Chemical Crystallography

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

Understanding of Space Groups and Miller Indices
Lecture – 13
Obtaining Equivalent Points by Shifting of Origin

Welcome back to the course of Chemical Crystallography. In the previous lecture, we were trying to understand how to do the stirrer projections of different space groups in two dimension and I have shown you how to do the origin shift in some specific cases and after that we started learning how to derive the equivalent points without drawing the space group diagrams. So, in that we have drawn a few space group diagrams which are we have derived some of these, equivalent points which do not involve origin shift.

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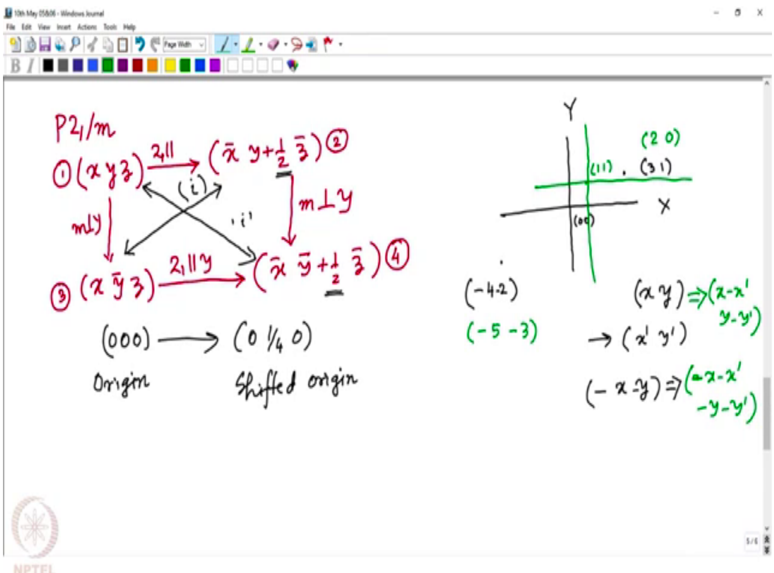

Let us see the situation with centrosymmetric space group P 2 1 by m. So, if we start in the same manner with the first point xyz and then we apply a 2fold parallel to y sorry, a 2 1 screw parallel to y, what we get is x bar y plus half z bar and we get the point number 2.

So, now if we apply a mirror perpendicular to y on point number one, what we would get is x y bar z and then we again apply 2 1 parallel to y on this point number 3 and we get x bar y bar plus half z bar is my point number 4. This can also be obtained by applying a mirror perpendicular to y on point number 2. Now, what we see is that the points one and four are inversely related of course, because they are x y z and x bar y bar z, but there is a translational component half associated with this inversion.

So, they are not exactly inversion related, but there is a translational component associated with it. Similarly, the points three and two are once again inversion related x y bar z becomes x bar y z bar, but we have a translational component of half which means the origin is not coinciding with the point of intersection of 2 1 screw and the mirror. So, what we need to do in that case is that we need to shift the origin from 0 0 0 to 0 onefourth 0; original origin was here and shifted origin is at this point. Now, what happens to those coordinates of 1 2 3 and 4? To understand that let us use a simple coordinate system x y.

And suppose, we have a point here which is 3 1 with respect to this origin at 0 0. Now, if I shift the origin from 0 0 to 1 1, what will be the coordinate of this new with this point, with respect to the new origin? The coordinate of this particular point with the new origin will become 2 0 right. On the other hand, if this particular point was on the negative side where suppose, it was at this point at minus 4 2 minus 4 minus 2 with respect to the new origin. This point would then become minus 5 minus 3.

So, if the coordinate has positive numbers and if we shift the origin to some positive numbers like x prime y prime the positive coordinate changes to x minus x prime y minus y prime, but if the coordinate was negative minus x minus y then also it changes to minus x minus x prime minus y minus y prime.

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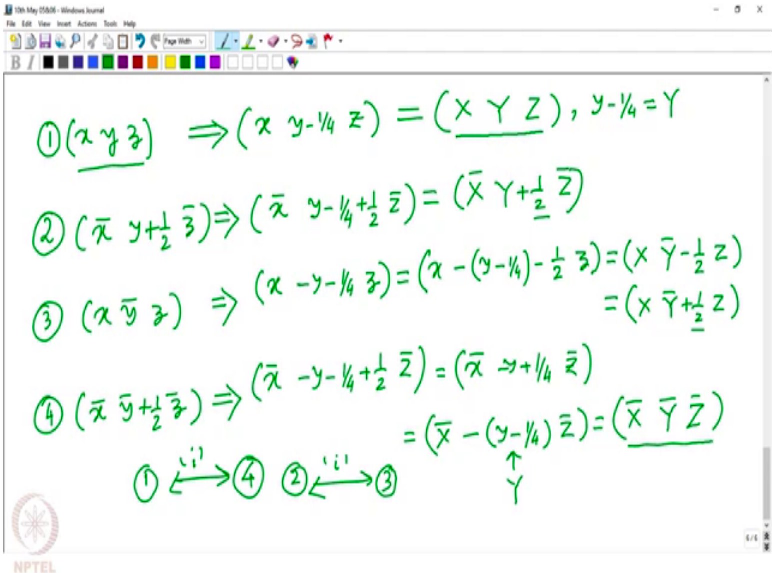

So, with this concept we should start rewriting these 4 points. So, what are the 4 points that we have got ? Four points are; x y z x bar y plus half z bar, point number 3 is x y bar z and point number 4 is x bar y bar plus half z bar. So with shift of origin, the first point transforms to x y minus one fourth z; we write this as capital X capital Y capital Z which means we are replacing y minus one fourth by capital Y and keeping the x and z as capital X and capital Z.

So, now if we do the same thing for point number 2, x bar remains as it is, y becomes y minus one fourth plus half z bar that can be written as x y bar plus half z. Now, that a situation with point number 3 is what we discussed towards the second part of the previous slide, where the coordinate is negative. So, this transforms to y bar, which means minus y minus one fourth z.

So, now I rewrite it as x, we take minus out y minus one fourth, what have I written? I have written minus of minus one fourth; that means, plus one fourth; but here, we have minus one fourth. So, we should have a component of half added here sorry, a component of half subtracted here and z so; that means, now, we can write x y bar minus half z and as I said now on y. I have minus half which means it is outside the unit cell. So, to bring it inside the unit cell, I rewrite it as x y bar plus half z by adding 1 along the y axis only.

So, as a result now, the point number 2 and point number 3 are inversion related. I am sorry, I am I made a mistake previously. This is x bar y plus half z bar and this is x y bar plus half z. Let us see what happens to the point number 4; x bar as it is minus y minus one fourth plus half and z bar. So, that simply means x bar minus y plus one fourth z bar which is equal to capital X bar minus y minus one fourth z bar, which we should write as X bar Y bar Z bar because this y minus one fourth is nothing, but y and then we have a minus sign; so, it makes it y bar. So, this point number 1 and 4 are inversion related, point number 2 and 3 are inversion related and the translational components are same.

So, in case of the point number one there was no translation, in case of point number 4 there is no translation. So, X Y Z it has become X bar Y bar Z bar X bar Y plus half Z bar has become X Y bar plus half Z and we get the four equivalent points for C 2 1 space group.

Now, let us try to get these equivalent points using a matrix method as we have already indicated that we can construct 3 by 3 matrix for different symmetry elements. For two fold and 2 1, we have already discussed about it.

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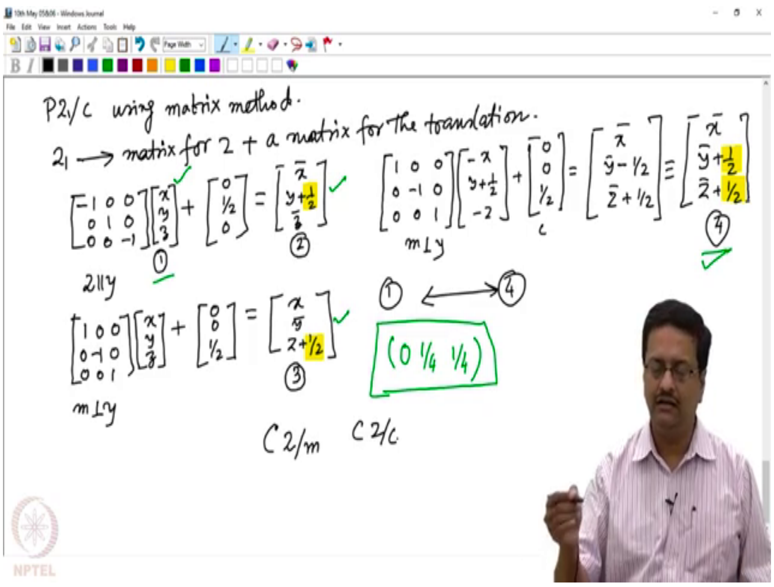

So, let us see how can we determine the equivalent points for P 2 1 by c space group using matrix transformation method or simply matrix method. So, when we are trying to write a matrix for 2 1, it is a matrix for 2 plus a matrix for the translation. So, now, if we have the matrix for 2 written as minus 1 0 0 0 1 0 0 0 minus 1, this is a matrix for 2 fold parallel to y. We multiply that with the coordinate xyz and then add a translation along y that is the half translation along y,What we end up getting are these points x bar y plus half z bar, We now, apply the c glide on the same point 1 c glide perpendicular to b would mean it is a combination of mirror, perpendicular to b which means it should be 0 0 1 0 0 0 minus 1 0 and 0 0 1 this is a matrix for mirror perpendicular to y. We multiply this with the coordinates xyz and then add the translation, which is a c glide translation; that means, the translation is along z.

So, 0 0 half is the translational component is added, we end up getting the points x y bar z plus half. Now, we once again apply a c glide on the point, we obtained here. So, this is our point number 1, this is the point number 2, this is the point number 3. Now, I am applying c glide on point number 2. So, c glide once again means that it is a matrix for a mirror and then I have the points which are minus x y plus half minus z and then, we apply the translational component 0 0 half, because it is a c glide; so, mirror and c. So, what we end up getting is x bar y bar minus half z bar plus half which is actually equivalent to x bar y bar plus half z bar plus half and that is my point number four.

So, if I look at now, the points 1 and 4 1 and 4, they are inversion related, but the, half translation is half zero; both along y and z. If we look at the points 2 and 3 what we see is they are also related by half translation in both y and z here, it is half with respect to nothing, here it is nothing and then half here which actually indicates that the origin has to be shifted at 0 one fourth one fourth. So, from this we see that a new origin has to be chosen at 0 one fourth one fourth and all these coordinates need to be rewritten with that transformed coordinates using the origin transformed values.

So, I would like to leave this exercise for you to do it yourself, then you will understand how these four points can be in further modified with a new origin and the translational components that are present between the point number 1 and point number 4 are removed. So, with this we would like to conclude this lecture, where we learnt a few complicated, things for example, we have learnt how to draw the space group diagrams for centrosymmetric and non centrosymmetric systems.

We have learnt how to draw the space group diagrams, where we do not have origin shift and centrosymmetric and then we have learnt how to do it for noncentrosymmetric for centrosymmetric with origin shift as well. So, as your take home exercise maybe to derive the equivalent points for c 2 by m and c 2 by c as well using both matrix method and by drawing the figure.