Solid State Chemistry
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Lecture - 13
Schonflies and Hermann-Mauguin Conventions

Now, I will give the 3rd lecture of week 3. In this lecture I will talk about two conventions which are used to describe the symmetries crystals. Later on we will see that this convention is also used to classify crystals. But at this point I just want to introduce these two conventions which are referred to as the Schonflies and the Hermann-Mauguin convention. These will be used just to describe the symmetry elements. So let us look at these two conventions.

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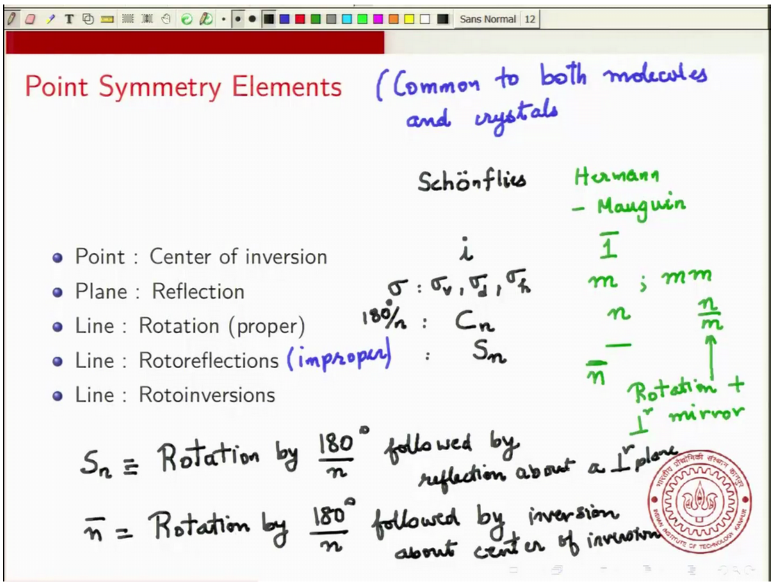

So, far we have seen the different point symmetry elements. And we remind ourselves that this point symmetry elements are common to both molecules isolated molecules. That means, if you just look at a molecule and you look at a symmetry of a molecule you can lookit will have these point symmetry elements. And crystals which are essentially infinite array of atoms and of atoms which consists of infinitely many atoms.

So, unlike molecules it just consists of a few atoms crystals consist of infinitely many atoms. And but they are arranged in a particular way. So there are symmetry elements called point we have seen this symmetry elements called point symmetry element ok.

what are the symmetry elements that we have seen? We have seen the point is a symmetry element the point is a the geometric point is a symmetry element.

And that generates a symmetry operation called the center of inversion. So, point can be a center of inversion so this process of inversion about the point is symmetry operation. You can have a plane and the symmetry operation can be reflection about this plane. You can have a line which is a symmetry element and the symmetry operation can be a rotation a simple rotation or a proper rotation about this point.

You can have a line of symmetry element which can be an axis of rotoreflections or rotations followed by a reflection. This is also referred to as improper rotations in especially in molecular in molecular group theory. This is referred to as an improper reflection in molecular symmetry. I can also have rotoinversions so this is the rotation followed by an inversion ok. So, so these are the different symmetry elements and various symmetries that we have ok.

Now there are two notations that are used ok. And I will show I will write them right here. So, the first is the notation for molecular group theory which is due to a person called Schonflies ok. And in the Schonflies notation the center of inversion is denoted by a letter i. So, if you have if a molecule has an inversion symmetry you refer to by i you refer to this operation of inversion about the centre.

So the other notation which is actually very commonly used which is more commonly used in crystallography is the Hermann-Mauguin notation ok. And in this Hermann-Mauguin notation the operation of inversion is referred to as a 1 bar. So, 1 bar referred to this operation of inversion. The next symmetry operation is reflection about a plane.

And again this in molecules can have several axis of reflection ok. They need not have only one axis of reflection several planes of reflection. So, now, the notation use for this reflection operations they so you typically use the symbol sigma to denote a reflection ok. And in molecular symmetry there are different kinds of reflections ok. So, you so you differentiate between the different kinds of reflections ok.

So, you might write sigma v or sigma d or sigma h; these are different reflections ok. They are defined with respect to the molecule ok. So, there is v d h stands for vertical diagonal and horizontal ok. I would not be discussing that in detail. But you will see symbols like sigma v sigma d and sigma h you might have already seen these when in other courses on molecular symmetry.

So, these are the this is the notation for with reflection symmetry operation. So, reflection in the Hermann-Mauguin notation are simply shown by the letter m m stands for a mirror ok. Simply shown by just one letter m ok. Now if there are multiple mirrors if there are if there are multiple mirrors in a crystal multiple mirror planes in a crystal. Then you can use m m or m m n and so on m m m and so on.

So, you can use multiple ms if we have multiple mirror reflection symmetries. Now coming to rotations the proper rotations in the molecular notation or the Schonflies notation are denoted by C with the subscript n ok. And remember this is rotation by this refers to rotation by 180 degrees divide 180 by n degrees degrees ok. So, 180 degrees by n rotation is denoted by C n.

So, if you have C2 it is a 90 degree rotation, if you have C3 it is a 60 degree rotation. In crystallographic notation in Hermann-Mauguin notation they are rotations are just denoted by the letter n. And in case you have a mirror ok and rotation whose axis is perpendicular to the mirror. Then often the symbol m by n is used a rotation and a perpendicular mirror is oftened sorry it is denoted by n by m n by m ok.

So, this refers to a rotation and a perpendicular mirror. So, this is a rotation plus perpendicular mirror ok. So, that is about these proper rotations ok. Now, additionally you have rotoreflections now these are not used in crystals, but in molecular notation these are donated these denoted by S n. S n means rotation by 180 by n degrees followed by a reflection in a plane perpendicular to the rotation axis.

So, S n write it down equal to this corresponds to rotation by an angle of 180 divided by n degrees followed by reflection about a perpendicular plane ok. So, S n refers to this to this particular symmetry operations and what should be noted is that S n axis is relevant when the individual axis when the individual operation of rotation or reflection is not a symmetry operation.

So, and, but S n is a symmetry operation so that is the interesting case. Now S n in Hermann-Mauguin notation we do not really use this ok. So, there is no symbol for it, but we use rotoreflections rotoinversions ok. So, this is the rotation followed by an inversion and this is denoted by n bar n with the bar on top refers to rotation followed by reflections about mirror about the plane, that is perpendicular to the rotation axis ok.

So, these are the two common notations and these are notations for the symmetry operations. So, these are either notations for symmetry operations or for symmetry elements. So, you can say that a crustal has a three axis of rotation ok. So, it has a threefold axis of rotation or you could say that it has a three bar axis ok. So that means, there is an axis where it has a rotoinversion axis ok.

So, it has a certain rotoinversion axis. So, it is a individual operations that are described by these symbols ok. So, I will just write for completeness n bar equal to rotation by 180 degrees divided by n followed by inversion about the center of inversion ok. When we saw that we saw in the case of a tetrahedron that some times that that tetrahedron has a C2 axis, but it has a 4 bar.

So, it has a twofold axis of rotation, but it has a fourfold inversion axis ok. So, sometimes these individual operations of rotation or inversion might not be a symmetry operation. But they their combination happens to be a symmetry operation.

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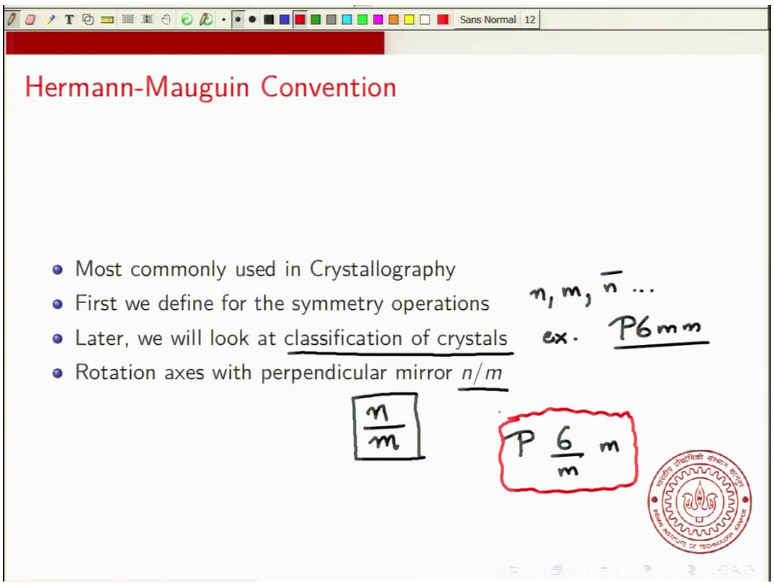

So, I will talk a little bit more about the Hermann-Mauguin convention. So, this is most commonly used in crystallography. So, we have already said this ok. And what is done is, first we find we use it to define the various symmetry operations and that we have already seen ok. So, we have we have things like n m n bar and so on.

And will see soon that we can also use it to classify the symmetry operations that are not point of symmetry operations. So, those are the translational symmetry operations ok. And later on we will see that the same Hermann-Mauguin convention is actually used to classify the different crystals ok. So, you will see things like example you can give for something like P6 m m ok.

So, this is a Hermann-Mauguin convention for a crystal ok. It is not a Hermann-Mauguin convention for a symmetry operation. But essentially it each of these names we will see later that how to understand the meaning of how to interpret such a name ok.

So, that convention is something that we look and I also already mentioned that if we have a rotation axis with a perpendicular mirror, you use the symbol n by m actually this m n divided by m ok. So, so it is they should be written one below the other ok.

So, for example, you can have something like P6 by m m you could have something like this to in the notation for the crystal ok. So, again we look at all these in more detail when we come to classification of crystals ok.

But for now I want each of you to realise that this Hermann-Mauguin convention is actually extremely important. And that is what will be used extensively in crystal in classifying crystals and identifying the various symmetry operations in crystals ok. So, I will conclude this lecture here and we will continue in the next lecture.

Thank you.