III Crystal symmetry

3-3 Point group and space group

A. Point group

1. Symbols of the 32 three dimensional point groups

General symbol	Triclinic	Monoclinic 1^{st} setting	Tetragonal	Trigonal	Hexagonal	Cubic
X	1	2	4	3	6	23
$\bar{X}$ even		$\bar{2} \equiv m$	$\bar{4}$		$\bar{6}$	
X + centre Include $\bar{X}$ odd order	$\bar{1}$	2/m	4/m	$\bar{3}$	6/m	m3 $\equiv$ 2/m $\bar{3}$
	Monoclinci 2^{nd} setting	Orthorhombic				
X2	2 $\equiv$ 12	222	422	32	622	432
Xm	m $\equiv$ 1m	mm2	4mm	3m	6mm	
$\bar{X}$2 or $\bar{X}$m even			$\bar{4}$2m		$\bar{6}$m2	$\bar{4}$3m
X2 + centre Xm +centre Include $\bar{X}$m odd order	2/m	mmm $\equiv$ 2/m 2/m 2/m	4/mmm $\equiv$ 4/m 2/m 2/m	$\bar{3}$m $\equiv$ $\bar{3}$ 2/m	6/mmm $\equiv$ 6/m 2/m 2/m	m3m $\equiv$ 4/m $\bar{3}$ 2/m

Rotation axis X

Rotation-Inversion axis $\bar{X}$

Ratation axis with mirror plane normal to it X/m

Rotation axis with diad axis (axes) normal to it X2

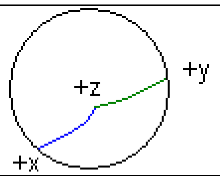
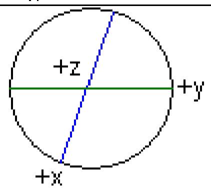
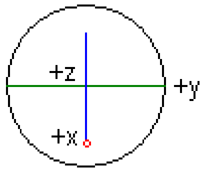
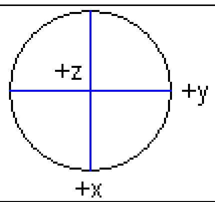
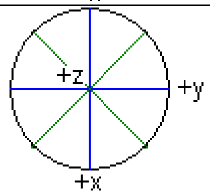
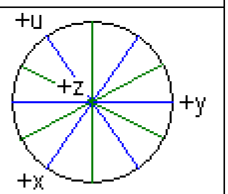
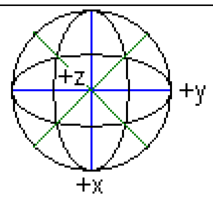
Rotation axis with mirror plane (planes) parallel to it Xm

Rotation-inversion axis with diad axis (axes) normal to it $\bar{X}$2

Rotation-inversion axis with mirror plane (planes) parallel to it $\bar{X}$m

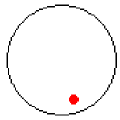
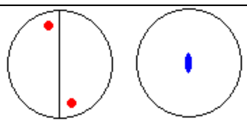
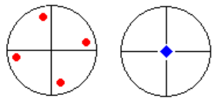
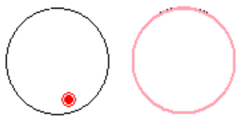
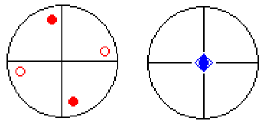
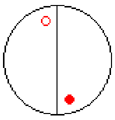
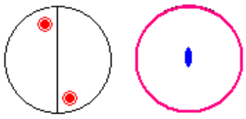
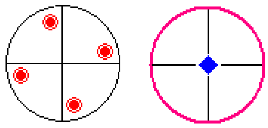
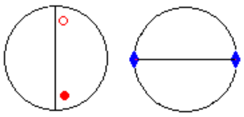
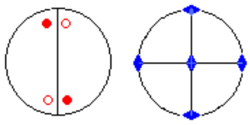
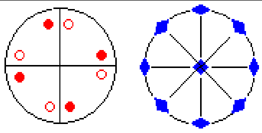
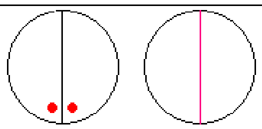
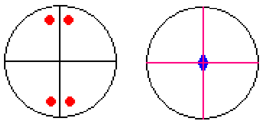
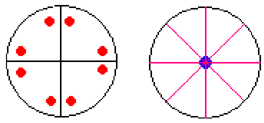
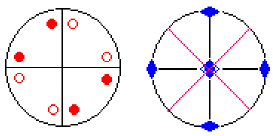
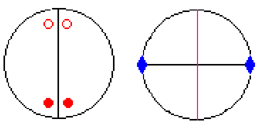
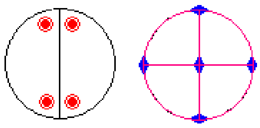
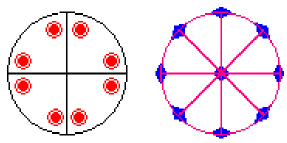
Rotation axis with mirror plane (planes) normal to it and mirror plane (planes) parallel to it X/mm

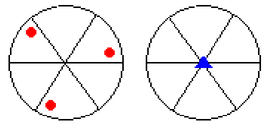
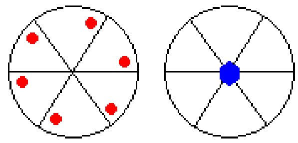
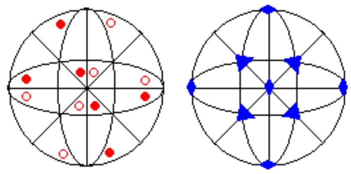
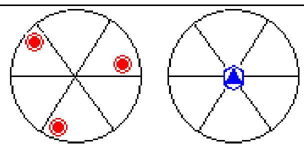
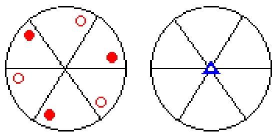
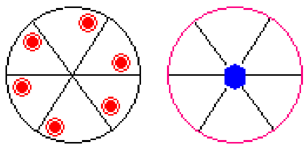
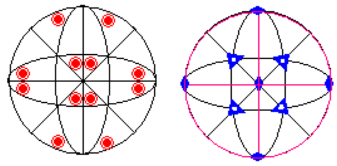
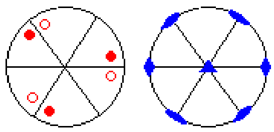
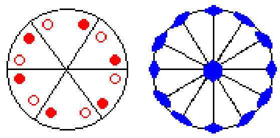
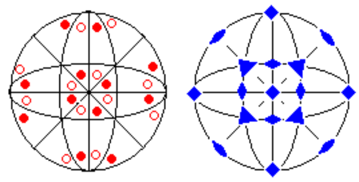
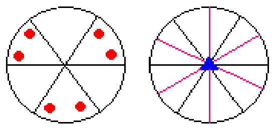
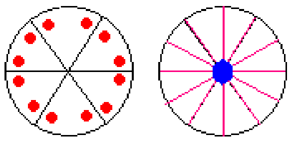
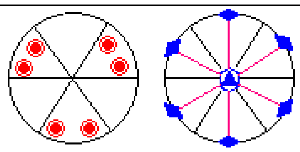
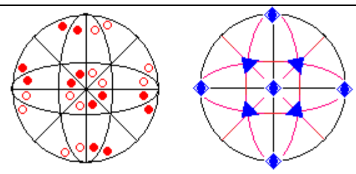
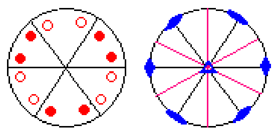
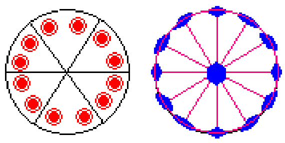
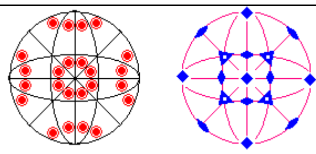
2. Order of positions in the symbols of the three dimensional point groups as applied to lattices

System and point group	Position in point group symbol			Stereographic representation
	Primary	Secondary	Tertiary	
Triclinic 1, $\bar{1}$	Only one symbol which denotes all directions in the crystal.			
Monoclinic 2, m, 2/m	The symbol gives the nature of the unique diad axis (rotation and/or inversion). 1st setting: z-axis unique 2nd setting: y-axis unique			 1st setting  2nd setting
Orthorhombic 222, mm2, mmm	Diad (rotation and/or inversion) along x-axis	Diad (rotation and/or inversion) along y-axis	Diad (rotation and/or inversion) along z-axis	
Tetragonal 4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}$2m, 4/mmm	Tetrad (rotation and/or inversion) along z-axis	Diad (rotation and/or inversion) along x- and y-axes	Diad (rotation and/or inversion) along [110] and [1$\bar{1}$0] axis	
Trigonal and Hexagonal 3, $\bar{3}$, 32, 3m, $\bar{3}$m, 6, $\bar{6}$, 6/m, 622, 6mm, $\bar{6}$m2, 6/mmm	Triad or hexad (rotation and/or inversion) along z-axis	Diad (rotation and/or inversion) along x-, y- and u-axes	Diad (rotation and/or inversion) normal to x-, y-, u-axes in the plane (0001)	
Cubic 23, m3, 432, $\bar{4}$3m, m3m	Diads or tetrad (rotation and/or inversion) along <100> axes	Triads (rotation and/or inversion) along <111> axes	Diads (rotation and/or inversion) along <110> axes	

The 32 three dimensional point groups

Stereograms of poles of equivalent directions and symmetry elements of the 32 point groups (z-axis is normal to the paper in all drawings)

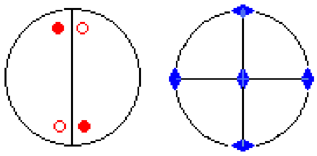
General Symbol	Triclinic	Monoclinic (1st setting)	Tetragonal
X	 1	 2	 4
$\bar{X}$ even		 m ≡ $\bar{2}$	 $\bar{4}$
X + centre $\bar{X}$ odd	 $\bar{1}$	 2/m	 4/m
	Monoclinic (2nd setting)	Orthorhombic	
X2	 2	 222	 422
Xm	 m	 mm2	 4mm
$\bar{X}$2 or $\bar{X}$m even			 $\bar{4}$2m
X2 + centre Xm +centre $\bar{X}$m odd		 Mmm =2/m 2/m 2/m	 4/mmm = 4/m 2/m 2/m

	Trigonal	Hexagonal	Cubic
X	 3	 6	 23
$\bar{X}$ even		 $\bar{6}$	
X + centre $\bar{X}$ odd	 $\bar{3}$	 6/m	 m3 =2/m $\bar{3}$
X2	 32	 622	 432
Xm	 3m	 6mm	
X̄2 or X̄m even		 6̄m2	 4̄3m
X2 + centre Xm +centre X̄m odd	 3̄m = 3̄ 2/m	 6/mmm = 6/m 2/m 2/m	 m3m = 4/m $\bar{3}$ 2/m

MS2041 lecture notes for educational purposes only

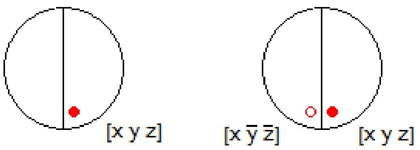
Examples of point group operation

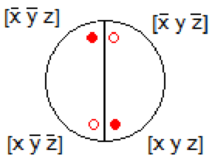
#1 Point group 222



(1) At a general position [x y z], the symmetry is 1

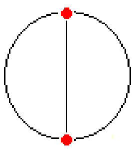
Multiplicity = 4





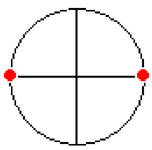
(2) At a special position [100], the symmetry is 2.

Multiplicity = 2



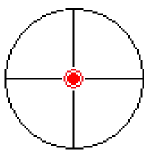
At a special position [010], the symmetry is 2.

Multiplicity = 2

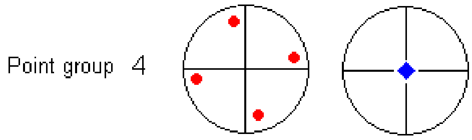


At a special position [001], the symmetry is 2.

Multiplicity = 2

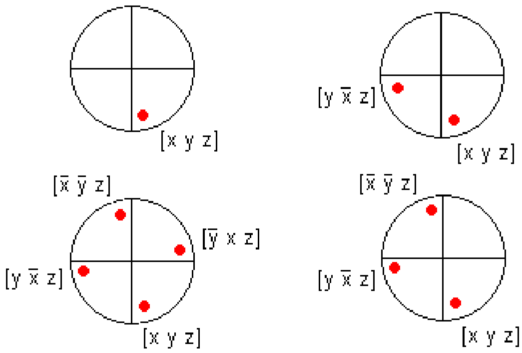


#2 Point group 4



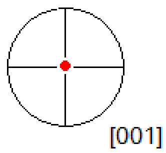
(1) At a general position [x y z], the symmetry is 1

Multiplicity = 4

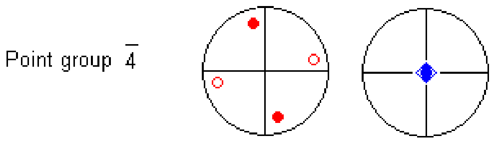


(2) At a special position [001], the symmetry is 4.

Multiplicity = 1

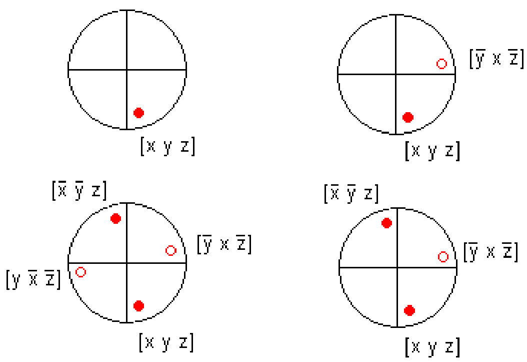


#3 Point group $\bar{4}$



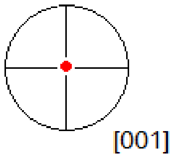
(1) At a general position [x y z], the symmetry is 1

Multiplicity = 4



(2) At a special position [001], the symmetry is $\bar{4}$.

Multiplicity = 1



3. Transformation of vector components

   Original vector is $\vec{P}=[p_1,\ p_2,\ p_3]=[x,y,z]$

   i.e.

$$\vec{P}=x\hat{x}+y\hat{y}+z\hat{z}$$

   When symmetry operation transform the original axes($\hat{x},\ \hat{y},\hat{z}$) to the new axes $(\hat{x}',\ \hat{y}',\ \hat{z}')$

   New vector after transformation of axes becomes $\vec{P'}=[p'_1,p'_2,p'_3]=[u,v,w]$

   i.e.

$$\vec{P'}=u\hat{x'}+v\hat{y'}+w\hat{z'}$$

   The angular relations between the axes may be specified by drawing up a table of direction cosines.

		Old axes		
		$\hat{x}$	$\hat{y}$	$\hat{z}$
New axes	$\hat{x'}$	$a_{11}=\cos\widehat{x'\hat{x}}$	$a_{12}=\cos\widehat{x'\hat{y}}$	$a_{13}=\cos\widehat{x'\hat{z}}$
	$\hat{y'}$	$a_{21}=\cos\widehat{y'\hat{x}}$	$a_{22}=\cos\widehat{y'\hat{y}}$	$a_{23}=\cos\widehat{y'\hat{z}}$
	$\hat{z'}$	$a_{31}=\cos\widehat{z'\hat{x}}$	$a_{32}=\cos\widehat{z'\hat{y}}$	$a_{33}=\cos\widehat{z'\hat{z}}$

   Then

$$u=x*\cos\widehat{x'\hat{x}}+y*\cos\widehat{x'\hat{y}}+\ z*\cos\widehat{x'\hat{z}}$$

   i.e.

$$p'_1=a_{11}*p_1+a_{12}*p_2+a_{13}*p_3$$

   In a dummy notation

$$p'_1=a_{1j}*p_j$$

   Similarly

$$p'_2=a_{2j}*p_j$$
$$p'_3=a_{3j}*p_j$$

i.e.

$$p'_i = a_{ij} * p_j$$

Moreover, by repeating the argument for the reverse transformation and we have

$$x = u * \cos\widehat{x'\hat{x}} + v * \cos\widehat{y'\hat{x}} + w * \cos\widehat{z'\hat{x}}$$
$$p_1 = a_{j1} * p'_j$$

Similarly,

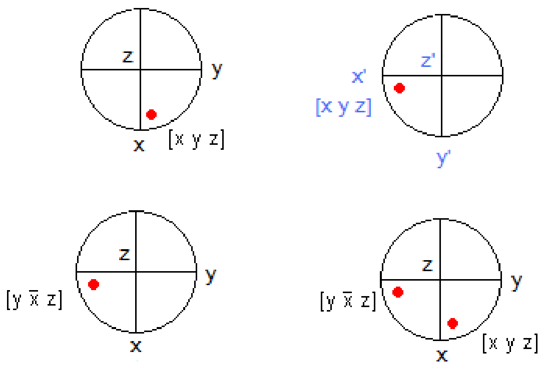
$$p_2 = a_{j2} * p'_j$$
$$p_3 = a_{j3} * p'_j$$

i.e. "old" in terms of "new"

$$p_i = a_{ji} * p'_j$$

For example:

#1 Point group 4



The direction cosines for the first operation is

		Old axes		
		$\hat{x}$	$\hat{y}$	$\hat{z}$
New axes	$\hat{x}' = -\hat{y}$	$a_{11} = 0$	$a_{12} = -1$	$a_{13} = 0$
	$\hat{y}' = \hat{x}$	$a_{21} = 1$	$a_{22} = 0$	$a_{23} = 0$
	$\hat{z}' = \hat{z}$	$a_{31} = 0$	$a_{32} = 0$	$a_{33} = 1$

After symmetry operation, the new position is [x y z] in new axes

We can express it in old axes by

$$p_i = a_{ji} * p'_j = p'_j * a_{ji}$$

$$\begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} y \\ \bar{x} \\ z \end{bmatrix}$$

Therefore, the new position is [y $\bar{x}$ z] in old axes.

B. Space group

1. List of the 230 crystallographic 3D space groups

(Adapted from Wikipedia, the free encyclopedia)

Class	#	Crystal systems and space groups							
		triclinic system							
1	1	P1							
$\bar{1}$	2	P$\bar{1}$							
		monoclinic system							
2	3-5	P2	P2_1	C2					
m	6-9	Pm	Pc	Cm	Cc				
$2/m$	10-15	P2/m	P2_1/m	C2/m	P2/c	P2_1/c	C2/c		
		orthorhombic system							
222	16-24	P222	P222_1	P2_12_12	P2_12_12	C222_1	C222	F222	I222
		I$2_12_12_1$							
mm2	25-46	Pmm2	Pmc2_1	Pcc2	Pma2	Pca2_1	Pnc2	Pmn2_1	Pba2
		Pn2_1	Pnn2	Cmm2	Cmc2_1	Ccc2	Amm2	Aem2	Ama2
		Aea2	Fmm2	Fdd2	Imm2	Iba2	Ima2		
mmm	47-74	Pmmm	Pnnn	Pccm	Pban	Pmma	Pnna	Pmna	Pcca
		Pbam	Pccn	Pbcm	Pnnm	Pmmn	Pbcn	Pbca	Pnma
		Cmcm	Cmce	Cmmm	Cccm	Cmme	Ccce	Fmmm	Fddd
		Immm	Ibam	Ibca	Imma				
		tetragonal system							
4	75-80	P4	P4_1	P4_2	P4_3	I4	I4_1		
$\bar{4}$	81-82	P$\bar{4}$	I$\bar{4}$						
4/m	83-88	P4/m	P4_2/m	P4/n	P4_2/n	I4/m	I4_1/a		
422	89-98	P422	P42_12	P4_122	P4_12_12	P4_222	P4_22_12	P4_322	P$4_32_1$2
		I422	I4_122						
4mm	99-110	P4mm	P4bm	P4_2cm	P4_2nm	P4cc	P4nc	P4_2mc	P4_2bc
		I4mm	I4cm	I4_1md	I4_1cd				
$\bar{4}$2m	111-	P$\bar{4}$2m	P$\bar{4}$2c	P$\bar{4}2_1$m	P$\bar{4}2_1$c	P$\bar{4}$m2	P$\bar{4}$c2	P$\bar{4}$b2	P$\bar{4}$n2

	122	$I\bar{4}m2$	$I\bar{4}c2$	$I\bar{4}2m$	$I\bar{4}2d$				
$4/mm$	123-142	$P4/mm$ $P4_2/m$ $I4/mm$	$P4/mm$ $P4_2/m$ $I4/mc$	$P4/nb$ $P4_2/n$ $I4_1/am$	$P4/nn$ $P4_2/m$ $I4_1/ac$	$P4/mb$ $P4_2/m$	$P4/nn$ $P4_2/m$	$P4/nm$ $P4_2/n$	$P4/nc$ $P4_2/n$
		rhombohedral (trigonal) system							
3	143-146	$P3$	$P3_1$	$P3_2$	$R3$				
$\bar{3}$	147-148	$P\bar{3}$	$R\bar{3}$						
32	149-155	$P312$	$P321$	$P3_112$	$P3_121$	$P3_212$	$P3_221$	$R32$	
$3m$	156-161	$P3m1$	$P31m$	$P3c1$	$P31c$	$R3m$	$R3c$		
$\bar{3}m$	162-167	$P\bar{3}1m$	$P\bar{3}1c$	$P\bar{3}m1$	$P\bar{3}c1$	$R\bar{3}m$	$R\bar{3}c$		
		hexagonal system							
6	168-173	$P6$	$P6_1$	$P6_5$	$P6_2$	$P6_4$	$P6_3$		
$\bar{6}$	174	$P\bar{6}$							
$6/m$	175-176	$P6/m$	$P6_3/m$						
622	177-182	$P622$	$P6_122$	$P6_522$	$P6_222$	$P6_422$	$P6_322$		
$6mm$	183-186	$P6mm$	$P6cc$	$P6_3cm$	$P6_3mc$				
$\bar{6}m2$	187-190	$P\bar{6}m2$	$P\bar{6}c2$	$P\bar{6}2m$	$P\bar{6}2c$				
$6/mm$	191-194	$P6/mm$	$P6/mc$	$P6_3/m$	$P6_3/m$				
		cubic system							
23	195-199	$P23$	$F23$	$I23$	$P2_13$	$I2_13$			
$m\bar{3}$	200-206	$Pm\bar{3}$	$Pn\bar{3}$	$Fm\bar{3}$	$Fd\bar{3}$	$I\bar{3}$	$Pa\bar{3}$	$Ia\bar{3}$	
432	207-214	$P432$	$P4_232$	$F432$	$F4_132$	$I432$	$P4_332$	$P4_132$	$I4_132$
$\bar{4}3m$	215-220	$P\bar{4}3m$	$F\bar{4}3m$	$I\bar{4}3m$	$P\bar{4}3n$	$F\bar{4}3c$	$I\bar{4}3d$		
$m\bar{3}m$	221-230	$Pm\bar{3}m$ $Im\bar{3}m$	$Pn\bar{3}n$ $Ia\bar{3}d$	$Pm\bar{3}n$	$Pn\bar{3}m$	$Fm\bar{3}m$	$Fm\bar{3}c$	$Fd\bar{3}m$	$Fd\bar{3}c$

Symmetry elements in space group

(1) Point group

(2) Translation symmetry + point group

Translational symmetry operations

A Symbol of symmetry planes

Symbol	Symmetry plane	Graphic symbol		Nature of glide translation
		Normal to plane of projection	Parallel to plane of projection	
m	Reflection plane (mirror)			None
a, b	Axial glide plane			a/2 along [100] or 2/b along [010]; or along <100>
c			None	c/2 along z-axis; or (a+b+c)/2 along [111] on rhombohedral axes
n	Diagonal glide plane			(a+b)/2 or (b+c)/2 or (c+a)/2; Or (a+b+c)/2 (tetragonal and cubic)
d	"Diamond" glide plane			(a±b)/4 or (b±c)/4 or (c±a)/4; Or (a±b±c)/4 (tetragonal and cubic) See Note #1

Note #1: In the "diamond" glide plane the glide translation is half of the resultant of the two possible axial glide translations. The arrow in the first diagram show the direction of the horizontal component if the translation when the z-component is positive. In the second diagram the arrow shows the actual direction of the glide translation; there is always another diamond-glide reflection plane parallel to the first with a height difference of 1/4 and the arrow pointing along the other diagonal of the cell face.

Glide planes

---- translation plus reflection across the glide plane

* axial glide plane (glide plane along axis)

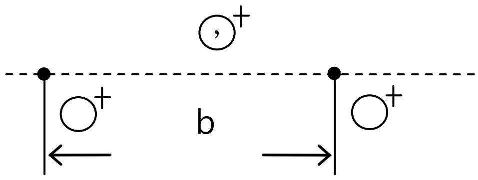
---- translation by half lattice repeat plus reflection

---- three types of axial glide plane

i. a glide, b glide, c glide (a, b, c)

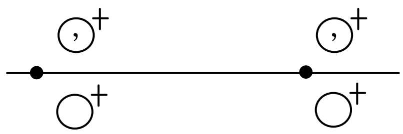
$\frac{1}{2}$ along line in plane $\equiv$ ($\frac{1}{2}$ along line parallel to projection plane)

e.g. b glide



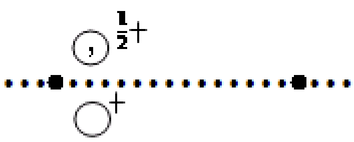
--- graphic symbol for the axial glide plane along y axis

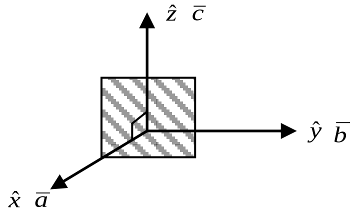
c.f. mirror (m)



— graphic symbol for mirror

*If the axial glide plane is $\frac{1}{2}$ normal to projection plane, the graphic symbol change to

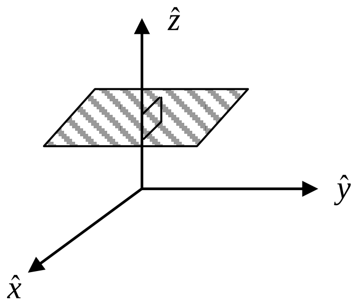




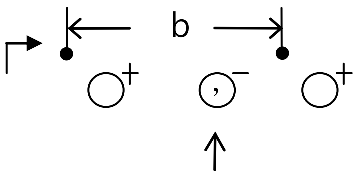
c glide

glide plane $\perp$ $\hat{z}$ axis

* If b glide plane is $\perp$ $\hat{z}$ axis,



glide plane symbol 



* c glide $\frac{c}{2}$ along z axis

or

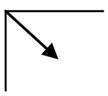
$\frac{a+b+c}{2}$ along [111] on rhombohedral axis

ii. Diagonal glide (n)

$\frac{a+b}{2}$ 、 $\frac{b+c}{2}$ 、 $\frac{a+c}{2}$ or $\frac{a+b+c}{2}$ (tetragonal, cubic system)

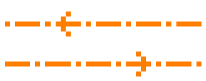
If glide plane is perpendicular to the drawing plane (xy plane), the graphic symbol is

If glide plane is parallel to the drawing plane, the graphic symbol is

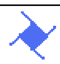
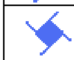
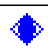
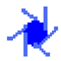
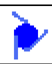
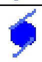
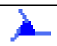
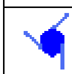
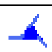
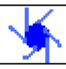


iii. Diamond glide (d)

$\frac{a+b}{4}$ or $\frac{a+b+c}{4}$ (tetragonal, cubic system)



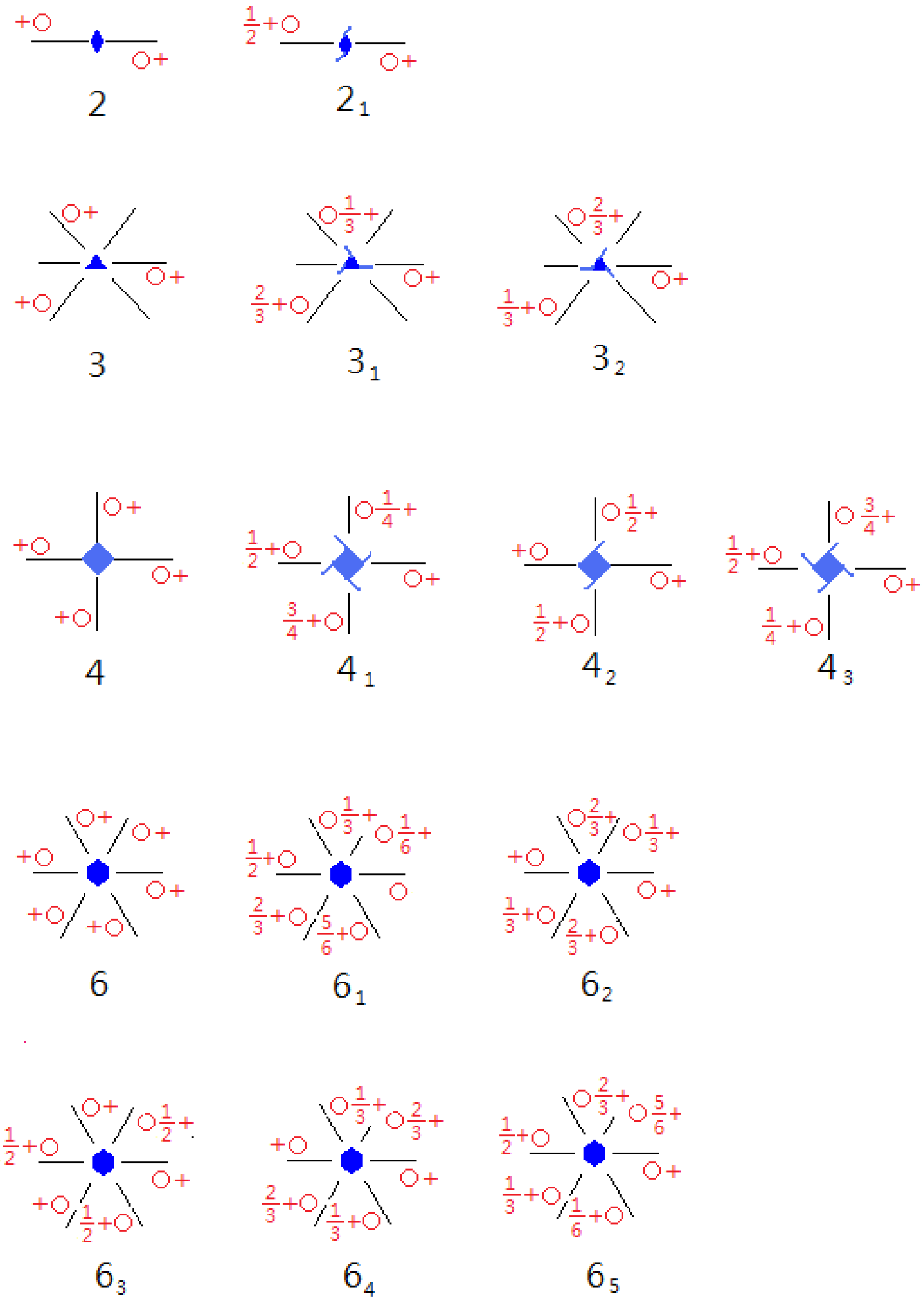
B Symbols of symmetry axes

symbol	Symmetry axis	Graphic symbol	Natur of right-handed screw translation along the axis	symbol	Symmetry axis	Graphic symbol	Natur of right-handed screw translation along the axis
1	Rotation monad	none	none	4	Rotation tetrad		none
$\bar{1}$	Inversion monad		none	4_1	Screw tetrads		c/4
2	Rotation diad	 Normal to paper	none	4_2			2c/4
				4_3			3c/4
		 Parallel to paper		$\bar{4}$	Inversion tetrad		none
2_1	Screw diad	 Normal to paper	c/2 either a/2 or c/2	6	Rotation hexad		none
		Parallel to paper		6_1	Screw hexads		c/6
				6_2			2c/6
3	Roation triad		none	6_3			3c/6
3_1	Screw triad		c/3	6_4			4c/6
3_2			2c/3	6_5			5c/6
$\bar{3}$	Inversion triad		none	$\bar{6}$	Inversion hexad		none

i All possible screw operations

*screw axis --- translation τ plus rotation

screw R_n along c axis
= counterclockwise rotation $(360/R)^{o}$ + translation $(n/R)\bar{c}$



Space group: 230

(1) Symmorphic space group is defined as a space group that may be specified entirely by symmetry operation acting at a common point (the operations need not involve τ) as well as the unit cell translation

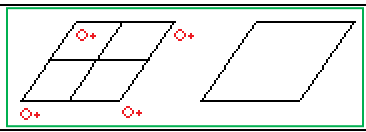
* 73 symmorphic space groups

Crystal system	Bravais lattice	Space group
Triclinic	p	P1, P$\bar{1}$
Monoclinic	P B or A	P2, Pm, P2/m B2, Bm B2/m (1st setting)
Orthorhombic	P C, A or B I F	P222, Pmm2, Pmmm C222, Cmm2, Amm2*, Cmmm I222, Imm2, Immm F222, Fmm2, Fmmm
Tetragonal	P I	P4, P$\bar{4}$, P4/m, P4mm P$\bar{4}$2m, P$\bar{4}$m2*, P4/mmm I4, I$\bar{4}$, I4/m, I422, I4mm I$\bar{4}$2m, I$\bar{4}$m2*, I4/mmm
Cubic	P I F	P23, Pm3, P432, P$\bar{4}$3m, Pm3m I23, Im3, I432, I$\bar{4}$3m, Im3m F23, Fm3, F432, F$\bar{4}$3m, Fm3m
Trigonal	P	P3, P$\bar{3}$, P312, P321*, P3m1 P31m*, P$\bar{3}$1m, P$\bar{3}$m1*
(Rhombohedral)	R	R3, R$\bar{3}$, R32, R3m, R$\bar{3}$m
Hexagonal	P	P6, P$\bar{6}$, P6/m, P622, P6mm P$\bar{6}$m2, P$\bar{6}$2m*, P6/mmm

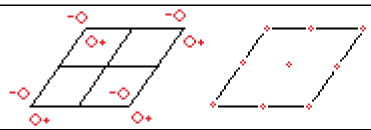
(2) Nonsymmorphic space group is defined as a space group involving at least a translation τ

Examples

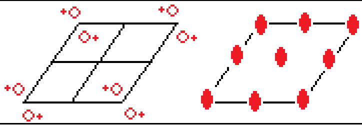
Space group P1

P1 C_1^1		No. 1	P1	1 Triclinic
				
			Origin on 1	
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
1	a	1	x, y, z	No conditions

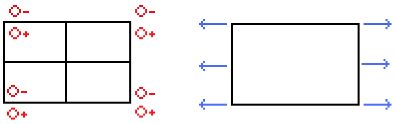
Space group $P\bar{1}$

$P\bar{1}$ C_i^1		No. 2	$P\bar{1}$	$\bar{1}$ Triclinic
				
			Origin on $\bar{1}$	
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
2	i	1	$x, y, z\ ;\ \bar{x}, \bar{y}, \bar{z}$	General: No conditions
1	h	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	Special: No conditions
1	g	$\bar{1}$	$0, \frac{1}{2}, \frac{1}{2}$	
1	f	$\bar{1}$	$\frac{1}{2}, 0, \frac{1}{2}$	
1	e	$\bar{1}$	$\frac{1}{2}, \frac{1}{2}, 0$	
1	d	$\bar{1}$	$\frac{1}{2}, 0, 0$	
1	c	$\bar{1}$	$0, \frac{1}{2}, 0$	
1	b	$\bar{1}$	$0, 0, \frac{1}{2}$	
1	a	$\bar{1}$	$0, 0, 0$	

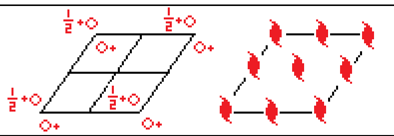
Space group P112

P112 C_2^1		No. 3	P112	2 Monoclinic
				
Ist setting			Origin on 2; unique axis c	
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
2	e	1	x, y, z; $\bar{x}$, $\bar{y}$, z	General: $\left\{\begin{matrix} hkl \\ hk0 \\ 00l \end{matrix}\right\}$ No conditions
1	d	2	$\frac{1}{2}$, $\frac{1}{2}$, z	Special: No conditions
1	c	2	$\frac{1}{2}$, 0, z	
1	b	2	0, $\frac{1}{2}$, z	
1	a	2	0, 0, z	

Space group P121

P121 C_2^1		No. 3	P121	2 Monoclinic
				
			Origin on 2; unique axis b	2^{nd} setting
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
2	e	1	x, y, z; $\bar{x}$, y, $\bar{z}$	General: $\begin{Bmatrix} hkl \\ h0l \\ 0k0 \end{Bmatrix}$ No conditions
1	d	2	$\frac{1}{2}$, y, $\frac{1}{2}$	Special: No conditions
1	c	2	$\frac{1}{2}$, y, 0	
1	b	2	0, y, $\frac{1}{2}$	
1	a	2	0, y, 0	

Space group $P112_1$

$P2_1$ C_2^2		No. 4	$P112_1$	2 Monoclinic
				
Ist setting			Origin on 2_1; unique axis c	
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
2	a	1	x, y, z; $\bar{x}$, $\bar{y}$, $\frac{1}{2}$ +z	General: hkl: No conditions hk0: No conditions 00l: l=2n

Explanation:

#1 Consider the diffraction condition from plane (h k 0)

Two atoms at x, y, z; $\bar{x}$, $\bar{y}$, $\frac{1}{2}$ +z

The diffraction amplitude F can be expressed as

$$
\begin{aligned}
F &= \sum_i f_i * e^{-2\pi i[h\ k\ l]*[x\ y\ z]} \\
&= \sum_i f_i * e^{-2\pi i[h\ k\ 0]*[x\ y\ z]} \\
&= f_i * e^{-2\pi i[h\ k\ 0]*[x\ y\ z]} + f_i * e^{-2\pi i[h\ k\ 0]*[\bar{x}\ \bar{y}\ 1/2+z]} \\
&= f_i * e^{-2\pi i(hx+ky)} + f_i * e^{-2\pi i(-hx-ky)} \\
&= f_i * \left(e^{-2\pi i(hx+ky)} + e^{2\pi i(hx+ky)}\right) \\
&= f_i * \left(2\cos\left(2\pi i(hx+ky)\right)\right) \\
&= 2f_i
\end{aligned}
$$

Therefore, no conditions can limit the (h, k, 0) diffraction.

#2 For the planes (00l)

Two atoms at x, y, z; $\bar{x}$, $\bar{y}$, $\frac{1}{2}$+z

The diffraction amplitude F can be expressed as

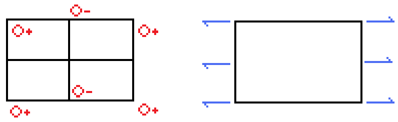
$$
\begin{aligned}
F &= \sum_i f_i * e^{-2\pi i[h\ k\ l]*[x_i\ y_i\ z_i]} \\
&= \sum_i f_i * e^{-2\pi i[0\ 0\ l]*[x_i\ y_i\ z_i]} \\
&= f_i * e^{-2\pi i[0\ 0\ l]*[x\ y\ z]} + f_i * e^{-2\pi i[0\ 0\ l]*[\bar{x}\ \bar{y}\ 1/2+z]} \\
&= f_i * e^{-2\pi ilz} + f_i * e^{-2\pi i\left(\frac{l}{2}+lz\right)} \\
&= f_i * e^{-2\pi ilz} * \left(1 + e^{-\pi il}\right) \\
&= f_i * \left(1 + e^{-\pi il}\right)
\end{aligned}
$$

If l=2n, then F=2f_i

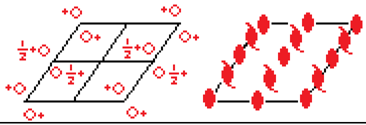
If l=2n+1, then F=0

Therefore, the condition l=2n limit the (0, 0 ,l) diffraction.

Space group $P12_11$

$P2_1$ C_2^2		No. 4	$P12_11$	2 Monoclinic
				
			Origin on 2_1; unique axis b	2^{nd} setting
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
2	a	1	x, y, z; $\bar{x}$, $\frac{1}{2}$+y, $\bar{z}$	General: hkl: No conditions h0l: No conditions 0k0: k=2n

Space group B112

B2 C_2^3		No. 5	B112	2 Monoclinic
				
Ist setting			Origin on 2; unique axis c	
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
4	c	1	x, y, z; $\bar{x}$, $\bar{y}$, z	General: hkl: h+l=2n hk0: h=2n 00l: l=2n
2	b	2	0, $\frac{1}{2}$, z	Special: as above only
2	a	2	0, 0, z	

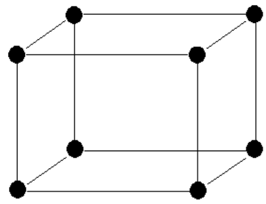
Space group P 4/m $\bar{3}$ 2/m

Pm3m O_1^h		No. 221	P 4/m $\bar{3}$ 2/m	m3m Cubic
Ist setting			Origin at centre; m3m	
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions	Condition limiting possible reflections
48	n	1	x,y,z; z,x,y; y,z,x; x,z,y; y,x,z; z,y,x; x, $\bar{y}$,z; z, $\bar{x}$,y; y, $\bar{z}$,x; x, $\bar{z}$, $\bar{y}$; y, $\bar{x}$, $\bar{z}$; z, $\bar{y}$, $\bar{x}$; $\bar{x}$, y, $\bar{z}$; $\bar{z}$, x, $\bar{y}$; $\bar{y}$, z,x$\bar{x}$; $\bar{x}$, z, $\bar{y}$; $\bar{y}$,x, $\bar{z}$; $\bar{z}$,y, $\bar{x}$; $\bar{x}$, $\bar{y}$,z; $\bar{z}$, $\bar{x}$,y; $\bar{y}$, $\bar{z}$,x; $\bar{x}$, $\bar{z}$,y; $\bar{y}$, $\bar{x}$, z; $\bar{z}$, $\bar{y}$,x; $\bar{x}$, $\bar{y}$, $\bar{z}$; $\bar{z}$,$\bar{x}$, $\bar{y}$; $\bar{y}$, $\bar{z}$, $\bar{x}$; $\bar{x}$, $\bar{z}$, $\bar{y}$; $\bar{y}$, $\bar{x}$, $\bar{z}$; $\bar{z}$, $\bar{y}$, $\bar{x}$; $\bar{x}$, y,z; $\bar{z}$, x,y; $\bar{y}$,z,x; $\bar{x}$, z, y; $\bar{y}$,x,z; $\bar{z}$,y,x; x, $\bar{y}$, z; z, $\bar{x}$, y; y, $\bar{z}$,x; x, $\bar{z}$, y; y, $\bar{x}$, z; z, $\bar{y}$, x; x, y, $\bar{z}$; z, x, $\bar{y}$; y, z, $\bar{x}$; x, z, $\bar{y}$; y, x, $\bar{z}$; z,y, $\bar{x}$;	General: $\left\{\begin{matrix}hkl\\hhl\\0kl\end{matrix}\right\}$No conditions
24	m	M	x,x,z; z,x,x; x,z,x; $\bar{x}$, $\bar{x}$, $\bar{z}$; $\bar{z}$, $\bar{x}$, $\bar{x}$; $\bar{x}$, $\bar{z}$, $\bar{x}$; x, $\bar{x}$, $\bar{z}$; z, $\bar{x}$, $\bar{x}$; x, $\bar{z}$, $\bar{x}$; $\bar{x}$, x, z; $\bar{z}$, x, x; $\bar{x}$, z, x; $\bar{x}$, x, $\bar{z}$; $\bar{z}$, $\bar{x}$, $\bar{x}$; $\bar{x}$, z, $\bar{x}$; x, $\bar{x}$, z; z, $\bar{x}$, x; x, $\bar{z}$, x; $\bar{x}$, $\bar{x}$, z; $\bar{z}$, $\bar{x}$, x; $\bar{x}$, $\bar{z}$, x; x, x, $\bar{z}$; z, x, $\bar{x}$; $\bar{x}$, z, $\bar{x}$;	Special: No conditions
24	l	M	$\frac{1}{2}$,y,z; z, $\frac{1}{2}$,y; y,z, $\frac{1}{2}$; $\frac{1}{2}$,z,y; y, $\frac{1}{2}$,z; z,y, $\frac{1}{2}$; $\frac{1}{2}$,$\bar{y}$, $\bar{z}$; $\bar{z}$, $\frac{1}{2}$, $\bar{y}$; $\bar{y}$, $\bar{z}$, $\frac{1}{2}$; $\frac{1}{2}$,$\bar{z}$, $\bar{y}$; $\frac{1}{2}$, $\bar{y}$,$\frac{1}{2}$, $\bar{z}$; $\bar{z}$, $\bar{y}$,$\frac{1}{2}$; $\frac{1}{2}$,y, $\bar{z}$; $\bar{z}$, $\frac{1}{2}$, y; y, $\bar{z}$, $\frac{1}{2}$; $\frac{1}{2}$,$\bar{z}$, y; y,$\frac{1}{2}$, $\bar{z}$; $\bar{z}$, y,$\frac{1}{2}$; $\frac{1}{2}$,$\bar{y}$, z; z, $\frac{1}{2}$, $\bar{y}$; $\bar{y}$, z, $\frac{1}{2}$; $\frac{1}{2}$,z, $\bar{y}$; $\bar{y}$,$\frac{1}{2}$, z; z, $\bar{y}$,$\frac{1}{2}$;	
24	k	M	0,y,z; z,0,y; y,z,0; 0,z,y; y,0,z; z,y,0; 0,$\bar{y}$, $\bar{z}$; $\bar{z}$, 0, $\bar{y}$; $\bar{y}$, $\bar{z}$,0; 0,$\bar{z}$, $\bar{y}$; 0, $\bar{y}$,0, $\bar{z}$; $\bar{z}$, $\bar{y}$,0; 0,y, $\bar{z}$; $\bar{z}$, 0, y; y, $\bar{z}$,0; 0,$\bar{z}$, y; y,0, $\bar{z}$; $\bar{z}$, y,0; 0,$\bar{y}$, z; z, 0, $\bar{y}$; $\bar{y}$, z,0; 0,z, $\bar{y}$; $\bar{y}$,0, z; z, $\bar{y}$,0;	
12	j	mm	$\frac{1}{2}$, x, x; x, $\frac{1}{2}$, x; x, x, $\frac{1}{2}$; $\frac{1}{2}$, x,$\bar{x}$; $\bar{x}$, $\frac{1}{2}$,x; x, $\bar{x}$, $\frac{1}{2}$; $\frac{1}{2}$, $\bar{x}$,$\bar{x}$; $\bar{x}$, $\frac{1}{2}$, $\bar{x}$; $\bar{x}$, $\bar{x}$, $\frac{1}{2}$; $\frac{1}{2}$, $\bar{x}$,x; x, $\frac{1}{2}$, $\bar{x}$; $\bar{x}$, x, $\frac{1}{2}$;	
12	i	mm	0,x,x; x,0,x; x,x,0; 0,x, $\bar{x}$; $\bar{x}$,0,x; x, $\bar{x}$,0; 0, $\bar{x}$, $\bar{x}$; $\bar{x}$,0, $\bar{x}$; $\bar{x}$, $\bar{x}$,0; 0,$\bar{x}$,x; x,0, $\bar{x}$; $\bar{x}$,x,0;	
12	h	mm	x, $\frac{1}{2}$,0; 0,x, $\frac{1}{2}$; $\frac{1}{2}$,0,x;x,0, $\frac{1}{2}$; $\frac{1}{2}$,x,0;0, $\frac{1}{2}$,x; $\bar{x}$, $\frac{1}{2}$,0; 0, $\bar{x}$, $\frac{1}{2}$; $\frac{1}{2}$,0, $\bar{x}$; $\bar{x}$,0, $\frac{1}{2}$; $\frac{1}{2}$, $\bar{x}$,0;0, $\frac{1}{2}$, $\bar{x}$	
8	g	3m	x,x,x; x,$\bar{x}$,$\bar{x}$; $\bar{x}$,x,$\bar{x}$; $\bar{x}$,$\bar{x}$,x; $\bar{x}$,$\bar{x}$,$\bar{x}$; $\bar{x}$,x,x; x,$\bar{x}$,x; x,x,$\bar{x}$	
6	f	4mm	x,$\frac{1}{2}$,$\frac{1}{2}$; $\frac{1}{2}$,x,$\frac{1}{2}$; $\frac{1}{2}$,$\frac{1}{2}$,x; $\bar{x}$,$\frac{1}{2}$,$\frac{1}{2}$; $\frac{1}{2}$,$\bar{x}$,$\frac{1}{2}$; $\frac{1}{2}$,$\frac{1}{2}$,$\bar{x}$	
6	e	4mm	x,0,0; 0,x,0; 0,0,x; $\bar{x}$,0,0; 0,$\bar{x}$,0; 0,0,$\bar{x}$	
3	d	4/mmm	$\frac{1}{2}$,0,0; 0,$\frac{1}{2}$,0; 0,0,$\frac{1}{2}$	
3	c	4/mmm	0,$\frac{1}{2}$,$\frac{1}{2}$; $\frac{1}{2}$,0,$\frac{1}{2}$; $\frac{1}{2}$,$\frac{1}{2}$,0	
1	b	m3m	$\frac{1}{2}$,$\frac{1}{2}$,$\frac{1}{2}$	
1	a	m3m	0,0,0	

The usage of space group for crystal structure identification

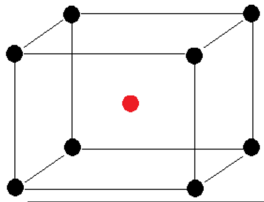
Space group P 4/m $\bar{3}$ 2/m

#1 Simple cubic



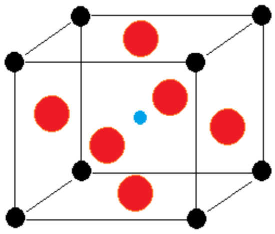
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions
1	A	m3m	0, 0, 0

#2 CsCl structure



atoms	Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions
Cl	1	a	m3m	0, 0, 0
Cs	1	b	m3m	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

#3 $BaTiO_3$ structure



atoms	Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions
Ba	1	a	m3m	0, 0, 0
Ti	1	b	m3m	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
O	3	c	4/mmm	$0, \frac{1}{2}, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{2}$; $\frac{1}{2}, \frac{1}{2}, 0$