Chemical Crystallography
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Understanding of Space Groups and Miller Indices
Lecture – 14
Representation of Orthorhombic and Tetragonal Space Groups

Welcome back to the course of Chemical Crystallography. We would start from the place where we ended in the last lecture, as if you remember, we were discussing about the 230 space groups and we were trying to draw the crystallographic projections for those space groups. So, we have done with some simple space groups, for example, we have worked on the triclinic system, we have done a number of space groups in monochronic system which are really simple in some cases it was difficult because we wanted to see how the space groups are drawn with shifting of origin in cases where there was involvement of 2 1 with m or 2 by c and so on.

And I gave you a couple of homeworks, I hope you have tried to solve those problems. So, now, let us try to see some of the orthorhombic space groups which we encounter every now and then.

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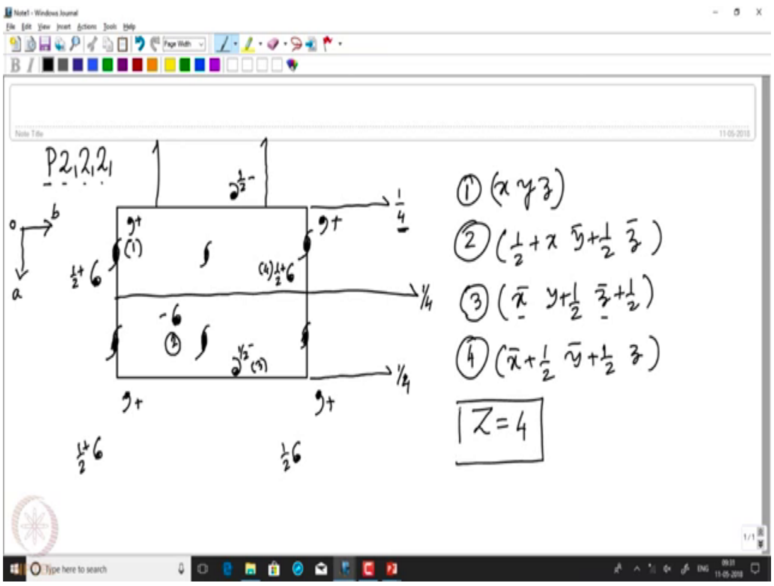

The most frequent orthorhombic space group that we encountere is P 2 1 2 1 2 1 what does it mean? It means that this space group represents a primitive orthorhombic lattice and there are 3 2 1 screw axis along x, y and z here, what I would like you to understand is that this is 3 2 1 screw axis do not intersect with each other; that means, the origin is not coinciding with these 2 1 screws.

So, the figure that I am going to draw will have a translational component associated with each of these 2 1 screws. So, here once again I am drawing the a b face of the orthorhombic unit cell, I am keeping the direction of the unit cell here, b is from left to right and a is from top to bottom with origin at the corner. So, as I indicated the 2 unscrews along a, b and c are all shifted one-fourth from the origin. So, the screw which is along b is drawn here and I write one-fourth indicating that this is not on the plane of projection rather it is one-fourth above the plane of projection. So, we have two such 2 1 screws.

In this, the second set of 2 1 which is parallel to a is again one-fourth shifted along a along b and then the third set of 2 1 screw which is parallel to c and the c axis is perpendicular to this plane of projection. So, the c axis screw a screw along the c or z axis appears at one fourth shifted from the origin. So, now, if we start drawing the object my favorite object as a comma plus when we apply a 2 1 screw parallel to z, we end up getting the object here with half elevated along c. So, now, this half elevated object is outside the unit cell, if I bring it inside the unit cell by adding one it should appear here.

If you remember, we have not here drawn these translation and related objects. So, the transmission related object for that should come out of the unit cell that should appear here and that should appear there as well. So, now, if I apply a 2 1 screw on this first point parallel to y which is here. So, the 2 1 screw rotates it and should have taken it here 2 and then it moves halfway and comes here with half negative because the 2 1 is here the object is here it rotates and goes below the plane so, we have it minus. So, now, if we translate that object inside the unit cell it appears at this point.

So, what we have got are the equivalent points for 2 1 screw. So, what we have done is we have done about that we have done about this and then we should do about the third to one which is parallel to a, if we do a 2 1 parallel to a, it should rotate here should come from this point to this is the twofold, but it is along a. So, it should be translated and it should have here at this point as minus.

So, now I have 4 points inside the unit cell, I can designate them now with the corresponding equivalent points corresponding x, y, z coordinates for that. So, point number one is x, y, z, point number 2 is half plus x y bar plus half z bar, point number 4 is x bar y plus half z bar plus half and part number 4 is x bar plus half y bar plus half and z.

So; obviously, inside the unit cell this is the point number 1, point number 2 has both y bar and z bar negative; that means, the 2 1 is parallel to x axis that is parallel to a. So, this point is nothing, but this one the coordinate 3 has x bar and z bar; that means, the 2 1 is parallel to y. So, we got the point which is parallel to y here. So, this point inside the unit cell is my third equivalent point and the fourth one has x bar and y bar which means it is parallel to z.

So, one we have got parallel to z here. So, inside the unit cell this is the point number four. So, these are the four equivalent points four; 3; 2 1, 2 1, 2 1 space group; that means, it has z equal to 4 and I have already mentioned that this is one of the chiral space groups because it does not have any mirror plane. Now let us see a c centred lattice in orthorhombic, let us see how one should draw C mm 2.

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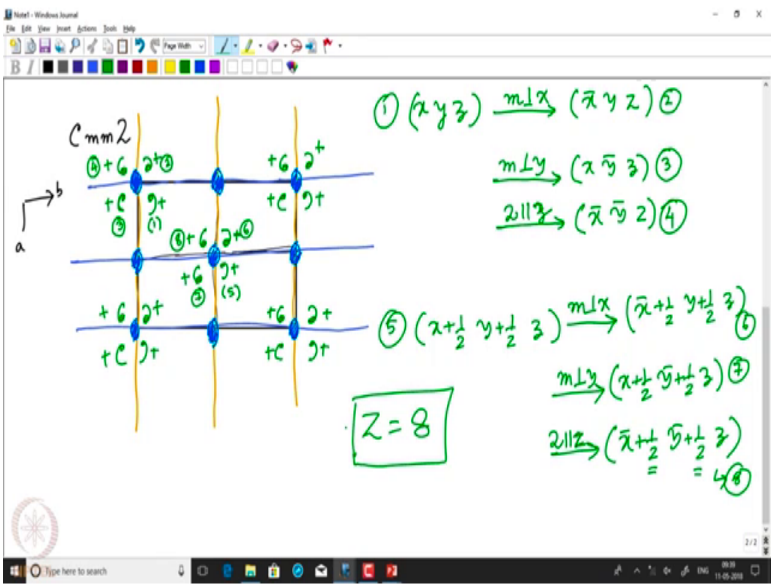

What does it mean? We have a C centred lattice, then we have a mirror perpendicular to x a mirror perpendicular to y and a twofold parallel to z so now for my easy understanding, I am making the rectangular divided into four parts because I need to place the atom which is related by C. So, this is my first point which I am translating and the point related to C centering is here.

So, if this is my point number 1; this I am designating; now as point number 5 as this will become the first point with C centering. So, point number 1 is x y z and point number 5 is x plus half y plus half z. So, now, I have mirrors where I have mirrors perpendicular to x. So, as a convention I have b and a like that. So, when I am saying I have a mirror perpendicular to x; that means the mirror is here.

So, if I apply a mirror symmetry on my point number 1, I get this the corresponding translational components are also drawn if I apply mirror on point number 5 I get this on applying mirror it does not change the side. So, on applying mirror the points above the plane still remain above the plane and that is why we put plus sign.

Now, the second mirror which is perpendicular to y is going like that. So, now, on applying this second mirror; what we get is another set of mirror images of point number 1. So, it becomes 2 and 3. So, if I write the corresponding translation related components, I have these points now what do we see here.

We can see that the point of intersection of these two mirrors m 1 and m 2 which are perpendicular to a and b respectively the point of intersection has become a twofold parallel to z, every point of intersection of the twofold has become every intersection of the mirror has become a twofold. So, we did do not have to draw any further equivalent points for the third symmetry of the space group C mm 2.

So, now the points 1, 2, 3 and 4 are corresponding to the 1, 2, 3 and 4 are corresponding to the first equivalent point that is x y z and 5, 6, 7 and 8 are equivalent points corresponding to the center atom. So, x y z, I apply a mirror perpendicular to x, I get x bar y z bar as my point number 2.

I apply a mirror perpendicular to y, I end up sorry this is x bar y z not z bar mirror perpendicular to y makes it x y bar z, this is my point number three and point number 4 is a twofold parallel to z making it x bar y bar z as my fourth point. So, if the same manner, if I apply it here mirror perpendicular to x gives me x bar plus half y plus half z that is point number 6, mirror perpendicular to y gives me x plus half y bar plus half z and then a two parallel to z gives me x bar plus half y bar plus half z.

See here when I am applying twofold parallel to z, it should have been minus x minus half minus y minus half z, but then I am directly writing plus half assuming that I am simultaneously adding one along x and one along y to get the final point. So, this is my point number 7 and this is the point number 8. So, in this case the z is 8.

I hope this is becoming clear to you when I am drawing it slowly, now we would like to see a couple of a trigonal space rules as well.

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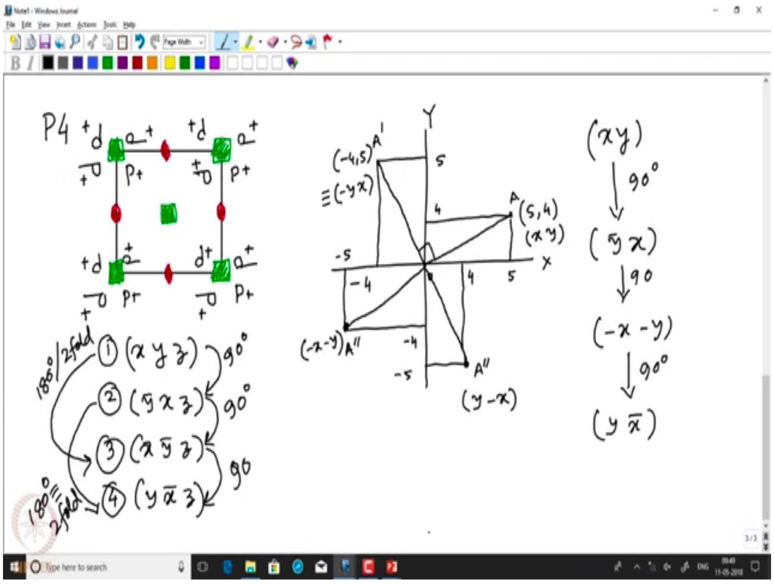

P 4 in tetragonal system as you all know a equal to b not equal to c and c which is parallel to z is the unique axis. So, we should draw a square which should represent the a b plane and the c axis is perpendicular to this plane of projection.

So, we should now start drawing it assuming that my c is perpendicular to the planar projection. So, what I am drawing is the c axis where we have a fourfold symmetry and I am putting the fourfold axis at 4 corners as usual and then the object that I am going to take is now a different object for easy understanding I am taking the letter P and as usual making it as plus because this is above the plane of projection.

So, now, if I am doing a fourfold rotation a 90 degree rotation of P makes it like that; another 90 degree rotation of P makes it like this and the third 90 degree rotation of P makes it like that and if we do it the same for all the four corners the figure should look like this.

Since in crystallography the translation is the most important symmetry element we should always draw the translation related objects wherever applicable or wherever possible. So, now, if we look at this figure carefully, what you can see is that the center of the unit cell, we have got another fourfold generated in addition we have twofold axis parallel to z got generated at the midpoint of these faces.

So, a P 4 which means you have fourfold axis parallel to z along the corners around the edges of the corners, there is a twofold axis in between the 2 fourfold axis. So, what are the equivalent points the equivalent points are very interesting here we have x, y, z as to start with the point number 2 is a 90 degree rotation about the z which makes it y bar x z.

Another 90 degree rotation makes it x bar y bar z and forth operation makes it y x bar z, you will be surprised; what is happening how come y is written in the place of x axis and x is written in the place of y axis, let us try to see with a physical example 5 comma 4 becomes there. So, o A becomes o A prime. So, this intercept was five this intercept was 4.

Now, on doing a 90 degree rotation, this intercept is 5 and the intercept here is minus 4. So, if we I had written it as x y, then the coordinate for that which is now minus 4, 5 can be written as minus y x. So, now, if I do another 90 degree rotation and bring it here which is a double prime then this is once again minus 5 this is minus 4.

So, if this was x y, this point is minus x minus y now if I do another 90 degree and the point comes here at a triple prime. So, this point becomes minus 5 and that point becomes plus 4 which means this point is nothing, but x coordinate is y which is 4 and y coordinate is minus 5 which is minus x. So, the points on doing a ninety degree rotation on a point x y changes like this.

This you make a 90 degree rotation, it becomes y bar x, another 90 degree rotation; it becomes minus x minus y another 90 degree rotation, it becomes y x bar; the same has been done here, this is a 90 degree rotation from there, it is a 90 degree rotation and from this to that is a ninety degree rotation remember that point number 1, 2, 3 is a 120 degree rotation which is equivalent to a twofold.

Similarly, point number 2 to 4 is 180 degree rotation which is equivalent to a twofold before we conclude this lecture, we would like to see one mode in tetragonal lattice and I then would leave it to you to draw other lattice other space groups of your choice, let us see what happens if we have I 4 what is I? I is body centered, 4 is a fourfold symmetry and it is in the tetragonal system.

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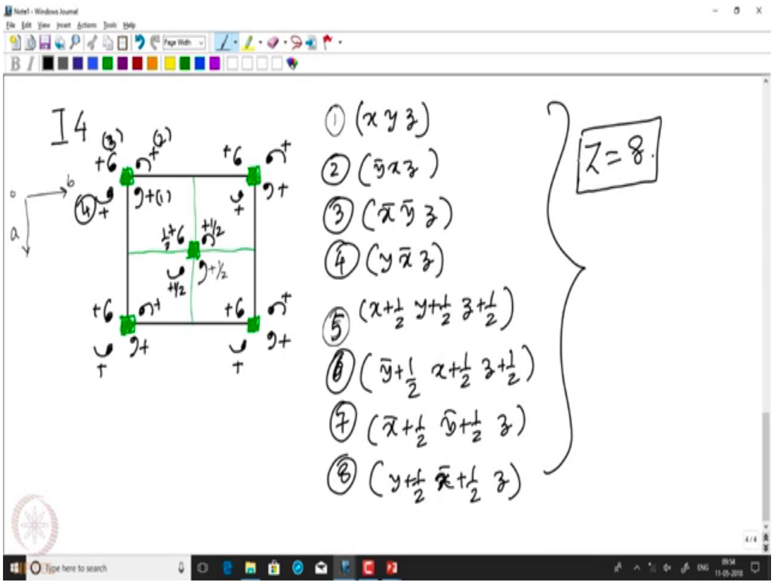

So, as usual, we should draw a square and since it is body centered lattice, let us first write my first object at x, y, z and the body centered object means if the original point is x, y, z, the body center point will be x plus half y plus half z plus half because it is at the center of the unit cell.

So, for my understanding, I am first dividing this square into 4 equal parts and then I am writing the point number 5 with plus half. So, it is simultaneously halfway along b, halfway along a and also lifted halfway along c from the plane of projection. So, if this is the point number 1, this is the point number 5 as before.

So, now as I said we have I 4; that means we have a fourfold symmetry, we apply that fourfold symmetry at all the 4 corners which means the edges parallel to z or parallel to c are the fourfold axis and simultaneously, there is a fourfold axis passing through the center of the unit cell. So, now, if we apply these symmetries it would get these points. So, by doing a 90 degree rotation you are getting these points.

So, now we look at the center atom also all will be plus half. So, as a result what we have in this are set of 8 equivalent points starting with x, y, z, we should have as before x bar y bar z which is the point number, sorry, I should not confuse you, I should start by doing it y bar x z and then point number 3 is x bar y bar z bar. So, this is 1, 2, 3, 4 the 4th point is y x bar z 5th point is the central point and you apply the same logic to get the points which are 6 as y bar plus half x plus half z plus half 7th point as x bar plus half y bar plus half z and the last point is y plus half x bar plus half z.

So, here we have z equal to 8; 8 equivalent points. So, today we have learned to draw a couple of orthorhombic space groups and a couple of tetragonal space groups their symmetry related objects and we have learned; how to do the co ordinate transformation in case of tetragonal lattice where we have a fourfold symmetry. So, in the next class, we will start learning what about the crystallographic planes direction, miller indices, etcetera.