Chemical Crystallography
Prof. Angshuman Roy Choudhury
Department of Chemical Sciences
Indian Institution of Science Education and Research, Mohali

Crystallographic Point Groups and Space Groups
Lecture - 08
Stereographic Projections of Point Groups

Welcome back to the course of Chemical Crystallography. In the previous lecture we just ended with the description of 32 crystallographic point groups where we talked about the symmetry elements and their orientations. And we have identified some of them with yellow lines with yellow highlights, and termed them as Laue groups.

So, now, we would like to discuss the stereographic projection of these 32 point groups. What we want to do is we want to we want to represent these 32 point groups in a 2 dimensional manner. So, for that we will follow the same type of procedure which we discussed in the previous lecture while drawing the projection for the roto inversion and roto reflection axis. First we would like to draw the point group 1.

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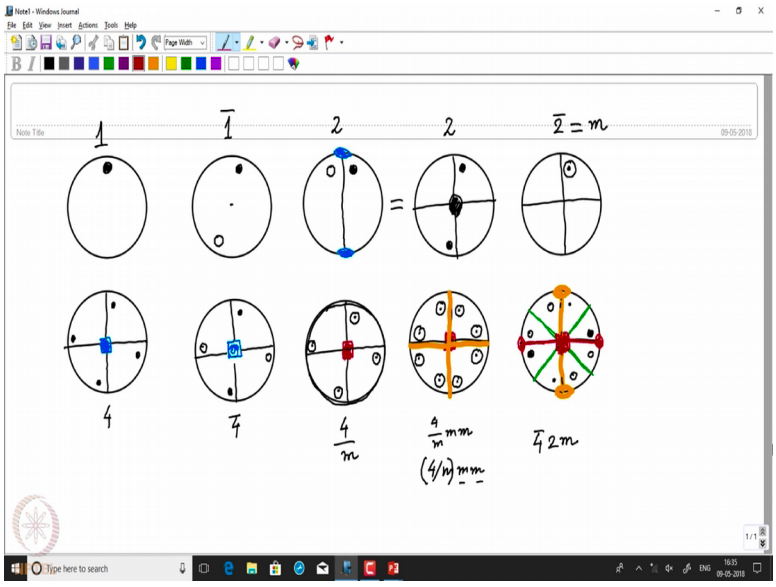

What is 1? We do not have any symmetry in 1 which means we should only draw a circle. Since, we will be needing this circle a few times now I am just making those circles available for us to draw these projections, one after another. So, the first thing that we would like to draw is the point group 1; space group 1 does not have any symmetry in

it so, only a 360 degree rotation can bring the same molecule or same object back to its original position. So, we just draw it as a closed circle and it is point blue 1.

When we say one bar it means it is a 360 degree rotation followed by inversion, which actually means just inversion. So, when we have one object which is a closed circle at the upper hemisphere we are trying to take its inverse and it comes to the lower hemisphere and the way the projection is understood as if you have a light at the top, you have the object here and the 2 positions one is up above the equator and the other one is below the equator of this imaginary sphere, are represented in 2 dimension. So, when we have a inversion center at the center, the inversion related object comes in the lower part of the sphere as open circle.

The next one that we would like to see is 2; there are 2 different ways one can draw a twofold if the twofold is in the plane of equator or in the equatorial plane, then what happens is if this is a sphere if a twofold is there from front to back the object which is here gets rotated by this twofold and comes to the lower hemisphere on the other side. So, the open circle sorry the closed circle on the right becomes open circle on the left by this twofold axis. One can consider the twofold to be along z, which means we may have the twofold in the middle of the plane of projection.

So, in that case we start from here. So, this is a twofold, my object is here when it rotates it still stays in the upper hemisphere, but comes to the other side of the upper circle. So, the object which is here on doing a twofold rotation comes there, and still remains a closed circle. So, this is another representation of 2; they are one and the same: what is 2 bar? A 2 bar operation means you have a twofold axis and inversion center. So, you start from one point here, do a twofold rotation followed by inversion takes it exactly below the original point. So, anything coming exactly below is equivalent to a mirror operation.

So, 2 bar should look like this, the closed circle and open circle are at same place because you have this twofold axis, you are rotating the point by 180 degree and taking the inversion it goes there. So, this inverted point comes at the same place of the original point, and that is why this 2 bar is equivalent to a mirror. Now let us see the point groups 4 and 4 bar one after another. When we say a point group 4 it indicates that it has a fourfold axis of symmetry at the middle, as a result the object is this is the fourfold axis the object is here it rotates by 90 degree 90 degree 90 degree and goes back to the

original position by 90 degree rotation and it always stays in the upper hemisphere. So, therefore, all the 4 positions are filled circles.

But in case of 4 bar the situation is slightly different, when you have this open close circle what do you do is rotate by 90 degree and simultaneously invert. So, it comes to the lower hemisphere. So, the closed circle after one round of 4 bar becomes open circle in the opposite side. So, from here the point should have come here as of the close circle, but then since this is a 4 bar which is a simultaneous operation. So, we do a fourfold rotation followed by inversion, it makes it as open circle.

Similarly, you rotate it by 90 degree and invert it, we started with open circle this must be a closed circle. Now, we start with this closed circle, rotate it about 90 degree and then invert it we started with closed circle so, this should become open circle. So, now you see 4 and 4 bar are different in their representation, what happens to 4 by m? The point to be noted here is when we say 4 bar it is roto inversion axis. So, rotation and inversion takes place simultaneously and then we identify the point, but when we write 4 by m, it means we have a fourfold axis and a mirror separately. So, we should have points corresponding to fourfold and then apply the mirror to all those fourfold those points generated by the same fourfold.

So, to do that we divide this circle in 4 parts write down the draw the fourfold in the middle, and then start with the closed circle we do a fourfold as we have done before on the left hand side and it generates those 4 points because of fourfold, and now when I am saying that 4 by m in the previous lecture I have talked about this 4 by m means a fourfold is along c, and mirror is perpendicular to that fourfold. So, the mirror plane is the plane of this particular circle. So, when you have mirror plane now in the plane of the circle, then all these 4 points which are closed circles will be reflected in the lower hemisphere. So, one open circle has to be drawn at the same place.

So, this then represents 4 by m what will be 4 by m m m? In the textbook you will see that it is written as 4 by m m m, it actually means it is a 4 by m operation and then there are 2 more mirrors perpendicular to that first mirror, which contain the fourfold axis. So, now, to identify that we first draw what we have seen in case of 4 by m. What we have seen in 4 by m is this which is there on your left. Now, when we are saying that there are 2 more mirrors containing the fourfold axis perpendicular to the previous mirror then the

2 mirror planes should be this one and that one. So, now if we try to operate these mirrors on the points that have been generated, we should simply get one more set of closed and open circle because of that mirror and because of this horizontal mirror, we get one point here and we get the corresponding point there. So, this represents 4 by mmm.

The next one in 4 we would like to discuss is 4 bar 2 m. So, now, it is a combination of 3 symmetry elements one is 4 bar which is along this j axis z axis, a twofold which is along a or b and mirror which we will see gets generated between the a and b like a diagonal plane that is sigma d. So, to start with what we should generate is before bar as we have seen in 4 bar here on the left, we should first generate the corresponding 4 bar. Now, I have a 2 which means this 2 is either along x or y. So, if I assume that 2 is along this direction which is here, what I end up getting is this twofold which we have thinking is along the equatorial plane and the point above the plane on application of this twofold goes below the plane.

So, as a result which is open circle here sorry closed circle here becomes open circle, this open circle goes to the other side and becomes closed circle, this open circle comes to the other side and becomes closed circle and this closed circle coming on the other side becomes open circle. See what has happened. By default by applying one twofold in one direction it has generated another twofold in a perpendicular direction, what else has happened it has generated a mirror plane bisecting these 2 twofold axis, 2 such mirror planes have already been generated.

So, we have 2 two folds one along x another along y, and then we have 2 mirrors bisecting the x and y direction as this and that. So, this particular diagram indicates the point group 4 bar 2 m, now we will try to see some of the point groups which involve 3 and 6.

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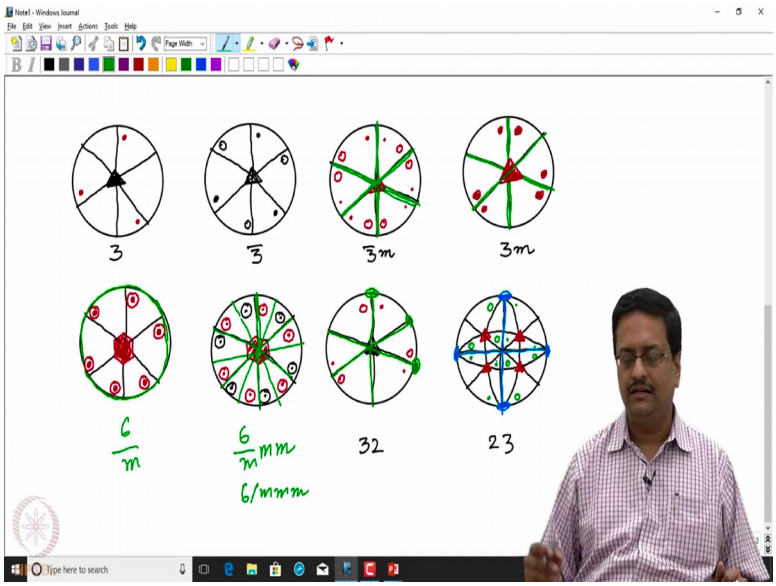

So, now let us start with simple 3 what is a threefold axis, it gives you at 120 degree rotation. So, whenever we try to draw 3 or 6 we should divide this circle in 6 parts; that means, we draw 3 lines like this. We have the threefold axis in the middle, we start with one object here and the threefold axis suppose these along z, then the point rotates like this by 120 degree and comes here by another 120 it comes here another 120 it goes there. So, by doing such operation it goes at those 3 places and it is just 3. The next one that we would like to draw is 3 bar what is the difference here? It is 3 and inversion simultaneously. So, one thing we should carefully divide the circle into 6 parts, and we should start with the closed circle.

So, now when we are doing it 3 bar, it should be a rotation followed by inversion and becoming an open circle this is my 3 bar axis. So, now, again we rotate from this point 120 degree rotation brings it at this point and then if we do an inversion we started with open circle we should end up getting a closed circle. Then we continue this operation 120 degree rotation followed by inversion becomes open circle start with open circle 120 degree rotation followed by followed by inversion becomes closed circle, once again 120 degree rotation followed by inversion becomes an open circle.

So, this is the representation of 3 bar what happens when we draw 3 bar m? We can straight away draw the 3 bar first, and when we are saying this as m this m is not perpendicular to 3 bar it is along the 3 bar. So, we can consider this m as one of these

lines when it is 3 by m, then it is perpendicular to threefold, but when it is 3 m or 3 bar m that mirror contains the threefold axis or 3 bar axis. So, by doing this mirror operation, what we get are just the mirror images of those points.

See what we have obtained by considering one mirror along one of those straight lines containing the threefold, and then applying the corresponding mirror, we have generated a mirror here and we have generated another mirror there. So, this particular diagram represents 3 bar m; what will happen if we want to draw 3 m? Once again we divide it into 6 parts, the threefold axis is in the center and then we would like to draw the points. So, first we draw 3 because these 2 are not simultaneous operations. So, we have judged on 3 and when we write m, it is the mirror containing the threefold axis. So, this could be a mirror like that.

So, this mirror reflects this point to the other side, this point on left hand side, this point on left hand side here. So, what is the result? As a result we see that it has given rights to these lines which we initially had drawn to make it 6 parts are also the corresponding mirror planes. Now let us try to draw 2 point groups 6 bar and 6 by mmm sorry we should draw 6 by m and 6 by m m m. So, when we again say it is 6 by m, it means we have a 6 fold axis along z. So, we again divide this into 6 parts the 6 fold axis that we are talking about is here. So, my object which is sitting at this point I am rotating it by 60 degree it goes, at all the places at rotation after rotation of 60 degree and it does not change its nature because it remains always in the upper hemisphere and then when we say by m the 6 fold is here and the by m mirror is perpendicular to it.

So, the mirror plane which we have here is the equatorial plane which is the boundary line of this circle as a result, these points will go below the equatorial plane after the mirror operation. So, the open circle and closed circle both will come at same place. So, now, we can easily understand that what will happen if we do 6 by mmm. So, we again divide it into 6 parts, the 6 fold axis is at the center, and then I will first draw 6 by m as it is drawn on the left hand side, and then the 2 mirrors that we are talking about are these 2 mirrors maybe even if we just draw one it will generate the other mirrors.

So, this one generates the object there, this mirror reflects it here the mirror reflection of this comes to the other side the mirror reflection from this point goes to the other are end, the mirror from here comes at this point, this mirror comes on this line. So, as a result

what has happened is it has generated the other mirrors as well and you can see there is a mirror in between. So, this is the representation of 6 by mmm, which in textbook you will see is written as 6 by mmm.

Now, we will do 2 space groups which are very similar, but they belong to 2 different crystal systems as you know 3 2 belongs to trigonal system, while 2 3 belongs to a cubic system. When we say 3 2 we first should draw a threefold; what is a threefold? We have already drawn it on the first left hand top corner. So, the threefold can be drawn very easily and the twofold axis that we are talking about is perpendicular this to this threefold, which is here and there are 3 such 2 folds which are like that.

So, now by doing this twofold operation, the closed circle becomes open circle this closed circle on this side becomes open circle this closed circle becomes open circle, on that side. So, this diagram represents a simple 3 2 point group, but 2 3 is different; 2 3 is a cubic point group and in a cube what you have are 4 threefold axis if you draw a cube, and then from every corner to the other body other corner along the body diagonal is your threefold and there are 4 such 3 folds, and the 2 folds that you have are along the faces the center of the faces you have these 2 folds along the center of faces.

So, drawing this 2 3 is slightly difficult. So, I am drawing it slowly for your easy understanding. First I am dividing it into 4 parts, then I am joining from top to bottom with a curved line I am joining again left to right with a curved line and then joining these points across. So, now, since we have 4 threefold axis along the body diagonals, we like those threefold axis at those 4 points of intersections of 4 lines. So, now, if we start putting our points the objects, suppose we have one object here we do a 3 threefold rotation the object comes here, we drew another threefold rotation the object comes there about that 3.

Now every one of those lines which we have drawn these lines correspond to a twofold axis. So, now, what has happened is the close circle on the right on 120 180 degree rotation becomes open circle on the left. So, this twofold do this this close circle on the light comes here and becomes open circle, and this comes here as open circle. So, the top portion is done. Now once again this particular line which we have drawn also represents a twofold.

So, when we do this twofold on all the 6 points that we have on the upper portion, the closed circles will become open circle and the open circles will become closed circles. So, then this particular diagram which we have now generated at the end is the stereographic projection of point group 2 3, I understand this is difficult and one can only draw it, when you have done this a many times. You should try to practice this 2 3 3 2 6 by mmm and all these point group drawings yourself to be able to draw it easily. So, in the next class we will continue with the crystallographic planes directions mirror indices etcetera.