

# CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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## Lecture 35: Derivation of 3D-Bravais Lattices

So, we have completed the development of all the 32 point groups in three dimensions, and in this lecture, we will now derive the three-dimensional Bravais lattices. Once this derivation is complete, we will subsequently combine the point groups and the Bravais lattices to develop the space groups in three dimensions.

The derivation of the three-dimensional Bravais lattices follows very similar lines to what we have already done for the two-dimensional plane lattices. In an analogous manner, we can extend the same logic to three-dimensional space lattices. Essentially, we ask what constitutes a three-dimensional space lattice. One approach is to begin with two-dimensional lattices, which possess only two translation vectors, and then add a third dimension by stacking these lattices to form a three-dimensional lattice. Let us examine how this procedure works.

We begin with an oblique lattice. Recall that an oblique lattice has no constraints on the unit cell parameters  $\bar{a}$  and  $\bar{b}$ , nor on the angle between the two vectors  $\bar{a}$  and  $\bar{b}$ . This corresponds to the plane group  $p1$ . Starting from this oblique lattice, we now introduce a third translation vector  $\bar{c}$ . This vector is added in an arbitrary direction. The vector  $\bar{c}$  makes an angle  $\alpha$  with the  $b$  axis, the angle between  $c$  and the  $a$  axes is  $\beta$ , and the angle  $\gamma$  is defined between the  $a$  and  $b$  axes. These are the conventional parameters  $\alpha$ ,  $\beta$ , and  $\gamma$ , taken in this order. With these definitions, we can complete the unit cell.

In this unit cell, there are no constraints on  $\bar{a}$ ,  $\bar{b}$ , or  $\bar{c}$ , since the  $\bar{c}$  vector has arbitrary direction and arbitrary length. Similarly, there are no constraints on the angles. The resulting three-dimensional lattice therefore has no symmetry, just like the oblique lattice with which we started. There are no constraints on the unit cell vectors  $\bar{a}$ ,  $\bar{b}$ , and  $\bar{c}$ , and no

constraints on the angles either. This situation is commonly written as  $a \neq b \neq c$ , where the inequality symbol indicates the absence of constraints rather than strict numerical inequality. If one refers to the list of Bravais lattices, this lattice is identified as a primitive triclinic unit cell.

Thus, the procedure followed was to start from the plane group  $p1$ , add a third translation, and obtain the three-dimensional space group  $P1$ . Here, we use a capital letter  $P$  to distinguish it from the plane group notation, which uses a lowercase  $p$ . In three-dimensional crystallography, capital letters are consistently used to designate whether a lattice is primitive, body-centered, end-centered, or face-centered, and we will maintain this convention throughout.

A natural question arises regarding which point groups the triclinic lattice can accommodate. The triclinic lattice clearly accommodates point group  $\bar{1}$ , which corresponds to the absence of symmetry. One may then ask whether it can accommodate

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**Start with an Oblique Lattice with no symmetry (plane group “ $p1$ ”)**

**Add an arbitrary third translation  $c$**

**Resulting 3D lattice – no symmetry**

No constraints on unit cell vectors  $a$ ,  $b$  and  $c$ :  $a \neq b \neq c$

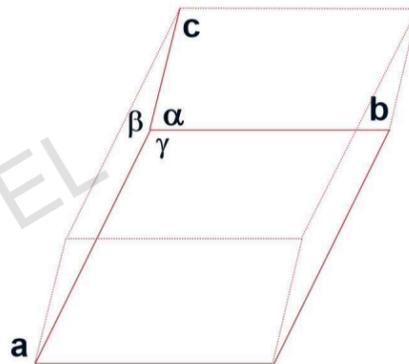
No constraints on angles:  $\alpha \neq \beta \neq \gamma$

**Primitive TRICLINIC unit cell**

**Started with Plane Group “ $p1$ ”. Added the third translation leading to the 3D Space Group “ $P1$ ”.**

**Which point group that the TRICLINIC lattice can accommodate?  $\bar{1}$**

Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	Simple Triclinic (P)
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any other symmetry. For now, we note that it can also accommodate an inversion center. As pointed out in an earlier lecture, all lattices, regardless of the crystal system to which they belong, possess an inversion center. When a motif is added, this inversion center may or may not be preserved in the resulting crystal structure. Consequently, any lattice can accommodate inversion symmetry. Even with inversion included, the lattice remains a primitive triclinic lattice.

Let us now consider another example, starting again from an oblique lattice, but this time with point group 2, corresponding to the plane group  $p2$ . The plane group  $p2$  consists of twofold rotational symmetries distributed at the corners, at the midpoints of the edges, and at the center of the unit cell. We now add a third translation vector to form a three-dimensional lattice.

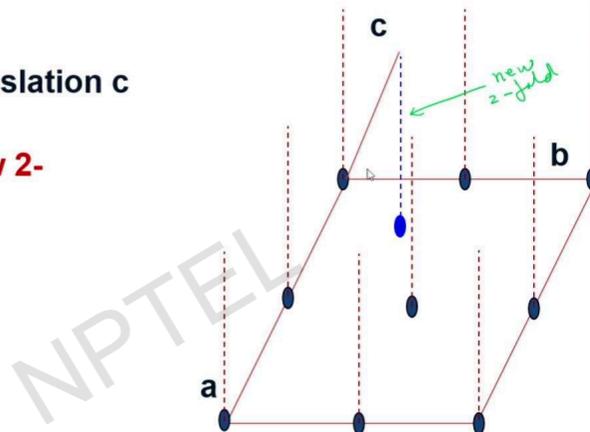
The key question is how this third translation vector should be added. Suppose we add it in the same way as before, namely in an arbitrary direction and with arbitrary length. The (Refer Slide Time: 07:11)

**Start with “ $p2$ ” plane group**

**Add an arbitrary third translation  $c$**

**Translation generates new 2-fold axes – not allowed**

All symmetry is destroyed



**Conclusion: arbitrary translation not allowed if the symmetry is to be preserved**

**Which translations  $c$  are permitted?**

dashed lines indicate extension into the third dimension, and the twofold axes extend into this dimension as well. When an arbitrary third translation  $c$  is added, the translation symmetry operates throughout space. As a result, the twofold axis is translated to a new position, producing an additional twofold axis. This new twofold axis, in turn, acts on the structure and generates further symmetry operations. Ultimately, this process destroys the original symmetry, leaving no well-defined symmetry at all. Therefore, this particular choice of translation is not allowed.

This leads to an important principle: when a third translation is added, it must not create any new symmetry elements. It must preserve the symmetry that existed in the original two-dimensional lattice. Hence, only certain translations are permitted.

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**Consider  $c = z$  (i.e., perpendicular to both  $a$  and  $b$ )**

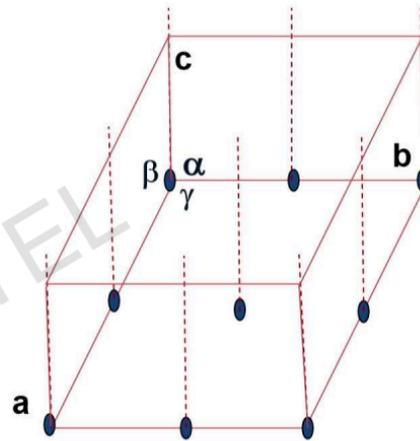
**No new rotation axes generated**

**This is an allowed translation**

**No constraints on unit cell vectors:**  
 $a, b$  and  $c$  ( $a \neq b \neq c$ )

**No constraint on  $\gamma, \alpha = \beta = 90^\circ$**   
 $\alpha = \beta = 90^\circ \neq \gamma$

**Primitive MONOCLINIC**



Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	Simple Monoclinic (P)

Consider a translation  $c$  parallel to the  $z$  direction, that is, perpendicular to the  $ab$  plane. In this case,  $c$  coincides with the twofold rotation axis. Adding this translation does not create any new rotational axes, and therefore it is an allowed translation. Completing the

unit cell yields a lattice in which there are no constraints on the magnitudes of  $\bar{a}$ ,  $\bar{b}$ , and  $\bar{c}$ . The angle  $\gamma$  remains unconstrained, as inherited from the oblique lattice. However, the angles  $\alpha$  and  $\beta$  must be  $90^\circ$ . Thus, we write  $\alpha = \beta = 90^\circ$ , with no constraint on  $\gamma$ . Referring again to the list of Bravais lattices, this lattice is identified as a primitive monoclinic lattice, often called simple monoclinic, and it is denoted by the capital letter *P*.

We may now ask whether other choices of  $c$  are possible that also preserve the original symmetry. Consider a translation vector defined as  $\bar{c} = \bar{a}/2 + z$ . This means that one moves halfway along  $\bar{a}$  and then translates a distance  $z$  in the third dimension. This vector terminates on a twofold axis, so that the twofold axis is translated onto another twofold axis located at the midpoint of an edge. As a result, the symmetry elements are superimposed, and no new symmetry is generated. This translation is therefore also allowed.

In this case, the resulting unit cell appears to have arbitrary vectors  $\bar{a}$ ,  $\bar{b}$ , and  $\bar{c}$ . However, we may redefine the unit cell to clarify its geometry. Starting from the same oblique lattice and extending the  $\bar{c}$  vector, we can define a new vector  $\bar{c}' = 2\bar{c} - \bar{a}$ . This construction yields a vector  $\bar{c}'$  that is perpendicular to the  $ab$  plane and aligned with the twofold axis. Completing the unit cell with  $a$ ,  $b$ , and  $c'$ , we again have  $a \neq b \neq c'$ , with  $\alpha = \beta = 90^\circ$  and  $\gamma$  unconstrained.

The difference between this case and the previous one lies in the distribution of lattice points. The translation by  $c$  moves the lattice point at the origin to a new position, which now lies at the center of a face of the unit cell. Upon completing the unit cell, there is also a lattice point at the center of the opposite face. Thus, the lattice has points at the corners and at the centers of two opposite faces. This lattice is therefore not primitive; it is a base-centered, or end-centered, monoclinic lattice.

In this construction, the face containing the additional lattice point is the  $B$  face, which lies in the  $AC'$  plane. Consequently, the lattice is described as base-centered monoclinic with centering  $B$ . If the lattice point were located on the rear face, it would be  $A$ -centered, and if it were on the top face, it would be  $C$ -centered. It is important to note that the base is an oblique parallelogram, whereas the vertical faces are rectangular. As a result, in an end-centered monoclinic lattice, lattice points can only appear on the vertical faces and not on the oblique base. This gives rise to two equivalent choices for defining an end-centered monoclinic lattice.

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**$c = a/2 + z$  ?**  
**No new rotation axes generated**  
**This is an allowed translation**

**Any other third translation?**

**A primitive cell is obtained (unit cell vectors appear arbitrary)**

**Consider an alternative**  
 $c' = 2c - a$

lattice point

$c'' = b/2 + z$

No constraints on  $a, b$  and  $c'$   
 No constraint on  $\alpha, \beta, \gamma$ ,  
 $\alpha = \beta = 90^\circ$   
 $\Rightarrow \alpha = \beta = 90^\circ \neq \gamma$

**End-Centred MONOCLINIC**

Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	Simple Monoclinic (P)
		Base Centred Monoclinic (B)

We may consider yet another possible translation, for example  $\bar{c} = \bar{b}/2 + z$ , which again produces an end-centered lattice, this time with the  $A$  face centered. Another alternative is to define  $\bar{c} = \bar{a}/2 + \bar{b}/2 + z$ , which terminates on the central twofold axis. This translation is also allowed. Extending this vector and redefining it as  $\bar{c}' = 2\bar{c} - \bar{a} - \bar{b}$  produces a unit cell in which  $a, b$ , and  $c'$  are unconstrained in length, with  $\alpha = \beta = 90^\circ$

and  $\gamma$  unconstrained. This construction yields a monoclinic lattice with a lattice point at the body center, suggesting a body-centered monoclinic lattice.

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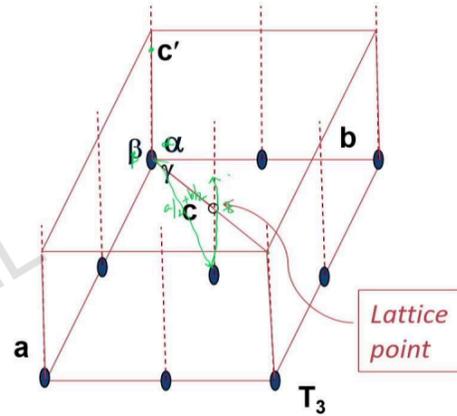
$c = a/2 + b/2 + z$  (allowed)

**Consider an alternative third translation:**

$c' = 2c - a - b$

The lengths of vectors  $a$ ,  $b$  and  $c'$  are not related

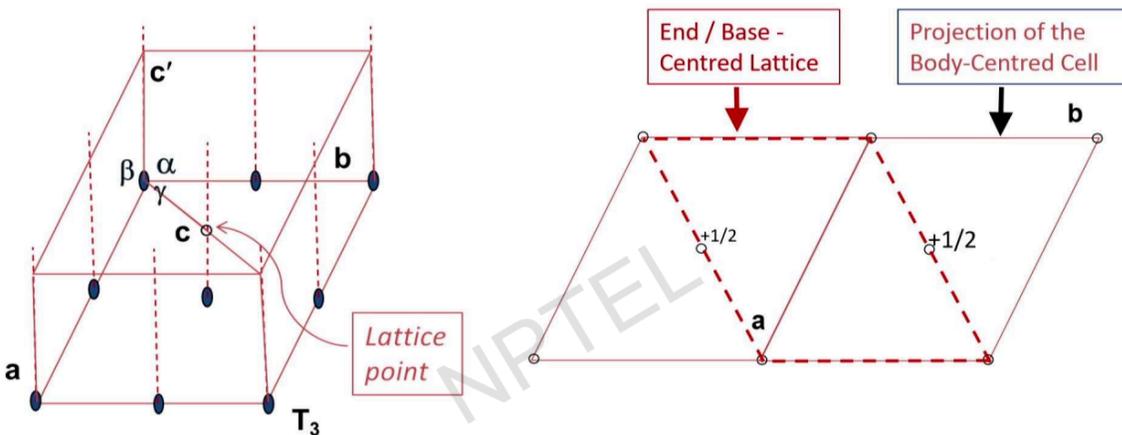
No constraint on  $\gamma$ ,  $\alpha = \beta = 90^\circ$   
 $\alpha = \beta = 90^\circ \neq \gamma$



**Body-Centred MONOCLINIC ?**

Monoclinic	$a \neq b \neq c$	Simple Monoclinic (P)
	$\alpha = \beta = 90^\circ \neq \gamma$	Base Centred Monoclinic (C)

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**Body-centred lattice can be represented by the base-centred lattice**

However, inspection of the list of Bravais lattices reveals that only two lattices exist in the monoclinic crystal system: the primitive monoclinic and the base-centered monoclinic lattices. To resolve this apparent contradiction, we examine the body-centered monoclinic lattice more closely. By projecting the lattice along the  $z$  axis, the lattice points, including the body-centered point, are projected onto the  $AB$  plane. The notation  $+ 1/2$  indicates that the body-centered point lies halfway along the  $c'$  axis. By considering adjacent unit cells and examining the projected arrangement, one finds that the body-centered lattice can be redefined as an end-centered lattice with centering on the  $B$ -face. Thus, the body-centered monoclinic lattice is not distinct from the base-centered monoclinic lattice and is therefore not listed separately among the Bravais lattices.

Nevertheless, it is worth noting that in the context of space groups, body-centered lattices in the monoclinic system do appear and are treated explicitly.

Now, let us take a different unit cell of the two-dimensional lattices. This time, let us consider a rectangular cell, and it has a mirror symmetry, which essentially means that we are considering the  $Pm$  plane group. In this  $Pm$  plane group, I now want to introduce a third vector. I am not going to draw a three-dimensional structure for this; rather, I will consider a projection. You can therefore imagine this as a projection with the mirror planes extended vertically upward. The third translation that I want to consider is  $\bar{c} = v\bar{b} + z$ , where  $v$  is simply a scalar value between 0 and 1. Thus, we move upward by a certain amount, travel along  $\bar{b}$ , and then the  $z$  component takes us upward. The projected vector  $\bar{c}$  would look something like this.

This is a projection of the translation  $c$ , but you should imagine that this translation vector actually lies upward and within the mirror plane, which is important. Since it lies in the mirror plane, it is allowed because it does not introduce any new symmetry. Consequently, there are again no constraints on  $a$ ,  $b$ , and  $c$ , because the vector  $c$  can have any length, and  $a$  and  $b$  were unconstrained to begin with. However, you will notice that

the angle  $\alpha$ , which is the angle between  $b$  and  $c$ , has no constraint, whereas the angles  $\gamma$  and  $\beta$  are  $90^\circ$ .

What kind of unit cell does this correspond to? This is essentially a primitive monoclinic unit cell, as you can see. The lengths  $a$ ,  $b$ , and  $c$  are unconstrained, and two of the angles are  $90^\circ$ , while the third angle is unconstrained. The only difference, if I compare this with the previous monoclinic diagrams that I have drawn, is that now the base of the cell is rectangular. The  $BC$  plane is a parallelogram, but the  $AC$  plane is also a rectangle. Thus, we again have two rectangular faces and one oblique, or parallelogram, face. The essential conclusion is that this construction leads to a primitive monoclinic cell.

Now, before proceeding further, note that the point groups  $2$ ,  $m$ , and also  $2/m$  can be associated with the monoclinic system. However, it is not possible to associate  $2mm$  with the monoclinic system. I will leave this as an exercise: start with the plane group  $2mm$  (Refer Slide Time: 22:22)

### Start with plane group $pm$ - rectangular net

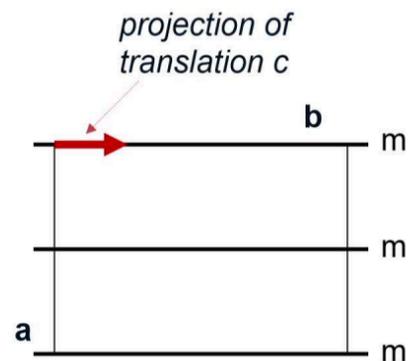
Permissible translation:  $c = vb + z$  ( $v$  is an arbitrary value between 0 and 1, i.e., the translation vector is in the mirror plane)

No constraints on  $a$ ,  $b$  and  $c$

No constraint on  $\alpha$ ,  $\gamma = \beta = 90^\circ$

**Base of the cell is rectangular;  $b$  and  $c$  form the parallelogram face.**

This simply leads to **Primitive Monoclinic !!**



Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$	Simple Monoclinic (P)
		Base Centred Monoclinic (C)

**Point groups:  $2$ ,  $m$  (and even  $2/m$ ) can be associated with Monoclinic System**

**Not possible to associate  $2mm$ . Why?**

**adding the third translation to the plane group  $p2mm$**

*(explore this by*

and add a third translation to see why this is not possible. The point group  $2/m$  is accommodated, and we will see a little later why  $2/m$  can be included.

Let us now take a different plane group belonging to the rectangular crystal system. This time, we consider a centered rectangular cell, which has the plane group  $Cm$ . We have already seen this in earlier lectures when discussing plane groups. Again, we consider a translation of the same form,  $v\bar{b} + z$ . This is again an allowed translation. You can see that  $A$ ,  $B$ , and  $C$  remain unconstrained, and among the angles, two are  $90^\circ$  while the third angle is unconstrained. Therefore, this must again be a monoclinic unit cell, but now the lattice is end-centered monoclinic because there is a lattice point at the base of the cell.

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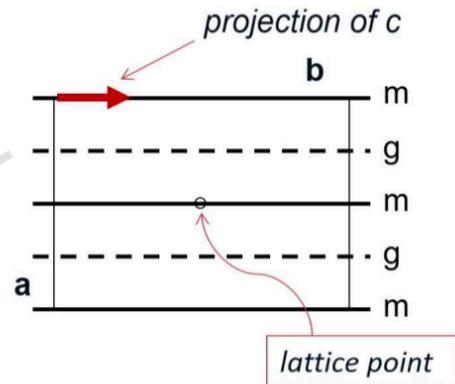
### Start with plane group $cm$ - centred rectangular net

Consider Translation  $c = vb + z$

No constraints on  $a$ ,  $b$  and  $c$

No constraint on  $\alpha, \gamma = \beta = 90^\circ$

**Base of the cell is rectangular;  $b$  and  $c$  form the parallelogram face.**



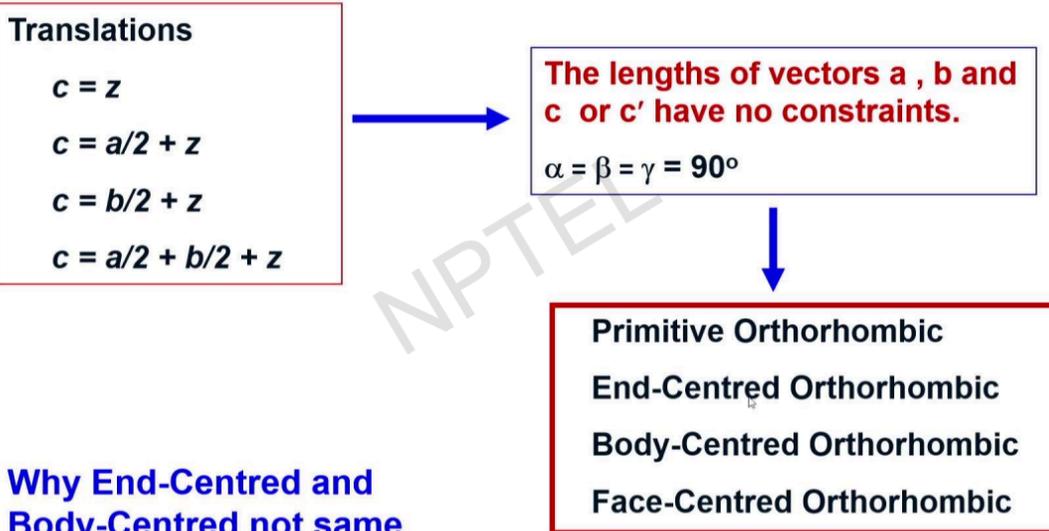
Lattice is end (or base)-centred monoclinic !!

In this way, we can continue taking other symmetries and other two-dimensional lattices to generate additional unit cells corresponding to the Bravais lattices. For example, one could consider the plane groups  $P2mm$ ,  $P2mg$ ,  $P2gg$ , and  $C2mm$ , and so on. One can add appropriate translations, and these translations are allowed by symmetry.

I am not going to go through all of these cases explicitly, but it will be instructive if you work through them yourself and draw the corresponding diagrams. By doing so, you can show that it is possible to obtain a primitive orthorhombic unit cell, an end-centered orthorhombic unit cell, a body-centered orthorhombic unit cell, and a face-centered orthorhombic unit cell. One should realize, however, that in the orthorhombic case, end-centered and body-centered lattices are not equivalent, unlike in the monoclinic case. Why should that be? You should try to reason this out.

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**Start with plane groups -  $p2mm$ ,  $p2mg$ ,  $p2gg$  and  $c2mm$**



**Why End-Centred and Body-Centred not same as in case of Monoclinic?**

Similarly, you can apply a third translation to plane groups such as  $P4$ ,  $P4mm$ , and  $P4gm$  to obtain either a primitive tetragonal or a body-centered tetragonal lattice. In this way, you can also reach the tetragonal crystal system. The point groups that can be associated with the tetragonal lattice are 4 and  $4mm$ . Since we started with a plane group having a square lattice, the fourfold symmetry is already present.

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**Apply third translation to plane groups –  $p4$ ,  $p4mm$  and  $p4gm$**

$$a = b \neq c$$
$$\alpha = \beta = \gamma = 90^\circ$$



**Primitive Tetragonal**  
**Body-Centred Tetragonal**

Point Groups that may be added to TETRAGONAL lattice:

-  $4$ ,  $4mm$

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**Start with plane group  $p3$**

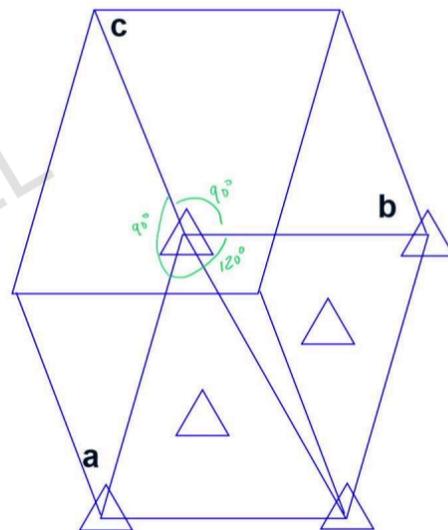
Consider  $c = z$  (i.e., straight up)

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$

**Primitive HEXAGONAL**

Above will also work for plane groups  $p3m1$ ,  $p31m$ ,  $p6$ ,  $p6mm$



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Now, let us take a very different plane group and start with the hexagonal case. We begin with a hexagonal two-dimensional lattice that has a threefold symmetry, namely the plane group  $P3$ . We add a third translation straight upward, which creates no new symmetry. This immediately gives  $a = b \neq c$ ,  $\alpha = \beta = 90^\circ$ , and  $\gamma = 120^\circ$ . This unit cell is therefore a primitive hexagonal cell in the three-dimensional Bravais lattice system.

However, there is another alternative construction starting again from the plane group  $P3$ . In this case, we add a translation of the form  $\frac{2}{3}\bar{a} + \frac{1}{3}\bar{b} + z$ . This defines a new third translation vector  $\bar{c}$ . Extending this vector repeatedly generates additional lattice points, leading to a unit cell containing three lattice points. Although this is a valid unit cell, it is not a Bravais lattice.

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**Translate plane group  $p3$  by**

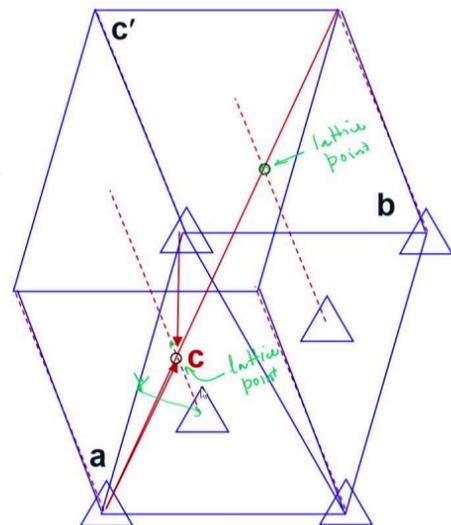
$$c = 2a/3 + b/3 + z$$

$$a = b \neq c$$

$$\alpha = \beta = 90^\circ, \gamma = 120^\circ$$

**Non-Primitive HEXAGONAL (3 lattice points per unit cell)**

**(not present in Bravais Lattice !!)**



By redefining the basis vectors as  $a''$ ,  $b''$ , and  $c''$ , one obtains a unit cell in which all three vectors have equal length and all three angles are equal but not equal to  $90^\circ$ . This

corresponds to a primitive rhombohedral lattice, with the constraint arising from the threefold rotational axis.

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**Select alternative coordinate system**

$$a'' , b'' \text{ and } c''$$

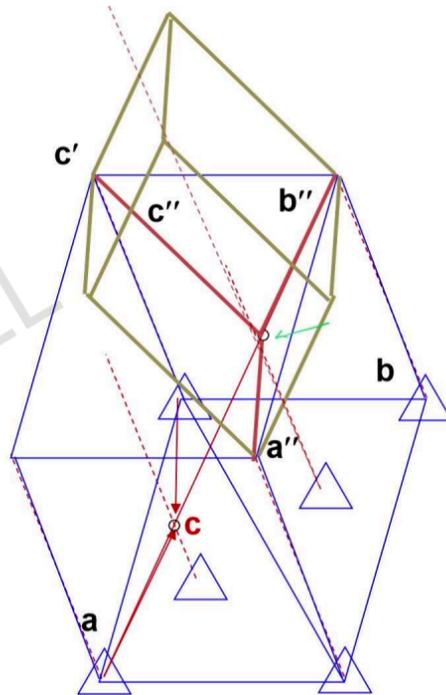
$$a'' = b'' = c''$$

$$\alpha = \beta = \gamma \neq 90^\circ$$

**Primitive Rhombohedral**

Point Groups that may be added to  
HEXAGONAL and RHOMBOHEDRAL  
lattices:

- 3, 3m, 6, 6mm



Inversion symmetry imposes no additional restrictions on lattice parameters because for every translation  $t$ , the translation  $-t$  is automatically present. Adding inversion to point group 2 leads to the point group  $2/m$ , which requires the same lattice constraints as 2. Thus, only a limited set of point groups needs to be considered to derive the Bravais lattices, namely the Laue groups, all of which contain inversion symmetry.

Although this approach yields eleven lattices, the cubic lattices can be obtained by starting from tetragonal or orthorhombic lattices and imposing additional rotational symmetries. In this way, one arrives at the simple cubic, body-centered cubic, and face-centered cubic lattices, completing the full set of fourteen Bravais lattices.

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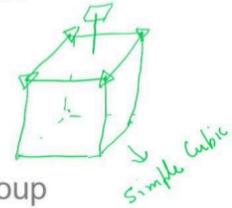
Inversion symmetry has not been considered.

Presence of inversion requires that for every translation  $\vec{t}$  there will be a translation  $-\vec{t}$

This is true for every space lattice

Therefore, inversion imposes no restriction

**Example:** add inversion to point group 2 leads to the point group  $2/m \Rightarrow$  Lattices required by  $2/m$  would be the same as those required by 2  $\Rightarrow$  MONOCLINIC  $\rightarrow 2, m, 2/m$



Conclusion

Only a few point group symmetries need to be considered for obtaining the 3D Bravais Lattices (Laue groups would be sufficient)

**For cubic lattices, consider the point groups 23 and 432**

**Take the Orthorhombic and Tetragonal Lattices: impose the 3-fold rotation axes along all body diagonals resulting in the three cubic unit cells**

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## Conventions for the unit cells

- Select the shortest translations in the lattice:  $a, b, c$
- If there is nothing special about any axis (as in the case of triclinic and orthorhombic):  $b > a > c$
- $c$  is generally defined as the unique direction
  - 4-fold axis in the tetragonal cell
  - 2-fold axis in the monoclinic cell
  - 3 or 6-fold axes in hexagonal cell)

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Finally, some conventions are used in defining unit cell parameters. The shortest translations are chosen as  $a$ ,  $b$ , and  $c$ . If no axis is unique, a conventional ordering of lattice parameters is adopted. If an axis is unique, such as the fourfold axis in tetragonal systems, the twofold or mirror-related axis in monoclinic systems, or the threefold or sixfold axis in hexagonal systems, it is conventionally chosen as the  $c$  axis. With this, the discussion concludes, and the development of three-dimensional space groups follows in the next lecture.