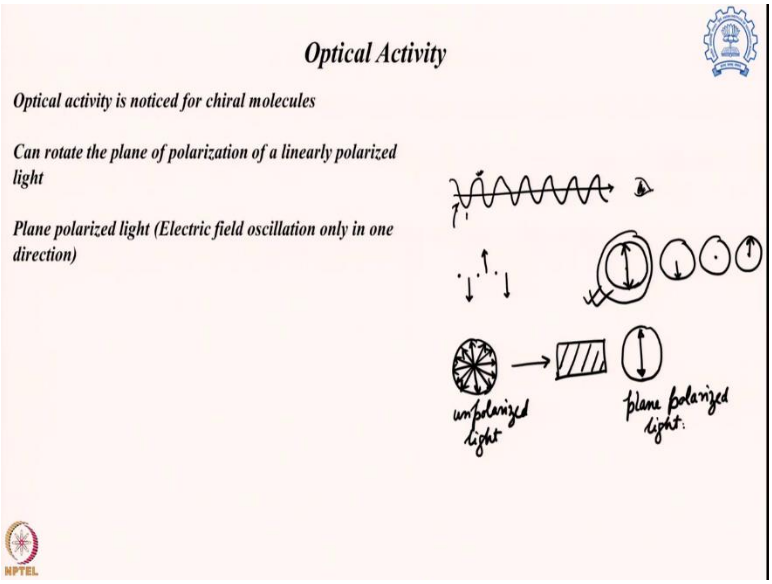
Concepts of Chemistry for Engineering
Professor Arnab Dutta
Department of Chemistry
Indian Institute of Technology, Bombay
Lecture 73
Optical activity, Conformational analysis, and absolute configuration of chiral transition metal Complexes

Hello, and welcome to this segment of optical activity. My name is Arnab Dutta and I am an Assistant Professor in Department of Chemistry IIT Bombay. Optical activity is mostly found for the chiral molecules. So, the chiral molecules can rotate the plane of the polarization of linearly polarized light to a particular direction and this particular phenomenon is known as the optical activity.

Now the question is why does a chiral molecule rotates the plane polarized light? And before that, what is a plane polarized or linearly polarized light. So, we will come into that first.

(Refer Slide Time: 00:53)

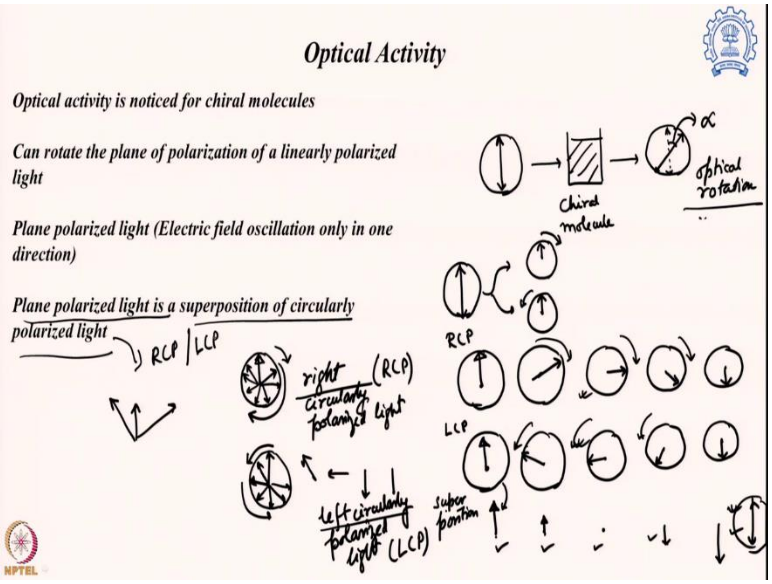


Optical Activity

Optical activity is noticed for chiral molecules

Can rotate the plane of polarization of a linearly polarized light

Plane polarized light (Electric field oscillation only in one direction)



Optical Activity

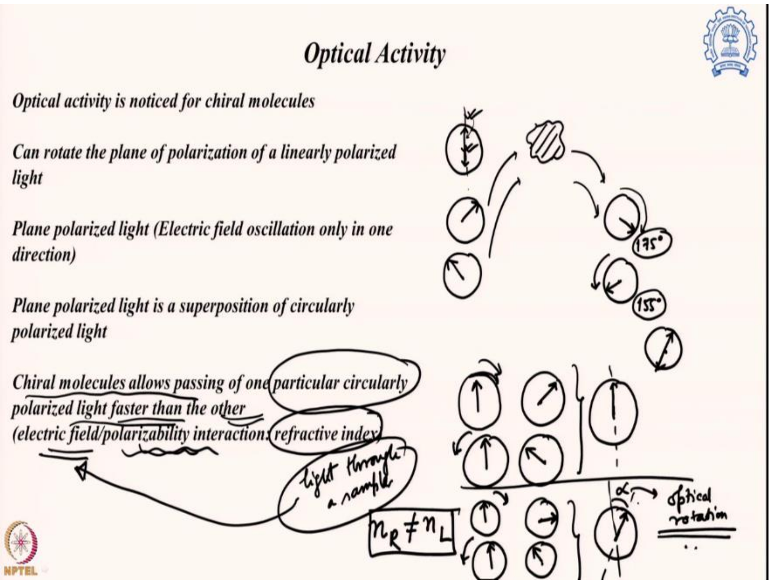
Optical activity is noticed for chiral molecules

Can rotate the plane of polarization of a linearly polarized light

Plane polarized light (Electric field oscillation only in one direction)

Plane polarized light is a superposition of circularly polarized light

---



Optical Activity

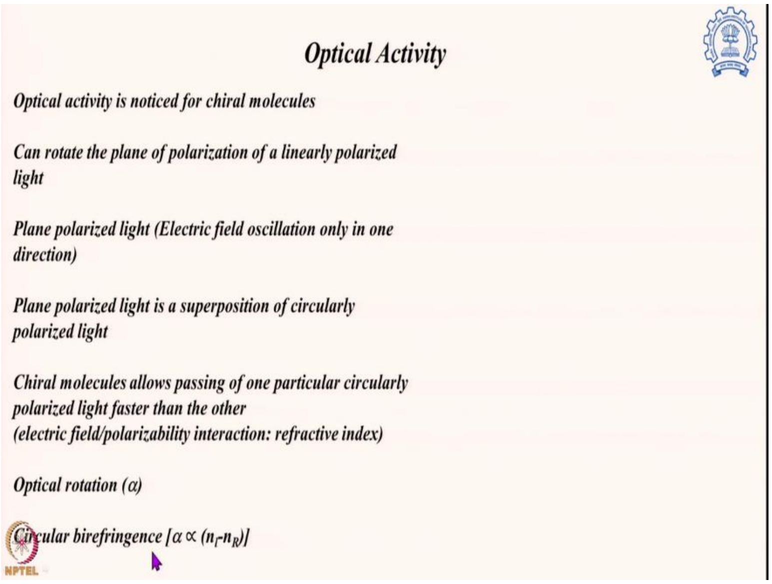
Optical activity is noticed for chiral molecules

Can rotate the plane of polarization of a linearly polarized light

Plane polarized light (Electric field oscillation only in one direction)

Plane polarized light is a superposition of circularly polarized light

Chiral molecules allows passing of one particular circularly polarized light faster than the other (electric field/polarizability interaction: refractive index)



Optical Activity

Optical activity is noticed for chiral molecules

Can rotate the plane of polarization of a linearly polarized light

Plane polarized light (Electric field oscillation only in one direction)

Plane polarized light is a superposition of circularly polarized light

Chiral molecules allows passing of one particular circularly polarized light faster than the other
(electric field/polarizability interaction: refractive index)

Optical rotation (α)

Circular birefringence [$\alpha \propto (n_L - n_R)$]

So, when we talk about light, the light generally travels in the form of a wave because it is electromagnetic wave. So, now this is how the light looks like when it is traveling if we are looking from the sideways but. If I try to look into that from the front, over here, how does the like would look like?

The light will look like as follows. Whenever it is at the center it will look like, this then it is going down, so it will be like this, then it is coming back and going back to zero again, then it is reaching the maximum, and so on and so forth. So, that is how it looks like.

So, if I put that all in the same place this will look like nothing but a line vibrotating like this. So, sometime it is going to be in this way, sometimes in the middle, sometime it is on the top. So, if we all combine them together this is how we say this is a light is coming through. So, this is what one particular plane. So, when the white light actually comes through it can show this behavior at any possible direction. So, this is known as the unpolarized light.

However, if we pass this unpolarized light through some special crystal which absorb all the different orientations of the light except the one, it will release the light which is vibrotating in one particular plane, and that is known as the plane polarized or linearly polarized light.

So now this plane polarized light, if it passes through a molecule which is chiral in nature, so say this is my plane polarized light where it started from, I pass this through a sample where I have a chiral molecule, and at the end when I am getting the final portion, so instead of being present in the original position we see it actually rotates. So, this particular rotation, if I put that as an alpha, is known as optical rotation. So, that is known as the rotation of the plane polarized light by a chiral molecule, and this is the optical rotation.

Now the question is how do we analyze this rotation is optical rotation? So, for that we have to go a little bit on details where we will see this plane polarized light, we are seeing is nothing but, it is a combination of two circularly polarized light, one which rotates right hand side, one which rotates on the left-hand side.

So, what do I mean by circularly polarized light? Circularly pressed light means when I start, I have my direction of the electrical field in this particular direction, then it starts rotates on the right hand side, and it continues to do so. So, the same electrical field it is going to do this rotation at the same place.

So instead of showing them in different places I can show them in one place. So, what we can see that this light is rotating in the same direction. So, it will be like this, this, this, and it will come back to the original position. So, that is, is the rotation.

When the rotation is happening on the right hand, side so you will say it is the right circularly polarized light. On the other hand there will be another component which rotates on the left hand side. So, like this, this, and so on and so forth, which can again be shown over here in the form of like this. So, now this one will be called the left hand circularly polarized light.

Now this right hand circularly polarized light and left hand circularly polarized light, they actually come together. So, you call them in short RCP, and this is called the LCP. They combine together and their combination or superposition is actually producing the linearly polarized light.

So how to understand that? So over here, on the top I am going to draw the RCP, then below that I am going to draw the LCP, and at the end, over there, I am going to show what is the superposition of those two systems.

So now, say, start over there, both of these are in the same direction so I should see a line like that if I super impose both of them. So, this is more of like a vector addition of this

RCP and LCP. Then RCP start moving on the right hand side, and the LCP moves the same amount but in the opposite direction. So, now if I combine these two how it will look like?

It will be the same position but with lower magnitude. Why? Because you can just imagine, one is this way one is that way, we get a vector over here. So, that is coming over here. The next one, this is rotated 90 degree, this one also rotated 90 degree. Now these two, if I combine them, they will cancel each other out so I should get nothing. Then it starts moving again.

And now as see one, but it is on the opposite direction because they also start rotating on the opposite direction. So, this is right hand, this is the left hand circularly polarized light. At the end they can go to the opposite end after full 180 degree rotation and this is what I get.

So now if we see the superpositions we are getting for each position it is nothing but, it is a plane polarized light in reality. So, it is nothing but a plane polarized light which is getting combined from this right hand and left hand circularly polarized light. So, that is why it is said that the plane polarized light is a superposition of circularly polarized light. By circularly polarized light we mean the RCP, the right hand circularly polarized light, and LCP the left hand circularly polarized light.

Now when a chiral molecule interacts with this plane polarized light it is actually interacting with both, right hand circularly polarized light and left hand circularly polarized light. And chiral molecule, because of the asymmetry present in the electronic environment that can detect the difference between RCP and LCP, the right hand and left hand circularly polarized light. And that is actually reflected in the form of optical rotation.

Let us connect those dots. So, say, I have my chiral molecule present over here and a plane polarized light is going through there. So, we can see actually it is not a simple plane polarized light but it is actually a combination of right hand circularly polarized light and left hand circularly polarized light, which are at the same phase. So, that is why I am always getting the plane polarized light over here.

Now what happens, once they both goes through the sample, one of them, say, the right hand circularly polarized light is moving faster than the left hand circularly polarized light.

So, previously they were in the same angle of rotation from the beginning. Now they are not.

So now say, it has moved, say 175 degree to the right hand side, in the left hand they rotate only 155 degree. So now what happens the right hand circularly polarized light and left hand circularly polarized light, their correspondent system is going to rotate from the original position where they are present.

So over here they are going to rotate on the right hand side because right hand circularly polarized light is moving more compared to the left hand side. So, coming back one more time, previously the right hand circularly polarized light and the left hand circularly polarized light started moving in the same direction in the same magnitude. So, that is why when you look into the resultant of their, they are always in the same position.

However, if one of them started moving more compared to the other, so say the right hand circularly polarized light is moving more than the left hand circularly polarized light what I am going to get is the resultant is now shifted, and that shifts from the original position and that is nothing but the optical rotation.

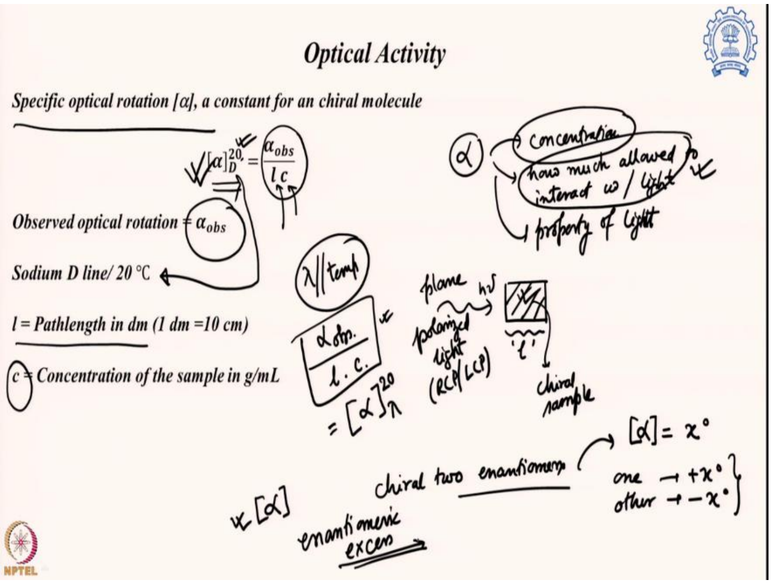
So, this optical rotation happens because the chiral molecule allows one of the circularly polarized light to move faster compared to the other. Now movement of light through a sample depends on the interaction of the light, that means an electromagnetic wave, the electrical field of it, and the electrons present in the molecule itself, the polarizability. So, they actually interact. And that interaction is given by the refractive index.

So, what we can say, the refractive index is given by n of the right hand circularly polarized light and the left hand circularly polarized light is not the same. And that is why the difference in the movement and that is why the resultant moves from the original position and we see an optical rotation.

So that is why the optical rotation is coming, and that is coming because of the difference in the left hand circularly polarized light refractive index and right hand circularly polarized light refractive index. And optical rotation is a function of their difference.

And this particular phenomenon is known as circular birefringence because it is creating a difference in refractive index, so that is why birefringence. And it is showing that on circularly polarized light, so that is why circular birefringence.

(Refer Slide Time: 13:40)



Optical Activity

Specific optical rotation $[\alpha]$, a constant for an chiral molecule

$$[\alpha]_D^{20} = \frac{\alpha_{obs}}{l\,c}$$

Observed optical rotation = α_{obs}

Sodium D line/ 20 ℃

l = Pathlength in dm (1 dm =10 cm)

c = Concentration of the sample in g/mL

Now when we talk about this optical rotation, and we understand why the optical rotation is happening, now this alpha value, the optical rotation will depend on how much concentration of the sample I have, how much sample is actually allowed to interact with the light, and the property of the light itself because light is giving the electromagnetic field, which is actually interacting.

So over here all these factors are actually combined over here in this equation, which says if you are taking optical rotation of a particular sample and say the measured optical rotation is lambda observed, and if we divided that by the path length of the system, so when we shine this plane polarized light, so this is the plane polarized light, which is nothing but a combination of two circularly polarized light, RCP and LCP, right hand and left side circularly polarized light, it is going through a sample where my chiral compound is.

So, it depends on how much path length I am allowing to get this interaction between this light and this sample. This is my chiral sample. And that is given by this particular term l, the path length. So, that is taken by, care of this factor, how much is allowed to interact with light.

So, what is the concentration? That will also depend. More the concentration of the sample more will be the number of molecule present over here, and that will have better interaction with the light. And that is taken care by this concentration term put over here.

Now we measure this optical rotation at a particular condition. So, generally it is at 20 degree centigrade so that is why this 20 term is given over here. And this D defined by sodium D line, which is actually a line coming from a sodium lamp at a particular wavelength.

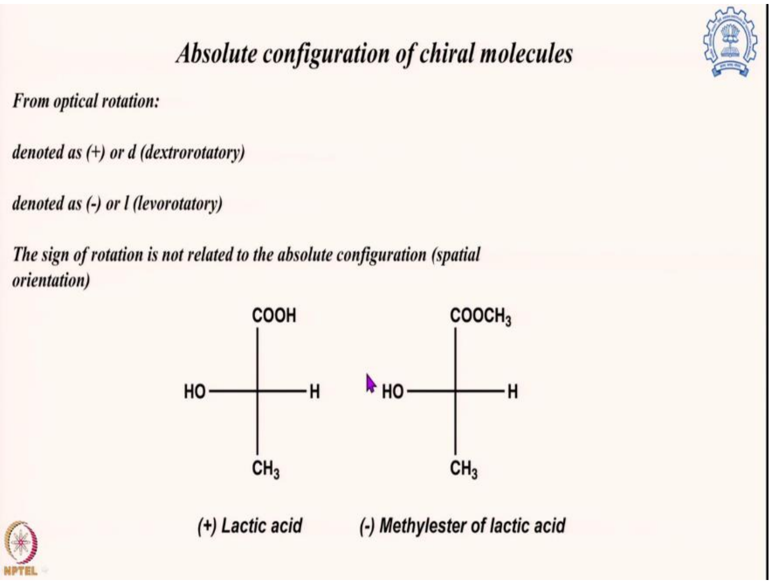
So, we measured that at a particular wavelength, at a particular temperature, and then if we have it observed optical rotation and I divided that by the path length and the concentration we get a value which will be a constant which is given over here. And generally we write the temperature and the lambda or the light which light we are using over here. So, this value is a particular constant value and for any particular chiral molecule it is, can be a signature value.

So now as we know any chiral molecule has two enantiomers, which are just mirror image of each other, so they will have alpha values exactly the same so it is x degree, they are rotating but for those two enantiomers, for one enantiomer it will be plus x the other one will be exactly same value but the opposite, minus x degree.

So that is why by taking a sample and measuring the optical rotation, and if we know the concentration and path length, we can figure it out what is the standard or specific optical rotation value. And not only that if we have a mixture of the samples, we can also find out what is the concentration of either of the enantiomer.

And we can find out the enantiomeric excess which is an important term when we discuss about producing an optically active or chiral compound and finding out their purity. So, we can do this experiment to find out how much is actually present with respect to one enantiomer.

(Refer Slide Time: 18:10)



Absolute configuration of chiral molecules

From optical rotation:

denoted as (+) or d (dextrorotatory)

denoted as (-) or l (levorotatory)

The sign of rotation is not related to the absolute configuration (spatial orientation)

(+) Lactic acid *(-) Methylester of lactic acid*

So now we have talked about this optical rotation, and as we just defined the optical rotation defines that how much is the plane polarized light rotates from its original position and it can be in the direction of the right hand side, which is taken as the plus sign, which is also defined as the ***d*** or dextro rotatory, over there, look into that carefully, the ***d*** is written in this particular way.

And over there the rotation on the left hand side is written as minus or ***l*** as levo rotatory. Levo means left hand, side dextro means right hand side. So, those are written over here in the lower case system which defines that it is an actual rotation of the plane polarized light when a particular chiral molecule is exposed with, to the plane polarized light.

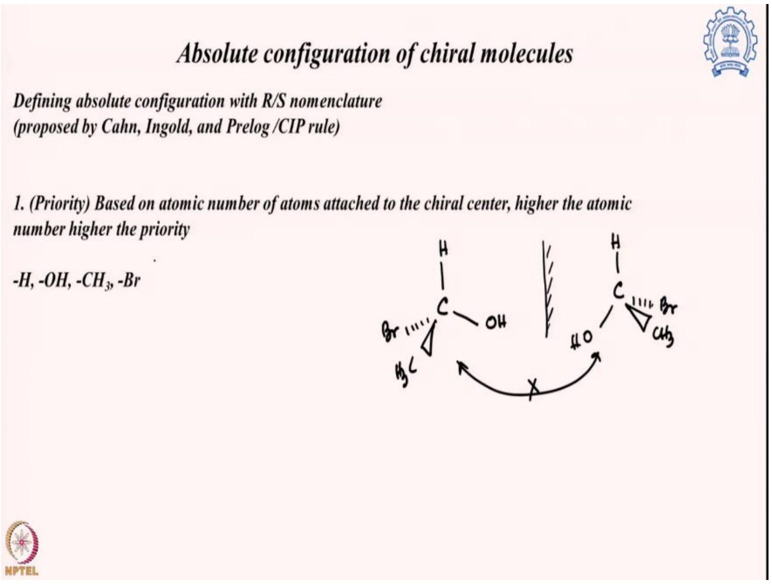
Now this plus or minus sign has nothing to do with the actual configuration of the molecule. The actual configuration of the molecule means how the molecule is actually oriented in three dimensions. So, for an example, the absolute configuration again means the spatial orientation of different groups present in the molecule.

And over here I am showing you two molecules. One is the lactic acid, this is the lactic acid present over here, I have drawn that in this particular configuration, where the carboxylic acid present over here, OH group over here, CH_3 over here, H over here. And this is found to rotate the plane polarized light in the right hand direction. So, it is denoted as plus or d molecule over here. So, it is written as plus lactic acid.

Now with the same configuration, keeping all the specific orientations, specific relative orientation same, I just change the carboxylate group to ester group, the methyl ester of it. And this molecule changes the direction of the optical rotation from plus to minus, although their actual absolute configuration in the same way.

So that means it says which particular direction the molecule is going to rotate is not directly correlated with the absolute configuration. So, just by doing an experiment and finding out that whether it is a plus or minus, I cannot really comment on the actual structure of the molecule. So, that is why we need a different nomenclature to designate the overall configuration or the absolute configuration of the molecule rather than just the direction of the optical rotation because they are not really correlated.

(Refer Slide Time: 20:45)

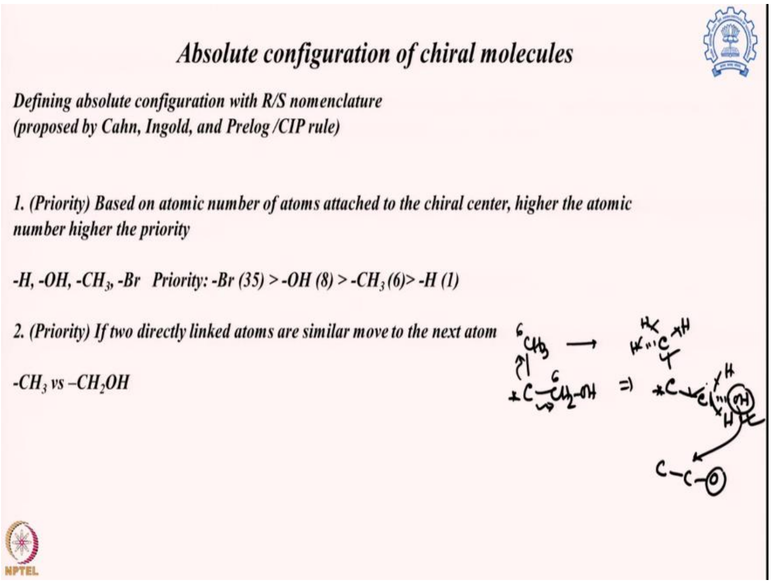


Absolute configuration of chiral molecules

Defining absolute configuration with R/S nomenclature
(proposed by Cahn, Ingold, and Prelog /CIP rule)

1. (Priority) Based on atomic number of atoms attached to the chiral center, higher the atomic number higher the priority

$-H$, $-OH$, $-CH_3$, $-Br$



Absolute configuration of chiral molecules

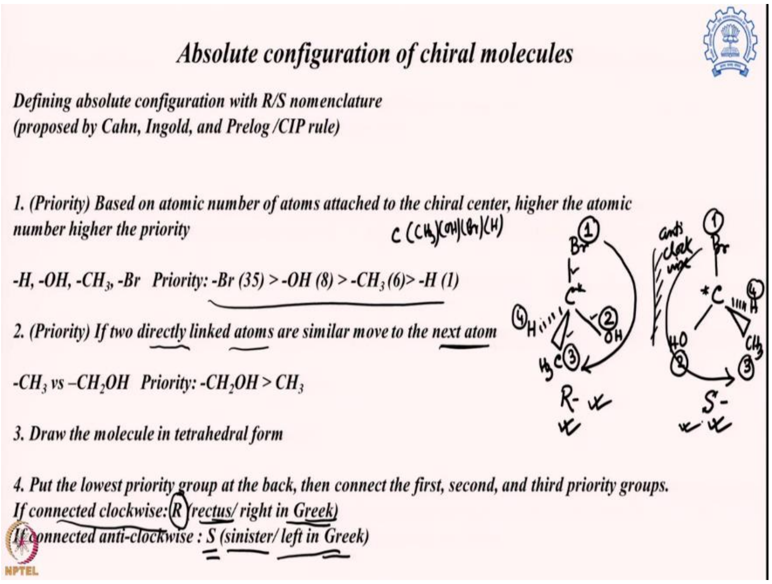
Defining absolute configuration with R/S nomenclature
(proposed by Cahn, Ingold, and Prelog /CIP rule)

1. (Priority) Based on atomic number of atoms attached to the chiral center, higher the atomic number higher the priority

$-H$, $-OH$, $-CH_3$, $-Br$ Priority: $-Br$ (35) > $-OH$ (8) > $-CH_3$ (6)> $-H$ (1)

2. (Priority) If two directly linked atoms are similar move to the next atom

$-CH_3$ vs $-CH_2OH$



Absolute configuration of chiral molecules

Defining absolute configuration with R/S nomenclature
(proposed by Cahn, Ingold, and Prelog /CIP rule)

1. (Priority) Based on atomic number of atoms attached to the chiral center, higher the atomic number higher the priority

$-H$, $-OH$, $-CH_3$, $-Br$ Priority: $-Br$ (35) > $-OH$ (8) > $-CH_3$ (6)> $-H$ (1)

2. (Priority) If two directly linked atoms are similar move to the next atom

$-CH_3$ vs $-CH_2OH$ Priority: $-CH_2OH > CH_3$

3. Draw the molecule in tetrahedral form

4. Put the lowest priority group at the back, then connect the first, second, and third priority groups.
If connected clockwise: R (rectus/ right in Greek)
If connected anti-clockwise : S (sinister/ left in Greek)

For defining an absolute configuration there is a nomenclature method which has been developed by these three scientists Cahn, Ingold and Prelog, and we call them as CIP rule by taking the first letter of each of their names, which is known as the CIP rule.

So, what is the CIP rule? So, in CIP rule we are going to prioritize the different groups bound to a chiral center. For an example a carbon center with four different groups bound to it. So, what, the first thing we are going to do, we are going to prioritize all those four different groups. And for that Cahn, Ingold and Prelog defined some rules.

The first rule is that we are going to define them with respect to their atomic number. So, for an example, I have a molecule over here. So, say, I have a molecule over here where I have a hydrogen, I have a OH group, I have a CH_3 group and I have a bromide group. So, all is present.

So, if I want to know if this particular structure, and if I take the mirror image of the system which will be the other enantiomer of it. So, the absolute configuration of these two molecules are actually not the same. They are different absolute configuration. But can I define actually the absolute configuration and nomenclature there. For that I need to find out what is the priority.

The priority is done with respect to the atomic number. And the atomic number, higher the atomic number, higher will be the priority, that is the simple rule. So, out of these four groups we can find the bromide is coming from bromine, has atomic number of 35, OH, the oxygen is directly connected to the carbon so we look into the atoms which are directly coordinated to the carbon, or the chiral center, so out of this O and H, oxygen is connected. So, we will take oxygen which has the atomic number of 8.

Then it bounds the methyl group and the carbon is directly connected, so that is why the carbon has atomic number of 6, and the end it is the hydrogen, 1. So, the priority will be 35 greater than 8 greater than 6 greater than 1 or the bromide greater than hydroxyl greater than the methyl greater than the hydrogen.

If there are two differently groups connected to it and both of them has the similar atoms bound first, we should go to the next atom. So, what does it mean? Now say, I have a molecule where I have a CH_3 group and a CH_2OH group present over there. Now directly it is connected to both carbons and both carbons has atomic number of 6. So, there is, not possible to prioritize them in this position.

So, for that we will go to the next one. So, the CH_3 molecule, so let me just draw this molecule little bit further away, is connected to three hydrogen. Whereas, this molecule is connected to two hydrogens and one O H group. So, over there you can see the next ones are all hydrogen, over there next one is hydrogen and one OH group. So, this, there is a carbon-carbon oxygen. So, this oxygen will get the preference. So, we go to the next one.

So, this is the chiral center. So, first one, it was unable to differentiate the prioritization. The next one actually allowed to do that. So, over here the OH group will be prioritized. So, the CH_2OH group has, have the highest priority because it has atomic number of 8.

Then we draw the molecule in tetrahedral form and at the end we are going to draw the molecule such a way that we are able to distinguish the difference.

For an example, let me take the example of that original molecule we have discussed about earlier. So, say, I am talking about this particular molecule, where carbon is connected to CH_3, and OH, a Br and H. So, over there what I am going to do is first draw this molecule such a way that the lowest priority group always go to the back.

So over there when you draw the lines, that means they are on the plane, this wedge bond means it is above the plane, and this dotted wedge bond means it is below the plane. So, out of these four groups hydrogen is always at the back. The rest of the group, we will just draw as it is. So, first the Br, then the OH, then say the CH_3. And then we number the priority. So, bromine is the number 1 priority, high atomic number, then the OH, the next one, and the CH_3, and hydrogen is 4, so it is on the back side.

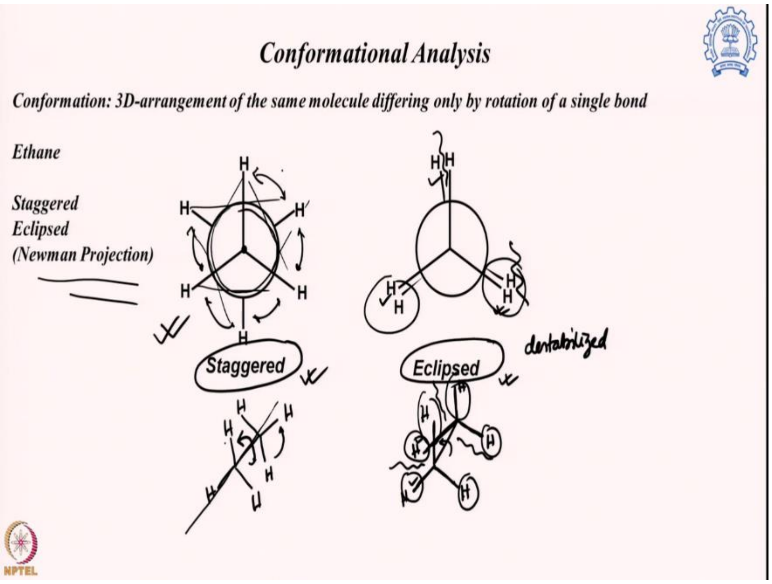
Now this 1, 2, 3, how they are connected to each other? You can see if I want to connect them by a line I have to rotate clockwise. So, if I have to rotate clockwise then the nomenclature gives by R. The R term come from the rectus, which is nothing but right in Greek.

Now if I draw the mirror image of this molecule, say the bromide, the OH now comes on this side, the CH_3 on this side, the hydrogen still remains on the back, again the prioritization is 1, 2, and 3, as per their atomic numbers, which is directly connected to the chiral carbon center. So, now you look 1, 2, 3, if I want to connect that, I have to rotate anti-clockwise, or a left hand side direction. So, that is, is going to nomenclature as S or sinister which means left in Greek. So, this is the R, this is the S.

So again, what we need to do to find the absolute configuration? First, find out all the groups connected to the chiral carbon with respect to the priority and the priority is defines by the higher atomic number. If the atoms linked to the chiral center is the same, move to the next atom until you find the difference.

Then draw the molecule in the tetrahedral orientation like this, put the number 4, or least priority group at the back, and then connect the 1, 2, and 3s. If it is a clockwise connection it is the R, if it is the left hand connection it is the S. So, by that we can define the absolute configuration of the molecule, how they are all each connected to each other.

(Refer Slide Time: 28:20)



Conformational Analysis

Conformation: 3D-arrangement of the same molecule differing only by rotation of a single bond

Ethane

Staggered

Eclipsed

(Newman Projection)

Now going to the next section, we also look into the conformation of different molecule. What is the conformation? Conformation means how a molecule is connected to different bonds, and if I rotate only a single bond, I go to a different orientation of the same molecule without changing the absolute configuration. And that is known as the conformation.

So, take an example. We take ethane. So, ethane is a molecule like this. So, over here, ethane is such a molecule. So, this is the hydrogen over here, this is a hydrogen over here, this hydrogen over there, on the back side there are the hydrogens on the other carbon.

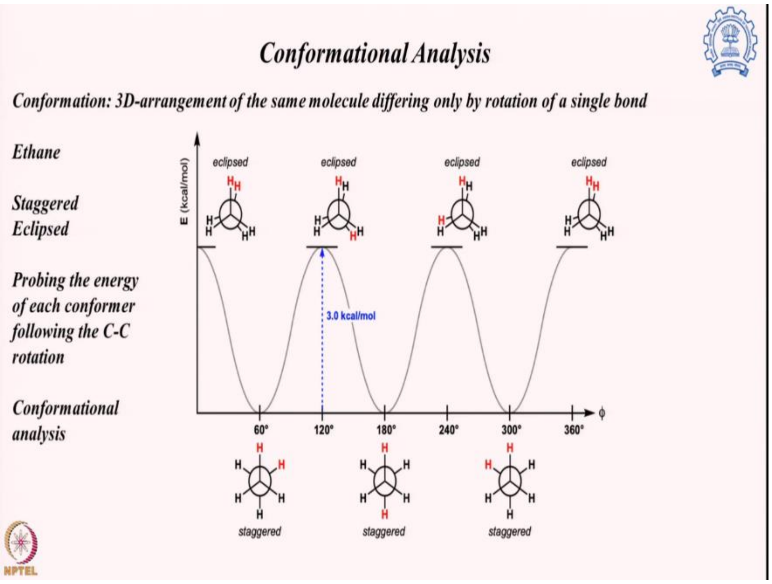
So now say, if I look through the molecule through this carbon-carbon bond, I will try to see this molecule in this way. The dot over here shows the first carbon, the circle on the back shows the second carbon. And that is how the molecule looks like. So, they look like this kind of trigonal structure if I look from the front, and that is how it looks like. And on the back that is also look like a trigonal structure. So, this is known as the Newman projection.

And now, over here if I rotate this carbon-carbon bond without changing anything else, so what I can achieve? So now say, I am rotating it, I am leaving the first carbon as it is, and by rotating it 120 degrees I will go to the same place. So, now say, I rotate only 60 degree, and I will rotate to this place where each of this hydrogen and each of the CH bond are actually almost on top of each other.

So, these are, kind of, we say, eclipsed to each other. So, that is known as the eclipsed form, whereas this one is known as the staggered form. And what is the difference between these two molecules? They are same molecule, ethane, C_2H_6, but the difference is how the, each of the bonds are oriented with respect to this carbon-carbon bond rotation. And depending on that I can have these two particular orientations. One is called the staggered, one is called the eclipsed.

Now if we try to find out what is the energy of the systems, now you can see because of this eclipsed interaction there is a possible steric hindrance coming over here because through the space the hydrogens are coming very close to each other and they can face some steric hindrance. So, that is why eclipsed is going to be destabilized and staggered from is the most stable from. The hydrogens are especially as far as possible you can get into this structure, 60 degree orientation.

(Refer Slide Time: 31:00)



Conformational Analysis

Conformation: 3D-arrangement of the same molecule differing only by rotation of a single bond

Ethane

Staggered
Eclipsed

Probing the energy of each conformer following the C-C rotation

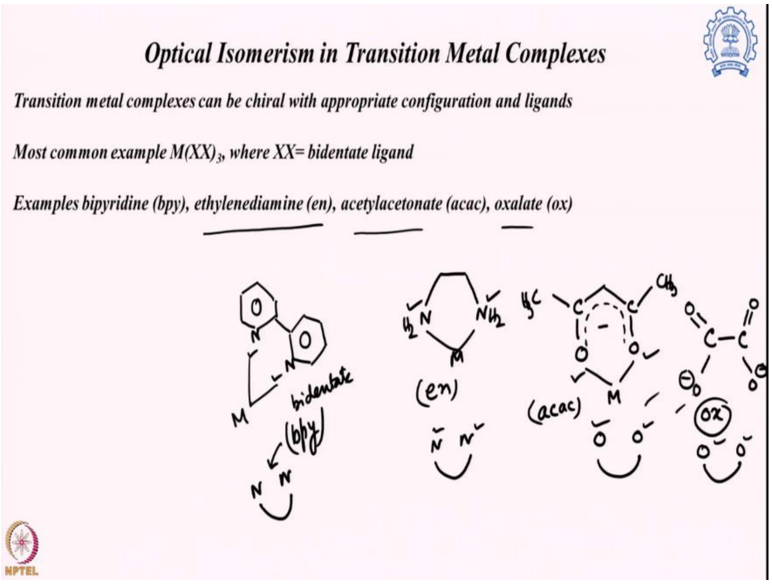
Conformational analysis

And then if I put this different orientation and that energy with respect to the angle of rotation of this C-C bond, I am going to get this kind of graph. So, this is where the staggered form, eclipsed from I begin with, so it is higher energy. Then I rotate this bond and I am following that with respect to this red circled hydrogen, the red colored hydrogens which is keeping the first one same, the back one I am rotating.

So, I rotate 60 degree and you can see now the energy is going down because they are going far away from each other, so it is getting stabilized. Now I am rotating further and this red one is rotating further coming to close to this hydrogen over here, and again it is facing eclipsed orientation, so it is going to higher in energy. And so on and so forth it goes back and forth.

So, finding out this kind of energy with respect to different conformer while I am rotating the C-C rotation, this is known as the conformational analysis of a particular molecule. So, this is one of the example how we can find out different conformers and how we can predict that energies. So, over there you can see the eclipsed form, because of this close interaction, steric interaction, it has three kilo cal per mole higher energy compared to the staggered one.

(Refer Slide Time: 32:15)

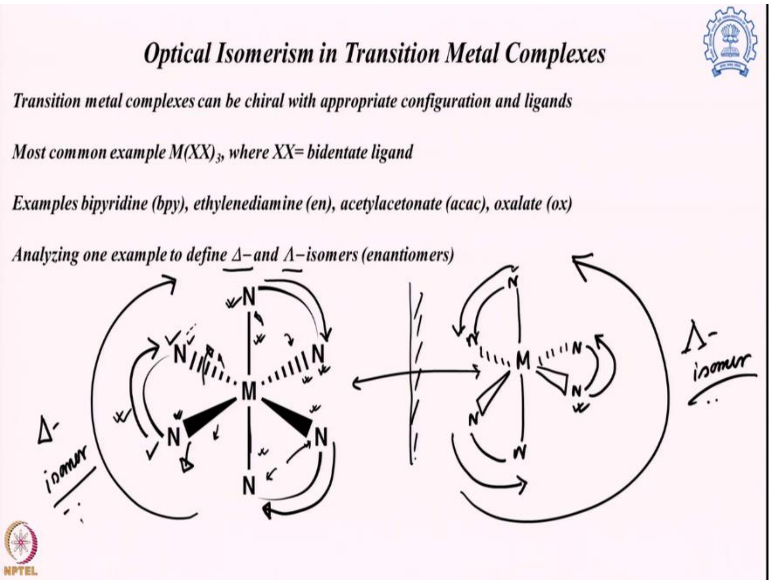


Optical Isomerism in Transition Metal Complexes

Transition metal complexes can be chiral with appropriate configuration and ligands

Most common example M(XX)$_3$, where XX= bidentate ligand

Examples bipyridine (bpy), ethylenediamine (en), acetylacetonate (acac), oxalate (ox)



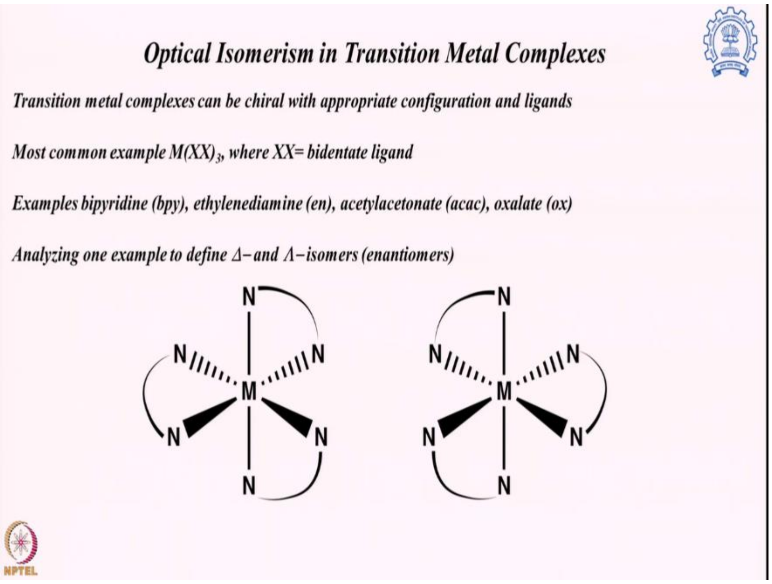
Optical Isomerism in Transition Metal Complexes

Transition metal complexes can be chiral with appropriate configuration and ligands

Most common example $M(XX)_3$, where XX= bidentate ligand

Examples bipyridine (bpy), ethylenediamine (en), acetylacetonate (acac), oxalate (ox)

Analyzing one example to define Δ−and Λ−isomers (enantiomers)



Optical Isomerism in Transition Metal Complexes

Transition metal complexes can be chiral with appropriate configuration and ligands

Most common example $M(XX)_3$, where XX= bidentate ligand

Examples bipyridine (bpy), ethylenediamine (en), acetylacetonate (acac), oxalate (ox)

Analyzing one example to define Δ−and Λ−isomers (enantiomers)

Now coming back to the last part of our discussion on optical activity, about the optical isomerism in transition metal complex. So, generally when we talk about optical activity or chiral complex we generally talk about the organic molecule where we have a carbon with four different groups. But transition metal complexes can also show chirality.

And the most common example of that, when we have a molecule in the form of a metal bound with XX ligand, where XX defines a bidentate ligand, that means a ligand which can bind the molecule with two different sites, and if three of them are present. So, altogether it has six coordination, and each of the ligand is giving two coordination each.

So, the examples of such bidentate ligands are given over here. So, one of them can be the bipyridine, which are two pyridine molecules connected to each other like in this way, where these two nitrogen's can come and bind with the metal. So, it can give a bidentate ligand. So, this is known as the bipyridine, in short from, bpy, and generally we write it as this way which shows that it is a bidentate ligand.

Then comes ethylenediamine. So, which is nothing but two amine groups connected with ethylene. So, this can also bind metal which is also again a bidentate ligand. Its short form is en, as shown over there. And this is also a bidentate ligand, and we generally also show that two nitrogen's binding with a connected form. So, it is another bidentate ligand form.

Then we can have acetylacetonate. We have a strong resonance coming over here with negative charge. And this is, can bind with another metal. So, this is also a bidentate ligand, and we show them generally in this particular direction. So, it is again a bidentate ligand.

Then we can have oxalates which can be shown over here. Similar way, bidentate ligand. And acetylacetonate, its short from his acac. So, these are the most common bidentate ligands which can bind a metal with two different sites. So, that is known as the bidentate ligand.

Now a metal binding to a bidentate ligand can have this particular structure. So, over here when we have formed this bidentate ligand, this is now a chiral molecule. If I draw the mirror image of this molecule, this will be the mirror image of this molecule. And we can see if we try to overlap these two molecules, they are not indistinguishable and superimposable. So, that means they are actually optically active compound.

So that means we need a nomenclature so that we can distinguish between those two enantiomers. So, for that we have a definition coming as delta and lambda isomer. How to do that? So now each particular bidentate ligand, we can see, there are two connection over here. And one of them is actually towards the observer, like us, and one of them is on the backhand side.

So, this is pretty straightforward for this particular group because this is wedge bond above the page, this is dotted bond below the page. So, that means this is towards you, this is backhand side.

Now this one over here, this is on the plane of the paper, this is backhand side, that means relatively this is towards us, this is on the backhand side. And between these two, this is on the plane of the paper, this is above, so this is again towards us, this is on the backhand side.

Now once we figure it out, which one is towards that and which one is backward among each of the set of the bidentate ligand, now you have to connect them. Connect them from the top to bottom. So, among these two, this is on top, this is at bottom. So, if we connect them, we have to go this direction. Similarly, between these two, this is top, this is bottom. Connect them we have to go this direction.

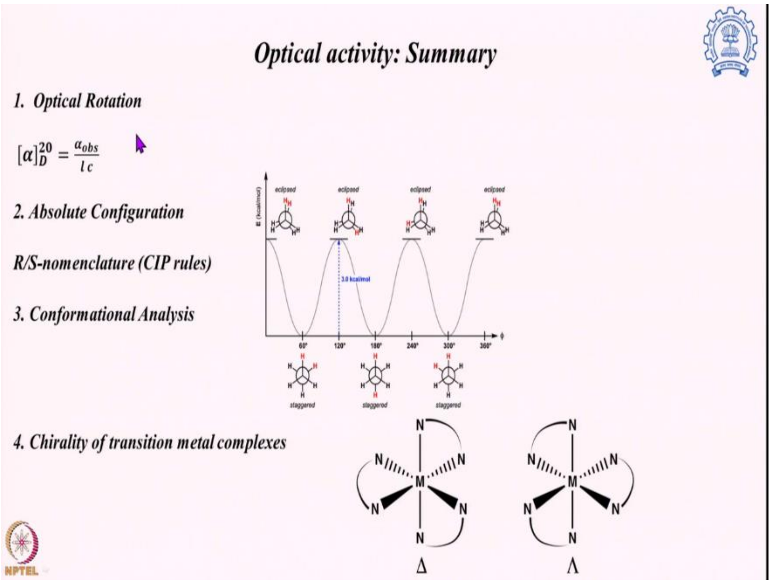
Similarly, for this, we have to go from this to this direction. So, over here you can see from the top to bottom, if I go from each of the bidentate ligand, I have to rotate right hand side altogether. So, this is known as the delta isomer, when I have to rotate right for going from the top to the bottom part of the same bidentate ligand.

What happens to its mirrored image? In the mirror image you can see, if I take this one, from top to bottom I am moving left hand side. This is top, this is bottom. So, again I am moving left hand side, again moving left hand side. So, this is, altogether, I am moving opposite side, and which is expected because this is the mirror image of each other. So, this is known as the lambda isomer.

So how to do that? Again, look into each of the bidentate ligand, find out which one is on the top, which one is the bottom, connect them. And find out for all three of them, and see which direction I am moving. If I am moving right hand rotation, it is delta, if we are moving left hand side, it is lambda.

So that is how we can distinguish between these two isomers present over here. So, delta and lambda. So, you can get an idea about this absolute configuration. Similarly, we get for the organic compound through R and S nomenclature.

(Refer Slide Time: 38:58)



Optical activity: Summary

1. Optical Rotation

$[\alpha]_D^{20} = \frac{\alpha_{obs}}{l\,c}$

2. Absolute Configuration

R/S-nomenclature (CIP rules)

3. Conformational Analysis

4. Chirality of transition metal complexes

So, in the summary, in this optical activity discussion we found how to define an optical rotation, and why it is happening. We found that optical rotation is connected with circular birefringence where the circularly polarized lights are actually have different refractive indexes. So, one of them move faster than the other. And that is why we see a difference in the plane polarized light, which is reflected by the optical rotation.

We can find a specific optical rotation, which is going to be a constant for a particular molecule measured at a particular temperature with a particular wavelength of light. We can also find out the absolute configuration of a molecule because, which is not directly correlated with the angle of rotation or the direction of the rotation.

The absolute nomenclature we can find by prioritizing the four different groups connected with the carbon which is a chiral in nature. And from there using the Cahn Ingold Prelog rules or CIP rules we can nomenclature them through R or S molecules.

We also discussed the conformational analysis, which is nothing but conformation of the different molecules which is nothing but a single bond rotation and we can find a different orientation of the molecule. And we can find how they are behaving with respect to the energy. And if we plot their energy versus different conformation we call them the conformational analysis, as we have discussed with the example of ethane.

Then we looked into the transition metal complex, whether they can be chiral or not. And we discussed one of the examples when a metal showing an octahedral coordination symmetry but bound with three different bidentate ligand, and over there they can show two different enantiomers, delta and lambda, and that we define with respect to how we can connect the frontier side and the back side of the same bidentate ligand.

If it is a right hand rotation for each of them, it is delta, if it is a anticlockwise rotation or left hand rotation, it is the lambda isomer. So, with respect to that, we like to conclude this section for the discussion about the optical activity. Thank you.