Chemical Crystallography
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Understanding of Space Groups and Miller Indices
Lecture - 17
Tutorial - 2

Welcome back to the course of Chemical Crystallography. This is a second tutorial after the end of second week. So, in the tutorial sheet you must have received some problem so, we will try to see how those problems can be solved.

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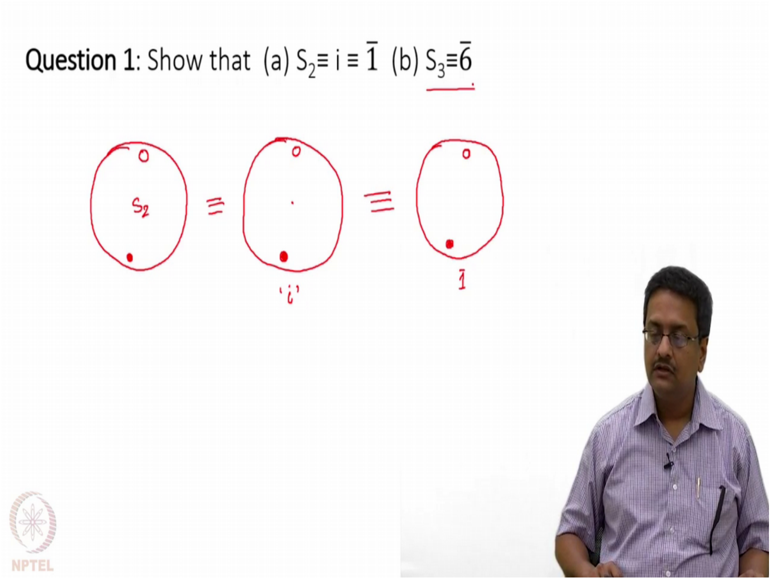

So, what we have asked is that. So, that S 2 is equivalent to i is equivalent to 1 bar to show that what is S 2 we should first draw a circle and then if I draw 1 open cycle inside the circle it is my object, and S 2 means rotation followed by reflection.

So, if I rotate by 180 degree and then reflect the open circle becomes the closed circle. So, this is S 2. What is i? I is inversion. So, if I have this object and if I invert; that means, the center of inversion whatever is above the plane should go to the below the plane and become the closed circle. So, open circle becomes a closed circle here. So, this indicates that this represents i; in the same manner if I try to draw 1 bar what is 1 bar? 1 bar is 360 degree rotation followed by inversion.

So, 360 degree rotation brings the open circle from the point where we started by doing 360 degree rotation, and inversion takes it to the lower hemisphere. So, again it becomes the same representation as we have seen for S 2 and i. So, these are equivalent. So, this is how you should solve these problems draw by trying the projection. So, I am not going to solve the second one for you I leave it to you to find the answer.

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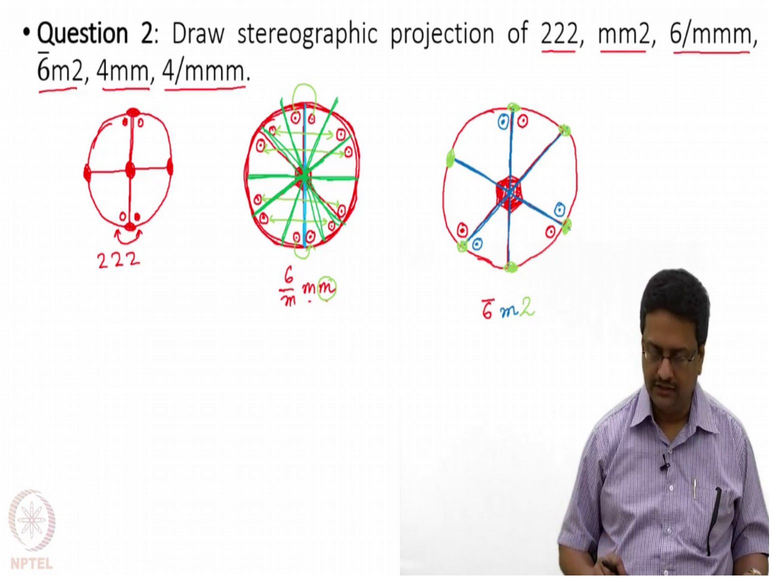

The second question in this assignment is asking you to draw some stereographic projections, some of which we probably have drawn during our regular class. So, today I will not draw all of them, but I will draw a few of them maybe 2 or 3. So, let us see what happens when it is 2 2 2. First we draw a circle, and for our easy understanding we divided into 4 parts and then put 1 open circle which represents my object.

So, now if I have a twofold passing through the centre; that means, perpendicular to the plane of projection, then this open circle should remain as open circle, because it stays in the upper hemisphere because this is a twofold the object is here it rotates like this and still stays in the upper hemisphere.

Then if I apply a twofold which is on the equatorial plane around the equator like that, then immediately what we would get is the open circle becomes a closed circle and this open circle on the other side becomes a closed circle. As a result one can observe that the central line that we had drawn earlier that central line also represents another twofold where these 2 points are translate rotated by 180 degree. So, this particular figure represents the 2 2 2 space group.

Let us see how it should be in case of 6 by mmm. As soon as we see that it is a 6 fold, we should draw 3 lines at 120 degree so, that we make these 6 parts, and we assume that the 6 fold axis is perpendicular to the plane of projection and then we start with open circle. When it is 6 fold so, at every 60 degree rotation you should have 1 open circle, when it is by m it means that the equatorial plane or the equator is your mirror plane, which is the circumference of the circle which I am making it bold. So, the circumference of the circle may becoming the mirror plane.

The open circle becomes closed circle and comes in the middle of the closed circle middle of the open circle and becomes like this, now when we have 2 mirrors these 2 mirrors are now parallel to the 6 fold axis and we can assume 1 of these lines to start with as mirror planes. So, I am drawing the mirror plane using a different color. So, if this line is a mirror plane, then the points should be reflected on either side of this plane. I hope this is clear because when we have 1 mirror it actually reflects all the points from one side to other. So, the mirror images are now drawn and I am marking them who is mirror image of what these 2 are mirror images.

These 2 are mirror images, here these 2 and again these simultaneously we can easily see that these ones are also mirror images. We do not need to draw any further mirror though we write a separate mirror like that because we can see by observation that the lines which we had drawn earlier are also representing mirror planes, and also in between these mirrors have been generated as well.

So, this is the diagram of 6 by mm m, I will only draw the other 6 bar 4 6 bar m 2 because it again may be difficult to imagine or understand. As usual we first draw the circle and divide it into 6 parts we take the 6 bar axis perpendicular to the plane of projection, and do it appropriately that the central zone is open circle and outer zone is a closed circle because it is a 6 bar axis.

What is 6 bar? 6 bar means it is the rotation followed by inversion. So, if we start at one point with open circle we rotate it by 60 degree, that brings a 6 fold, but then we have to do inversion it should become a closed circle, rotate it by 60 degree and then do one inversion it should become an open circle, rotate it by 60 degree take an inversion becomes that. Again rotate by 60 degree take the inversion so, the closed circle remains closed circle, then on inversion becomes open circle then open circle rotated by 60 degree and then inverted becomes the closed circle. So, what we have done is now just the 6 bar.

Now, we need to do m. If we take this plane as the mirror then what we would get are this points, which actually indicates that the other lines which are drawn are also corresponding mirror planes. And if you observe carefully what you can find is that the 2 fold is already generated along those 3 mirrors. So, this is the stereographic projection of 6 bar m 2, I leave other point will be space the point groups for you to draw yourself and you should check if the correctness of with the answers that will be given at a later stage.

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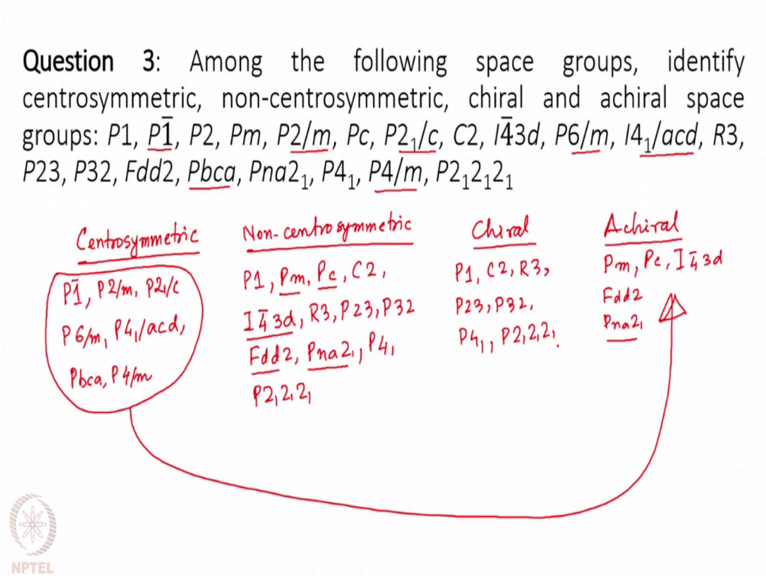

Now, comes the question which has a little more involvement to identify the space groups and classify them at as different types of space groups. So, the question is among the following space groups identify centrosymmetric non centrosymmetric chiral and achiral space groups. So, we should first write 4 classes; centrosymmetric, non centrosymmetric, chiral and achiral. So, from these space groups we can find out where that we have the center of inversion or not.

For example if we see P 1 bar 1 bar it means it has inversion center. So, P 1 bar is the centro symmetric space group, similarly you know that 2 by m here also it is 2 by m these are centrosymmetric space groups we can write as P 2 by m and P 2 1 by c or centrosymmetric space groups, this 6 by m this 1 is 4 by mmm where I am talking about the corresponding point groups are also centrosymmetric. Then we have Pbca which is mmm point group, P 4 by m. So, Pbca P 4 by m, these are centric centrosymmetric space groups. So, as immediately it is clear that the remaining are non centrosymmetric space group. So, we should classify them as non centrosymmetric. See I 4 3 d is m 3 4 3 m it is not a centrosymmetric space group. So, these are P 4 1 and P 2 1 2 1 2 1 are non centrosymmetric space groups; so, now, among them which are chiral and which are not chiral.

Of course all centrosymmetric space groups or a chiral space groups no doubt about it, plus the space groups which are non centrosymmetric, but contain a mirror plane like P m P c I 4 bar 3 d F d d 2 P na 2 1 these are a chiral space groups. So, we can write those as well along with the centrosymmetric space groups P m P c I 4 bar 3 d F d d 2 P na 2 1. These are non these are non centrosymmetric, but a chiral space group simply because we have this have at least a mirror or a glide plane. The planes the this space groups which do not have any mirror plane in them, at those space groups are called a chiral space groups. So, the chiral space groups are here P 1 C 2 R 3, P 2 3, P 3 2, P 4 1 and P 2 1 2 1 2 1.

So, one can conclude from here that the all chiral space groups are non-centrosymmetric, but not all non centrosymmetric space groups are chiral a part of non-centrosymmetric space groups which contained a mirror plane are a chiral and also one can say that all centrosymmetric space groups are a chiral, a centrosymmetric space group cannot be a chiral space group.

Why? Because a chiral compound a pure enantiomer cannot have its mirror image crystallize together in the crystal structure. If a chiral compound crystallizes in a structure it always goes in chiral space group and do not have its mirror image in the structure. If a racemic mixture crystallizes, it can crystallize in centrosymmetric or in non centrosymmetric space group but it has to crystallize in any of those a chiral space groups.

It may be a centrosymmetric space group or it may be a non-centrosymmetric, but a chiral space group. So, this is how one should understand the space groups which are possible for a chiral compound and which are possible for a racemic mixture.