through a solution of an asymmetric organic compound would tilt it direct will tilted direction and the direction would be either to the right or to the left which depends uh on the asymmetric compound that i have dissolved in the solution now what you would see that the plane of the plane polarized light is now rotated or it is tilted which can actually be detected

so the detector can also have a polarizer kind of compound which can detect the angle by which this has now tilted

so there can be detector that is able to do this and find that the plane of the plane polarized light has changed one side

so these molecules which are able to do this are said to be optically active because they do something to light

so therefore asymmetric organic molecules are symmetric molecules in general you would find most of them to be organic compounds

so asymmetric molecules asymmetric organic molecules are compounds that are optically active

so they are able to rotate the plane of the plane polarized light either towards the right or to the left now if the rotation is to the right that is clockwise when i look at it then it is called dextro rotatory and if it is to the left or in the anticlockwise direction it is called lever rotatory

so these two terms are from greek which means that rotating to the right or rotating to the left

so these are the terms that are used by organic ms

so if i say that i have an asymmetric compound and it is dextro rotatory that simply means that if i make a solution of that compound it would rotate the plane of the plane polarized light towards the right and dextro rotator is normally indicated by the sign d which stands for dextro or you can also represent it using a plus sign this is just to say that the light tills in the positive direction and the lever rotator is represented by l or a minus sign that means it rotates in the negative direction

so these are conventions that were used ah from the time they were observed now how how it again becomes important is if an asymmetric compound is

dextrorotatory that means if an asymmetric compound you are given an asymmetric compound that means this is a compound whose mirror image does not superimpose

so the compound and its mirror image are different now if the compound that is given to you is able to rotate the plane of plane polarized light to the right then of course its mirror image which is a different compound would be able to rotate the plane of the plane polarized light to the left and now if you take solutions having equal concentrations of both these molecules that means the original molecule and its mirror image the angle by which the light is rotated would also be same except that they would be in the opposite directions

so therefore such molecules which are mirror images of each other and are able to rotate the plane polarized light in opposite directions are called enantiomers

so enantiomers as i have written here

so you can see the time on the screen

so this can also be described as a symmetric carbon atoms which

so an enantiomers are those compounds whose mirror images are not super impossible on each other

so if you have a compound whose mirror image is not super impossible on the actual structure then that means they are they form enantiomers and they would be optically active and they both would rotate the plane polarized light to equal but opposite directions

so these compounds are therefore also called optical isomers

so if you hear the time optical isomers ah mentioned with respect to a compound that simply means that the compound is asymmetric and that particular compound would rotate the plane of the plane polarized light in one direction and its mirror image would rotate the plane of the plane polarized light in the opposite direction

so that is the point

so we have instruments which can actually be used to detect in which direction the light is being rotated and such instruments are called polarimeters

so polarimeter is normally found in organic chemistry labs where the research is being done

so if you find a molecule being synthesized if you synthesize a molecule then one of the steps is to go and check what is the polarity of the molecule or to check whether the more compound is asymmetric by looking at in which direction the light is rotated the plane polarized light is rotated ok

so now to come back to this optically active compounds that I was telling you the requirement is that you should have molecules which are mirror images of each other and which are not super impossible

so this was an example that we discussed these are mirror images and you can see that they are not super impossible on each other

so now I would ask you to concentrate on the screen where I have these molecules here

so I have an example here which is 2-butanol

so now if you look at this compound there is a carbon atom on this and it is attached to four different units one CH_3 which is given in pink an ethyl group which is given in green a hydrogen in blue and an OH in red now here I have separated the two molecules through a line through the middle and this actually let us assume that it is a mirror and the mirror image is on the other side we can see everything is same except that they look like exact mirror images now if I rotate this molecule and try to put it on top of that try to superimpose them I would find that they do not superimpose you have already seen that with the models

so as long as the four substituents are different they will not be able to superimpose on each other

so these are therefore called enantiomers

so what I have here are enantiomers of 2-butanol

so these are enantiomers of 2-butanol and they are not super impossible on each other

so they are optically active the compound 2-butanol is therefore asymmetric

so it can have two isomers and the isomers are only distinguished by their stereochemical orientation their orientation of the groups in space

so that they are distinguished from their mirror images

so we can say that the compound is optically active

so I also have another structure here which is just propanol

so so propane to 1-propanol now 1-propanol is the immediate relative of butane also it is a lower analogue now if I have to show that molecule

so this is probably how I can show

so let us assume that these two white balls here are the hydrogens at or let us call them as the CH_3 atoms and then if you assume that one of them is OH and the other one is CH_3 other one is a hydrogen

so so this is the compound here

so this compound is different from the previously asymmetric compounds that they discussed because they have two of the group similar and a symmetric carbon atom had all the four functional groups different

so this has two of them same

so now if I take these two molecules and if I try to make a mirror image of this this is what I get now you can see that if I try to superimpose it like this it does not work but of course I can rotate this molecule and then superimpose it you see the two hydrogens are on top of each other the two CH_3 s are on top of each other and the two red balls

so let's call them as red black and white balls

so you can see that the white balls are super impossible around exactly on top

of each other

so are the black and the red

so if if any of the two functional groups on a carbon atom are same then the carbon is no more asymmetric

so propanol propane two all is such an example and you can see that their mirror images are super impossible and therefore the molecule is not optically active

so these are the two examples now

so we have seen that a solution of one enantiomer

so solution of one of the stereoisomers would rotate the plane polarized light in one direction now what will happen if i mix it with the other isomer

so that means if i take a solution that contains both the isomers that means the original compound and its mirror image equal amounts

so if that happens what will happen is the original compound would rotate the line to plane polarized light to the right the other one rotate to the left the net result would be that it does not rotate in any direction and i will see that the plane polarized light comes straight

so therefore that kind of mixtures which are now optically inactive although the solution has optically active compounds in them the both the isomers are in equal amounts and then effectively turning them into optically inactive and such mixtures are called racemic mixtures

so a racemic mixture is a mixture of two enantiomers of a compound in equal amounts in solution

so now ah normally

so when you want to represent a molecule as a receiving mixture we do not direct d or l instead we write d and l together

so if you say that a compound is a dl mixture that tells you that it is a mixture of both the enantiomers and therefore it is optically inactive they can also be represented with a plus or minus sign plus on top minus on bottom normally inside a bracket

so a plus or minus sign in front of the name of a compound of an optically active compound suggest that the sample that is given to you is actually a mixture of both the enantiomers in equal amounts and therefore not optically active

so this stem racemic mixture is only used for asymmetric compounds compounds that do not have symmetry or compounds that are optically active but when they say when they are mentioned as racemic mixes they are equal mixtures of both the enantiomers now it is also possible that you start with an enantiomer you are given an enantiomer and you carry out a chemical reaction and during the process of the reaction if ah the optically active compounds converts into optically inactive compounds or probably because the asymmetric center remains there but however you end up having both the enantiomers pro formed as products then such process are called resume session product processes or resume session reaction

so your reaction is said to undergo racimization if the if a pure asymmetric starting material is converted into equal mixtures of enantiomers that means a reaction that gives equal mixtures of enantiomers from a single enantiomer are called are said to have undergone racimization ok

so now we will try to put these all things into perspective and then we would try to explain the different terms that are associated with the reaction of asymmetric compounds

so here in this particular screen what you see here is i have a compound which has a carbon atom that is attached to an ethyl methyl a hydrogen atom and an xo let us say there is an alkyl halide

so now this alkyl halide is

so it is actually a two hollow butane derivative because there are four carbon atoms an ethyl group methyl group and a carbon that is attached to a halogen and hydrogen now if

so i have three arrows going in all the direction in three directions

so these three arrows represent three different reactions

so now let us assume that the reaction is with a nucleophile y with something y

so now during the process of the reaction now let us have a look at the one that is to the right side

so now when this reaction happens if x is replaced by y but that does not affect the molecule at all

so only thing that happened is the carbon x bond broke and y came exactly from the same side and form a new mode

so then what you get is the stereochemistry of the molecule remains same

so so i could i could show you that

so if imagine that this is the molecule that i am talking about

so if this is the x atom that is supposed to go out now imagine that if this goes out and a new thing comes out here

so when this happens i have replaced this with this but nothing happened to this part of the molecule it did not undergo an inversion or anything from where the x atom left the y atom has come and joined

so if that happens then we say that the molecule has retained its configuration or we say that the reaction underwent retention

so the reaction has the retention as a stereo chemical outcome that is whatever was the optical activity of this compound that stays

so the optical activity or the symmetric nature of the molecule is not changed then it is called retention now there can be another thing that is where you remove this atom and the new atom comes from the back side

so this is exactly what happened in an sn2 reaction

so one of the atom goes out but the new atom comes from the opposite direction

so that is represented to the left side

so this would result that here you can see that in this particular molecule the x is to the left side but in the newly formed molecule a x is pointed ah to the right side

so from the left side at c x bond we get a right sided c y bond now if x and y are same i can actually put a mirror here and you would find that this structure a and the actual structure are mirror images provided x and y are same

so in this particular reaction the molecule has undergone an inversion it is as if the y has come from the side opposite to where the x was and gave us this molecule

so this kind of reactions where the stereochemistry of the compound is inverted are said to have undergone an inversion

so these are terms that we use when we talk about the reaction of asymmetric organic molecules

so now when a symmetric organic molecule undergoes a reaction in which the stereochemistry is retained in which the configuration of the asymmetric carbon atom is retained then we say the reaction is undergone a retention now if the configuration of the asymmetric carbon atom is inverted if the configuration was become something that is similar to the mirror image of the original one then we say that the reaction has undergone an inversion now there can be a third type

so in the third type what happens is when the reaction happens i get a mixture of products in equal amounts

so that means if ah if my starting material here gives a mixture of a and b in equal amount then we say the reaction is undergone resume session

so these are the three terms that you would come across when we talk about the

reaction of asymmetric organic molecules either retention retaining the stereochemistry inversion inverting the stereochemistry that means getting the mirror image or resonance where there is half retention and half inversion

so these are the three things now we should also note that any reaction

so have a look at the last reaction i have on the screen

so if you look at this reaction you see there is an alcohol and we have seen that alcohols can be converted into the corresponding halo compounds on treating with thionyl chloride SOCl_2

so this is the reaction we have learnt while we are learning the preparation of haloalkanes now what happens the carbon oxygen bond breaks and the carbon chloride bond forms now this molecule that they are given here is optically active because it has a carbon atom that i am highlighting now this carbon atom is attached to four different groups one is $\text{CH}_2\text{CH}_2\text{OH}$ another is hydrogen and ethyl group and a CH_3 but the reaction actually happened on this carbon atom which is not the asymmetric carbon which is not the stereocenter and therefore the product is formed with absolute retention of configuration because we have not touched the asymmetric carbon at all

so the terms inversion retention and resonance have real sense only when the reaction is happening at the asymmetric carbon atom otherwise the reaction would always retain its stereochemistry because it the reaction does not recognize an asymmetric carbon at all it is happening somewhere else in the molecule

so therefore such reactions would we could easily say that they retain

so they undergo retention

so it is not even worth mentioning because ah there the symmetric carbon is not part of not a part of the reaction that is taking place now with this particular idea let us have a relook at nucleophilic substitution reactions

so the first reaction that we discussed is $\text{S}_\text{N}2$ reactions which lead to inversion of configuration

so we said that this reaction generally undergoes an inversion

so the molecule i have here is 2-bromooctane

so 2-bromooctane is you can see there is a six carbon chain and there is a CH_3 and bromine is attached to the second carbon

so the carbon is attached to four different groups it is optically active and this isomer that i have drawn here is the minus isomer that is this is the levorotatory molecule now if i take minus 2-bromooctane that means ah the one that is levorotatory and treat it with an hydroxide anion and if the reaction undergoes an $\text{S}_\text{N}2$ reaction which it would then the product is plus octanol plus octane-2-ol

so therefore the stereochemistry of the molecule has inverted i started with one enantiomer which had a particular optical activity and the product has the opposite optical activity and br minus comes out therefore $\text{S}_\text{N}2$ reactions we can easily say that $\text{S}_\text{N}2$ reactions always follow inversion now let us have a look at $\text{S}_\text{N}1$ reaction in an $\text{S}_\text{N}1$ reaction

so this is something we discussed today if we take 2-bromooctane

so it is sorry the molecule i have here is 2-bromobutane

so this is an error here

so if you take 2-bromobutane and in an $\text{S}_\text{N}1$ reaction i would first form this particular carbocation

so this is 2-bromobutane and 2-bromobutane forms this carbocation we said that the carbocation is planar

so this is this species that i have shown here this is a planar molecule

so it has CH_3 , C_2H_5 and H now this planar molecule is the one which is then going to react with hydroxide anion now the planar molecule has two lobes of p orbital now the orange minus can come either from this side or it can come from

this side now if the o h minus is coming from the right side then the rest of the molecule would bend backwards

so you can see how my hand would tend

so initially i have a carbon atom at the middle of my pump and hydrogen atoms on three sides now when the o h minus comes to form a bond the the rest of the molecule would bend in the opposite direction forming a tetrahedral carbonate now if it comes from the other side they will bend in this direction forming a tetrahedral carbon atom

so now once that happens the os has this liberty of coming from either of the sides

so what we are going to get we have a planar intermediate

so the planar intermediate is going to give me two compounds

so it would be a mixture of ah plus two butanol and minus two butanol or plus two butane two all and minus two butane two volt

so this reaction when an sn1 reaction happens because the intermediate is planar i would get two products

so that means the reaction undergoes the resume session

so sn1 reactions proceed with rasimization just because the reaction is able is going through an intermediate which is no or asymmetric

so once the reaction takes a root in which an asymmetric carbon atom is turned into a planar compound into a symmetric compound then the products would be forming in equal amounts even if the products are supposed to be asymmetric you would get both the enantiomers formed in equal amounts and therefore you get a recimic mixture

so this particular reaction sn1 leads to resume session whereas sn 2 leads to inversion of configuration okay

so with this i will move into the next reaction of alkyl halides which is elimination reaction

so elimination reaction of halo alkynes result in the formation of alkenes

so the reaction can best be represented by what they have shown here

so there is a base

so which is normally hydroxide anion which is able to pick up a proton from the carbon that is adjacent to the carbon bearing a halogen atom

so i have a ch2 br bond

so this is the halo alkene part and it has a carbon that is attached to a hydrogen

so this hydrogen is a requirement for an elimination reaction

so now the hydroxide anion will pick this hydrogen and then the electrons that were between the carbon and hydrogen could be found between this carbon and this carbon forming a new double bond and an hbr comes out

so the br minus would go out and the o h would take the edge forming water

so the reaction can be represented like this this is normally done by taking the halo alkene in alcoholic potassium hydroxide and gently warming the reaction mixture now what is the most interesting part about this reaction is that

so it is a pretty simple reaction to see

so if there is a carbon atom attached to a halogen atom and if the adjacent carbon atom has a hydrogen then the base will pick that hydrogen the halogen will leave forming a double bond between these two carbon atoms and the carbon bearing the halogen atom is called as alpha and the adjacent carbon atom is called as beta

so therefore this reaction which forms this double bond are also called as beta elimination reactions because the two groups are going from alpha and beta from the adjacent carbon atom

so these are called as beta elimination reactions or they are in short

elimination reactions of haloalkanes now we have a look at this cyclic structure that I have drawn here

so if you look at this particular structure you can see that I have an iodine attached to a carbon atom and this carbon atom has one two three there are three carbon atoms adjacent to this particular carbon to which iodine is bonded and all these three carbon atoms have hydrogens

so I have shown these hydrogens as beta one beta two and beta two because these two hydrogens are same because they are in the ring and there is another hydrogen atom on a CH_3 that is going out

so I am considering an iodide and the iodide is on the carbon alpha and then there are three beta carbon atoms out of the three beta two of them are similar which are called beta two and on these three beta carbon atoms there are hydrogens

so therefore the iodine can go out now either by taking the hydrogen from beta 1 or by taking hydrogen from beta 2.

so what I would get is a mixture of products the one which is shown here

so in this particular compound which I am highlighting now the hydrogen has gone from the beta 2 carbon atom and in this one the hydrogen has gone from the beta one carbon atom now when this reaction is actually carried out you will find that the major product is the one where hydrogen is lost from the beta two carbon atom and the other product where hydrogen is lost from the beta 1 carbon is the minor product

so this forms a rule

so this is a general observation it is you would find this happening in all sorts of compounds and the rule that what does the rule say is this is called as a set of rule which is named after the Russian chemist Alexander Saytzeff

so it has to be pronounced that says

so people also write the name differently and say itself

so what Saytzeff's rule tells you is that when you have this kind of compounds that can give you mixture of alkenes normally the alkene that is most substituted forms

so you while studying the chemistry of alkenes you would have learned that the more an alkene is substituted the alkene becomes more and more stable

so stability of an alkene is associated with the extent of substitution

so therefore when there can be two products from the same alkene you would find that the product that gives you the most substituted alkene is the most stable

so in this case this alkene it has three substitutions

so if I have to name them one two and three you can see that there are three substituents on this alkene

so it is more stable whereas in this alkene there are substitutions only on one of the carbon atoms the other carbon atom is a CH_2

so this is less stable a more clearer example is here

so if I take 2-bromopentane and treat it with an alkoxide now there are hydrogen atoms on this carbon as well as on this carbon now therefore it can give me two products and in reality when you carry out this reaction you would find that the pentene where the double bond starts from the second carbon is formed in 81 percentage whereas the other one is formed only in 19 percentage that means this is the minor product and if you look at the substitution pattern on both the alkenes that are formed you the one that is more substituted that means there are two substitutions on the double bond is formed in more amount than the one where there is only one substitution

so this is a di substituted alkene is a mono substituted alkene and you will

see that the mono substituted alkene is formed less

so that is the sets of fruit

so this is the main point to be remembered in elimination reactions now we have learnt two reactions here substitution raises elimination in substitution we have a nucleophile coming and replacing the halogen atom and in elimination we have a base that is picking up the proton now in the example that i have already talked about the elimination we had an o h minus coming and picking up the proton

so now o h minus is a nucleophile you know that and it is also a base sodium hydroxide is a base but the orange minus is also a nucleophile now what will it like to do whether it would like to react in a nucleophilic substitution reaction or whether it would like to give you an elimination reaction by abstracting a proton

so this is a choice the molecule has the reaction has now

so so therefore always there will be a competition between a substitution and an elimination reaction that is whether the nucleophile has to act as a base or to act as a nucleophile

so therefore this is something of a conflict and whichever reaction is the easiest to happen that happens

so therefore sometimes we may end up having mixtures of elimination and substitution products

so there are certain rules that we can write down and read out

so one of them is that a bulkier nucleophile prefer to act as a base and abstract a proton because if the nucleophile is very big

so i have the example here you have a look at this structure

so in this particular case i have bromide

so this is isopropyl bromide or two bromopropane and the nucleophile i am trying to use here is tertiary butoxide

so it is an alkoxide which is attached to a tetrabutyl group this is a bulky nucleophile now this nucleophile will find it very difficult to reach the carbon atom to which bromine is bonded

so it may not reach here instead it is easier for this tertiary butoxide this alkoxide to pick a proton

so my nucleophile in this case is bulkier

so it prefers to act as a base and carry it pick out this proton and then make a double bond

so bulkier nucleophiles would act as bases now a primary alcohol alkyl halide prefers the center reaction now if my alkyl halide is primary then of course there is no hindrance whatsoever

so um sn2 reactions are very easy now when i go into a secondary alkyl halide

so the the example that we discussed here is two bromo propane is the secondary highlight now if i use a secondary halo alkane where the bromine is attached to a secondary atom

so have a look at the substitution reaction that is on the right side now if i use methoxide anion as the nucleophile or the base this is something that can easily attack here and give me an sn2 reaction now if my base becomes bulkier it would then give me an elimination reaction

so when you have secondary alkyl halides there is a choice either it can go for sn1 or sn2 or it can go for elimination and that now depends on the strength of the nucleophile and size a larger base a larger nucleophile would act as a base

so therefore in secondary alkyl halide cases we might end up having mixes of sn1 sn2 products and some names elimination sn1 when sometimes your nucleophile is not very strong and it is also not a strong base then it cannot give you elimination but over a period of time it can give you an sn1 reaction now

tertiary alkyl halides always prefer S_N1 or elimination reactions

so they do not give you S_N2 reaction

so they first form the carbocation and now the carbocation can either lose a proton from a beta carbon atom and form an alkene or it can also give you an S_N1 substitution and test and they can also undergo reactions where the base directly picks the proton from the beta carbon and the alkyl halide bond breaks

so this is how we can summarize them

so we can say that primary alkyl halides will give you S_N2 secondary alkyl halides can give you nucleophilic substitution reactions as well as eliminations and tertiary also can do the same thing now a bulkier nucleophile in general prefers to give you an elimination reaction okay

so with this we would come to the last of the reactions of halo alkenes that we would like to discuss here

so now this particular reaction is reactions of halo alkenes with metals now we know that a carbon halogen bond generally is polarized

so we have a negative charge on the halogen atom and a positive charge on the carbon now when such compounds are treated with certain metals what the metals would do is metals would break the carbon halogen bond because halide anions are stable they want to be associated with metals in many cases

so then what we would get is a metal halide that is formed along with a carbon metal bond and in many cases this carbon metal bond that is formed would be considerably covalent

so that means it is directional they do not stay as ion carbonyl do not stay as a carbonyl in all the cases it would normally be linked to the metal that is being used

so we can say that if a compound contains metal carbon bond of some sort then they are called as organometallic compounds

so organometallic compounds are compounds where there is a carbon metal bond and normally certain metals are good in this because they would form stabler bonds directional bonds just like a covalent bond with the carbon atom and such compounds are called as organometallic compounds now the most discussed and the first and most recognized organometallic compound is a grignard reagent

so this is named after victor grignard who discovered these molecules in 1900

so you can see that it is more than 100 years that this compound has been discovered

so now how he did that was when he take an alkyl halide

so in this case i have written bromoethane and if it is treated with magnesium metallic magnesium in dry ether

so the solvent that is being used should be something that will not react with the metal

so when when an halo alkene is treated with magnesium in a solvent such as dry ether it would give a product where there is a metal carbon bond a magnesium carbon bond and a magnesium bromine bond now the $MgBr$ is actually an ionic bond

so it is most likely an Mg^{+} and a Br^{-}

so they it can be treated as any of the salts of magnesium with any halogen atom

so it is mostly an ionic bond whereas the carbon magnesium bond is covalent in nature

so the carbon magnesium bond carbonyl magnesium are associated together with the Br^{-} around

so the magnesium effectively can be said to be in plus two oxidation state where most of the negative charge is centered on the carbon atom and bromine atom and magnesium bears these two positive charge

so although the metal carbon bond in a grignard reagent is directional is

mostly covalent that is highly polarized

so it is polarized to such an extent that the carbon can almost be assumed as to be bearing a negative charge in that

so it is a negatively charged carbon atom positively charged magnesium linked through a covalent bond a rather covalent bond and then there is a δ^-

so this is exactly opposite to what can happen to an alkyl halide

so in the alkyl halide we have seen that the carbon has a positive charge and the halogen has a negative charge here it is the opposite now therefore these compounds are very reactive

so a grignard reagent is not something that you can take outside you can something that you can keep on a table or anything because exposed to air because it reacts with moisture it reacts with alcohols it reacts with anything that has an exchangeable hydrogen

so i have represented that with the reaction here

so if you take grignard reagent and treat this one with thin alcohol what happens is the carbon metal bond breaks with the negative charge on the carbon reacting with the proton of the alcohol and giving in this case because we have used an ethyl magnesium bromide it reacts with the hydrogen of the roh and gives me ethane plus MgORx where or is the alkoxide anion

so now this compound MgORx is rather a salt where magnesium is bonded to a halogen halide anion as well as to an alkoxide anion

so it gives a salt along with a hydrocarbon

so this is what would happen even unintentionally if a grignard reagent is exposed to an alcohol or just to moisture

so if you keep it open the moisture from the atmosphere is enough to make this reaction happen and therefore this reaction would go ahead and start giving us this product okay now similarly there is another reaction called as woods reaction

so this particular reaction is normally used to prepare hydrocarbons not

so much of synthetic applications per say because it is a rather violent reaction now what does the reaction do is if you take alkyl halide in the presence of sodium metallic sodium the carbon halogen bond breaks sodium takes out the halide unlike magnesium sodium can only have one valency

so sodium would take out the halide and therefore what we would have is a naked carbon atom which was earlier attached to the halogen atom

so two such alkyl groups would combine together and give us a hydrocarbon with double the number of carbon atoms to the halo alkane that we started with

so it can be represented with the reaction that is written here

so if you take an alkyl halide two molecules of the alkyl halide would react with two atoms of sodium giving us a hydrocarbon that has an extended carbon chain which is twice the number of total carbon atoms in the halo alkane plus two molecules of sodium halide

so this reaction is called as a woods reaction can be considered as a coupling reaction where two alkyl groups can be coupled together you start with the alkyl halide you clip off both the halogen atoms they go out as a salt with sodium and then the two alkyl groups are coupled together to give us a hydrocarbon

so this is a reaction of halo alkynes with metal

so two important reactions out of which the grignard reagent is always the most important because it gives us a reagent that has a negatively charged carbon atom whereas the woods reaction only gives you a product which is a hydrocarbon

so its they are limited with respect to that ok

so with this we would be able to summarize the reactions of halo alkene

so there are three reaction main classes of reactions that we studied one of them was substitution reactions which follows $\text{S}_{\text{N}}1$ and $\text{S}_{\text{N}}2$ second one was

elimination reactions and third one was reaction with metals now substitution reactions can be used to make a large number of functionalized organic molecules depending on the nucleophile that we use now their reaction pathway is generally sn_1 or sn_2 sn_1 follows a path which would result in racemization if the halo alkane is asymmetric sn_2 would result in inversion that means if we start with the particular configuration of an asymmetric carbon atom we get the opposite configuration in the product then of course these reactions can also have led to the formation of alkenes and once alkenes are formed we get the alkene that is most substituted which is called as the site of fruit halo alkanes can also form grignard reaction the grignard reagents that is the important thing about the third class of reactions that we discussed

so with this i would stop here and in the next class that we would have on this topic we will talk about the reactions of halo alkanes which are actually different from the reaction of halo alkanes thank you very much you