Group Theory Methods in Physics
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Lecture – 12
Symmetries of Molecule, Schoenflies Notation

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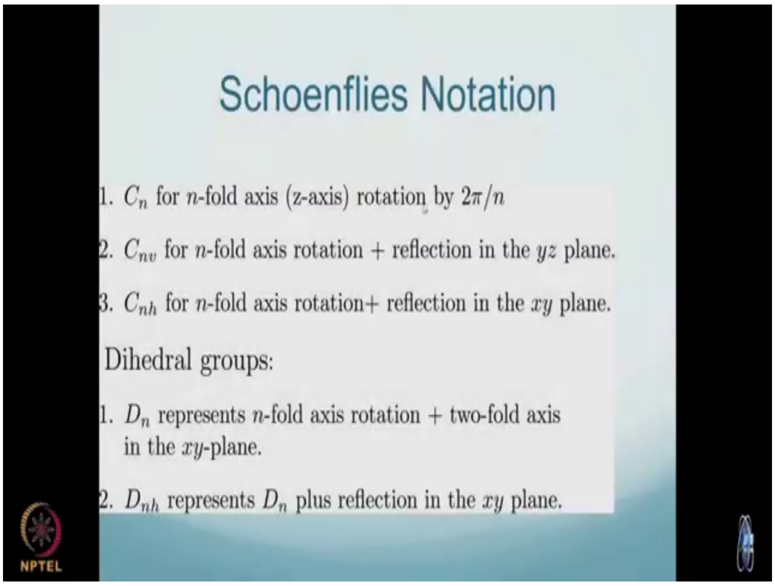

So, just to put in this notation which just like SI units or your periodic table with elements having some symbols, there is some notation called Schoenflies Notation. C n is for an n-fold z axis rotation by 2 pi by n. C nv, in this case C 2 I have written C 2 v, for an n-fold rotation plus reflection in the yz plane. C nh is an n-fold axis rotation plus reflection in the xy plane. I am going to take the access to be along the z axis. This is what I was explaining in the last lecture before we did.

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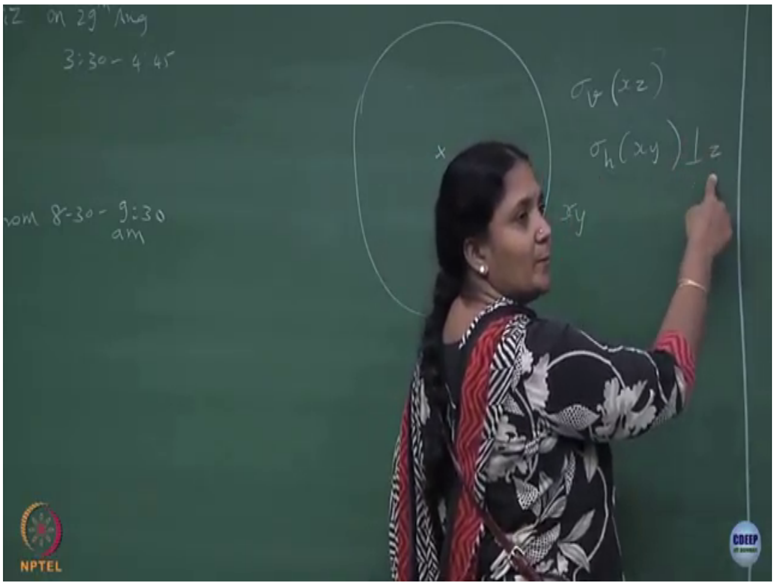

So, I am going to take the plane of the molecule to be the xy plane, this board plane of the board to be the xy plane, I am going to take the axis to be coming out of the board that I am taking it to be the z axis, is that clear. So, if I want to say sigma v plane, sigma v plane should have the z axis, axis of rotation is taken to be along the z axis, the principal axis of rotation and sigma v plane will be always in the involving either xz or yz, it should have the z axis. Sigma h plane will be only in the xy, because it has to be perpendicular to the z axis the plane has to be perpendicular. Here it should contain the z axis that is the definition, is that clear, ok.

So, those are the shorthand notations and each one is a point group, ok. C n is a point group, C nv has C n as a subgroup and C nh has C n subgroup again, right. The question for you is can we write C nv as C n cross sigma v. Always, in the C 2 v we wrote it. And that is question with something which you have to look at the ammonia molecule; take the ammonia molecule. What does the ammonia molecule?

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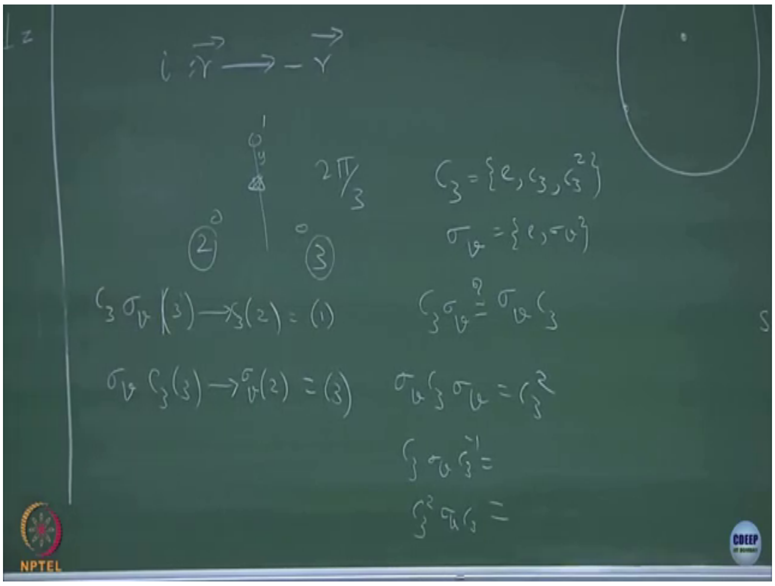

You have the 3 hydrogens or you can take the nitrogen through which you can put a triangular 3-fold axis and rotate it, right rotate it by 2 pi by 3. So, this has C 3 symmetry, ok. You can also put a plane, you can put a plane containing this axis let us call this to be y axis, right. And then what happens? If you put a plane through this then you have a sigma v, a question is a C 3 sigma v question mark, is it same as sigma v C 3, ok. So, these are questions which will tell you whether it is a direct product group or semi direct product group or these are only generators by which you can write the group.

To see a semi direct product you have to see whether there is an invariant subgroup, is that clear. So, is this happening is the question. So, if I do mirror symmetry, let us keep the mirror here, let me number the atoms, ok. So, when I put the mirror and let us concentrate on the atom 3, atom 3 goes to atom 2, right.

So, let us do that sigma v on atom 3 it goes to atom 2, ok. And now I want to do a C 3 on it, C 3 on this C 3 on that will give you atom 1, right. If you do C 3 on 3, right, what happens? This goes to the 2 pi by 3 rotation about this axis should take the 3 to 2, right. And then I want to do sigma v. Sigma v will go to, right. What does this tell us? It is not commute, ok.

So, you can figure it out this way that this group is a non-abelian group, unlike this which is abelian and then you have to see once its non-abelian you know it cannot be written as a direct product of C 3 and sigma v, and then if you can see whether there is an invariant subgroup what will be the order of this groups. So, the order of this group this is generator, right. So, order of the group you can just multiply because we have to multiply every element by every other elements, so there will be 6 elements. So, you can write the elements of C 3 v which is another point group and this is the point group symmetry of ammonia molecule, ok.

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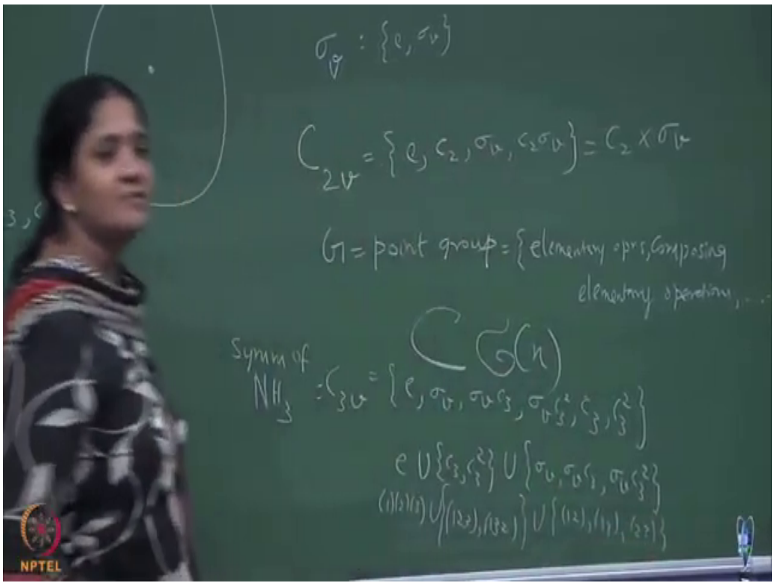

Symmetry of ammonia molecule is C 3 v, and the elements are e, sigma v, sigma v C 3, sigma v C 3 squared and then C 3, and C 3 square. Am I right? Anything I am left? I have just multiplied the sigma v with C 3 and C 3 squared and without sigma v. Now, can you see any subgroups of your symmetric group to which this will be isomorphic? Which one?

Student: C nv in terms of a b (Refer Time: 08:10).

In terms of a b you can see the same symmetry and you can also rewrite this as can we, right it also as a class structure identity element, union, C 3 and C 3 squared is the belongs to the class and then this is sigma v, sigma v C 3, sigma v C 3 square. There are 3 classes. To see that it is a class you can also do sigma v C 3, sigma v here and check it out. C 3 will go into C 3 squared. You can check it out even here by operating whatever I have done, you can show that sigma v C 3 sigma v will be C 3 squared, and you can show that C 3 sigma v C 3 will be some answer and then you will also find C 3 squared sigma v C 3 sorry inverse this is inverse and C 3 minus 2 which is nothing, but which is C 3 what is that, ok.

So, you can try out this and check that it can be broken up into conjugacy classes, ok, which will also tell you that in the planes of symmetry, you could try to say that you can have another plane going through this access, but containing you know it can be like this. You can call this plane as sigma v; you can call this plane as sigma v prime, and similarly this plane a sigma v double prime, ok.

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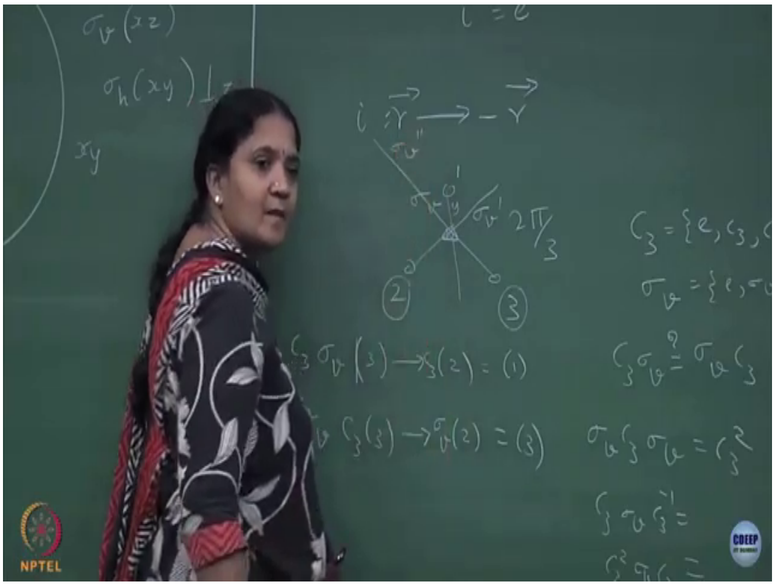

So, there are 3 planes of symmetries equivalently. These 3 elements which I wrote can be independently written as if this molecule has 3 planes of symmetry, each of these planes has the principal axis; it contains a principal axis, so they are all vertical planes. So, there are 3 planes of symmetries and one principal axis. So, you can show that if you have a principal axis and 3 planes, the 3 planes will be related by a similarity transformation. So, they will all be conjugate to each other. So, that is why the set of elements which are the 3 mirror planes will be conjugate to each other and C 3 and C 3 squared will also the conjugacy class, ok.

And once I write it this way as she has already pointed it out that you can write this to be like b and b square and then this is a, a b and a b square or you can write it in the permutation group of 3 objects that it is going to be this one will be like a 1 2 3 and a 1 3 2, right. This is identity which is 1, 2 and 3, these two are in the same class and then this one will be a 1 2 plane, 1 3 plane and a 2 3 permutation, transposition.

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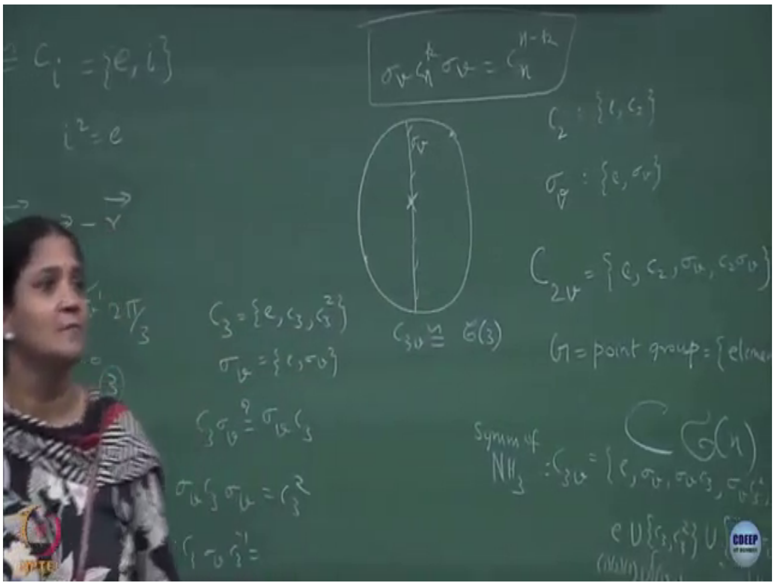

So, these two are isomorphic to; so, C 3 v is isomorphic to symmetric group of degree 3, ok. Whatever we did in the earlier lecture is formalism, now you can see to be applied to looking at the molecular symmetries, ok. So, I also briefly said we call it dihedral groups.

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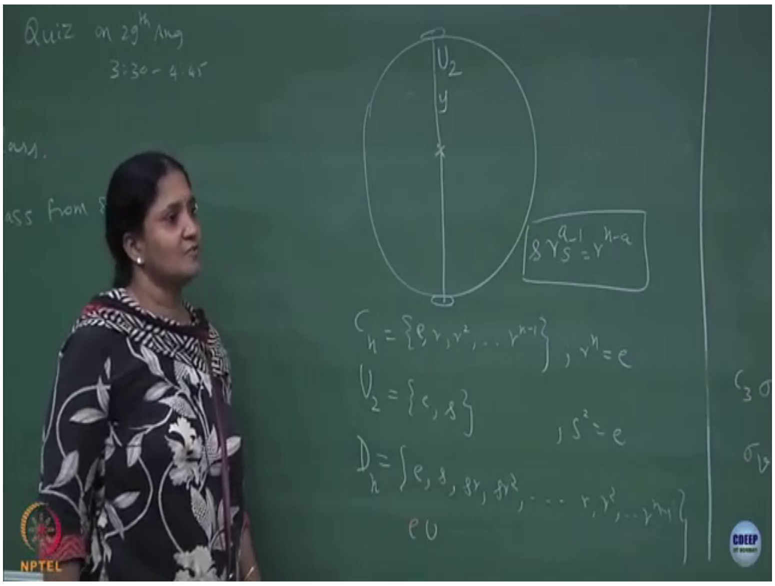

In the picture of these molecules, in the picture of these molecules besides the principal axis of rotation you could also have a two-fold axis of rotation let us say it is the y axis. It is not a plane it s still a proper rotation you can have a two-fold axis of rotation. What is two-fold axis? 180 degree rotation, ok.

So, if you have that additional two-fold axis of rotation over on top of this principal axis which is an n-fold, you can call that two-fold axis of rotation as U 2, you will have a C n group for the principal axis of rotation, you will have an U 2 group which is similar to what we saw. This one was one identity r, r squared, r to the power of n minus 1. I did briefly mention about the dihedral groups. This one is identity and s.

So, r to the power of n is identity here, s squared is identity and then we try to combine all possible terms and I said that is the dihedral group which is denoted as D n which will be made of how many elements. What will be the order of the group? This as order.

Student: n.

n, and this has order 2. When you take these two together and write the whole set it will be order 2 n, right. You will have 2 n order elements, ok. So, you will have identity s, then s with r, s with r squared and so on, and then r, r square, n minus 1. Conjugacy class, we did this there, there was very simple, but here you need to see what are the conjugacy class, ok

So, these are things which requires some more information that if you have a principal axis and if you have a two-fold axis perpendicular to the principal axis, then you can show that r a should be same as r n minus a, should be conjugate to. So, I should say that there exists an element s s inverse which will give you r n minus a, in such situations you will have this.

Here also I should say that even though we did C 3 v, even if you had an n-fold axis symmetry here and if you had a plane which contains, by plane I mean is sigma v plane, do not confuse the sigma v plane with this axis. The two-fold axis we show it by this symbol. The sigma v plane here or if you want you can put a like I said it is a mirror. If you have a sigma v plane with containing the principal axis, here also you can show that sigma v C 3 k sigma v a C 3 sorry not C 3 C n in general, ok. What does this mean? C n k is conjugate to C n n minus k that is why C 3 and C 3 squared are conjugate elements. So, I am not proving it for you, but you can show that whenever you have a mirror plane containing the principal axis then you can show that C n k any power k power, C n n is identity so, they will be conjugate to each other, ok.

So, you can use those properties here and try and do how to break this into conjugacy class, and will it depend on when n is odd when n is even. So, some of these questions if you can think over it we can discuss the structures; so, D n group.

Student: (Refer Time: 17:33) U 2.

U 2 is the two-fold axis symmetry, two-fold axis symmetry.

Student: (Refer Time: 17:41).

Rotation by y axis by 180 degrees, ok.

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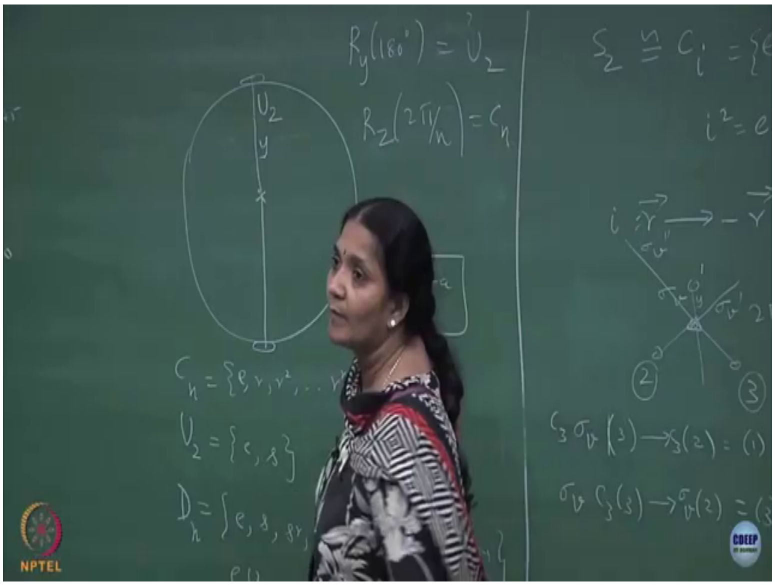

Student: What is the (Refer Time: 17:58).

The principal axis will be a rotation about z axis by 2 pi by n, clear. Yeah, ok. So, that is what I am mentioning on the screen. D n represents n-fold axis rotation plus a two-fold axis in the xy plane which is perpendicular to the z axis that is what I mean, ok. So, this is this can be rotation not only in the y axis it could be in the xy plane in general axis could be, but it should make perpendicular to the principal axis. So, that is the dihedral group.

In the earlier, lecture I just gave it as generators and I asked you to generate the set, but now you have a physical interpretations on molecules which have these kinds of symmetries. That is why these terms start coming up when you ask people in chemistry working on symmetries of molecules, ok.

And then it goes on, you can have a D n and then you all can also have a D n is a proper group, only pure rotations, but D nh is on top of D n you also add a mirror plane in the xy plane. So, you will have more elements, ok; so, D n plus a reflection in the xy plane. So, this is the way the notation continues, ok.

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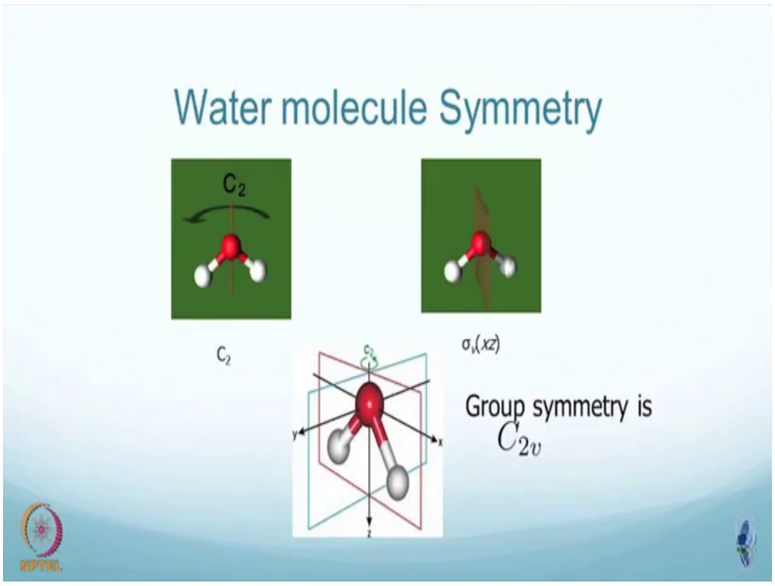

So, this I have already explained to you.

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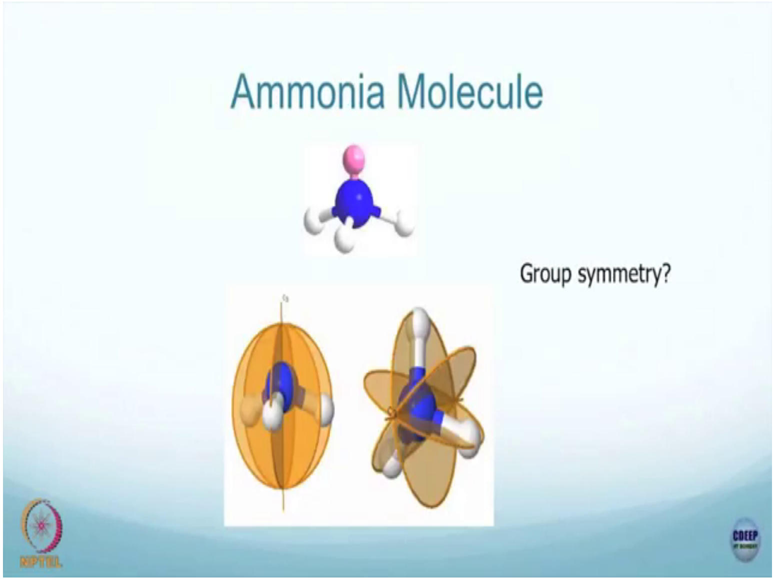

I have shown the planes of symmetry and axis of symmetry.

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And then I said find out what is the symmetry of this. This is very now simple to you to see what are the allowed symmetry. You can start seeing does it have only pure rotations, can it have some more reflection planes, all these things you have to make it maximal. It may have a subgroup. Like here what the molecule has a C 2 symmetry which is a subgroup, but you have to make it maximal that beyond that you cannot add any more symmetries. So, C 2 v is the symmetry of the water molecule which includes rotations and the reflections.

Similarly, for the methane molecule you can show that it is C 4 v, because all the 4 hydrogen atoms can be rotated amongst each other, you can start putting reflection planes, and so on, ok.