PROFESSOR: Let the minutes of the proceeding show that I re-entered the room at 3:00 and 12 seconds, true to my word. OK, I wanted to give you one example of a screw axis that you're probably familiar with in everyday life. That was a telephone pole that I was very familiar with when I was a little kid because we used to love to wait until it got dark and our parents couldn't see us.

And then, we'd climb up the thing. And wow, you could see all over the whole neighborhood. I'm surprised nobody said, what? They had electricity when you were a little kid? Yes, they did. But now it's all underground. So kids, I don't know what they do for recreation these days.

OK, let me pursue this question of screw axes. We've seen what a 2 sub 1 screw access looks like. I just erased it. But it consists of objects of the same chirality extending left and right on either side of the principal axis.

The symbol for a twofold axis is this. The symbol for a twofold screw axis is the symbol for a twofold access with alternate sides extended like a propeller, a very descriptive symbol. The thing is rotating around. And you can think of these as the little ribbons that you used to have on the handle bars of your bike when you were a little kid. And as you pedaled along, these things fluttered out behind, and it was really cool.

OK, let's move on to the next family of screw axes. And let me look at an operation A2 pi over 3 with a translation component, tau. And these things are going to get awfully cumbersome to draw. So let me use a device-- I wish I could claim credit for it. But actually, a student in my class one year said, hey, I've got a really cool way to draw these things for you.

Let's imagine that this is a screw axis. We put a cylinder of paper around the screw. And then, let's divide up the surface of the paper in terms of end segments. So if this were a threefold screw axis, these would be 120 degrees segments.

And then, let's draw horizontal lines on the sides of the cylinder. Then, if we want to see how the screw axis reproduces a pattern from a given motif, you just fill in these boxes. And then when you're all done, cut the cylinder and you can draw the pattern quite nicely on a two dimensional surface.

So this is what I call the unrolled cylinder device. Somebody very imaginative invented it. His name, unfortunately, is lost to history. But I didn't want to claim credit for it myself. So what is the pattern of a threefold screw axis going to be?

Let's let the difference between boxes be the translation component, tau. And so what we will do is take an initial motif, rotate it 120 degrees, slide it up by tau relative to the axis about which we're rotating. Performing the operation again would involve rotating 120 degrees, sliding up by tau. Doing it yet get again brings us back down full circle. So this would be the translational periodicity along the direction of the screw axis. And this would be the value of tau equal to 1/3 of the translation.

So that is what a threefold screw access would look like. And the pattern obviously, if we would keep repeating it, would do something like this-- so perfectly interpretable, easy to draw. But things are actually more interesting and more complicated than this.

We are stating two things about this operation. We're specifying a translation. But then the other thing that we're specifying is the translation component tau. And why should we be constrained to say that tau can only be one nth of the translation?

If we do the operation n times, then doing the operation n times would give us a total translation of n tau. But there's no reason why that has to be one translation. Why not two? Why not three? Why not four?

So the only real constraint is that n tau has to be some integer, m, times the translation that is parallel to the screw axis. And this means that the value of tau is not just equal to 1 nth of-- restricted to 1 nth-- of t. Tau can be m/n times T.

And that is perfectly compatible. You do the operation n times. You're going to be directly above where you started. That's going to be a translation vector. But why

not two translations, or three translations, or four translations? So there are infinitely more screw axes than just the n subscript something translations. So let's look at some of the possibilities.

For a threefold screw axis, tau could be equal to 0T Tau could be equal to 1/3 of T. Tau could be equal to 2/3 of a translation. Tau could be equal to 3/3 of the translation, 4/3, 5/3, and so on, on and on and on. We could fill the whole board with possible screw axes having different values of tau.

Now, let me convince you, hopefully easily, that if tau is equal to 3/3 t, tau would be an integral number of translations-- in this case, one. Down here, 6/3 t would be two translations. We're already going to have those operations in the pattern when tau was equal to 0T.

So let me show you what I mean if it's not clear. Here's a trio of objects on either side of the rotation part of the operation. So what I'm saying is tau would be equal to two translations. That would, for some perverse reason, defining this as the pitch of the screw. Is it clear that that is going to be an operation that I already have when I say there's a threefold axis and a translation, T, parallel to that threefold axis? That's going to give all sorts of screw operations. But they are going to be integral multiples of the translation that's parallel to the axis.

So the rule is that we can always subtract off one translation from any of these definitions of tau and reduce it to something smaller. So we can always define tau less than or equal to T without any change or artificial restrictedness on the nature of the pattern. So that says that for a threefold screw, for a threefold screw axis, there are only three that we should consider.

Tau equal to 0, and that's a pure threefold rotation axis. tau could be equal to 1/3 of a translation. And now, we introduce the notation used to designate screws. If n tau was equal to mT, the symbol for the screw axis is n, the rank of the axis, with m as a subscript. So the pattern that we just drew here would be designated 3 subscript 1. And that's says automatically that the value of tau was equal to 1/3 of the translation that's parallel to the axis.

So the only other ones we have to consider besides 3 and 3 sub 1 is 3 sub 2, where tau would be equal to 2/3 of T. Let's see what that looks like by quickly drawing it out again using this dandy little unrolled cylinder device. Let's let this be my first motif. And I'll take this as the value of tau, two boxes up.

So I rotate, slide up by tau, rotate, slide up by tau, rotate, slide up by tau, and I'm back up here. And here is my translation. tau is equal to 2/3 of a translation. And my translation, then, should be equal to 3/2 times tau.

But this is supposed to be the translation. And there's nothing in this box. OK, this introduces another very important aspect of the patterns produced by screw axes. And it's sufficiently important we must use first the basic screw operation, A alpha tau and the translation in terms of which we have defined tau.

So use the spiral that you have defined by stating A alpha tau is the basic operation. But then, don't quit. You're saying another thing, that tau is a certain fraction of a translation. And you have to use that translation to generate additional objects in the pattern.

So in this pattern that we've drawn here, this is supposed to be a translation. So I have to take this one and slide it up by T. I have to take this one and slide it up by T. I have to take this one and slide it down by T. So I'm using a different kind of shading to indicate the ones I produced by A alpha tau and the ones that I produced from that helix by using the translation, T.

So this is the final pattern. It has a basic screw operation that's equal to 2/3 of the translation. And it has a translation that's 3/2 of tau. So everything's fine. Yeah?

AUDIENCE: For the very top one where you have it colored in, [? should that stay ?] outside the box?

PROFESSOR: Yeah, well, it's supposed to be another row.

AUDIENCE: Shouldn't that be a box lower [INAUDIBLE]?

PROFESSOR: Yes, it should indeed. Thank you. When your nose is right in the middle of the thing, sometimes you don't notice that as readily as somebody in the audience. OK, so that's the pattern of 3 sub 2. And now, if we realize that we must use both the basic operation, A alpha tau, and translation to fill things in, it's clear that if we try to have tau greater than the translation, the translations, when we apply them, would give us a screw that had the possibility of being redefined in terms of a shorter tau.

OK, one thing that is apparent if you look at this pattern is that 3 sub 2 produces the same sort of helix but in an enantiomorphic sense. This one is a spiral that goes this way. And this one increases when we rotate in a clockwise fashion.

So are they distinct? Yeah, they really are because you can have both the left handed spiral and the right handed spiral together in the same space group. I don't remember whether that's true for the threefold screw axes or not. I'm not sure. I have to check that. Yes?

AUDIENCE: So really [INAUDIBLE] enantiomorphic because they're all left handed. So it's just minus 1, isn't it?

PROFESSOR: Good for you. I was about to make that point. The sense of the spiral is enantiomorphic in the sense that this one is a right handed spiral. This one is a left handed spiral. But they're not truly enantiomorphic patterns because if we start with a right handed motif, this one also has a right handed motif. So I should qualify that statement, which I was about to do. It's the sense of the spiral which is enantiomorphic. This is not to say that one has motifs of one chirality and the other one has to have the opposite chirality.

AUDIENCE: Couldn't you just [INAUDIBLE] being minus 1? Just [INAUDIBLE] minus 1?

PROFESSOR: Yeah, I could do that, I could do that. And remember that we can add or subtract a translation at will from tau. And if I took a full translation and subtracted it from 3 sub 1, I would get-- I get tau equal to minus 2. Nope, doesn't work that way.

AUDIENCE: [INAUDIBLE]?

PROFESSOR: Yeah, it's the same tau but in the opposite sense, yeah. OK, so what comes out of this is that there are three kinds of axes that involve a 120 degree rotation. Three, which we can view as 3 sub 0, 3 sub 1, 3 sub 2.

The symbols that are used for them now, we know and love the triangle that represents the locus of a threefold axis. Four 3 sub 1 and 3 sub 2, what one does is to extend the edges of the triangle. There's the streamers on the bike handle again.

And if you look down on the pattern and use a right handed spiral, then you extend the streamers, the edges of the triangle, that goes down into the board this way. And 3 sub 2 would-- if it was in the same pattern-- you would indicate by extending the opposite pair of the opposite set of edges.

AUDIENCE: So would they be different space groups? [INAUDIBLE]?

PROFESSOR: Yes, there is a P3 sub 1. And there is a P3 sub 2. And they are distinct space groups.

AUDIENCE: So how can you distinguish [INAUDIBLE]?

PROFESSOR: You would find out where the atoms sit. And in one case, the spiral would occur in a right handed fashion. And in the other one, from a left handed fashion. You can determine the position of the atoms unambiguously.

OK, let's do one that's more interesting where the rank of the rotation part of the operation is higher. And let's look at fourfold screw axes. So here, we would consider tau equal 0, tau equals 1/4 of a translation, tau equal to 2/4 of a translation, and tau equal to 3/4 of a translation.

So let's take our cylinder that was formerly wrapped around the rotation access, straighten it out. And I won't bother to draw the pattern for a fourfold access. But for a 4 sub1 1 screw axis, this would be tau. And that would be one, two, three, one quarter of a translation that's parallel to tau. Or conversely, so T is equal to 4 tau. Or conversely, how is equal to one quarter of the translation.

So start with a first motif, rotate 90 degrees, slide up by one quarter of the

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translation. Rotate and slide, rotate and slide. Now I've come full circle. Rotate and slide. So this, then, is the pattern for the screw axis that I'll label as 4 sub 1 by analogy to what I've done with threefold screw axes.

Over here, let me immediately jump to 4 sub 3. I'm going to have to be a little more stingy with the spacing of my boxes or I'm going to run out of room. So if this is 4 sub 3, turns out that tau should be equal to 3/4 of a translation. And conversely, the translation should equal to 4/3 of tau. So that's the situation that I would obtain if one, two, three boxes gives me the length of tau and four boxes give me the length of the translation.

OK, so again I'll use different sorts of shading to indicate which way I have gotten this. I would rotate 90 degrees. I would jump up one, two, three boxes. So here's the next one. Rotate, one, two, three boxes up brings me to here. Rotate, one, two, three boxes brings me up to here. Rotating again, sliding up three boxes brings me to here.

OK, so there's the basic helix. And how is indeed equal to 4/3 of the translation. But I can't quit yet. I've used the basic operation, A alpha tau. Now, I've got to fill in with translation. And according to my rule, the translation should be equal to 4/3 of-- I'm sorry, this should be the translation is 4/3 of tau. So this should be the translation running up one, two, three, four boxes.

So that's-- I'll use a different shading here. That would fill in one here. One, two, three, four boxes up brings me to here. One, two, three, four boxes up would bring me to here. Go down by four-- one, two, three, four-- brings me to here. And let me use still a different shading here. One, two, three, four brings me down to here.

Filling in quickly, one, two, three, four. Another one would sit here. One, two, three, four, another one would sit here. One, two, three, four, another one would sit here. And you can see what is happening here, that 4 sub 3 looks exactly like 4 sub 1 but in the opposite sense. So it's the same relation as between 3 sub 1 and 3 sub 2.

What do we use as symbols? This is a 4 sub 1 screw. And again, if we look down on

the pattern from the top, use a right handed rule and extend every edge of the square, that would be the symbol for 4 sub 1. 4 sub 3 is the same sort of spiral, but in the opposite direction. So we will, with a right handed rule and going between neighboring closest motifs, we would extend this, extend this, and extend this. So that's the symbol for 4 sub 3.

With that, we come back over to here. And that is everything except 4 sub 2. And again, I'll mark up a cylinder that's been split into quadrants, draw reference horizontal lines. This is 4 sub 2. And we define this as tau.

Then, the translation, this should be equal to 1/4 of the translation parallel to the axis. And conversely, the translation should be four halves. So let's draw the pattern.

This was the first one. Rotate, slide up by tau. This is the next one. Rotate and slide, rotate and slide. Rotate and slide begin, rotate and slide. So this turns out to be the nature of the helix that is produced by A pi over 2 tau.

But this is not yet a pattern that has the translational periodicity that I have claimed. That's supposed to be the translation, twice tau, up to here. So I would have two slide this one up to here. I'd have to slide this one up to here. I'd have to slide this one up to here. And something's wrong here-- one, two, three, four. I think I went too far up for one of them. This one was one, two, three. This one, I went up too far. I skipped one. What did I do wrong?

AUDIENCE: You did the rotation wrong.

PROFESSOR: Hm?

AUDIENCE: The two [INAUDIBLE].

PROFESSOR: OK, let me do this all over again. Again, I can't see standing right on top of it. It's not a very good attempt to make it look easy. Let's split this up into four quadrants.

If this one comes out quite differently, I'll make sure I have it right. So this is my translation, one, two, three. This is the translation. And that should be equal to four

halves of tau. So this, then, is my value of tau. It should go up two boxes to here.

And that should be equal to 1/2 of T. So I want to rotate, slide up two boxes, rotate, slide up two boxes, rotate, slide up two boxes, rotate, slide up two boxes, rotate, and slide up two boxes. And now, I have to fill in with translation. So I will take this one and go up one, two, three, four translations. That's what I did wrong.

I'll take this one and go down one, two, three, four translations. Take this one and go up one, two, three, four translations. Take this one and go one, two, three, four translations. Take this one and go one, two, three, four translations. And now, lo and behold, what I have is one, two, three, four.

Curious sort of thing-- I have two motifs at every level. And they are 180 degrees apart. So a 4 sub 2 screw axis produces a pattern that looks like this. Pair of motifs like this 180 degrees apart, pair of motifs skewed by 90 degrees to that pair, another pair translationally equivalent to the first.

But what is the chirality of this spiral? 3 sub 1 was right handed. 4 sub 1 was right handed. 4 sub 3 was left handed. 4 sub 2 was right in the middle. Is that right handed or left handed?

The answer is it's both. It's both. There's one spiral that goes up this way. And there's another spiral that goes up in the opposite sense. So it's both. It's a left handed spiral and a right handed spiral together in the same pattern.

And the pattern for this screw axis, the symbol for this screw axis if it occurs in a pattern, is every other edge of the square extended. Which do you extend? Well, it really doesn't matter because it's both left handed and right handed simultaneously. So you can use either one. Yes, a couple questions?

AUDIENCE: Can you explain why you explain you did that shading?

PROFESSOR: I just wanted to differentiate the ones that I used. They're all the same. And where they come from doesn't affect what the basic pattern looks like. But I tried to make clear which ones I got by using the operation A alpha tau.

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And for 4 sub 2, which I just did twice, once correctly and once incorrectly, these with shading were produced by the operation of rotating and sliding up by 1/2 of the translation. The other ones, the ones for which I used this shading, I filled in by using what the translation was, namely twice tau. So it's just a way of keeping track of what operations I used to produce everything that's in the pattern. And for 4 sub 3, I had to use three kinds of shading. Yes, sir?

AUDIENCE: Should I [INAUDIBLE] the fact that this was actually two superimposed twofold axis separated by 1/2 T?

PROFESSOR: Yes, you could read that into it. And you would be very observant because a 4 sub 2 screw axis contains a twofold rotation as a subgroup.

AUDIENCE: [INAUDIBLE].

PROFESSOR: And since you were shrewd enough to deduce this-- we ask the question with glide planes when we're dealing with two dimensional plane groups. Is a glide plane a candidate location for a special position? In other words, if I move the atom directly onto a glide plane, is there coalescence?

The answer was no. Suppose I asked the same question now of a screw axis. Is a screw axis a candidate location for a special position? The answer is sometimes yes, sometimes no.

AUDIENCE: Well, only if you have [INAUDIBLE].

PROFESSOR: Yeah, so actually if I move the atom, the first atom, onto the locus of the rotation part of the operation, I get pairwise coalescence. And instead of getting all of these, I'll have just a string of single atoms separated by half a translation, half as many. So that's a special position. I don't get the full number out when I throw one into the space group.

Now, there are an infinite number of screw axes. My old friend, the saguaro cactus, which has a 19 to maybe 23-fold rotational component to its symmetry, does not, if I look at it carefully, have the same thing on every one of these ribs because the tufts

of spines spiral up like this. So a saguaro cactus, if I take the spines into account, doesn't have 22-fold rotational symmetry. It has some sort of 22-fold screw axis. And I've never been determined enough to risk puncturing my finger by going down around a saguaro and seeing if there's some other tuft at the same level and whether it's a 22 subscript 3 or 22 subscript 2 screw axis. But a saguaro cactus does have a screw axis as its symmetry element.

OK, let us generalize on the basis of what we've done so far. For any screw axis whatsoever, crystallographic or not, we will have an n sub 1 screw, an n sub 2 screw, where tau is equal to 1 nth of a translation, tau equal to 2 nths of a translation. And we will go all the way up n sub n minus 1, n sub n minus 2.

And always, regardless of n, the ones at either end tend to be spirals in an enantiomorphic sense. And n sub 2 and an n sub n minus 2 are spirals.

If you end up with an odd one in the middle, this has no chirality to the spiral. There's a left handed one and a right handed one. On the other hand, for something like two and four and six, the ones at opposite ends of the series are enantiomorphs in the sense of the rotation. For any six-fold screw axis-- and I will pass out the nature of the pattern without taking time to draw it-- 6 sub 1 and 6 sub 5 are enantiomorphous.

6 sub 2 and 6 sub 4 are enantiomorphous. And 6 sub 3 stands alone. 6 sub 3 consists of a pattern of three objects on a triangle pointing in one sense, three on a triangle pointing in the opposite sense. This is the value of tau. And that is equal to 3/6 of the translation. So no left handed or right handed sense.

6 sub 2 consist of pairs of objects separated by 60 degrees. 6 sub 4, exactly the same pairs, but they go in the opposite sense. 6 sub 1 is just a single spiral going up with atoms at intervals of 1/6 of the translation. 6 sub 5, a spiral in the opposite sense.

OK, with that, let me pass out a sheet that has patterns done in a decent fashion for all of the crystallographic screw axes. Bear in mind that there are fascinating,

interesting, and intriguing patterns for non-crystallographic screw axes. And let me say a few words about the symbol used in the space group for glide planes.

Any questions on this, by the way? I don't want to have beat it into the ground. Yes?

AUDIENCE: I have a question on symbols. How do you know which way the arrows point on the triangle or the squares?

PROFESSOR: Oh, here?

AUDIENCE: Yeah.

PROFESSOR: OK. Probably the best thing to do is to look at the patterns that I just passed around if you got one yet. If you look at 3 sub 1 and look down on it from the top and indicate the sense of rotation that gets you from the one above to the one that's directly below, your hand will curl around in a clockwise fashion. And the little tails on the symbol for the threefold axis trail out behind the way in which you're rotating.

If you look at 3 sub 2 and look down on it, you would have to, using your right hand, rotate in a counterclockwise sense. And therefore, the streamers go out again in the opposite direction. Same for 4 sub 1. There, every edge of the square is enclosed. If you look at how you have to rotate to get from the one on top to the one immediately below using your right hand, again, you have to rotate in a clockwise sense. And therefore, the edges that are elongated trail out in the opposite direction.

And finally, drawn in a decent fashion are 6 sub 1, 6 sub 5, which are spirals in the opposite sense. 6 sub 2, 6 sub 4, pairs of things at each level. And the level is 1/3 of the translation. 6 sub 3, triangles of objects at intervals that are equal to 1/2 of T, 3/6 of T. OK, does that answer? That is really a convention of some higher order. But nevertheless, it is a convention and it is consistent. Other questions about screw axes? Yeah?

AUDIENCE: So in nature, is there a difference between the right handed screw [INAUDIBLE]?

PROFESSOR: That's like asking is there something like a Coriolis effect in crystals. You know the

Coriolis effect that if you're in the southern hemisphere, the water gurgles down the drain one direction. If you're in the northern hemisphere, the opposite direction?

There was actually a very famous scientist, what was his name? I think it was Serret. Serret, so famous I can't think of his name. I remembers his name, Serret He developed a very famous theorem in kinetics, and that was thermal migration, migration driven not by a chemical potential gradient but by a temperature gradient.

And it's very difficult to measure. And only recently have people been testing that theory and making measurements. He asked this very same question. And he said, I think it was potassium chlorate that he looked at which has no mirror plane or inversion in it. So it occurs in left handed and right handed forms.

He asked, is there something like a Coriolis effect that would give you more right handed crystals in the northern hemisphere and more left handed crystals in the southern hemisphere? So what he'd do, he drew a lot of crystals. And he started counting. And he counted, and he counted, and counted. And he couldn't tell if there was a difference. And counted, counted, counted. And still, after lots and lots of counting, still could not get a result that was statistically significant.

And he went nuts. Sorry to tell you this. So I think it remains to be seen whether there is indeed a Coriolis effect in crystal shapes. And that's true. It's tragic. We're all laughing at the poor guy. But he actually just couldn't stand it. He counted so many crystals, poof! That's a true, unfortunate story. No, I don't think there is any difference between left handed crystals or right handed crystals.

Remember my story about sugar and its chirality and the little bugs that can only eat one chirality. Other questions of the less frivolous nature? That was not frivolous. That was a good question. OK, well let's say a little bit about glide planes and how they appear in space groups.

Things were very easy in two dimensions because the glide plane was a glide line. And everything had to be confined to a two dimensional space. So we used a solid line to indicate a mirror plane, the locus of the operation, sigma. And we use a

dashed line to indicate the locus of an operation, sigma tau. And tau was in the direction of the dashes.

Well, I've given it all away with the little diagram that I passed around. Things are much more complicated in three dimensions. If this is the locus of a glide plane and this is the direction of tau in a space group, we could be looking at that glide plane in a total of four different ways.

We could be looking at the glide plane from the side, edge on, and perpendicular to tau. We could be looking at the glide plane edge on and along the direction of tau. Or we could be between these two orientations and looking at the glide plane edge on but in between normal to tau and parallel to tau. And finally, we could look at the glide plane down from the top.

If we view the glide plane from above, for example suppose we have a monoclinic crystal and we put a glide plane in the base of the cell which has tau in this direction, the way you indicate that is with a little chevron off to the side. And if this is the direction of tau, you put a little barb on the chevron that indicates the direction of tau.

So the three possibilities for a monoclinic crystal is that how could be this way, in which case you use a chevron like this. Or how could be in this direction. And then, you use a chevron with a barb attached like this. Or how could be a diagonal glide, in which case the atoms would be up and opposite chirality and down and back up again. In that case, you add a little barb in between the two directions to indicate the direction of tau.

We put some labels on this, this a and this b. This situation would be a tau that is equal to 1/2 of b. In this case, how would be equal to 1/2 of a. In this case, how would be equal to 1/2 of a plus b.

This is designated as a b glide. And rather than having the symbol n appear in the symbol for the space group, a b would appear. This is an a glide. And the a would appear in the symbol. And this is a diagonal glide. And that, for reasons that I have

never found anyone able to explain to me, is called an n glide. I know of no language in which the word for diagonal begins with an n. But that's what it's called.

Now, those same glides can be viewed from directions that are parallel to the plane of the glide plane. Looking normal to tau is exactly the same situation we had in plane groups. So one uses the dash.

If you're looking along the glide plane end on but in the direction of tau, you use a dotted line. It's easy to keep straight which is which. If there's a little arrow in there and you look at it from the side, you see a line segment. If you look at it from the end, you see a dot. So it's easy to remember this convention.

If you're neither perpendicular to nor parallel to the glide plane, you just mix the two symbols. So you use a dashed dot line. So those are the symbols for glide. Glide plane is something like a piece of wood. It's got grain to it. The direction of the grain is the direction of tau, if you'd like.

All right, in the hand out, I give you some examples of the way in which a pattern of objects that has glide in it would be interpreted in terms of a geometric symbol. At the bottom right of the page, the left hand diagram has atoms related by a glide plane in the base of the cell where tau is running left to right. And so you have a chevron with an arrow on the right hand branch.

If you have atoms alternately left handed, right handed at a level and 1/2 plus that elevation, then you're looking at a glide plane edge on and down along the direction of tau. So you would indicate the locus of that glide plane by a series of dots.

What other type of glide plane is possible, not for monoclinic, but for lattices that have a centered lattice point in the middle of the cell? So this takes a special type of Bravais lattice. And this would be a lattice, for example, that had lattice points at the corners of the cell and another lattice point in the middle of the cell. One face of the cell is centered.

Then, you have not only translations a, b, and a plus b, which can serve as directions for glide. But you have another translation that is not present in the

primitive lattice. And this is 1/2 of a plus 1/2 of b. And if that's a translation, you could have a glide plane parallel to the base of the cell and have tau equal to 1/2 of 1/2 of a plus b, namely have this little vector in here be tau.

And the symbol for that kind of glide is d. And I do know what that stands for. That stands for a diamond glide because diamond, one of the very simple structures for an element or any compound and one of the early structures to be determined experimentally, does have a d glide in it. So the name of the compound, diamond, gave its name to the type of glide plane.

OK, I've got still 10 more minutes. What I would like to do next is to look at some of the other monoclinic space groups and also examine the way in which this information is presented for you in the international tables. So I've got a big, fat pack of material that shows you all of the monoclinic space group, that is the space groups derived from point group two, the space groups with point group m, and the space groups with point group 2/m.

And we've done a few of these. But what we haven't looked at is the Shcoenflies notation for the result or the way in which this information is presented in the international tables. To introduce you to these gradually, this is the monoclinic space group-- these are the monoclinic space groups as presented in the old international tables for x-ray crystallography.

A little bit later, I will pass out to you a few higher symmetry space groups that are represented in both the old international tables and the new international tables. And as I indicated somewhat disparagingly earlier on, there is so much information in the new version that they're very, very hard to use.

But OK, if you open the hand out, you find space group P2. So that's a twofold axis added to a primitive monoclinic axis. You see on the left hand page this situation, this ridiculous situation, that exists only for monoclinic crystals the first setting, where the axes are a on the left hand side running down, and b on the top running from left to right, and c coming straight up out of the page.

And the second setting, where the unique axis is b, and that means if you're going to draw the space group with c coming up, a down, and b to the right, b now is the direction of the twofold axis. So the diagram looks completely different. But it's the same space group except that the first setting is tilted on its side so that a comes down, b is from left to right, and c, which is now not a direction of the twofold axis, comes out.

So there's some jargon here, that geometric jargon. The atoms occur at different elevations. So in these two cases, the atoms occur only at elevations plus z or minus z. And you see next to the little circles that represent the symmetry equivalent positions for the general position a plus. And that means elevation plus z.

And for the first setting, all the atoms occur at an elevation plus z for the general position. For the second setting in the right hand diagram, you're looking at the twofold axis from the side. And therefore, one atom is at plus z. The one that's related by symmetry gets rotated down to minus z. So you see a little plus next to one atom, a little minus next to the next to it.

We need a symbol for a view down along the locus of a twofold axis. And that's the little pointed oval that we became familiar with with the plane groups. When you're looking at the twofold axis from the side, how are you going to indicate that? Well, the convention is to use an arrow. And that's what you see on the right hand side for the second setting of P2.

If this were not a twofold axis but a 2 sub 1 screw axis, it would be a one-sided barb. So looking down at these two axes with rotations of 180 degrees, this is the symbol for two viewed from the side. And a one-sided barb would be the symbol for a 2 sub 1 screw axis. Mercifully, these are the only screw axes that need to be depicted in a view from the side. So there's no standard symbol for a sixfold access or a fourfold axis looked at from the side.

In boldface, in the outer corner of these pages, you see the international symbol, which is what we used for the plane groups, the symbol for the lattice type, primitive, except now we use uppercase symbols for the lattice type to distinguish the space

groups from the plane groups. Underneath it, you see a C2 superscript 1. This is the Schoenflies symbol. You'll recognize C2 as the Schoenflies symbol for a twofold axis.

Schoenflies' symbol for the space group was to add a superscript, namely the first one that old [? Artur ?] got, the second one that [? Artur ?] got from this point group, the third one he got from the point group, and so on. So it's pretty much an arbitrary order, except he starts with, as you'll see, a twofold access, then replaces the twofold axis with a screw access.

So if you turn to the next page, you see symbols for not twofold axes, but 2 sub 1 screw axes along the edges of the cell. You see now a different sort of symbol alongside the atoms. There's one at plus z. That's the representative one at x, y, z. If you repeat it by a screw rotation, you rotate it 180 degrees and slide it up by 1/2 of [? c. ?] So you see the symbol 1/2 plus. So plus is plus z. 1/2 plus is 1/2 plus z.

Over to the second settings, trying not to sneer too vigorously, you'll see pointed barbs. That's the symbol for a twofold axis viewed from the side. And then, one of them is plus. The one that's a little long parallel to the 2 sub 1 screw axis goes to the other side and goes from plus z down to the minus z.

Let me ask you a question which people usually don't think about. If you look at the first setting and ask, what are the lengths of the translations? That's a. And that's so many angstroms. And that's b. That's so many angstroms. If I ask you that for the second setting, the answer is a little trickier.

What is the length of this translation? That's b. What is the length of this translation? I'm sorry, that's c. And this translation is a, right?

Wrong. That is no longer a. And the reason for that is that when you have a cell with non-orthogonal angles in it, let me indicate for the most general case for a triclinic crystal. So this is a. This is b. And then the third translation normal to that plane is c.

And if we have a structure with atoms in these locations and we want to project the structure along c, you do exactly that. You don't plop the atoms down onto the base

of the cell when you project it because if you did so, the atom that is up in the neighboring unit cell would come down to a different location. And you would not have a pattern that was periodic based on a lattice.

You get that only if, when you're projecting in an oblique lattice, you project along the translation. And then, and only then, can you end up with a pattern that looks like it has translational periodicity and really does. So if a cell is oblique, you do not project just by plopping the atoms down on the base of the cell. You project them parallel to the translation that extends up above the direction onto which you're projecting.

So if our cell in the second setting is monoclinic and this is a and this b and c comes up, if we look at that cell from the side as is done in the depiction on the right hand, then we let this be the direction of b. So that is b. But the thing that is at right angles to b is going to be a times the cosine of beta. And it's not a itself.

So this is a right angle. But this is not the lattice translation. It is the lattice translation times a trigonometric function. The triclinic case is a hairy beast. To calculate the length of these axes and projection, it's clear what they are. But to get these values involves alpha and beta and gamma. And it's a very, very complicated function.

AUDIENCE: So the angle between a and c in general is not 90 degrees in monoclinics?

PROFESSOR: The angle between depends on how you label your axes. For monoclinic, if you do the first setting, then by definition this is a, and this is b, and this is c. So these are always by definition 90 degrees.

If you use the second setting, then this is the direction of b. And this is the direction of a. And this is the direction of c. That keeps the system right handed. Then, this is a right angle and this is a general angle.

AUDIENCE: But all you're doing is taking that top one and just [? tilting it over ?].

PROFESSOR: No, I'm doing more than that because if there were a twofold axis, that would be the

direction of the twofold axis. Now, this is the direction of the twofold axis. The other thing that happens is the symbols for the glides change.

So if you look at space group number seven, which is a case where the mirror plane has been replaced by a b glide in the first setting, and that means the glide is perpendicular to the twofold axis. If the twofold axis is now the direction of b, the glide plane turns into a b glide.

But let's just thumb through them quickly. And then, we're actually two minutes past my promised quitting hour. First one, P2. Then, replace the twofold access by a 2 sub 1 screw. So that's Schoenflies symbol C2 superscript 2. Then, do this with centered lattices. The international table chooses to use a side centered cell. So that's the third one you can get from a twofold axis. So Schoenflies calls it C subscript 2 superscript 3.

And if you add that to a side centered lattice, you get screw axes interleaved between the twofold axes. Put it on its side, it stays C2 superscript 3 in the Schoenflies notation. But the side centered d become side centered c because it's b that comes out of the oblique net.

So the international symbol tells you exactly what you have. The Schoenflies symbol is arbitrary. It tells you the point group and it tells you the order in which Schoenflies derived them. But that non-informative nature to the symbol has a blessing. And that is it doesn't change with different labellings of a, b, and c. It doesn't change with a being shortest, b being shortest. It just sits there and its dumb, uninformative fashion. And that is nice. So both of them have survived.

OK, so could we get another space group out of this by replacing the twofold axis by a 2 sub 1? No, because we've already got 2 sub 1 screw axes in C2 superscript 3. So then, Schoenflies moves on and begins to work with symmetry planes.

So number six puts a mirror plane in the primitive monoclinic lattice. That becomes CS. That's the Schoenflies symbol for point group m. And it's the first thing you can get.

Another piece of convention for displaying the representative pattern of atoms, in the first setting, the two atoms sit directly above one another. So there are two new things here. A vertical line through the atom indicates that there are two of them that are superimposed in projection. And moreover, the little tadpole has appeared inside the frog eggs in the left hand part.

So this says on the right hand side of that split circle, the atom is at plus z. On the left hand side with the comment to indicate an enantiomorph is 1 at minus z that sits directly below the first one. And you'll notice in the diagram of the symmetry elements is a chevron working off the lower right hand corner of the cell. And that's the symbol for a mirror plane that's being viewed directly from above.

And then I'll just go a couple more. You could replace the mirror plane with a glide plane. And that's a b glide. Now, you can see the atoms going up at plus z, slide along by 1/2 z, and popped down to minus z, going down to an enantiomorph, so there's a comma inside the circle.

The chevron in the lower right hand corner of the diagram of symmetry elements now has acquired an arrow, a barb, that indicates the direction of tau. The second setting, again, flops the thing on its side so that you're looking now down along the b glide. And so you see a dotted line that indicates a glide plane viewed edge on in the direction of tau.

Then, you can put a mirror plane for number eight into a side centered b lattice. And that gives you another space group. And then, you can put a glide plane into the b lattice. And that, interestingly, gives you a different space group.

Number eight has an alternating mirror plane with an axial glide. Number nine has an alternating axial glide alternating with a diagonal glide-- two glide planes. Not a mirror plane and a glide, but two different kinds of glide planes. And then, you've used up all the tricks you can pull there.

So now, we take the last monoclinic point group, 2/m, drop it into a primitive lattice. Replace the twofold axis with a 2 sub 1 screw axis. That gives you P2 sub 1 over m.

Then, leave the twofold axis alone and leave the plane alone and put 2/m in a side centered cell. And then, replace the mirror plane by a glide. That's number 13. And then finally, the summa cum ultra, replace the twofold axis y a 2 sub 1 screw and replace the mirror plane with a glide, number 14. And then, do the same thing in a centered lattice.

So we get a total of 13 different space groups from two lousy kinds of lattices and three possible point groups. You get 13 different distinct space groups. OK, that's a quick overview.

Notice that just as was the case for the plane groups, the tables go on to list the way in which atoms are related by symmetry and the number per cell and the site symmetry just as in the plane groups. And the way a three dimensional structure is going to be described to you is exactly analogous to what we did with two dimensions. Magnesium in position 3b, symmetry 6/m, oxygen in position 12d, symmetry 1. And then, the tables give you the coordinates of all the symmetry S atoms.

OK, thank you for your patience. That was a long stretch in one shot. I'll say a little bit, very little, next Tuesday about the convention for orthorhombic space groups because there, no one direction is any more or less special than any other. So the symbol for the space group changes all over the place when the axes take on different lengths, relative lengths. But the symmetry is exactly the same. So we'll see you--