晶体衍射与结构分析

Lec-03

Crystal Diffraction and Structure Analysis

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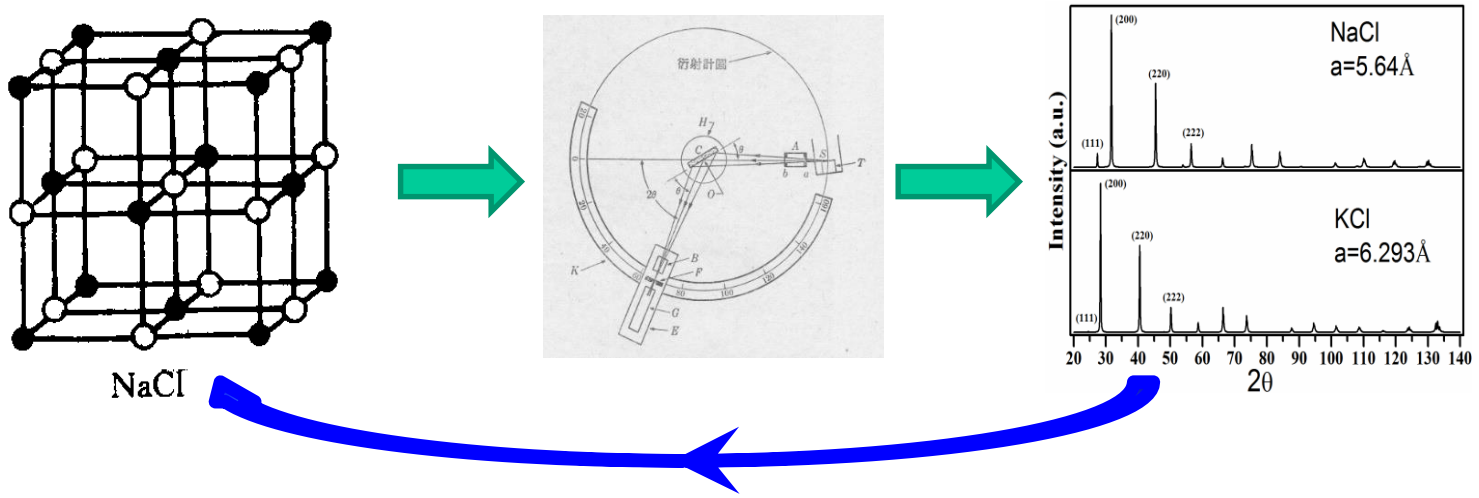

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1.5 空间群

1.6 国际晶体学表

晶体结构 ↔ 空间点阵＋结构基元

Structure ↔ Lattice + Basis

晶系名称	特征对称	晶胞形状
立 方	四个3次轴	a=b=c, α=β=γ=90°
六方	一个6次轴	a=b≠c, α=β=90°,γ=120°
四方	一个4次轴	a=b≠c, α=β=γ=90°
三方	一个3次轴	a=b=c, α=β=γ≠90°
正交	三个互相垂直的2次轴或对称面或它们的组合，而无更高次轴	a≠b≠c, α=β=γ=90°
单斜	只具有一个二次轴或对称面或它们的组合，而无更高次轴	a≠b≠c, α=γ=90°≠β
三斜	不具有对称轴和对称面，只能含一次对称轴和对称中心	a≠b≠c, α≠β≠γ

晶系名称	晶胞形状	国际符号位序	位序所代表的方向与基矢方向的关系	所属点群
立 方	a=b=c, α=β=γ=90° 	1 2 3	[100][010][001] [111] … [110]…	23； m $\bar{3}$; 43; $\bar{4}$ 3m; m $\bar{3}$m;
六方	a=b≠c, α=β=90°,γ=120° 	1 2 3	[001] [100] [010] [120]…	6; $\bar{6}$; 6/m $\bar{6}$m2;622 6mm;6/mmm

四方	a=b≠c, α=β=γ=90°.	1 2 3	[001] [100] [010] [110]…	4; $\bar{4}$; 4/m $\bar{4}$m2;422 4mm;4/mmm
三方 (R点阵)	a=b=c, α=β=γ≠90°	1 2	[111] [1-10]	3次轴对应 a+b+c方向
三方 H点阵	a=b≠c, α=β=90°, γ=120°	1 2 3	[001] [100] [010] [120] [210]	3; $\bar{3}$; 3m1 321; $\bar{3}$m1

正交	a≠b≠c, α=β=γ=90°	1 2 3	[100] [010] [001]	222 mm2 mmm
单斜	a≠b≠c, α=γ=90°≠β	1	[010]	2; m ; 2/m
三斜	a≠b≠c, α≠β≠γ	1	[000]	1; $\bar{1}$

晶 体 结 构

晶体结构中

微观空间对称元素及组合，空间群

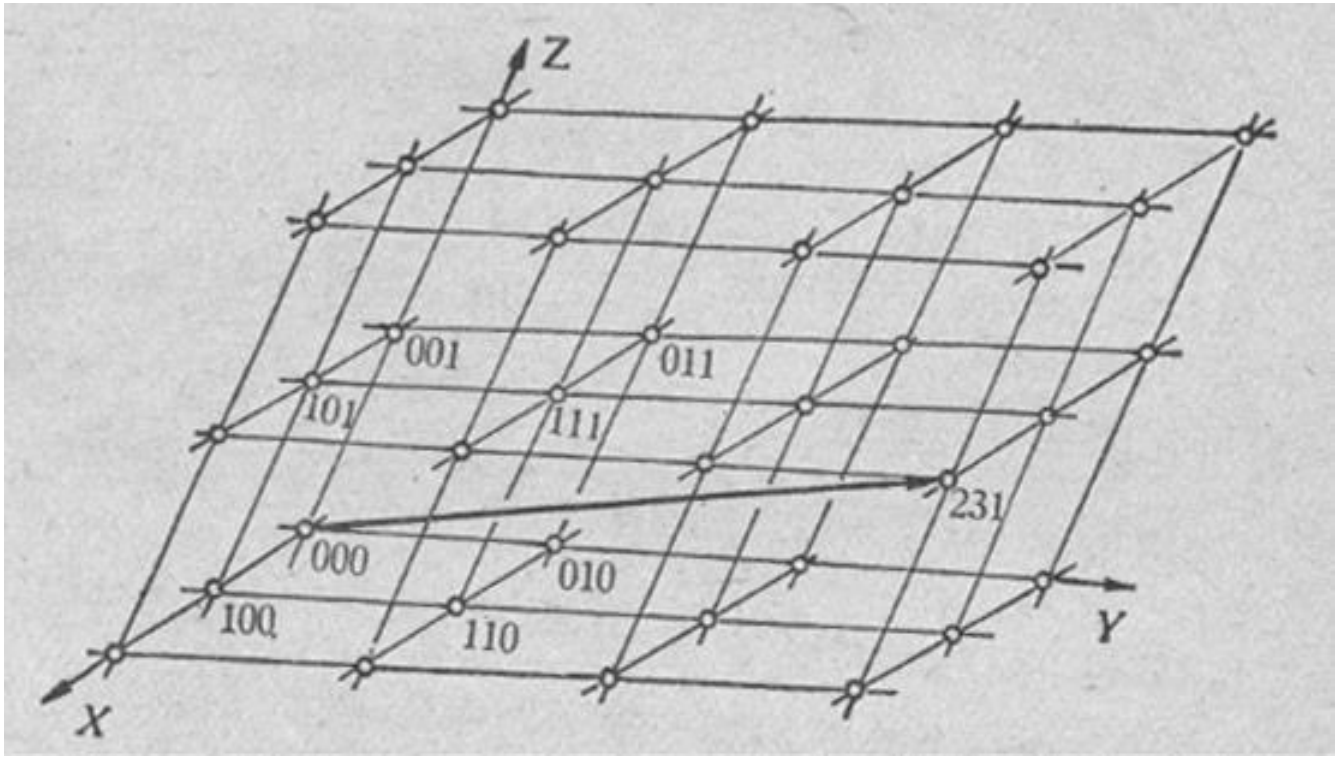
关键：平移对称性

晶体结构 ↔ 空间点阵＋结构基元

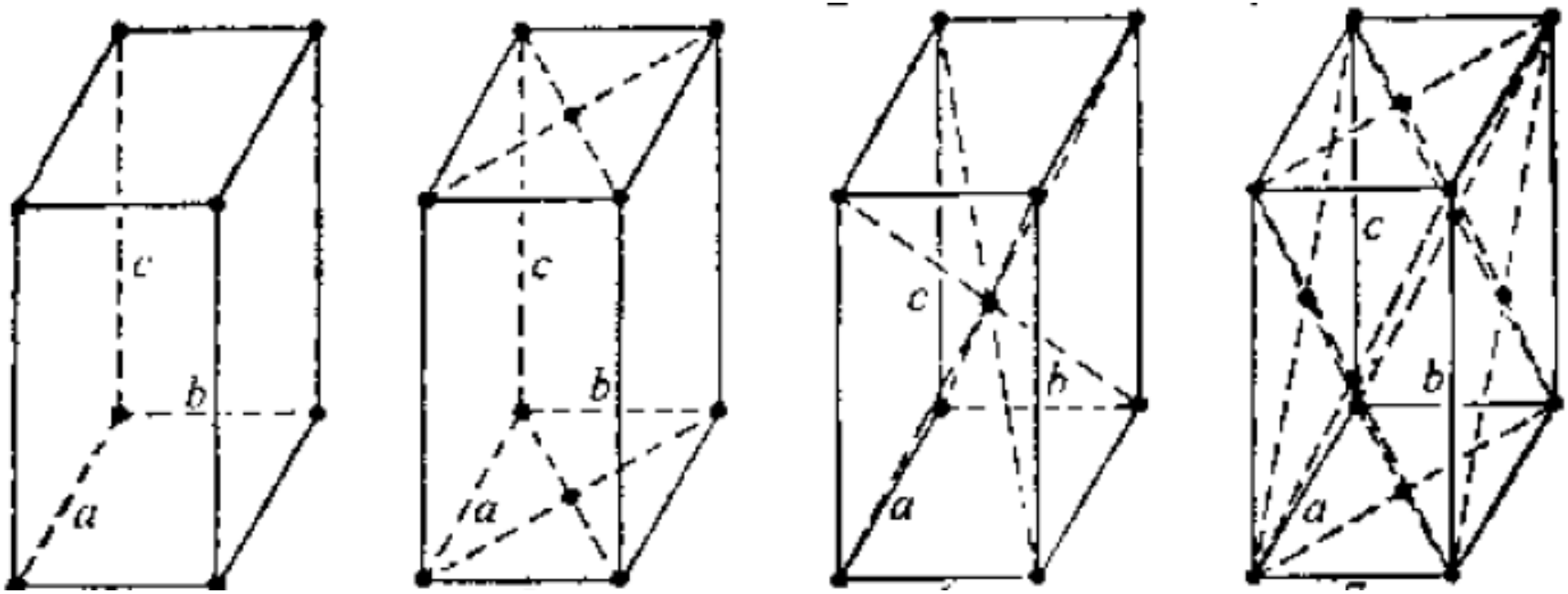
Structure ↔ Lattice + Basis

1.5.1 微观空间对称元素

初基平移 $T = m\boldsymbol{a} + n\boldsymbol{b} + l\boldsymbol{c}$

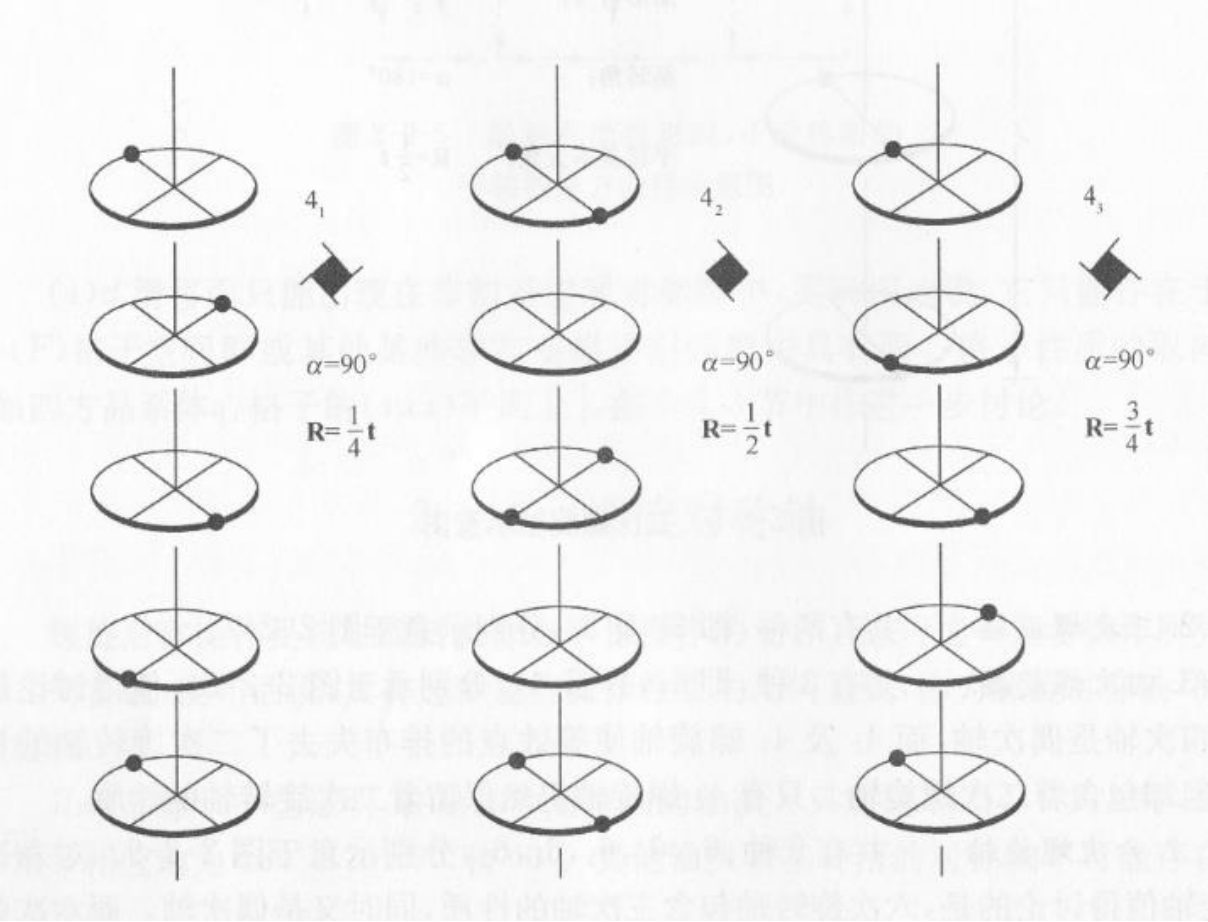


非初基平移 $T = m\boldsymbol{a} + n\boldsymbol{b} + l\boldsymbol{c}$



Primitive P　　c-centred C　　body-centred I　　face-centred F

螺旋轴是旋转与平移的复合操作



$2_1,3_1,3_2,4_1,4_2,4_3,6_1,6_2,6_3,6_4,6_5$.

Rutile (金红石型结构)

金红石，TiO_2，

空间群$P4_2/mnm$

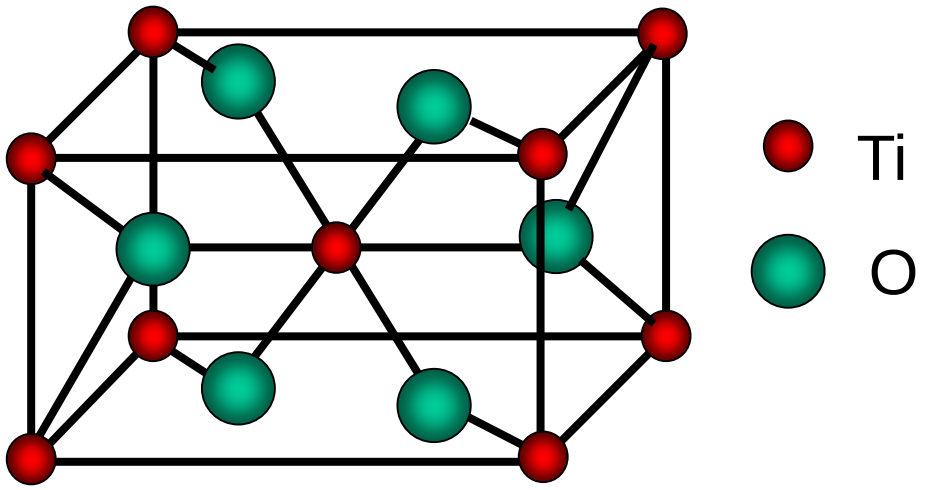
a=4.593, c=2.959Å

单位晶胞内有4个O^{2-}，

2个Ti^{4+}，Z=2。

Ti 2a (0, 0, 0)

O 4f (0.302, 0.302, 0)



滑移面为反映面和平移的复合操作。

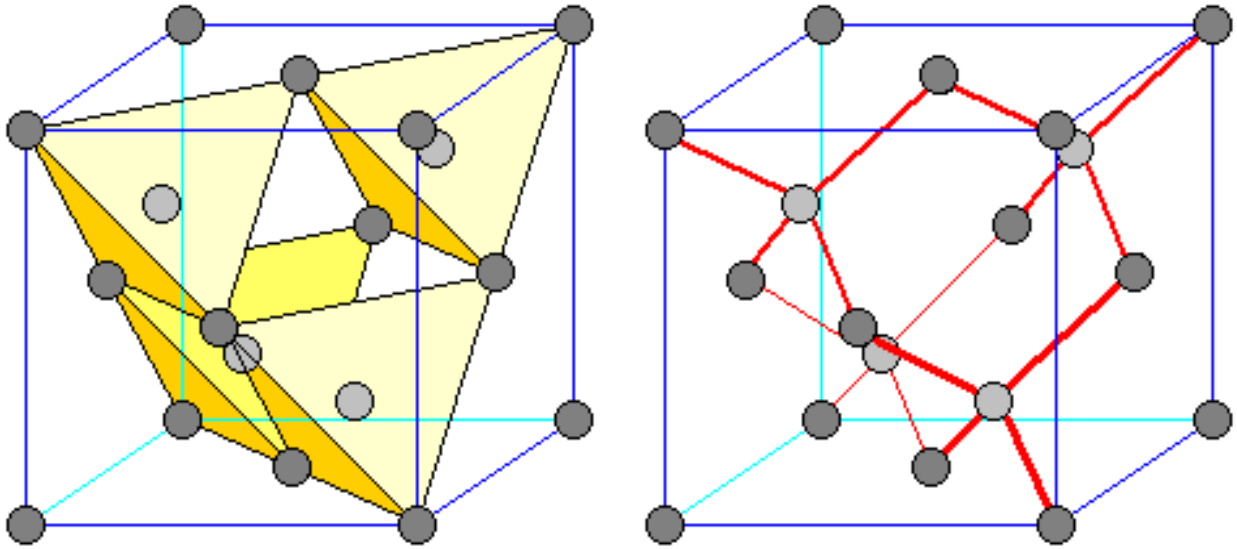
滑移面有5种类型，a,b,c,n,d。

滑移面a,b,c的对称操作分别为点阵图像经滑移面反映后分别沿平行于基矢***a,b,c***方向平移a/2,b/2,c/2，使点阵图像的等同部分重合。

滑移面n为经反映后平移（a+b）/2, 或(b+c)/2,或(c+a)/2。

滑移面d为经反映后平移（a+b）/4, 或(b+c)/4,或(c+a)/4

Diamond (金刚石型结构)

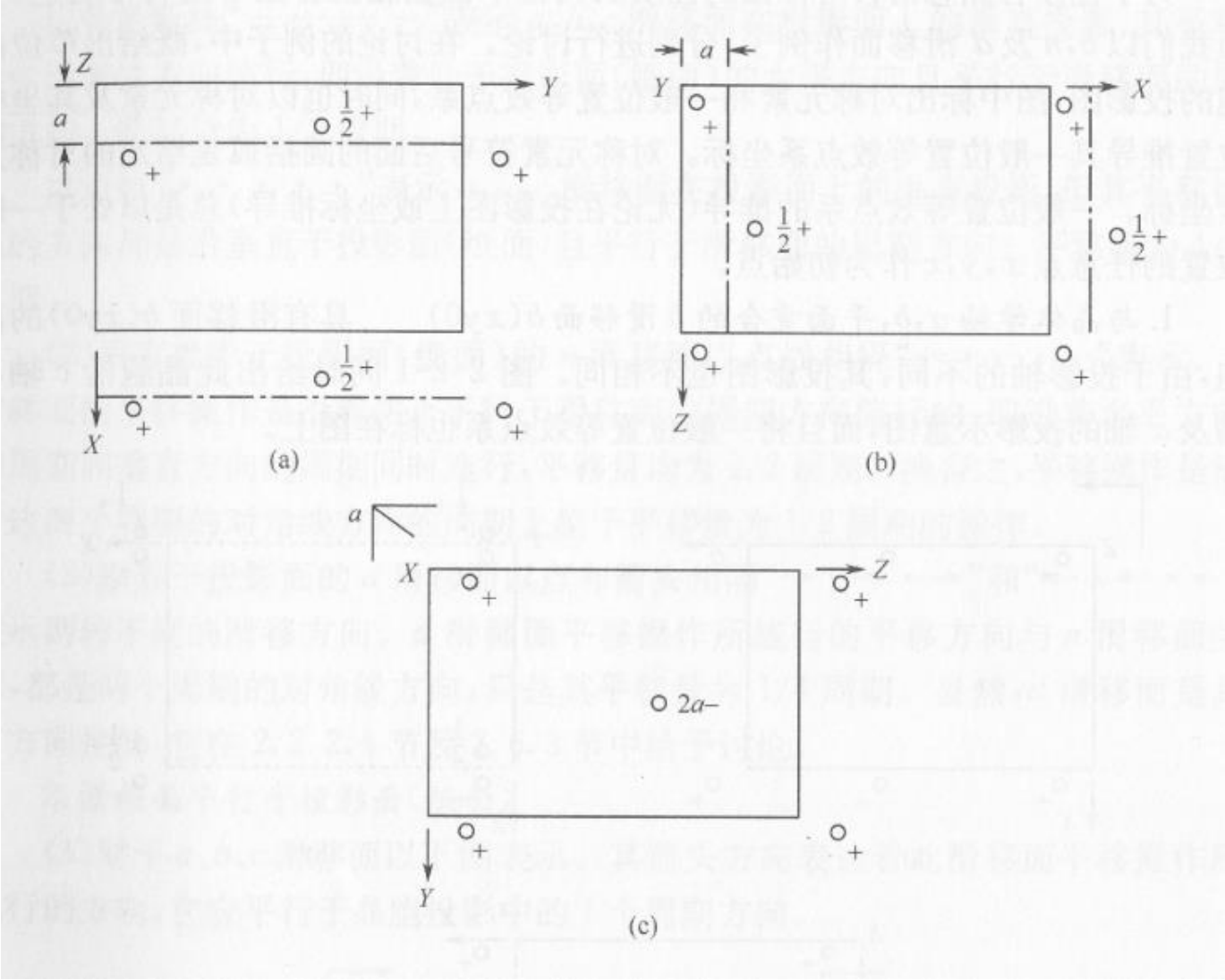


Fd3m , a=3.570 Å

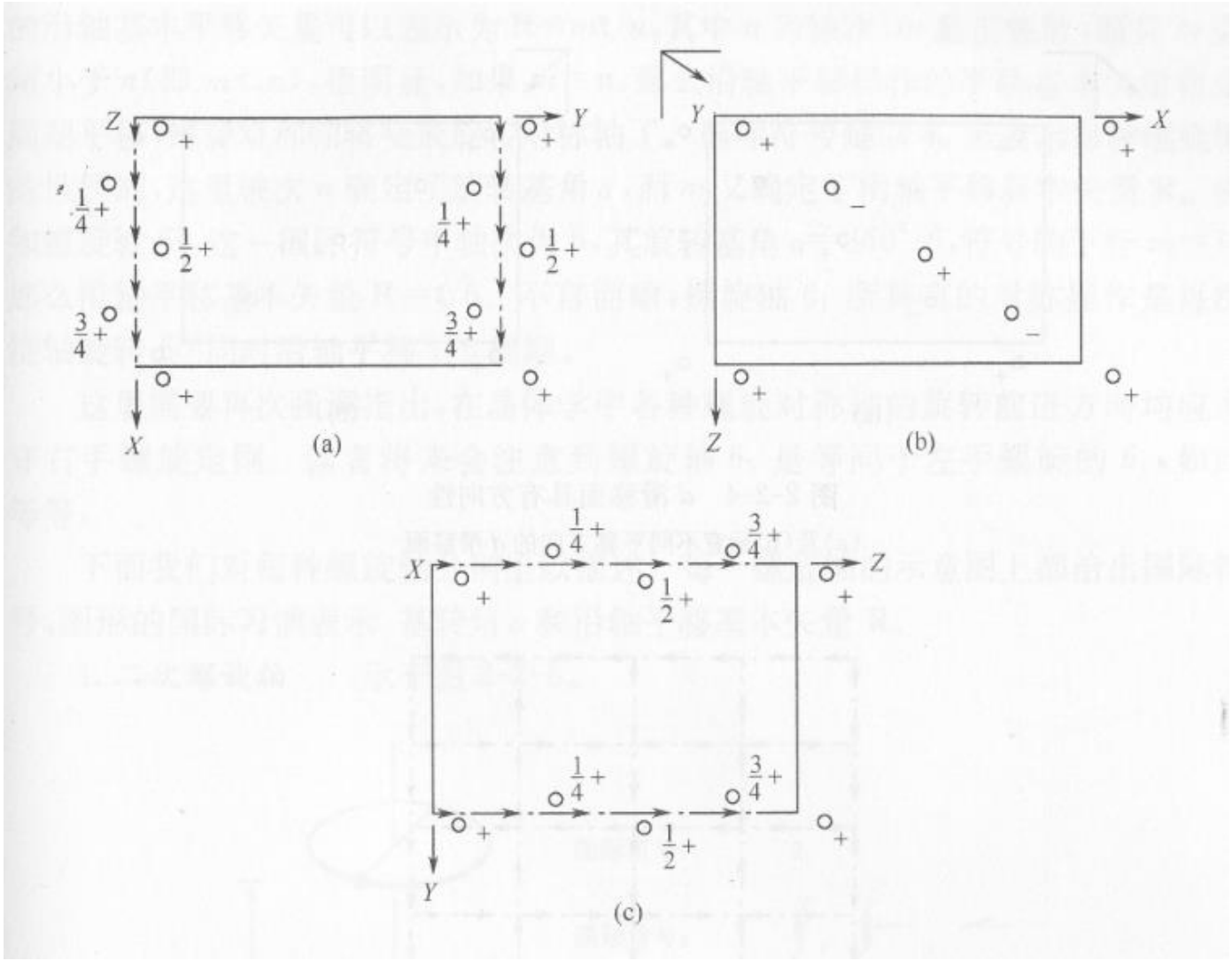
C 8a (0,0,0) (3/4,1/4,3/4)

Z=8

晶胞中微观对称元素表示方法



晶胞中微观对称元素表示方法



1.5.2 空间群

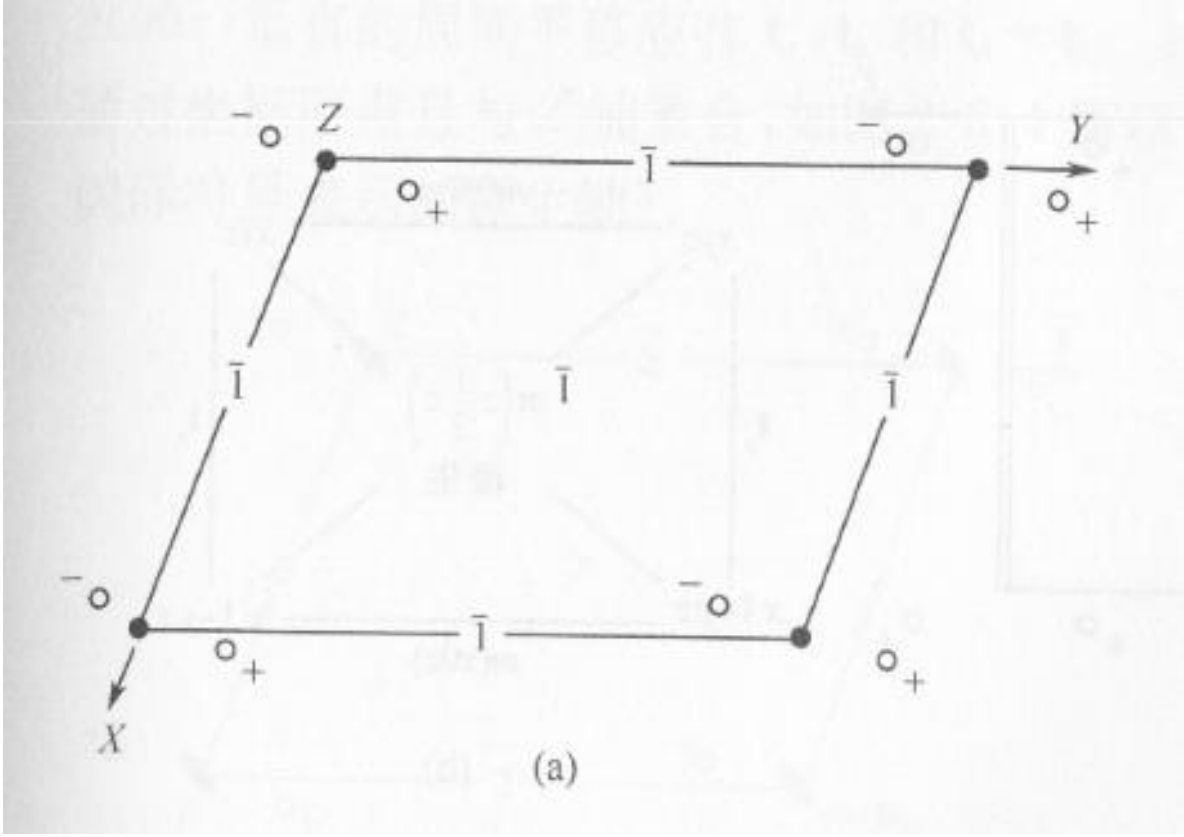
微观空间对称元素共有下列26种。

$$1, \bar{1}, m, a, b, c, n, d$$

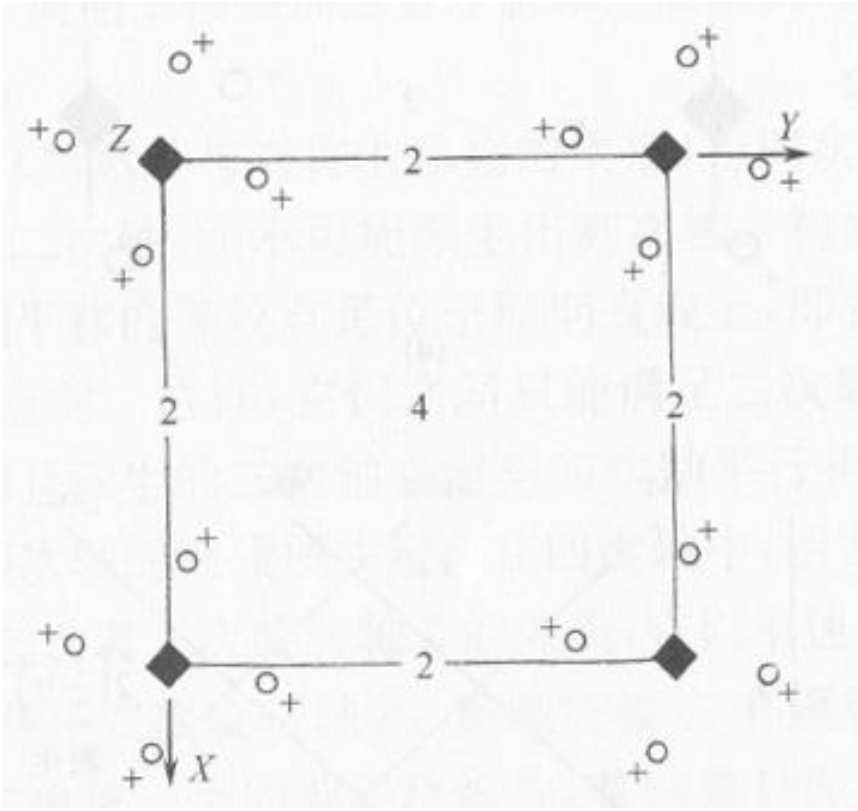
$$2, 2_1, 3, \bar{3}, 3_1, 3_2, 4, \bar{4}, 4_1, 4_2, 4_3, 6, \bar{6}, 6_1, 6_2, 6_3, 6_4, 6_5$$

在晶体内部微观结构中，上述26种微观对称元素，以及初基平移（P）、非初基平移的共同组合（I，C，F）称为空间对称群，简称空间群。在晶体微观结构中可能存在的空间群共有230中。

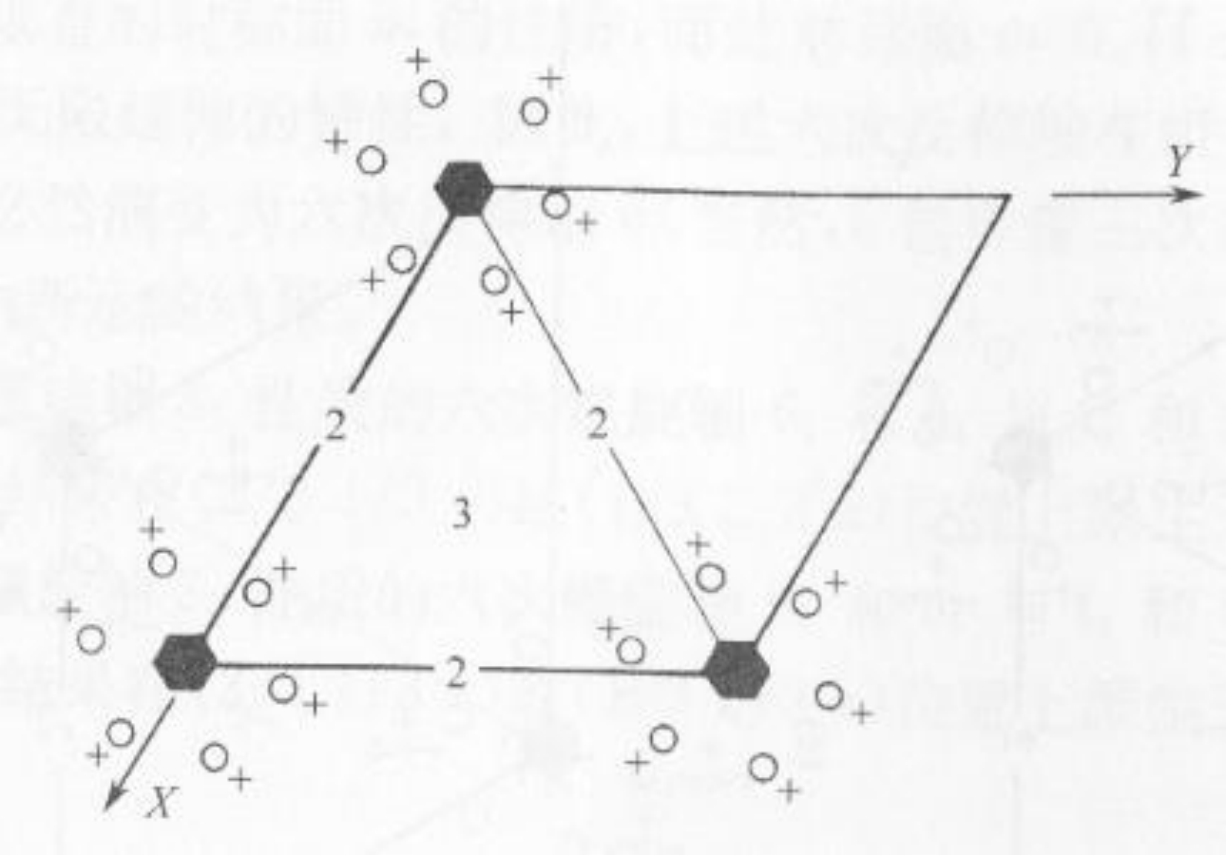
晶体的微观空间对称元素与周期平移的组合



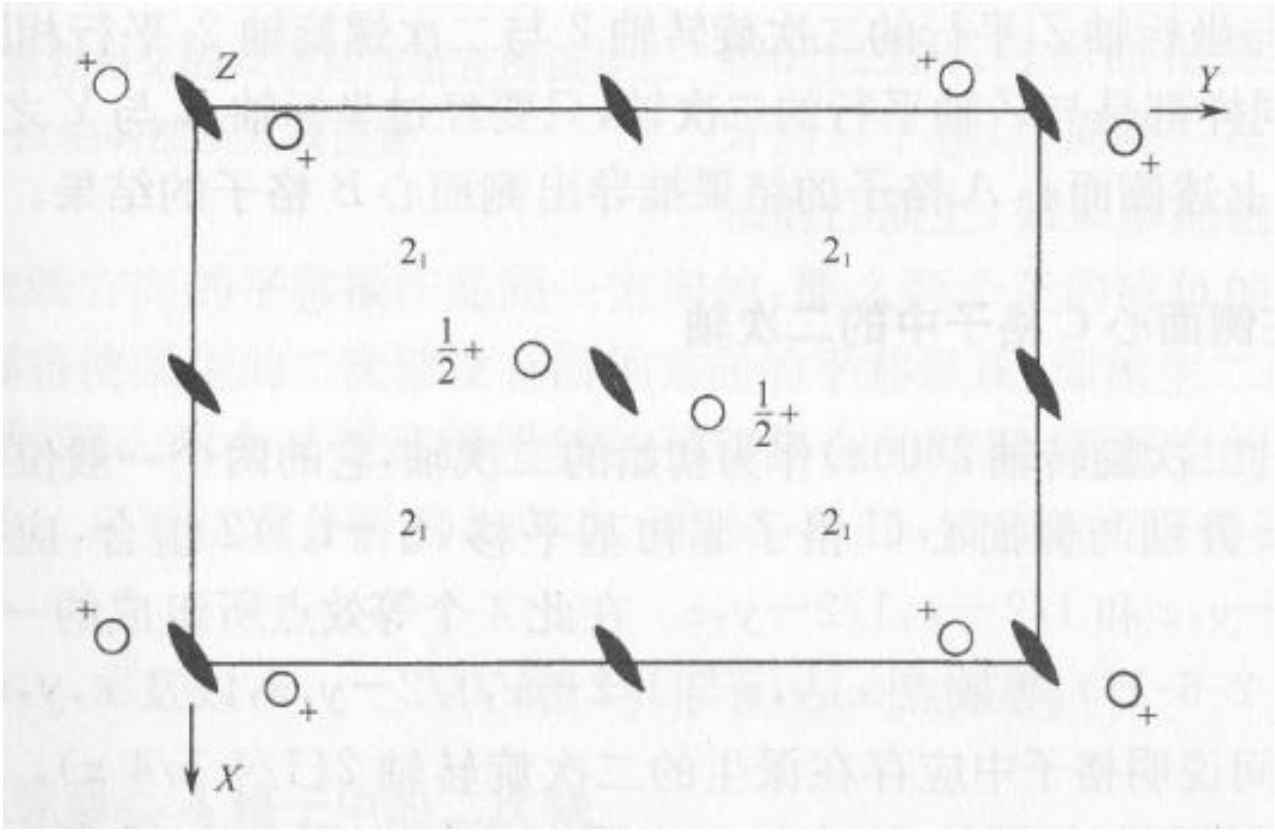
晶体的微观空间对称元素与周期平移的组合



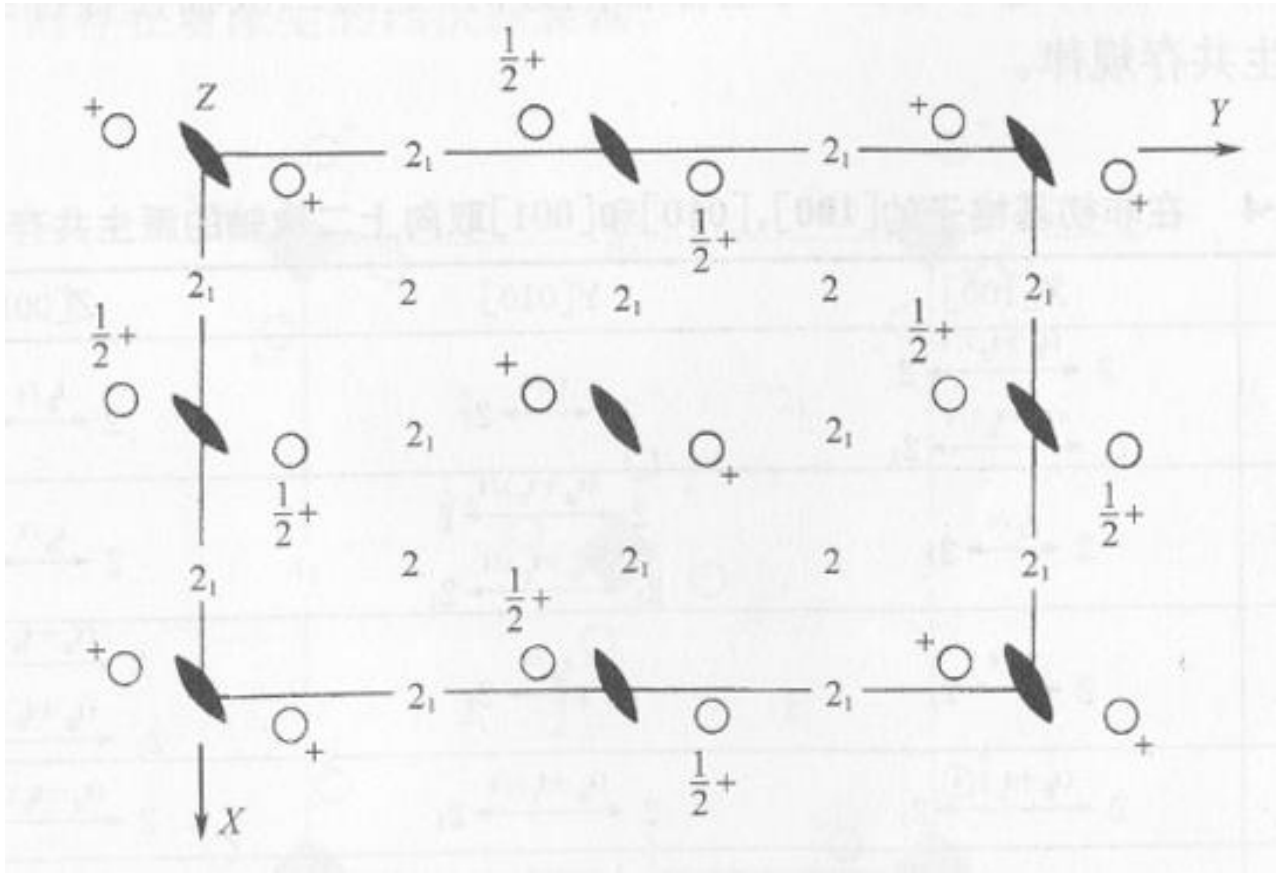
晶体的微观空间对称元素与周期平移的组合



晶体的微观空间对称元素与非初基平移的组合



晶体的微观空间对称元素与非初基平移的组合



1.6　晶体学国际表，等效点系

International Tables for Crystallography

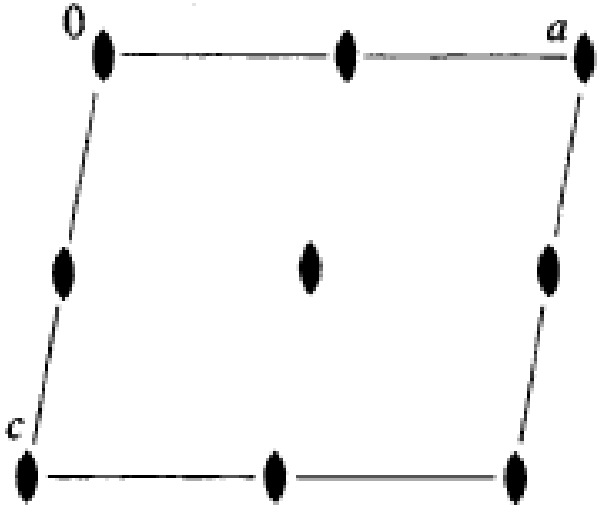
A,B,C,D,E,F,G　seven Volumes

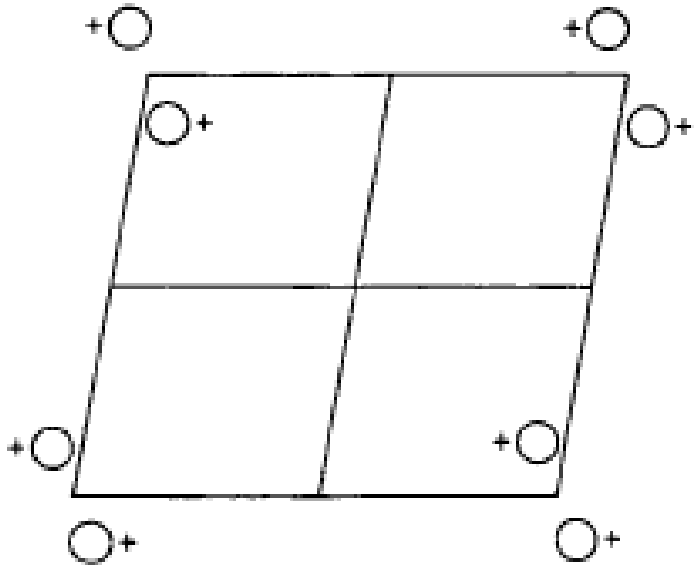
Position

$P2$ C_2^1 2 Monoclinic

No. 3 $P121$ Patterson symmetry $P12/m1$

UNIQUE AXIS b

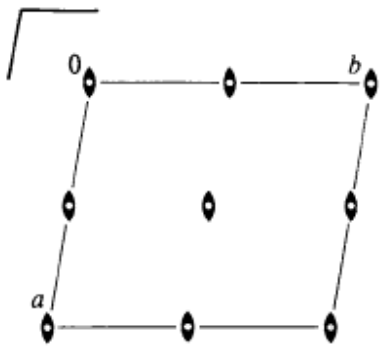


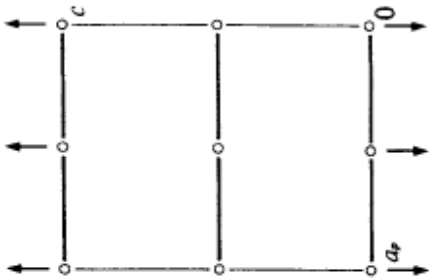


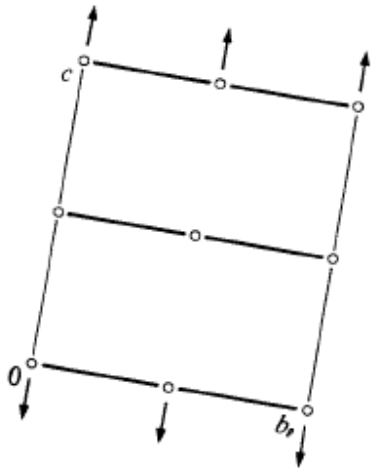
$P2/m$ C_{2h}^1 $2/m$ Monoclinic

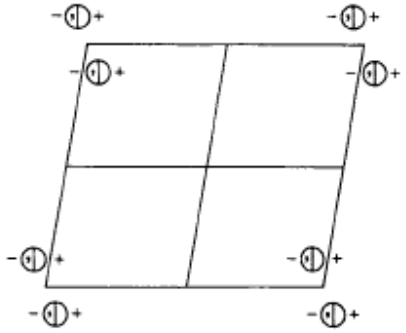
No. 10 $P112/m$ Patterson symmetry $P112/m$

UNIQUE AXIS c



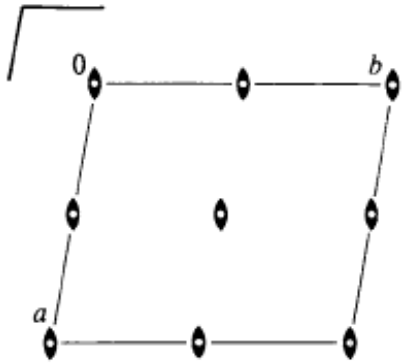


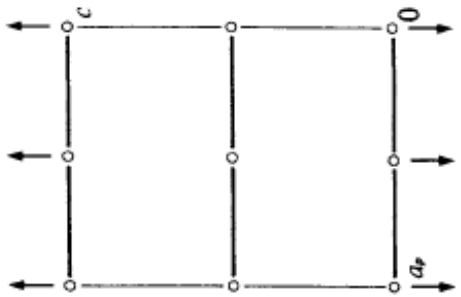


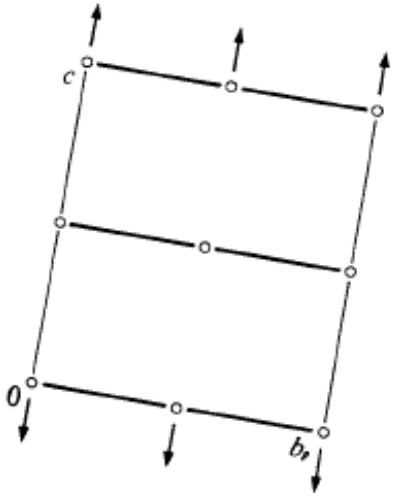


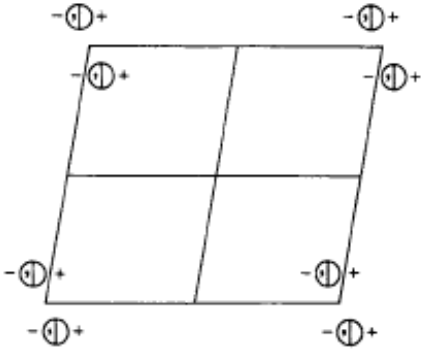
P2/m International Tables for Crystallography

UNIQUE AXIS *c*









P2/m International Tables for Crystallography

Origin at centre $(2/m)$

Asymmetric unit $0 \le x \le 1; \quad 0 \le y \le \frac{1}{2}; \quad 0 \le z \le \frac{1}{2}$

Symmetry operations

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

Maximal isomorphic subgroups of lowest index

IIc [2] $P1\,1\,2/m$ ($c' = 2c$) ($P2/m$, 10); [2] $P1\,1\,2/m$ ($a' = 2a$ or $b' = 2b$ or $a' = a - b, b' = a + b$) ($P2/m$, 10)

Minimal non-isomorphic supergroups

I [2] $Pmmm$ (47); [2] $Pccm$ (49); [2] $Pmma$ (51); [2] $Pmna$ (53); [2] $Pbam$ (55); [2] $Pnnm$ (58); [2] $Cmmm$ (65); [2] $Cccm$ (66); [2] $P4/m$ (83); [2] $P4_2/m$ (84); [3] $P6/m$ (175)

II [2] $A1\,1\,2/m$ ($C2/m$, 12); [2] $B1\,1\,2/m$ ($C2/m$, 12); [2] $I1\,1\,2/m$ ($C2/m$, 12)

P2/m Crystallographic site（等效点系）

International Tables for Crystallography

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	o	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,y,\bar{z}$
2	n	m	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$		
2	m	m	$x,y,0$	$\bar{x},\bar{y},0$		
2	l	2	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$		
2	k	2	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$		

P2/m

Crystallographic site（等效点系）

2	j	2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$
2	i	2	$0,0,z$	$0,0,\bar{z}$
1	h	$2/m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
1	g	$2/m$	$\frac{1}{2},\frac{1}{2},0$	
1	f	$2/m$	$\frac{1}{2},0,\frac{1}{2}$	
1	e	$2/m$	$0,\frac{1}{2},\frac{1}{2}$	
1	d	$2/m$	$0,\frac{1}{2},0$	
1	c	$2/m$	$\frac{1}{2},0,0$	
1	b	$2/m$	$0,0,\frac{1}{2}$	
1	a	$2/m$	$0,0,0$	

P2/m International Tables for Crystallography

Symmetry of special projections

Along [001] $p2$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2mm$
$\mathbf{a}' = \mathbf{b}_p$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2mm$
$\mathbf{a}' = \mathbf{c}$ $\mathbf{b}' = \mathbf{a}_p$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

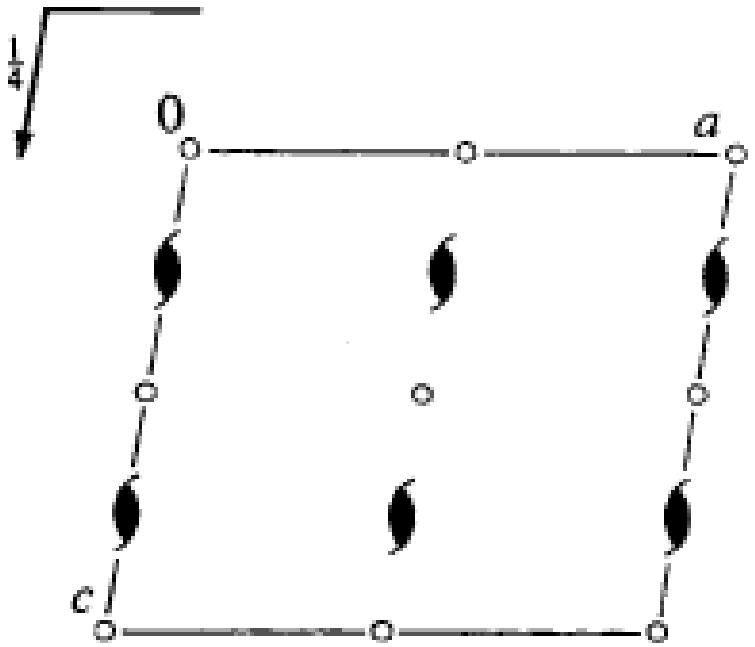
I [2] $P\,1\,1\,m$ (Pm, 6) 1; 4
[2] $P\,1\,1\,2$ ($P2$, 3) 1; 2
[2] $P\,\bar{1}$ (2) 1; 3

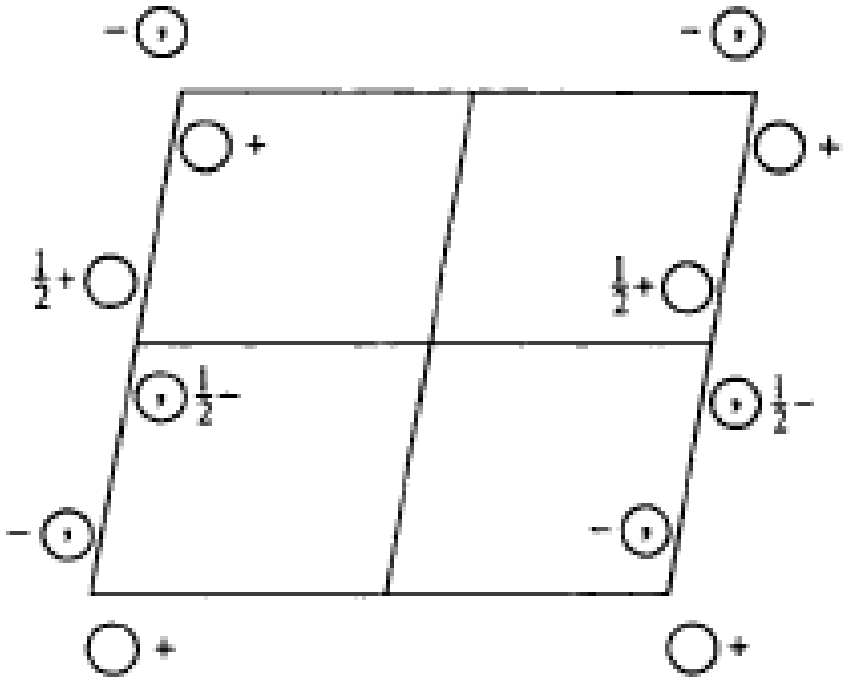
IIa none

IIb [2] $P\,1\,1\,2_1/m$ ($\mathbf{c}' = 2\mathbf{c}$) ($P2_1/m$, 11); [2] $P\,1\,1\,2/a$ ($\mathbf{a}' = 2\mathbf{a}$) ($P2/c$, 13); [2] $P\,1\,1\,2/b$ ($\mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $C\,1\,1\,2/e$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) ($P2/c$, 13); [2] $A\,1\,1\,2/m$ ($\mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [2] $B\,1\,1\,2/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12); [2] $F\,1\,1\,2/m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}, \mathbf{c}' = 2\mathbf{c}$) ($C2/m$, 12)

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$





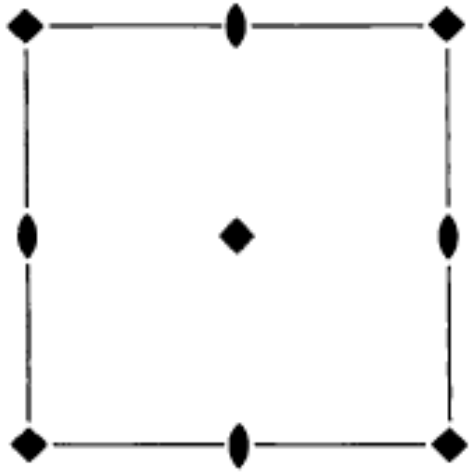
$P2_1/c$ Crystallographic site（等效点系）

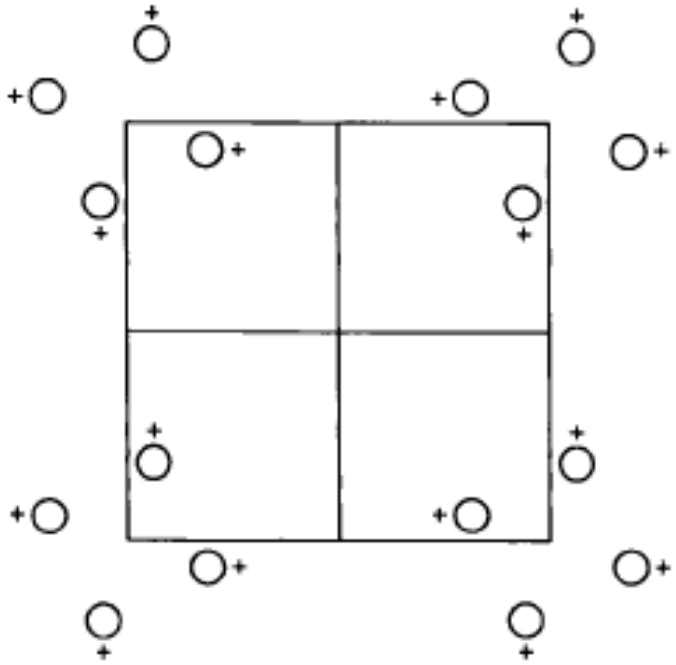
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*e*	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$
2	*d*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		
2	*c*	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$		
2	*b*	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
2	*a*	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$		

$P4$ C_4^1 4 Tetragonal

No. 75 $P4$ Patterson symmetry $P4/m$





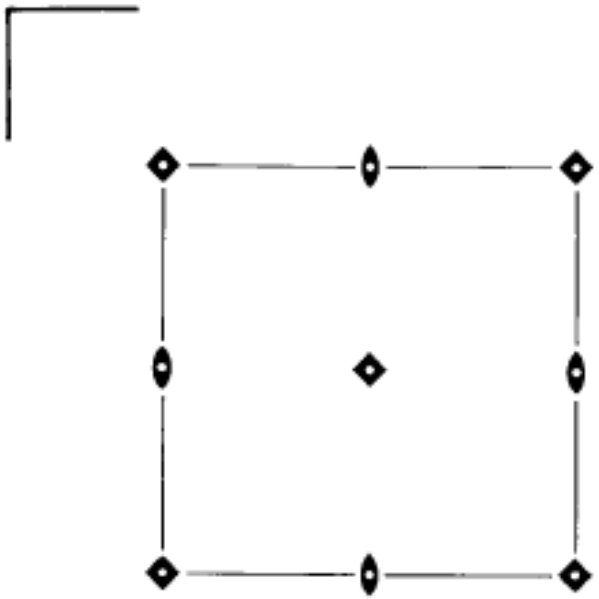
P4 Crystallographic site（等效点系）

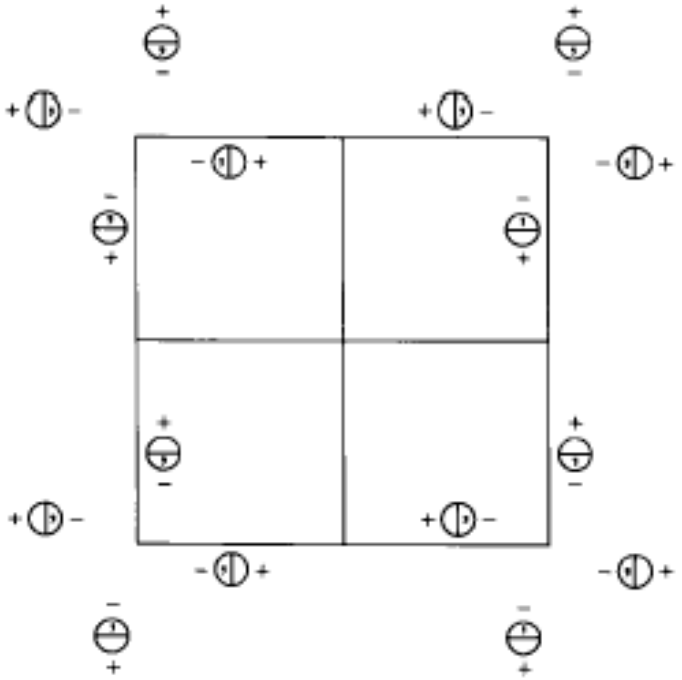
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	*d*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
2	*c*	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$		
1	*b*	4 . .	$\frac{1}{2},\frac{1}{2},z$			
1	*a*	4 . .	$0,0,z$			

$P4/m$ C_{4h}^{1} $4/m$ Tetragonal

No. 83 $P4/m$ Patterson symmetry $P4/m$





P4/m Crystallographic site（等效点系）

Positions

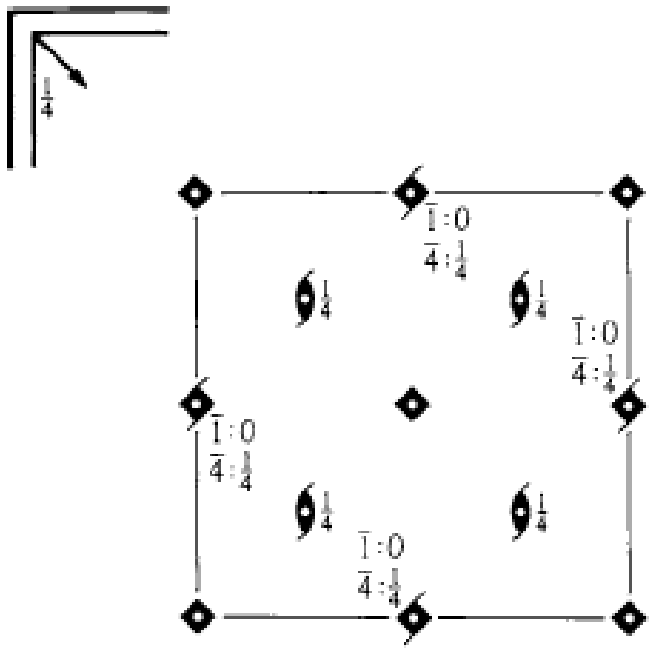
Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	l	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$
4	k	m . .	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{y},x,\frac{1}{2}$	$y,\bar{x},\frac{1}{2}$
4	j	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$
4	i	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$
2	h	4 . .	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$		
2	g	4 . .	$0,0,z$	$0,0,\bar{z}$		

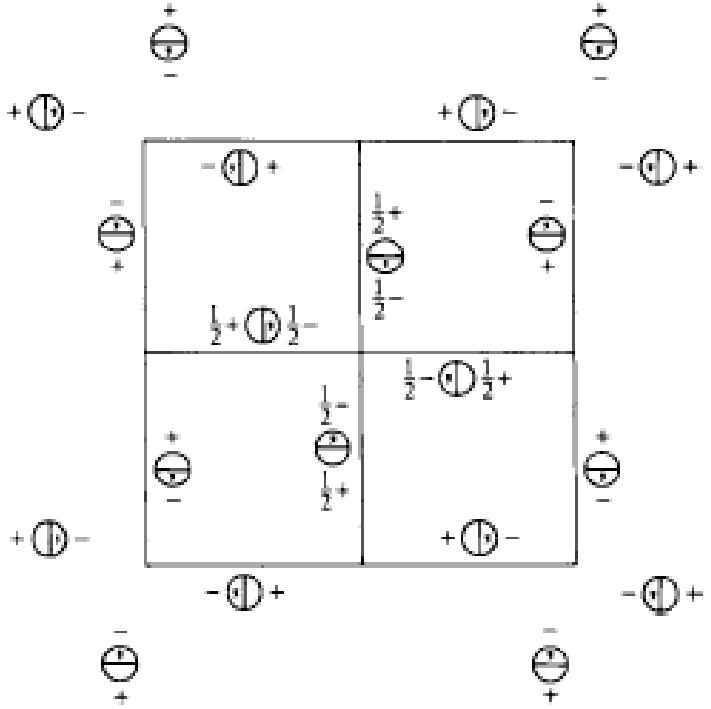
P4/m Crystallographic site（等效点系）

2	*f*	2/*m* . .	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$
2	*e*	2/*m* . .	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$
1	*d*	4/*m* . .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
1	*c*	4/*m* . .	$\frac{1}{2},\frac{1}{2},0$	
1	*b*	4/*m* . .	$0,0,\frac{1}{2}$	
1	*a*	4/*m* . .	$0,0,0$	

$I4/m$ C_{4h}^5 $4/m$ Tetragonal

No. 87 $I4/m$ Patterson symmetry $I4/m$





I4/m Crystallographic site（等效点系）

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$			
16	i	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{y},x,z$ (7) $y,\bar{x},\bar{z}$	(4) $y,\bar{x},z$ (8) $\bar{y},x,\bar{z}$
8	h	m . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$
8	g	2 . .	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$

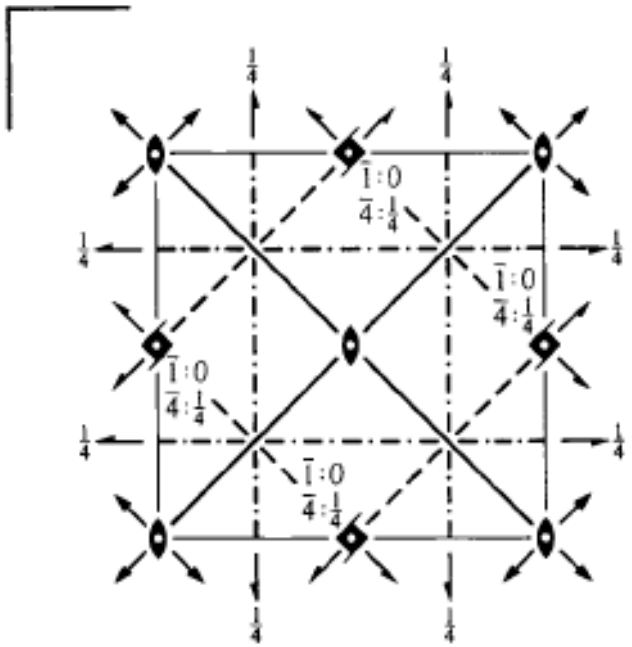
I4/m Crystallographic site（等效点系）

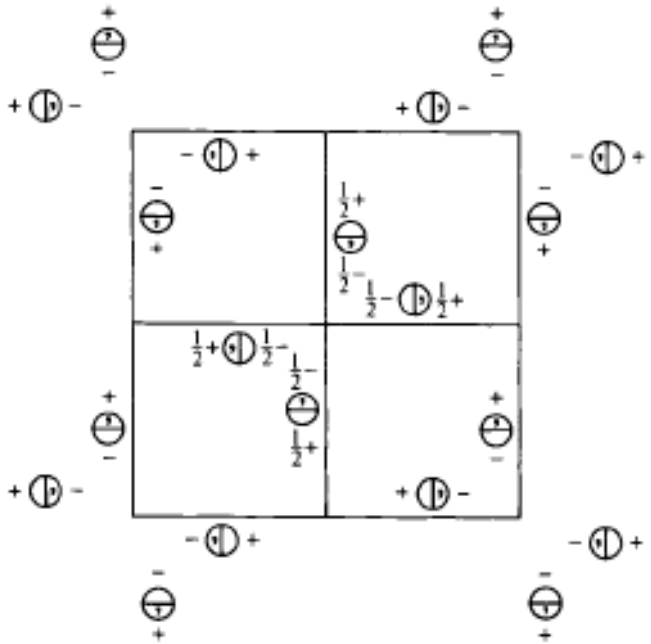
8	f	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$
4	e	$4\,.\,.$	$0,0,z$	$0,0,\bar{z}$		
4	d	$\bar{4}\,.\,.$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$		
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$		
2	b	$4/m\,.\,.$	$0,0,\frac{1}{2}$			
2	a	$4/m\,.\,.$	$0,0,0$			

$P4_2/mnm$ TiO2

$P4_2/mnm$ D_{4h}^{14} $4/mmm$ Tetragonal

No. 136 $P\ 4_2/m\ 2_1/n\ 2/m$ Patterson symmetry $P4/mmm$





$P4_2/mnm$ Crystallographic site（等效点系）

Positions

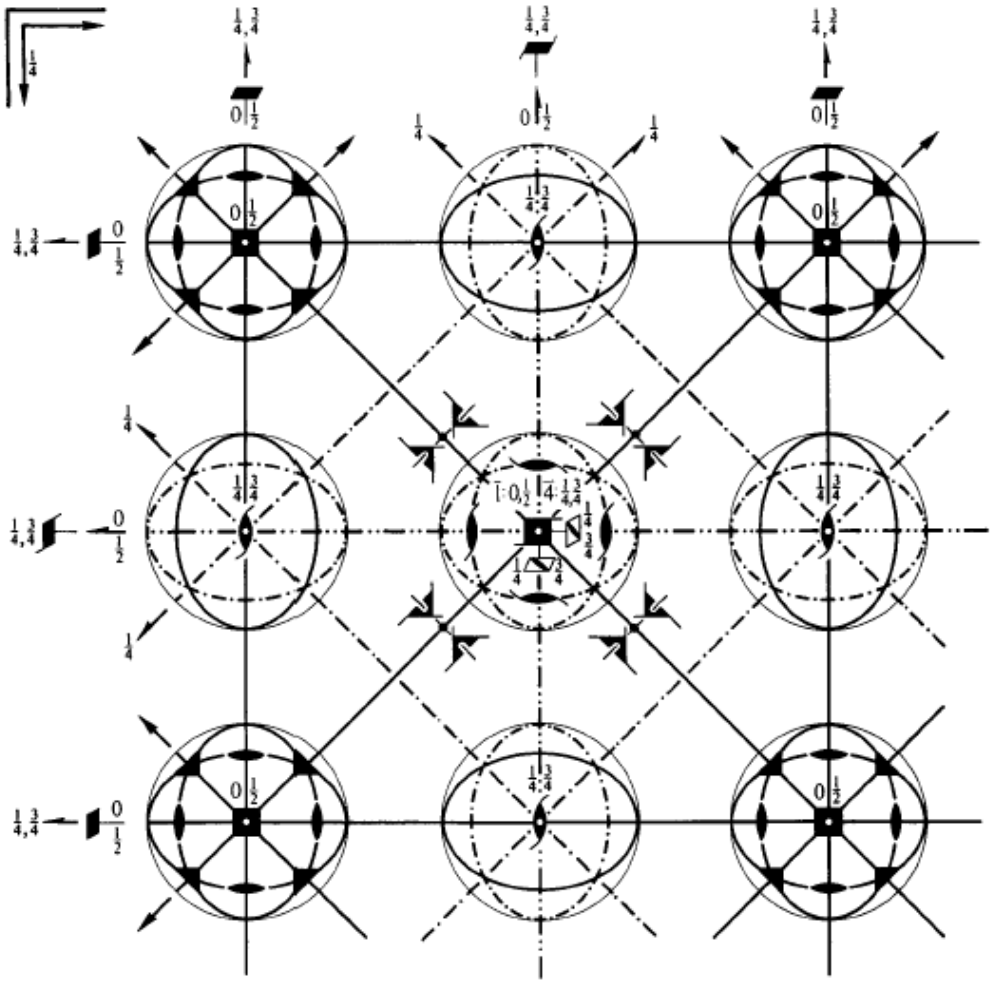
Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
16	*k*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	(4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $y,x,\bar{z}$	(8) $\bar{y},\bar{x},\bar{z}$
			(9) $\bar{x},\bar{y},\bar{z}$	(10) $x,y,\bar{z}$	(11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	(12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	(15) $\bar{y},\bar{x},z$	(16) y,x,z
8	*j*	. . *m*	x,x,z	$\bar{x},\bar{x},z$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$
8	*i*	*m* . .	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$y+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$
			$\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$	$y,x,0$	$\bar{y},\bar{x},0$
8	*h*	2 . .	$0,\frac{1}{2},z$	$0,\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,\bar{z}$
			$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$\frac{1}{2},0,z+\frac{1}{2}$	$\frac{1}{2},0,z$

$P4_2/mnm$ Crystallographic site（等效点系）

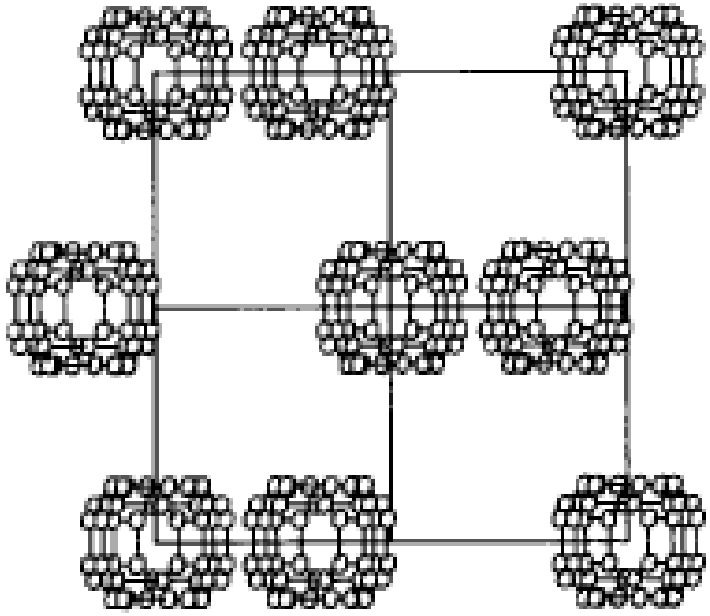
4	g	$m\,.\,2m$	$x,\bar{x},0$	$\bar{x},x,0$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$
4	f	$m\,.\,2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$
4	e	$2\,.\,mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$
4	d	$\bar{4}\,.\,.$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$
2	b	$m\,.\,mm$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		
2	a	$m\,.\,mm$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		

$F\,m\bar{3}\,m$ O_h^5 $m\bar{3}\,m$ Cubic

No. 225 $F\ 4/m\ \bar{3}\ 2/m$ Patterson symmetry $F\,m\bar{3}\,m$



Fm3m



Fm3m Crystallographic site（等效点系）

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates			
		$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
192	*l* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
		(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
		(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
		(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
		(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
		(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
		(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$
		(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
		(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$
		(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
		(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$
		(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

Fm3m Crystallographic site（等效点系）

96	*k*	. . *m*	x,x,z $\bar{z},\bar{x},x$ $x,x,\bar{z}$ $\bar{x},\bar{z},\bar{x}$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$ $\bar{x},\bar{x},\bar{z}$ $x,\bar{z},x$	$\bar{x},x,\bar{z}$ x,z,x $x,\bar{x},z$ $z,x,\bar{x}$	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$ $\bar{x},x,z$ $z,\bar{x},x$	z,x,x $x,\bar{z},\bar{x}$ $x,z,\bar{x}$ $\bar{z},x,x$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$ $\bar{x},z,x$ $\bar{z},\bar{x},\bar{x}$
96	*j*	*m* . .	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$ $0,z,y$ $\bar{z},\bar{y},0$
48	*i*	*m* . *m*2	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$
48	*h*	*m* . *m*2	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
48	*g*	2 . *mm*	$x,\frac{1}{4},\frac{1}{4}$ $\frac{1}{4},x,\frac{3}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$ $\frac{3}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},x,\frac{1}{4}$ $x,\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$ $\bar{x},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},x$ $\frac{1}{4},\frac{1}{4},\bar{x}$	$\frac{3}{4},\frac{1}{4},\bar{x}$ $\frac{1}{4},\frac{3}{4},x$

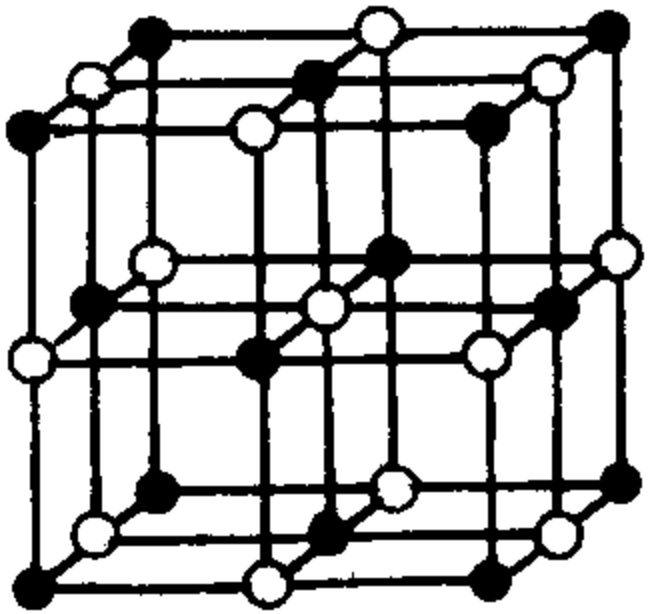
1.7　晶体学国际表，等效点系的简单应用举例

晶胞中原子位置（坐标）的猜测与确定

32	*f*	. 3 *m*	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$		
24	*e*	4 *m* . *m*	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
24	*d*	*m* . *mm*	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$
8	*c*	$\bar{4}$ 3 *m*	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$				
4	*b*	*m* $\bar{3}$ *m*	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
4	*a*	*m* $\bar{3}$ *m*	$0,0,0$					

Fm3m
a=5.640 Å
Na 4a (0,0,0)
Cl 4b (0.5,0.5,0.5)
Z=4
NaCl型结构

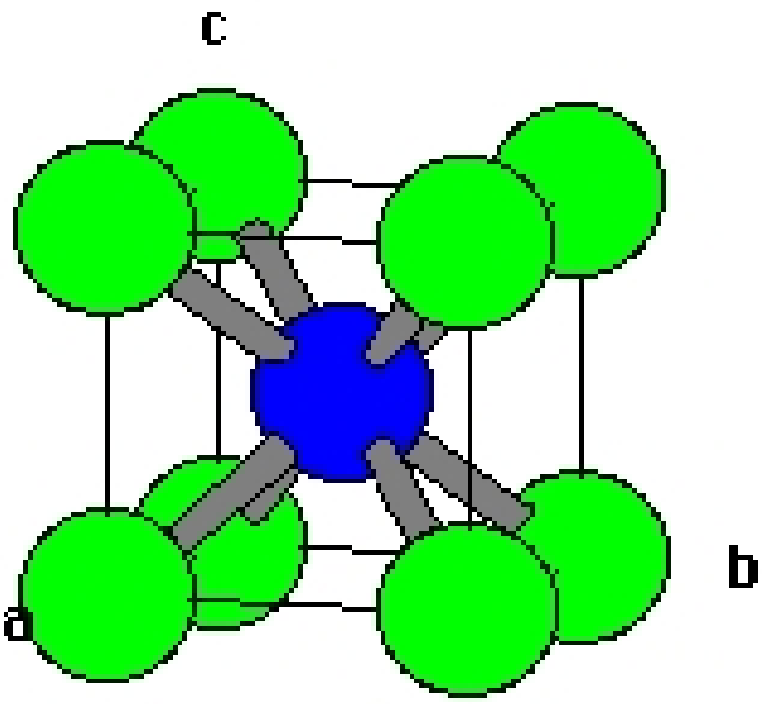
KCl: a=6.2901Å



NaCl

密度

CsCl型结构



Pm3m

a=4.11 Å

Cl 1a (0,0,0)

Cs 1b (0.5,0.5,0.5)

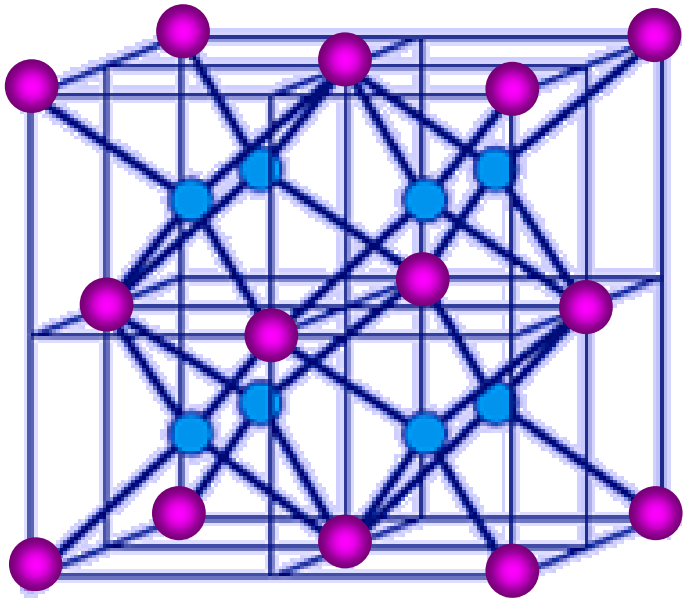
Z=1

CsCl型结构

Pm3m

3	*d*	$4/m\,m\,.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$
3	*c*	$4/m\,m\,.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
1	*b*	$m\,\bar{3}\,m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
1	*a*	$m\,\bar{3}\,m$	$0,0,0$		

Fluorite（萤石型结构）



Ca $^{2+}$

F $^{-}$

Fluorite:CaF_2

Fm3m

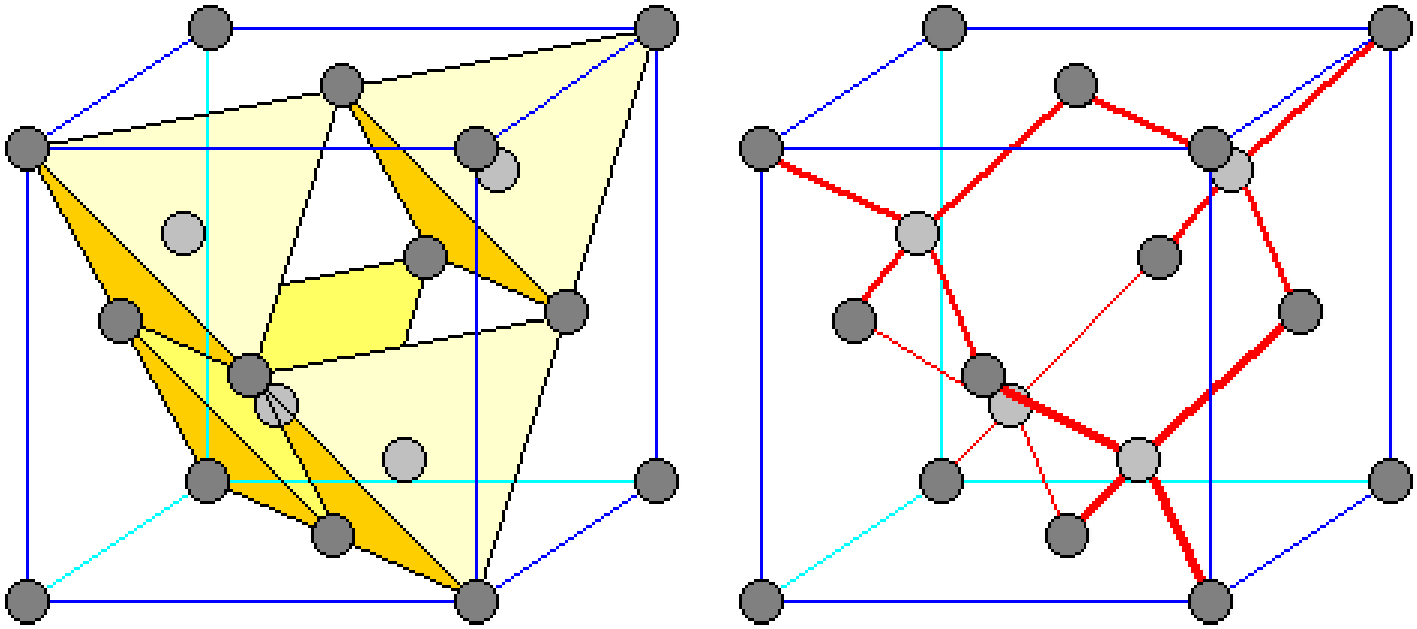
a=5.450 Å

Ca 4a (0,0,0)

F 8c(0.25,0.25,02.5)

Z=4

Diamond (金刚石型结构)



Fd3m , a=3.570 Å

C 8a (0,0,0) (3/4,1/4,3/4)

Z=8

Fd3m

32	*e*	. 3 *m*	x,x,x		$\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	
			$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$		$x+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$	
			$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$		$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$	
			$x+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$		$\bar{x}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$	
16	*d*	. $\bar{3}$ *m*	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{7}{8}$
16	*c*	. $\bar{3}$ *m*	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{3}{8}$
8	*b*	$\bar{4}$ 3 *m*	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$		
8	*a*	$\bar{4}$ 3 *m*	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$		

Rutile (金红石型结构)

金红石，TiO_2，

空间群$P4_2/mnm$

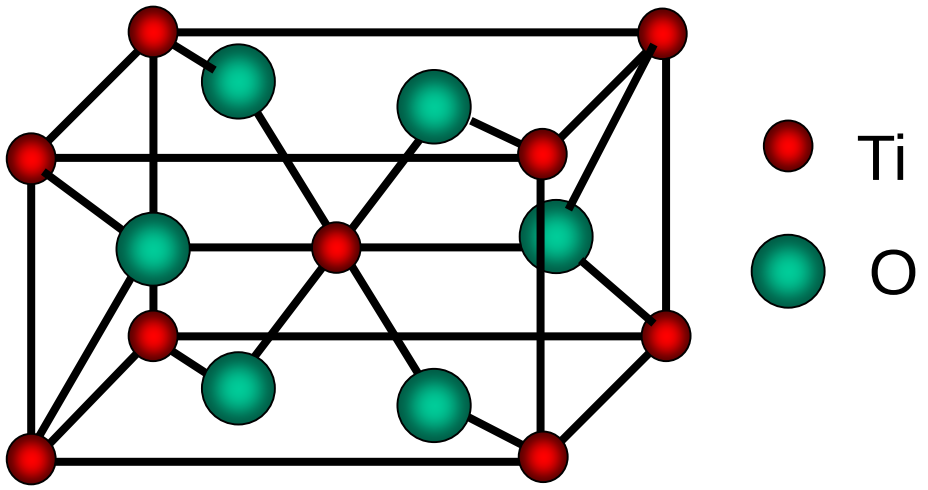
a=4.593, c=2.959Å

单位晶胞内有4个O^{2-}，

2个Ti^{4+}，Z=2。

Ti 2a (0, 0, 0)

O 4f (0.302, 0.302, 0)



$P4_2/mnm$

4	g	$m\,.\,2m$	$x,\bar{x},0$	$\bar{x},x,0$	$x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$
4	f	$m\,.\,2m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$
4	e	$2\,.\,mm$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$
4	d	$\bar{4}\,.\,.$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},0,\frac{3}{4}$
4	c	$2/m\,.\,.$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},0,0$
2	b	$m\,.\,mm$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		
2	a	$m\,.\,mm$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		

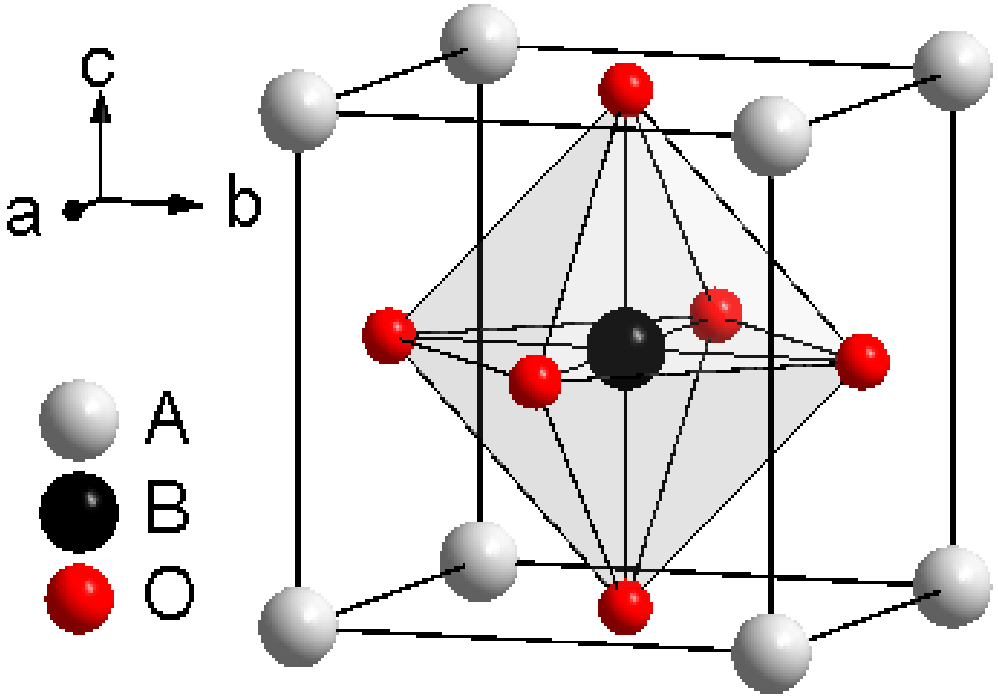
Ti 2a (0,0,0)

O 4f (0.302,0.302,0)

Perovskite Structure

钙钛矿型结构 ABO3：

超导，巨磁电阻，铁电，铁磁，负膨胀 离子导体，太阳能电池



Pm3m 钙钛矿型结构 ABO3

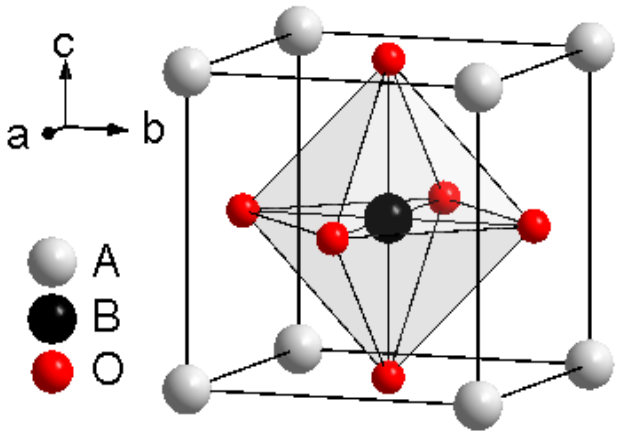
3	*d*	$4/m\,m\,.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$
3	*c*	$4/m\,m\,.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
1	*b*	$m\bar{3}\,m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
1	*a*	$m\bar{3}\,m$	$0,0,0$		

A：1a 0, 0, 0

B: 1b 0.5, 0.5, 0.5

O: 3c 0, 0.5, 0.5

Z=1

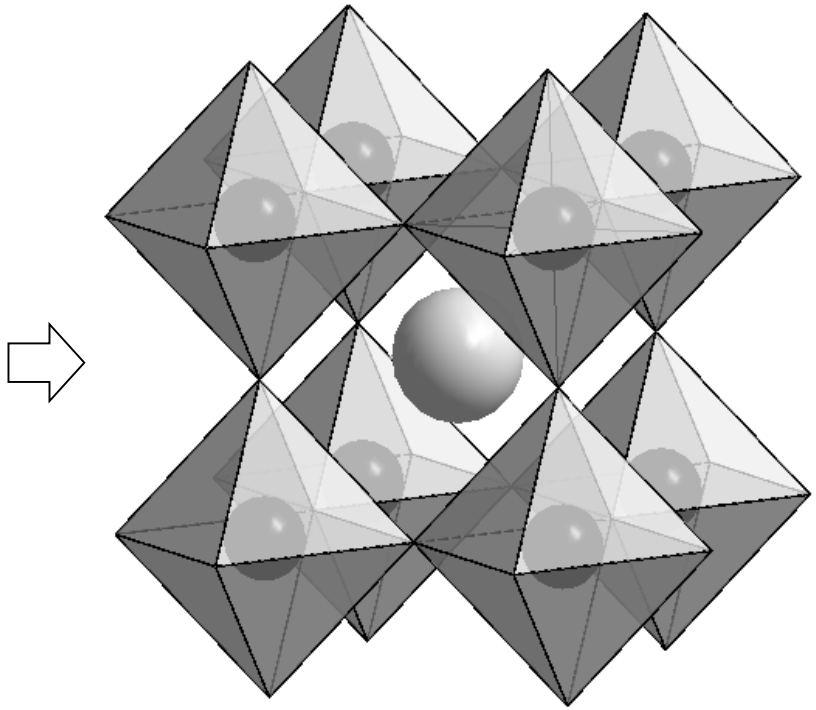


Perovskite Structure

$A^{2+}B^{4+}O_3$	$CaTiO_3$	$BaTiO_3$
$A^{1+}B^{5+}O_3$	$NaTaO_3$	$AgNbO_3$
$A^{3+}B^{3+}O_3$	$LaCoO_3$	$AdGaO_3$
A_xBO_3	$Gd_{0.333}TaO_3$	Na_xTaO_3
ABO_{3-x}	$CaMnO_{3-x}$	$SrVO_{3-x}$

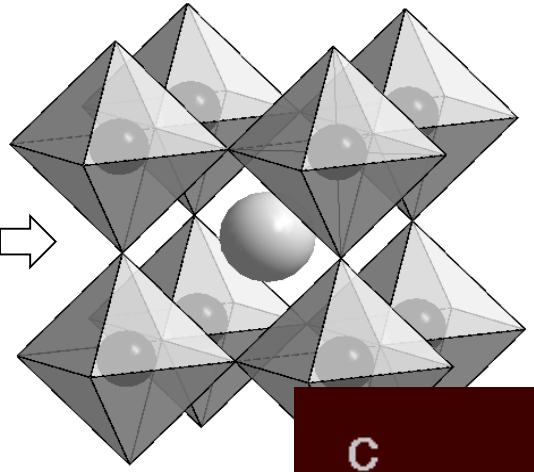
Perovskite Structure

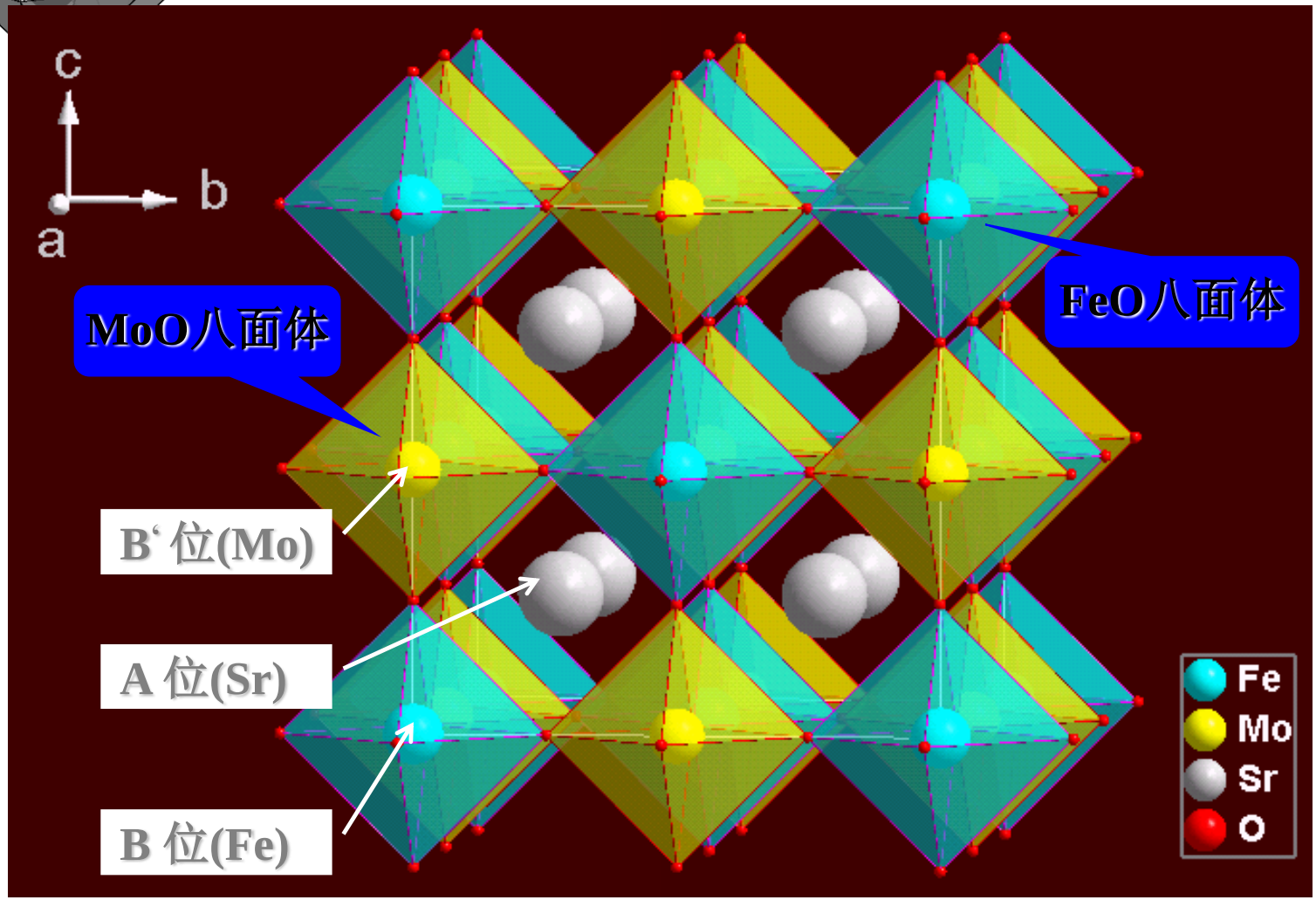
$A^{2+}(B^{3+}_{0.67}\ B^{6+}_{0.33})O_3$	$Ba(Al_{0.67}\ W_{0.33})O_3$
$A^{2+}(B^{2+}_{0.33}\ B^{5+}_{0.67})O_3$	$Ba(Co_{0.33}Nb_{0.67})O_3$
$A^{2+}(B^{3+}_{0.5}\ B^{5+}_{0.5})O_3$	$Ba(Er_{0.5}Re_{0.5})O_3$
$A^{2+}(B^{2+}_{0.5}\ B^{6+}_{0.5})O_3$	$Ba(Ca_{0.5}W_{0.5})O_3$
$A^{2+}(B^{1+}_{0.5}\ B^{7+}_{0.5})O_3$	$Ba(Li_{0.5}I_{0.5})O_3$
$A^{2+}(B^{1+}_{0.25}\ B^{5+}_{0.75})O_3$	$Ba(Na_{0.25}Ta_{0.75})O_3$
$A^{3+}(B^{2+}_{0.5}\ B^{4+}_{0.5})O_3$	$La(Mg_{0.5}Ti_{0.5})O_3$
$A^{2+}(B^{3+}_{0.5}\ B^{4+}_{0.5})O_{2.75}$	$Ba(In_{0.5}U_{0.5})O_{2.75}$
$A^{2+}(B^{2+}_{0.5}\ B^{5+}_{0.5})O_{2.75}$	$Ba(Fe_{0.5}Mo_{0.5})O_{2.75}$



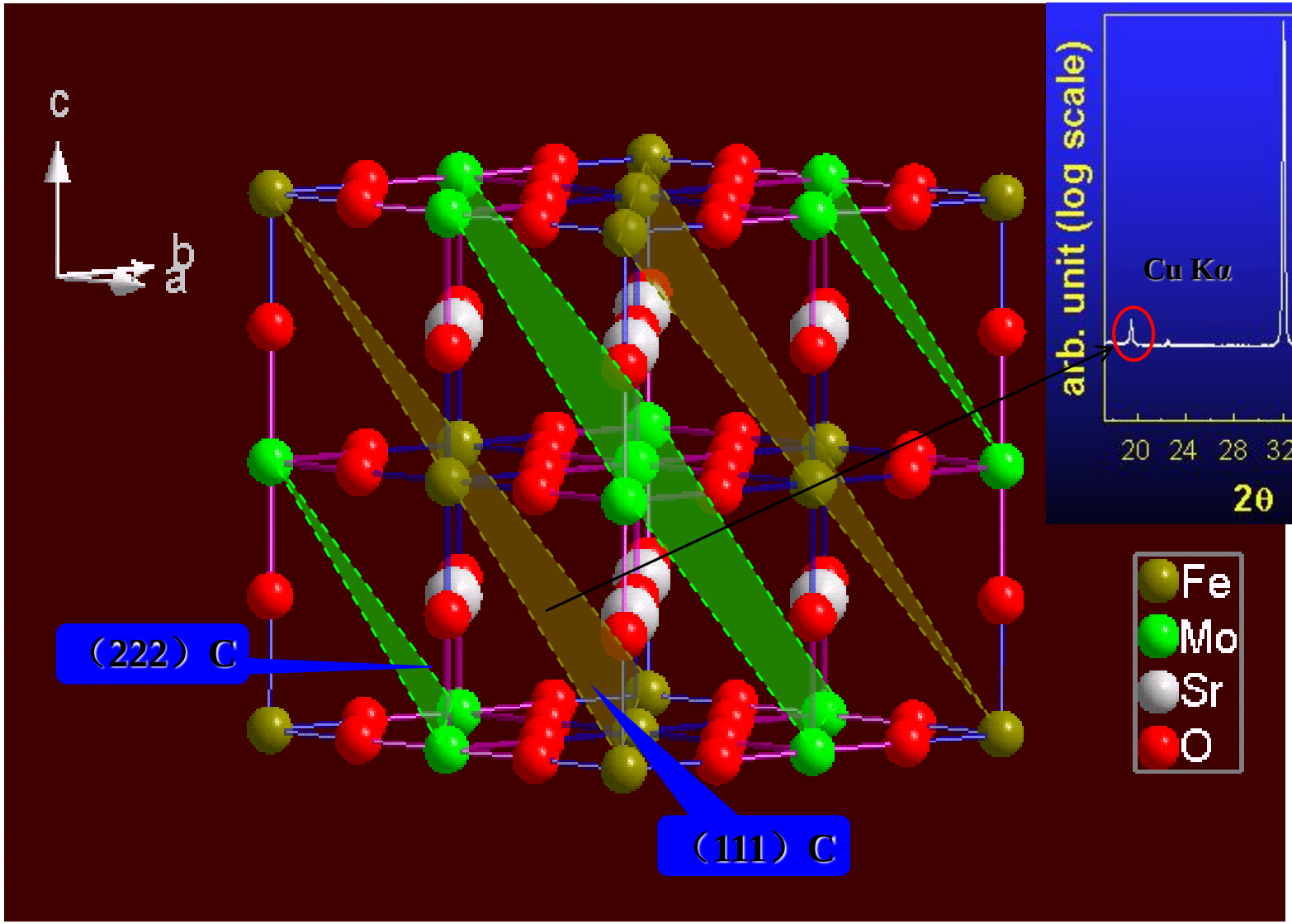
BO_6八面体骨架

Double Perovskite Structure





Double Perovskite Structure



Pm3m

48	*n*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

Pm3m

24	*m*	. . *m*	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$
24	*l*	*m* . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$z,\frac{1}{2},y$	$z,\frac{1}{2},\bar{y}$
			$\bar{z},\frac{1}{2},y$	$\bar{z},\frac{1}{2},\bar{y}$	$y,z,\frac{1}{2}$	$\bar{y},z,\frac{1}{2}$	$y,\bar{z},\frac{1}{2}$	$\bar{y},\bar{z},\frac{1}{2}$
			$y,\frac{1}{2},\bar{z}$	$\bar{y},\frac{1}{2},\bar{z}$	$y,\frac{1}{2},z$	$\bar{y},\frac{1}{2},z$	$\frac{1}{2},z,\bar{y}$	$\frac{1}{2},z,y$
			$\frac{1}{2},\bar{z},\bar{y}$	$\frac{1}{2},\bar{z},y$	$z,y,\frac{1}{2}$	$z,\bar{y},\frac{1}{2}$	$\bar{z},y,\frac{1}{2}$	$\bar{z},\bar{y},\frac{1}{2}$
24	*k*	*m* . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$

Pm3m

12	j	m . $m2$	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$
12	i	m . $m2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
12	h	m m 2 . .	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},\bar{x}$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},x$
8	g	. 3 m	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$		
6	f	4 m . m	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	4 m . m	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$

Pm3m

3	*d*	$4/m\,m\,.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$
3	*c*	$4/m\,m\,.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
1	*b*	$m\,\bar{3}\,m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
1	*a*	$m\,\bar{3}\,m$	$0,0,0$		

ABO3 CaTiO3

$Sr_2Fe_xMo_{2-x}O_6$

对于立方相，本文参考Sr_2FeMoO_6的高温立方相，选择了

$$Fm\bar{3}m \quad (2a_p \times 2a_p \times 2a_p)$$

Wyckoff位置：Sr 8*c*、Fe 4*a*、Mo 4*b*、O 24*e*

对于$Sr_2Fe_xMo_{2-x}O_6$（$0.8 \le x \le 1.5$）四方相，结果*I4/mmm*

（a_p为原始立方钙 钛矿的晶格参数） **Z=2**

Wyckoff位置：Sr 4*d*、Fe 2*a*、Mo 2*b*、O1　8*h*、O2　4*e*

I4/mmm

4	*e*	$4\,m\,m$	$0,0,z$	$0,0,\bar{z}$
4	*d*	$\bar{4}\,m\,2$	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$
4	*c*	$m\,m\,m\,.$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$
2	*b*	$4/m\,m\,m$	$0,0,\frac{1}{2}$	
2	*a*	$4/m\,m\,m$	$0,0,0$	

I4/mmm

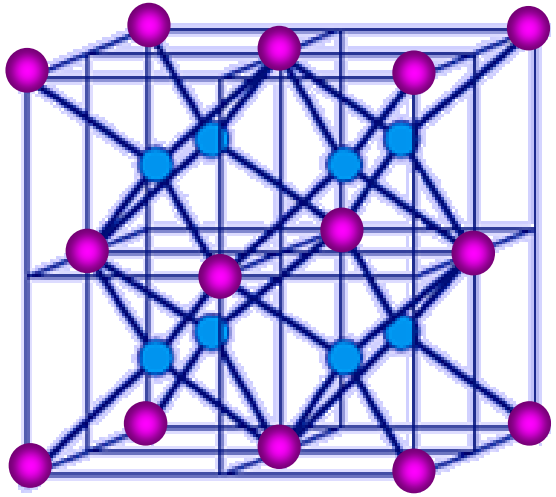
8	j	$m\,2\,m.$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$
8	i	$m\,2\,m.$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$
8	h	$m\,.\,2\,m$	$x,x,0$	$\bar{x},\bar{x},0$	$\bar{x},x,0$	$x,\bar{x},0$
8	g	$2\,m\,m.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$	$0,\frac{1}{2},\bar{z}$	$\frac{1}{2},0,\bar{z}$
8	f	$..\,2/m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$

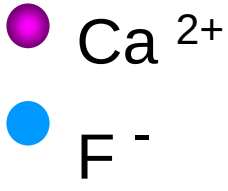
I4/mmm

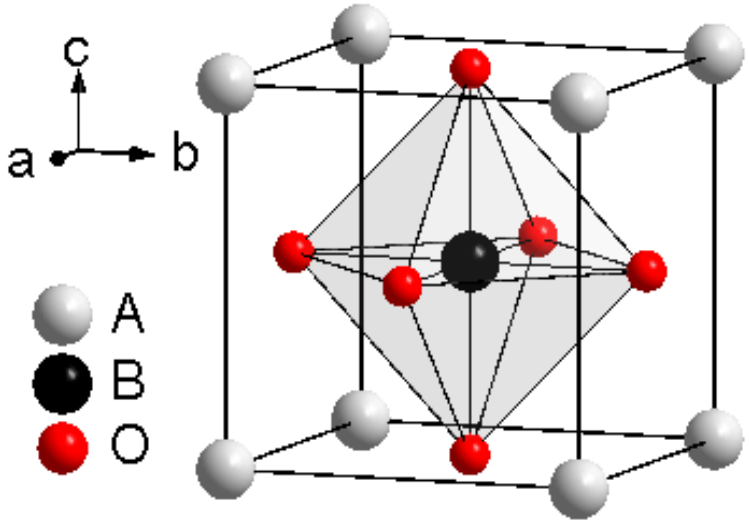
16	n	$.m.$	$0,y,z$	$0,\bar{y},z$	$\bar{y},0,z$	$y,0,z$
			$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$y,0,\bar{z}$	$\bar{y},0,\bar{z}$
16	m	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$
			$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$
16	l	$m..$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{y},x,0$	$y,\bar{x},0$
			$\bar{x},y,0$	$x,\bar{y},0$	$y,x,0$	$\bar{y},\bar{x},0$
16	k	$..2$	$x,x+\frac{1}{2},\frac{1}{4}$	$\bar{x},\bar{x}+\frac{1}{2},\frac{1}{4}$	$\bar{x}+\frac{1}{2},x,\frac{1}{4}$	$x+\frac{1}{2},\bar{x},\frac{1}{4}$
			$\bar{x},\bar{x}+\frac{1}{2},\frac{3}{4}$	$x,x+\frac{1}{2},\frac{3}{4}$	$x+\frac{1}{2},\bar{x},\frac{3}{4}$	$\bar{x}+\frac{1}{2},x,\frac{3}{4}$

晶胞中原子位置、配位多面体与对称要素的关系

四面体　SiO4　　八面体　TiO6







等大球最紧密堆积，面心立方，

四面体空隙，八面体空隙　　数目比：n:2n:n

Crystal structure of $Ba_9Sc_2Si_6O_{24}$

Atom	Site	x	y	z
Ba1	3a	0	0	0
Ba2	18f	0.0269	0.6704	0.1087
Ba3	6c	1/3	2/3	0.0031
Sc	6c	0	0	0.1645
Si	18f	0.3386	0.0259	0.0763
O1	18f	0.3568	0.0764	0.0068
O2	18f	0.4889	0.1656	0.1144
O3	18f	-0.0102	0.1666	0.1060
O4	18f	0.1334	0.4721	0.0927

$Ba_9Sc_2Si_6O_{24}$

R-3

a = 9.8716

c = 21.9376 Å

Z = 3

27 Ba, 6 Sc

18 Si, 72 O

from
边柳的博士学位论文

晶胞中原子位置、配位多面体与对称要素的关系

$Ba_9Sc_2Si_6O_{24}:Eu^{2+},Mn^{2+}$　R-3