Symmetry and Structure in the Solid State
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Lecture - 06
Details of Stereographic Projections

So, in the last class, we stopped at the discussion of having three mutually perpendicular 2 fold axis generating the 222 combination as a possible point group.

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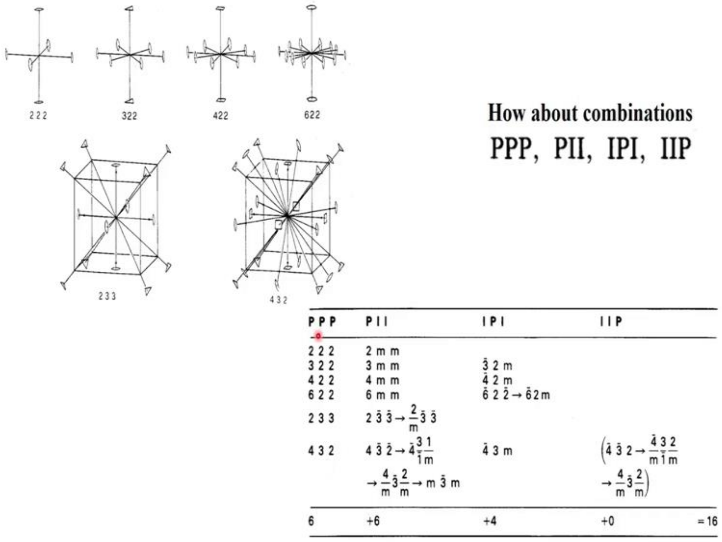

How about combinations
PPP, PII, IPI, IIP

PPP	PII	IPI	IIP	
222	2mm			
322	3mm	$\bar{3}2m$		
422	4mm	$\bar{4}2m$		
622	6mm	$\bar{6}2\bar{2} \rightarrow \bar{6}2m$		
233	$2\bar{3}\bar{3} \rightarrow \frac{2}{m}\bar{3}\bar{3}$			
432	$4\bar{3}\bar{2} \rightarrow \bar{4}\frac{3}{\bar{1}}\frac{1}{m}$ $\rightarrow \frac{4}{m}\bar{3}\frac{2}{m} \rightarrow m\bar{3}m$	$\bar{4}3m$	$\left(\bar{4}\bar{3}2 \rightarrow \frac{\bar{4}}{m}\frac{3}{\bar{1}}\frac{2}{m}\right.$ $\left.\rightarrow \frac{4}{m}\bar{3}\frac{2}{m}\right)$	
6	+6	+4	+0	=16

2mm is another point possible point group and so on and with respect to 3 fold, 4 fold, 6 fold and then also the combination of 233 and 432 giving rise to access in different directions. We find that there are 6 plus 6, so, 12 additional point group symmetry is which come up. We have to therefore, consider the other combination. We see here it is a proper, improper, improper axis, here we at considered an improper axis with a proper axis; obviously, by the satisfaction of the Euler's theorem it has to be IPI, we can also have IIP.

So, that these combinations now we will give rise to a newer possible point groups and those are listed here. We are not going to find out how they come up and how to derive it and so on. The best way to do that would be to take a course on group theory and if someone is interested, there are group theory courses also available in this program. So, if they take the group theory course, there will be a possibility to understand how to get to the other. This is not in the scope of our course. But what we note is here is that this will introduce four new symmetry. So, this 2mm or m2m is one on the same; see again I will repeat, 222 gives rise with PII, we get 2mm.

Now; that means, that there is a twofold axis along this direction let us say and m and m in these two directions. Now, if I go to IPI; that means, I should have m2m. So, the symmetry will be m2m because there are 90 degrees with respect to each other and we have a very nicely define rectangular coordinate system in this particular case with 90 degree angles between them whether we have a mirror here or a mirror there or a mirror there, it does not matter and. So, also the presence of the 2 fold axis.

And therefore, m2m and here in this case mm2, they become one and the same as 2mm. So, there is no need to have additional point groups coming in this combination. On the other hand, in this combination and additional one comes because $\bar{3}$ is something different from $\bar{2}$ because $\bar{2}$ becomes m where as in case of $\bar{3}$ it is different and it is a standalone symmetry and therefore, you get $\bar{3}$2m.

Similarly, $\bar{4}$2m, $\bar{6}$2m and you also have in this case $\bar{4}$3m. So, there four additional things will come in. On the other hand, if you have IIP combination, all these combinations PII will be there will be repeated here and in this case also it is repeated and therefore, we do not get any additional point group symmetries. So, we have therefore, 13 plus 16 that comes to 32. So, that comes to 29, not 32.

So, what is happening what is it we are missing because we, we want 32 point groups and we have now getting 29, what happened to the other three? The other three will come as a simultaneous presence of proper and improper.

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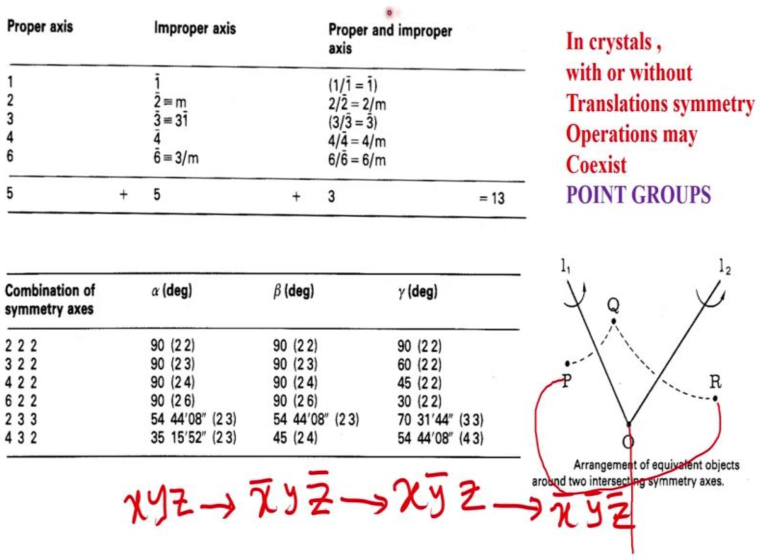

Proper axis		Improper axis		Proper and improper axis	
1		$\bar{1}$		$(1/\bar{1} = \bar{1})$	
2		$\bar{2} \equiv m$		$2/\bar{2} = 2/m$	
3		$\bar{3} \equiv 3\bar{1}$		$(3/\bar{3} = \bar{3})$	
4		$\bar{4}$		$4/\bar{4} = 4/m$	
6		$\bar{6} \equiv 3/m$		$6/\bar{6} = 6/m$	
5	+	5	+	3	= 13

In crystals ,
with or without
Translations symmetry
Operations may
Coexist
POINT GROUPS

Combination of symmetry axes	α (deg)	β (deg)	γ (deg)
2 2 2	90 (2 2)	90 (2 2)	90 (2 2)
3 2 2	90 (2 3)	90 (2 3)	60 (2 2)
4 2 2	90 (2 4)	90 (2 4)	45 (2 2)
6 2 2	90 (2 6)	90 (2 6)	30 (2 2)
2 3 3	54 44′08″ (2 3)	54 44′08″ (2 3)	70 31′44″ (3 3)
4 3 2	35 15′52″ (2 3)	45 (2 4)	54 44′08″ (4 3)

Arrangement of equivalent objects around two intersecting symmetry axes.

$$xyz \rightarrow \bar{x}y\bar{z} \rightarrow x\bar{y}z \rightarrow \bar{x}\bar{y}\bar{z}$$

You see in the previous slide, we had this proper and improper axis simultaneously present. So, we have to therefore considered the combination of proper and improper axis.

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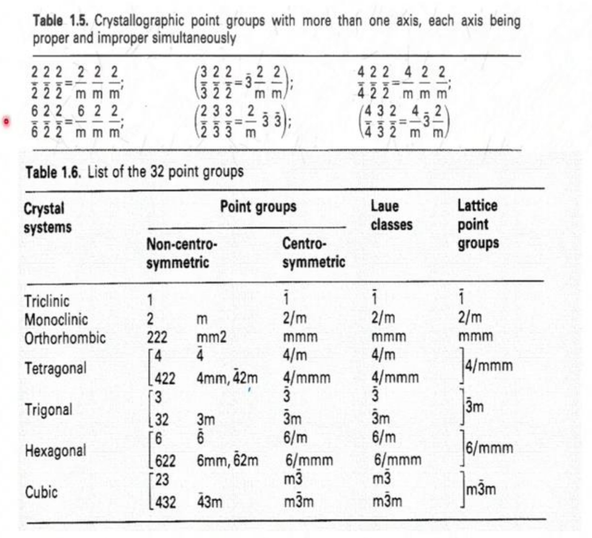

Table 1.5. Crystallographic point groups with more than one axis, each axis being proper and improper simultaneously

$$\frac{2}{\bar{2}}\frac{2}{\bar{2}}\frac{2}{\bar{2}} = \frac{2}{m}\frac{2}{m}\frac{2}{m}; \qquad \left(\frac{3}{\bar{3}}\frac{2}{\bar{2}}\frac{2}{\bar{2}} = \bar{3}\frac{2}{m}\frac{2}{m}\right); \qquad \frac{4}{\bar{4}}\frac{2}{\bar{2}}\frac{2}{\bar{2}} = \frac{4}{m}\frac{2}{m}\frac{2}{m};$$

$$\frac{6}{\bar{6}}\frac{2}{\bar{2}}\frac{2}{\bar{2}} = \frac{6}{m}\frac{2}{m}\frac{2}{m}; \qquad \left(\frac{2}{\bar{2}}\frac{3}{\bar{3}}\frac{3}{\bar{3}} = \frac{2}{m}\bar{3}\,\bar{3}\right); \qquad \left(\frac{4}{\bar{4}}\frac{3}{\bar{3}}\frac{2}{\bar{2}} = \frac{4}{m}\bar{3}\frac{2}{m}\right)$$

Table 1.6. List of the 32 point groups

Crystal systems	Point groups			Laue classes	Lattice point groups
	Non-centro-symmetric		Centro-symmetric		
Triclinic	1		$\bar{1}$	$\bar{1}$	$\bar{1}$
Monoclinic	2	m	2/m	2/m	2/m
Orthorhombic	222	mm2	mmm	mmm	mmm
Tetragonal	4	$\bar{4}$	4/m	4/m	4/mmm
	422	4mm, $\bar{4}$2m	4/mmm	4/mmm	
Trigonal	3		$\bar{3}$	$\bar{3}$	$\bar{3}$m
	32	3m	$\bar{3}$m	$\bar{3}$m	
Hexagonal	6	$\bar{6}$	6/m	6/m	6/mmm
	622	6mm, $\bar{6}$2m	6/mmm	6/mmm	
Cubic	23		m$\bar{3}$	m$\bar{3}$	m$\bar{3}$m
	432	$\bar{4}$3m	m$\bar{3}$m	m$\bar{3}$m	

So, being simultaneously present and if we consider that, we get these additional three possible point groups. For example, if you take 2/2, 2/$\bar{2}$, 2/$\bar{2}$, 2/$\bar{2}$ this is proper-improper, proper- improper, proper- improper, you get a new point group symmetry which is 2/ m 2/ m 2/ m which is not present in this combination, because 2/m, 2 / m, 2/ m is not generatable by these operations.

And therefore, 2/m 2/m 2/m is a new point group. So, on the other hand, 6/m 2/m 2/m is also a new point group and with 622 and with 422 also we will get an additional point group, the rest of them do not appear. And as a consequence, we have 3 more crystallographic point groups with more than one axis each axis being proper and improper simultaneously, that is what this table says and this particular table therefore, now concludes that we have 29 plus 3 which is now 32 point group.

So, these are the various ways in which we represent the 32 point groups. So, let me recount. We can go back here with set of proper axis 1, 2, 3, 4 and 6, we get the combination of $\bar{1}$ $\bar{2}$ $\bar{3}$ $\bar{4}$ $\bar{6}$ which is now the improper axis associated with the proper axis. Whenever we associate an improper axis with proper axis, we get a new point group and therefore, this is 5 plus 5.

We can also have proper and improper axis simultaneously operating at a point and that gives rise to three more which is 13 and then we see the combinations that are possible, we consider not just the PPP, we consider the additional PII, IPI, IIP and these combinations will give rise to another 16 of them. So, 13 plus 16 give us 29 and then they aspect that we can combine both proper and improper axis is simultaneously gives us the three more and that for we get the total 32 point groups.

Now, comes the beauty. Now, comes something which we have not anticipated or not bother to understand over the years. When people said that there are 7 crystal systems, we believe that there are 7 crystal systems and that was a belief rather than actually a proof and we also knew of course, there are 32 point groups. Most of us in the college days, we learn to presence of 32 point groups, but now what happens sees that if you now take this point groups and clarify classify them, classify them if you classify them into various classes where the importance of the angles between them becomes crucial, sorry the importance of the angles between the axis becomes crucial, then you see that we can clarify classify them into different crystal systems.

So, this gives rise to these so called seven crystal systems. The first one is the triclinic system where we have a non-centrosymmetric possibility; that means, there is no centre of inversions that is present with this unit cell, but this unit cell can exist by itself. So, the symmetry that is associated with this is one. And then, the when we combine this with the centro symmetry combination the center of inversion is put in we get a $\bar{1}$.

We will not write now worry about this so called Laue class or the lattice point group nor worry about the geometry of these seven crystal systems because the geometry of the seven crystal systems we will automatically get as we see in the next class maybe or even today later in the today's class. But what is important is that the 7 crystal classes have the point group identification with them associated with them is identified here. For example, if you take a monoclinic system, you can have a twofold symmetry or a mirror symmetry which is $\bar{2}$.

Now, both of them do not represent a centrosymmetric system. Now, I am going to clarify this issue because you may say that, you know the $\bar{2}$ is a combination of 2 fold and an inversion centre. So, how come it is non-centro symmetric? It is non centrosymmetric because you now examine your equivalent points. If you examine the equivalent points, sorry if you examine the equivalent points in case of the mirror symmetry, it is x y z and x $\bar{y}$ z.

We operate x $\bar{y}$ z mirror again, we go back to x y z we do not see the presence of the inversion centre. Even though mirror in principle is a combination of the 2 fold and the inversion centre, it does not generated inversion centre. That is very important and therefore, we see that the so called non-centro symmetric systems where there is no centre of symmetry automatically coming into the crystal system, this is either 2 or mirror and in case centrosymmetry it is 2/ m.

Orthorhombic symmetry, we already saw that it is 222 and the combination mm2 is allowed and mmm is allowed, mmm is actually 2/m 2/m 2/m, we will prove all these issues with respect to the fact that the geometry of these crystal systems why these geometry now defines incorporating the point groups. So, the presence of the point group forces the crystal system to go into these crystal systems, forces the molecule to crystallize in these crystal systems.

So, the molecule when it crystallizes is first is the point groups, hopefully, we do not know is a chicken and egg problem whether the molecule decides to do what kind of crystal it should go in to or the crystal system decides what molecule should come into it is crystal system, that is an answer problem even though there are indications that the way in which the molecules associate themselves will decide ; that means, the functional groups or molecular molecules will decide what kind of a crystal system they go in to.

But that is something which is not an equivocally established. What happens in a when you crystallize a given material is that there is what is known as the nucleus which is formed initially and this nucleation how it is formed and why it is formed at what rapidity it forms and so on has never been understood.

So, crystallization phenomena even though you control temperature pressure and so on and crystallized the materials. It is a kinetic way of crystallization is governed by the kinetics of the situation kinetics of the way in which we grow the crystals either from made it or from solvent evaporation or whatever techniques we used to grow crystals, it is a kinetic process. This is something which is not fully understood because we do not know what is the nucleation process that involves the crystallization protocol.

Anyhow, let us go further. So, we therefore, now distribute the point groups, this is a very important list very important table in which we now classify the point groups into various crystal systems. As we saw in this diagram, the moment we have the 222, we identify orthorhombic system. So, we there is no other system which can have a point group symmetry is associated with 222, tetragonal the trigonal systems will have 322, tetragonal systems will have a four-fold symmetry and hexagonal system will have a 6 fold symmetry.

So, when we actually decide how these symmetry elements distribute themselves in the 3 dimensional lattice, we will see how the nature of these orientation of the axis decides the nature of it is crystal system ; that means, in the case of just give you an example, you already know this result from your earlier college days, but we have never put 2 and 2 together. For example, in the case of a triclinic system, we say a is not equal to b is not equal to c and interactional angles are not equal.

Now, the only symmetry element that can be present in a unit cell of that type is either 1 or $\bar{1}$. That is because it is a point operation. The moment we bring in an axis operation, we will have to bring in additional symmetry that is associated with the lattice. So, in a triclinic system in other words, you cannot have any axis of rotation. In a triclinic system, you cannot have a mirror plane. In a triclinic system, you cannot have three-fold rotation, fourfold rotation and so on.

Because triclinic systems are restricted to either by themselves or the maximum they can have maximum symmetry, they can have a is a centre of symmetry as is shown here and. In fact, that is what is referred to as the Laue class. This is the maximum symmetry to which it refers to and this is what you will find when you do the x ray diffraction experiment which we will learn later on. And then, what also is indicated here is the maximum symmetry that will get associated with this system which is this so called lattice point groups. We will work out these two issues as I mentioned later on one once we do the diffraction theory.

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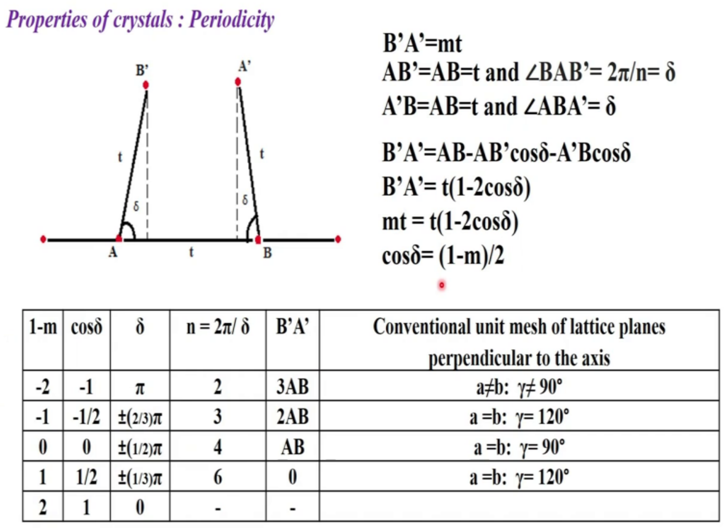

Properties of crystals : Periodicity

$B'A' = mt$

$AB' = AB = t$ and $\angle BAB' = 2\pi/n = \delta$

$A'B = AB = t$ and $\angle ABA' = \delta$

$B'A' = AB - AB'\cos\delta - A'B\cos\delta$

$B'A' = t(1 - 2\cos\delta)$

$mt = t(1 - 2\cos\delta)$

$\cos\delta = (1-m)/2$

1-m	cosδ	δ	n = 2π/ δ	B'A'	Conventional unit mesh of lattice planes perpendicular to the axis
-2	-1	π	2	3AB	a≠b: γ≠ 90°
-1	-1/2	±(2/3)π	3	2AB	a =b: γ= 120°
0	0	±(1/2)π	4	AB	a =b: γ= 90°
1	1/2	±(1/3)π	6	0	a =b: γ= 120°
2	1	0	-	-	

So, at this particular stage therefore, we have now done the following we have found that in a periodic system, we get this periodicity only because of the fact that we restrict our ourselves to 5 axis of rotation and then the restrict ourselves to a point about which we can have a centre of inversion and we also restrict ourselves to the fact that whatever combination of symmetries, we can have is restricted to these many.

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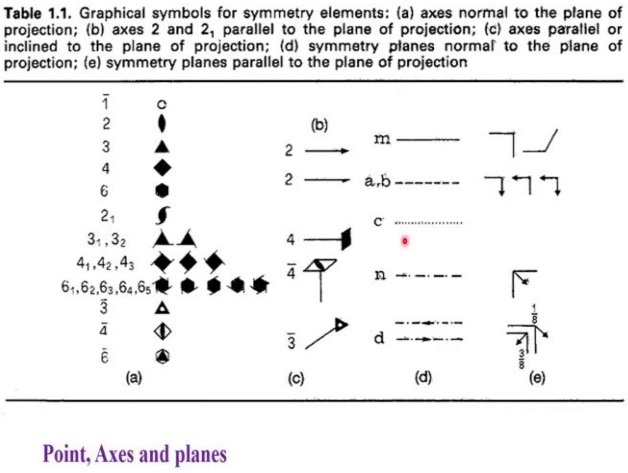

Table 1.1. Graphical symbols for symmetry elements: (a) axes normal to the plane of projection; (b) axes 2 and 2_1 parallel to the plane of projection; (c) axes parallel or inclined to the plane of projection; (d) symmetry planes normal to the plane of projection; (e) symmetry planes parallel to the plane of projection

Point, Axes and planes

And as a consequence, we found out that these many operations in crystals with or without translational symmetry, living out the screw operations and the glide planes.

Their operations will coexist and this gives rise to the so called point groups. So, if the operations are independent like this, the proper axis we have five point groups, five point groups coming with improper axis proper axis and improper axis combinations will give rise to 3 of them and then if you have more than one, they follow the Euler's symmetry, more than one symmetry intersects at a given point O, then the third one is automatically invoked and based on that, we will get additional possible point groups and therefore, the there are totally 32 point groups. You see that as the as the lattice nature changes, you will see more and more increasing number of point groups which can be associated with it.

So, the moment you have a tetragonal system, you always have a fourfold symmetry. You have a trigonal system, you always have a threefold symmetry, hexagonal system will always be a 6 fold symmetry. Cubic system, as we saw there is no 90 degree angle information here. So, you will have a threefold symmetry along the diagonal. So, the presence of the 3 fold symmetry along the diagonal distinguishes a cubic system from a trigonal system where the trigonal system has a threefold axis about one of the axis.

So, these are some of the issues we will discuss more and more as we go into the 3 dimensional lattices and then from this point groups, how we can go to 3 dimensional space. What is that which generates combination of point groups with the crystal systems and the behavior of the translational periodicity that is associated with the crystal systems, which generates eventually what we call as the space groups.

So, we will then see how the distribution of the symmetry elements goes to the symmetry in order to this space groups information. Keeping this part in mind, we should always be reminded and that is why it is next slide.

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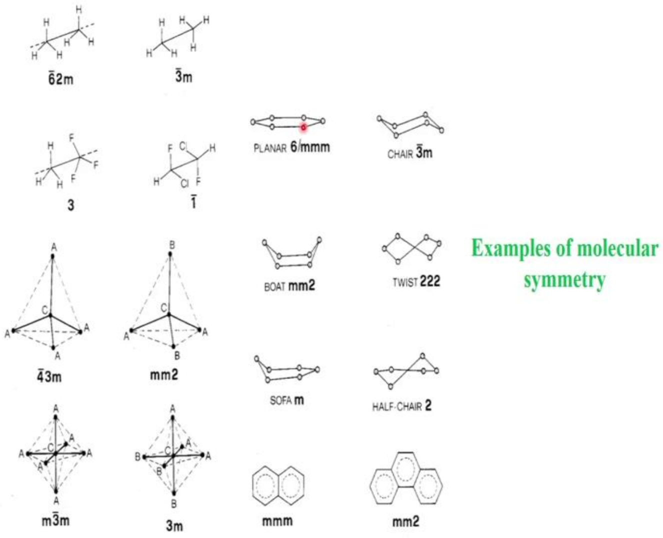

Examples of molecular symmetry

We should always be reminded that the crystal symmetry and the molecular symmetry are different from each other. It is not necessary that a molecule with a certain symmetry should crystallize with the same symmetry in the crystal system. For example, if there is a system which is now like this, this has a very high symmetry, I this is the point group symmetry which are which is indicated for each of these molecules.

So, we can identify the symmetry that is associated with each one of these molecules. Take for example, this case this particular compound which has a Fluorine in up there and a fluorine down here is having a centre of inversion at that point. The presence of the centre of inversion at that point will make this molecule process the centre of symmetry. What crystal system it goes into is unknown, it depends upon what kind of interactions that this particular molecule which has a centro symmetry develops with it is neighbors in the three dimensional lattice.

So remember, that in a crystal when you grow a crystal it is a three dimensional unit, so the basic repeat motif is this molecule. So, this molecule now let us say crystallizes in some space group. It is not necessary that it should crystallize only in a triclinic system. It can have a higher crystal system depending upon the way in which this is packed inside the unit cell. This takes you back to the (Refer Time: 17:32) diagram, you know you remember we talked about the (Refer Time: 17:33) diagram and in the (Refer Time: 17:35) diagram, one issue we put in very strongly that is the close packing.

So, when these kind of molecules back into the crystal lattice there, remember that they should pack closely and the nature of the close packing is crucial and way in which the close packing is decided depends upon the interactions this particular molecule develops with it is neighbours and these are known as intermolecular interactions. We will be spending some time towards the end of the course on understanding these intermolecular interactions based upon the nature by in which these molecules are assembled themselves.

At this stage, I was already referring to the work of Kitaigorodsky. Kitaigorodsky said that if the molecule has a symmetry and this particular symmetry will be found and must be found in the crystal structure as well. Invariably the molecular symmetry will find itself very comfortable is settling down in a crystal system which has one bar symmetry it does not mean that it should crystallize this particular molecule should crystallize in a monoclinic system. I would suggest that you refer to literature and see this particular molecule and see what crystal system it goes into. Just to keep the curiosity alive.

Similarly, what happens to this planar 6/m m m which is the symmetry that is associated with benzene? Benzene is not going to crystallize in a hexagonal space group. Find out where benzene crystallizes under what conditions benzene crystallizes. So, this opens up the possibility of molecules crystallizing in more than one possible crystal system and this is where the interest comes in pharmaceutical industry.

Because pharmaceutical industry wants molecules to crystallize in different crystal systems because the physical properties associated with the crystal depend upon how the molecules pack inside their crystal lattice. The physical properties by which I mean the melting point, the solubility, this so called bioavailability which is very crucial pharmaceutical materials, they need to have the molecular symmetry and the crystal symmetry go hand in hand.

Because of the fact that the molecules, they are very clever the keep that symmetry, benzene cannot cannot be other than having a planar 6/mmm symmetry, but for example, a cyclohexane can have boat it can have a sofa configuration, it can have a half chair configuration, it can have a twist chair configuration, it can also have a chair configuration. So, depending upon the type of substituents you put on this particular crystals they of this molecule, it will decide which kind of a minimum energy configuration it would like to adapt. So, it has this flexibility whereas, here there is no flexibility.

Now, because of the fact that there is no flexibility here, it does not mean that it should crystallize in a system which has this 6/mmm space group 6/m2/m2/m space group. So, this space group in which it crystallizes once again, I suggest you refer to the literature find out in which crystal system benzene goes into and under what circumstances because we although that benzene is a liquid at room temperature. So, when you crystallize, you have to do some tricks either by reducing them reducing the temperature or by applying pressure and then find out what happens to the crystal structure.

So, this therefore, gives rise to the possibility and innumerable number of possibilities particular line pharma industries to design what they called as polymorphic modifications. So, each and every molecule shown here can have different kinds of polymorphs and the presence of polymorphism is crucial for the pharmaceutical industry. So, there is an application potential right away coming up for the industry people this is also true with materials because depending upon the type of molecule and the molecular property, the material property will be decided once again by the nature in which it packs itself inside the crystal lattice.

So, the crystals therefore, not necessarily should have the property of the molecule, but the molecular property can be tuned to the property of that could be displayed in the crystal system. So, this therefore, opens up the possibility of studying more than one crystal structure of a given molecule. And so, polymorphism issues both in material science and pharmaceutical industry become example important. So, that is why I showed some examples of molecular symmetry here, just to tell you that for example, the presence of mm2 symmetry in this does not mean that this molecule will crystallize only in the orthorhombic symmetric. It can crystallize in many other symmetry. So, the symmetry of the molecule is not necessarily the symmetry of the crystal structure.

So, the this is what I was telling that if there is a tetrahedral carbon with A B A B substitution, there is a tetrahedral combination with all a is kind of substitution, you see that the point group symmetry are different, the crystal symmetry may be more very much different. So, this may crystallize in a tetragonal system, this may also crystallize in a tetragonal system, but the molecular symmetry is still kept intact. When the molecular symmetry is found to have a certain information which it can use in the crystal system, when the crystallization takes place the crystallization will be in such a way that the molecular symmetry is kept intact.

And therefore, it is very likely that these symmetry in the molecule is not destroyed. What is destroyed is the way in which the molecules are arranged inside the unit cell. So, the question of minimization of energy comes in. This is how prediction of crystal structures has become a very big issue because you know unless you make a crystal and solve the crystal structure. It is not possible to a priori you predict what crystal system it is molecule can go in to and this has been an exercise which has been practiced over the years and it I must mention that this stage that we have not achieved anything significantly appealing in order to say that wow, I can predict the crystal structure given the molecule. People have done this exercise, this is area is called crystal structure prediction and this crystal structure prediction area is now a very flourishing area where people are taking the molecules and then predicting the possible crystal structures into which they can go based on various thermodynamic and kinetic parameters. They are trying to control both thermodynamic and kinetic parameters as because I already mentioned that crystallization is a kinetically driven phenomenon.

So, based on that energy minimization of energy is performed in a possible unit cell which then is modified such that the minimized energy configuration eventually results for the closed packed crystal structure where we have the molecules closely packed in the unit cell. So, the unit cells are define and the possible structure are predicted. For example, structures of very many pharmaceutical compounds are earlier predicted, but the problem is that it either goes into one of the possible predictions or it will never go in to one of the possible prediction.

So, the conclusions drawn from crystal structure prediction are still to be testing. So, this approach of crystal structure prediction using molecular dynamics simulations and so on is a upcoming field, but it is not a field where we can have hundred percent success at this moment. So, there is a lot of improvement required, there is a lot of advances that they one has to look at in terms of calculations particularly to get to the final prediction of how a molecule can go into a crystal structure.

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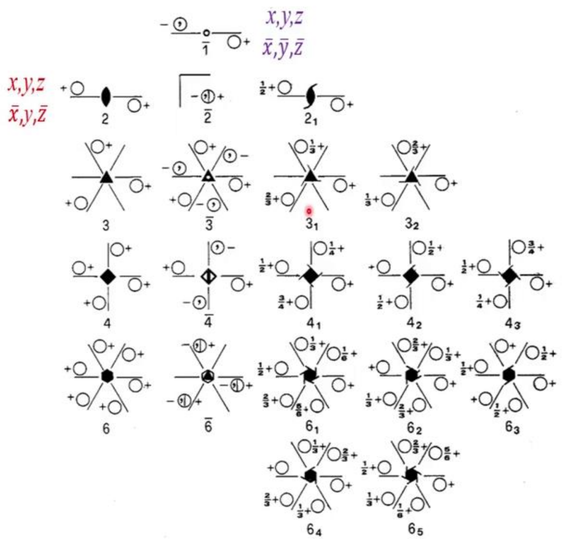

Now, we come to the operation itself, the symmetry operation itself. We are still not out of the understanding of the symmetry operations. So, the way in which this particular slide is prepared and demonstrated is to show what happens to the objects when they find themselves in a situation where they see these point groups. For example, if a if an object the object is referred to by this big circle with a positive and the object is referred to a circle with a comma, whenever this subject in wards itself we put a comma inside the object. So, whenever the object is inverted we put a comma inside the object and when it is coming towards you, this is shown as plus when it is going inwards it is shown as minus.

So, in this example for we have illustrated the suppose we take the coordinate of this point as x y z, then the coordinate of this particular point is -x -y -z; that means, these two now are related by a centro symmetry and the centre of symmetry symbol is used here the little circle, open circle and the symmetry is illustrated below. So, all possible symmetries which we have discussed with respect to the 2, 3, 4 and 6 are given in this list. So, this particular list therefore, has all the possible ways in which you can generate now objects in this 3 dimensional lattice. Here is only issue which I will discuss and probably stop today that is to discuss, what happens if this object is here?

So, suppose the object now decides to come to the position of the centro symmetry, then what happens to this particular object? So, this then will be moved here and then it has to generate x y z to $\bar{x}$ $\bar{y}$ $\bar{z}$. Suppose, this is now also the origin of the crystal system 0 0 0, then it will make an image of itself on 0 0 0 ; that means, we will have to show this something like what is shown here ok.

In the case of a $\bar{6}$ symmetry, you take this picture imagine this fellow to be moved at to that particular position and that is exactly what will happen; that means, now if this is representing a molecule, the molecule now must have a centrosymmetry because it has to sit on the centre of symmetry and then this particular molecule which sits on the centre of symmetry is related to itself.

So, the diagram now will look like taking out this fellow and pushing it to the one bar position. Such a position such a situation is referred to as a special position in this condition. So, whenever there is a object which sits on the symmetry element itself, it becomes a special position in any given system. So, any point group which we have discussed so far, if this sits on a special position, then it becomes a sits on the symmetry element it becomes a special position.

So, in this particular case, the number of equivalent points generated will become only one because 0 0 0 will give rise to -0 -0 -0. So, it is half and half. So that means, the occupancy of this particular position when we are sitting at the centre of symmetry becomes half.

So, in this case, the occupancy is full this becomes half. So, there are two independent possible positions for this particular compound or the object in this particular case molecule; one is related to the other by inversion centre; however, the number being 2 will reduce to 1 in case this sits on this is the inversion centre and that is how the possibility of having a centre of symmetric molecule occupy central a molecule with a with an inversion centre, how it can go and sit at the inversion center.

So, the molecules now will be repeated on through itself and therefore, we will get now only one equivalent point here. There were two equivalent points, it becomes only one equivalent point and the occupancy of that position now becomes half. So that means, only half the molecule if there is a molecule of the type we discussed before, suppose this particular molecule is sitting at the at that $\bar{1}$ position, then this half of the molecule will be related to the other half. So, when you have to worry about is to determine only one half of the molecule.

So, that way this is called the occupancy. So, the occupancy of that position becomes half. So, please note the whole idea of the first few classes which you have gone so far as I mentioned also earlier is to learn the grammar; we are actually learning the grammar one once we have identified the alphabets the so called point groups and all that will form the alphabetical notation in crystallographic language.

And what we are trying to do is to develop the grammar, the various ways in which we can have an adverb, the way in which we can have an adjective in a language. So, the crystallographic language therefore, has several new words introduced. Today for example, may introduce equivalent points we introduce the various symmetry elements called the inversion centre, we set special positions, we set the occupancy, all these are individual grammatical terms which are necessary to develop a crystallographic knowledge. At this stage, we will stop today and then we will go for forward in the coming classes.

Thank you.