Symmetry, Stereochemistry And Application

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Lecture No-54
Symmetries in X-ray Crystallography

Welcome back to the course entitled symmetric stereochemistry and applications. In the previous lecture we started discussing about the aspects of crystallographic symmetry and in that context we were talking about what happen when you apply a crystallographic symmetry on an object located in space.

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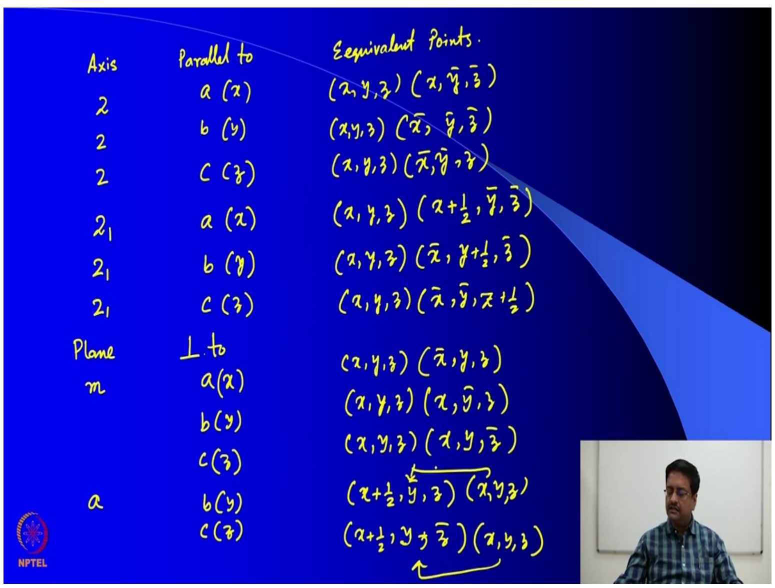

So we had just written what happens to the coordinates of an object kept at x, y, z with and then you apply a 2fold axis parallel to a. So, if we continue in that direction we talked about axis the axis is parallel to some axis and we get some equivalent points. So, I just wrote if it is a 2fold axis parallel to a, which means parallel to x axis then the coordinate x, y, z would get converted to x, y bar z bar.

Similarly 2 fold parallel to b which means parallel to y would make x, y, z to x bar y z bar and a 2 fold parallel to c which means parallel to z will make x, y, z to become x bar y bar z. So, then when it is a question of a 2_1 screw axis parallel to a that means parallel to x axis x, y, z coordinate when you rotate the object about a y and z becomes negative and when i say 2_1 screw parallel to a that means the motion is along the direction of a.

So, the coordinate of a, which is x is added with plus half y becomes minus and z becomes minus. So, similarly 2_1 parallel to b means it is parallel to y. So, for that x, y, z would eventually become x bar y plus half z bar because the rotation is about y and the translation is along y direction. Similarly 2_1 parallel to c or parallel to z would mean the transformation of x, y, z coordinates to x bar y bar z plus half, right.

Similarly when we talk about different planes and that plane has to be perpendicular to some axis or some direction then what will be the corresponding equivalent points. Suppose if it is a mirror plane perpendicular to a will make the points x, y, z to get converted to x bar, y, z because the mirror is perpendicular to the direction of a or perpendicular to x axis as a result it gets converted to x gets converted to x bar.

So, mirror perpendicular to b that means y would indicate x, y, z to get converted to x y bar, z and mirror perpendicular to c that is z axis will make x, y, z get converted to x, y, z bar. Similarly I just do it for a glide perpendicular to b that is y and perpendicular to c that is z. So, when it is perpendicular to b it means the translation is along a, because it is a glide and reflection is perpendicular to b that means it is y bar. So, it should become x plus half y bar z.

Similarly in this case the translation is again along x reflection is perpendicular to z. So, y remains as y and it becomes z bar. So, this is how you should try to convert these different glide planes and draw the corresponding equivalent points of course it is x, y, z which is always there which gets converted to the new coordinate because of that applied symmetry. So, when you try to apply these symmetry elements you generate the other objects or other molecules in the unit cell.

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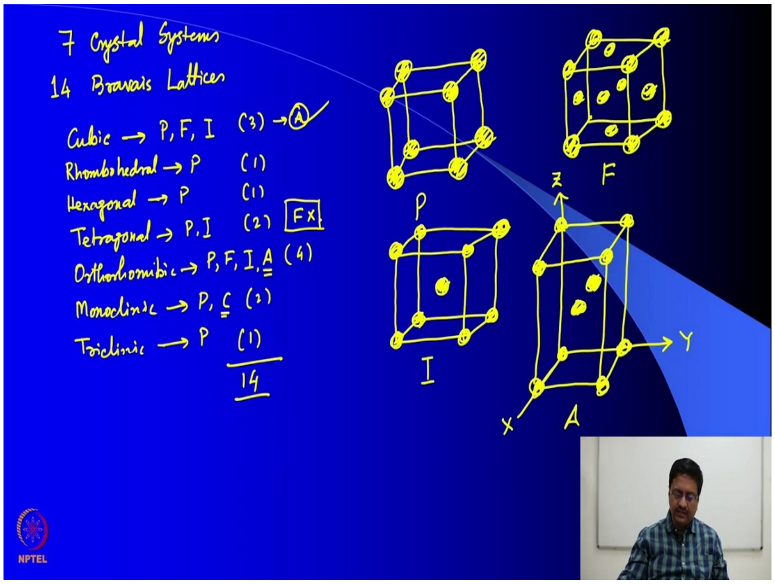

So, now when you try to think about applying these symmetry elements in addition to what we had as 7 crystal systems there can be 14. So, what are those 14 bravais lattices, for a cubic system you can have a primitive lattice you can have face center lattice and you can have body centered lattice. In case of rhombohedral you can have only primitive lattice in case of hexagonal one can only have a primitive lattice tetragonal one can have primitive and I centred lattice orthorhombic system can have everything primitive face centered body centered and one of the faces centered.

Monoclinic can have primitive and c centered and triclinic can have a primitive lattice. So, here you have 3 plus 1, 4 plus 1, 5 plus 2, 7 plus 4, eleven plus 2, 13 plus one total 14 previous lattices that are possible in the solid state in crystal systems. You may be wondering what these lattices mean I am quickly trying to draw a cubic lattice and explain the possible variations. So, if this is a cubic lattice you have atoms associated at 8 corners is called a primitive lattice.

So, this is called a primitive or P lattice when you have a cubic system with atoms at 8 corners and 6 faces that is called a face center lattice which I am trying to draw now. And then the other possibility is a body centered lattice where you have atoms at 8 corners plus atom at the center of this unit cell remember that when you say primitive phase centered or body centered all the atoms that are related by centricity they are all of same type.

So, here all the atoms are of same type. So, this is the body centered or I lattice. In case of orthorhombic, you see there is something called a which means if you remember in case of orthorhombic A and A, B, C are not same. So, if we draw an orthorhombic lattice like this if this direction is x if this direction is y and that is said the plane which is perpendicular to x axis is the A direction. So, A center lattice means you will have atoms at 8 corners and atoms at the center of the faces which is perpendicular to A.

So, this is the A center lattice. So, similarly in monoclinic C-C center is occupied and that is a C lattice. So, what you note here is in case of tetragonal there is no F in case of cubic there is no A because all these faces are equivalent. So, in case of cube if you make one face center then all the faces get centered and in case of tetragonal if you try to make a face center tetragonal lattice you will see yourself that there is a possibility of having a smaller volume body center tetragonal lattice and that is considered as the Bravais lattice and not the face center tetragonal lattice.

So we have a restriction on number of different possible crystal systems and different possible bravais lattices.

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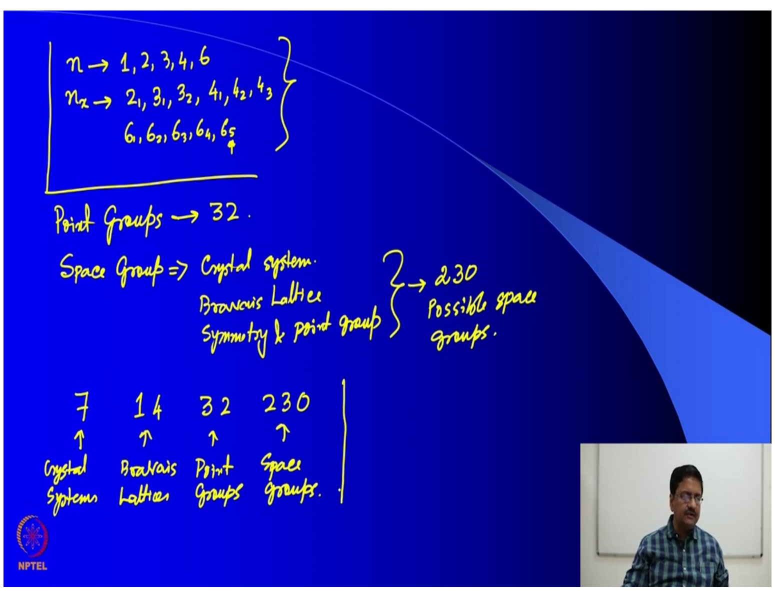

And then in addition we have a restriction on the number of rotational axis that is n which is restricted to 1, 2, 3, 4 and 6. Nx that is the glide plane can be 2_1, 3_1 and 3_2, 4_1, 4_2 and 4_3, 6_1, 6_2, 6_3, 6_4 and 6_5 here remember this 5 means 5 by 6 translation it is not axis. So, because of these restrictions that there cannot be more number of symmetry axis like n equal to 5 or 8 or whatever the total number of point groups.

In X-ray crystallography is restricted to 32 there are only 32 point groups and then when you combine the point group along with the lattice centering and the crystal system you generate an unique nomenclature for every crystal that you get and that unique nomenclature is called the space group. It is a combination of the information from crystal system bravais lattice the information of symmetry and point group.

All these are included in one notation called the space group and there are 230 possible space groups in crystallography. So, you see these numbers 7, 14, 32 and 230 are 4 very very important numbers in x-ray crystallography we have 7 crystal systems 14 bravais lattices 32 point groups and 230 space groups. So, here we now come to a point that we need to slowly understand how this symmetry elements can be applied or are actually applied to generate a 3 dimensional lattice.

So, when we try to understand a 3 dimensional lattice to start we need to see what are the possibilities of 1D lattice and then we extend our knowledge from 1D to 2D and then one can extend to 3D and we will certainly not go up to 3D. But we will discuss about the concept of 1D lattices in a few moment.

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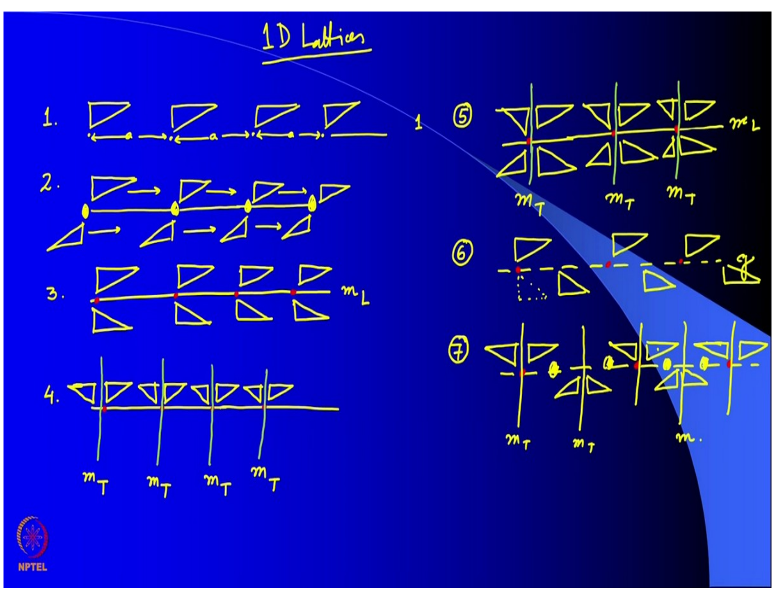

So, the 1D lattices that can be considered are a certain number of restricted lattices and they are numbered as one 2 3 4 and 5 like that up to 7. So, the first type of one d lattice has only translational symmetry which means the object is only translated in one particular direction the way i am. So, from the point to point to point to point the translation is same. So, here you have only one full axis of symmetric that is translational symmetry the second one is something where you apply a 2 fold axis and that 2 fold axis is translated at a certain distance and the original object is translated always as usual.

So, when you apply a 2 fold screw sorry 2 fold axis about this point here you generate the object like this you see that these fellows are translated these rotated objects are also translated. So, this has a 2fold axis of symmetry this is the second type of 1D lattice the third type of 1D lattice can have a longitudinal mirror. So, suppose if this is the line of translation your object is here and this object has a translational component at this particular distance as a result your translation related objects come at its own place.

So, this is same as one now if this line is a mirror plane and we call it as a longitudinal mirror or m L the reflection generates the object like this right. So, this is the third type of lattice the 4th type of lattice has a mirror which is perpendicular to the direction of this translation. So, this translation as usual is in the direction from left to right and the object is here. Now there is a mirror passing through this point.

So, the mirror related object the mirror image of this object should appear here. So, this mirror is called the transverse mirror or m T. So, this is the 4th type of lattice that one can think of in one dimensional symmetry. The fifth type of 1D lattice can be considered when you have the combination of mL and m T. So this is my mL and the translational components are at these points and i am drawing the object first.

So, now if you apply the longitudinal mirror related mirror symmetry you get these objects. Then if you apply the corresponding transverse mirror just like before it would generate the other set of objects like this. So, you have both longitudinal and transverse mirrors in this case. The next or 6th type of lattice that one can think of in 1D is a glide. So, if I draw a glide plane like this then the object which may be here has the translation from this point to that point to that point.

So, we draw the object at every one unit translation and the right relation is like as I already have shown this is reflection followed by half translation makes the object here. So, this is the glide related one dimensional lattice. And the 7th and last type of 1D lattice is a combination of glide and a translational symmetry element which is which I am now trying to draw. So if I draw first my object and I have the corresponding transverse mirrors here.

So, I am now first drawing the transverse mirror related object and then we apply glide plane on both. So, when you apply glide plane here it goes to this point and this comes here generating a transverse mirror in between. Similarly this object comes here and that mirror related object comes there and generates a transverse mirror in between and what we see is between the 2 transverse mirrors a 2-fold axis has got generated.

So, these are the 7 possible 1D lattices that one can think of. So, from here we will continue in the next class.