X-ray Crystallography: Lecture 3:

Crystal Symmetry: Crystal System, Symmetry elements, Non-primitive Lattices, Space groups, Systematic Absences

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Primitive Unit Cell

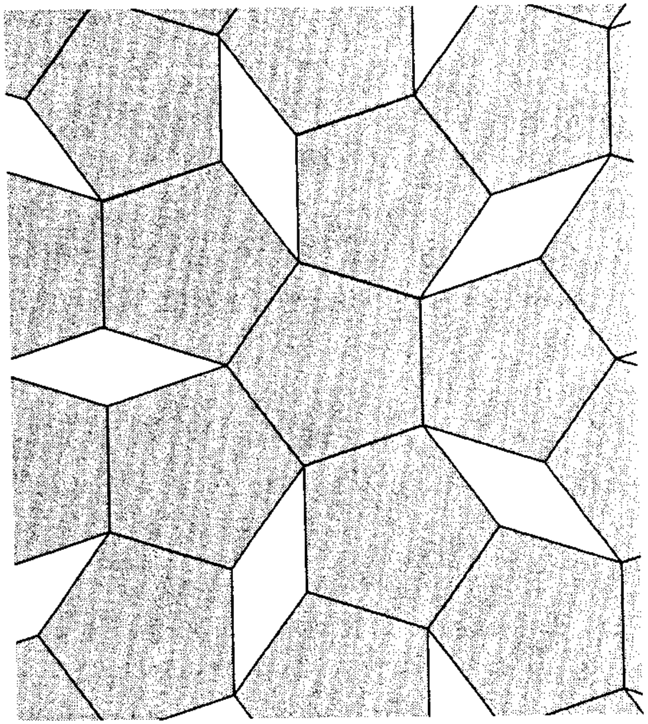
- A **primitive cell** or **primitive unit cell** is a volume of space that when translated through all the vectors in a Bravais lattice just fills all of space without either overlapping itself or leaving voids.
- A primitive cell must contain precisely one lattice point.

Fundamental Types of Lattices

- Crystal lattices can be mapped into themselves by the lattice translations **T** and by various other symmetry operations.
- A typical symmetry operation is that of rotation about an axis that passes through a lattice point. Allowed rotations of : 2 π, 2π/2, 2π/3,2π/4, 2π/6
- (Note: lattices do not have rotation axes for 1/5, 1/7 …) times 2π

Five fold axis of symmetry cannot exist

Figure 7 A fivefold axis of symmetry cannot exist in a periodic lattice because it is not possible to fill the area of a plane with a connected array of pentagons. We can, however, fill all the area of a plane with just two distinct designs of "tiles" or elementary polygons. A quasicrystal is a quasiperiodic nonrandom assembly of two types of figures. Quasicrystals are discussed at the end of Chapter 2.



Two Dimensional Lattices

- There is an unlimited number of possible lattices, since there is no restriction on the lengths of the lattice translation vectors or on the angle between them. An **oblique lattice** has arbitrary **a1** and **a2** and is invariant only under rotation of π and 2 π about any lattice point.

Symmetry Elements

- The ***identity*** operation.
- The ***reflection*** operation about a plane
- The ***inversion*** operation. If the resulting object is *indistinguishable* from the original, is because the inversion center is inside the object.
- The ***rotation*** operations (both *proper* and *improper*) occur with respect to a line called the rotation axis.
- *a)* A *proper* rotation is performed by rotating the object 360°/*n*, where *n* is the order of the axis.
  b) An *improper* rotation is performed by rotating the object 360°/*n* followed by a reflection through a plane perpendicular to the rotation axis

Point Group Symmetry

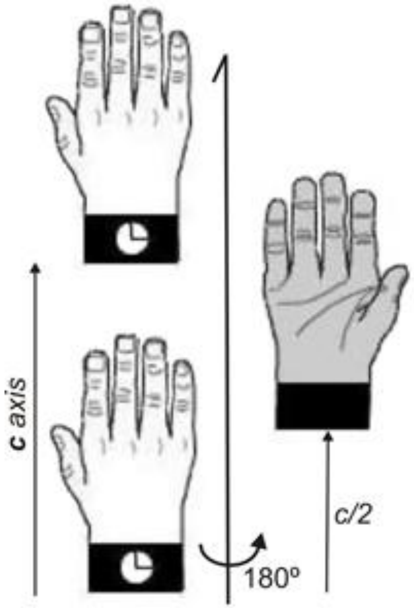
- Point group symmetry is when all symmetry operations act on a point, i.e. no translational symmetry.

- There are many ***symmetry point groups***, but in crystals they must be consistent with the crystalline periodicity thus **5**-fold and **7**-fold axes are not possible in crystals and therefore only ***32 point groups*** are allowed in the crystalline state of matter. These ***32 point groups*** are also known in Crystallography as the ***32 crystal classes***

Translational Symmetry Elements

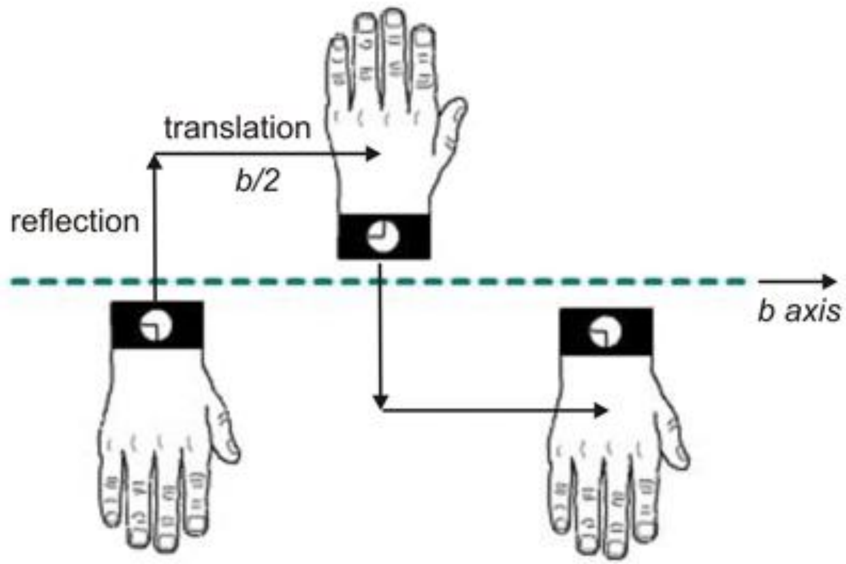
- Combining the rotation axes and the mirror planes with the characteristic translations of the crystals, new symmetry elements appear with some "sliding" components: ***screw axes*** and ***glide planes***.

Screw Axes



A $\mathbf{2_1}$ screw axis in the ***c*** direction. A rotation of 180 followed by a translation of *c*/2 along the ***c*** axis. In general the notation for a crew axis is n_m where n is the order of the rotation axis and **m/n** is the amount of translation along a unit cell axis.

Glide Planes



A mirror plane is reflection in a plane followed by translation in a direction parallel to the plane is called a glide plane (in this case an ***a*** glide plane). The glide plane is designated as ***a***, ***b***, or ***c*** if the translation is ***a***/2, ***b***/2, or ***c***/2 and ***n*** if it is (***a*** + ***b***)/2, (***a*** + ***c***)/2, or (***b*** + ***c***)/2.
There is also a diamond (d) glide plane which only occurs in face of body centered unit cells. In this case the translation is: (***a*** + ***b***)/4, (***a*** + ***c***)/4, or (***b*** + ***c***)/4.

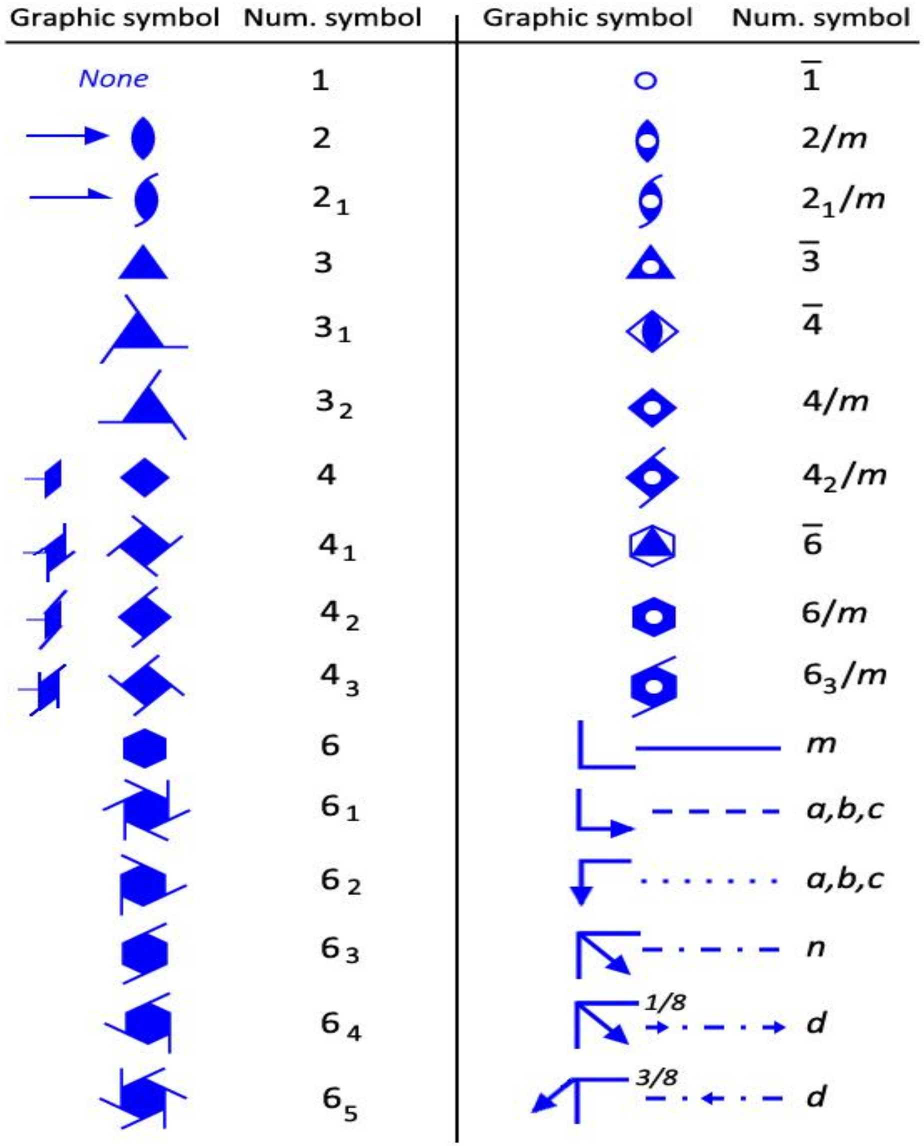
Symmetry Elements and Equivalent Positions

- In order to discuss the effect of symmetry we have to consider its effect on the general (arbitrary) position, ***x, y, z***.
- The operation acts to produce new coordinates for equivalent positions, i.e. sites identical in all respects as seen by the molecule.
- This is shown by the following tables.

TABLE 3.2 Some Symmetry Elements and Their Equivalent Positions

		Equivalent Positions	
Axis 2	Parallel to a	x, y, z	$x, \bar{y}, \bar{z}$
2	b	x, y, z	$\bar{x}, y, \bar{z}$
2	c	x, y, z	$\bar{x}, \bar{y}, z$
2_1	a	x, y, z	$x+\frac{1}{2}, \bar{y}, \bar{z}$
2_1	b	x, y, z	$\bar{x}, y+\frac{1}{2}, \bar{z}$
2_1	c	x, y, z	$\bar{x}, \bar{y}, z+\frac{1}{2}$
Plane m	Perpendicular to a	x, y, z	$\bar{x}, y, z$
m	b	x, y, z	$x, \bar{y}, z$
m	c	x, y, z	$x, y, \bar{z}$
a	b	x, y, z	$x+\frac{1}{2}, \bar{y}, z$
a	c	x, y, z	$x+\frac{1}{2}, y, \bar{z}$
b	a	x, y, z	$\bar{x}, y+\frac{1}{2}, z$
b	c	x, y, z	$x, y+\frac{1}{2}, \bar{z}$
c	a	x, y, z	$\bar{x}, y, z+\frac{1}{2}$
c	b	x, y, z	$x, \bar{y}, z+\frac{1}{2}$
n	a	x, y, z	$\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$
n	b	x, y, z	$x+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$
n	c	x, y, z	$x+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$
d	a	x, y, z	$\bar{x}, y+\frac{1}{4}, z+\frac{1}{4}$
d	b	x, y, z	$x+\frac{1}{4}, \bar{y}, z+\frac{1}{4}$
d	c	x, y, z	$x+\frac{1}{4}, y+\frac{1}{4}, \bar{z}$

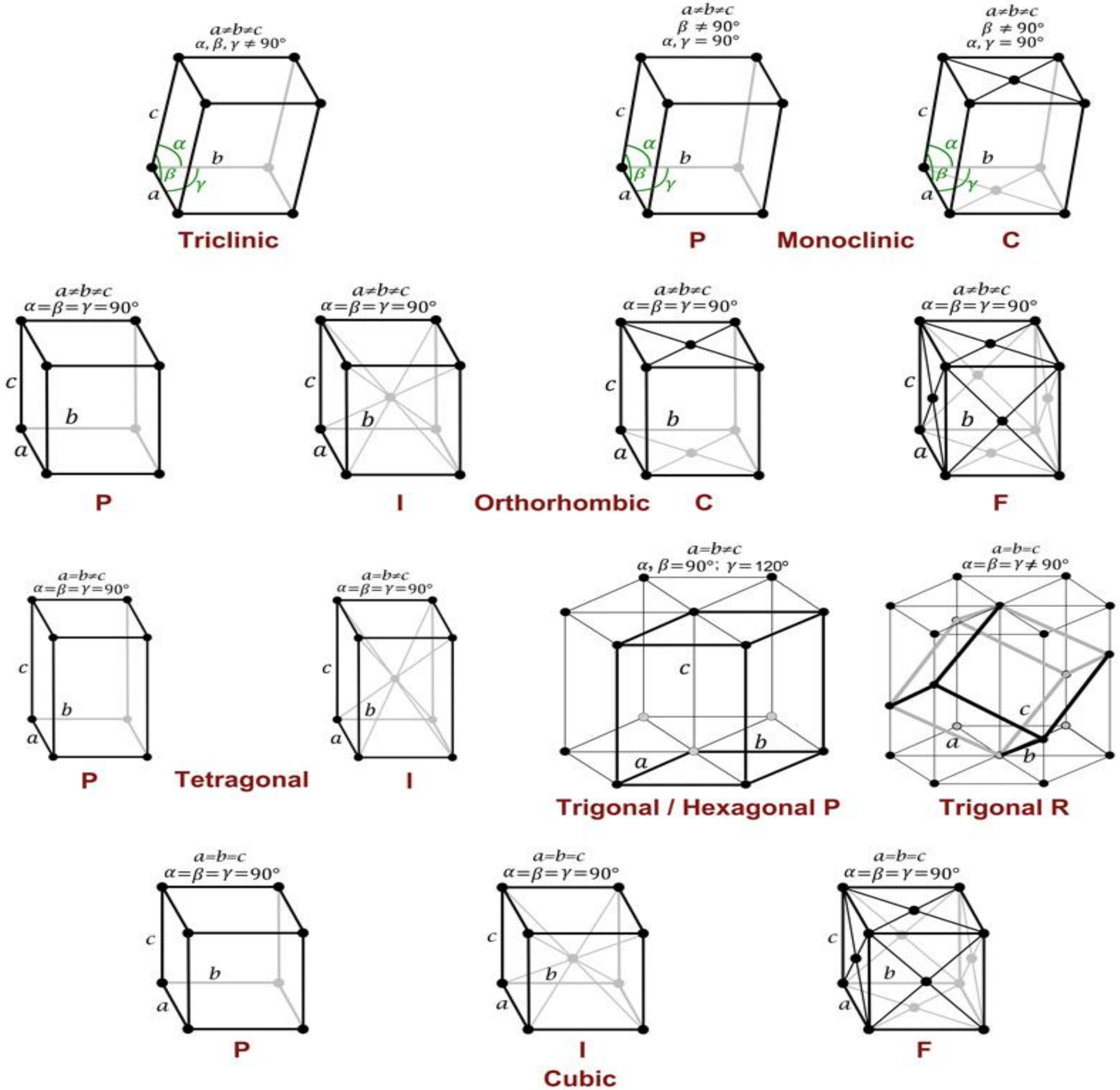
Symbols for Space Groups



Bravais Lattices

- In addition, the repetition modes by translation in crystals must be compatible with the possible point groups (the 32 crystal classes), and this is why we find only ***14 types of translational lattices*** which are compatible with the crystal classes. These types of lattices (translational repetition modes) are known as the ***Bravais lattices.***

14 Bravais Lattices



Primitive vs Non-Primitive Lattices

- There are 7 primitive and 7 non-primitive Bravais lattices.
- In any array of lattice points it is always possible to choose a primitive triclinic cell regardless of the symmetry present.
- However this neglects simplification provided by symmetry.
- Cardinal rule is to choose the cell so that it conforms to symmetry actually present.
- In addition there are some conventions to bring a degree of standardization to the choice of cell.
- This is illustrated in the next slide.

I vs C in Monoclinic Cells

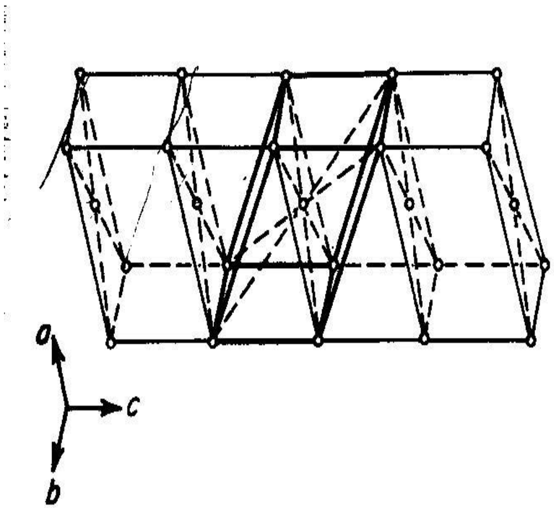


Figure 3.14. Choice of *C* or *I* unit cells in monoclinic lattices.

In this example the unit cells outlined by light grid lines have their *ab* faces centered and thus correspond to a *C* lattice.

An alternative (and equally good) set of unit cells is illustrated by the cell outlined in heavy lines

Those points formerly at the centers of the *ab* faces are now at the body center of the new cell and thus this cell would be designated as *I.*

By convention the C cell is chosen.

However sometimes *I* is chosen for convenience of structural reasons (choice of axes by diffractometer to make *β* as close to 90 as possible).

Space Groups

- Space groups are designated by the type of Bravais lattice symbol (***P, A, B, C, I,*** or ***F***) along with symbols representing the necessary and sufficient symmetry operations to define the group.
- Combining the 32 allowed point groups with the 14 Bravais lattices leads to 230 space groups.
- We will look start with the simplest case and build up to more complex cases.

Space Groups from Point Group 1: **P1** SG #1

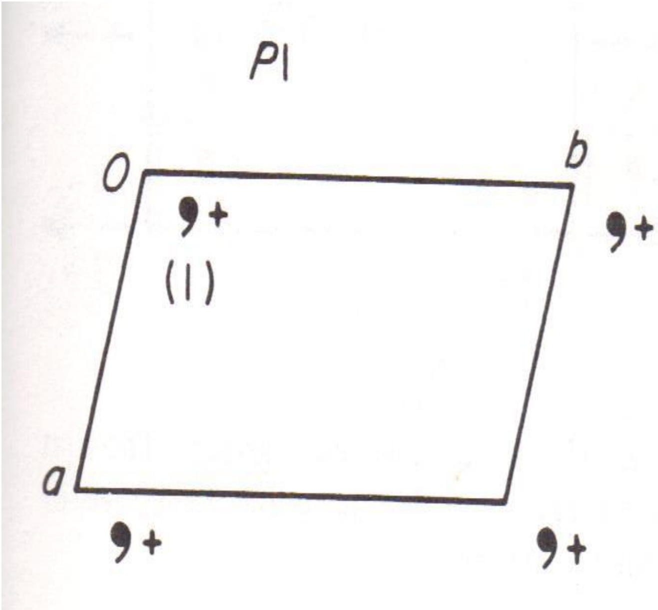


Figure 3.23. *P*1, equivalent positions *x*, *y*, *z*.

Unit cell is always drawn with the origin at the top right hand corner, the ***b*** axis to the right and the ***a*** axis down the page.
We use a motif (**,**) to symbolize a general position in the unit cell and then use the symmetry elements to generate equivalent positions
Since the diagram is 2-D we use (**+**) to symbolize position along the z axis.
All lattice points have to be equivalent by definition.
We note that there is only one lattice point inside the unit cell so the general multiplicity of this SG is 1.

From Point Group -1: **P-1** SG #2

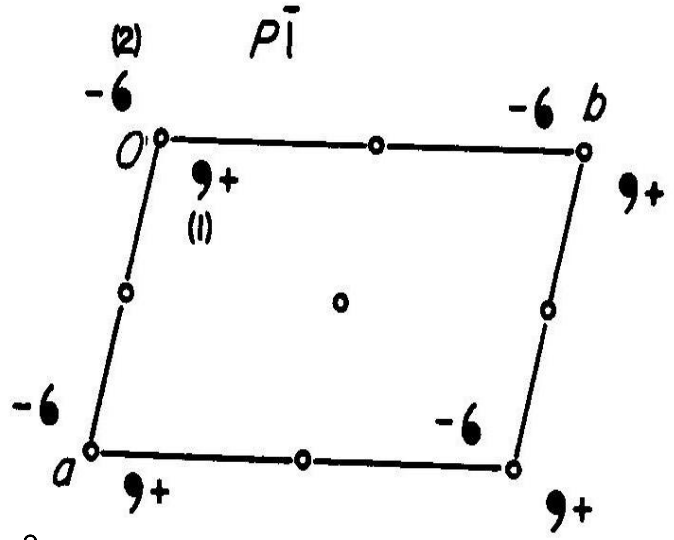


Figure 3.24. $P\bar{1}$, equivalent positions (1) x, y, z; (2) $\bar{x}, \bar{y}, \bar{z}$.

Centers of inversion are represented by °.
Since the environment of all lattice points must be the same these centers must occur at every corner, half way along each edge, at the center of each face, and the body center.
We start with the motif at position (**1**) and then use the symmetry to generate position (**2**).
The general position and its equivalent are given.
We note that there are two lattice points inside the unit cell boundary even though one of them is marked by (-) which means it is outside the cell boundary.
However adding 1 to this z coordinate would bring it inside the unit cell so the general multiplicity of this SG is 2.

Space Groups from Point Group 2, m or 2/m

- The next three point groups either have a 2-fold axis, a mirror plane or both.
- These are inconsistent with the triclinic system but are consistent with the monoclinic system.

P2 SG #3

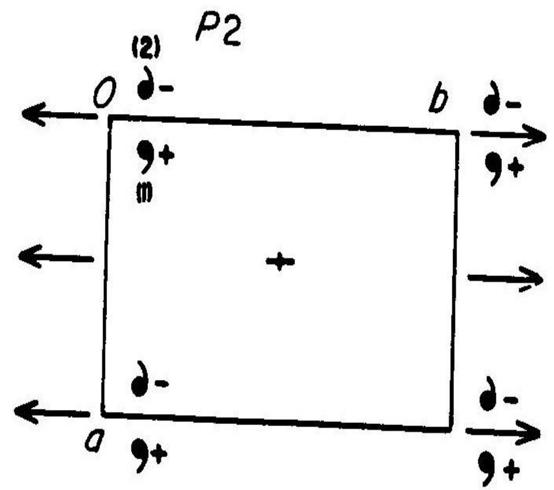


Figure 3.25. *P*2, equivalent positions (1) x, y, z; (2) $\bar{x}, y, \bar{z}$.

Note the use of → and ← to symbolize the 2-fold symmetry along the ***b*** axis. Commencing with position (**1**) we use this symmetry to generate position (**2**).

All other motifs are generated using the fact that the environment about each lattice point has to be identical.

The general position and its symmetry equivalent are listed.

We note that there are two lattice points inside the unit cell boundary so the general multiplicity of this SG is 2.

Space group #4; **$P2_1$**

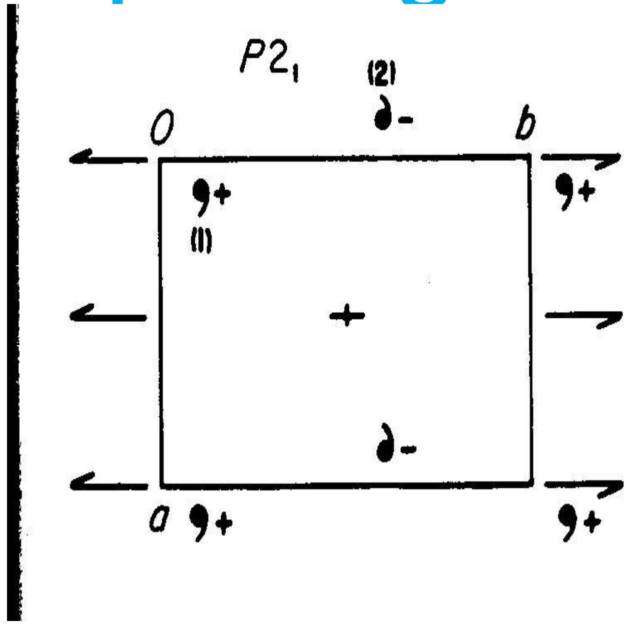


Figure 3.26. $P2_1$, equivalent positions (1) x, y, z; (2) $\bar{x}, y+\frac{1}{2}, \bar{z}$.

Note the use of symbols to designate the ***2_1*** axis in the ***b*** direction
Starting from position (**1**) we generate position (**2**) by rotating about the ***b*** axis followed by translation of ***b***/2 in the ***b*** direction.
All other motifs are generated using the fact that the environment about each lattice point has to be identical.
The general position and its symmetry equivalent are listed.
We note that there are two lattice points inside the unit cell boundary so the general multiplicity of this SG is 2.

SG #5: **C2**

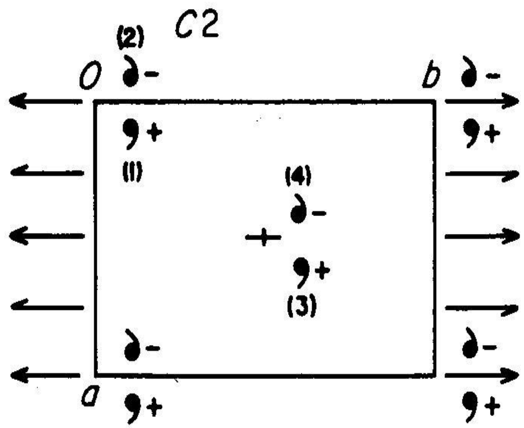


Figure 3.27. $C2$, equivalent positions (1) x, y, z; (2) $\bar{x}, y, \bar{z}$; (3) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (4) $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$.

This is a non-primitive ***C***-centered lattice so for every ***x, y, z*** position there will be an equivalent ***½+x, ½+y, z*** position.
The combination of ***C***-centering and the 2-fold rotation axis leads to the presence of $\boldsymbol{2_1}$ axes at ***a***/4 and 3***a***/4, midway between the 2-fold axes.
This will be seen as we generate all the equivalent positions using both the ***C***-centering and ***2***-fold axes.
From (***1: x, y, z***) using the 2-fold we get (***2: -x, y, -z***).
Then using the ***C***-centering we get (***3: ½+x, ½+y, z***).
Then using the 2-fold at ***a***/2 we get (***4: ½-x, ½+y, -z***).
But we can go from (***1***) to (***4***) directly by using the $\boldsymbol{2_1}$ at ***a***/4.
Thus we have ***proved the existence of this addition symmetry element*** by combining ***C***-centering with a 2-fold rotation axis.

Point Group m, SG #6 **Pm**

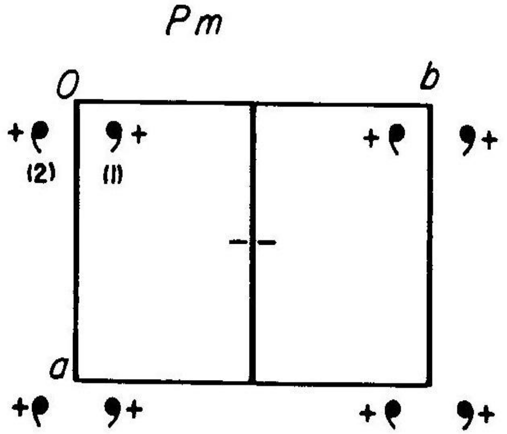


Figure 3.29. *Pm*, equivalent positions (1) x, y, z; (2) $x, \bar{y}, z$.

Mirror planes have to be perpendicular to ***b*** axis and are shown as heavy lines with one at ***b***/2.

Position (**2**) generated from position (**1**) by the mirror plane.

Two motifs inside cell and 2 general positions.

SG #7: **Pc**

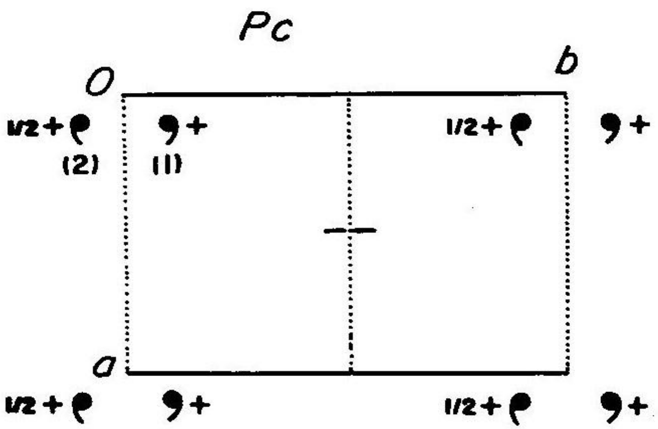


Figure 3.30. *Pc*, equivalent positions (1) x, y, z; (2) $x, \bar{y}, z+\frac{1}{2}$.

This space group is similar to the diagram for ***Pm*** except that the ***c*** glide planes (shown as dotted lines) replace the mirror planes.

Position (**2**) from position (**1**) by the ***c*** glide. We note the reflection through mirror followed by translation of ***c***/2

Two motifs inside boundaries of cell thus two general positions.

SG #8: **Cm**

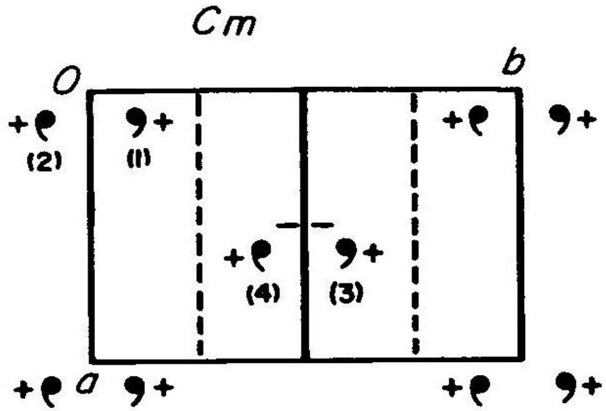


Figure 3.31. Cm, equivalent positions (1) x, y, z; (2) $x, \bar{y}, z$; (3) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (4) $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$.

This space group combines ***C***-centering with mirror planes coincident with ***B*** faces and at ***b***/2.

The combination of ***C***-centering and mirror planes generates a glide planes at ***b***/4 and 3***b***/4.

Starting from position (**1**), position (**2**) is generated by the mirror plane, then position (**3**) is generated by the ***C***-centering, followed by position (**4**) due to the mirror plane at ***b***/2.

It can be seen that going directly from (**1**) to (**4**) requires the presence of an ***a*** glide at ***b***/4 and thus proves the existence of this symmetry element.

In this space group there are 4 general positions.

SG #9: **Cc**

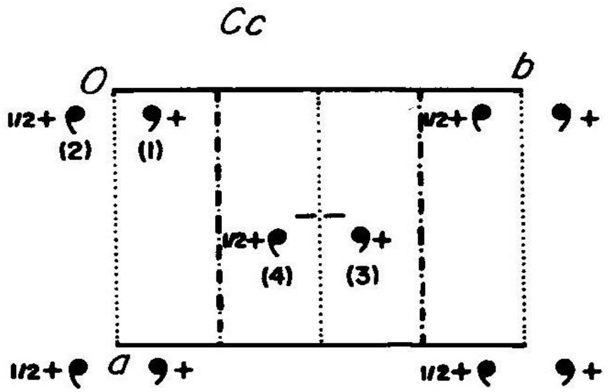


Figure 3.32. *Cc*, equivalent positions (1) x, y, z; (2) $x, \bar{y}, z+\frac{1}{2}$; (3) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (4) $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$.

The **B** faces contain the ***c*** glide planes indicated by the dotted lines.
The combination of ***C***-centering with ***c*** glide planes produces n glide planes at ***b***/4 and 3***b***/4.
Starting with the general position (**1**), position (**2**) is generated by the ***c*** glide plane.
From (**1**), position (**3**) in generated by the ***C***-centering.
From position (**3**), position (**4**) is generated by the ***c*** glide plane at ***b***/2
Position (**4**) is related to position (**1**) by the ***n*** glide plane.
There are 4 motifs inside the boundaries of the box leading to 4 general positions in this space group.

Point Group 2/m

- Combining 2/m with a P lattice leads to SG’s P2/m, $P2_1/m$, P2/c and $P2_1/c$.
- The symmetry elements 2/m correspond to a center of symmetry so these SG’s are centrosymmetric.
- Choosing the 2-fold axis coincident with b and the mirror planes coincident with B faces places the center of symmetry at the origin.
- We will only discuss SG’s P2/m and P21/c

SG #10: **P2/m**

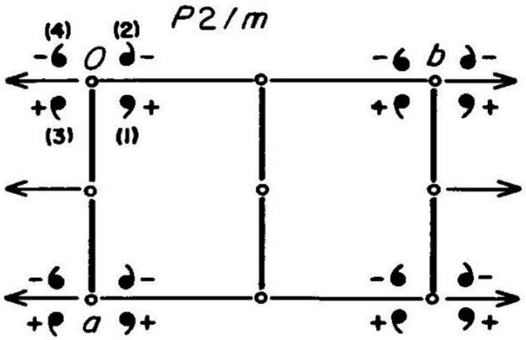


Figure 3.33. $P2/m$, equivalent positions (1) x, y, z; (2) $\bar{x}, y, \bar{z}$; (3) $x, \bar{y}, z$; (4) $\bar{x}, \bar{y}, \bar{z}$.

Center of symmetry at origin, 2-fold axes along ***b*** axis and at ***a***/2.

Mirror planes in ***B*** face and at ***b***/2.

These elements generate positions (**2**), (**3**), and (**4**) from position (**1**)

Four motifs inside boundaries so general multiplicity of 4 for this SG.

SG's **P2$_1$/m**, **P2/c** & **P2$_1$/c**

- For crystallographic computing reasons the origin is usually chosen to be a center of symmetry if possible.
- For these SG's the centers do not lie at intersection of planes and axes because both 2_1 and c involve translations.
- We have to move these elements to allow the center to be the origin.
- This is shown on next slide.

Shift of Origin

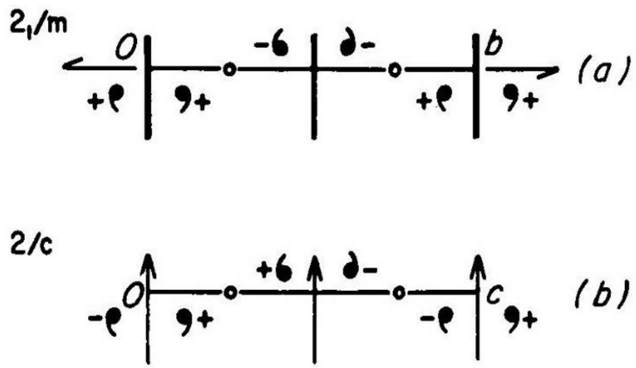


Figure 3.34. (*a*) $2_1/m$ with screw in *b* direction and mirrors at $b = 0, \frac{1}{2}$. (*b*) $2/c$ with *c*-glide perpendicular to *b* and axes at $c = 0, \frac{1}{2}$.

In diagram (a) the $\boldsymbol{2_1}$ is along ***b*** with mirror planes in ***B*** face and at ***b***/2.

Centers are seen at ***b***/4 and 3***b***/4 and mirror planes at ***b*** = 0 and ***b*** = ½.

Shifting the center to the origin by the translation of ***b*** = -½ will put the mirrors at ***b***/4 and –***b***/4 (equivalent to 3***b***/4).

For ***2/c*** In diagram (b) shows center at ***c***/4 and 4***c***/4 with 2-fold axes at ***c*** = 0 and ***c*** = ½.

Shifting the center to the origin by the translation of ***c*** = -½ will put the 2-fold axes at ***c***/4 and –***c***/4 (equivalent to 3***c***/4).

For $\boldsymbol{2_1/c}$ a similar origin shift will place the $\boldsymbol{2_1}$ axes at ***c***/4 and 3***c***/4

SG #14: **$P2_1/c$**

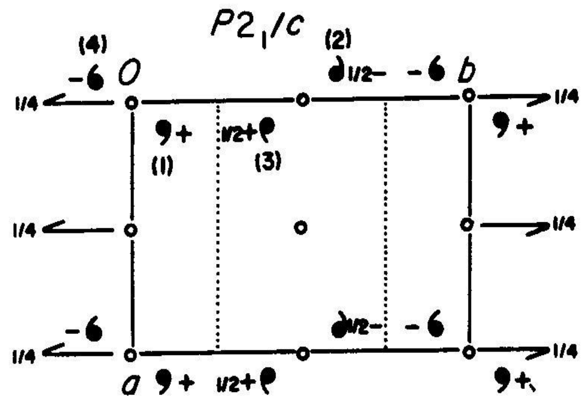


Figure 3.37. $P2_1/c$, equivalent positions (1) x, y, z; (2) $\bar{x}, y+\frac{1}{2}, \bar{z}+\frac{1}{2}$; (3) $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$; (4) $\bar{x}, \bar{y}, \bar{z}$.

Note that the ***2_1*** axes are at ***c***/4 (and 3***c***/4).

Thus going from (**1**) at *x, y, z* to (**2**) will be at *–x, y* + *½, ½* - *z* using the ***2_1*** at ***c***/4.

From (**2**) to (**3**) we use the center at ***b***/2 or to go from (**1**) to (**3**) we use the ***c*** glide at ***b***/2.

To go from (**1**) to (**4**) we use the center at the origin.

Space groups

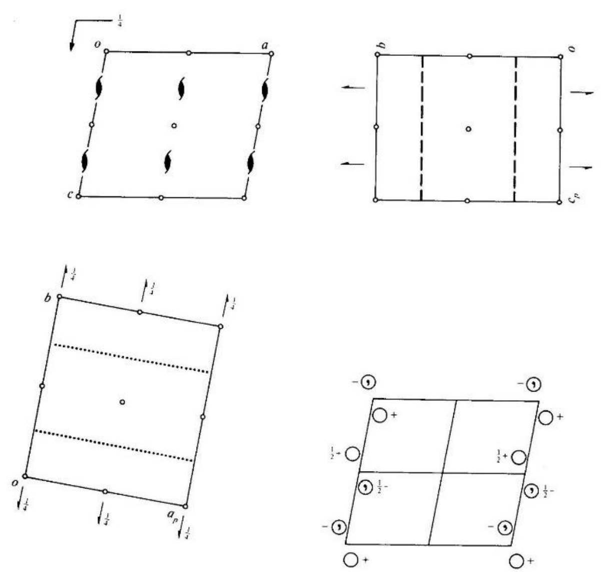
- All 230 Space groups are listed in **International Tables for Crystallography Volume A** in the standard setting as well as some non-standard settings for the more common space groups.
- There is much useful information for each SG.
- The pages for ***$P2_1/c$*** are shown next.

$P2_1/c$ Page 1

$P\,2_1/c$ C_{2h}^5 $2/m$ **Monoclini**

No. 14 $P\,1\,2_1/c\,1$ Patterson symmetry $P\,1\,2/m$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \leq x \leq 1$; $0 \leq y \leq \frac{1}{4}$; $0 \leq z \leq 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{2},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ $0,0,0$ (4) c $x,\frac{1}{4},z$

$P2_1/c$ Page 2

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
4 e 1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
					Special: as above, plus
2 d $\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2 c $\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2 b $\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2 a $\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

Symmetry of special projections

Along [001] $p\,2gm$
$\mathbf{a}'=\mathbf{a}_p$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $p\,2gg$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$
Origin at $x,0,0$

Along [010] $p\,2$
$\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2]$P\,1\,2_1\,1\,(P\,2_1)$ 1; 2
[2]$P\,\bar{1}$ 1; 3
[2]$P\,1\,c\,1\,(P\,c)$ 1; 4

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3]$P\,1\,2_1/c\,1\,(\mathbf{b}'=3\mathbf{b})(P\,2_1/c)$; [2]$P\,1\,2_1/c\,1\,(\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a},\mathbf{c}'=2\mathbf{a}+\mathbf{c})(P\,2_1/c)$

Minimal non-isomorphic supergroups

I [2]$Pnna$; [2]$Pmna$; [2]$Pcca$; [2]$Pbam$; [2]$Pccn$; [2]$Pbcm$; [2]$Pnnm$; [2]$Pbcn$; [2]$Pbca$; [2]$Pnma$;
[2]$Cmca$

II [2]$C\,1\,2/c\,1\,(C\,2/c)$; [2]$A\,1\,2/m\,1\,(C\,2/m)$; [2]$I\,1\,2/c\,1\,(C\,2/c)$; [2]$P\,1\,2_1/m\,1\,(2\mathbf{c}'=\mathbf{c})(P\,2_1/m)$;
[2]$P\,1\,2/c\,1\,(2\mathbf{b}'=\mathbf{b})(P\,2/c)$

Information of Page 2

- Note the General Multiplicity of the SG and the equivalent positions
- Note the systematic absences that determine the SG (more about systematic absences later)
- Note the special conditions, their coordinates and their site symmetry.

Crystal System Frequency

Crystal System	**Frequency**
Triclinic	20.91%
Monoclinic	*53.16%*
Orthorhombic	20.98%
Tetragonal	2.33%
Trigonal	1.62%
Hexagonal	0.53%
Cubic	0.47%

Space Group Frequency in CSD

Symbol	SG No	Frequency
$P2_1/c$	**14**	**36.0%**
P-1	2	19.9%
$P2_12_12_1$	19	9.2%
C2/c	15	7.3%
$P2_1$	3	5.8%
Pbca	61	3.9%
Pnma	62	1.6%
$Pna2_1$	33	1.6%
Cc	9	1.0%
P1	1	1.0%

Systematic Absences

- Translational symmetry elements, i.e. nonprimitive lattices, screw axes and glide planes give diffraction patterns in which certain classes of reflections are absent.
- In some cases these can be used to unambiguously determine the SG.
- However there are many SG's which are not uniquely defined by their systematic absences.
- Fortunately the 6 most common SG's are uniquely defined by their systematic absences.

Translational Symmetry and Extinctions

TABLE 5.2 Translational Symmetry Elements and Their Extinctions

Symmetry Element	Affected Reflection	Condition for Systematic Absence of Reflection
2-fold screw (2_1) along a	$h00$	$h = 2n + 1 = $ odd
4-fold screw (4_2) along b	$0k0$	$k = 2n + 1$
6-fold screw (6_3) along c	$00l$	$l = 2n + 1$
3-fold screw ($3_1, 3_2$), 6-fold screw ($6_2, 6_4$) along c	$00l$	$l = 3n + 1, 3n + 2$, i.e., not evenly divisible by 3
4-fold screw ($4_1, 4_3$) along a	$h00$	$h = 4n + 1$, 2, or 3
b	$0k0$	$k = 4n + 1$, 2, or 3
c	$00l$	$l = 4n + 1$, 2, or 3
6-fold screw ($6_1, 6_5$) along c[a]	$00l$	$l = 6n + 1$, 2, 3, 4, or 5
Glide plane perpendicular to a		
Translation $b/2$ (b glide)	$0kl$	$k = 2n + 1$
$c/2$ (c glide)		$l = 2n + 1$
$b/2 + c/2$ (n glide)		$k = l = 2n + 1$
$b/4 + c/4$ (d glide)		$k + l = 4n + 1$, 2, or 3
Glide plane perpendicular to b		
Translation $a/2$ (a glide)	$h0l$	$h = 2n + 1$
$c/2$ (c glide)		$l = 2n + 1$
$a/2 + c/2$ (n glide)		$h + l = 2n + 1$
$a/4 + c/4$ (d glide)		$h + l = 4n + 1$, 2, or 3
Glide plane perpendicular to c		
Translation $a/2$ (a glide)	$hk0$	$h = 2n + 1$
$b/2$ (b glide)		$k = 2n + 1$
$a/2 + b/2$ (n glide)		$h + k = 2n + 1$
$a/4 + b/4$ (d glide)		$h + k = 4n + 1$, 2, or 3
A-centered lattice (A)	hkl	$k + l = 2n + 1$
B-centered line (B)		$h + l = 2n + 1$
C-centered lattice (C)		$h + k = 2n + 1$
Face-centered lattice (F)		$h + k = 2n + 1$, $h + l = 2n + 1$, $k + l = 2n + 1$ } i.e., h, k, l not all even or all odd
Body-centered lattice (I)		$h + k + l = 2n + 1$

[a] Note that in the crystal classes in which 3- and 6-fold screws occur as cell axes, these conventionally assigned to be c, so only the $00l$ reflections need be considered.

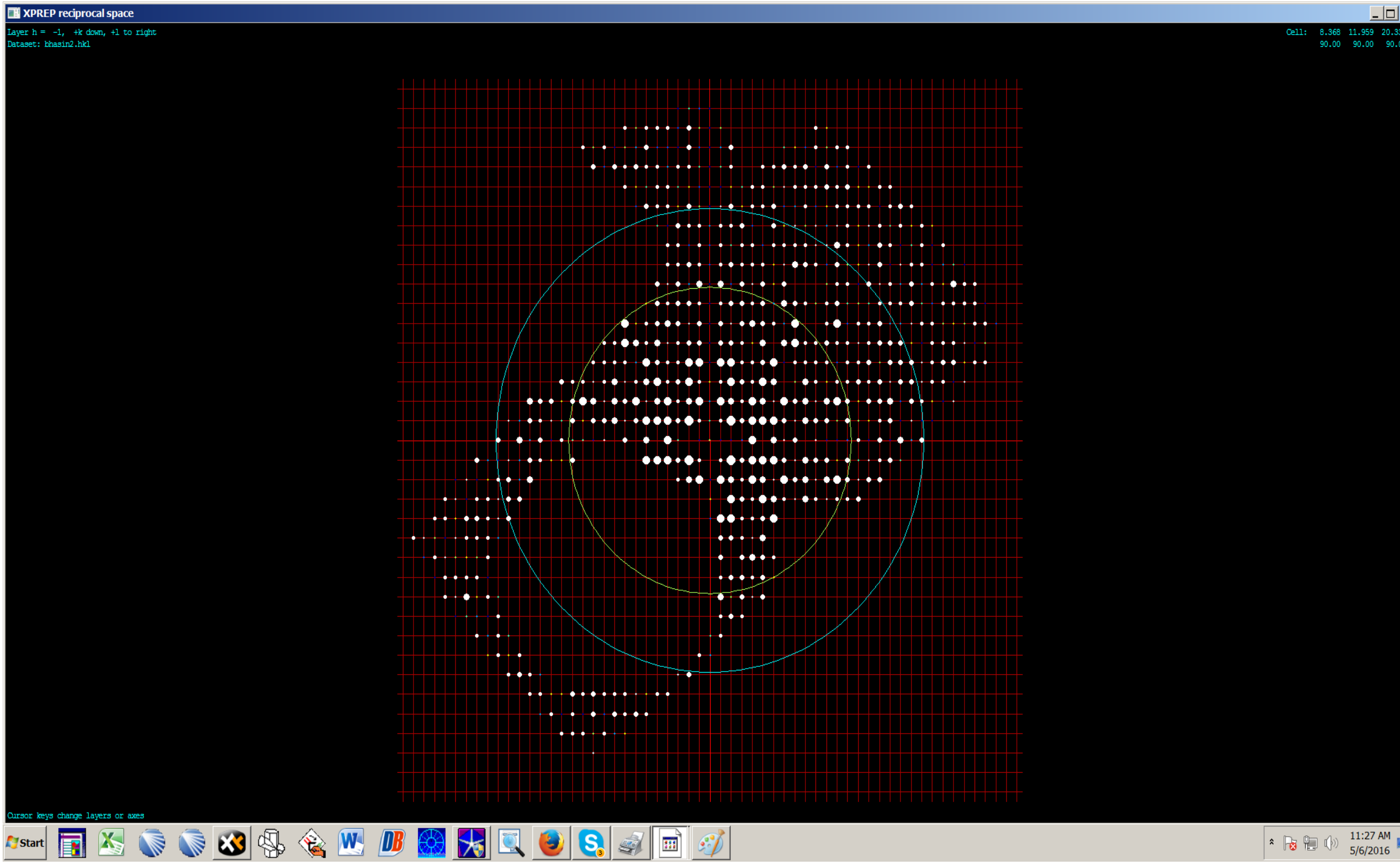
Determining SG from Absences

1. Determine lattice type from general reflections (***hkl***).

2. Find glide planes from ***hk0***, ***h0l***, and ***0kl*** classes.

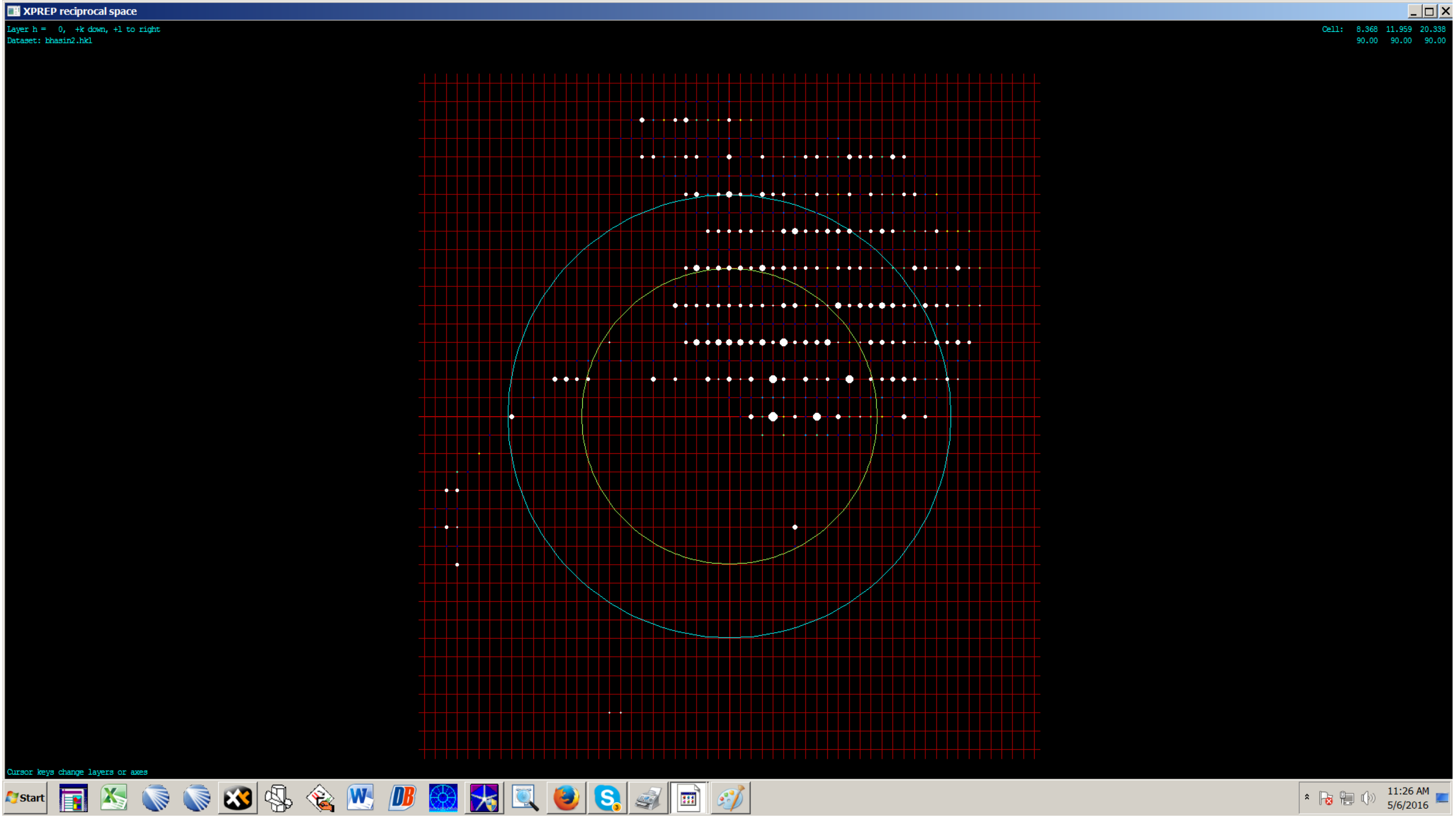
3. If no glide planes, find screw axes from ***h00***, ***0k0***, and ***00l*** classes.

hkl reflections



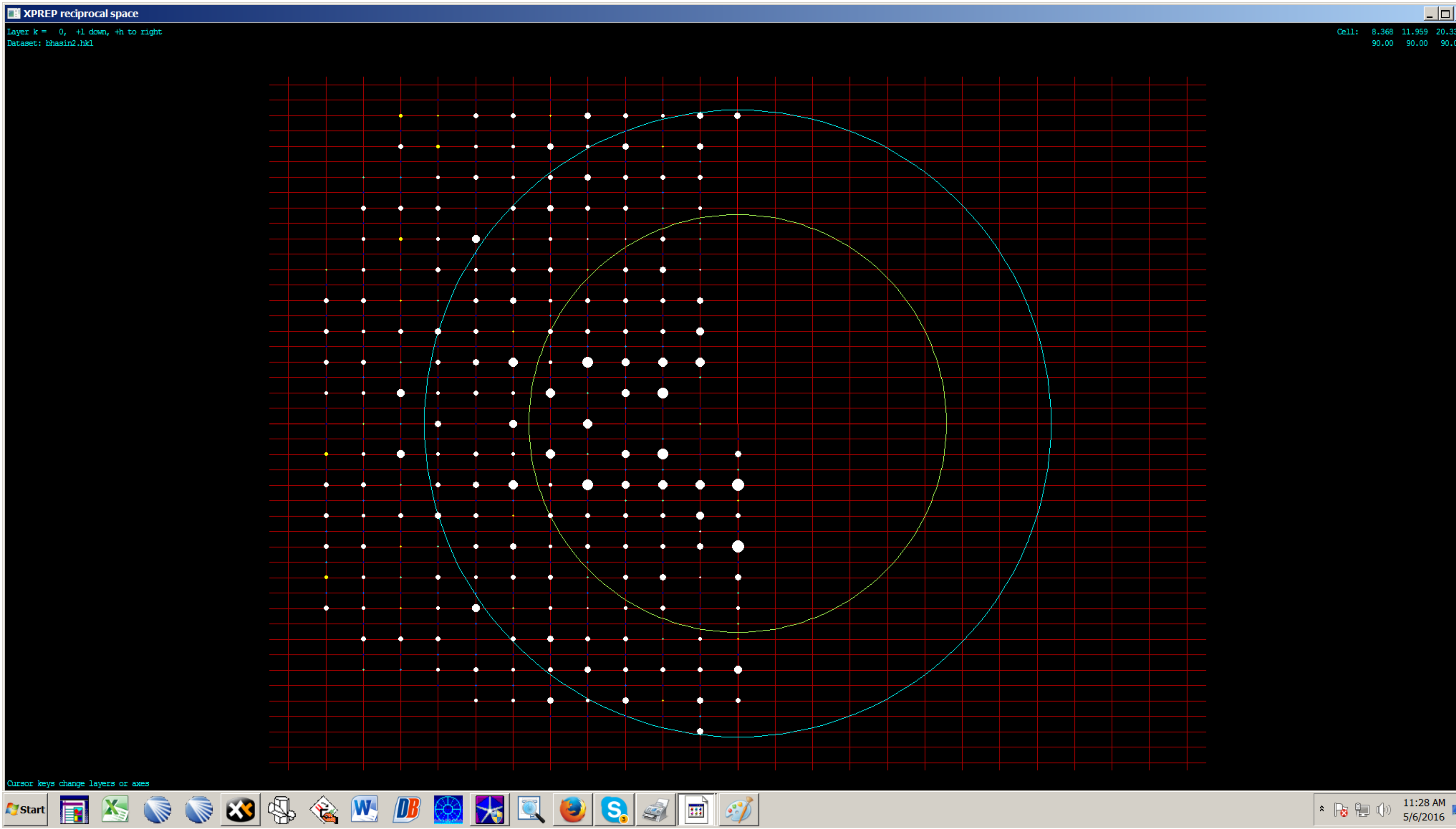
Individual reflections are missing but no systematic absences → ***P*** lattice

0kl reflections



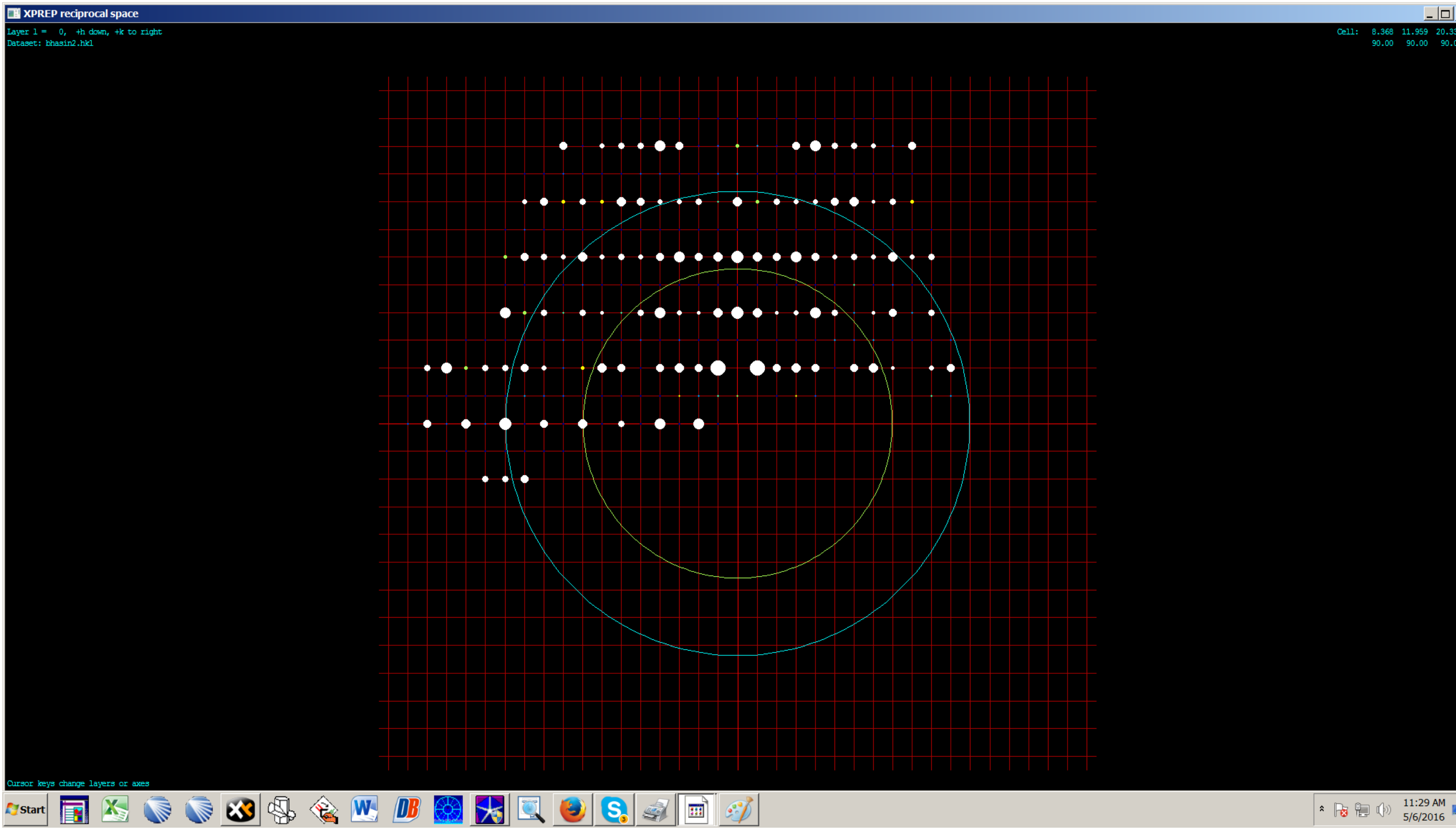
Note that every odd row of ***k*** reflections is systematically absent for the ***hkl*** layer where ***h*** = 0 → indicates the presence of a ***b*** glide plane.

h0l reflections



For ***hkl*** reflections where ***k*** = 0, all odd rows where ***l*** is odd is absent → indicates the presence of a ***c*** glide plane.

hk0 reflections



For the ***hkl*** reflections where ***l*** = 0, all rows where ***h*** is odd are absent → indicates the presence of an ***a*** glide plane

Space group determination

- From ***hkl*** reflections → ***P*** lattice
- From ***0kl*** reflections → ***b*** glide
- From ***h0l*** reflections → ***c*** glide
- From ***hk0*** reflections → ***a*** glide

- Space group → ***Pbca*** which is uniquely determined, i.e. no other possible SG for these absences.