B. Space group

1. The 230 crystallographic 3D space groups

(You may find detailed information in Wikipedia, the free encyclopedia)

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)

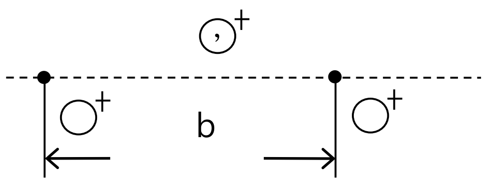
---- translation by half lattice repeat plus reflection

---- 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

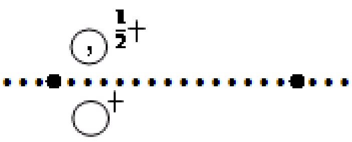


--- graphic symbol for the axial glide plane along y axis

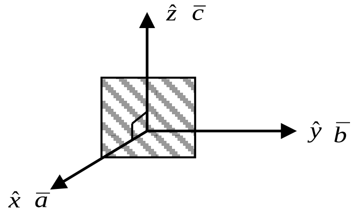
c.f. mirror (m)

— graphic symbol for mirror

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

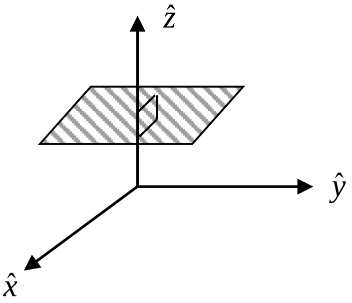


c glide

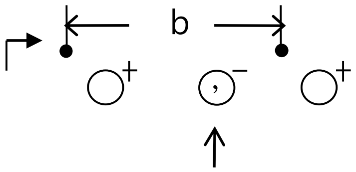


glide plane $\perp$ $\hat{z}$ axis

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



glide plane symbol 



underneath the glide plane

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

or

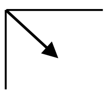
$\frac{a+b+c}{2}$ along [111] on rhombohedral axis

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)

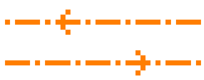
If glide plane is perpendicular to the drawing plane (xy plane), the graphic symbol is

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

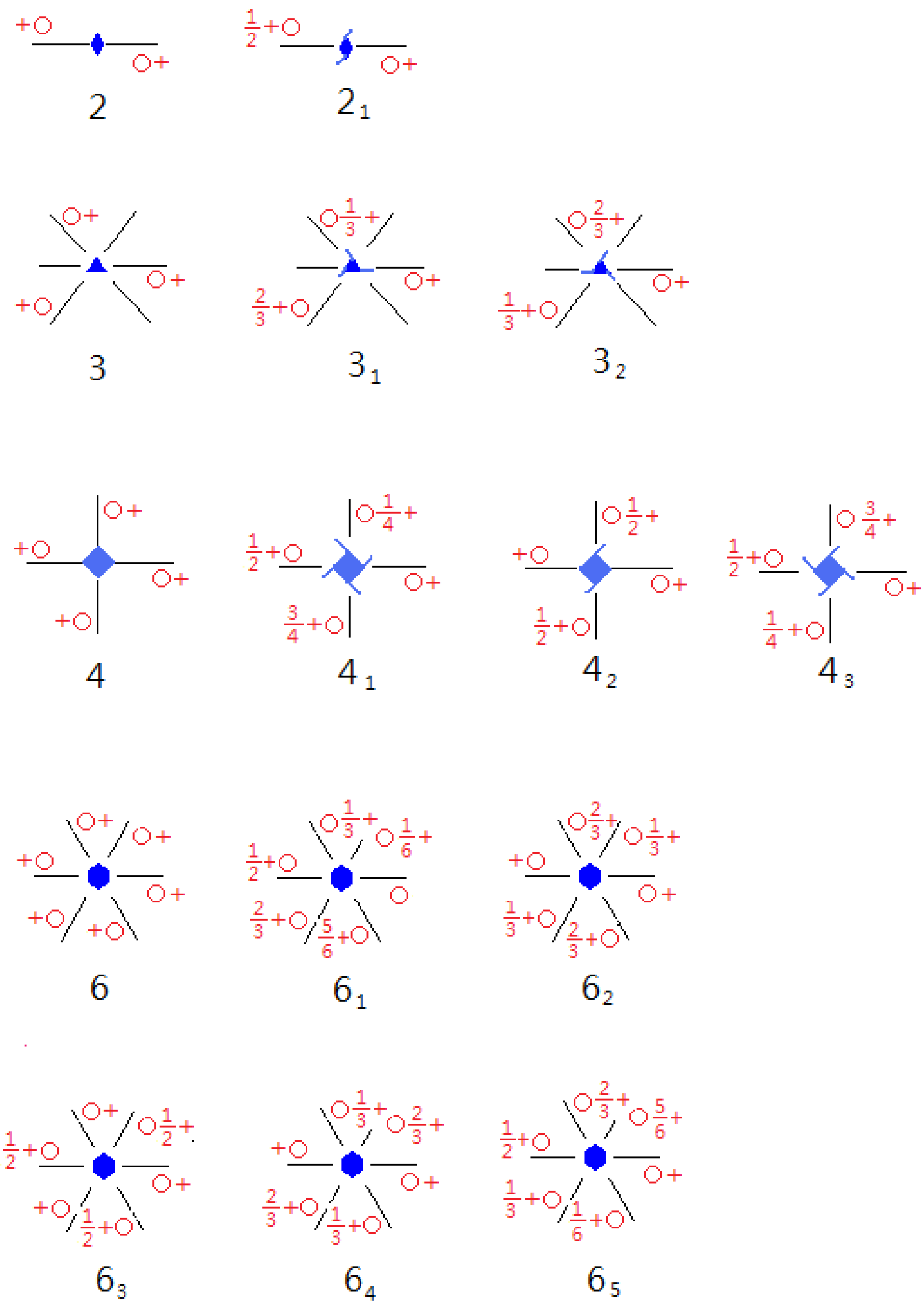
symbol	Symmetry axis	Graphic symbol	Natur of right-handed screw translation along the axis	symbol	Symmetry axis	Graphic symbol	Natur of right-handed screw translation along the axis
1	Rotation monad	none	none	4	Rotation tetrad		none
$\bar{1}$	Inversion monad		none	4_1	Screw tetrads		c/4
2	Rotation diad	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

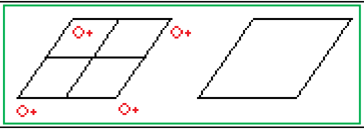
Crystal system	Bravais lattice	Space group
Triclinic	p	P1, $P\bar{1}$
Monoclinic	P B or A	P2, Pm, P2/m B2, Bm B2/m (1st setting)
Orthorhombic	P C, A or B I F	P222, Pmm2, Pmmm C222, Cmm2, Amm2*, Cmmm I222, Imm2, Immm F222, Fmm2, Fmmm
Tetragonal	P I	P4, $P\bar{4}$, P4/m, P4mm $P\bar{4}2m$, $P\bar{4}m2$*, 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

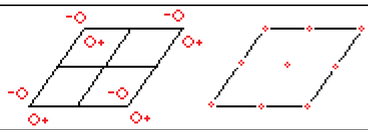
Examples

(All the space groups in the following pages are adapted from the International Tables for Crystallography and replotted in the color form for educational purposes.)

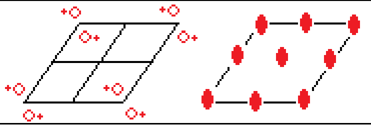
Space group P1

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

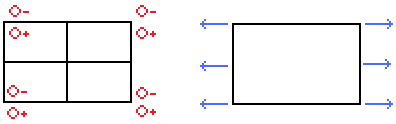
Space group $P\bar{1}$

$P\bar{1}$ 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	

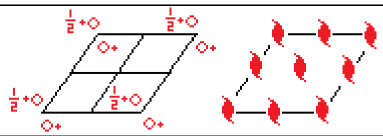
Space group P112

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: $\begin{Bmatrix} hkl \\ hk0 \\ 00l \end{Bmatrix}$ 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	2nd 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

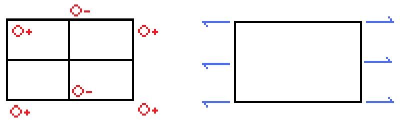
$$
\begin{aligned}
F &= \sum_i f_i * e^{-2\pi i [h\ k\ l]*[x_i\ y_i\ z_i]} \\
&= \sum_i f_i * e^{-2\pi i [0\ 0\ l]*[x_i\ y_i\ z_i]} \\
&= f_i * e^{-2\pi i [0\ 0\ l]*[x\ y\ z]} + f_i * e^{-2\pi i [0\ 0\ l]*[\bar{x}\ \bar{y}\ 1/2+z]} \\
&= f_i * e^{-2\pi i l z} + f_i * e^{-2\pi i \left(\frac{l}{2}+lz\right)}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

If l=2n, then F=2f_i

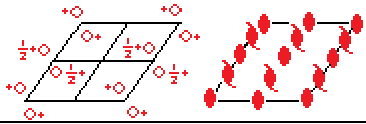
If l=2n+1, then F=0

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	

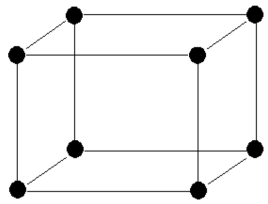
Space group P 4/m $\bar{3}$ 2/m

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: $\left.\begin{cases}hkl\\hhl\\0kl\end{cases}\right\}$ 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

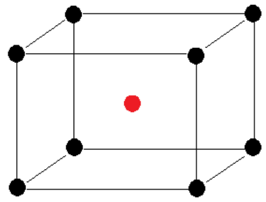
Space group P 4/m $\bar{3}$ 2/m

#1 Simple cubic



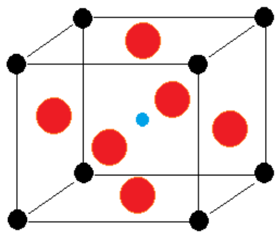
Number of positions	Wyckoff notation	Point symmetry	Coordinates of equivalent positions
1	A	m3m	0, 0, 0

#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	$0, \frac{1}{2}, \frac{1}{2};$ $\frac{1}{2}, 0, \frac{1}{2};$ $\frac{1}{2}, \frac{1}{2}, 0$