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Essentials of Unit Cells, Symmetry & Space Groups

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This document contains some tables, diagrams and exercises to enhance your understanding of the concepts and some of the terms concerning symmetry and space groups. This includes, unit cells, lattice points, lattice planes, Miller indices, crystal systems, Bravais lattices, Laue groups, symmetry operators, systematic absences and equivalent positions. The standard reference on crystallographic symmetry is *International Tables for Crystallography, Volume A* (*http://it.iucr.org*). An affordable introduction, with many of the most important features, is the special *Teaching Edition of Volume A*.

The recommended steps for determining which of the 230 space groups is adopted by a structure are summarized below. Of course, we now have excellent software to help and the ability of *SHELXT* to solve the structure and deduce the space group without knowing anything except the correct crystal system relieves us of this effort a lot of the time. Nonetheless, there will always be cases where such automatically obtained results are ambiguous, so it is important to be able to work systematically through all steps of space group determination.

Initially, especially when starting a data collection, if there is any doubt it is wise to consider the lowest likely symmetry first, otherwise only part of the diffraction data may be measured or analyzed. It is always safest to collect at least a hemisphere of data whenever there is doubt.

a. Derive any information possible from the morphology of the crystals or from knowledge that the compound in the crystals must be chiral.
b. Determine the size, shape and volume of the unit cell, which might suggest the crystal system, although this is not yet definitive as only the diffraction symmetry can confirm this.
c. Determine the diffraction symmetry of the crystal (check for the highest Laue class with a low R_{int}) and the Bravais lattice (*P*, *A*, *B*, *C*, *I*, *F* or *R*).
d. Use the 18 Å^3 rule and the known (expected) composition of the crystals to determine how many formula units (*Z*) there are per unit cell. Unusual values suggest that the compound is not what is expected or that solvent molecules might be present. Space groups incompatible with *Z* can be eliminated (*e.g.* a space group with four symmetry-equivalent positions in a unit cell cannot be possible for an asymmetric molecule if there is only room in the unit cell for two of them).

Beyond this point, if there is any doubt, start with the highest possible symmetry first and work downward, only trying lower symmetry when forced to do so. Otherwise, effort may be wasted finding two "independent" molecules, which are actually related, and refining the resulting excess parameters.

e. Determine any symmetry operations which involve translation and are indicated by special conditions for some classes of data (*i.e.* analyze the systematic absences).
f. Use International Tables to check whether a space group has now been determined uniquely. If not, then…
g. Examine the intensity statistics to see whether symmetry operations not involving translation are indicated (centrosymmetric versus non-centrosymmetric and rotation axes).
h. During refinement, pay attention to validation alerts about missed symmetry; check these carefully.

Unit cells

Smallest structural unit from which the entire crystal can be built by *translation only*

Figure 2.1. Regular two-dimensional array.

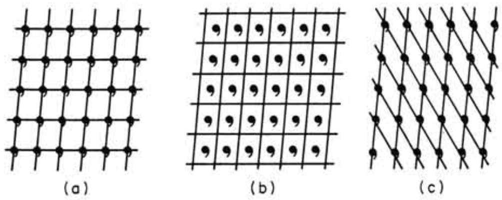


Figure 2.2. Three different grid systems referred to the array of Fig. 2.1.

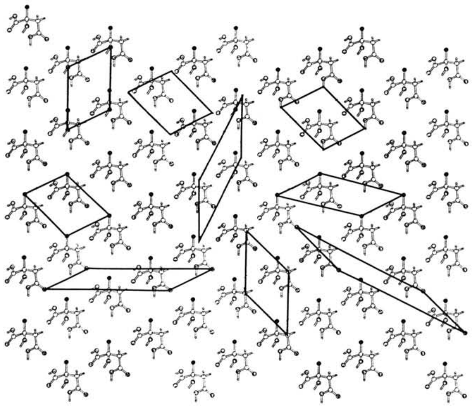


FIGURE 4.1 (cont'd). (b) Diagram illustrating choices of a two-dimensional unit cell from a crystal structure. Each choice encompasses the equivalent of one molecule.

Many choices of shape and origin as long as the volume is completely filled when the “boxes” are stacked in 3 dimensions.

The lattice is a notional grid that is built from stacking the unit cells.

Most figures taken from Stout & Jensen, X-ray Structure Determination – A Practical Guide, 1989

Unit cells and their defining parameters

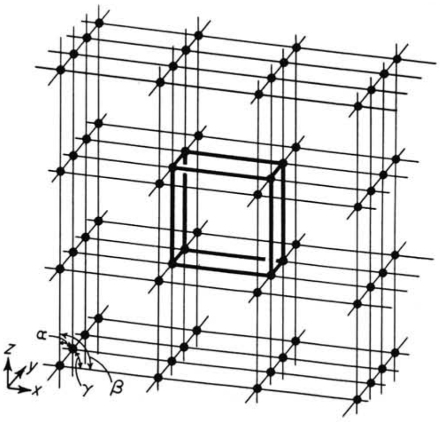


Figure 2.3. Three-dimensional lattice, showing unit cell (heavy lines).

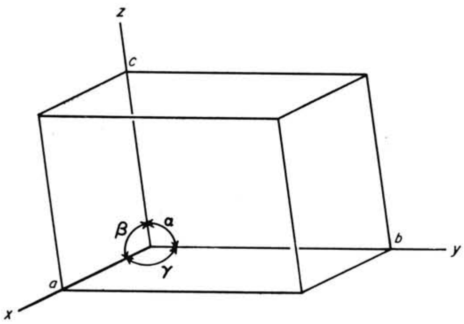


Figure 3.1. Unit cell.

A lattice point is the intersection of the lattice grid or corners of the unit cell (additional lattice points occur in non-primitive unit cells). The view from any lattice point is identical to that from any other lattice point.

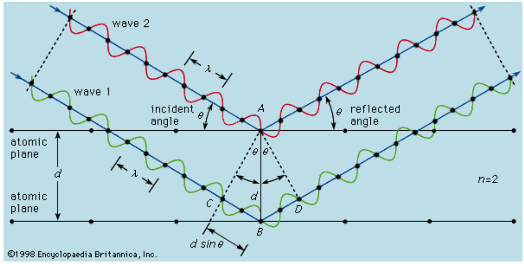
The unit cell edges are ***a***, ***b***, ***c***

The angles between edges are α, β, γ where α is at the intersection of edges ***b*** and ***c***, etc.

Lattice planes

- Families of parallel planes passing through the lattice
- Every lattice point must lie on a member of the family
- Indexed with Miller Indices according to the inverse of the intercept of a plane on the unit cell axes
- Planes parallel to an axis have index 0 for that direction
- Examples at right:
  (1,1) [or (–1,–1)]
  (1,3) [or (–1,–3)]
  (–2,1) [or (2,–1)]

Lattice planes are important because they are notionally what X-rays “reflect” from in the Bragg theory; *e.g.*, the 111 reflection arises from the (111) lattice planes.



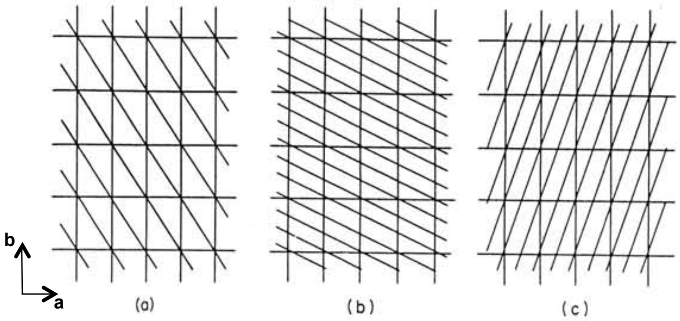
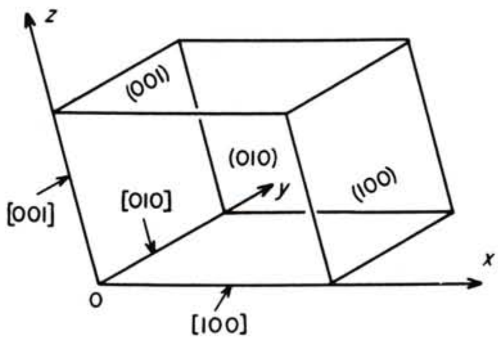


Figure 2.5 Three families of lattice “planes” in a two-dimensional lattice.

Nomenclature of Miller Indices

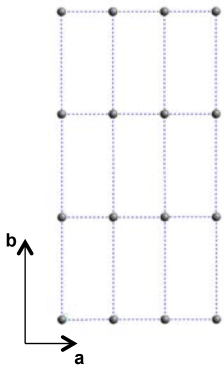
- Vectors are in square brackets, [ ]. [100] is a vector along the *x* axis.
- Lattice planes are in parentheses, ( ). (100) is a family of planes which lies in the *bc*-plane and intersects the *x* axis at 0, *a*, 2*a*, ...
- Families of lattice planes that are related by symmetry are in braces, { }. For a cubic unit cell, {100} depicts the planes corresponding to all unit cell faces, but in a triclinic unit cell {100} refers only to (100) and (–100).
- (*h*00) is a family of planes which lies in the *bc*-plane and intersects the *x* axis at 0, *a*/*h*, 2*a*/*h*, ...

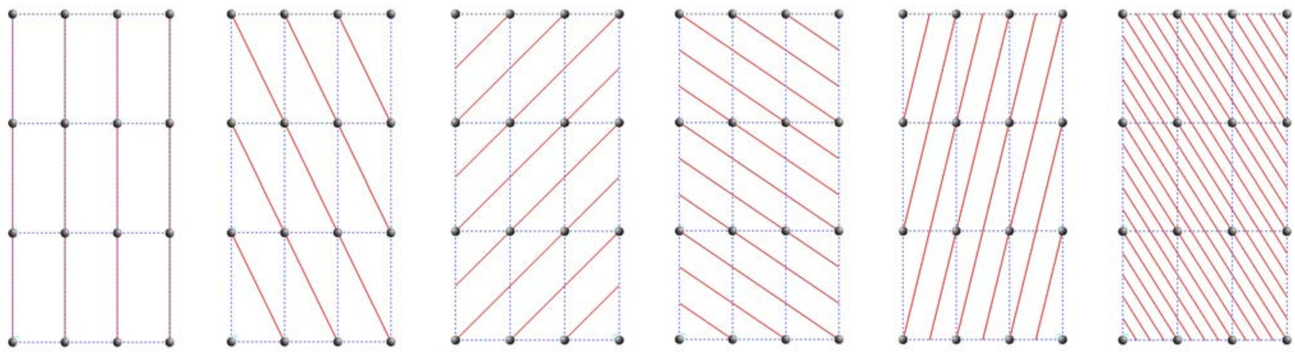


- In general, (*hkl*) is a family of lattice planes which intersects the unit cell axes at *n*(*a*/*h*, *b*/*k*, *c*/*l*), where *n* is an integer.
- (*hkl*) can also refer to a single plane at (*a*/*h*, *b*/*k*, *c*/*l*).

Miller Indices exercise

Given the two-dimensional lattice shown to the right, for each of the six sets of lattice planes shown below, write below the diagram the Miller Indices of that set of lattice planes.





The 7 Crystal Systems

– defined by their rotational symmetry elements, ***not*** the unit cell dimensions

Crystal system	Constraints on unit cell dimensions	Rotational symmetry
Triclinic	$a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$	none
Monoclinic	$a \neq b \neq c$; $\alpha = \gamma = 90°$; $\beta > 90°$	2-fold axis parallel to b
Orthorhombic	$a \neq b \neq c$; $\alpha = \beta = \gamma = 90°$	3 perpendicular 2-fold axes parallel to a, b, c
Tetragonal	$a = b \neq c$; $\alpha = \beta = \gamma = 90°$	4-fold axis parallel to c; two 2-fold axes perpendicular to c
Trigonal		
rhombohedral lattice	$a = b = c$; $\alpha = \beta = \gamma \neq 90°$	3-fold axis along body diagonal
hexagonal lattice	$a = b \neq c$; $\alpha = \beta = 90°$; $\gamma = 120°$	3-fold axis parallel to c
Hexagonal	$a = b \neq c$; $\alpha = \beta = 90°$; $\gamma = 120°$	6-fold axis parallel to c; two 2-fold axes perpendicular to c
Cubic	$a = b = c$; $\alpha = \beta = \gamma = 90°$	3-fold axes along all body diagonals; 4-fold axes parallel to each crystal axis

Lattice symmetry of unit cells

Apply a symmetry operation to an object, or a grid of lattice points, and the object/grid looks the same as before.

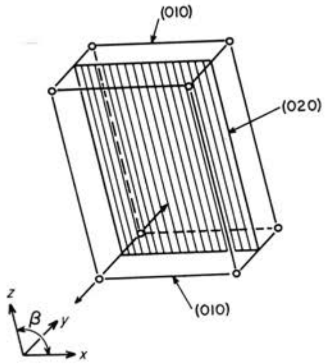


Figure 3.7. Monoclinic unit cell showing two planes of the set (010) and one axis the set [010]. The interleaving mirror plane (020) is also shown.

Monoclinic: one 2-fold axis parallel to the unique axis (**b**-axis)
Mirror plane perpendicular to this axis
➔ 2/*m* symmetry

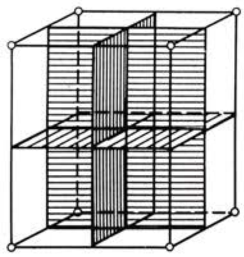


Figure 3.8. Unique mirror planes in an orthorhombic unit cell.

Orthorhombic: three mutually perpendicular mirror planes and three 2-fold axes perpendicular to these
➔ 2/*m* 2/*m* 2/*m* = *mmm*

Tetragonal: one 4-fold axis parallel to the unique axis (**c**-axis)
Mirror plane perpendicular to this axis
→ 4/*m* symmetry

Additionally:
One mirror plane parallel to **c** and to the *ac* cell face; the 4-fold generates a second mirror → designated *m* symmetry

One diagonal mirror plane parallel to **c**; the 4-fold generates a second mirror → *m* symmetry

➔ Overall lattice symmetry: 4/*m m m* = 4/*mmm*

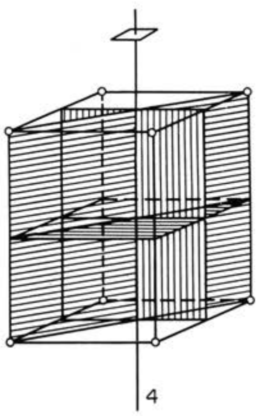
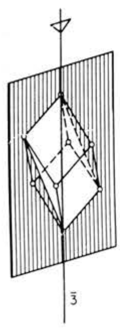


Figure 3.9. Unique mirror planes in a tetragonal unit cell. Other planes present are generated from these by symmetry.



Rhombohedral: one 3-fold rotary inversion axis along the body diagonal

One unique mirror parallel to this; the 3-fold axis generates two other mirrors

➔ –3*m*

Hexagonal: one 6-fold axis parallel to the unique axis (**c**-axis)
Mirror plane perpendicular to this axis
→ 6/*m* symmetry

Additionally:
One diagonal mirror plane parallel to **c**; the 6-fold generates 5 more mirrors every 60° → designated *m* symmetry

One mirror plane parallel to **c** rotated 30° from the above mirror; the 6-fold generates 5 more mirrors every 60° → *m* symmetry

➔ Overall lattice symmetry: 6/*m m m* = 6/*mmm*

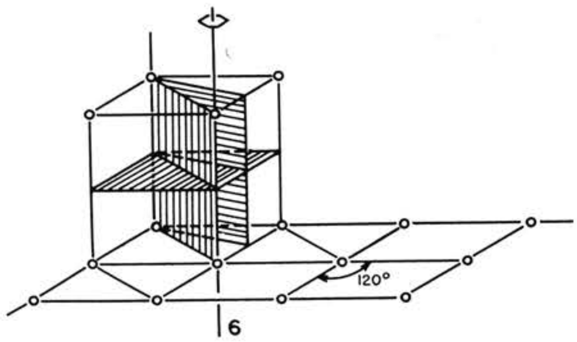


Figure 3.11. Unique mirror planes in a hexagonal unit cell. Other planes present are generated from these by symmetry.

Cubic: three mutually perpendicular mirror planes parallel to the cell axes and three 4-fold axes perpendicular to these
→ 4/*m* symmetry

Additionally:
A 3-fold rotary inversion axis along each of the four body diagonals of the unit cell
→ –3 symmetry

Mirrors along each of the 6 face diagonals and 2-fold axes perpendicular to these through opposite cell edges
→ 2/*m* symmetry

➔ Overall lattice symmetry: 4/*m* –3 2/*m* = *m*–3*m*

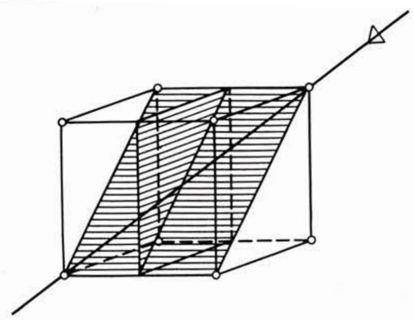


Figure 3.12. Unique mirror planes in a cubic unit cell. Other planes present are generated from these by symmetry.

Primitive and non-primitive unit cells – Bravais Lattices

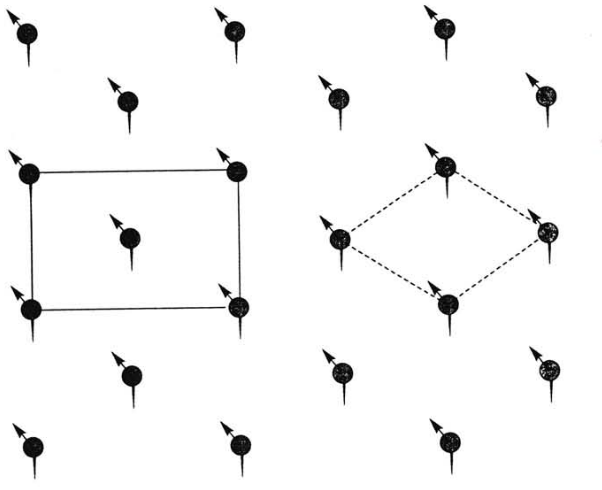


FIGURE 4.1. (a) Symmetry in a repeating pattern. One possible unit cell, indicated by broken lines contains one object per unit cell and is described as "primitive." Another possible unit cell, indicated by solid lines, contains two objects per unit cell and is said to be "centered" (and therefore "nonprimitive"). Thus, while the simplest unit cell is not rectangular, a larger unit cell with higher symmetry, which in this case is rectangular, can readily be picked out from the arrangement of objects.

We aim for the unit cell which uses the most symmetry to describe the structure – it simplifies the structure model and calculations!

The 14 Bravais Lattices

- We add non-primitive unit cells to the 7 crystal systems
- Non-primitive unit cells have additional lattice points to those at the corners
- Non-primitive unit cells simplify description and calculations by allowing increased symmetry to describe more of the unit cell contents

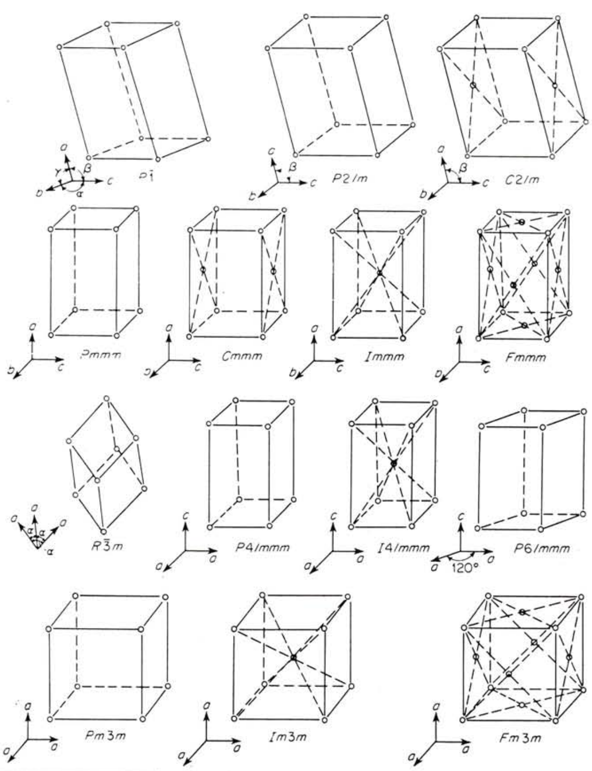


Figure 3.13. The 14 Bravais lattices.

Triclinic	P	
Monoclinic	P C	(C may also be A or I; C is chosen by convention)
Orthorhombic	P C F I	(C may also be A or B)
Tetragonal	P I	
Hexagonal	P	
Rhombohedral	P (usually designated R)	
Cubic	P F I	

Rules for the best unit cell & Bravais Lattice

Transform the unit cell to the one with the highest metric symmetry, provided…

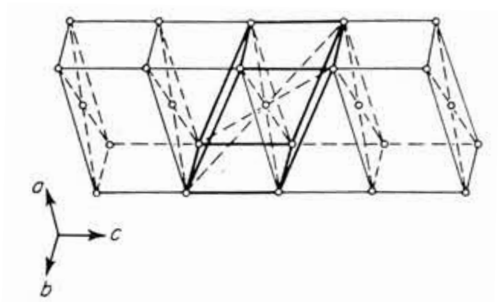
- If the cell volume stays the same, the Bravais lattice cannot change (primitive remains primitive). Example transformation matrix: [1 0 0 / -1 1 0 / 0 0 1].
- If the cell volume increases (double, triple…), the Bravais lattice MUST become non-primitive. If it doesn't, the transformation is invalid.
- If the cell volume and Bravais lattice changes, but the crystal system remains the same, the transformation has not improved the overall symmetry displayed by the unit cell, so the transformation is invalid.
- The transformation must be one of the 44 Niggli matrices.

Tips…

- Primitive triclinic or monoclinic unit cells with two sides equal and the corresponding angles equal, but not 90°, can always be transformed into a C-lattice in the next higher crystal system (volume doubles).

  Example transformation matrix: [1 -1 0 / 1 1 0 / 0 0 1].
- A rhombohedral cell with all angles 60° is more likely to be cubic.

Monoclinic *C* and *I* lattices are equivalent. Choose the one that gives β closest to 90°.



Monoclinic *B* and tetragonal *C* lattices do not increase the symmetry − keep *P*.

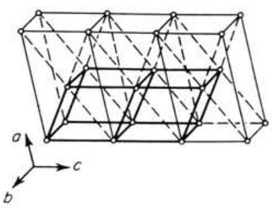


Figure 3.15. Relationship between monoclinic *B* and *P* lattices.

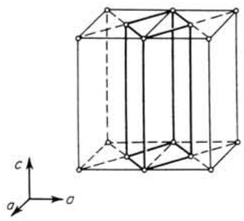


Figure 3.16. Relationship between tetragonal *C* and *P* lattices.

Hexagonal can be described using an "orthohexagonal" orthorhombic *C* lattice. Useful in special cases or for structure comparisons.

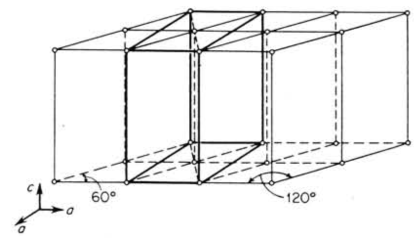
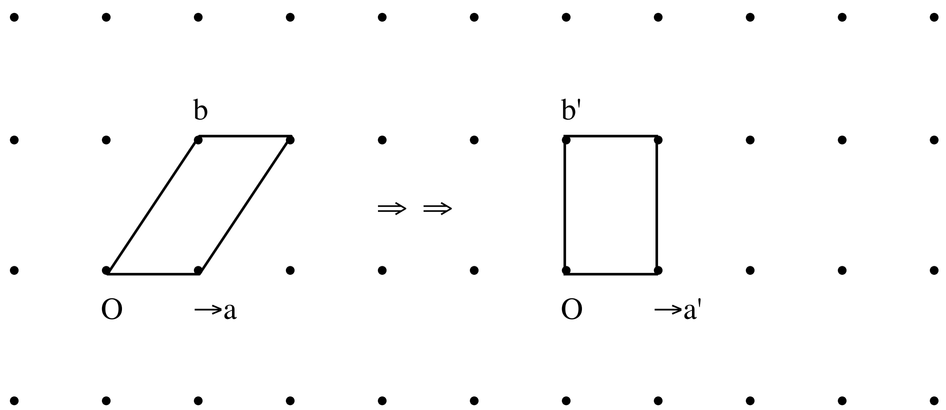


Figure 3.17. Possible choice of an orthorhombic unit cell in the hexagonal system.

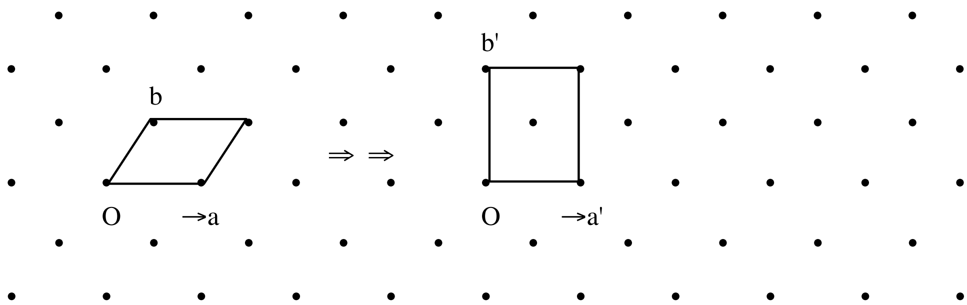
Bravais Lattice exercise

For all of the following, the c-axis comes directly out of the page.

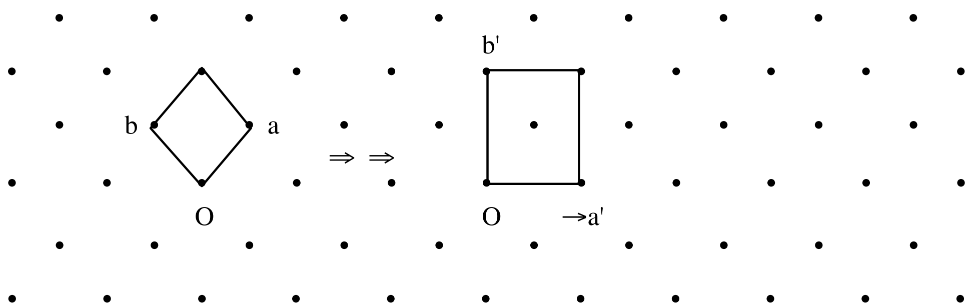
1. Transformation allowed as monoclinic becomes orthorhombic, but the volume remains the same, so the Bravais lattice remains primitive. a' = , b' = , c' = .
Matrix: [/ /].



2. Transformation allowed as monoclinic becomes orthorhombic. Volume doubles and Bravais lattice becomes non-primitive (C). a' = , b' = , c' = .
Matrix: [/ /].

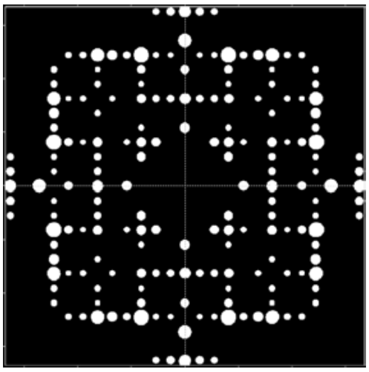


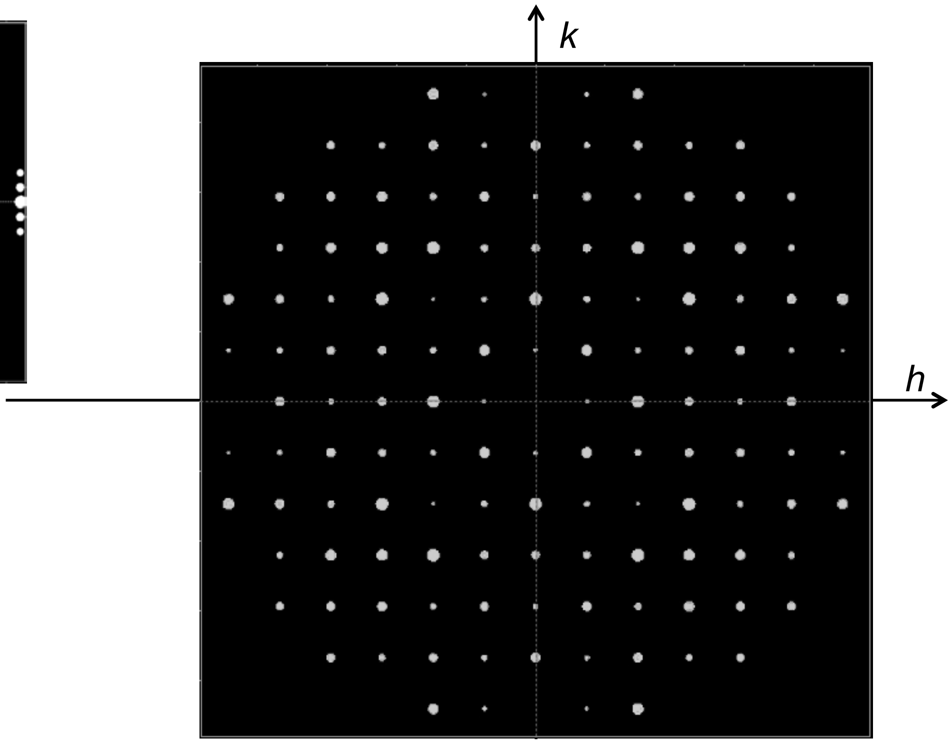
3. The same lattice as previously, just the initial primitive cell was chosen differently. Transformation allowed as monoclinic becomes orthorhombic. Volume doubles and Bravais lattice becomes non-primitive (C). a' = , b' = , c' = .
Matrix: [/ /].



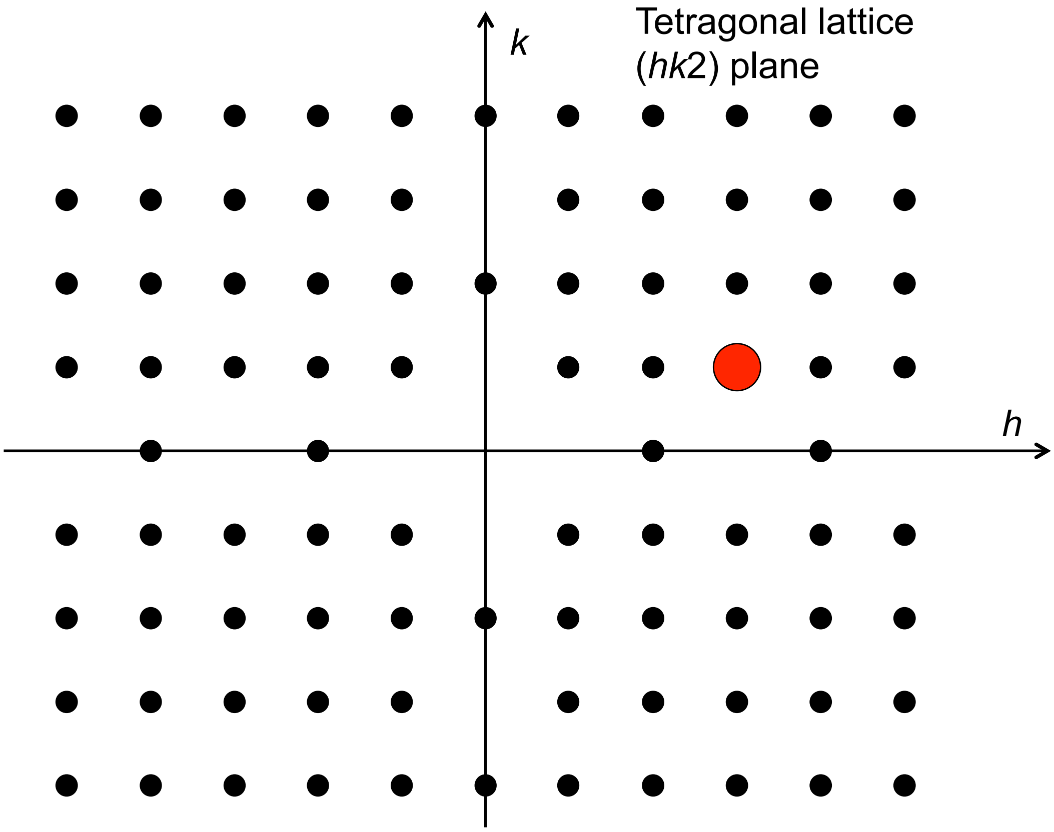
Laue Symmetry

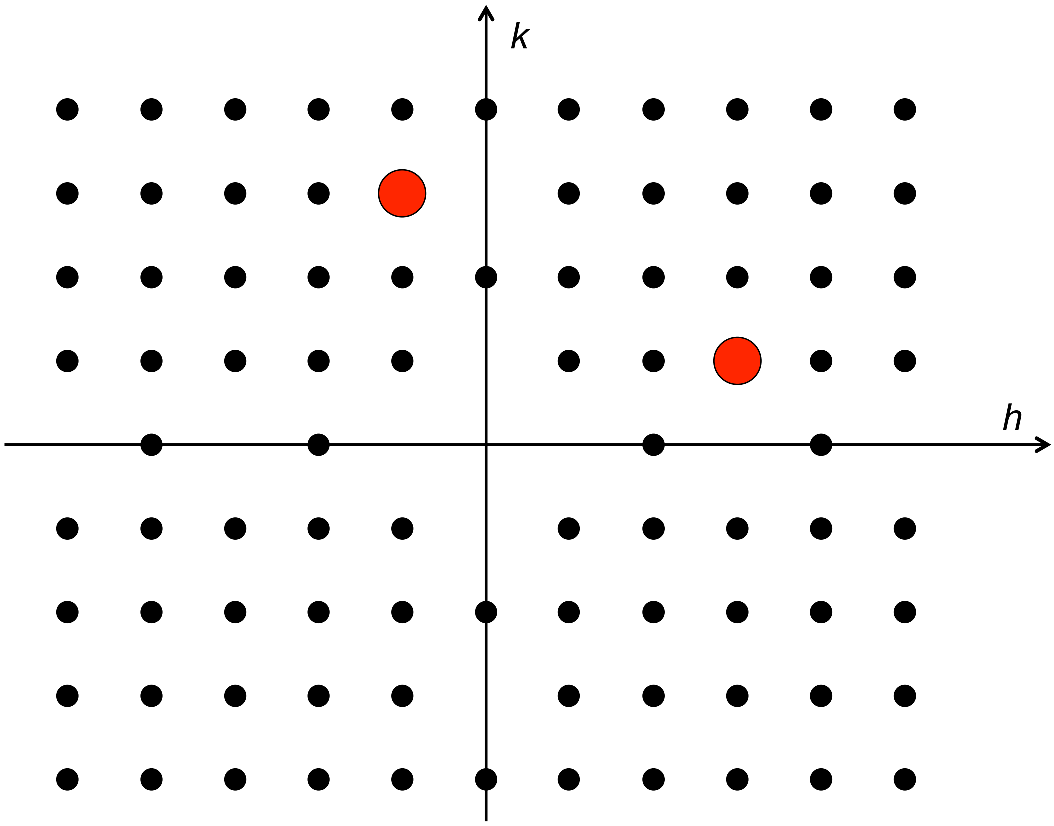
In reciprocal space, the diffraction pattern mimics the lattice symmetry in terms of reflection positions and their intensities. Diffraction comes from lattice planes and if sets of lattice planes are related by symmetry, the diffracted beams from these lattice planes will have the same relationships.



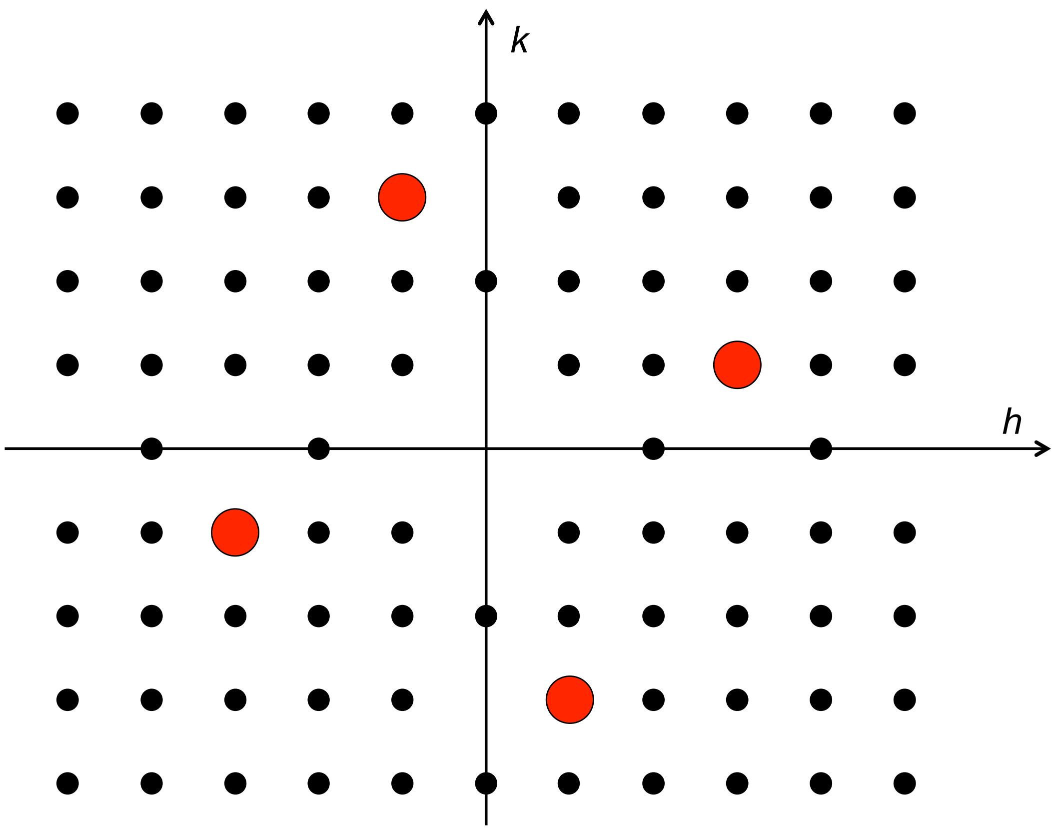


As an example, consider the diffraction from a tetragonal lattice.



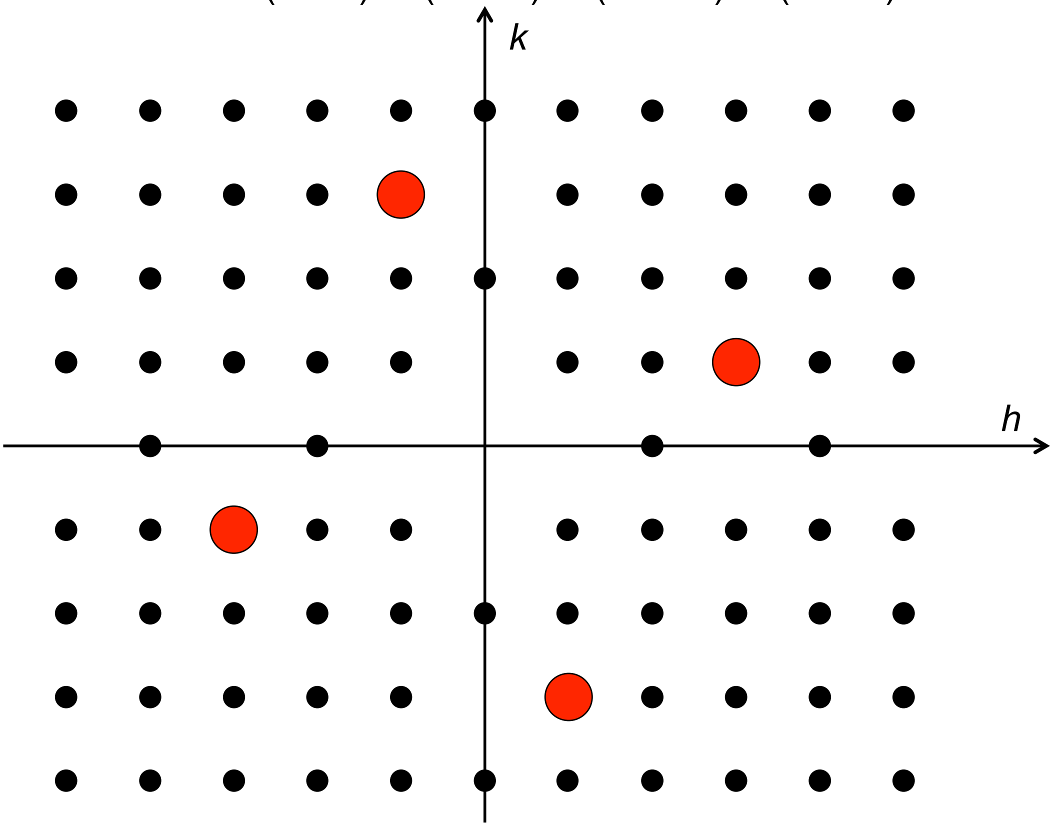


Apply 4-fold axis

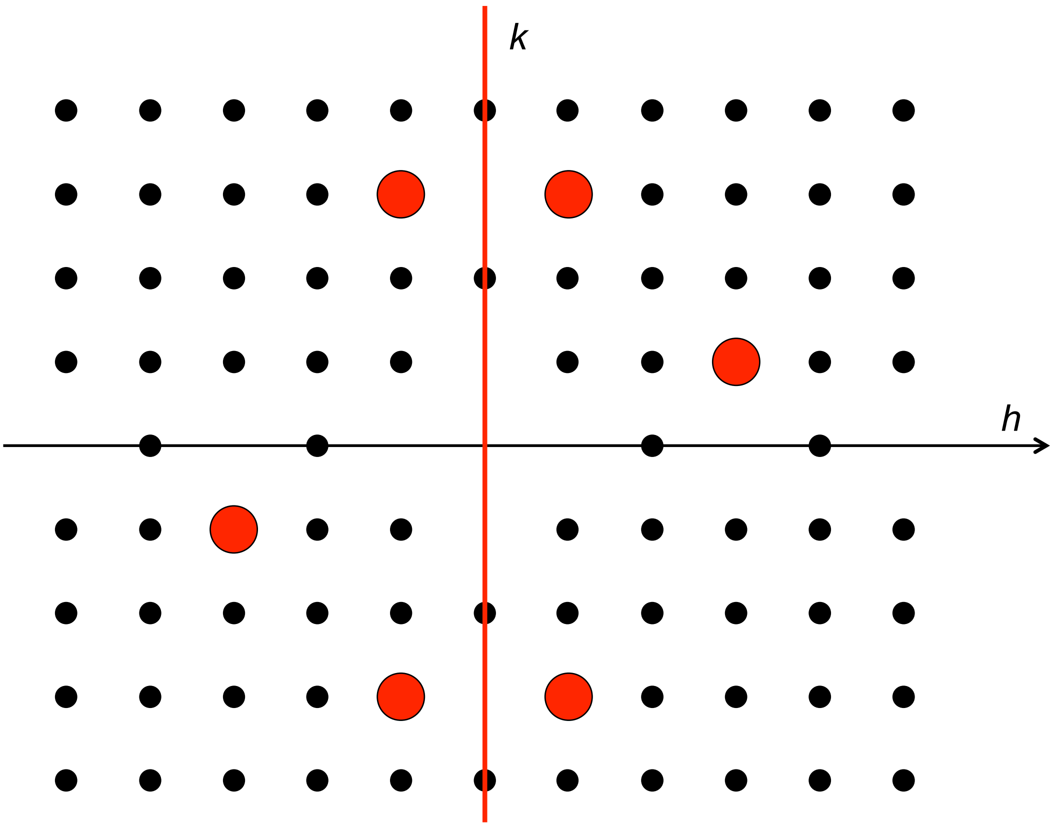


4-fold axis: I(3 1 2) = I(-1 3 2) = I(-3 -1 2) = I(1 -3 2)

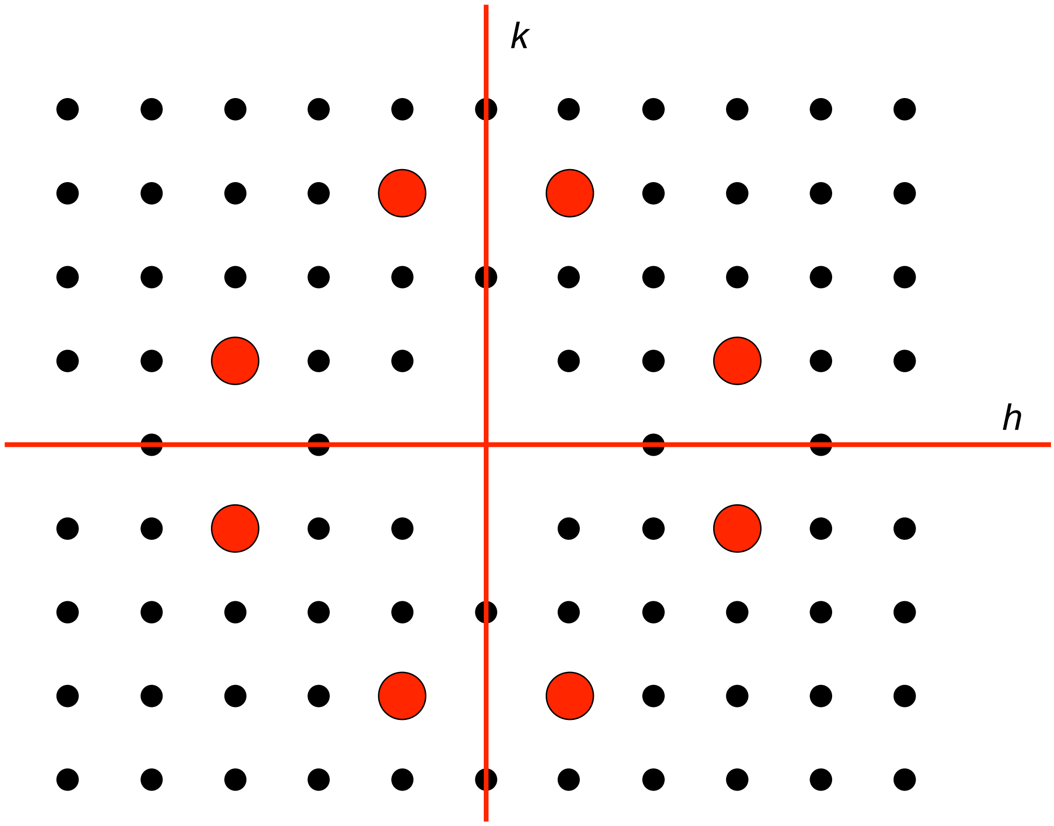
4-fold axis: I(3 1 2) = I(-1 3 2) = I(-3 -1 2) = I(1 -3 2)



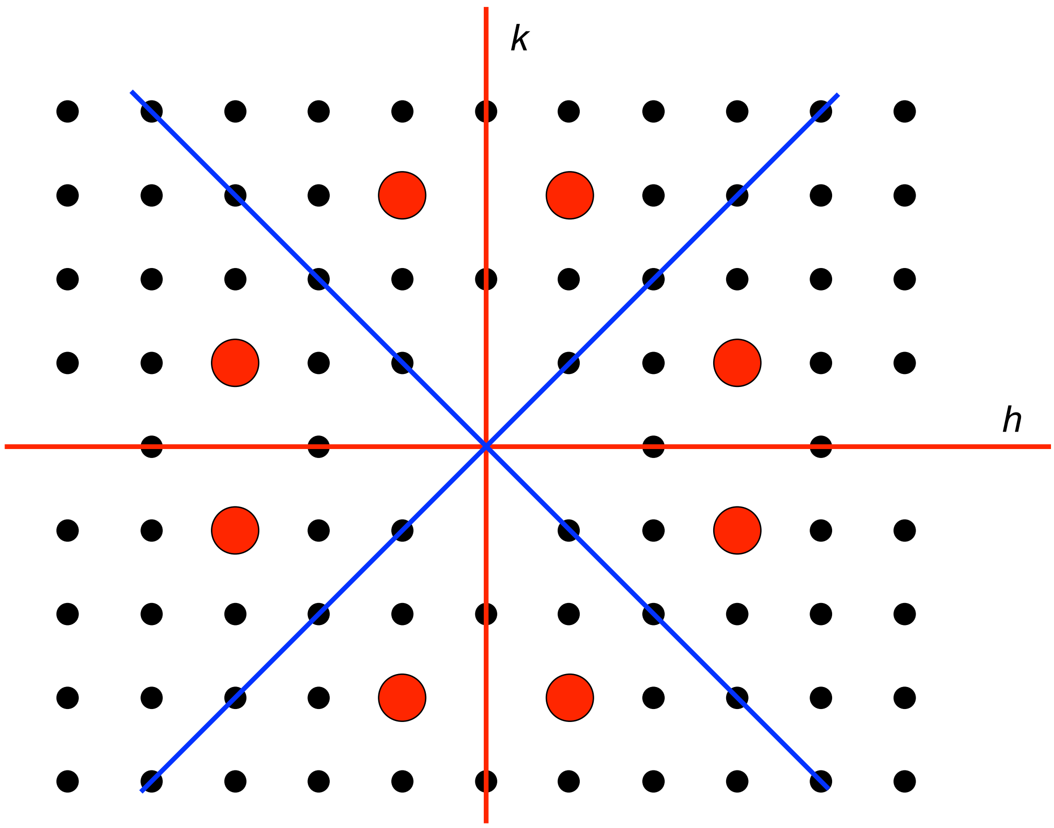
In tetragonal there is a mirror perpendicular to the 4-axis (4/*m*), so additionally I(*hkl*) = I(*hk* –*l*): ➔ 4/*m* Laue symmetry



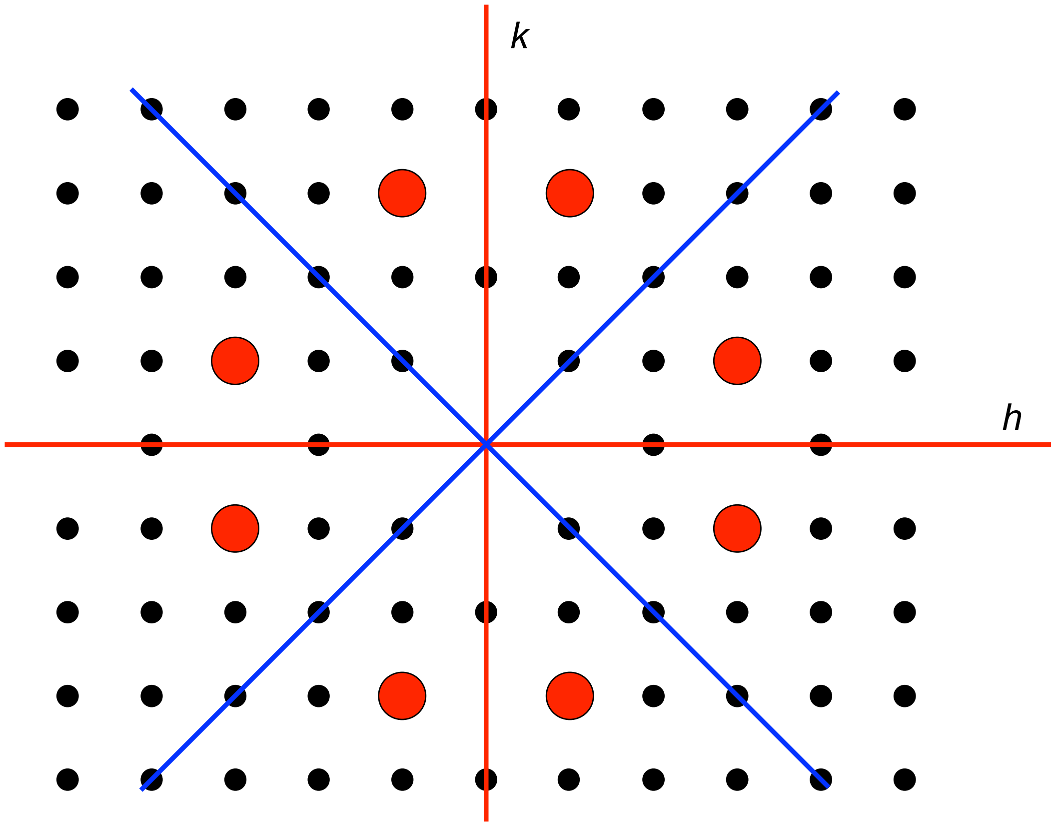
Add a mirror: I(3 1 2) = I(1 3 2) = I(-1 3 2) = I(1 -3 2) = I(-1 -3 2), *etc.*



4-fold enforces second mirror:
I(3 1 2) = I(1 3 2) = I(3 -1 2) = I(-3 1 2) = (-1 -3 2), *etc.* ➔ 4*m*



This generates another set of mirrors: ➔ 4*mm*



In tetragonal there is a mirror perpendicular to the 4-axis (4/*m*),
I(*hkl*) = I(*hk* –*l*): ➔ 4/*mmm* overall Laue symmetry

Laue symmetry – equivalent reflections (have same intensity)

Reflections with equivalent intensities for a given diffraction symmetry

diffraction group (with related chiral group)	conditions for	$I(hkl) \equiv$	$I(\bar{h}\bar{k}\bar{l}) \equiv$	multiplicity of centrosymmetric general data
$\bar{1}$ (1)	---	---	---	2
2/*m* (2)	$\bar{1}$ (1)	$I(\bar{h}k\bar{l})$	$I(h\bar{k}l)$	4
mmm (222)	2/m (2)	$I(h\bar{k}\bar{l}),I(\bar{h}\bar{k}l)$	$I(\bar{h}kl),I(hk\bar{l})$	8
4/*m* (4)	$\bar{1}$ (1)	$I(\bar{h}\bar{k}l),I(\bar{k}hl),I(k\bar{h}l)$	$I(hk\bar{l}),I(k\bar{h}\bar{l}),I(\bar{k}h\bar{l})$	8
4/*mmm* (422)	4/*m* (4)	$I(\bar{h}k\bar{l}),I(h\bar{k}\bar{l}),I(\bar{k}\bar{h}\bar{l}),I(kh\bar{l})$	$I(\bar{h}kl)),I(h\bar{k}l),I(khl),I(\bar{k}\bar{h}l)$	16
$\bar{3}$ (3)	$\bar{1}$ (1)	$I(kil), I(ihl),$	$I(\bar{k}\bar{i}\bar{l}),I(\bar{i}\bar{h}\bar{l})$*	6
$\bar{3}m1$ (321)	$\bar{3}$ (3)	$I(\bar{k}\bar{h}\bar{l}),I(\bar{h}\bar{i}\bar{l}),I(\bar{i}\bar{k}\bar{l})$	$I(hil), I(khl),I(ikl)$	12
$\bar{3}1m$ (312)	$\bar{3}$ (3)	$I(kh\bar{l}),I(hi\bar{l}),),I(ik\bar{l})$	$I(\bar{k}\bar{h}l),I(\bar{h}\bar{i}l),I(\bar{i}\bar{k}l)$	12
6/*m* (6)	$\bar{3}$ (3)	$I(\bar{h}\bar{k}l),I(\bar{k}\bar{i}l),I(\bar{i}\bar{h}l)$	$I(hk\bar{l}),I(ihl),I(ki\bar{l})$	12
6/mmm (622)	6/*m* (6)	$I(\bar{k}\bar{h}\bar{l}),I(\bar{h}\bar{i}\bar{l}),I(\bar{i}\bar{k}\bar{l})$ $I(kh\bar{l}),I(hi\bar{l}),),I(ik\bar{l})$	$I(hil),I(khl),I(ikl)$ $I(\bar{k}\bar{h}l),I(\bar{h}\bar{i}l),I(\bar{i}\bar{k}l)$	24
$m\bar{3}$ (23)	*mmm* (222)	$I(klh),I(k\bar{l}\bar{h}),I(\bar{k}l\bar{h}),I(\bar{k}\bar{l}h)$ $I(lhk),I(l\bar{h}\bar{k}),I(\bar{l}h\bar{k}),I(\bar{l}\bar{h}k)$	$I(\bar{k}\bar{l}\bar{h}),I(k\bar{l}h),I(\bar{k}lh),I(kl\bar{h})$ $I(\bar{l}\bar{h}\bar{k}),I(\bar{l}hk),I(l\bar{h}k),I(lh\bar{k})$	24
$m\bar{3}m$ (432)	$m\bar{3}$ (23)	$I(l\bar{k}h),I(lk\bar{h}),I(\bar{l}\bar{k}\bar{h}),I(\bar{l}kh)$ $I(\bar{k}\bar{h}\bar{l}),I(\bar{k}hl),I(kh\bar{l}),I(k\bar{h}l)$ $I(\bar{h}\bar{l}\bar{k}),I(\bar{h}lk),I(h\bar{l}k),I(hl\bar{k})$	$I(lkh),I(l\bar{k}\bar{h}),),I(\bar{l}k\bar{h}),I(\bar{l}\bar{k}\bar{h})$ $I(khl),I(\bar{k}\bar{h}\bar{l}),I(\bar{k}\bar{h}l),I(k\bar{h}\bar{l})$ $I(hlk),I(\bar{h}\bar{l}k),I(\bar{h}l\bar{k}),I(h\bar{l}\bar{k})$	48

**In trigonal and hexagonal crystals, i=-h-k.*

Centrosymmetric space groups:
I(*hkl*) = I(−*h* −*k* −*l*)
Friedels Law holds

Non-centrosymmetric space groups:
I(*hkl*) ≠ I(−*h* −*k* −*l*)
because of anomalous scattering; the effect might be small, though.

When merging equivalent reflections, ensure only the truly equivalent sets of reflections are merged.

Symmetry operators and elements

The basic symmetry operations are translation, rotation and reflection. All other symmetry operations result from a combination of these.

Mirror planes, *m*

An object with two halves related by a mirror, or two objects related by a mirror. Applying the operation twice returns to the starting position.

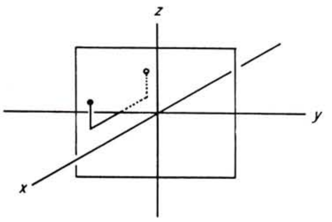


Figure 3.3. A mirror plane.

n-fold rotation axes, where *n* = 1, 2, 3, 4, 6

An object with *n*-fold rotation symmetry, or objects related by an *n*-fold rotation axis, will appear identical after rotation through 360/*n* degrees. Applying the operation *n*-times returns to the starting position.

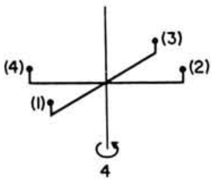


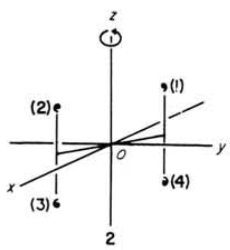
Figure 3.2. A 4-fold rotation axis.

Point symmetry operators

At least one point in space remains unchanged on application of a point symmetry operator.

These include *n*-fold rotation axes, mirror planes and their combination:

A centre of inversion, $\bar{1}$, is a combination of a 2-fold rotation and then reflection in a plane perpendicular to the 2-fold axis. Applying the operation twice returns to the starting position.



n-fold rotary inversion axes (*n*-bar), where $n = \bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}$ ($\bar{2} = m$)

An object with *n*-fold rotary inversion symmetry, or objects related by an *n*-fold rotary inversion axis, will appear identical after rotation through 360/*n* degrees and then inversion. Applying the operation *n*-times returns to the starting position.

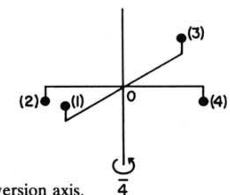


Figure 3.5. A 4-fold rotary inversion axis.

Point symmetry operators

n-fold rotation axes and *n*-fold rotary inversion axes are known as proper and improper rotations, respectively.

proper rotations		"improper rotations"	
Int.	*Schoenflies*	*Int.*	*Schoenflies*
1	C_1 (identity)	$\bar{1}$	S_2, C_i or I (inversion)
2	C_2	$\bar{2}$ or m	S_1, C_s or σ (reflection)
3	C_3	$\bar{3}$	S_6
4	C_4	$\bar{4}$	S_4
6	C_6	$\bar{6}$	S_3 or C_{3h}

Improper rotations, mirror symmetry and glide planes change the "handedness" of an object. Chiral or enantiopure objects (molecules) cannot crystallise in a space group possessing such a symmetry element. This can only occur if the objects are a racemic mixture.

Point groups

There are just 32 possible combinations of *n*-fold rotation axes, *n*-fold rotary inversion axes and mirrors. These are the three-dimensional point groups.

Crystal Systems, Diffraction Symmetries and Point Groups

system	*diffraction symmetry*	*corresponding lower symmetries*
triclinic	$\bar{1}(C_i)$	$1(C_1)$*
monoclinic	$2/m\ (C_{2h})$	$m(C_s)$, $2(C_2)$*
orthorhombic	$mmm\ (D_{2h})$	$mm(C_{2v})$, $222(D_2)$*
tetragonal	$4/m\ (C_{4h})$	$4(C_4)$*, $\bar{4}(S_4)$
	$4/mmm\ (D_{4h})$	$4mm(C_{4v})$, $422(D_4)$*, $\bar{4}m2(D_{2d})$
trigonal	$\bar{3}\ (S_6)$	$3(C_3)$*
	$\bar{3}m\ (D_{3d})$	$32(D_3)$*, $3m(C_{3v})$
hexagonal	$6/m\ (C_{6h})$	$6(C_6)$*, $\bar{6}(C_{3h})$
	$6/mmm\ (D_{6h})$	$6mm(C_{6v})$, $622(D_6)$*, $\bar{6}m2(D_{3d})$
cubic	$m\ \bar{3}\ (T_h)$	$23(T)$*
	$m\ \bar{3}m\ (O_h)$	$432(O)$*, $\bar{4}3m(T_d)$

* point groups possible for optically pure, chiral structures.

The 32 crystallographic point groups

Crystal System and Bravais Lattices	*Point groups* *Internat.*	*Schönflies*	*Space group numbers*	*Symmetry along* *a* [100]	*b* [010]	*c* [001]	*order*[1]	*E,P,C*[2]
triclinic	1	C_1	1	1	1	1	1	E, P
P (= *C*, *I*, *F*)	$\bar{1}$	C_i	2	$\bar{1}$	$\bar{1}$	$\bar{1}$	2	C
monoclinic	2	C_2	3-5	1	2	1	2	E, P
P	*m*	C_s	6-9	1	*m*	1	2	P
C (= *I*, *F*)	2/*m*	C_{2h}	10-15	$\bar{1}$	2/m	$\bar{1}$	4	C
orthorhombic	222	D_2	16-24	2	2	2	4	E
P, *C*, *I*, *F*	*mm*2	C_{2v}	25-46	*m*	*m*	2	4	P
	mmm	D_{2h}	47-74	2/*m*	2/*m*	2/*m*	8	C
				c	***a* & *b***	***ab* [110]**		
tetragonal	4	C_4	78-80	4	1	1	4	E, P
	$\bar{4}$	S_4	81-82	$\bar{4}$	1	1	4	-
P (= *C*)	4/*m*	C_{4h}	83-88	4/*m*	$\bar{1}$	$\bar{1}$	8	C
I (= *F*)	422	D_4	89-98	4	2	2	8	E
	4*mm*	C_{4v}	99-110	4	*m*	*m*	8	P
	$\bar{4}2m$*	D_{2d}	111-122	$\bar{4}$	2	*m*	8	-
	$\bar{4}m2$*			$\bar{4}$	*m*	2		
	4/*mmm*	D_{4h}	123-142	4/*m*	2/*m*	2/*m*	16	C
trigonal	3	C_3	143-146	3	1	1	3	E, P
	$\bar{3}$	S_6	147-148	$\bar{3}$	$\bar{1}$	$\bar{1}$	6	C
P or *R*	321*	D_3	149-155	3	2	1	6	E
	312*			3	1	2		
	3*m*1*	C_{3v}	156-161	3	*m*	1	6	P
	31*m**			$\bar{3}$	1	*m*		
	$\bar{3}m1$*	D_{3d}	162-167	$\bar{3}$	2/*m*	$\bar{1}$	12	C
	$\bar{3}1m$*			$\bar{3}$	$\bar{1}$	2/*m*		
hexagonal	6	C_6	168-173	6	1	1	6	E, P
	$\bar{6}$	C_{3h}	174	$\bar{6}$	1	1	6	-
P	6/m	C_{6h}	175-176	6/*m*	$\bar{1}$	$\bar{1}$	12	C
	622	D_6	177-182	6	2	2	12	E
	6*mm*	C_{6v}	183-186	6	*m*	*m*	12	P
	$\bar{6}2m$*	D_{3d}	187-190	$\bar{6}$	2	*m*	12	-
	$\bar{6}m2$*			$\bar{6}$	*m*	2	12	-
	6/*mmm*	D_{6h}	191-194	6/*m*	2/*m*	2/*m*	24	C
				a*, *b* & *c	***abc* [111]**	***ab* [110]**		
cubic	23	*T*	195-199	2	3	1	12	E
	$m\bar{3}$	T_h	200-206	2/*m*	$\bar{3}$	$\bar{1}$	24	C
P, *I*, *F*	432	*O*	207-214	4	3	2	24	E
	$\bar{4}3m$	T_d	215-220	$\bar{4}$	3	*m*	24	-
	$m\bar{3}m$	O_h	221-230	4/*m*	$\bar{3}$	2/*m*	48	C

[1] Multiplied by 2 for *I* or *C* lattices, by 3 for *R* and by 4 for *F*.

[2] Enantiomorphous, Polar or Centrosymmetric.

* In these point groups, different space groups occur because of the different possibilities for the arrangement of the symmetry elements.

Space symmetry operators

Operations which include a translation component – no point remains unchanged on application of that operator

n-fold screw axes, n_r, where $n = 1, 2, 3, 4, 6$ and $r < n$

Rotation of $n/360$ degrees followed by a translation of r/n along a unit cell axis.

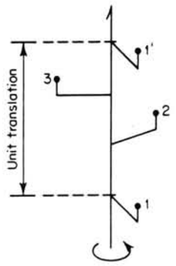


Figure 3.20. Screw axis 3_1.

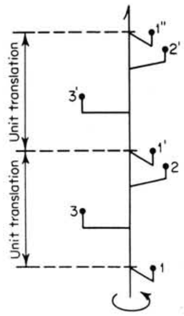


Figure 3.21. Screw axis 3_2.

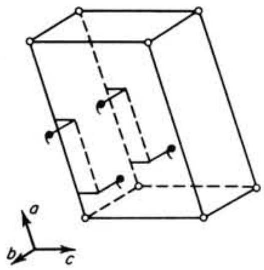
After *n* applications of the operation, the starting position is reached, but in the r^{th} unit cell further along the translation direction.

Screw axes do not change the handedness of a chiral object.

Glide planes, *a*, *b*, *c*, *n*, *d*, *e*

a, *b*, *c* glides: mirror operation followed by a translation parallel to the reflecting plane of 0.5 along a unit cell axis.

The orientation of the mirror plane is ambiguous:
for an *a*-glide, the reflection plane could be perpendicular to *b* or *c*.
The actual symmetry operators must be inspected to resolve this.



Glide planes change the handedness of a chiral object ➔ racemic mixture

Figure 3.22. Glide plane *a*.

n-glide: mirror operation followed by a translation parallel to the reflecting plane of 0.5 along a unit cell face diagonal.

n is even more ambiguous; mirror could be perpendicular to *a*, *b*, or *c*.

After 2 applications of an *a*, *b*, *c* or *n* operation, the starting position is reached, but in the next unit cell along the translation direction.

d-glide (diamond-glide): mirror operation followed by a translation parallel to the reflecting plane of 0.25 along a unit cell face diagonal or body diagonal.

The orientation of the mirror for *d* is also ambiguous.

After 4 applications of a *d* operation, the starting position is reached in the next unit cell along the translation direction.

A mirror of order two is incompatible with a translation component of order 4, unless after two operations of the *d*-glide there is a lattice point, so the unit cell must be either face-centred or body-centred, *F* or *I*.
e.g. *Fddd*

e-glide ("double" glide plane): one mirror operation followed by *two* perpendicular glide vectors related by a centred lattice translation.

After 2 applications of an *e*-glide operation, the starting position is reached in the next unit cell along the translation direction.

The unit cell must be centred: *A*, *C*, *F* or *I*.

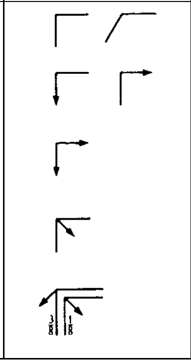
Symbol introduced in 1992 to reduce ambiguity.

Graphical symbols for symmetry operators

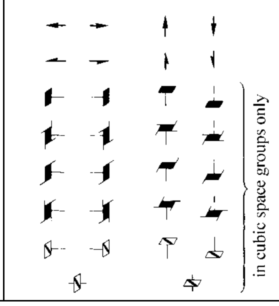
1.4.1. Symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)

Symmetry plane or symmetry line	Graphical symbol	Glide vector in units of lattice translation vectors parallel and normal to the projection plane	Printed symbol
Reflection plane, mirror plane Reflection line, mirror line (two dimensions)		None	*m*
'Axial' glide plane Glide line (two dimensions)		$\frac{1}{2}$ lattice vector along line in projection plane $\frac{1}{2}$ lattice vector along line in figure plane	*a*, *b* or *c* *g*
'Axial' glide plane		$\frac{1}{2}$ lattice vector normal to projection plane	*a*, *b* or *c*
'Double' glide plane* (in centred cells only)		*Two* glide vectors: $\frac{1}{2}$ along line parallel to projection plane and $\frac{1}{2}$ normal to projection plane	*e*
'Diagonal' glide plane		*One* glide vector with *two* components: $\frac{1}{2}$ along line parallel to projection plane, $\frac{1}{2}$ normal to projection plane	*n*
'Diamond' glide plane† (pair of planes; in centred cells only)		$\frac{1}{4}$ along line parallel to projection plane, combined with $\frac{1}{4}$ normal to projection plane (arrow indicates direction parallel to the projection plane for which the normal component is positive)	*d*

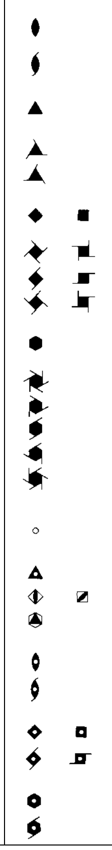
1.4.2. Symmetry planes parallel to the plane of projection

Symmetry plane	Graphical symbol*	Glide vector in units of lattice translation vectors parallel to the projection plane	Printed symbol
Reflection plane, mirror plane		None	*m*
'Axial' glide plane		$\frac{1}{2}$ lattice vector in the direction of the arrow	*a*, *b* or *c*
'Double' glide plane† (in centred cells only)		*Two* glide vectors: $\frac{1}{2}$ in either of the directions of the two arrows	*e*
'Diagonal' glide plane		*One* glide vector with *two* components $\frac{1}{2}$ in the direction of the arrow	*n*
'Diamond' glide plane‡ (pair of planes; in centred cells only)		$\frac{1}{2}$ in the direction of the arrow; the glide vector is always half of a centring vector, *i.e.* one quarter of a diagonal of the conventional face-centred cell	*d*

1.4.6. Symmetry axes parallel to the plane of projection

Symmetry axis	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Twofold rotation axis		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Fourfold rotation axis		None	4 (2)
Fourfold screw axis: '4 sub 1'		$\frac{1}{4}$	4_1 (2_1)
Fourfold screw axis: '4 sub 2'		$\frac{1}{2}$	4_2 (2)
Fourfold screw axis: '4 sub 3'		$\frac{3}{4}$	4_3 (2_1)
Inversion axis: '4 bar'		None	$\bar{4}$ (2)
Inversion point on '4 bar'-axis		–	$\bar{4}$ point

1.4.5. Symmetry axes normal to the plane of projection and symmetry points in the plane of the figure

Symmetry axis or symmetry point	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Identity	None	None	1
Twofold rotation axis Twofold rotation point (two dimensions)		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Threefold rotation axis Threefold rotation point (two dimensions)		None	3
Threefold screw axis: '3 sub 1'		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'		$\frac{2}{3}$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)		None	4 (2)
Fourfold screw axis: '4 sub 1'		$\frac{1}{4}$	4_1 (2_1)
Fourfold screw axis: '4 sub 2'		$\frac{1}{2}$	4_2 (2)
Fourfold screw axis: '4 sub 3'		$\frac{3}{4}$	4_3 (2_1)
Sixfold rotation axis Sixfold rotation point (two dimensions)		None	6 (3,2)
Sixfold screw axis: '6 sub 1'		$\frac{1}{6}$	6_1 $(3_1, 2_1)$
Sixfold screw axis: '6 sub 2'		$\frac{1}{3}$	6_2 $(3_2, 2)$
Sixfold screw axis: '6 sub 3'		$\frac{1}{2}$	6_3 $(3, 2_1)$
Sixfold screw axis: '6 sub 4'		$\frac{2}{3}$	6_4 $(3_1, 2)$
Sixfold screw axis: '6 sub 5'		$\frac{5}{6}$	6_5 $(3_2, 2_1)$
Centre of symmetry, inversion centre: '1 bar' Reflection point, mirror point (one dimension)		None	$\bar{1}$
Inversion axis: '3 bar'		None	$\bar{3}$ $(3, \bar{1})$
Inversion axis: '4 bar'		None	$\bar{4}$ (2)
Inversion axis: '6 bar'		None	$\bar{6} \equiv 3/m$
Twofold rotation axis with centre of symmetry		None	$2/m$ $(\bar{1})$
Twofold screw axis with centre of symmetry		$\frac{1}{2}$	$2_1/m$ $(\bar{1})$
Fourfold rotation axis with centre of symmetry		None	$4/m$ $(\bar{4}, 2, \bar{1})$
'4 sub 2' screw axis with centre of symmetry		$\frac{1}{2}$	$4_2/m$ $(\bar{4}, 2, \bar{1})$
Sixfold rotation axis with centre of symmetry		None	$6/m$ $(\bar{6}, \bar{3}, 3, 2, \bar{1})$
'6 sub 3' screw axis with centre of symmetry		$\frac{1}{2}$	$6_3/m$ $(\bar{6}, \bar{3}, 3, 2_1, \bar{1})$

1.4.7. Symmetry axes inclined to the plane of projection (in cubic space groups only)

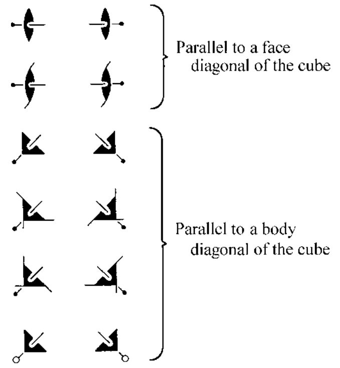
Symmetry axis	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Twofold rotation axis		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Threefold rotation axis		None	3
Threefold screw axis: '3 sub 1'		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'		$\frac{2}{3}$	3_2
Inversion axis: '3 bar'		None	$\bar{3}$ $(3, \bar{1})$

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	$x+\frac{1}{4}, y+\frac{1}{4}, \bar{z}$

Symmetry restrictions on atoms on special positions

If an atom is located exactly on a point symmetry site, it is said to occupy a special position. This is caused by degeneracy of the equivalent positions, *i.e.* application of the symmetry operators of the space group concerned to the coordinates of a special position generates two or more identical atomic coordinates. The parameters of the atom are constrained in accordance with the point group of the site. There are three types of parameter to consider: the site multiplicity, the positional parameters *x*, *y* and *z*, and the tensor describing the atomic displacement ellipsoid, *Uij*.

The site multiplicity: an atom in a general position, unrestricted by symmetry, is said to have a multiplicity of 1, whatever the number of equivalent atoms in the unit cell. If an atom is in a special position, its multiplicity is the reciprocal of order of the point group of the site. Thus, an atom on a site of *mmm* symmetry (order = 8) in any space group is said to have a multiplicity of $^1/_8$.

The positional parameters: these are unrestricted only for atoms in general positions. Otherwise, they are restricted as follows, where 0 is any fixed point; e.g. possibly also ½ or ¼:

a) restricted to a plane (site symmetry *m*):

plane normal to:	[100]	[010]	[001]	[011]	[101]	[110]
atom restricted to:	0,*y*,*z*	*x*,0,*z*	*x*,*y*,0	*x*,*y*,*y*	*x*,*y*,*x*	*x*,*x*,*z*

b) restricted to a line (site symmetry 2, 3, 4, 6, *mm*2, 3*m*, 4*mm*, 6*mm*):

axis parallel to:	[100]	[010]	[001]	[011]	[101]	[110]	[111]
atom restricted to:	*x*,0,0	0,*y*,0	0,0,*z*	0,*y*,*y*	*x*,0,*x*	*x*,*x*,0	*x*,*x*,*x*

c) any other point group, the atom is fixed to a point, such as 0,0,0 or ½, ½, ½.

Symmetry restrictions on atoms in special positions

The atomic displacement parameters: there are five possibilities for restrictions on the tensor that describes the displacement ellipsoid. These correspond to the constraints on unit cell parameters.

a) shape and orientation unrestricted: (triclinic) point groups 1 and $\bar{1}$: 6 independent parameters.

b) shape unrestricted, one of the principal axes of the ellipsoid is parallel to a given direction, and the others are normal to it; (monoclinic) point groups 2, *m*, 2/*m*: 4 parameters

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
[100]	A	B	C	D	0	0
[010]	A	B	C	0	D	0
[001]	A	B	C	0	0	D
[011]	A	B	B	C	D	D
[101]	A	B	A	C	D	C
[110]	A	A	B	C	C	D

c) shape unrestricted, orientation fixed (orthorhombic) point groups 222, *mm*2, *mmm*: 3 param.

[100], [010], [001]	A	B	C	0	0	0
[100], [011], [01-1]	A	B	B	0	C	C
[010], [101], [10-1]	A	B	A	C	0	C
[001], [110], [1-10]	A	A	B	C	C	0

d) shape restricted to one circular cross section (tetragonal, trigonal, hexagonal): 2 parameters

[001]	A	A	B	0	0	0
[111]	A	A	A	B	B	B

e) shape restricted to a sphere (cubic) − isotropic: 1 parameter: A, A, A, 0, 0, 0

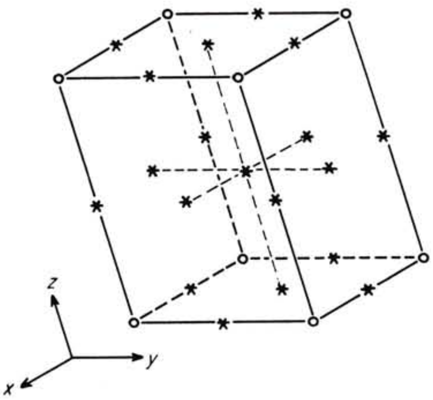
Internal symmetry versus lattice symmetry

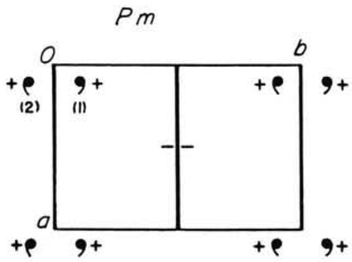
The internal symmetry displayed by an assembly of objects generates the entire lattice symmetry if the origin is chosen correctly.

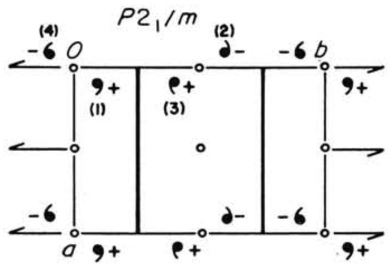
Examples:

Local centres of inversion correspond with the symmetry of the entire lattice if one of them is placed at the origin (corner) of the unit cell.

Local mirror planes are mirrors in monoclinic and orthorhombic lattices only if they intersect the axis they are perpendicular to at 0, ½, 1 or at ¼, ¾.







Equivalent positions

Given an object (e.g. atom) at any point *x*, *y*, *z* in the unit cell and the space group symmetry operators, where are additional copies of this object that are related by an exact symmetry operation?

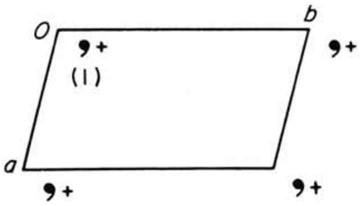


Figure 3.23. $P1$, equivalent positions x, y, z.

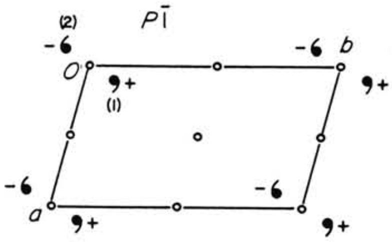


Figure 3.24. $P\bar{1}$, equivalent positions (1) x, y, z; (2) $\bar{x}, \bar{y}, \bar{z}$.

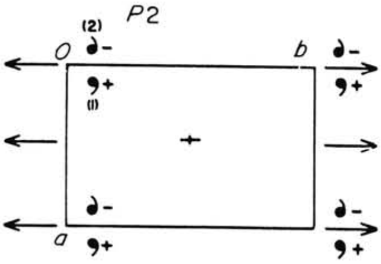


Figure 3.25. $P2$, equivalent positions (1) x, y, z; (2) $\bar{x}, y, \bar{z}$.

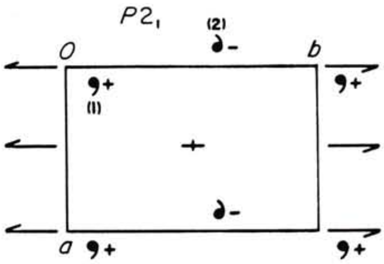


Figure 3.26. $P2_1$, equivalent positions (1) x, y, z; (2) $\bar{x}, y+\frac{1}{2}, \bar{z}$.

Equivalent positions

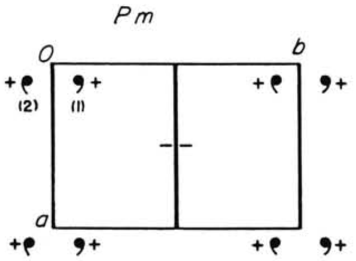


Figure 3.29. *Pm*, equivalent positions (1) x, y, z; (2) $x, \bar{y}, z$.

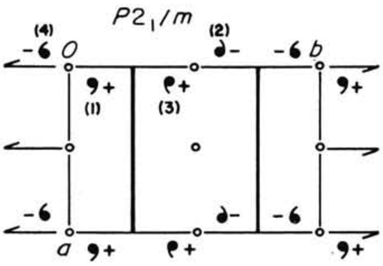


Figure 3.35. $P2_1/m$, equivalent positions (1) x, y, z; (2) $\bar{x}, y+\frac{1}{2}, \bar{z}$; (3) $x, \bar{y}+\frac{1}{2}, z$; (4) $\bar{x}, \bar{y}, \bar{z}$.

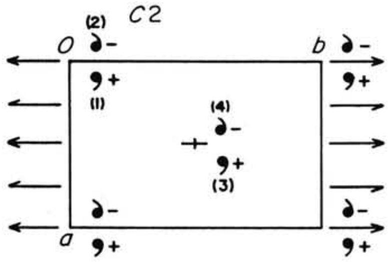


Figure 3.27. *C*2, equivalent positions (1) x, y, z; (2) $\bar{x}, y, \bar{z}$; (3) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (4) $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$.

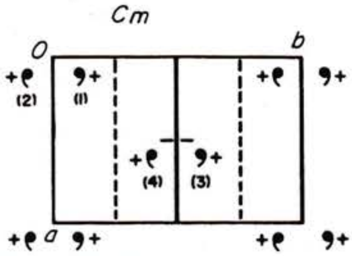


Figure 3.31. *Cm*, equivalent positions (1) x, y, z; (2) $x, \bar{y}, z$; (3) $x+\frac{1}{2}, y+\frac{1}{2}, z$; (4) $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$.

The logic of space group symbols

The form of the space group symbol as usually given is often an abbreviation, but may simply be described as follows. It consists of the Bravais lattice type followed by the point group symbol altered to indicate the translational symmetry elements present. The rules for doing this are:

triclinic: no translational symmetry: space groups *P*1 and $P\bar{1}$.

monoclinic: symmetry along *b* given as 2, *m* or 2/*m*, altered to show 2_1 axes and *a*, *c*, or *n* glide planes.

orthorhombic: symmetry along the *a*, *b* and *c* axes. 2/*m* is abbreviated to *m*.

tetragonal, *trigonal* and *hexagonal*: symmetry along *c* ([001]) is shown first, then, if there is any higher than $\bar{1}$, along *a* & *b* ([100] & [010]), and finally along the *ab*-diagonal ([110]).

cubic: symmetry is given first along *c*, *a* & *b*, then along the body diagonals ([111)] and finally, if there is any higher than $\bar{1}$, along the face diagonals ([110] and permutations thereof).

Systematic absences

A consequence only of translation components in symmetry operators; lattice centering, screws and glides

Table 5. Centred Lattices and conditions for data

Bravais Lattice	Symbol	Points equivalent to 0,0,0	Condition for data *hkl*	Fraction present
Primitive	*P*	none	none	1
A-centred	*A*	0,½,½	*k+l=2n*	½
B-centred	*B*	½,0,½	*h+l=2n*	½
C-centred	*C*	½,½,0	*h+k=2n*	½
Body centred	*I*	½,½,½	*h+k+l=2n*	½
Face centred	*F*	{0,½,½; ½,0,½; ½,½,0}	{*h,k,l* all odd or all even}	¼
Rhombohedral	*R*	$^1/_3, ^2/_3, ^2/_3$ $^2/_3, ^1/_3, ^1/_3$	*-h+k+l* =3*n*	$^1/_3$

	Reflections	Conditions for observation	Type of lattice or symmetry element	Translations
General reflections = lattice centering	*hkl*	$h+k+l=2n$	I lattice	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
		$h+k=2n$	C lattice	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$
		$h+l=2n$	B lattice	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$
		$k+l=2n$	A lattice	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$
		h, k, l all even or all odd	F lattice	$\frac{1}{2}(\mathbf{a}+\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{c}), \frac{1}{2}(\mathbf{b}+\mathbf{c})$
		$-h+k+l=3n$	R lattice (*inverse*)	$\frac{1}{3}(2\mathbf{a}+\mathbf{b}+\mathbf{c}), \frac{1}{3}(\mathbf{a}+2\mathbf{b}+2\mathbf{c})$
		$h-k+l=3n$	R lattice (*obverrse*)	$\frac{1}{3}(\mathbf{a}+2\mathbf{b}+\mathbf{c}), \frac{1}{3}(2\mathbf{a}+\mathbf{b}+2\mathbf{c})$
Zonal reflections = glide planes	0*kl*	$k=2n$	b glide plane, (100)	$\frac{1}{2}\mathbf{b}$
		$l=2n$	c glide plane, (100)	$\frac{1}{2}\mathbf{c}$
		$k+l=2n$	n glide plane, (100)	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$
		$k+l=4n$	d glide plane, (100)	$\frac{1}{4}(\mathbf{b}+\mathbf{c})$
	*h*0*l*	$h=2n$	a glide plane, (010)	$\frac{1}{2}\mathbf{a}$
		$l=2n$	c glide plane, (010)	$\frac{1}{2}\mathbf{c}$
		$h+l=2n$	n glide plane, (010)	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$
		$h+l=4n$	d glide plane, (010)	$\frac{1}{4}(\mathbf{a}+\mathbf{c})$
	*hk*0	$h=2n$	a glide plane, (001)	$\frac{1}{2}\mathbf{a}$
		$k=2n$	b glide plane, (001)	$\frac{1}{2}\mathbf{b}$
		$h+k=2n$	n glide plane, (001)	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$
		$h+k=4n$	d glide plane, (001)	$\frac{1}{4}(\mathbf{a}+\mathbf{b})$
	hhl	$l=2n$	c glide plane, $(1\bar{1}0)$	$\frac{1}{2}\mathbf{c}$
		$2h+l=2n$	n glide plane, $(1\bar{1}0)$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
		$2h+l=4n$	d glide plane, $(1\bar{1}0)$	$\frac{1}{4}(\mathbf{a}+\mathbf{b}+\mathbf{c})$

Axial reflections = screw axes

Reflections	Conditions for observation	Symmetry element; orientation	Translations
$h00$	$h = 2n$	$2_1, 4_2$ screw axes; [100]	$\frac{1}{2}\mathbf{a}$
	$h = 4n$	$4_1, 4_3$ screw axes; [100]	$\frac{1}{4}\mathbf{a}$
$0k0$	$k = 2n$	$2_1, 4_2$ screw axes; [010]	$\frac{1}{2}\mathbf{b}$
	$k = 4n$	$4_1, 4_3$ screw axes; [010]	$\frac{1}{4}\mathbf{b}$
$00l$	$l = 2n$	$2_1, 4_2, 6_3$ screw axes; [001]	$\frac{1}{2}\mathbf{c}$
	$l = 3n$	$3_1, 3_2, 6_2, 6_4$ screw axes; [001]	$\frac{1}{3}\mathbf{c}$
	$l = 4n$	$4_1, 4_3$ screw axes; [001]	$\frac{1}{4}\mathbf{c}$
	$l = 6n$	$6_1, 6_5$ screw axes; [001]	$\frac{1}{6}\mathbf{c}$
$hh0$	$h = 2n$	2_1 screw axis; [110]	$\frac{1}{2}\mathbf{c}$

Systematic absences tables from D. Schwarzenbach, *Crystallography* (1996).

Mathematical explanation of the systematic absence condition

The structure factor for any reflection hkl is given as

$$F(hkl) = \sum_{j=1}^{N} f_j \, exp[2\pi i(hx_j + ky_j + lz_j)]$$

summed over all (N) atoms in the unit cell at their respective fractional atomic coordinates x, y, z.

Rewrite as two parts each summed over half of the atoms:

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + ky_j + lz_j)] + \sum_{j=\frac{N}{2}+1}^{N} f_j \, exp[2\pi i(hx_j + ky_j + lz_j)]$$

For a **glide plane** along c, half of the atoms in the unit cell are related to the other half by the symmetry operation. In the case of the mirror component of the operation being perpendicular to b, the equivalent positions are x, y, z and $x, -y, ½+z$. We only need to consider half of the atoms (the asymmetric unit) and substitute the symmetry operator for the other half. The above becomes:

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + ky_j + lz_j)] + \sum_{j=1}^{N/2} f_j \, exp\{2\pi i[hx_j + k(-y_j) + l(z_j + \tfrac{1}{2})]\}$$

For the special case where $k = 0$ (the $h0l$ reflections):

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + lz_j)] + \sum_{j=1}^{N/2} f_j \, exp\{2\pi i[hx_j + l(z_j + \tfrac{1}{2})]\}$$

Since the exponent of a sum is the product of the individuals exponents, this can be rewritten as:

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + lz_j)] + \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + lz_j)] \, exp[2\pi i(l/2)]$$

and then factorized to:

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + lz_j)] \, [1 + exp(\pi i l)]$$

if l is odd, $exp(\pi il) = -1$, so $F(h0l) = 0$ (strictly zero for all l odd)
if l is even, $exp(\pi il) \neq -1$, so $F(h0l)$ can have any value.

For a **screw axis**, the same logic can be applied.

For a 2_1 screw axis along b, the equivalent positions are x, y, z and $-x, \frac{1}{2}+y, -z$, so again we only need to consider half of the atoms in the unit cell and can write:

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + ky_j + lz_j)] + \sum_{j=1}^{N/2} f_j \, exp\{2\pi i[-hx_j + k(y_j + \tfrac{1}{2}) - lz_j]\}$$

For the special case where $h = 0$ and $l = 0$ (the $0k0$ reflections):

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp(2\pi iky_j) + \sum_{j=1}^{N/2} f_j \, exp[2\pi ik(y_j + \tfrac{1}{2})]$$

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp(2\pi iky_j) + \sum_{j=1}^{N/2} f_j \, exp(2\pi iky_j) \, exp[2\pi i(k/2)]$$

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp(2\pi iky_j) \, [1 + exp(\pi ik)]$$

> In all cases, this term arises solely from the *translation* component and is the term responsible for cancelling the intensity when the index is odd.

if k is odd, $exp(\pi ik) = -1$, so $F(0k0) = 0$ (strictly zero for all k odd)
if k is even, $exp(\pi ik) \neq -1$, so $F(0k0)$ can have any value.

For **lattice centring**, we can proceed exactly the same way.

For example, for an I lattice, the equivalent positions are x, y, z and $\frac{1}{2}+x, \frac{1}{2}+y, \frac{1}{2}+z$, which leads to:

$$F(hkl) = \sum_{j=1}^{N/2} f_j \, exp[2\pi i(hx_j + ky_j + lz_j)] \, \{1 + exp[\pi i(hx_j + ky_j + lz_j)]\}$$

Thus, if and only if the sum $h + k + l$ is odd, $exp[\pi i(hx_j + ky_j + lz_j)] = -1$, so $F(hkl) = 0$.

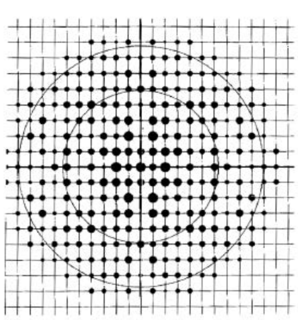
Centrosymmetric or non-centrosymmetric? – intensity statistics

When several space groups have the same systematic absences, intensity statistics can help verify the presence or absence of an inversion centre, but are statistical, so only give a hint.

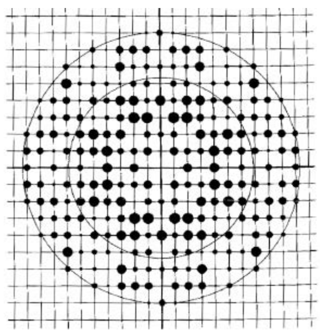
We use normalised structure factors: $|E|^2(hkl) = |F|^2(hkl)/\langle|F|^2\rangle_\theta$,

which should have a mean value of $\langle|E|^2\rangle = 1$ for all values of $sin\theta$.

The distribution of E-values about the mean differs according to the centricity. In non-centrosymmetric structures, intensities differ little from a mean value and the diffraction pattern will look quite featureless. In centrosymmetric structures, the relationship between atoms in pairs will tend to give more very weak and very strong intensities.



Acentric intensity distribution:
Ammonium oxalate monohydrate: *h*1*l*



Centric intensity distribution:
Ammonium oxalate monohydrate: *h*0*l*

Intensity statistics

In terms of the probability *P*(E) of a reflection having a particular value of |*E*|, the distributions may be given as:

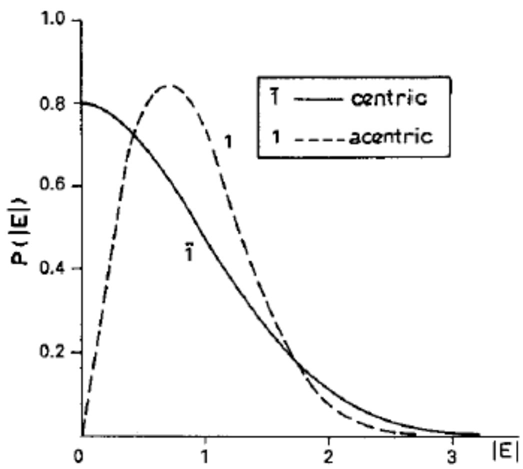
acentric: $P(|E|) = 2|E|\exp(-|E|^2)$

centric: $P(|E|) = (2/\pi)^{½}\exp(-|E|^2/2)$

Calculate the expectation value, $\langle|E^2-1|\rangle$

~ 0.97 for centrosymmetric structures
~ 0.75 for non-centrosymmetric

A suggestion of non-centricity is more reliable than one of centricity; a pseudo-centrosymmetric structure, or one in which only the heavy atoms have a centrosymmetric arrangement, may skew the statistics towards centric values.



Heavy atoms on special positions and twinning tend to lower $\langle|E^2-1|\rangle$.
Pseudo translational symmetry tends to increase this value.

Intensity statistics

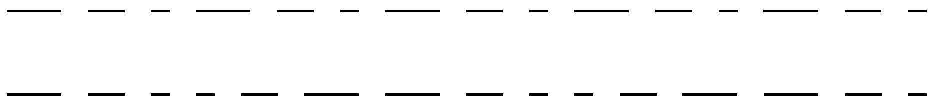
The intensity statistics of axial and zonal reflections can indicate if one or another projection of a non-centrosymmetric structure onto a plane has a centrosymmetric appearance, thereby being able to distinguish between two non-centrosymmetric space groups with the same systematic absences, such as *P*2 and *Pm.*

Distribution statistics and symmetry enhancements

Symmetry element	General data (*h k l*)		Perpendicular zone (*h k* 0)		Parallel row (0 0 *l*)	
	Dist.	Enh.	Dist.	Enh.	Dist.	Enh.
1	A	1	A	1	A	
$2, 2_1$	A	1	C	1	A	2
$3, 3_1, 3_2$	A	1	A	1	A	3
$4, 4_1, 4_2, 4_3$	A	1	C	1	A	4
$6, 6_1, 6_2, 6_3, 6_4, 6_5$	A	1	C	1	A	6
$\bar{1}$	C	1	C	1	C	1
$\bar{2}$ (m, a, b, c, n, d)	A	1	A	2	C	1
$\bar{3}$	C	1	C	1	C	3
$\bar{4}$	A	1	C	1	C	2
$\bar{6}$	A	1	A	2	C	3

A, acentric; C, centric—elements assumed parallel to *c*.

The Symmetry of Repeating Patterns in One Dimension



in each pattern, find:

a) the unit cell (the smallest repeating unit) and its dimension (*a*)

b) the symmetry operations (which relate one part of a cell to another)

c) the asymmetric unit (the smallest symmetry independent unit)

d) the general multiplicity (the number of asymmetric units per cell)

e) special positions (locations which have lower multiplicity and higher symmetry)

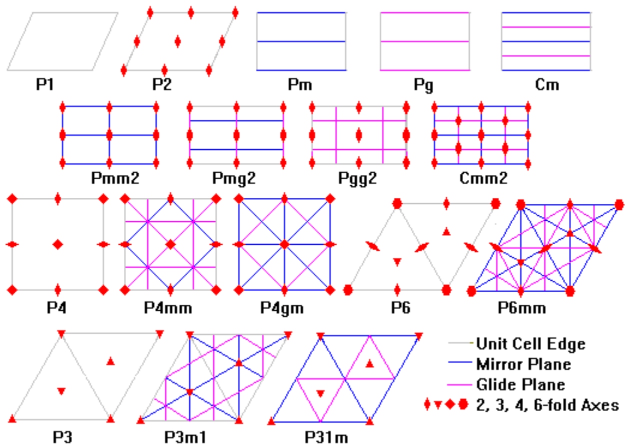
The Symmetry of Repeating Patterns in Two Dimensions

p d p d p d p
p d p d p d p
p d p d p d p
p d p d p d p

For each pattern, draw in the unit cell box and symmetry elements, then assign the plane group from the table below.

p d p d p d
b q b q b q
p d p d p d
b q b q b q

The 17 Plane Groups



Centred Lattices in Two Dimensions

```
p   p   p   p   p   p   p             p   q   p   q   p   q   p
b   b   b   b   b   b   b             b   d   b   d   b   d   b
  p   p   p   p   p   p   p           q   p   q   p   q   p   q
  b   b   b   b   b   b   b           d   b   d   b   d   b   d
p   p   p   p   p   p   p             p   q   p   q   p   q   p
b   b   b   b   b   b   b             b   d   b   d   b   d   b
```

```
          +----------------------------------------------------------+
          |    Space Group Determination and Data Initialisation    |
          +----------------------------------------------------------+


Total no. of intensity data =  66170

hkl limits are:
    -12 =< h =<  11
    -25 =< k =<  25
    -30 =< l =<  24

Lattice exceptions          P     A     B     C     I     F    Obv    Rev    All
 Total no of reflections    0 33110 33089 33117 33116 49658  44086  44141  66170
 Total  with I>3*sig(I)     0 17156 17280 17132 17444 25784  23355  23367  35095
 Mean intensity for all     0     5     5     5     5     5      5      5      5
 Mean intensity I>3*sig(I)  0    10     9     9     9     9      9      9      9

 (Obv and Rev refer to R type cells)

Preferred lattice type is P

Unit cell:
 a =    9.9870(0.0002)          alpha=  90.00(0.000)
 b =   19.8289(0.0004)          beta =  90.00(0.000)
 c =   23.4870(0.0004)          gamma=  90.00(0.000)

Niggli reduced cell:   9.987 19.829 23.487   90.00   90.00   90.00

Niggli matrix:         99.7402     393.1852     551.6392
                        0.0000       0.0000       0.0000

Transformation matrix:      1.00     0.00     0.00
                            0.00     1.00     0.00
                            0.00     0.00     1.00

Niggli matrix indicates orthorhombic cell of type P
```

General reflections, *hkl.*
No class has very few reflections with I>3σ(I), so no absence conditions.
Deduce lattice is P

Unit cell looks to be metrically orthorhombic.

This is no guarantee that it really is orthorhombic

Checking Laue class from equivalent reflections:

Laue class	R(int)	n	Rmeas	PCV
-1	0.050	18215	0.090	0.119
2/m	0.054	10633	0.092	0.136
mmm	0.054	5909	0.092	0.142
4/m	0.455	7499	0.566	0.530
4/mmm	0.448	4303	0.564	0.532
-3	0.557	11540	0.759	0.650
-3m	0.599	7151	0.931	0.925
6/m	0.547	6415	0.751	0.646
6/mmm	0.596	4106	0.922	0.901
m-3	0.526	3404	0.775	0.782
m-3m	0.590	2023	0.958	1.076

Check R_{int} to determine Laue class. Highest symmetry Laue class with a low R_{int} is the correct one (the furthest down the list). Here it is mmm
➔ confirms orthorhombic

Check for higher symmetry

Checking for higher metric symmetry via LePage method:

Possible 2-Fold Axes - 2-Axis Crit = 0.50, Exp. Error = 0.30 Deg., LATT = P:

Nr	D	N	Rows Direct	Rows Recip	Products Dot	Products Delta	Angle Between Two Direct Axes 1	2	3	4	5	6	7	8	9
1	9.987	2	1 0 0	1 0 0	1	0.000	0.	90.	90.						
2	19.829	2	0 1 0	0 1 0	1	0.000	90.	0.	90.						
3	23.487	2	0 0 1	0 0 1	1	0.000	90.	90.	0.						

Transformation Matrix: Input (a,b,c) to Conventional Cell(a', b', c'):
(a') (1.00 0.00 0.00) (a) (x') (1.00 0.00 0.00) (x) Metrically
(b') = (0.00 1.00 0.00) (b). (y') = (0.00 1.00 0.00) (y). orthorhombic
(c') (0.00 0.00 1.00) (c) (z') (0.00 0.00 1.00) (z) FOM: 0.000

	Latt	a	b	c	Alpha	Beta	Gamma	Volume
Input Cell	P	9.987	19.829	23.487	90.00	90.00	90.00	4651.16
Reduc Cell	P	9.987	19.829	23.487	90.00	90.00	90.00	4651.19
Conv. Cell	oP	9.987	19.829	23.487	90.00	90.00	90.00	4651.16

No alternative metric symmetry detected.

Check systematic absences

Reflection class		For this condition <F^2>	No of reflns	For the reverse <F^2>	No of reflns	Probability
hkl:	k+l=2n	41.9113	18980	41.7514	18975	0.126
hkl:	h+l=2n	38.8383	19015	44.8363	18940	0.100
hkl:	h+k=2n	39.6968	19032	43.9782	18923	0.107
hkl:	h+k+l=2n	40.1476	18944	43.5092	19011	0.111
hkl:	h+k,k+l=2n	36.7967	9536	43.5207	28419	0.096
hkl:	-h+k+l=3n	41.8586	12640	41.8178	25315	0.125
hkl:	h-k+l=3n	41.8586	12640	41.8177	25315	0.125
hkl:	h-k=3n	44.9562	12685	40.2628	25270	0.147
0kl:	k =2n	115.2899	1136	1.1060	1204	0.972
0kl:	l =2n	44.9548	1148	67.6953	1192	0.064
0kl:	k+l=2n	44.9334	1168	68.1047	1172	0.063
0kl:	k+l=4n	42.3558	578	61.1914	1762	0.068
h0l:	h =2n	33.1576	556	88.3164	596	0.020
h0l:	l =2n	32.8670	560	88.9639	592	0.020
h0l:	h+l=2n	123.5405	572	0.7018	580	0.983
h0l:	h+l=4n	117.2448	288	43.1778	864	0.390
hk0:	h =2n	118.9381	464	0.0920	500	0.998
hk0:	k =2n	50.2180	468	63.9742	496	0.085
hk0:	h+k=2n	48.1080	488	66.7155	476	0.074
hk0:	h+k=4n	64.6011	246	54.7930	718	0.158
h00:	h =2n	359.3501	12	0.5916	12	0.995
h00:	h =4n	44.1875	6	225.2320	18	0.004
0k0:	k =2n	812.6345	22	0.1555	24	0.999
0k0:	k =4n	919.9577	10	241.1697	36	0.497
00l:	l =2n	368.1109	28	-0.1829	28	1.000
00l:	l =3n	164.4744	20	194.7915	36	0.096
00l:	l =4n	669.4493	14	22.1355	42	0.907
00l:	l =6n	329.1777	10	152.3958	46	0.319
hhl:	l =2n	49.8828	530	88.7771	528	0.047
hhl:	l =4n	75.4162	262	67.2779	796	0.148
h-hl	l =2n	49.8828	530	88.7771	528	0.047

Look only at those relevant for the already confirmed crystal system and Bravais Lattice.
Here, orthorhombic P.

Look for classes with low mean F^2 when the condition is not met ("for the reverse" columns).

Check systematic absences

Reflection class	For this condition <F^2>	No of reflns	For the reverse <F^2>	No of reflns	Probability
hkl: k+l=2n	41.9113	18980	41.7514	18975	0.126
hkl: h+l=2n	38.8383	19015	44.8363	18940	0.100
hkl: h+k=2n	39.6968	19032	43.9782	18923	0.107
hkl: h+k+l=2n	40.1476	18944	43.5092	19011	0.111
hkl: h+k,k+l=2n	36.7967	9536	43.5207	28419	0.096
hkl: -h+k+l=3n	41.8586	12640	41.8178	25315	0.125
hkl: h-k+l=3n	41.8586	12640	41.8177	25315	0.125
hkl: h-k=3n	44.9562	12685	40.2628	25270	0.147
0kl: k =2n	115.2899	1136	1.1060	1204	0.972
0kl: l =2n	44.9548	1148	67.6953	1192	0.064
0kl: k+l=2n	44.9334	1168	68.1047	1172	0.063
0kl: k+l=4n	42.3558	578	61.1914	1762	0.068
h0l: h =2n	33.1576	556	88.3164	596	0.020
h0l: l =2n	32.8670	560	88.9639	592	0.020
h0l: h+l=2n	123.5405	572	0.7018	580	0.983
h0l: h+l=4n	117.2448	288	43.1778	864	0.390
hk0: h =2n	118.9381	464	0.0920	500	0.998
hk0: k =2n	50.2180	468	63.9742	496	0.085
hk0: h+k=2n	48.1080	488	66.7155	476	0.074
hk0: h+k=4n	64.6011	246	54.7930	718	0.158
h00: h =2n	359.3501	12	0.5916	12	0.995
h00: h =4n	44.1875	6	225.2320	18	0.004
0k0: k =2n	812.6345	22	0.1555	24	0.999
0k0: k =4n	919.9577	10	241.1697	36	0.497
00l: l =2n	368.1109	28	-0.1829	28	1.000
00l: l =3n	164.4744	20	194.7915	36	0.096
00l: l =4n	669.4493	14	22.1355	42	0.907
00l: l =6n	329.1777	10	152.3958	46	0.319
hhl: l =2n	49.8828	530	88.7771	528	0.047
hhl: l =4n	75.4162	262	67.2779	796	0.148
h-hl l =2n	49.8828	530	88.7771	528	0.047

Look for classes with low mean F^2 when the condition is not met ("for the reverse" columns).

Suggested absences:

```
0kl:    k =2n+1
h0l:  h+l=2n+1
hk0:    h =2n+1
h00:    h =2n+1
0k0:    k =2n+1
00l:    l =2n+1
```

From systematic absence tables, only one space group has these absences: *Pbna*. Non-standard setting of *Pbcn*.

3. DETERMINATION OF SPACE GROUPS

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* (2/*m* 2/*m* 2/*m*) (*cont.*)

Reflection conditions								Laue class *mmm* (2/*m* 2/*m* 2/*m*)		
								Point group		
hkl	0*kl*	*h*0*l*	*hk*0	*h*00	0*k*0	00*l*	Extinction symbol	222	*mm*2 *m*2*m* 2*mm*	*mmm*
		h + *l*		*h*		*l*	*P*–*n*–		**$Pmn2_1$** (31)	
									$P2_1nm$ (31)	*Pmnm* (59)
		h + *l*	*h*	*h*		*l*	*P*–*na*		*P*2*na* (30)	***Pmna*** (53)
		h + *l*	*k*	*h*	*k*	*l*	*P*–*nb*		$P2_1nb$ (33)	*Pmnb* (62)
		h + *l*	*h* + *k*	*h*	*k*	*l*	*P*–*nn*		*P*2*nn* (34)	*Pmnn* (58)
	k				*k*		*Pb*– –		*Pbm*2 (28)	
									$Pb2_1m$ (26)	*Pbmm* (51)
							Pb–*a*		$Pb2_1a$ (29)	*Pbma* (57)
	k		*k*		*k*		*Pb*–*b*		*Pb*2*b* (27)	*Pbmb* (49)
	k		*h* + *k*	*h*	*k*		*Pb*–*n*		*Pb*2*n* (30)	*Pbmn* (53)
	k	*h*		*h*	*k*		*Pba*–		***Pba*2** (32)	***Pbam*** (55)
	k	*h*	*h*	*h*	*k*		*Pbaa*			*Pbaa* (54)
	k	*h*	*k*	*h*	*k*		*Pbab*			*Pbab* (54)
	k	*h*	*h* + *k*	*h*	*k*		*Pban*			***Pban*** (50)
	k	*l*			*k*	*l*	*Pbc*–		$Pbc2_1$ (29)	***Pbcm*** (57)
	k	*l*	*h*	*h*	*k*	*l*	*Pbca*			***Pbca*** (61)
	k	*l*	*k*		*k*	*l*	*Pbcb*			*Pbcb* (54)
	k	*l*	*h* + *k*	*h*	*k*	*l*	*Pbcn*			***Pbcn*** (60)
	k	*h* + *l*		*h*	*k*	*l*	*Pbn*–		$Pbn2_1$ (33)	*Pbnm* (62)
	k	*h* + *l*	*h*	*h*	*k*	*l*	*Pbna*			*Pbna* (60)
	k	*h* + *l*	*k*	*h*	*k*	*l*	*Pbnb*			*Pbnb* (56)
	k	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*Pbnn*			*Pbnn* (52)
	l					*l*	*Pc*– –		$Pcm2_1$ (26)	
									*Pc*2*m* (28)	*Pcmm* (51)
	l		*h*	*h*		*l*	*Pc*–*a*		*Pc*2*a* (32)	*Pcma* (55)
	l		*k*		*k*	*l*	*Pc*–*b*		$Pc2_1b$ (29)	*Pcmb* (57)

Search reflection conditions ALWAYS in the columns left to right.

Progressively narrow the possibilities.

No entry means no absences for that class of reflections.

```
0kl:   k =2n+1
h0l:  h+l=2n+1
hk0:   h =2n+1
h00:   h =2n+1
0k0:   k =2n+1
00l:   l =2n+1
```

Search reflection conditions ALWAYS in the columns left to right.

Progressively narrow the possibilities.

No entry means no absences for that class of reflections.

Table 3.1.4.1. *Reflection conditions, diffraction symbols and possible space groups* (*cont.*)

ORTHORHOMBIC, Laue class *mmm* (2/*m* 2/*m* 2/*m*) (*cont.*)

Reflection conditions								Laue class *mmm* (2/*m* 2/*m* 2/*m*) Point group		
hkl	0*kl*	*h*0*l*							*mm*2 *m*2*m* 2*mm*	*mmm*
		h + *l*							$Pmn2_1$ (31)	
									$P2_1nm$ (31)	*Pmnm* (59)
		h + *l*							*P*2*na* (30)	***Pmna*** (53)
		h + *l*							$P2_1nb$ (33)	*Pmnb* (62)
		h + *l*							*P*2*nn* (34)	*Pmnn* (58)
	k								*Pbm*2 (28)	
									$Pb2_1m$ (26)	*Pbmm* (51)
	k		*h*	*h*	*k*				$Pb2_1a$ (29)	*Pbma* (57)
	k		*k*		*k*				*Pb*2*b* (27)	*Pbmb* (49)
	k		*h* + *k*	*h*	*k*		*Pb*		*Pb*2*n* (30)	*Pbmn* (53)
	k	*h*		*h*	*k*		*Pba*–		***Pba*2** (32)	***Pbam*** (55)
	k	*h*	*h*	*h*	*k*		*Pbaa*			*Pbaa* (54)
	k	*h*	*k*	*h*	*k*		*Pbab*			*Pbab* (54)
	k	*h*	*h* + *k*	*h*	*k*		*Pban*			***Pban*** (50)
	k	*l*			*k*	*l*	*Pbc*–		2_1 (29)	***Pbcm*** (57)
	k	*l*	*h*	*h*	*k*	*l*	*Pbca*			***Pbca*** (61)
	k	*l*	*k*		*k*	*l*	*Pbcb*			*Pbcb* (54)
	k	*l*	*h* + *k*	*h*	*k*	*l*	*Pbcn*			***Pbcn*** (60)
	k	*h* + *l*		*h*	*k*	*l*	*Pbn*–		$Pbn2_1$ (33)	*Pbnm* (62)
	k	*h* + *l*	*h*	*h*	*k*	*l*	*Pbna*			*Pbna* (60)
	k	*h* + *l*	*k*	*h*	*k*	*l*	*Pbnb*			*Pbnb* (56)
	k	*h* + *l*	*h* + *k*	*h*	*k*	*l*	*Pbnn*			*Pbnn* (52)
	l					*l*	*Pc*– –		$Pcm2_1$ (26)	
									*Pc*2*m* (28)	*Pcmm* (51)
	l		*h*	*h*		*l*	*Pc*–*a*		*Pc*2*a* (32)	*Pcma* (55)
	l		*k*		*k*	*l*	*Pc*–*b*		$Pc2_1b$ (29)	*Pcmb* (57)

Pbna is a non-standard setting of *Pbcn*. Transform unit cell to the standard setting. Transformation matrix:
[0 0 1 / 1 0 0 / 0 1 0] = axes *cab*

As an exercise find which orthorhombic space groups exhibit the following conditions under which reflections are observed:

1: *h*00, *h* = 2*n*; 0*k*0, *k* = 2*n*

2: 0*kl*, *k* = 2*n*; *h*0*l*, *l* = 2*n*; *hk*0, *h*+*k* = 2*n*;
*h*00, *h* = 2*n*; 0*k*0, *k* = 2*n*; 00*l*, *l* = 2*n*

3: *hkl*, *h*+*k* = 2*n*;
0*kl*, *k*,*l* = 2*n*; *h*0*l*, *h*,*l* = 2*n* *hk*0, *h*+*k* = 2*n*,
*h*00, *h* = 2*n*; 0*k*0, *k* = 2*n*; 00*l*, *l* = 2*n*

4: *hkl*, *h*+*k* = 2*n*, *h*+*l* = 2*n*, *k*+*l* = 2*n*;
0*kl*, *k*,*l* = 2*n*; *h*0*l*, *h*,*l* = 2*n* *hk*0, *h*,*k* = 2*n*,
*h*00, *h* = 2*n*; 0*k*0, *k* = 2*n*; 00*l*, *l* = 2*n*

Which monoclinic space group?

h	k	l	I	sig(I)
2	0	0	2171.64	26.68
3	0	0	274.28	11.15
4	0	0	240.69	11.82
5	0	0	155.15	10.38
6	0	0	5107.39	23.15
7	0	0	235.41	7.37
8	0	0	2384.91	15.85
9	0	0	539.23	10.21
0	3	0	5.42	8.48
0	3	0	1.86	12.00
0	4	0	8595.96	31.56
0	4	0	8213.34	31.14
0	5	0	-3.01	9.85
0	5	0	5.90	9.78
0	6	0	1272.11	12.29
0	6	0	3310.68	18.63
0	7	0	0.46	9.31
0	8	0	390.04	7.81
0	9	0	-3.49	10.31
0	0	3	-3.22	14.74
0	0	4	1636.64	23.32
0	0	5	3.15	12.05
0	0	6	248.34	12.79
0	0	7	9.05	10.77
0	0	8	1504.68	15.02

h	k	l	I	sig(I)
1	0	2	87.28	15.07
2	0	2	4585.57	31.14
3	0	2	1043.06	16.20
4	0	2	3.02	6.72
5	0	2	671.88	10.00
1	0	3	-3.04	13.92
2	0	3	1.70	12.46
3	0	3	-4.76	10.58
4	0	3	-3.87	9.43
5	0	3	-0.32	8.24
1	0	4	570.30	16.03
3	0	4	405.88	9.88
4	0	4	1471.07	13.31
5	0	4	448.25	10.16
1	0	5	-4.33	11.48
2	0	5	-3.55	10.93
3	0	5	4.16	10.04
4	0	5	1.57	9.09
5	0	5	-10.21	8.17
1	0	6	3752.04	24.13
2	0	6	2345.81	18.91
3	0	6	654.73	12.37
4	0	6	1307.56	12.07
5	0	6	168.16	9.17

Which orthorhombic space group?

h	k	l	I	sig
2	0	0	37	18
3	0	0	4	14
4	0	0	8	16
5	0	0	1	15
6	0	0	68	14
7	0	0	0	12
8	0	0	545	22
2	1	0	626	30
3	1	0	1879	40
4	1	0	350	20
5	1	0	24	14
6	1	0	2980	40
7	1	0	6	12
8	1	0	548	20
0	2	0	1755	38
1	2	0	184	16
2	2	0	241	19
3	2	0	207	15
4	2	0	18	14
5	2	0	2562	37
6	2	0	24	14
7	2	0	104	17
8	2	0	560	22
0	3	0	-1	14
1	3	0	779	22
2	3	0	555	18
3	3	0	1502	28
4	3	0	527	20
5	3	0	130	15
6	3	0	2809	35
7	3	0	48	16
8	3	0	109	14
0	4	0	715	18
1	4	0	3	13
2	4	0	282	16
3	4	0	364	14
4	4	0	247	15
5	4	0	1402	25
6	4	0	64	14
7	4	0	92	14
8	4	0	305	19

h	k	l	I	sig
0	5	0	4	9
1	5	0	1356	22
2	5	0	656	18
3	5	0	600	18
4	5	0	48	13
5	5	0	368	16
6	5	0	122	14
7	5	0	1031	22
8	5	0	47	14
0	6	0	0	12
1	6	0	312	15
2	6	0	360	15
3	6	0	63	9
4	6	0	217	11
5	6	0	786	19
6	6	0	483	17
7	6	0	138	14
8	6	0	349	17
0	7	0	0	8
1	7	0	770	18
2	7	0	192	13
3	7	0	70	9
4	7	0	51	9
5	7	0	215	14
6	7	0	468	13
7	7	0	798	17
8	7	0	233	15
0	8	0	660	16
1	8	0	906	18
2	8	0	126	13
3	8	0	341	14
4	8	0	74	13
5	8	0	543	16
6	8	0	63	13
7	8	0	253	15
8	8	0	-0	13
2	0	1	7	17
3	0	1	600	24
4	0	1	7	13
5	0	1	923	24
6	0	1	-4	15

h	k	l	I	sig
7	0	1	7	12
8	0	1	0	15
0	2	1	5	17
0	3	1	3	10
0	4	1	648	20
0	5	1	0	12
0	6	1	176	13
0	7	1	1	11
0	8	1	216	13
1	0	2	-20	16
2	0	2	4	16
3	0	2	11	10
4	0	2	6	13
5	0	2	-0	13
6	0	2	277	16
7	0	2	5	12
8	0	2	1234	24
0	2	2	4526	55
0	3	2	3	14
0	4	2	294	17
0	5	2	2	12
0	6	2	216	11
0	7	2	12	11
0	8	-2	290	14
1	0	3	865	25
2	0	3	1	11
3	0	3	3924	42
4	0	3	11	10
5	0	3	8	9
6	0	3	-0	13
7	0	3	11	12
8	0	3	4	13
0	1	3	-1	13
0	2	3	499	19
0	3	3	16	10
0	4	3	16	9
0	5	3	4	8
0	6	3	3	8
0	7	3	-2	8
0	8	3	7	8

h	k	l	I	sig
0	0	4	7338	67
1	0	4	3	11
2	0	4	822	23
3	0	4	-6	15
4	0	4	1596	26
5	0	4	13	13
6	0	4	782	17
7	0	4	7	8
8	0	4	1726	25
0	1	4	8	16
0	2	4	1834	32
0	3	4	5	14
0	4	4	1145	21
0	5	4	13	13
0	6	4	374	13
0	7	4	7	12
0	8	4	1	12
0	0	5	26	16
1	0	5	4	10
2	0	5	8	10
3	0	5	4418	37
4	0	5	4	13
5	0	5	213	15
6	0	5	2	13
7	0	5	1	9
8	0	5	4	13
0	1	5	10	15
0	2	5	1175	26
0	3	5	9	9
0	4	5	655	16
0	5	5	7	9
0	6	5	12	9
0	7	5	3	12
0	8	5	15	8
0	0	6	4196	42
1	0	6	3	10
2	0	6	402	15
3	0	6	-5	14
4	0	6	1344	20
5	0	6	1	13
6	0	6	1308	19

h	k	l	I	sig
7	0	6	14	13
8	0	6	1841	25
0	2	6	1524	25
0	3	6	6	14
0	4	6	937	19
0	5	6	-0	9
0	6	6	1302	19
0	7	6	10	12
0	8	6	6	12
0	0	7	3	10
1	0	7	190	16
2	0	7	7	10
3	0	7	2867	30
4	0	7	15	13
5	0	7	12	9
6	0	7	1	9
7	0	7	9	9
8	0	7	3	13