

PROFESSOR: That I know of that derives two-dimensional symmetries. And so, what I will give you instead is a set of notes-- nothing fancy, just handwritten-- but which will carry out each of the derivations in detail, so you'll have something to fall back on if it seems overly complicated. Any questions on what we've done to this point?

We've really set forth the ground rules and components of our final step. And that, as I mentioned earlier, is to combine one or more of these collections of symmetry elements around a fixed point in space, with one of the five two-dimensional lattices that can accommodate them.

And when we find a successful, feasible combination, we will have derived something that we could call the two-dimensional crystallographic space groups. These are collections of operations which really pick up everything-- the whole space-- move it, tumble it end over end, and throw it back down into coincidence with itself.

So hence the term space group, rather than point group, where it's only a point that's left invariant at worst. OK, so what we're going to do then is to take each of the point groups in turn, and combine each of them, when possible, with one of the five lattice types. And I remind you that those are the oblique lattice or parallelogram lattice.

And this was what was required by two and one, no symmetry at all. Then there was the primitive rectangular net, and the symmetry element that required that was a mirror plane, or we could have, depending on how the mirror plane was aligned relative to the translation, we could also have a lattice that was non-primitive, a double cell. And that was a centered rectangular net.

And either of those was compatible with a mirror plane. Then we had a square cell-- square net or square cell-- and that was what was required by a 4-fold axis. And then the hexagonal net, and that could be required by either a 3-fold or a 6-fold.

Well, if you add up the number of point groups that we've listed here, there are only six, but there are 10 crystallographic point groups. So what about the ones that we have not yet considered adding to a lattice, and these are the nets of the form Cnv . So let's consider, in turn, each of those point groups and see what they would require of the lattice that could accommodate them.

But let's do 2MM first. 2MM, the 2 is compatible with an oblique net. The mirror plane wants either a rectangular net or a centered rectangular net. So all we can do is to add this to a rectangular or centered rectangular net. Let's put a 2-fold axis at the lattice point. The mirror plane has to be aligned along the edge of a rectangular net.

If there are two of them, you just put one along each of the edges of the rectangular net. A mirror plane in a net could either go in like this, or could go, for the centered net, in like this. So what we're saying, 2-fold doesn't care, add a mirror plane, it means that the parallelogram has to become a rectangle.

You can put the two mirror planes of 2MM in along the two edges of the rectangle, or do this equally well with a centered rectangular net, put the mirror plane in parallel to the edges, just like we did in CM, put the 2-fold axis in at the lattice points. So there's a lattice point at the corner, and also a lattice point in the middle of the cell.

So for the rectangular net, we could put in either M or 2MM in both of these rectangular nets, the primitive and the centered. 4-fold access requires that the net become still more specialized and have the shape of a square.

AUDIENCE: Professor?

PROFESSOR: Hmm?

AUDIENCE: We can't see on this side.

PROFESSOR: Oh, I'm sorry. I'll pace back and forth, which I usually do. Then everybody will get equal time. OK, so I'm glad you spoke up. 4-fold axis requires a square net. There

are two mirror planes, 45 degrees apart, and those mirror planes have to be along the edges of a rectangular net.

Put one of them in this orientation, and that surely is along the edge of a rectangular net, along the edge of a net that's not only rectangular but square. But it has a higher symmetry, and that's fine. Looks as though this diagonal mirror plane might cause troubles, but let's note that if we look at the diagonal translations in this lattice, that they will define a centered rectangular net, so putting the other mirror plane in this way puts it along the edge of a centered rectangular net.

So this mirror plane is perfectly happy as well. So in the square lattice we could pop either symmetry 4 or 4MM. 3-fold is an interesting one. That's the odd symmetry that does strange things. Here is a hexagonal net, and that's what a 3-fold axis requires. Two translations, identical in magnitude, and in terms of what goes on along them, in exactly 120 degrees apart.

Now, I don't readily see any rectangle along the edge of which I could align the mirror plane in 3M. But it's the oblique shape of this net that throws you off. Let's notice that if I draw several unit cells side by side, here is a double cell that has a rectangular shape. OK? Take $2T_1$ plus T_2 as one edge of the cell, and leave the other one as T_2 , and we have defined a cell where that is identically a 90-degree angle.

So one of the mirror planes of 3M could go in this orientation, and the other one would be 30 degrees away. So this would be the orientation of the two mirror planes. So we're putting in 3M with M perpendicular to the translations that define the primitive hexagonal cell, T_1 and T_2 .

But there's another way you can do it. Let me draw the same net, the same hexagonal net, and look at a different kind of double cell. OK, here's my hexagonal net, two translations, T_1 and T_2 , with a 3-fold axis at the lattice point. And now I will again draw a couple of extra cells-- double T_1 , and let's double T_2 .

And then let me point out that I can put in the mirror plane this way and along this

way, and here is a double cell, and I can put the mirror plane along this direction and this direction. So this is crazy. This is the same lattice and the same point group, but there are two different ways I can align the point group in the lattice.

I can put the mirror plane in such that it's perpendicular to a cell edge, or put the mirror plane in 30 degrees away from that orientation such that it is along the edge of a centric rectangular net. So I could add 3M as well with the mirror plane aligned parallel to the translations in the net. So lots of funny permutations here.

Here I have one symmetry element, two different lattices that I can combine with it. Here I have one point group, 3M, but two different ways in which I can set it relative to the edges of the cell. Yes?

AUDIENCE: Why are you putting two mirror planes in each of those figures when you really only could do one mirror plane?

PROFESSOR: Actually, I need-- well, there are going to be a radiating sheaf of mirror lines coming out of that 3-fold axis.

AUDIENCE: An angle of 60 degrees.

PROFESSOR: They are at an angle of 60 degrees. It has to be 60 degrees, and that is indeed what I have here. I've just drawn part of 3M, and if I draw the remaining mirror planes, they would do this. OK, I think that's fairly intelligible. Another reason for notes is to draw these diagrams when they're reasonably complex.

On a blackboard, when you're rushing to get through it, is something that's easier said than done, even though you may have done it a number of times. So there is the job that we've laid out for ourselves. Five lattices, 10 point groups, and we can drop each of the point groups into one or more of the lattices of the five that we have determined.

As soon as we combine things, we're going to have the situation that we've encountered before. In general, if I have an operation number one that produces one transformation of coordinates, and combine it with an operation number two

which has another change of coordinates, there must automatically arise some third operation.

And we can write it in terms of the language of operators by saying operation number one followed by operation number two is equivalent to an operation number three. And in terms of the pattern, this says that whenever you throw two symmetry transformations together, a third one pops up. You can't push it down. It's going to be there once you add the first two combinations.

You may have to be really clever to see where it is and what it is, but it's going to be there. It's going to be there. It comes in automatically. So this general class of statement, this equality in operations, is something that I like to call, for short, a combination theorem.

And we've seen several examples of this already, notably the one in the last hour that said whenever you combine two mirror lines at an angle μ , you automatically create, like it or not, a rotation operation of a 2μ . So as soon as we start making these combinations, we're going to find a new operation arising.

So let's start with the simplest one. Add a 1-fold axis to a general oblique net. So there is T1, there is T2, we don't put anything in it, it's just a simple array of translations with lattice points that we can put at the terminal point of these translations. There's no symmetry. If we put in one atom, that atom hangs on every lattice point, and that's all there is to it.

It's so simple it's not only uninteresting, it's ugly. It's just a simple atom arranged in a periodic array. As with everything we've done so far, it's convenient to have a notation to indicate which particular plane group one has, and the symbol here is to give side by side the type of lattice as the first part of the symbol, and then the point group that you have added.

So what do we have here? We've taken a primitive oblique lattice, and we've added no symmetry at all, a 1-fold axis. And here people who have derived symmetry theory assume that the reader knows something. And so you're going to get a lot of

respect when you show your colleagues that you know what this notation means.

All you have to do, if you know the symmetry, is to state whether the lattice is primitive, as it has to be for an oblique net, or whether it's centered, in the case of the rectangular net. Three dimensions is a lot more complicated. If the lattice is cubic, it could be primitive, it could be face-centered, it could be body-centered.

So you need a symbol that tells the type of lattice. In this case it's primitive, and the point group that we've added is 1, so this rather boring ugly thing here is called P1. Another bit of code. We're going to do eventually the same thing in three dimensions. We're going to take just a general oblique three-dimensional lattice, and not adorn it with any sort of symmetry at all, and that will also be called P1.

But to distinguish the two, capital P1 means a three-dimensional lattice, and we won't be working with those for a while. We haven't even enumerated them. A lowercase p, that is the symbol for a two-dimensional net. In other words, a plane group rather than a space group. So here's the first, P1, and it really doesn't give shivers running up and down my spine to look at it.

So let's do one that's a little more interesting. Let's take a 2-fold axis and combine it first with a primitive rectangular net. I'm sorry, what am I saying? I want an oblique net. So the symbol-- and I'm assuming this is going to be unique, and we haven't seen anything with a 2-fold axis in it, so it is.

So this would be P for a primitive lattice, 2 for the symmetry that you've added to the lattice. And since you are all cognoscenti, I don't have to tell you it's an oblique lattice, because you know, don't you, deep down in your heart, that a 2-fold axis requires only that the lattice be an oblique lattice. Nothing special is required.

So what we will do is to take this general oblique lattice with two translations, T1 and T2, and to this-- remember, we don't deal with symmetry elements. We have to do this operation by operation. So what we're doing is taking the operation A_{π} , the only non-trivial operation contained in a 2-fold axis, and putting that in at a lattice point.

OK. Bells ring and whistles go off. We don't know what happens when we make this combination. And let me do this in more general terms, so we can derive the theorem once and for all. Here's a translation, and let me add to the end of that translation a rotation operation A_α . In this case, it would be the operation A_π .

What's the net result of rotating and then translating? That's a non-trivial question. So if I'm doing this for a general rotation of α , let me take a translation, and I'm going to make my construction in the following way, because I'm really clever. And I'm going to put this translation T at one half of α on one side of the perpendicular to T .

And then I'll let that rotation go to work. And it'll take the translation and move it to $\alpha/2$ on the other side of the perpendicular. And now I'll let the translation move to this rotated translation, and if it does so, it's going to move the translation over to here. Here's a motif hanging on this translation. It's rotated over to here, and then gets slid over to here.

This one is right-handed, this one is right-handed, this one is right-handed. How do I get from this one to this one? Only two ways, translation or rotation. If we rotate, about what point are we rotating? Now I'm going to use a definition which seemed trivial. I said, a symmetry element is the locus of points that is unmoved by the operation.

And if we decided, because these two motifs are not parallel to one another and have the same chirality, that the rotation-- has to be a rotation that relates the two. When asked finally the question, what point is left unmoved? Ha. It's this point where these two translations come together at a single point. That's the point that's left unmoved by rotating from here to here and then sliding over by the translation T .

And I can say exactly where that rotation is. It's going to be along the perpendicular bisector of my original translation. And where is it going to be located? This line makes an angle of $\alpha/2$ with respect to the perpendicular to T . So that angle is also $\alpha/2$.

This line and this line both make an angle of $\alpha/2$ relative to the normal to the translation, so this angle is also $\alpha/2$. And look how this has turned out. The combination of a rotation with a translation is another rotation, B , about a different point but through the same net amount α as the original translation.

On top of that, really to nail this down, where should we look? This distance in here is $T/2$, and the tangent of α is $T/2$ over this distance x . And if I just solve for that distance, x is equal to $T/2$ -- I'm sorry. I got this garbled. $T/2$ over x is equal to the tangent of α . That's what I wanted to do.

So if I solve for x , that distance x is $T/2$ over the tangent of α , and I can write that as $T/2$ times the cotangent of $\alpha/2$. So here it is, done properly at last. Go up a distance x along the perpendicular bisector of T , and you go up a distance $T/2$ times the cotangent of $\alpha/2$.

So this is a general result for any rotation operation. Combine a rotation operation A α with a perpendicular translation-- perpendicular to the rotation axis A -- and the result is a new rotation operation through the same angle, but at a different location. It's at a distance x , which is equal to $T/2$ times the cotangent of $\alpha/2$ along the perpendicular bisector of T .

So this is a general theorem. This is a fact of two-dimensional life that is always going to be true regardless of α . And the only constraint is that the translation has to be added perpendicular to the locus of the rotation axis, and that has to be the case in two dimensions, because the rotation axis has to always be normal to the space, the two-dimensional space.

In three dimensions, we'll have to generalize this to make the translation have arbitrary orientation relative to the rotation axis, but we've got enough to chew on at the moment. Yes.

AUDIENCE: [INAUDIBLE]

PROFESSOR: The distance x is the distance up along the perpendicular bisector. I'm sorry. I said it

but I didn't write it in. OK? Let me go through it again since we've got everything on the board. We start with the original object, rotate it by α , and then we then further map it to a new location by the translation T .

Both motifs are right-handed, but they're not parallel, so therefore, they have to be related by a rotation. If we ask what is the locus about which this location has occurred, we use the fact that the locus of a rotation axis is the only point that's left unmoved by the net transformation, and the place where this translation intersects the translation that has been shifted over by T is a point that sits up along the perpendicular bisector of the translation by a distance T over 2 times the cotangent of α over 2.

So that's in the abstract. Let's now look at a particular application of this to our addition of a 2-fold rotation to a translation. So here's the translation T . We're going to put a 2-fold axis and the only operation which it possesses, namely $A \pi$. And according to our theorem, up along the perpendicular bisector of T by distance x equals T over 2 times the cotangent of α over 2 should be a new operation $B \pi$.

So in this case, this would be T over 2 times the cotangent of π over 2. Cotangent of 90 degrees is 0. So this says that you go 0 of the way along the perpendicular bisector, which means you stay right at the midpoint of T . So this says that if you rotate through 180 degrees, follow that by this translation, you should find that the net effect is a rotation of π over 2 about this point.

Boggles the mind, but let's show that it works. Here is an initial point, initial motif number 1, and it is right-handed. We rotate by 180 degrees. Here's number 2, it stays right-handed, and I pick it up and I move it by this translation, and it moves from here to here. Here's number 3, it stayed right-handed, and the way I get from 1 to 3 in one shot is to rotate 180 degrees about the midpoint of the translation.

How about that? People are so astounded that they're stunned, except for the people who couldn't see what I was doing, and they're moving back and forth frantically trying to see what I wrote. I'll let you catch your breath, and then let's do this, use this to derive the two-dimensional space group, the plane group that

results when we add a 2-fold axis to an oblique net.

And it's turned out very simply, because if I've got the operation $B\pi$ here, that implies that I've got a 2-fold axis, because that's the only operation that exists within a 2-fold axis. So I'll start by putting in a 2-fold axis here. I'll combine $A\pi$ with this translation $T1$, I get a new rotation operation, $B\pi$, in the middle of this translation, so there's a new 2-fold axis there.

The 2-fold axis here hanging at this lattice point as well, and at these other lattice points. Combine the rotation $A\pi$ with this translation $T2$, I get a new operation, $B\pi$, sitting in the middle of this translation, so I've got all I need to say that there's a 2-fold axis there. That 2-fold axis will get translated down here by $T1$.

This 2-fold axis will be translated over to here by $T2$. Then the only other thing that I have to combine this translation with is the translation $T1$ plus $T2$, and that combined with $A\pi$ says I should have $B\pi$ in the middle of that translation as well, so I'll get another 2-fold axis in the middle of the cell. And that's it. We've got our first nontrivial two-dimensional space group.

And what do we call this? Confusing as hell, some might say, but crystallographers would say that it's a primitive lattice combined with a 2-fold axis, this is $P2$. I don't have to tell you that it's an oblique net, because you know that that is all that a 2-fold axis requires, that the net be oblique.

What does the pattern look like? I'll say another thing that's so simple, it takes a while for it to sink in. The pattern of a plane group is the pattern that is generated by the point group merely hung at every lattice point in the net. So if this is what a 2-fold axis does, relates a pair of motifs like this, a pattern for $P2$ is this pair hung at every lattice point.

So all of the objects are of the same chirality, all either left-handed or right-handed. I've got the same pair at every corner of the cell. And notice that these new symmetry elements that popped up just like what we found in the point groups, the new mirror planes that came arose as a consequence of the combination that we

had made.

And they were independent in most cases, 3M being the one case where they weren't. These additional three 2-fold axes are independent 2-fold axes. They're different kinds of 2-fold axes than the ones at the corner. Not only are they not equivalent by translation, but they do different things relative to the motifs that are in the pattern.

This 2-fold axis has a different relation relative to the two closest motifs than does this one, than does this one. They relate different objects pairwise in the pattern. And no two of these 2-fold axes describe the same pairwise relationship. So these are independent 2-fold axes.

Independent in the sense that they do different things relative to the motifs in the pattern, different in the sense that there is no other operation that throws this one into this one, and therefore, of necessity, would require that the pair about this 2-fold axis be the same as the pair about this 2-fold axis. OK. So there is a first nontrivial two-dimensional space group.

I should mention-- probably an obvious fact-- that this also has a cousin in three dimensions. If I just imagine all of these 2-fold axes extending out through space perpendicular to the plane of the blackboard, and take another translation that is also perpendicular to the blackboard, I would have the three-dimensional space group which has the same symbol except capital P, indicating that it's a space lattice.

So almost at no extra charge, we've done all the work to determine one of the three-dimensional space groups. Yes?

AUDIENCE: If you change the order of the combination of the translation rotation, do we get the same operation?

PROFESSOR: OK. That is a good question. I really meant to mention it earlier in connection with the point groups. Does interchange of the order of the operations in a combination change the result, or change, in other words, the symmetry element that is

equivalent to the net combination of the two? How many think yes, it does change?

AUDIENCE: Could you say that again?

PROFESSOR: OK, if we have two operations A and B, is operation A followed by B the same result as the operation B followed by A? Does the order make a difference? And how many say yes--

AUDIENCE: The order makes a difference?

PROFESSOR: The order does make a difference. How many say no? Well, this is one of these happy occasions where I can say you're all right. Sometimes yes, sometimes no. So let's ask when does it make a difference and when does it not. Let's look at one of our point groups.

Let me take a non-trivial point group. This would be point group 4MM. OK? So those are all mirror planes of two different kinds. And let me quickly sketch in the pattern. The pattern is just a pair of things hanging on the mirror plane, and that pair is rotated by 90 degrees.

OK. Suppose we look at the operation A π over 2, a 90-degree rotation in a counterclockwise direction, and let the other operation be σ_1 , this reflection plane here. Suppose we reflect and follow that by A π over 2. We reflect to here and then we rotate by 90 degrees, and that's going to give us the number 3 sitting up here. So we reflect it and then rotate it.

How about if we first rotate that same object by A π over 2 and follow it by σ_1 . So we'll rotate number 1 to here, so this is 2 prime, and you can see we're already in trouble. If we now reflect along σ_1 , this is 3 prime. So in one case we ended up here, in the other case we ended up here. So the order did make a difference.

Let us look at another example. Let's look at 2MM. So here's an operation σ_1 , here's an operation σ_2 , so let's first do σ_1 followed by A π . So here's object 1, reflect to here, and then we rotate by 180 degrees, and this is number 3.

Now let's do the operation A_{π} and follow it by σ_1 . So we'll take number 1 and rotate it up to here. So here's number 1 prime. And then we reflect by σ_1 , and 3 and 3 prime are exactly the same. So it didn't make a difference. So the answer is sometimes yes, sometimes no, which is interesting, but even more interesting is how can you tell? Yeah, you have a question?

AUDIENCE: In that first identity you drew--

PROFESSOR: Yep.

AUDIENCE: The right side, it seems like your commas are drawn backwards and that just affects--

PROFESSOR: Could be. Mm, no, they're-- ah, these are drawn backwards. They should all have their tails pointing in. No, it doesn't work, actually, because even if I screwed up on the orientation, the positions are different. Again, first time I reflected, and then rotated, so this is 3. If I rotate and then reflect, I'm way over here.

So this is one location, this is another location, and even if I screwed up by having the tails pointed the wrong orientation, still not the same. But here, clearly, reflecting and rotating is the same as rotating and reflecting. I end up in the same place. So how can you tell?

It's a very difficult thing to prove that this is the case, but you can interchange the order of operations when the two symmetry operations that are involved leave each other untransformed. And if the two symmetry operations move one another, then changing the order changes the net result.

It doesn't change the nature of the operation, but it does change the locus about which it operates. Let me show you what I mean. Here's $2MM$. The 2-fold axis takes this mirror plane, turns it upside down. It takes this mirror plane and flips it over. The mirror plane is left unchanged in both cases.

The mirror plane has the 2-fold axis sitting right on it, so it doesn't change the location of the 2-fold axis when it acts on it. And similarly, this mirror plane takes this

mirror plane and reflects it, and it doesn't change anything. So all of these operations-- the three independent operations, σ_1 , σ_2 , and A_{π} -- all leave their locus of operation unchanged.

Whereas that, clearly, is not the same for a 4-fold axis and a mirror plane. The mirror plane, when it acts on the 4-fold axis, leaves it unchanged, but the 4-fold axis, when it acts on the mirror plane, moves it into a new, entirely different location. And when that is the case, the order does make a difference.

So I can take that corny joke of the mathematicians, what is purple and commutes? An Abelian grape. I can say, what is purple and commutes? It's a purple 4-fold axis in a mirror plane, a purple 4MM. OK, what other aspect of the plane groups and three dimensional space groups is an analytic representation of the way the plane group maps atoms around?

And I see that it is five of the hour, so let me just make one final statement to indicate what I'm going to talk about next time. Here's the arrangement of 2-fold axes, and if you have an atom sitting in here, and this is T1 and T2, and we use this as the basis of a coordinate system, so this atom sits at a location x along T1 and y along T2.

And then they ask, what other atoms are related to it? Well, that 2-fold axis will move x to minus x , and move y to minus y , and those are the only two atoms I get. So a characteristic of this plane group, if I were describing to you a crystal structure which had this symmetry, I might say something like a lithium in a position with coordinates xy , and therefore minus x minus y would also have to occur.

I have an oxygen at a different number, x' y' , and that must then also occur at minus x' minus y' . And it looks as though any time you throw in an atom at a location xy , you get a symmetry related companion to it with negative coordinates. And this is what is called the general position of the space group.

There's nothing special about it, and you put in an atom here, you get another atom here. This is going to be a nice economical way of describing an atomic

arrangement, particularly if you realize that there are almost 150 atoms that appear in the unit cell for some of the cubic symmetries. Drop in one, wow, all hell breaks loose, 150 other ones.

But what you can do is codify the coordinates of all these symmetry-related atoms. And that is a great utility in describing crystal structures, because I only have to give you the coordinates of one representative atom. But this is not the only thing that happens. This is the general position because it's general relative to its location with respect to the symmetry elements.

If x and y were both 0, I would have one atom moving to the origin to coincide with the second one. And if I put one in at 0, 0, that's all I'm going to get. The 2-fold axis is just going to twirl it around, and the translation will repeat it to the other lattice points. So if I put in an atom at 0, 0, that's all I'm going to get.

And the same thing would occur for any of these four independent 2-fold axes. If I let x and y migrate to 0, $1/2$, this atom will join together with this atom, and I would get just one atom sitting there. So there's a position also of the form 0, $1/2$, and a position $1/2$, 0, and a position $1/2$, $1/2$ that are the location of these four distinct 2-fold axes.

OK, to have a shorthand way of referring to the general position in these positions, which are called special positions-- what's special about them is that they're right on top of a symmetry element, and whenever that happens, the number per cell is a sub-multiple of the number in the general position, because coalescence has occurred.

And so they're three independent 2-fold axes, so there are four locations where you get only one atom per cell rather than two. And then to give you a way of referring to these positions readily, they are labeled starting with the most specialized, just going through the alphabet, position a, position b, position c, position d, position e, which is the general position.

And then another piece of information that's almost trivial here, but is not for more

complicated symmetries, what's called the rank of the position, and that is the number that you get per cell, one per cell, one per cell, and for the general position you get two. So the rank of the position is just the number per cell.

And then, if it's a special position, the atom has to sit at a site of some symmetry, and in this case, the atoms all sit at 2-fold axes for the special position. The general position always has site symmetry 1 always. So that's the characteristics of the way in which this symmetry can move atoms around.

And this is of great utility in interpreting structures. For example, suppose our motif was not an individual atom, but was a molecule. And suppose you had one molecule per cell. That would tell you the molecule has to fit in a special position. And the special positions are all 2-fold axes.

So if the molecule has to sit on a 2-fold axis, the configuration of that molecule has to have at least a 2-fold symmetry, or else you can't fit in one per cell in this particular plane group. So you can use this information to determine structures.

I'm going to give you a problem a little bit later on when we get to three-dimensional crystallography, and I'm going to give you the magnitude of the cell edge and the density of rock salt. And from that, in 10 minutes, you can find out that there's only one possible structure for rock salt.

The Braggs fiddled around for the better part of a year doing x-ray experiments and trying to calculate what the intensities would be for different atomic positions. You, in another two weeks, can get the same answer in 10 minutes knowing only the lattice constant and the density and the space group.

So a lot of physical consequences of the nature of the structure, the confirmation of the molecule, the extent or absence of solid substitution of one species for another, can be dredged out of the properties of the space group.

OK, I've run 2 minutes over, but we took our break two minutes later, so let's call it a day and I shall see you on Thursday, hopefully armed with pictures so that I can personally present each one of you with your corrected problem sets.

