PROFESSOR: Any questions about where we left off-- up to where we left off? OK, what I'll do then is give you a few more examples of the combinations in 22 to show which ones we have to retain as frameworks for crystallographic point groups and which ones exist as groups but which involve rotational symmetries that are not permitted to a lattice. So we've seen a combination of three orthogonal twofold axes and then projection that would look like this. And the international symbol for that point group is just a running list of the different axes that are present, 222. The next group in the sequence would be 3 2 2, where we took a 120 degree rotation. We combine that with a twofold axis perpendicular to it and the new twofold axis comes out and reminds you again of things that are quite clear but which are easy to forget-- that this angle here is 1/2 of 2 pi over 3. Don't forget that 1/2. So the neighboring twofold axis is 60 degrees away and then if we allow these axes to operate on each other, the net symmetry consistent set of axes looks like this.

But let us look at a solid that has this symmetry. And such a solid would be a trigonal-- triangular prism. And again we can use the corners of this polyhedron as the reference locations of our motifs. So let us put a first motif here, number 1. Let's rotate it by 120 degrees to get a second motif here. And then let us rotate that one down by a twofold axis coming out of one of the edges. That will give us number 3 that is down here or of the same chirality. And how do we get from 1 to 3 directly in one shot? And the answer is about a twofold axis that comes out of the face of the prism. So again the prism that we've used as our reference is a prism that looks like this. We've got one twofold axis coming out of the face. The next twofold axis is the one that is equivalent to a threefold rotation followed by a twofold rotation.

Now here we hit a situation in deciding on the name for the combination that is analogous to what we found in two-dimensional plane groups for 3mm. We saw that only one mirror plane was distinct. We look at this arrangement of axes-- this was axis a, alpha, this was axis b, beta. But if I repeat one of these twofold axes by 120 degree rotations, this one is the opposite end of this one, this one is the opposite end of this one, and this one is the opposite end of this one. So there are only three kinds of-- there are three, twofold axes and they are related by the 120 degree rotation. Another way of saying that is that if we look at a trigonal prism, each of the twofold axes comes out of an edge and out of the opposite face. So there they all do the same thing in this regular prism-- twofold axes extend between corners of the opposite face. So there are only-- there's only one kind of twofold axis present in terms of being symmetry independent. So just as we called 3mm, 3m, and we call this one 3 2 because all the twofold axes are symmetry equivalent.

The next one that is crystallographic would be a combination of a 90 degree rotation with a pair of twofold axes that are normal to it and separated by 1/2 of pi over 2, the [? throw ?] of a fourfold axis. And the symbol for this one would be a fourfold and now there are two different kinds of twofold axes. And if we look at a regular square prism, we can again show that what we've been demonstrating for these other prisms is true. One twofold axis would come out of the face, the other twofold axis would come out of the midpoint of an edge, and the fourfold axis would come up here. And a 90 degree rotation, from here to here, followed by a twofold rotation about this axis, gives us as a net effect a 1, 2, 3. And that rotation from 1 to 3 about this twofold axis gives us the combined mappings.

Notice that the order in which we do them is unimportant. For example we could do the same thing but do two 180 degree rotations about the twofold axes. Let's say we start by doing a rotation about this twofold axis. From here down to here. And then we do a twofold axis about the-- twofold axis that comes out the face and that would take number 2, and rotate it up to number 3. And the way we get from 1 to 3 directly is by a rotation of C pi over 2 about the square face of the prism. So do them in any order you like-- two 180 degree rotations, or a 90 degree rotation, one of the two full rotations with 90 is the other twofold-- the other type of twofold axis. The 90 degree rotation plus the second type of the twofold axis is the same as the first. So the result can be permuted and turns out to be the same combination.

The next one that we would hit if we proceed systematically is non-crystallographic. And this would be a fivefold axis. And I'm foolhardy to even start trying to sketch this in three dimensions. Nevertheless, nothing ventured, nothing gained. Start with a twofold axis out of one of the edges and rotate from 1 down to 2. Follow that by a twofold rotation about the twofold axis that comes out of the face. And that gives us one number 3 up here, and lo and behold, the way you get from 1 to 3 directly is by a rotation through 1/5 of 2 pi. So this would be the non-crystallographic point group, 5- well it's not going to be 5 2 2. And that has a whole bunch of twofold axes separated by 1/10 of 2 pi. And just as in 3 2, twofold axes here all come out of the face and out of the opposite edge. So this would be called 522. A nice symmetry but not crystallographic, so we can promptly forget about.

So what comes out of this is a family of groups that are all of the form n 2 2. The crystallographic ones are 222, 32, 422 which we've looked at in detail, and one that I won't draw because there's so much symmetry it get's messy. This is 622. There is a Schoenflies notation. You remember the language that we encountered for our two dimensional point groups. We used m for mirror in the international notation. We used C standing for cyclic group, subscript s standing for Spiegel in the Schoenflies notation. The Schoenflies notation for all of this family of symmetry is Dn, and the D stands for dihedral. And the reason for that name is that the difference between all of these groups, besides the n-fold axis, is this angle between adjacent twofolds and this is a dihedral angle. I have a set of planes passing through a common axis; the angle between those planes is termed a dihedral angle. So this is called D for dihedral and then a subscript that gives the rank of the axis. So Dn generically. This is D2, this is D3, this is D4, and this is D6.

Comments or debate? Yes, sir.

AUDIENCE: [INAUDIBLE]

PROFESSOR: [INAUDIBLE] --out of this face. So I got from here down to the diametrically opposed axis. And I rotate it about the adjacent one which comes out of an edge and-- what did I do here. Here I did A pi over 2 from 1 to 2, and then I did B pi, where this is B pi, and they turned out to be C pi, which is this one here. So going from here to here down to number 3 is the same as going from 1 to 3 in one shot about a twofold axis normal to the face. And actually I'm courageous to try to do this in three dimensions.

We could do it in projection and then things are used-- this for a point that's up, and use this for a point that's down. And then what we've done is to go from 1 that's up, to 2 that's up, and then we rotate it about this twofold axis. That was 3, that's down. So when we get into complicated symmetries where you just can't do a proper job drawing them in an orthographic drawing, we'll do them in projection and use a solid dot for something that's up and an open circle for something that's down.

Is there any other way we can combine things? Well what you would have to do is use these three relations, and plug and chug your way through all of the combinations which were enumerated in the handout. And I'll save ourselves a lot of work by saying that there are only two more combinations. And these are combinations of axes at angles that have relevance to directions in a cube. One of them is a twofold axis with a threefold axis with a threefold rotation. Again remember these are not equations in symmetry elements. This is really A pi, combined with B 2 pi over 3, combined with C 2 pi over 3. And the angles that fall out of this are all crazy things like 109 point something degrees and they make no sense whatsoever. They're not nice things like some multiples of 2 pi, 90 degrees or 120 degrees. And they make no sense at all until you refer them to directions in a cube. And this one, 2 3 3, consists of a twofold axis coming out of the face of the cube, a 120 degree rotation, so this is B 2 pi over 3, this is A pi. And the other one, C2 pi over 3, corresponds to a threefold axis coming out of another body diagonal.

I don't know if I want to be gutsy enough to try to illustrate that that really works. But one thing that we should do is to let these axes go to work on one another, and see what comes out. First thing we can say is that this threefold axis-- if we extend it, it comes out of the bottom diagonal of the cube. This one, if we extend it, will come out of this diagonal of the cube. So there's a threefold here, and a threefold here. The twofold axis gives us a threefold axis that will come down this way. So there's a threefold axis here and a threefold axis coming out here. And then the twofold axis will rotate this threefold axis over to the remaining pair of corners.

So we have created this by looking at a twofold rotation, combined with the threefold axis, combined with the rotation of another threefold axis. But in point of fact, if you let the twofold axis operate on the threefold axis coming out of one body diagonal, you get threefold axes automatically out of all body diagonals. So this is given the international symbol 2 3, because if you start with one twofold axis out of a face normal and one threefold axis out of-- along a body diagonal, the twofold axis, acting on that threefold axis gives you one along every body diagonal. And the threefold axis-- let me point out that a cube standing up on its body diagonal, with a threefold axis coming out here and these faces sloping down into the blackboard.

If I have a twofold axis coming out of one face, the threefold axis puts a twofold axis on this face and rotates again 120 degrees and puts a twofold axis on this face. So the threefold axis relates all twofold axes coming out normal to the cubed face. And they were really just two independent axes in this combination. So 2 3 is the international symbol-- one kind of twofold axis, one kind of threefold axis-- inclined at these crazy angles that are in a cube. The Schoenflies notation for this is T, and that stands for tetrahedron. And let me try to convince you that if I look at a tetrahedron, that that is the arrangement of pure rotation axes in a tetrahedron.

And the way to show a tetrahedron is to inscribe it in a cube. So if I connect these two faces together and these two faces together, that will define for me a solid that has four triangular faces. Easier to recognize it when we put it up on one face. So this is a tetrahedron. Schoenflies symbol is T. And I love to get to this part of the semester and be at this point at the end of the hour, because if I draw a stereographic projection of the twofold axes, in this symmetry, I can take a couple of more twofold axes and add it to this combination which destroys the group. But lets me wish everybody a happy Halloween and exit to a stunned silence at the end of the hour. So this is a nice point group for October.

There is one more and that is the highest symmetry of all. And this is a combination of a rotation-- A pi over 2, a 90 degree rotation, with a rotation B 2 pi over 3, rotation through one third of the circle, and the rotation C pi. And the directions between the axes that come out there don't come out some multiples of 2 pi. Again they are crazy angles that make no sense at all unless you refer them to directions that occur in a cube. The fourfold axis is in the direction that corresponds to the normal to a face. The twofold axis corresponds to a direction out of one of the edges. And the threefold axis corresponds to a direction that is a body diagonal.

So again this is a mess. If we let those axes work on one another however, we will produce, more readily appreciated in a stereographic projection, fourfold axes along the directions that correspond to face normal. So the cube, threefold axes coming out of the body diagonals and twofold axes in between all of the fourfold axes in directions that correspond to the lines from the center of the cube out through the edges. So this is a group which would be called 4 3 2. There's one kind of fourfold axis related to all the others by the other rotation axes that are present. One kind of threefold axis that is related to all of the other threefold axes along the body diagonal by other rotation axes that are present. And twofold axes, one kind, all coming out of the edges.

So this is the group that, in international tables, is called 4 3 2. And the Schoenflies notation, this is called O. And that is the general reaction when one sees this lovely combination. You go ooh and O is what it's called. But the O doesn't stand for a gasp, it stands for an octahedral. This is the symmetry of an octahedron-- rotational symmetry of an octahedron. So that's it. That is the bestiary of ways in which you can combine crystallographic rotation axes in space about a fixed point of intersection. And there are eleven of them. There are the axes by themselves-- 1, 2, 3, 4, and 6. There are the dihedral groups, 222, 32, 422, and 622.. And then the two cubic groups, T and O. In the international notation, I'm mixing metaphors. These are 23 and 432.

I call to your attention the insidious similarity of the two combinations of axes, 32 and 23. When the 3 comes first, this is a group of the form n22. When the 2 comes first, that is the tetrahedral group. So if you count them all up, there are 4, 2 is 6, and 5. There are eleven axial combinations. Quite a few more than the situation in two dimensions where we just had single rotation axes 1, 2, 3, 4, 6. Now we have those as in two dimensions but the dihedral groups and the two cubic arrangements of axes as well. So we don't have to stretch our vocabulary too much more to be all inclusive here. OK, comments? Takes your breath away, doesn't it?

All right, let me indicate the next step in outline. What we will next do is introduce our remaining two symmetry operations into the picture. We have the eleven axial combinations. As I said, we can regard these as a framework that we can decorate with mirror planes and or the inversion center, which has not appeared until this point because inversion is inherently a three dimensional transformation. So what we're going to do is to take these axial combinations and add another symmetry operation to the group. And this as-- we used the term earlier, this is an extender. We have something that constitutes a group by itself then we muck things up by adding another operation. Remember in all of this we are combining operations, not symmetry elements. So we'll take an axial combination and add the reflection sigma, a reflection operation sigma. Or take a rotation and combine it with the operation of inversion as an extender.

So let's itemize the sorts of extenders we should consider. And the ground rules are that the extender should leave the arrangement of rotation axes invariant. Because if it doesn't, we are going to create a rotation operation that does not conform to the constraints that we used in Euler's construction. So for example, if we take 222, which contains the operations A pi, B pi, C pi and identity, that's the group 222. If we would add to the arrangement 222 a mirror plane that snaked through some arbitrary fashion like this, that mirror plane is going to reproduce the twofold axis over to here. And that is either going to not constitute a group because this twofold, this twofold, and this twofold don't conform to Euler's construction. Or alternatively, if we put it in carefully at 45 degrees with this twofold axis, we're going to get twofold axes that are 45 degrees apart and that's going to change this into a fourfold axis.

So if the addition of a mirror plane does not leave the arrangement of rotation axes-- rotation operations-- invariant, we're either going to get something that's impossible and does not constitute a group. Or else we're going to get a combination of rotation operations of higher symmetry which we've already found because we went through that process of combination using Euler's construction in an exhaustive fashion. So the rule then is that if we add the reflection operation sigma, then the arrangement of rotation operations must be left invariant.

OK let's look at the single axes. If there's an n-fold axis, the ways we can add a reflection operation to that axis is to pass the reflection operation through the axis. And this is going to look very much like the two dimensional point groups of the form nmm except that rather than having a mirror line, imagine the whole works as extending upwards along the rotation axis and space. So this extender is called a vertical mirror plane. The other way we could add a mirror plane to an n-fold rotation axis is to put the mirror plane in an orientation that's perpendicular to the rotation axis. That didn't exist in two dimensions because that plane that's perpendicular to the axis is the plane of our paper. And unless we wanted to have a two-sided group that was on both the top of the paper and the bottom of the paper, and we make up the rules since it's our ball game.

And that could be a group and these would be the two-sided plane groups, a plane point groups, but we didn't do that here. Adding the mirror plane, the reflection operation sigma, in a fashion that is normal to the rotation operation, A 2 pi over n, is another distinct combination. And this is called, very descriptively a horizontal mirror plane. That looks like about all you can do except for the cases where we have more than one kind of rotation axis present. So let me use 422 as an example. We could add a horizontal mirror plane perpendicular to the principal axis of symmetry, and that would be the horizontal sigma.

We could add a vertical mirror plane. And now there are two ways we can do it. We could put the mirror plane, the operation sigma, through the fourfold axis and in a fashion that was perpendicular to the twofold axis. And we will retain the term of vertical sigma for that addition. But the other thing that we could do would be to put the reflection operation interleaved between the twofold axes. That's going to take this one and flip it into this one, this one flip it into this one, flip these back and forth, and that doesn't create any new reflection. And this is referred to as a diagonal reflection plane. Diagonal to what? Diagonally interleaved between the twofold axes. And these are distinct additions and they will lead to different groups.

In as far as addition of reflection operations is concerned, that's about all we can do that's distinct. And notice that this is for the groups Dn, and tetrahedral, and octahedral only. The distinction here is not defined for just a single axis. So there are three possible extenders here-- a vertical mirror plane, a horizontal mirror plane, a diagonal mirror plane, added to each of the eleven arrangements of rotation axes. And then the final extender that we could add is to add inversion. And the symbol for the inversion operation is 1 bar. And obviously if one point in space is going to be left invariant, you either add this on a single axis, and that is what you'd have to do for the groups Cn, or at the point of intersection. And that would be the case if more than one axis, and that's the groups of the form n22, T, and O.

That's it. That's the job. So we should consider each of these possible additions of an extender systematically. I don't propose to do every single one independently. If we do a couple, you'll get the general idea. And I think because I have an honest face, and you've come to trust me, I can just describe the remaining results to you and we won't grind through every single one.

Now the enormity of what I've proposed becomes apparent when I say that we now are going to have need of a number of different-- what I call combination theorems, that let us complete the group multiplication table. And deduce, as a consequence, which symmetry operations must come into being because of these additions. So we'll want to know what happens when you add a vertical sigma to a rotation operation, A 2 pi over n. We'll want to know what happens when you add a horizontal sigma to a rotation operation, A 2 pi over n. And we're going to want to know what happens when you add a diagonal mirror plane, this really is a special case of the vertical mirror plane. And we'll want to know what happens when you add an inversion center to a rotation axis.

So let me do a few of these and then next time we can start off and start driving the three dimensional symmetries. So let's just repeat the ones that we've already done. We said that if we have a rotation operation A alpha, and we put a reflection plane through it, that A alpha followed by a reflection plane passing through it-- let me call this sigma V-- because this is the so-called vertical, up orientation. We've already seen that in two dimensions. This is a vertical mirror plane, sigma prime, that is going to be alpha over 2 away from the first. So that is something that we've already seen in it's entirety in the two dimensional point groups. There was m sigma, there was 2mm, and that was C2V, 3m, that's C3V, 4mm, and that was C6V, and 6mm, and that's C4V, and that's C6V. So that is the result that we obtained for two dimensions. And you can see now the reason for distinguishing the mirror plane by saying it is a vertical mirror plane because this is in the three dimensional sense. It's vertical parallel to and passing through the rotation axis-- no longer a rotation point but a rotation axis. So we've got those theorems.

What happens if we take a rotation operation, A pi, and put a horizontal reflection operation through it normal to that axis? So I'll call this sigma h, a horizontal operation. OK what we have to do is draw it out once and for all. Here's the first one, let's say it's right-handed. We'll rotate by A pi to get a second one which stays right-handed. And then we'll reflect it down in the horizontal mirror plane to get a third one which is left-handed. And now the question is, how is number one related to number three?

Anybody want to hazard a guess? We've got to go from a right-handed one to a left-handed one. But these two guys are oriented anti-parallel to one another. So how do we relate the first one to the third one? I heard somebody mumble softly enough to remain anonymous. Inversion. Right. So as we go along making these combinations, if we had not been bright enough to think of the operation of inversion as a general transformation where the sense of all three coordinates is changed, we would have stumbled over headlong right here. Combine a rotation operation, A pi, with a mirror reflection that is perpendicular to the axis. The way you get from one to three in one shot is by inversion through a point that is at the intersection between the rotation axis and the mirror plane. So rotation followed by rotation in a vertical mirror plane that's perpendicular to the axis is the operation of inversion at the point of intersection.

So again, if we had not been clever enough to invent it or tell you about in advance, there it is. When we start forming the group multiplication table, we would have had to have defined this operation to describe this relation.

AUDIENCE: Is that sigma sub h?

PROFESSOR: Ah yeah. Let me write that, sigma h. I thought that V didn't look like a V, so I changed it so it looked like a V but it shouldn't be a V. That's a horizontal mirror plane.

OK this is a new combination and if we see what operations are going to be present in the group, we've got the two operations of the twofold axis, 1 and A pi. And what we have added is sigma h as an extender. So 1 and A pi, this little box here is the subgroup that we know and love as the twofold axis. And then we'll write sigma h here and now let's fill in the group multiplication table. Doing the identity operation twice is identity. Doing the identity operation followed by A pi is A pi. Identity followed by sigma h is sigma h. Identity followed by A pi, sigma h, lets me fill in those boxes. Do a rotation twice, that's the identity operation. Do a rotation of A pi and follow that by a reflection, A pi followed by reflection. This is the inversion operation.

And so I should add inversion to my list of operations since it's come up. So 1 followed by inversion is inversion. A pi followed by inversion is the horizontal reflection. Horizontal reflection followed by A pi is the same as inversion. Horizontal reflection followed by horizontal reflection is the identity operation-- brings me back to where I started from. And a horizontal reflection followed by inversion is the same as A pi. So I'll have another object down here to complete the three dimensional arrangement. And this is the group for operations-- A pi, inversion, horizontal reflection, and the identity operation.

So what do we call this one? The operation A pi plus a horizontal reflection operation gives rise to a group that is a twofold axis of its operations, perpendicular to a mirror plane. And this written as a fraction means that the 2 is perpendicular to the mirror plane rather than being parallel and in the plane of the mirror plane. So two codes for writing symbols. A 2 followed on the same line by the m means that the m is parallel to 2. We know that when we write them as a fraction, that will be our way of designating that this mirror plane is perpendicular to a twofold axis. OK it's the witching hour, 4 o'clock exactly. That's when we ought to quit, so let's stop there.