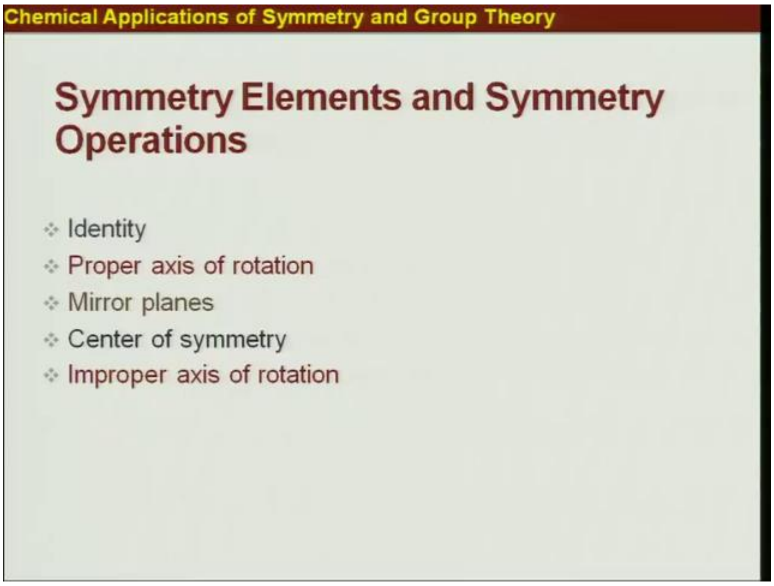
Chemical Applications of Symmetry and Group Theory
Prof. Manabendra Chandra
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture – 03

Hello everyone, welcome to the day three of first look up this course. So, in the last class we learnt about symmetry elements and symmetry operations. So, we learnt about the definition of symmetry operations as well as symmetry elements. So, we know that to any given movement of a body that brings the body back to an indistinguishable structure that is called a symmetry operation. And the symmetry operations are taking place about some point or about an axis or a plane which may or may not been included in the body, and this points or planes or axis they are known as symmetry elements, and if you look at on the screen. So, we can see we have outlined all the symmetry elements that are possible for any given object.

(Refer Slide Time: 01:12)



So, we have 5 different symmetry elements, identity element and proper axis of rotation then mirror planes and center of symmetry or the inversion symmetry and lastly the improper axis of rotation. And in the last class, we learnt about the identity which is symmetry operation and also we learnt about a proper axis rotation. So, we showed you some examples of proper axis of rotation there.

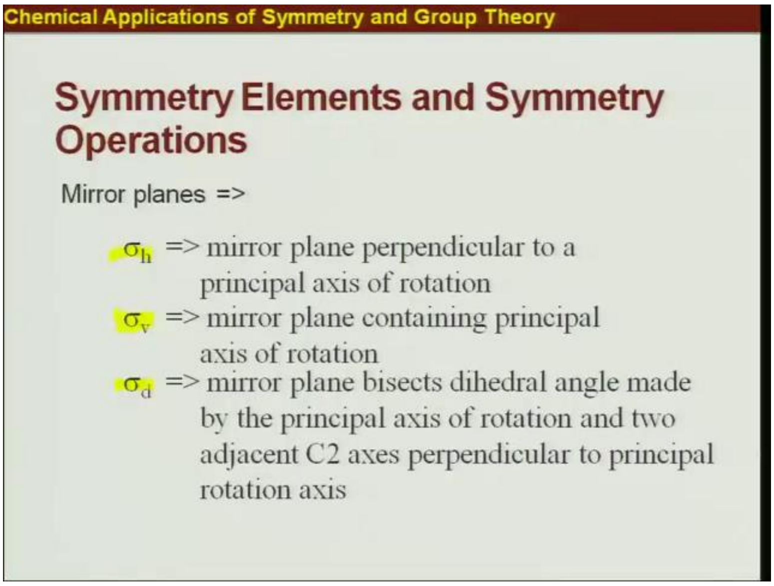
(Refer Slide Time: 01:57)

Today I will just show you, one with the help of 1 model that we make things lot clear for you, OK. So, you can see the model that I am holding you can think it like a model for chloroforms c h c l 3. So, this white one corresponds to c c l bond and the red ones each one corresponds to c h bonds sorry c h c l 3 I said. So, this white one will be c h bond and red the ones will be c c l bonds.

Now, you can imagine an axis which passes through this c h bond and about that if I give a rotation. So, this particular c c l bond is toward you now I give a 120 degree rotation. So, now, you have another configuration. So, you can see that this 2 are indistinguishable and these axis is c 3 if I operate once more, then I end up having another indistinguishable structure of c l c l 3. So, this axis is known as c 3 axis, OK. And this is the proper axis of rotation, and c 3 it gives you back the indistinguishable structure of the original molecule.

Now, we looked at also another example of so, benzene and I think ammonia also. So, I will request you to try to form some model, if you can buy from market any book shop will have this models boil and stick model or you can make some models by yourself, which is not so difficult and try out finding out difference symmetry elements because, that will really help you and understanding how you can find out the symmetry elements, because when you look at any molecular structure on pen and paper at the beginning, it may not be so apparent for certain molecules it will be very easy, but for some molecular structures it will be little difficult without having a particular model.

(Refer Slide Time: 04:24)



So, let us move on to the next symmetry element which is the mirror plane. So, plane of symmetry is defined as follows, like, if I have plane within the body, not outside the body, suppose I have a molecule say for example, I have a molecule the same molecule that I showed earlier that is c h c l 3 and if I can imagine at plane through this body, about which I can have reflection of any given point or any side of the plane. Suppose the coordinate of that particular point is x y z then after reflection through this particular plane I will get an indistinguishable you know structure on the other side in this indistinguishable point. So, the plane will be such that for any such point on this body will find an equivalent point on the other side of the plane. Then I will call that particular plane within the body of the molecule as a plane of symmetry or a reflection plane, OK.

So, let us have a look at this particular molecule again. So, can you tell is there any plane which can be called a plane of symmetry? The answer is; obviously, yes. So, if you imagine a plane through one h c and a c l this plane. So, this is the plane this will cut the structure into half two-half's. So, one-half contains this part and the half contains this part correct, and one is the mirror image of the other exactly. So, if I take choose a point here the reflection through this point will find another point which is exactly equivalent to the first point. So, this acts as a mirror plane. Now you can see since I am talking about this particular structures there is not only 1 plane, there are multiple plane since I you know choose 1 h c c l plane, but I can actually choose any other c h c c l plane and the third-one is this one. So, I can have three planes of symmetries and these where of symmetry is, denoted as a sigma, OK.

So, sigma is the symbol of plane of symmetry now very often we will come across with different types of sigma's for example, like sigma h, sigma v and sigma d. These three are mainly used and many operations you will also find like you know sigma v, sigma v prime, sigma v double prime or sigma d, sigma d double prime, sigma 3 double prime and so on. Now this all like sigma h or sigma d or sigma v or you can with the primes, they are all sigma planes there is nothing special about it, but this you know subscribes h d and v they are used to distinguish you know certain type of you know mirror plane, but they are you know functions are exactly the same, just to reflects certain points from one side of the molecule to another to give an indistinguishable structure.

So, what is sigma v first place? So, sigma v like you can see the definition of sigma v on your screen, so sigma if I convert this. So, sigma v is here. So, sigma v is the mirror plane which contains the principal axis of symmetry, we have learnt about principal axis of symmetry. So, for example, here this c h bond and if I have an axis through the c h bond that is my principal axis of symmetry in this particular is a c 3. So, if 3 is any sigma plane containing this axis I we call it as a sigma v. So, although planes that I showed you just few minutes back they are all sigma v. So, this plane is a sigma v plane, this plane is another sigma v plane and this plane is also another sigma v plane, OK.

Now let us have a look at what is sigma h? So, sigma h is the sigma plane, which is perpendicular to the principal axis of rotation. So, suppose I would have a sigma plane which is perpendicular to this axis that is why in this plane? That would be all sigma h plane. But you can see here is there any sigma explain, answer is no. Because, this is my principal axis of symmetry and if I have a perpendicular plane perpendicular to this principal axis of symmetry, then I really do not have any equivalent structure or indistinguishable structure when I reflect any point from this side on to this plane right, because I will not find a counter part for this point on the other side. So, is this one or this one? So, there is no such sigma h plane in this particular molecule, but you can actually have sigma h plane, if you consider certain other molecules.

(Refer Slide Time: 10:13)

Say for example, this all of you know what this model transfer right. This is a benzene molecule so, all 6 carbons and 6 hydrogen’s.

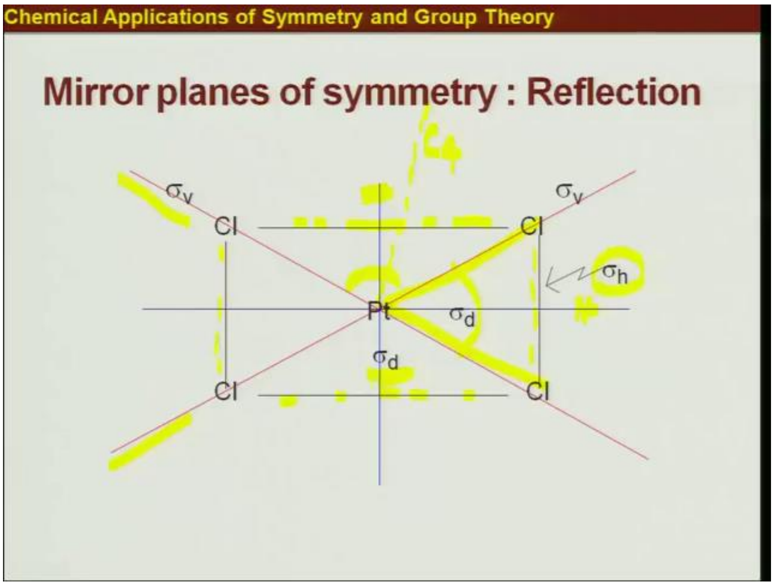
So, now I can easily figure out what will be the principal axis of symmetry. So, if I have an axis just passing through the middle of this benzene ring and I can rotate it by 60 degree I get another you know indistinguishable structure, we dealt with this in last week. Now if that is the principal axis of symmetry 12 have a sigma h plane look at it carefully, this is a planar molecule right. So, I just reorient it toward you now say this is my axis this is c 6 perpendicular to this will be just the benzene plane.

Now, you can easily imagine a plane through this benzene ring containing the carbons and hydrogen’s. So, if you reflect any object here it will finally, indistinguishable you know structure after the reflection because the plane will cut all these atoms into exact half right. So, therefore, any point on this side will have a counterpart on the other side. So, I will have a sigma plane really in this plane and this sigma plane which is perpendicular to this c 6 axis the principal axis of rotation this is a sigma h plane.

Now, what about sigma d? That is the other type of plane of symmetrical. So, sigma d is also a plane which contains the principal axis of symmetry, but it is different from sigma v in a slight you know in a certain way, what is that let us have a look at it. So, now, we have all ready figured out what will be the principal axis of symmetry here, this thing and then if I have a plane you can imagine we have already figured out sigma h so, forget about it.

Now, let us find out sigma v in this case. So, if I have in this direction a plane then I have you know this particular hydrogen a counterpart here, similarly this one has a counterpart here, this one as a counterpart here sorry this one will be cut into half this and this one. So, I have a sigma plane similarly a plane passing through this hydrogen carbon this carbon and this hydrogen will also form a plane and this is another plane. Now I can have another plane, another type of plane which will actually cut the angle that is form the dihedral angle to the precise which is formed by taking the principal axis of symmetry that is the this particular axis and this carbon and this carbon which contains those sigma v. So, I have an angle like this and this and the dihedral angle as this. So, if I have a plane, which bisects this dihedral angle and the plane if it acts as a symmetry plane then I will call that particular sigma plane as the sigma d is that clear.

(Refer Slide Time: 13:54)



So, you can see the actual definition clearly we can on a screen, OK, all right. So, now, let us take another example through which you can clearly see what is sigma d? Sigma v and sigma h, so p t c l chloral takes a chloral platinum if I ignored the charges then I have a just square plane complex so, platinum and 4 chlorine are at 4 corners of a square if I can imagine right, all of you know the structure. So, here if you have a look at on your screen you can see a there can be a mirror plane which contains all the chlorine atoms and the platinum atom meaning that molecule of plane itself can act as a symmetry plane, because the molecular plane will cut all the atoms into half. So, you can get a symmetry plane and that will be a sigma h why because, this is the square planar complex and you can imagine rotational symmetry axis perpendicular to this plane passing through the platinum atom right. And you can give a 90 degree rotation you can get an indistinguishable structures so; that means, you have an c 4 axis right and that is the you know highest order rotation axis that you can find for this particular molecule because other once are c 2 that also you can easily figure out, because we have learnt how to find the c 2s also using that d f 3 examples that we gave in the last class.

Now, we have found you know c 4 axis there that is principal axis of symmetry and the molecular plane which can act as a sigma plane also is perpendicular to the c 4 so, therefore, we will designate that particular plane which is also you know guided by this you know square kind of structure. So, this is our sigma h right. On the other hand if you follow these red lines which are also in the sigma planes because you can produce indistinguishable structure through reflection by reflection through these planes. This 2 contain the principal axis of symmetry. So, this is a sigma v plane.

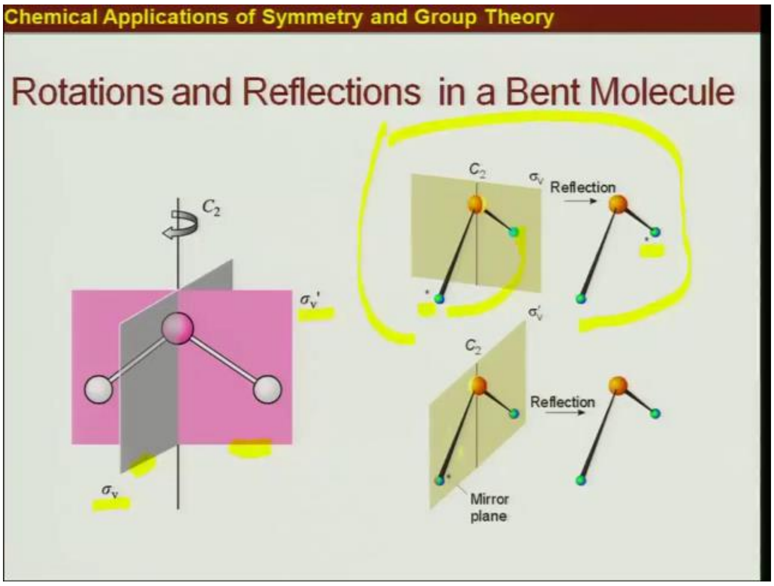
Now, you can have two other types of planes also which is shown here using the blue colors right. So, this 2 contains the principal axis of symmetry that is c 4 and also it bisects the dihedral angle. So, this dihedral angles are formed essentially by a 2 sigma v is right 2 adjacent sigma v’s day form this you know dihedral angle and it bisects that and matter of that, this dihedral angle is also formed by the intersection of 2 c 2 axis. So, the 2 c 2 axis they intersect and you take the principal axis of symmetry we form the same dihedral angle.

So, this is the dihedral angle. And if you can imagine say this is c 4 then this you know dihedral angle is the 1 that we are talking about and this sigma plane shown in blue color the bisects this plane similarly, this is happening in this particular case also right. So, these 2 are sigma d planes. So, I hope by now you know exactly what a sigma planes and what are their functions and what are the different types of sigma planes and how to know each one is what now. So, far we have learnt identity we have learnt rotations and we just now have learnt the reflection. These are the symmetry operations so; we learnt identity elements we learnt about the rotational axis and sigma plane or mirror plane.

Now, you can combine you know this operations which I will talk about may be 2 to 3 classes later now on this screen if you look at I have tried to show you the rotation and reflection symmetries for a single molecule. Because our aim is to you know classify molecule in terms of the symmetries, we have been talking about this structure is more symmetric than this structure, but how. So, we found out there are certain things like symmetry element and symmetry operations by which you can somehow quantify.

So, depending on how many symmetry operations are there how many symmetry elements are there and how many symmetry operations can be generated using those symmetry elements that will decide which molecule is have been higher symmetry then another molecule.

(Refer Slide Time: 19:27)



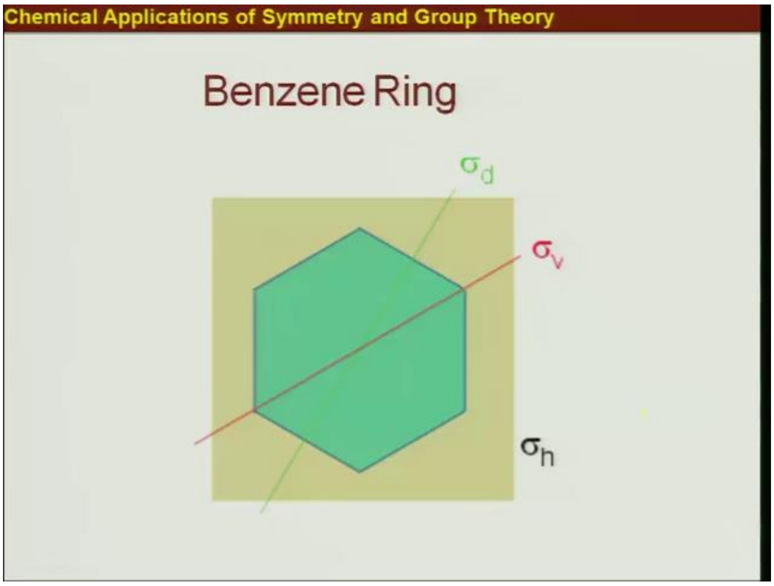
So, we should be able to find out all the symmetry elements that are present in a given molecule. So, now, if you have a look at on your screen you will see we have given an example of water molecule and you should be able to easily find out the rotational axis which is c 2 right, because we can have 180 rotation by an axis passing through oxygen and which can you know which is on the plane of h o h bond h o h molecule. So, that one is the c 2 axis.

Now, in the same structure I have tried to show two different planes. So, this is 1 which is in somewhat like a pink color and another is in you know grey color, so, these 2 planes if you can imagine and is very easy to see here right because this is one of the simplest structures that you can have. So, this 2 planes instead of them you will produce indistinguishable you know structure of these molecule water when we operate you know this reflection. Now you can see here that I have given sigma v and sigma v prime rotations to this 2 plane and mention that, you may come across this kind of symbol is in that is you know not only that sigma v, sigma d, sigma h, but also sigma d, sigma prime sigma d prime or here sigma b, sigma b prime this is just to differential because if I call both of them sigma v then when you 1 to 2 something further mathematically or they are the quantitatively he will end up in trouble because, if you I am distinguishing two different series that sigma v is right and 2 different sigma v’s will have different functions like here you look at the structure again sigma v will cut this molecules into two-half's where each half will have 1 some portion of this oxygen half portion of oxygen and 1 h.

Similarly, the other half will have the same thing, but the sigma v prime plane that cuts the molecule into half in such a way that each half gets half of each atoms right. So, those 2 are different right. So, later on we will see that those 2 will have certain different characters. We will know about this term particular the character in a later stage. So, in order to distinguish them we have given 2 different symbols sigma v and sigma v prime. Now on the same screen you can see that I am putting this c 2 and you know sigma v there and you can see how the operations will you know transform the molecule so, in the first case this is the top part if you look at we will see there is a star mark hydrogen atom which moves from here to here right. So, if you look at this molecule it has gone here so, c 2 will move this molecule this hydrogen atom over here. Now if you have a sigma v acting there, sigma v essentially which will cut this h o h angle into half then this star will now be reflected here. So, here for some reason this star is not been shown up. So, not this star will be somewhere here right.

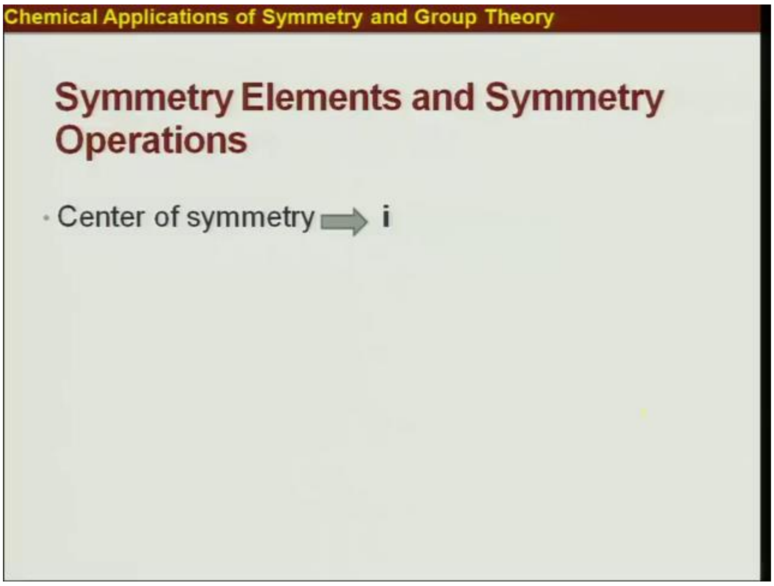
So, now we can see that this sigma v and c 2, they produce the same result that is pretty amazing thing and in many cases you will see that you will see that you know some symmetry operations will produce the same structure operating on the molecule. And also I will mention here that, we will see you know successive operations successive application of this symmetry operations, 2 or more than 2 can produce and structure which one can actually get by applying 1 single symmetric operation. All those things will come from the combination of the symmetry operations that we will see the probably the following week, but I just a wanted to mention that, so, that we are aware of that band.

(Refer Slide Time: 24:04)



So, here on the screen you have this benzene ring at is difference between sigma v, sigma h and sigma d they are shown and I have already showed you using this model if you remember exactly. So, that is all I wanted to talk about regarding plane of symmetry, well let us move on to next symmetry elements that we need to know and to learn that is center of symmetry also called inversion center that is written on the screen.

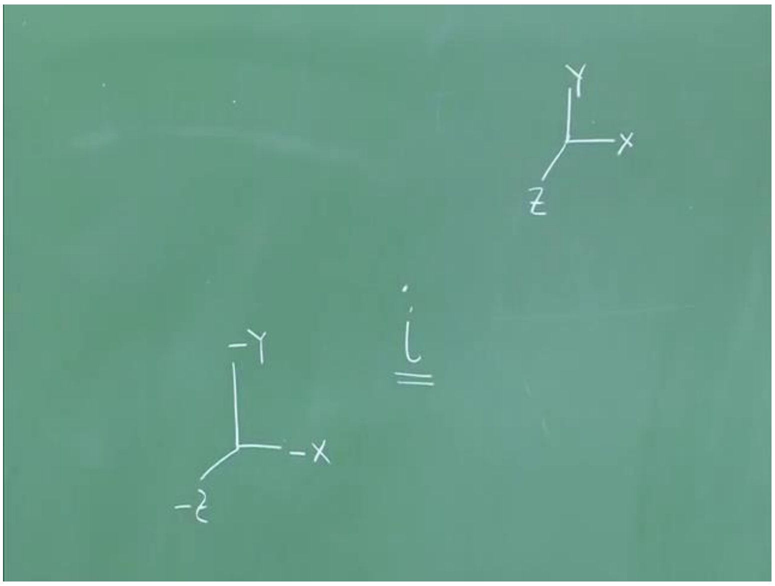
(Refer Slide Time: 24:34)



So, how do we define center of inversion for any given structure or molecular structure if you if you can produce and you know equivalent point by passing by taking a point on the object and passing through a particular point and getting the equivalent point on the other side so, then that origin, will be known as center of inversion.

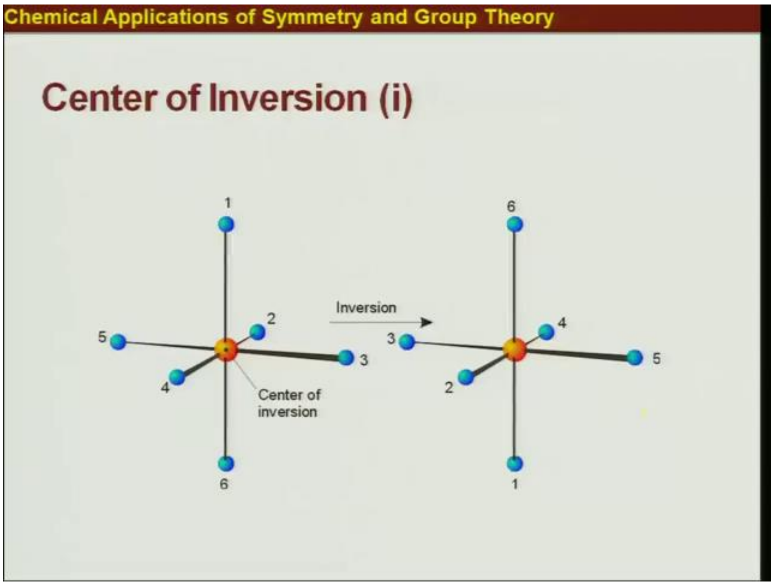
So, let me try to explain this in little bit later way. So, suppose I have say let me try to use the board here.

(Refer Slide Time: 25:47)



So, suppose this is my space which I characterizes any particular molecule now I take any particular point and the coordinate of that point is this that is x y and z. Now if I take this point which coordinates x y z and can find an equivalent point here whose coordinate will be minus x minus z y and minus z then the origin of this system will be the point of inversion or center of inversion. So, this particular point here will be the center of inversion i. So, we will explain what is the center of inversion is a using and the model and you know I will also I have prepared some presentation regarding that one.

(Refer Slide Time: 26:54)



So, let us take this particular molecule on your screen, which resembles octahedral molecule like, s 8, 6. So, we will use this particular molecule to explain the center of inversion in the next class. So, we will stop here today, and will come back in the day 4 of this course with this inversion center and many more days.

Thank you very much.