Symmetry and Structure in the Solid State
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Lecture – 53
Patterson Method 1

The symmetry that is required in a Patterson synthesis. As we have just seen that the Patterson is always centrosymmetric, it loses all the information on the translational components, which are associated with the space group. So, 2 1 screws is off, the glide planes are off, so the space group now will be the one which trips of all these translational components.

So, it is space group is 2 1, 2 1, 2 1 as we already mentioned is the corresponding Patterson symmetry will be p 2 by m, 2 by m, 2 by m abbreviated as p m m m. But as well as the centering is concerned, we see that the centering is still intact that means, if there is a c centered lattice c 2 2, 2 1, it is corresponding Patterson symmetry will be c 2 by m, 2 by m, 2 by m. So, the seen centering information is not lost with respect to the lattice that is with respect to the Bravais lattice. Bravais lattice information is maintained in the Patterson, the translational components symmetry is lost.

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Vitamin B_{12} (C_{63} H_{88} N_{14} O_{14} P Co. 8 H_2O was solved although Admittedly with great difficulty, using initial the phases from the Cobalt atom (Z^2 ratio = 0.17).

TABLE 12.1 Some Harker Lines and Planes

2-Fold axis ∥ *a*, *b*, *c*	$0vw$; $u0w$; $uv0$
2-Fold screw ∥ *a*, *b*, *c*	$\frac{1}{2}\,u\,w$; $u\,\frac{1}{2}\,w$; $u\,v\,\frac{1}{2}$
m plane ⊥ *a*, *b*, *c*,	$u00$; $0v0$; $00w$
a glide ⊥ *b*, *c*	$\frac{1}{2}\,v\,0$; $\frac{1}{2}\,0\,w$
b glide ⊥ *a*, *c*	$u\,\frac{1}{2}\,0$; $0\,\frac{1}{2}\,w$
c glide ⊥ *a*, *b*	$u\,0\,\frac{1}{2}$; $0\,v\,\frac{1}{2}$

However, Harker came up with a very nice suggestion that is to examine this Patterson maps very very carefully. When the Patterson maps are examined very carefully and one looks at projection as well as the axial regions of the vector map, since the vectors are redefining, now u, v, w is defined as x 1 minus x 2, y 1 minus y 2, z 1 minus z 2 the inter atomic vectors.

The property of the vectors will be in such a way that they will also follow the symmetry, because the Patterson as retained the symmetry. The only issue is now is there any way, we can find out whether the system was associated with a 2-fold screw or a 2-fold axis. So, if one looks at the projections of these Patterson map, so we can do a three-dimensional Patterson map and look at the projections of that along x, y and z.

So, if we put now a situation where we have the projection down the x axis, 0 v w, if one looks at 0 v w, the 2-fold axis is parallel to a, b and c. So, as a result we end up with what is known as a Harker plane. So, the Harker plane will have information about the 2-fold axis, there will be a peak corresponding to v and w in the projection down 0 that means, we now look at this plane 0 v w in the vector map, it will give us the solution for v and w for every atom in the Patterson.

And if there is a heavy atom, the u w coordinates of the heavy atom or embedded in the 0 v w, if we are looking down looking at a case where we have a 2-fold axis which is parallel to a. That means if the crystal system is p 2 let us say and the 2-fold axis is now parallel to a that means, we have now looking at the projection 0 v w. So, this is the vector map.

So, in the vector map v is y 1 minus y 2, w is z 1 minus z 2, but in the vector map if there is a 2-fold axis in the system. Let us take the example of p 2 2 2 2 in orthorhombic system, where we have 2-fold axis parallel to a, parallel to b and as well as parallel to c. In that case, we have three projections 0 v w; u 0 w; u v 0. So, all these three projections will give us the values of u and w corresponding to each inter atomic vector.

So, suppose there is a heavy atom in the structure the heavy atom in the structure will give rise to a very heavy peak and that particular heavy peak will correspond to v and w. And therefore, the when we do this projection of the Patterson map and then plot it up, we will see that there is a particular value of v and a particular of value of w with now satisfies the v w that should correspond to the heavy atom position.

So, we therefore get the solution to the two coordinates. So, we will get therefore v is y 1 minus y 2, w is z 1 minus z 2. So, we get information on not just the z 1 and z 2, we will also get information on y 1 and y 2 and this will be uniquely found. So, the projection plots will carry the symmetry information. So, if there is a 2-fold symmetry, the 2-fold symmetry information even though last on the main Patterson, it will be present on the 2-fold screw position corresponding to parallel to a, parallel to b, parallel to c we have these positions.

So, if we now look at the section half, you will get solutions for u and w. So, we will see that with examples as we go further, but essentially they Harker planes will now correspond to positions associated with either 2-fold or 2-fold axis or any other axis, which are now with respect to the Patterson, they have a projection possibility that means, 3–fold axis is possible, 4–fold axis is possible and so on and along with the screws. So, where did I have given only the 2-fold example here for our; for making it simple, so what is done is we if we now have this system p 2 2 2 here, we look at these three projections and we get solutions for u w, u v w, u w and u v. So, if the system is p 2 2 2, then there are 2 2-fold axis perpendicular to each other just as an example.

Then we have the coordinate the solution for v and w for the heavy atom position, it will be very large value u and w for the heavy atom position and u and v for the heavy atom position. So, you see that between the three projections, between these two u is common, between these two w is common and between 1 and 3 v is common. So, we get a unique solution for u, v, w. One once we have u, v, w; then it is in principal possible to get the coordinates of the heavy atom.

So, the heavy atom presence will be easily identified by looking at these projections and also the identity associated with the symmetry information. So, even though symmetry is not there in the main Patterson, the overall Patterson; the projection reflections carry and information associated with the translational component. So, if there is a 2-fold, we have to examine the sections passing through x, y and z at half, half, half.

So, take for example 2 1, 2 1, 2 1 you will uniquely solve for u, v and w, because you look at these three now projections and you get solutions for u, v and w. So, if there is a heavy atom, then the heavy atom position in terms of u, v, w vectors is possible to be found. So, therefore, this gives the examination of Harker planes therefore, gives us an opportunity to identify, where the heavy atoms are. And also to associate the symmetry that is associated with that particular space group. So, if the space group is P 2 1, 2 1, 2 1 in we compute the Patterson. The Patterson we know is p 2 by m, 2 by m, 2 by m, but the three projections associated with the x, y and z directions which is parallel to a, b and c will tell us about the possibility of locating the heavy atom positions to start with.

And secondly, it will also tell us what is the possible translational component that is associated with that particular symmetry operation. So, if we take 2 1, 2 1, 2 1 it is quite uniquely all three 2 1 axis can be determined by looking at the three projections and looking at a high values of the u w, u w and u v which appear in those projection plots. The similar argument goes for the Harker lines. So, in case of the mirror and the glide planes, you will instead of getting Harker planes, you get a Harker lines.

So, there will be lines of symmetry about which you will get information about for example, if there is a mirror plane, perpendicular to a, perpendicular to b or perpendicular to c; the corresponding Harker lines will be u 0 0, 0 v 0, 0 0 w. So, you have to look along the axis u v and w. And if there is an a glide, it will now have to have a half component here. So, we look at half v w, if the a glide is parallel to perpendicular to b; and if the a glide is perpendicular to c, we get half 0 w and so on.

So, basically what they take home lesson from this table is that we compute a Patterson, and using the Patterson, we can now determine the space group as well as the heavy atom position if we make use of Harker lines and planes. In fact, the Harker idea we came up for the location of the heavy atom in a totally different context. It came up with the idea that if we have a protein solution and in that protein solution; we now introduce a heavy atom containing die. So, like for example, we have a green sweater and blue sweater. Essentially, you put dice into these sweaters, sweater is a fibrous protein, it is made up of material, which is a protein.

There is no change in the structure of the protein, the wool remains wool, but what happens is the colour changes, because your put a dye; that means, the dye has been incorporated into the silk structure in the into the wool structure, which is the protein. In such a way that the actual structure and associated properties of the material has not changed, because of the fact that in a protein we have lots of empty space, which is occupied by solvent water and so on, it is possible to introduce dies without changing the overall configuration or confirmation of the protein molecule. So, this process where we can put a dye into the system and depending upon the nature of the dye, the nature of the structure of the dye and so on, it may occupy different positions around the protein and still leave the protein as such.

Suppose the dye contents of heavy element. The heavy element will dye will now also be going into the protein; and that particular heavy element therefore, can be located by Patterson synthesis. The process, which was develop by Harker is known as isomorphous replacement method. And using that one can find out the structure of the protein, we can solve the structure of the protein is not within the scope of our current discussion. But essentially one should know that it is possible to determine the structure using the heavy atom approach of a big large protein. And their of course, the issue of z square ratio will be very ominously low. So, still one can determine the structure using this isomorphous replacement.

So, essentially depending upon the different kinds of heavy atoms and their derivatives, which are now going into the protein structure. So, what you do is you take the dye solution, soak the protein in the dye solution, then you will dye will get incorporated. So, the colour will change, but the crystals which come out of this now will contain the heavy element as well along with the structure of that small molecule into which we have put the protein in.

Similarly, depending upon the size and nature of the heavy atom and the surroundings, the position at which the heavy atom goes will also change. So, this is known as multiple isomorphous replacement, because you will have different positions for the atoms to occupy within the framework of the protein structure. In such a way that the crystal structure of the protein still remains the same that means, the space group remains the same, there is no alteration in any other expect except that we have now different positions of the heavy atoms that can be used to reconstruct the protein structure. And this is known as the multiple isomorphous replacement that is again due to Harker.

So, Harker as contributed immensely to the Patterson synthesis do the normalize this isomorphous replacement method and MIR which is multiple isomorphous replacement method, which is very commonly used by protein cryptographers around the world now. Programming and things like that also become easier to determine the heavy atom position following which one can determine the structure of the protein. The other aspect which Harker has contributed to we will discuss after when we go to the direct methods. There he developed the required inequalities to start with which eventually became of course equalities of probabilities and those expressions where utilized in order to develop the so called direct method by means which we can solve the structure.

So, essentially we have now a Patterson calculatable probably the possible Patterson can be calculated. The Patterson will be divide of the face problem. If there is a heavy atom, it is possible to use the Patterson to locate the heavy atom. And the symmetry that is associated with the space group is sort of (Refer Time: 14:28) into these Harker lines and planes through, which we can extract the information not only about the position of the heavy atom very straightforward and easy way, but also identify the translational components that are associated with this particular space group.

So, the symmetry again as you see plays a major role in controlling how the Patterson vectors appear, and how they get aligned in Harker lines or in Harker planes with respect to the heavy atom position determination. These now serve as guidelines to solve the crystal structure to get the heavy atom and then one once we have the heavy atom difference Fourier techniques will allow us to solve the structure right.

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One heavy atom in the asymmetric unit of $P\bar{1}$

Equivalent points :

x, y, z $\quad$ $-x, -y, -z$

Vectors for two atoms in $P\bar{1}$.

$P\bar{1}$	x, y, z	$-x, -y, -z$
x, y, z	$0,0,0$	$-2x, -2y, -2z$
$-x, -y, -z$	$2x, 2y, 2z$	$0,0,0$

So, we will take some examples. So, the case of the first one is p 1 bar, I will take the case of p 1 bar equivalent points x, y, z, minus x, minus y, minus z. So, this is the position of the atom let us say in p 1 bar. Then what happens we, we make a matrix of this kind on the right side where we take x, y, z combine it with itself, which is the self vector and that is 0, 0, 0. Then take the second vector and combine it with this one which gives us minus 2 x, minus 2 y, minus 2 z; and with x, y, x minus x, minus y minus z or the x bar, y bar, z bar, we get 2 x, 2 y, 2 z and 0, 0, 0.

So, that means, if you compute the Patterson now in the Patterson diagram, we will get suppose there is a heavy atom in the structure, the heavy atom is associated let us see with x, y, z and x bar, y bar, z bar is automatically there in the space group p 1 bar. The x, y, z position can be determined, because we get two vectors one at minus 2 x minus, 2 y minus, 2 z, and the other at 2 x, 2 y, 2 z. So, since we get two vectors one at 2 x, 2 y, 2 z, other at minus 2 x, minus 2 y, minus 2 z we could look for a solution for x, y, z.

So, in principle we are able to find out the position of the heavy atom. So, we have these two corresponding peaks appearing one at 2 x, 2 y, 2 z and the other at minus 2 x, minus 2 y, minus 2 z. So, use this two to find out x, y, z so that means, you divide this by 2 that by 2 divide that by 2. And this one again divide by 2 divide by 2 divide by 2, but do a x bar, y bar, z bar to go over to x, y, z then you will get a unique solution for the heavy atom.

So, p 1 bar system is fairly straight forward. So, we can use this in this right hand side 2 by 2 matrix in this particular case the equivalent points and the 2 by 2 matrix is developed this way. Using this matrix you will get solution for x, y and z. So, we find the heavy atom position. The discussion now on the Patterson is limited only to the heavy atom method, because we are not going into the possibility of using Patterson as a general technique to determine the structure which can be done, but that is again for a way into the advance crystallographic course which we are not now going through.

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One heavy atom in the asymmetric unit of $P2_1$

Equivalent points :

$x, y, z \qquad -x, ½+y, -z$

Vectors between general positions in $P2_1$.

$P2_1$	x, y, z	$-x, ½+y, -z$
x, y, z	0,0,0	$-2x$, ½, $-2z$
$-x, ½+y, -z$	$2x$, ½, $2z$	0,0,0

So, the next space group we can consider is P 2 1, where we have equivalent points are x, y, z, x bar half plus y z bar. Remember that there is a P 2 1 here. So, when once you see P 2 1 as the space group, you expect a Harker line. So, you expect a Harker line or a Harker section, which one you expect, you expect a Harker section. Harker lines comes for glide planes and mirror and Harker section comes for the screw axis. So, you expect a Harker plane. So, you see here you get a solution to the heavy atom, there by taking vector between general positions, x, y, z, x bar half plus y z bar I am writing general position because P 2 1 has a special position 2.

So, general positions x, y, z, minus x, half plus y, minus z so, if you do the same operation as we did before with p 1 bar, we will get two sets of vectors 0, 0, 0. And this gives me minus 2 x, half, minus 2 z, notice the half here ok and then you get 2 x, half, 2 z, because y is equal to half in both these examples, you get solution to x and z. So, in a space group like P 2 1, y can be anywhere, y is arbitrary, because it is along a 2-fold axis. So, we can fix your y coordinate everywhere along the 2 1 direction. So, 2 x and 2 z will solve for x and z. You easily identify now the Harker sections which are this as well as that corresponding to y equals half.

So, you have now therefore in the projection, which you do down the y axis at half you see that you will get a solution corresponding to 2 x, 2 z, minus 2 x, minus 2 z. So, you plot now the value of v equals half ok. And then you will see a centrosymmetric related two peaks which are very heavy corresponding to the heavy atom. So, those will be 2 x, 2 z and minus 2 x, minus 2 z, that is why say centro symmetrically in the plane. So, the plane which you are considering now is half which tells you automatically that there is a 2 1 screw axis that is present in the system. So, this is the Harker section.

What you can do also is one once you have found the solutions for x, z and then arbitrary y, y you can fix anywhere in P 2 1. So, let us say we fix the y value at 0, then you can look for 2 x, 2 y, 2 z, there will be a p corresponding to 2 x, 2 y, 2 z for the solutions which you have arrived for x and z. So, here we get solution for x and z, we find the coordinates of x and z. The coordinate of y can be fixed arbitrarily, because there is no a region fixation along the 2 1 screw axis, where it can be anywhere all along the line of the screw axis, it can still have the screw property.

So, you fix decide to fix where the y should be conveniently and therefore, we have this option. So, you see the importance of the Harker section which is developing here with v equals half. We straightaway see the solution 2 x and z, we get 2 x, 2 z and therefore, we get x and z. So, we have the x and z coordinates of the heavy atom, y we are fixing. So, we get the corresponding 2 y with depending on where we fix the y value, and therefore, we get the position of the heavy atom.

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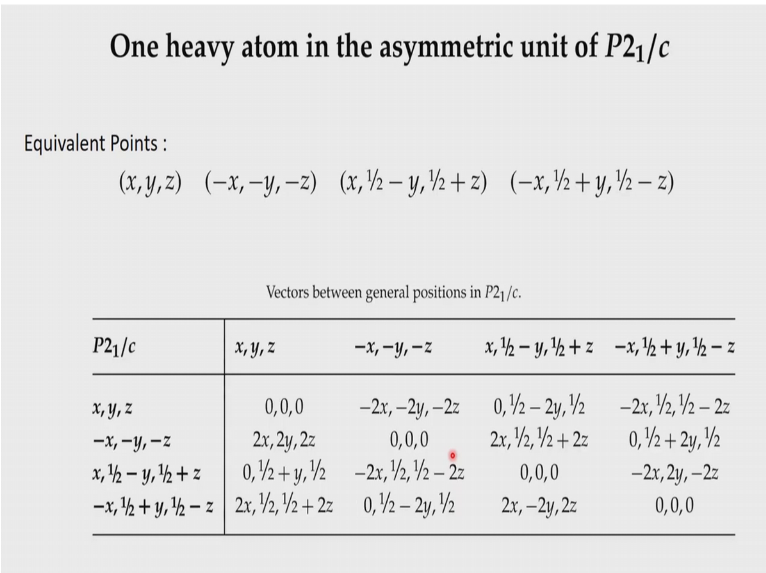
One heavy atom in the asymmetric unit of $P2_1/c$

Equivalent Points :

(x, y, z) $(-x, -y, -z)$ $(x, ½ - y, ½ + z)$ $(-x, ½ + y, ½ - z)$

Vectors between general positions in $P2_1/c$.

$P2_1/c$	x, y, z	$-x, -y, -z$	$x, ½ - y, ½ + z$	$-x, ½ + y, ½ - z$
x, y, z	0,0,0	$-2x, -2y, -2z$	$0, ½ - 2y, ½$	$-2x, ½, ½ - 2z$
$-x, -y, -z$	$2x, 2y, 2z$	0,0,0	$2x, ½, ½ + 2z$	$0, ½ + 2y, ½$
$x, ½ - y, ½ + z$	$0, ½ + y, ½$	$-2x, ½, ½ - 2z$	0,0,0	$-2x, 2y, -2z$
$-x, ½ + y, ½ - z$	$2x, ½, ½ + 2z$	$0, ½ - 2y, ½$	$2x, -2y, 2z$	0,0,0

So, P 2 1 is a fairly straight forward case, we now go to P 2 1 upon c which is the most common system we come across. So, here we have four equivalent points x, y, z, x bar, y bar, z bar, the x, half, minus y, half plus z, and x, half plus y, half minus z. So, we have we have to now do a Patterson between them. So, x minus x is 2 x, y minus y is 2 y, z minus z is 2 z, which comes here. So, you write the four equivalent points, you write the four equivalent points and make the matrix of this. So, this matrix will give you 0, 0, 0 here; 0, 0, 0 here; 0, 0 along the diagonal it is all 0's. And then you get a symmetric this position of 2 x, 2 y, it is 2 z, 0 half plus y half, 0 half minus y half, 2 x half.

So, corresponding to the 2 1 screw axis yeah. So, we now are looking at the vectors which come from symmetry operations of P 2 1 upon c. So, if one looks at P 2 1 upon c, we have four equivalent points. These two equivalent points are generated by the center of symmetry. These two equivalent points are generated by the center of symmetry, These to these is a glide operation, then these to these is also incorporating the center of symmetry equivalent glide operation. So, there is a relationship between these four, which tells us the presence of 2 1 as well as the c glide perpendicular to the 2 1 axis.

How does it reflect on the Patterson vectors, this is where the beauty of Harker sections and Harker lines come up, because using this we get a unique solution for the heavy atom position in P 2 1 upon c. So, we compute the Patterson, Patterson of course, as we know will going to be p 2 by m. So, it is not going to give us much information on the translational component as we know. However, if you look at this matrix; examine the matrix where we go now write the four equivalent points here and four equivalent points there and then make the combinations of those.

So, if you take x, y, z and itself, it is 0, 0, 0; you take x, y, z to minus x etcetera we get minus 2 x, minus 2 y, minus 2 z. You see that this position to this position, the it is related by a center of symmetry, the corresponding vectors are also centrosymmetrically related, so minus 2 x, minus 2 y, minus 2 z will generated 2 x, 2 y, 2 z. So, these two are now centrosymmetrically related. So, we get solutions for x, y and z by examining the come to two components 2 x, 2 y, 2 z and 2 x, 2 y, 2 z minus of the two vector. So, we look at this vector end and this vector end and see whether the peaks that are associated with this are corresponding to the product of the heavy atom.

So, if the heavy atom is bromine, these two vectors should be very close to 35.5 square after the scaling factor is taken into account. It will not be exact, but it will have a very high value compared to the rest of the vectors, you find in the Patterson space. So, you pick up these two. So, the way you practically do Patterson is you compute the Patterson of a heavy atom structure and then arrange the vectors in a descending order and see whether they follow any kind of symmetry.

So, if the follow symmetry, then you identify the symmetry and also try to solve for the x, y, z from the set of vectors. So, we have therefore, here 2 x, 2 y, 2 z, 2 x, 2 y, 2 z and we get a x, y, z keep it aside. And now take the third one, which will now give us with respect to this 0, half plus y, half; now this is a glide operation and therefore, we have to look here under the glide operation you get 0, half minus 2 y, half. So, this is a Harker line and this is also a Harker line.

So, if we look at the Harker line, you get a unique solution for y. This should be half plus 2 y here; there is a mistake, it should be half plus 2 y. So, you get half plus 2 y, half minus 2 y, you get a solution for y; you have solution for x, y and z already here, compare that y with this y, it should be the same. So, you therefore, now conclude that the value of y is for the heavy atom system has been completely determined. You go to the last one which is 2 x, half, half plus 2 z, you will find this minus 2 x, half, half minus 2 z, which is now the previous one was a Harker line this is a Harker section. This is a Harker section, because we are looking at the c glide operation, this is a Harker section, because we are looking at the two one screw operation Harker line this Harker line is due 2 1 screw operation, this Harker section is due to the c glide operation.

So, we see all the symmetries which are coming here. So, you do not have to worry that Patterson is not giving you any cemetery information. The symmetry information that is coming up is essentially coming from the equivalent points, which are present in the crystal structure and they are depicted in terms of their vector relationships in the Patterson map. So that way we can identify these matrix set up this matrix get all these coordinates and we can uniquely solve for x, y and z. So, we get the position of x, y, z which is corresponding to the heavy atom in a very straightforward way if we analyze these sections, the Harker section as well as the Harker planes, along with that look at the vectors corresponding to 2 x, 2 y, 2 z.

So, you would see that there is no other set of vectors which will be present here either they are related by center of sub symmetry or by the operation of the 2-fold like here. For example, if you look at these 2 x bar, y bar, z bar and the third one, you see that it is 2 x, 2 y, 2 z and here it is minus 2 x, 2 y, minus 2 z. So, that is the operation of a 2-fold about the y direction. And here it is half plus y therefore, it adds on a half value to the y 2 half plus 2 y it should be.

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One heavy atom in the asymmetric unit of *Pbca*

Equivalent Points :

x, y, z
$\frac{1}{2}+x, \frac{1}{2}-y, -z$
$\frac{1}{2}-x, -y, \frac{1}{2}+z$
$-x, \frac{1}{2}+y, \frac{1}{2}-z$
$-x, -y, -z$
$\frac{1}{2}-x, \frac{1}{2}+y, z$
$\frac{1}{2}+x, y, \frac{1}{2}-z$
$x, \frac{1}{2}-y, \frac{1}{2}+z$

Vectors between general positions in *Pbca*.

Pbca	x, y, z
x, y, z	$0, 0, 0$
$\frac{1}{2}+x, \frac{1}{2}-y, -z$	$\frac{1}{2}, \frac{1}{2}+2y, 2z$
$\frac{1}{2}-x, -y, \frac{1}{2}+z$	$\frac{1}{2}+2x, 2y, \frac{1}{2}$
$-x, \frac{1}{2}+y, \frac{1}{2}-z$	$2x, \frac{1}{2}, \frac{1}{2}+2z$
$-x, -y, -z$	$2x, 2y, 2z$
$\frac{1}{2}-x, \frac{1}{2}+y, z$	$\frac{1}{2}+2x, \frac{1}{2}, 0$
$\frac{1}{2}+x, y, \frac{1}{2}-z$	$\frac{1}{2}, 0, \frac{1}{2}+2z$
$x, \frac{1}{2}-y, \frac{1}{2}+z$	$0, \frac{1}{2}+2y, \frac{1}{2}$

So, essentially we get a unique solution in case of 2 1 by c. There is one other example in all these cases one thing which we have talking about is that we are looking at only one heavy atom. It is not necessary that we should have only one heavy atom, we can have more than one heavy atom. I have given this table and I have given the Patterson vectors, which between general positions in Pbca. You can verify yourself that you can put this into a kind of a matrix, which we put in the earlier two cases. I am not going to put that. You can this is an exercise, which one goes through we will get a hang of how to set up those matrices, so which are essentially required to identify and solve the vector position.

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One heavy atom in the asymmetric unit of $P2_12_12_1$

Equivalent Points :

x, y, z $\quad$ $\frac{1}{2}+x, \frac{1}{2}-y, -z$ $\quad$ $\frac{1}{2}-x, -y, \frac{1}{2}+z$ $\quad$ $-x, \frac{1}{2}+y, \frac{1}{2}-z$

Vectors between general positions in $P2_12_12_1$.

$P2_12_12_1$	x, y, z	$\frac{1}{2}+x, \frac{1}{2}-y, -z$	$\frac{1}{2}-x, -y, \frac{1}{2}+z$	$-x, \frac{1}{2}+y, \frac{1}{2}-z$
x, y, z	$0,0,0$	$\frac{1}{2}, \frac{1}{2}-2y, -2z$	$\frac{1}{2}-2x, -2y, \frac{1}{2}$	$-2x, \frac{1}{2}, \frac{1}{2}-2z$
$\frac{1}{2}+x, \frac{1}{2}-y, -z$	$\frac{1}{2}, \frac{1}{2}+2y, 2z$	$0,0,0$	$-2x, \frac{1}{2}, \frac{1}{2}+2z$	$\frac{1}{2}-2x, 2y, \frac{1}{2}$
$\frac{1}{2}-x, -y, \frac{1}{2}+z$	$\frac{1}{2}+2x, 2y, \frac{1}{2}$	$2x, \frac{1}{2}, \frac{1}{2}-2z$	$0,0,0$	$\frac{1}{2}, \frac{1}{2}+2y, -2z$
$-x, \frac{1}{2}+y, \frac{1}{2}-z$	$2x, \frac{1}{2}, \frac{1}{2}+2z$	$\frac{1}{2}+2x, -2y, \frac{1}{2}$	$\frac{1}{2}, \frac{1}{2}-2y, 2z$	$0,0,0$

The for the 2 1 2 1 2 1 anyway I have given this matrix. So, P b c a you can find out what should be the matrix. So, it means you have to reorganize this in the form which is coming up here. So, you write a eight equivalent points and then generated in case of P b c a. So, the size of the matrix keep going up, but these solutions become more and more unique. So, you get a solution for example, from looking at the peak 2 x, 2 y, 2 z, you get a solution from looking at 2 x, half minus 2 y, 0. We will also get information from 0, 0, half plus z and so on.

So, essentially you get x, y, z from various possibilities and the common x, y, z, which comes up from a looking at all these vectors will be the one which you identify as the heavy atom position. Obviously, all these peaks will have to stand out, so these are therefore, the highest peaks in the Patterson. So, it is becomes very easy computationally, because one once you compute the Patterson you rearrange the peaks in a descending order. And look at the possibility of assigning these peaks to the various where the peaks appear and when you see where the peaks appear, you will get the various Harker sections and Harker lines. So, essentially you can solve the heavy atom position fairly straight forward way.

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As a practical example of locating an atom from Patterson data, the bromine atom in methyl micromerol bromoacetate[8] (space group $P2_12_12_1$) was located from three Harker sections, each calculated over only its unique area. Thus

(a) Section at $u = 48/96$, with $v = 0 \rightarrow 50/100$, w; $0 \rightarrow 50/100$.
Peak found at 48/96, 11/100, 21/100.
Assigned $\frac{1}{2}, \frac{1}{2} - 2y, 2z$, so $y = 19.5/100$, $z = 10.5/100$.

(b) Section at $v = 50/100$, with $u = 0 \rightarrow 48/96$, $w = 0 \rightarrow 50/100$.
Peak found at 34/96, 50/100, 29/100.
Assigned $2x, \frac{1}{2}, \frac{1}{2} - 2z$, so $x = 17/96$ ($\frac{1}{2} - 2z = 29/100$ as required).

(c) Section at $w = 50/100$, with $u = 0 \rightarrow 48/96$ and $v = 0 \rightarrow 50/100$.
Peak found at 14/96, 39/100, 50/100.
General form $\frac{1}{2} \pm 2x, \pm 2y, \frac{1}{2}$. The peak found corresponds to $\frac{1}{2} - 2x, 2y, \frac{1}{2}$.

The complete set of symmetry-related bromine atoms for this example is

Br_1	17/96, 19.5/100, 10.5/100	x, y, z
Br_2	31/96, −19.5/100, 60.5/100	$\frac{1}{2} - x, -y, \frac{1}{2} + z$
Br_3	65/96, 30.5/100, −10.5/100	$\frac{1}{2} + x, \frac{1}{2} - y, -z$
Br_4	−17/96, 69.5/100, 39.5/100	$-x, \frac{1}{2} + y, \frac{1}{2} - z$

So, this is a gist of overall operation of the Patterson synthesis. And I know I have restricted through, but here is a practical example to make you convinced and how you get exactly the heavy atom position.