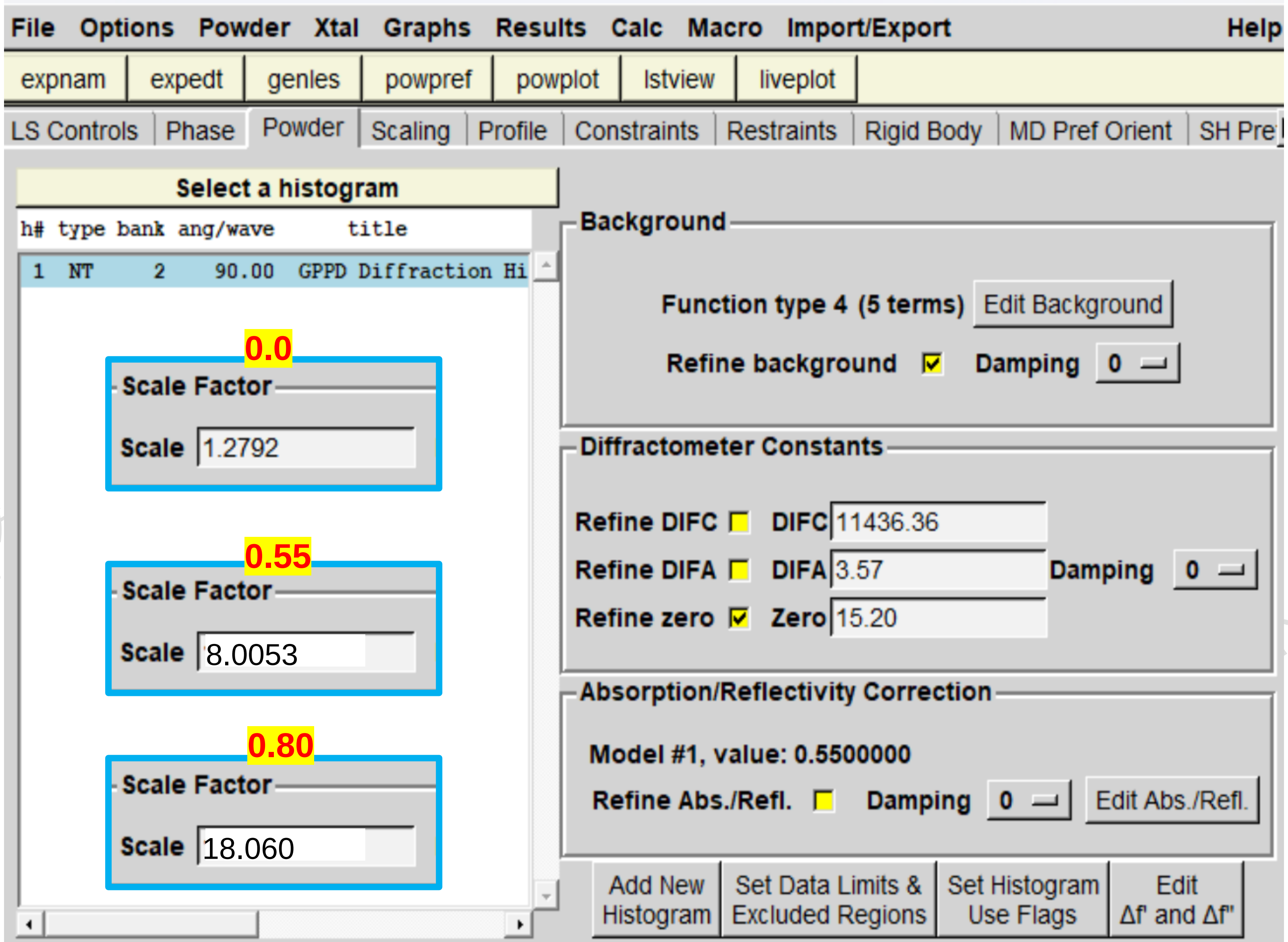
刘鹏飞

1. 对于Powder选项的Refine zero和Profile里面的shft (function is type 3)，这两项似乎不能同时精修，那么对于峰形函数有偏离的时候，修那个比较好？还是一个一个来？

2. 在选择Absorption Coefficient时候，黄老师直接填了一个数值0.55，但这一项是可以选择Refine Abs./Refl.进行精修的，那么我们是直接填值进行尝试好还是直接精修？



```
h# type bank ang/wave        title
 1  NT    2    90.00  GPPD Diffraction Hi
```

0.0

Scale Factor

Scale 1.2792

0.55

Scale Factor

Scale 8.0053

0.80

Scale Factor

Scale 18.060

Background

Function type 4 (5 terms)

Refine background ☑ Damping 0

Diffractometer Constants

Refine DIFC ☐ DIFC 11436.36

Refine DIFA ☐ DIFA 3.57 Damping 0

Refine zero ☑ Zero 15.20

Absorption/Reflectivity Correction

Model #1, value: 0.5500000

Refine Abs./Refl. ☐ Damping 0

晶体结构空间对称群的架构及应用

THE FRAME AND APPLICATION OF SPACE GROUP OF CRYSTAL STRCTURE

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HUANG QINGZHEN

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China Spallation Neutron Source

结构报告

Table I. Refined structure parameters for $Eu_{1.2}Ce_{0.8}Sr_2RuCu_2O_{9.63}$ at 295 K. Space group I4/mmm (#139). a=3.8427(3) Å and c=28.555(2) Å. V=421.7(1) Å^3, z=2.

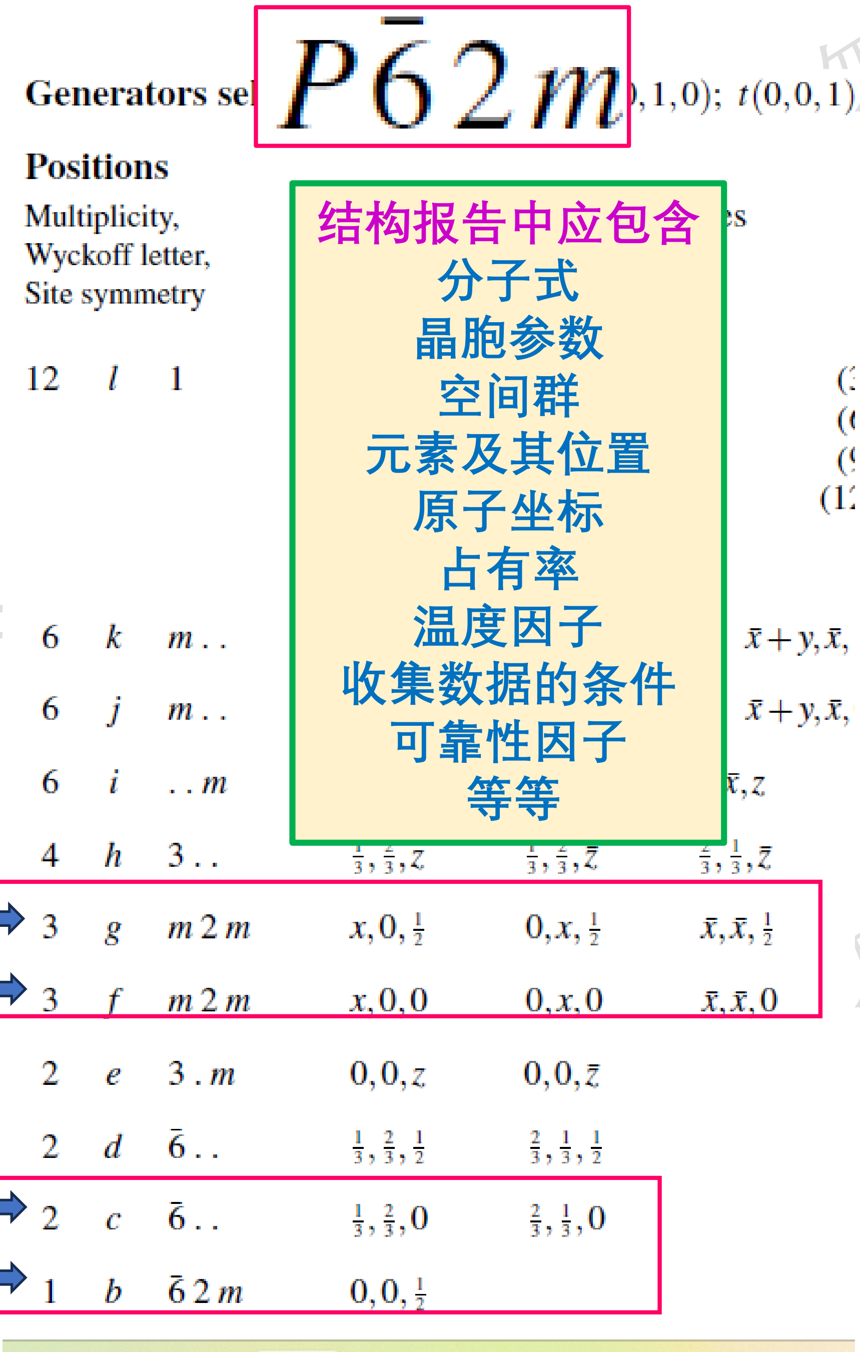
Atom	site	x	y	z	n	B(Å^2)
Eu/Ce	4*e*	0	0	0.2953(3)	0.6/0.4	0.5(1)
Sr	4*e*	0	0	0.4227(3)	1	1.0(1)
Ru	2*a*	0	0	0	1	0.4(2)
Cu	4*e*	0	0	0.14323(3)	1	0.4(1)
O1	8*j*	0.117(3)	1/2	0	0.45(2)	1.4(5)
O2	4*e*	0	0	0.0672(3)	0.92(3)	0.80(2)
O3	8*g*	0	1/2	0.1495(2)	1	0.9(1)
O4	4*d*	0	1/2	1/4	1	0.8(1)

wRp=6.39%, Rp=4.34%, χ^2=1.09.

结构报告中包含的信息

Table 2. Structural parameters of $Mn_{1.1}Fe_{0.9}P_{0.8}Ge_{0.2}$ at 239 K under pressure 0.69 GPa applied. Space group $P\bar{6}2m$. Atomic positions: Mn: $3g$ (x, 0, 1/2); $Fe_{0.928(3)}$ /$Mn_{0.072(1)}$: $3f$ (x, 0, 0); $P_{0.81(1)}$ /$Ge_{0.19(1)}$ (1):$1b$ (0, 0, 1/2); $P_{0.736(6)}$ /$Ge_{0.264(6)}$(2): $2c$ (1/3, 2/3, 0).

Atom	Parameters	0 GPa		0.69 GPa	
		PMP	FMP	PMP	FMP
		19.8(1)%	80.2(1) %	26.5(1)%	73.5(1)%
	a (Å)	6.059(4)	6.1515(4)	6.052(1)	6.1455(4)
	c (Å)	3.47(3)	3.3555(3)	3.445(1)	3.3473(3)
	V (Å^3)	109.6(1)	109.96(2)	109.30(4)	109.48(2)
Mn	x	0.64(1)	0.596(2)	0.599(6)	0.603(2)
	B(Å^2)	0.77(2)	0.77(2)	0.6 (1)	0.6(1)
	M (μ_B)		4.4(3)		4.0(2)
Mn/Fe	x	0.243(5)	0.2550(8)	0.253(3)	0.2538(8)
	B(Å^2)	0.7(1)	0.7(1)	0.6(1)	0.6(1)
	M (μ_B)		1.0(2)		1.0(2)
P/Ge(1)	B(Å^2)	0.5(1)	0.5(1)	0.6(1)	0.4(1)
P/Ge(2)	B(Å^2)	0.5(1)	0.5(1)	0.6(1)	0.4(1)
	R (%)	2.44		2.35	
	wR (%)	3.13		2.94	
	χ^2	2.433		2.129	



$P\bar{6}2m$

Generators sel ,1,0); $t(0,0,1)$

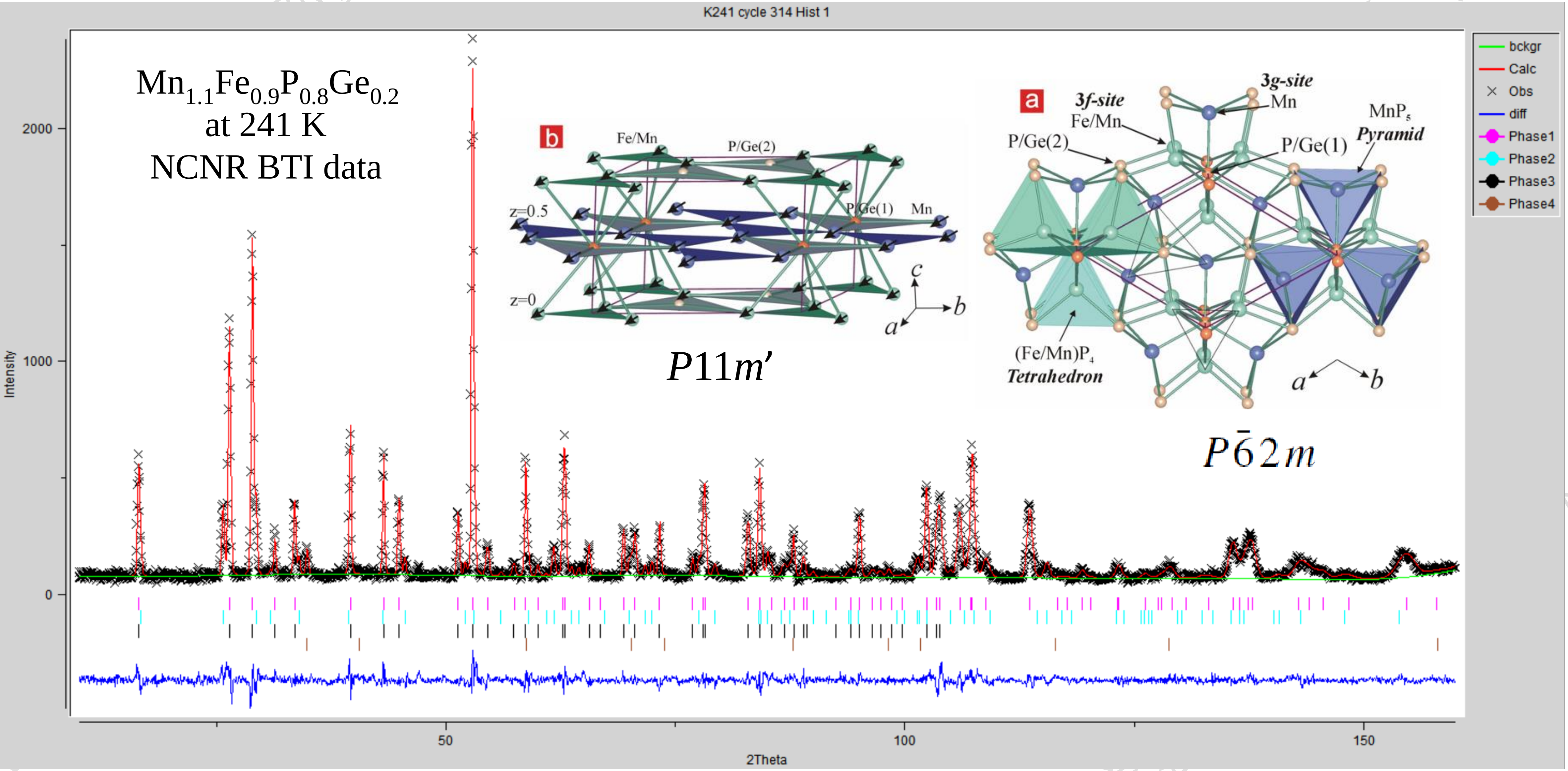
Positions

Multiplicity,
Wyckoff letter,
Site symmetry

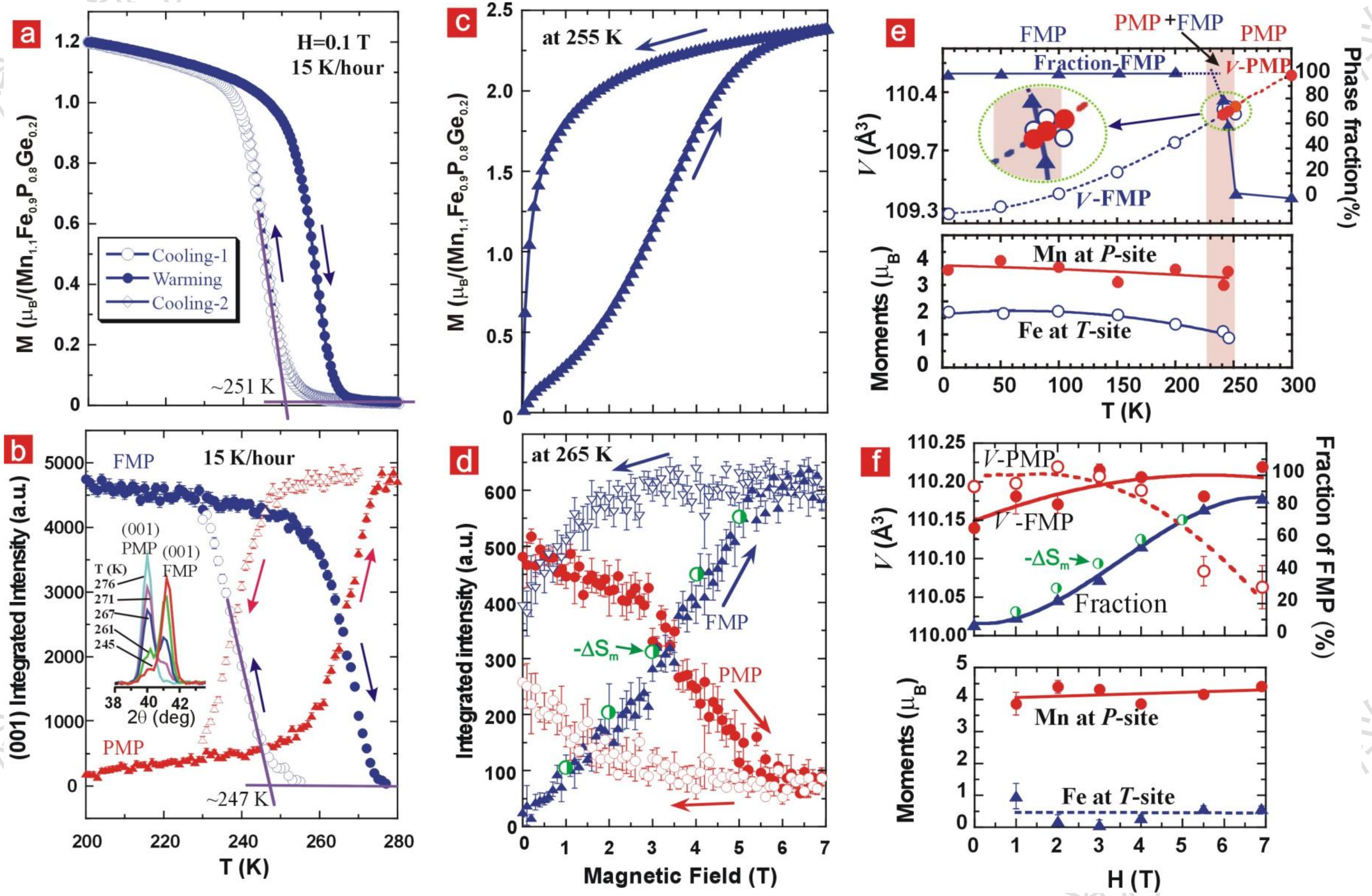
12	l	1			
6	k	$m\,.\,.$			$\bar{x}+y,\bar{x},$
6	j	$m\,.\,.$			$\bar{x}+y,\bar{x},$
6	i	$.\,.\,m$			$\bar{x},z$
4	h	$3\,.\,.$	$\frac{1}{3},\frac{2}{3},z$	$\frac{1}{3},\frac{2}{3},\bar{z}$	$\frac{2}{3},\frac{1}{3},\bar{z}$
3	g	$m\,2\,m$	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$
3	f	$m\,2\,m$	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$
2	e	$3\,.\,m$	$0,0,z$	$0,0,\bar{z}$	
2	d	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},\frac{1}{2}$	$\frac{2}{3},\frac{1}{3},\frac{1}{2}$	
2	c	$\bar{6}\,.\,.$	$\frac{1}{3},\frac{2}{3},0$	$\frac{2}{3},\frac{1}{3},0$	
1	b	$\bar{6}\,2\,m$	$0,0,\frac{1}{2}$		

结构报告中应包含
分子式
晶胞参数
空间群
元素及其位置
原子坐标
占有率
温度因子
收集数据的条件
可靠性因子
等等

结构报告中常提供的信息



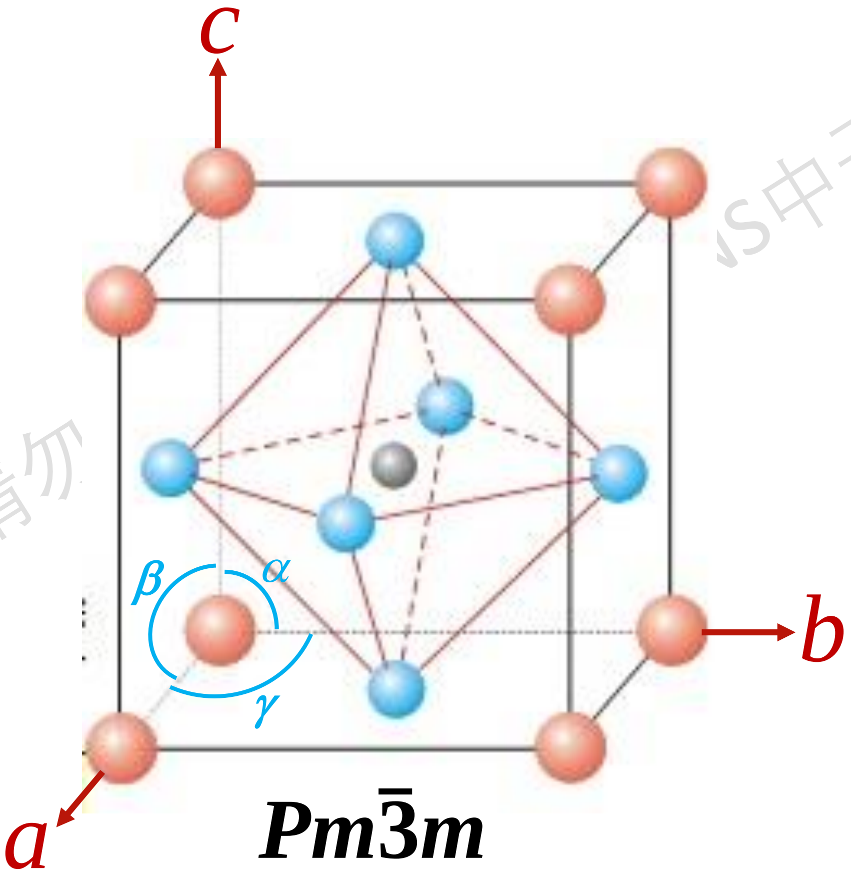
结构与性能的关联


a
H=0.1 T
15 K/hour
M (μ_B/(Mn$_{1.1}$Fe$_{0.9}$P$_{0.8}$Ge$_{0.2}$)
1.2
1.0
0.8
0.6
0.4
0.2
0
Cooling-1
Warming
Cooling-2
~251 K
b
FMP
15 K/hour
(001) Integrated Intensity (a.u.)
5000
4000
3000
2000
1000
0
(001)
PMP
(001)
FMP
T (K)
276
271
267
261
245
38
40
42
2θ (deg)
PMP
~247 K
200
220
240
260
280
T (K)
c
at 255 K
M (μ_B/(Mn$_{1.1}$Fe$_{0.9}$P$_{0.8}$Ge$_{0.2}$)
2.5
2.0
1.5
1.0
0.5
0
d
at 265 K
Integrated intensity (a.u.)
600
500
400
300
200
100
0
-ΔS$_m$
FMP
PMP
0
1
2
3
4
5
6
7
Magnetic Field (T)
e
FMP
PMP +FMP
PMP
Fraction-FMP
V-PMP
V-FMP
V (Å^3)
110.4
109.7
109.3
Phase fraction(%)
100
80
60
40
20
0
Moments (μ_B)
4
3
2
1
0
Mn at P-site
Fe at T-site
0
50
100
150
200
250
300
T (K)
f
V-PMP
V-FMP
-ΔS$_m$
Fraction
V (Å^3)
110.25
110.20
110.15
110.10
110.05
110.00
Fraction of FMP (%)
100
80
60
40
20
0
Moments (μ_B)
5
4
3
2
1
0
Mn at P-site
Fe at T-site
0
1
2
3
4
5
6
7
H (T)

空间群—晶体结构中全部对称要素的集合

单位晶胞结构中的对称性等结构信息可由空间群描述，空间群共有230个。空间群包含有：七大晶系，14个Bravais点阵，11个劳埃群，32个点群，对称元素组合，对称元素组合投影图，阵点的对称性及位置，等效点位置和衍射条件等等。

- 单位晶胞
- 单位晶胞是一个六面体，是晶体中的最小的重复单元在晶体中无间隙地组合；单位晶胞大小与形状由晶胞参数 *a, b, c, α, β, γ* 表示， *a, b, c* 为六面体边长， *α, β, γ* 分别是 *bc, ca, ab* 所组成的夹角。
- 晶胞里包含描述晶体结构所需的最基本的结构信息，包括点阵，对称性和阵点的位置以及内容。
- 这些结构的基本信息可以用空间群完整地表示。

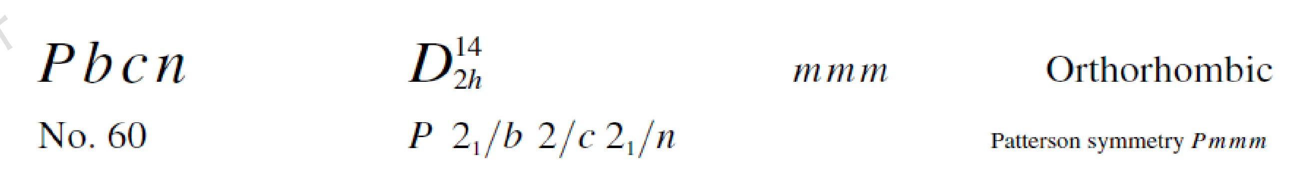


Pm$\bar{3}$*m*

* 空间群

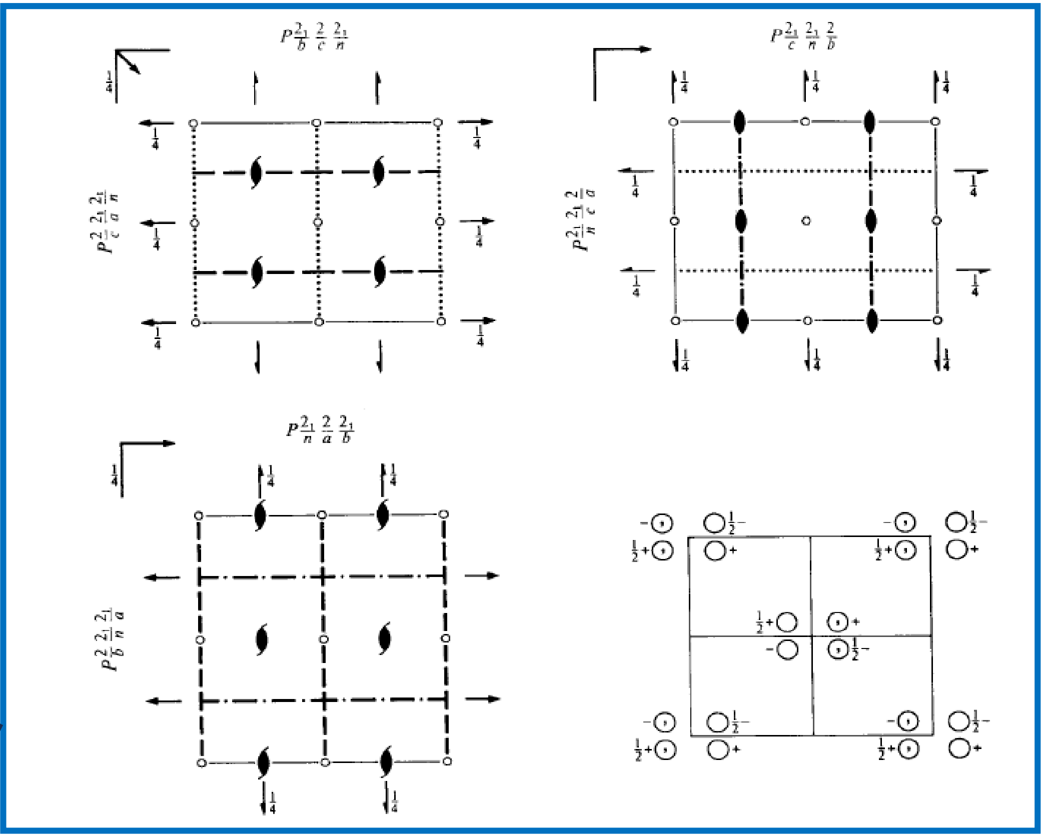
空间群的标记是通过结合一个描述点阵类型的大写字母和确定对称要素的记号来定义的。空间群的对称要素除了旋转轴和镜面，可能包含更复杂的对称要素，包括螺旋轴（screw axis-旋转和平移的组合）和滑移面（glide plane-镜面反射和平移的组合），加上不同的点阵，从而衍生出230不同的空间群。一个空间群表示一个晶胞里所有的对称性。

空间群-I
点阵和对称性


International Tables for Crystallography (2006). Vol. A, Space group 60, pp. 294–295.

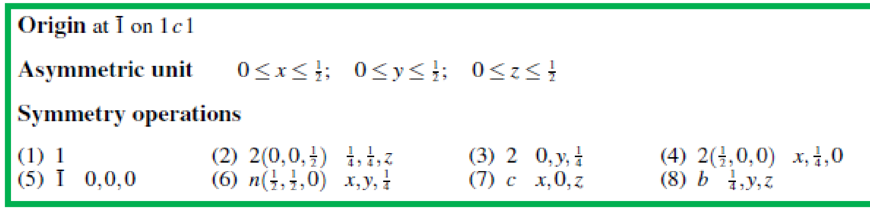
$Pbcn$	D_{2h}^{14}	mmm	Orthorhombic
No. 60	$P\ 2_1/b\ 2/c\ 2_1/n$		Patterson symmetry $Pmmm$

- 空间群序号 (No.60)
- 空间群符号 (*Pbcn*) [包括点阵 (*P*) 和对称操作元素 (*bcn*)]
- 熊弗里斯（Schoenflis）符号（D_{2h}）
- 完整的空间群符号 (*P* $2_1/b$ $2/\overset{14}{c}$ $2_1/n$)
- 点群 (*mmm*)
- Patterson 群 (*Pmmm*)
- 晶系 (Orthorhombic)



a, *b*, *c*三个方向的对称性的对称元素投影平面图

(1) *Headline*
(2) *Diagrams* for the symmetry elements and the general position (for graphical symbols of symmetry elements see Chapter 1.4)
(3) *Origin*
(4) *Asymmetric unit*
(5) *Symmetry operations*


Origin at $\bar{1}$ on $1c1$

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

Symmetry operations

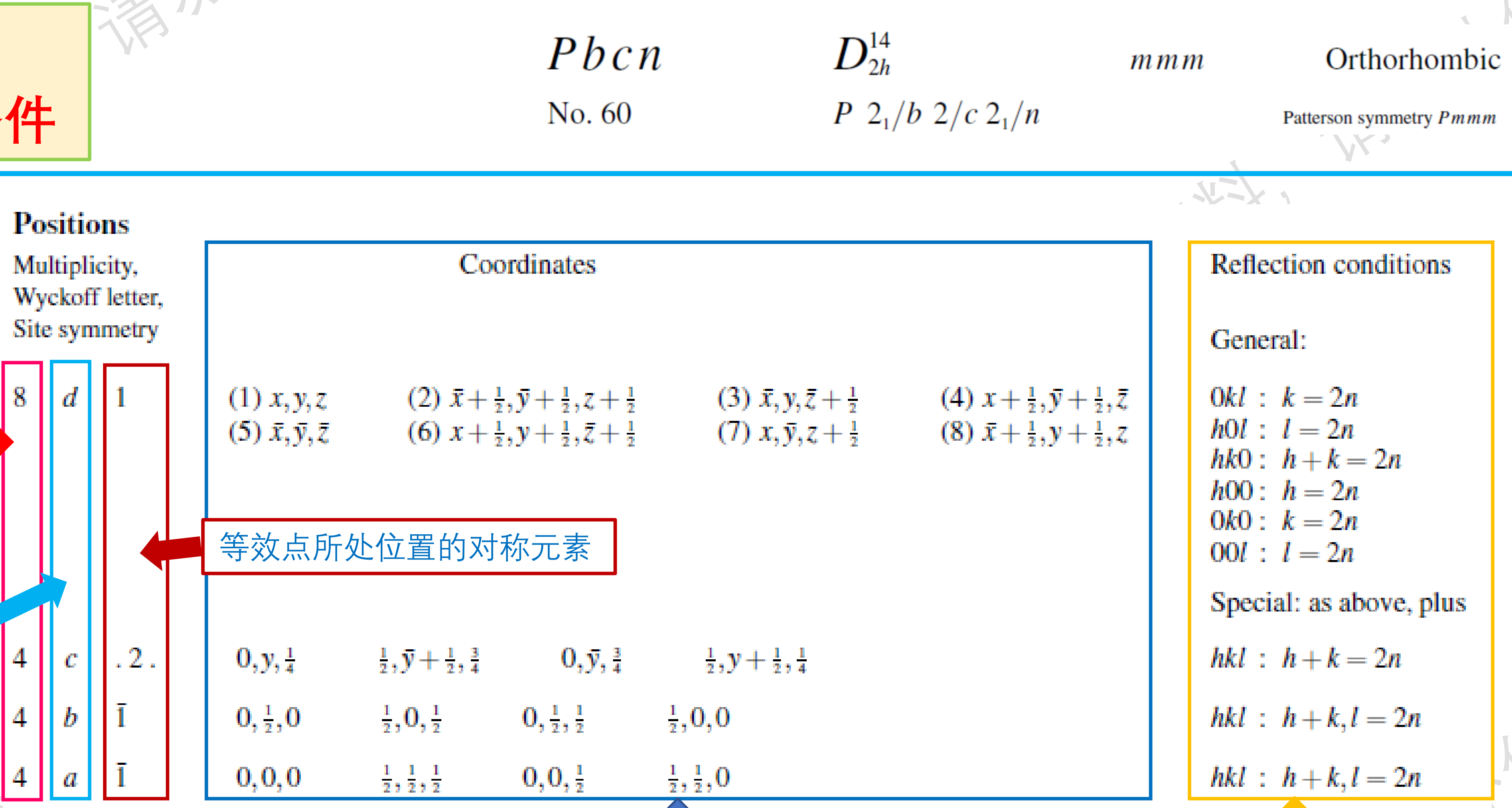
(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},\frac{1}{4},z$	(3) 2 $0,y,\frac{1}{4}$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},0$
(5) $\bar{1}$ 0,0,0	(6) $n(\frac{1}{2},\frac{1}{2},0)$ $x,y,\frac{1}{4}$	(7) c $x,0,z$	(8) b $\frac{1}{4},y,z$

原点，非对称单元，和对称性操作

空间群-II
结构参数与衍射条件

等效点数目，表示由空间群的所有对称元素的操作联系起来的一组点的数目。有一般和特殊等效点系。一般等效点系是经过空间群的全部对称元素操作得到的全部点。等效点位置的对称性最低（1次轴），数目最多。该空间群的一般等效点数目为“8”。 特殊等效点系的点处于特殊位置，处于等效元素上得到的一组点，数目比一般等效点数目少。

Wychoff 等效点系符号，如在此空间群中“*c*” 表示该等效点数目“**4**”，等效点系位于***b***方向的“**2**”次轴上，以及对应的等效点坐标。在描述结构表中以“4c”表示。



$Pbcn$ D_{2h}^{14} mmm Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	$0kl$: $k=2n$ $h0l$: $l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	
							Special: as above, plus
4	c	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{3}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{4}$	hkl : $h+k=2n$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$	hkl : $h+k,l=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+k,l=2n$

等效点所处位置的对称元素

对应的等效点系的全部等效点的位置坐标。对应着有边的反射条件。例如，如果晶胞里的原子全部占据“**4c**”位置，那么就只有晶面 *hkl* 中 ***h+k=2n*** 的结构因子F_{hkl}不等0.

产生衍射峰的条件。也就是通常说的系统消光规律。系统消光是由于点阵和微观对称的存在而使某一类晶面衍射的结构因子F_{hkl} = 0。

(6) *Headline* in abbreviated form;
(7) *Generators selected*; this information is the basis for the order of the entries under *Symmetry operations* and *Positions;*
(8) General and special *Positions*, with the following columns: *Multiplicity, Wyckoff letter, Site symmetry*, given by the oriented; site-symmetry symbol, *Coordinates, Reflection conditions.*

空间群-III
子群和超群

$Pbcn$ D_{2h}^{14} mmm Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$

Symmetry of special projections

Along [001] $c2mm$
$\mathbf{a}' = \mathbf{a}$ $\mathbf{b}' = \mathbf{b}$
Origin at $0,0,z$

Along [100] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{b}$ $\mathbf{b}' = \mathbf{c}$
Origin at $x,0,0$

Along [010] $p2gm$
$\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I	[2] $P2_1cn$ ($Pna2_1$, 33)	1; 4; 6; 7
	[2] $Pb2n$ ($Pnc2$, 30)	1; 3; 6; 8
	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 2; 7; 8
	[2] $P2_122_1$ ($P2_12_12$, 18)	1; 2; 3; 4
	[2] $P112_1/n$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P2_1/b11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P12/c1$ ($P2/c$, 13)	1; 3; 5; 7
IIa	none	
IIb	none	

8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

(9) *Symmetry of special projections* (not given for plane groups)
(10) *Maximal non-isomorphic subgroups*
(11) *Maximal isomorphic subgroups of lowest index*
(12) *Minimal non-isomorphic supergroups*

Maximal isomorphic subgroups of lowest index

IIc [3] $Pbcn$ ($\mathbf{a}' = 3\mathbf{a}$) (60); [3] $Pbcn$ ($\mathbf{b}' = 3\mathbf{b}$) (60); [3] $Pbcn$ ($\mathbf{c}' = 3\mathbf{c}$) (60)

Minimal non-isomorphic supergroups

I none

II [2] $Cmcm$ (63); [2] $Aema$ ($Cmce$, 64); [2] $Bbeb$ ($Ccce$, 68); [2] $Ibam$ (72); [2] $Pbmn$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($Pmna$, 53); [2] $Pbcb$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}$) ($Pcca$, 54); [2] $Pmca$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($Pbcm$, 57)

空间群-I

对称性部分

$Pbcn$ D_{2h}^{14} mmm Orthorhombic

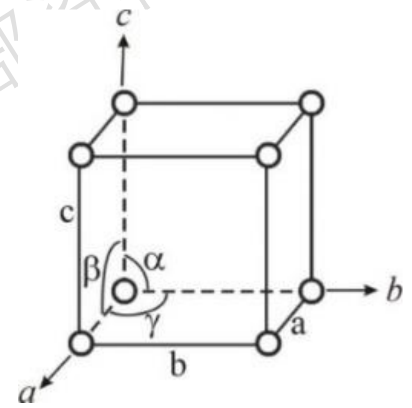
No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$

晶系：Orthorhombic (正交)

Crystal families

7 crystal systems and unit cell conditions imposed on cell geometry

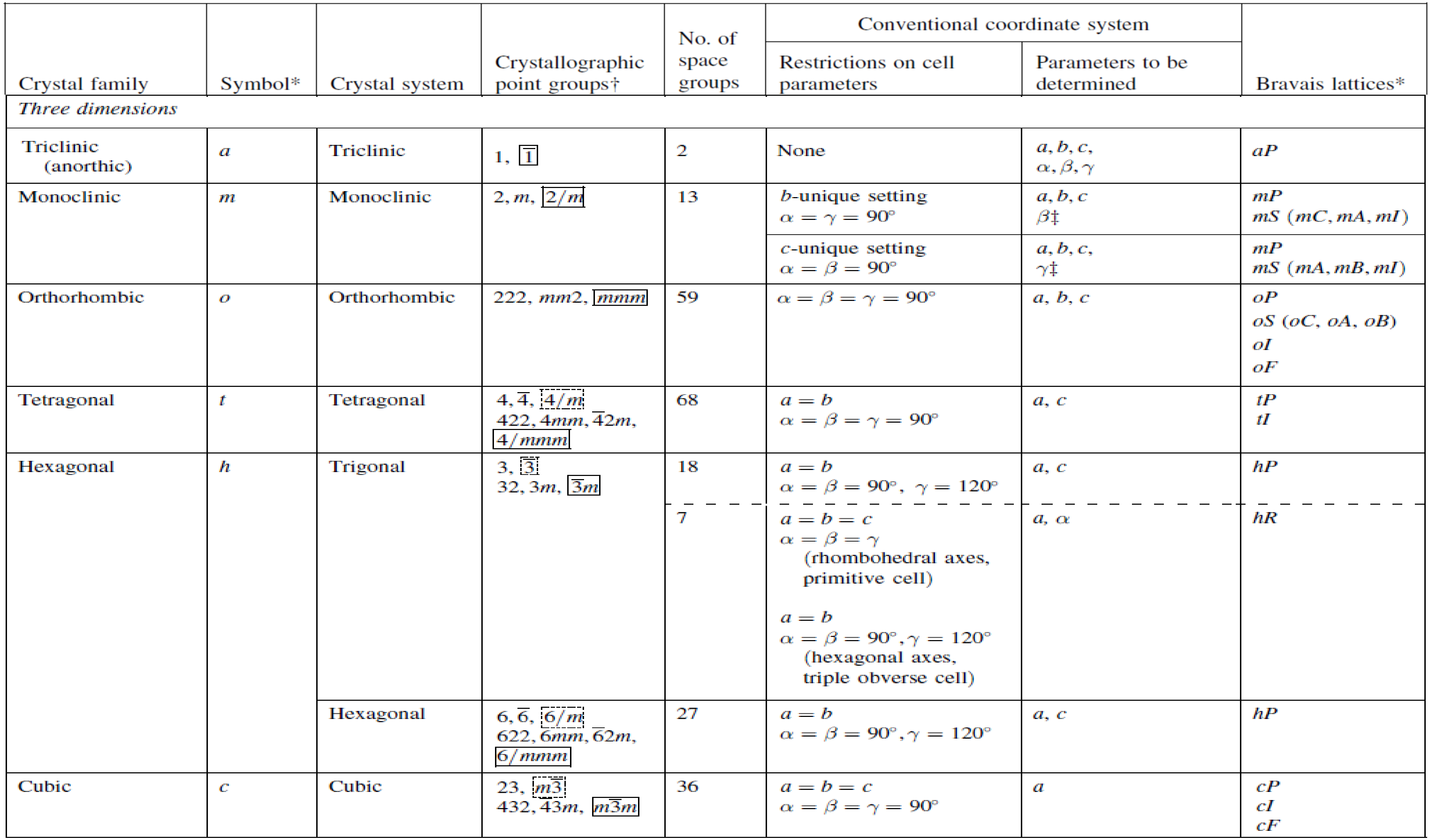
Symbol	Crystal system	Conditions imposed on cell geometry
a	Triclinic 1-2*	None
m	Monoclinic 3-15	$\alpha=\gamma=90°, \beta\neq 90°,$ (*b* unique) $\alpha=\beta=90°, \gamma\neq 90°$ (*c* unique)
o	Orthorhombic 16-74	$a\neq b\neq c,\ \alpha=\beta=\gamma=90°$
t	Tetragonal 75-142	$a=b\neq c, \alpha=\beta=\gamma=90°$
h	Trigonal 143-167	$a=b\neq c; \alpha=\beta=90°\ ; \gamma=120°$ (H-setting) $a=b=c, \alpha=\beta=\gamma$ (R-setting)
h	Hexagonal 168-194	$a=b\neq c, \alpha=\beta=90°, \gamma=120°$
c	Cubic 195-230	$a=b=c, \alpha=\beta=\gamma=90°$



六面体单位晶胞的定义

- The crystal families are symbolized by the lower-case letters *a*, *m*, *o*, *t*, *h*, and *c*.
- All ‘hexagonal’, ‘trigonal’ and ‘rhombohedral’ space groups are contained in one family, the hexagonal crystal family.
- 包含的空间群的序号

Table 2.1.2.1. *Crystal families, crystal systems, conventional coordinate systems and Bravais lattices in three dimensions.*



Crystal family	Symbol*	Crystal system	Crystallographic point groups†	No. of space groups	Conventional coordinate system		Bravais lattices*
					Restrictions on cell parameters	Parameters to be determined	
Three dimensions							
Triclinic (anorthic)	a	Triclinic	$1, \boxed{\bar{1}}$	2	None	$a, b, c,$ α, β, γ	aP
Monoclinic	m	Monoclinic	$2, m, \boxed{2/m}$	13	b-unique setting $\alpha = \gamma = 90^\circ$	a, b, c β‡	mP mS (mC, mA, mI)
					c-unique setting $\alpha = \beta = 90^\circ$	$a, b, c,$ γ‡	mP mS (mA, mB, mI)
Orthorhombic	o	Orthorhombic	$222, mm2, \boxed{mmm}$	59	$\alpha = \beta = \gamma = 90^\circ$	a, b, c	oP oS (oC, oA, oB) oI oF
Tetragonal	t	Tetragonal	$4, \bar{4}, \boxed{4/m}$ $422, 4mm, \bar{4}2m,$ $\boxed{4/mmm}$	68	$a = b$ $\alpha = \beta = \gamma = 90^\circ$	a, c	tP tI
Hexagonal	h	Trigonal	$3, \boxed{\bar{3}}$ $32, 3m, \boxed{\bar{3}m}$	18	$a = b$ $\alpha = \beta = 90^\circ, \ \gamma = 120^\circ$	a, c	hP
				7	$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell) $a = b$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$ (hexagonal axes, triple obverse cell)	a, α	hR
		Hexagonal	$6, \bar{6}, \boxed{6/m}$ $622, 6mm, \bar{6}2m,$ $\boxed{6/mmm}$	27	$a = b$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	a, c	hP
Cubic	c	Cubic	$23, \boxed{m\bar{3}}$ $432, \bar{4}3m, \boxed{m\bar{3}m}$	36	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	a	cP cI cF

International Tables for Crystallography (2006). Vol. A, Chapter 2.1, p. 15.

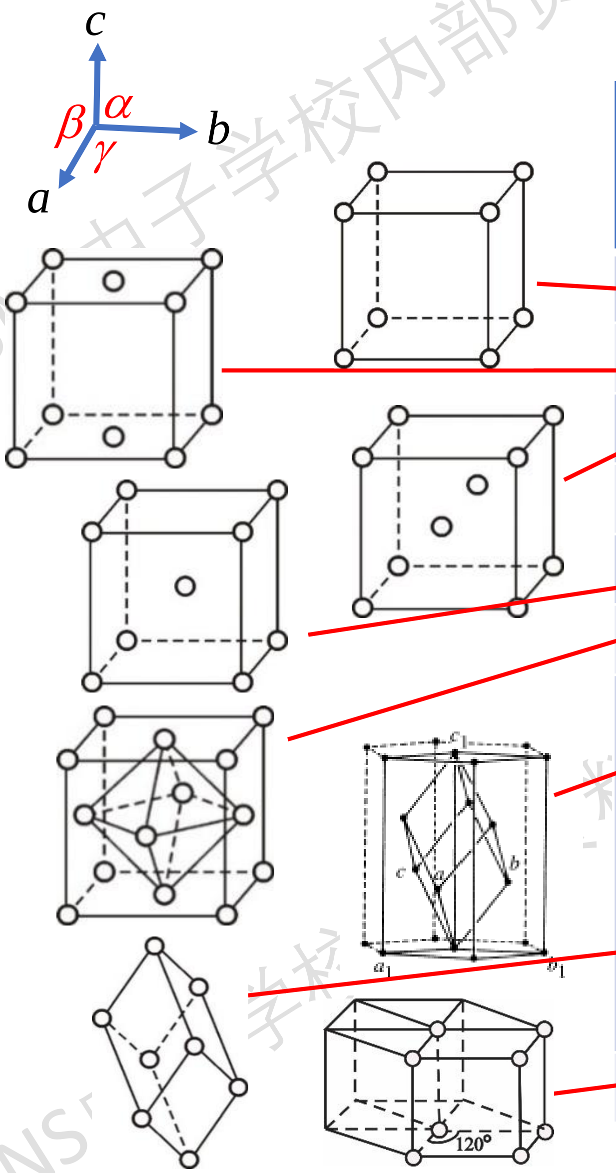
点阵 Lattice
Three-dimensional cells

P b c n

Pbcn D_{2h}^{14} *mmm* Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry *Pmmm*

Printed symbols for the conventional centring types of three-dimensional cells



Printed symbol	Centering type of cell	Number of lattice points per cell	Coordinates of lattice points within cell
P	Primitive	1	0,0,0
C	*C*-face centred	2	0,0,0; ½,½,0
A	*A*-face centred	2	0,0,0; 0,½,½
B	*B*-face centred	2	0,0,0; ½,0,½
I	Body centred	2	0,0,0; ½,½,½
F	All-face centred	4	0,0,0; ½,½,0; 0,½,½; ½,0,½
R	Rhombohedrally centred *(description with 'hexagonal axes')*	3	0,0,0; $^{2}/_{3},^{1}/_{3},^{1}/_{3}$; $^{1}/_{3},^{2}/_{3},^{2}/_{3}$ ***(obverse setting)*** 0,0,0; $^{1}/_{3},^{2}/_{3},^{1}/_{3}$; $^{2}/_{3},^{1}/_{3},^{2}/_{3}$ ***(reverse setting)***
	Primitive *(description with 'rhombohedral axes')*	1	0,0,0
P (H)	Hexagonal centred	3	0,0,0; $^{2}/_{3},^{1}/_{3}$,0; $^{1}/_{3},^{2}/_{3}$,0

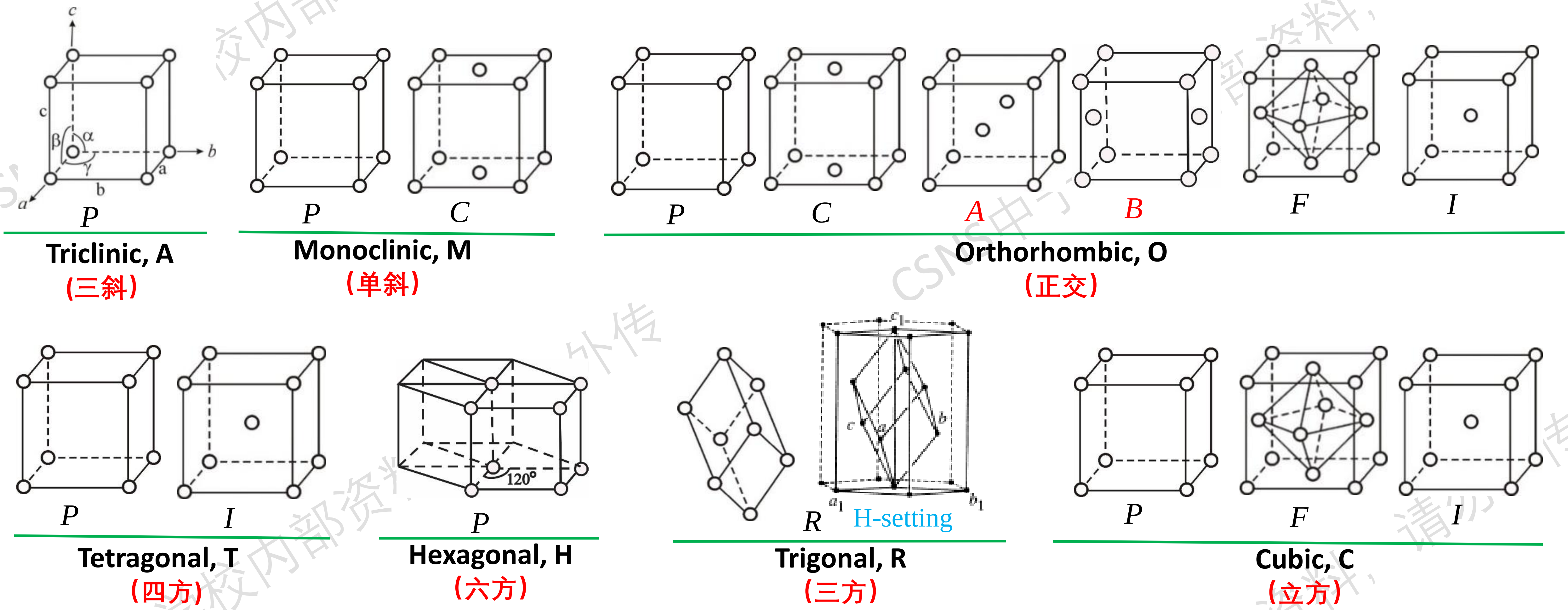
***International Tables for Crystallography* (2006). Vol. A, Chapter 1.2, p. 4.**

空间群-I
对称性部分

点阵 Lattice
The 14 crystal Bravais lattices

P （点阵类型） $Pbcn$ No. 60 D_{2h}^{14} mmm Orthorhombic

$P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$



Triclinic, A
（三斜）

Monoclinic, M
（单斜）

Orthorhombic, O
（正交）

Tetragonal, T
（四方）

Hexagonal, H
（六方）

Trigonal, R
（三方）

Cubic, C
（立方）

Bravais在1850年提出并总结出三维晶格只有14种可能，称作Bravais点阵。由于七个晶系中对晶胞形状的定义不同，各个晶系中可能有的点阵类型也不一样。在三斜晶系中只可能有一种简单点阵P，而正交晶系中可能有 P，C，F，I 共4种点阵。

空间群-I
对称性部分

Trigonal, *R*（三方）

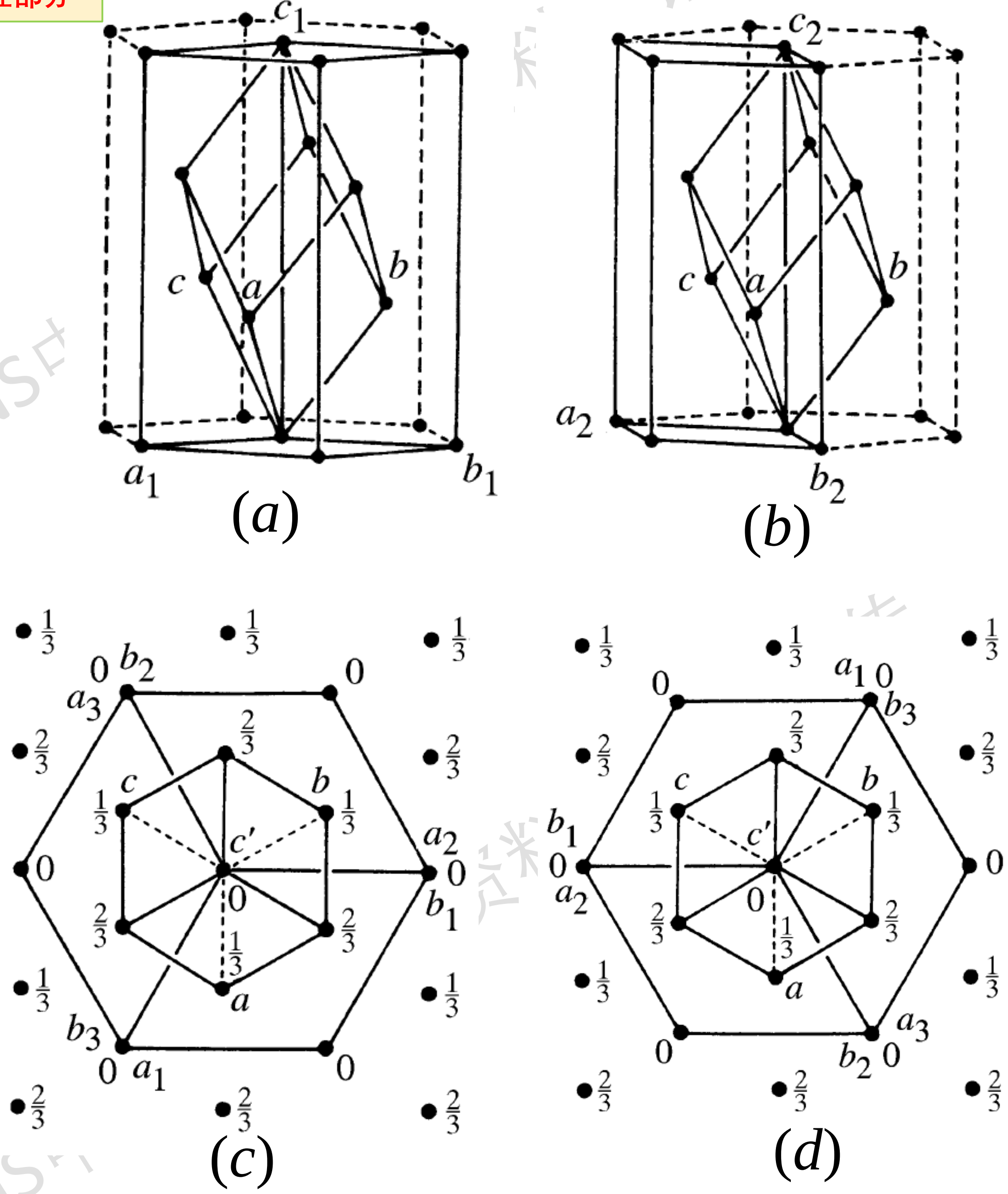
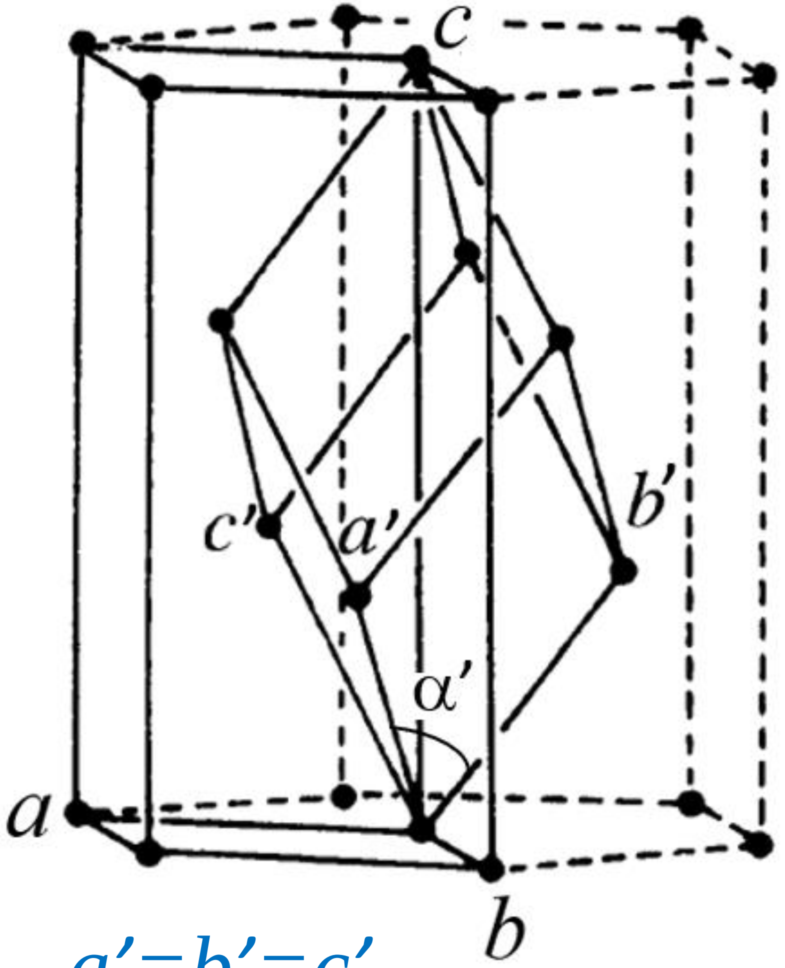


Fig. 5.1.3.6. Unit cells in the rhombohedral lattice: same origin for all cells. The basis of the rhombohedral cell is labelled *a*, *b*, *c*. Two settings of the triple hexagonal cell are possible with respect to a primitive rhombohedral cell: The *obverse setting* with the lattice points 0, 0, 0; 2/3, 1/3, 1/3; 1/3, 2/3, 2/3 has been used in *International Tables* since 1952. Its general reflection condition is $-h+k+l=3n$. The *reverse setting* with lattice points 0, 0, 0; 1/3, 2/3, 1/3; 2/3, 1/3, 2/3 was used in the 1935 edition. Its general reflection condition is $h-k+l=3n$. (*a*) Obverse setting of triple hexagonal cell a_1, b_1, c_1 in relation to the primitive rhombohedral cell *a*, *b*, *c*. (*b*) Reverse setting of triple hexagonal cell a_2, b_2, c_2 in relation to the primitive rhombohedral cell *a*, *b*, *c*. (*c*) Primitive rhombohedral cell (- - - lower edges), *a*, *b*, *c* in relation to the three triple hexagonal cells in obverse setting a_1, b_1, *c*; a_2, b_2, *c*; a_3, b_3, *c*. Projection along *c*. (*d*) Primitive rhombohedral cell (- - - lower edges), *a*, *b*, *c* in relation to the three triple hexagonal cells in reverse setting a_1, b_1, *c*; a_2, b_2, *c*; a_3, b_3, *c*. Projection along *c*.

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, Chapter 5.1, p84 (2005)

The relations between the cell parameters *a*, *c* of the triple hexagonal cell and the cell parameters *a′*, of the primitive rhombohedral cell.



a′=b′=c′

$$a = a'\sqrt{2}\sqrt{1-\cos\alpha'} = 2a'\sin\frac{\alpha'}{2}$$

$$c = a'\sqrt{3}\sqrt{1+2\cos\alpha'}$$

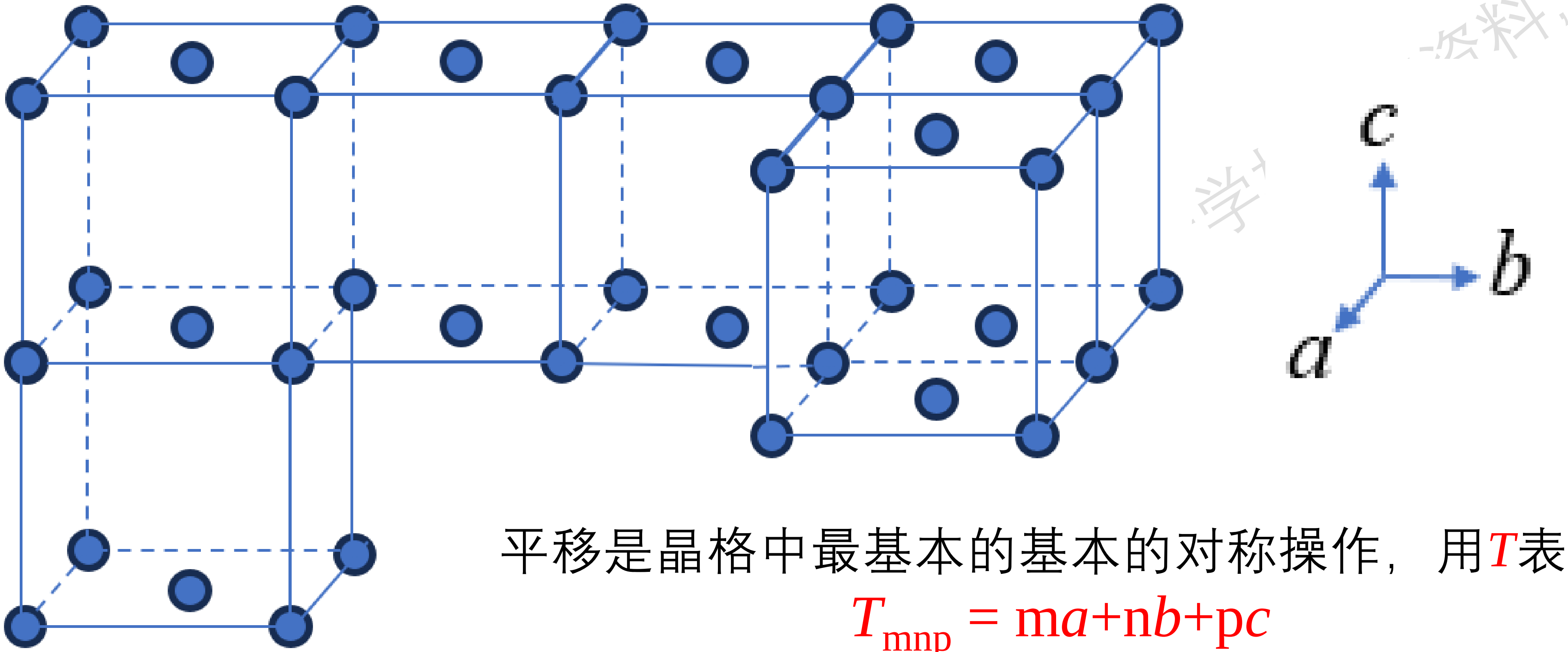
$$\frac{c}{a} = \sqrt{\frac{3}{2}}\sqrt{\frac{1+2\cos\alpha'}{1-\cos\alpha'}} = \sqrt{\frac{9}{4\sin^2(\alpha'/2)}-3}$$

$$a' = \tfrac{1}{3}\sqrt{3a^2+c^2}$$

$$\sin\frac{\alpha'}{2} = \frac{3}{2\sqrt{3+(c^2/a^2)}} \quad \text{or} \quad \cos\alpha' = \frac{(c^2/a^2)-\frac{3}{2}}{(c^2/a^2)+3}$$

INTERNATIONAL TABLES FOR CRYSTALLOGRAPHY, Chapter 2, p16 (2005)

点阵—平移操作



平移是晶格中最基本的基本的对称操作，用*T*表示：

$$T_{mnp} = ma+nb+pc$$

这里m，n，p为任意整数。T_{mnp}表示在晶体的三维点阵上，点阵阵点在*a*，*b*，和*c*方向分别平移m, n, 和p单位后，点阵结构仍能复原。

Pbcn 空间群中的对称要素及其操作

1. 晶体的对称性反映在晶格对称性上，分为2大类：a) 具有分子对称性的4种类型的对称要素和对称操作，称作宏观对称要素；b) 具有与平移有关的3种对称要素和对称操作，称作微观对称要素。
2. 旋转轴（Rotation axes），反演旋转轴 (Inversion axes） 和螺旋轴（Screw axes）的轴次只能为1， 2， 3， 4， 6；
3. 如果晶格绕1个旋转轴转动 $\alpha=2\pi/n$ （n为整数）角度，称旋转轴为n重旋转轴；
4. 螺旋轴和滑移面的滑移量只能符合点阵结构中平移量。

宏观对称要素

(不含平移操作的对称元素，没有衍射消光)

(1) 对称中心：i； (2) 对称面: m

(3) 旋转轴：1, 2, 3, 4, 6

(4) 反演旋转轴(旋转+反演)：$\bar{1}, \bar{3}, \bar{4}, \bar{6}$

微观对称要素

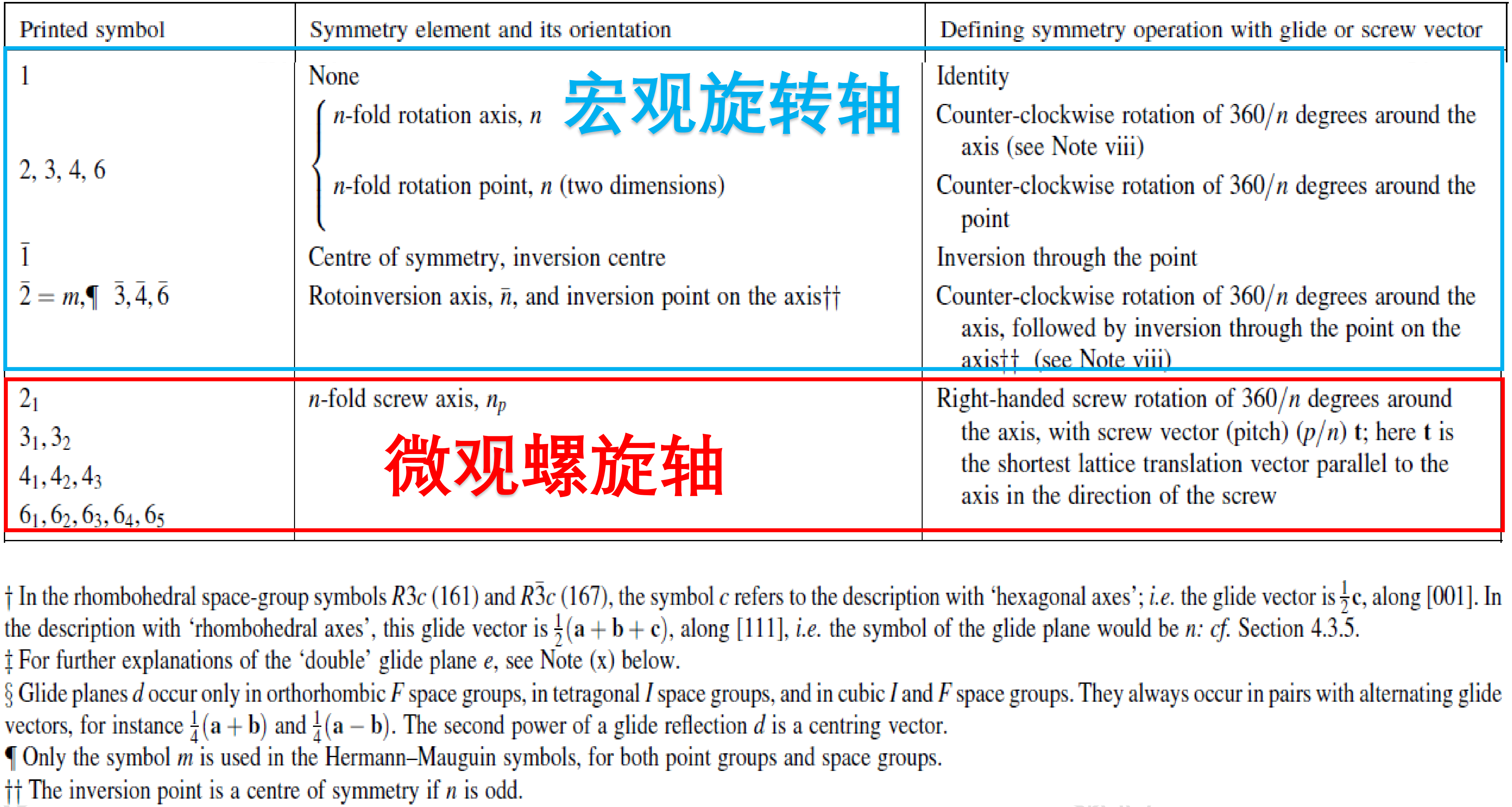
(部分宏观对称元素+平移操作的对称元素，有衍射消光)

(1) 点阵：平移

(2) 滑移面：a, b, c, e, n, d

(3) 螺旋轴:$2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5$

1.3.1 *continue*



Printed symbol	Symmetry element and its orientation	Defining symmetry operation with glide or screw vector
1	None	Identity
2, 3, 4, 6	*n*-fold rotation axis, *n*	Counter-clockwise rotation of 360/*n* degrees around the axis (see Note viii)
	n-fold rotation point, *n* (two dimensions)	Counter-clockwise rotation of 360/*n* degrees around the point
$\bar{1}$	Centre of symmetry, inversion centre	Inversion through the point
$\bar{2} = m$,¶ $\bar{3}, \bar{4}, \bar{6}$	Rotoinversion axis, $\bar{n}$, and inversion point on the axis††	Counter-clockwise rotation of 360/*n* degrees around the axis, followed by inversion through the point on the axis†† (see Note viii)
2_1 $3_1, 3_2$ $4_1, 4_2, 4_3$ $6_1, 6_2, 6_3, 6_4, 6_5$	*n*-fold screw axis, n_p	Right-handed screw rotation of 360/*n* degrees around the axis, with screw vector (pitch) (*p*/*n*) **t**; here **t** is the shortest lattice translation vector parallel to the axis in the direction of the screw

宏观旋转轴

微观螺旋轴

† In the rhombohedral space-group symbols $R3c$ (161) and $R\bar{3}c$ (167), the symbol *c* refers to the description with 'hexagonal axes'; *i.e.* the glide vector is $\frac{1}{2}\mathbf{c}$, along [001]. In the description with 'rhombohedral axes', this glide vector is $\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$, along [111], *i.e.* the symbol of the glide plane would be *n*: *cf.* Section 4.3.5.

‡ For further explanations of the 'double' glide plane *e*, see Note (x) below.

§ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a}+\mathbf{b})$ and $\frac{1}{4}(\mathbf{a}-\mathbf{b})$. The second power of a glide reflection *d* is a centring vector.

¶ Only the symbol *m* is used in the Hermann–Mauguin symbols, for both point groups and space groups.

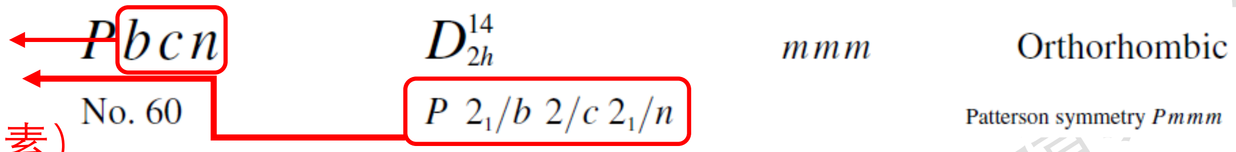
†† The inversion point is a centre of symmetry if *n* is odd.

International Tables for Crystallography (2006). Vol. A, Chapter 1.3, pp. 5–6.

Lattice Symmetry Direction

bcn

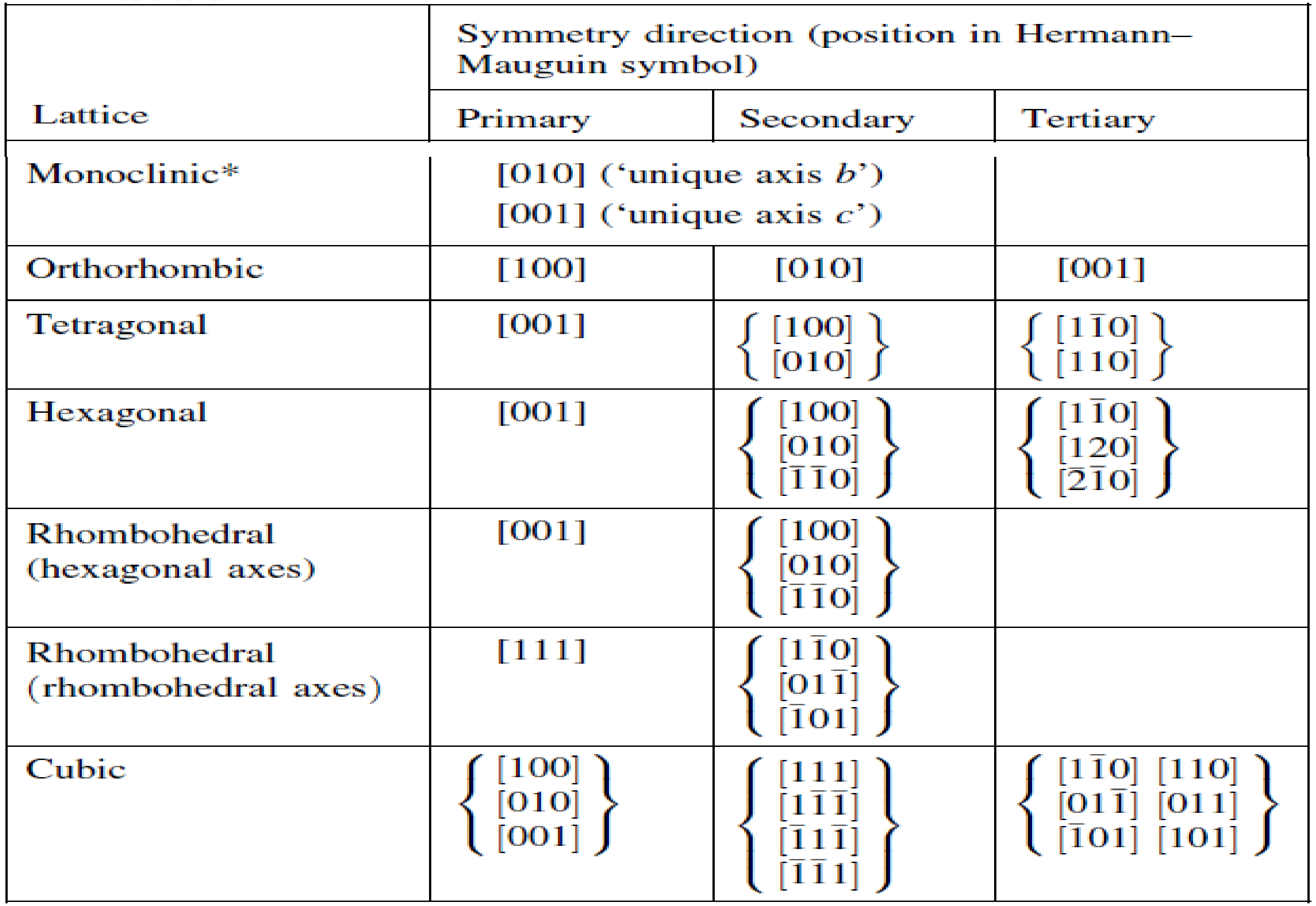
（对称性元素）



Pbcn D_{2h}^{14} *mmm* Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry *Pmmm*

Table 2.2.4.1. *Lattice symmetry directions for three dimensions.* Directions that belong to the same set of equivalent symmetry directions are collected between braces. The first entry in each set is taken as the representative of that set.



Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Monoclinic*	[010] (‘unique axis *b*’) [001] (‘unique axis *c*’)		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	{[100] [010]}	{$[1\bar{1}0]$ [110]}
Hexagonal	[001]	{[100] [010] $[\bar{1}\bar{1}0]$}	{$[1\bar{1}0]$ [120] $[\bar{2}\bar{1}0]$}
Rhombohedral (hexagonal axes)	[001]	{[100] [010] $[\bar{1}\bar{1}0]$}	
Rhombohedral (rhombohedral axes)	[111]	{$[1\bar{1}0]$ $[01\bar{1}]$ $[\bar{1}01]$}	
Cubic	{[100] [010] [001]}	{[111] $[1\bar{1}\bar{1}]$ $[\bar{1}1\bar{1}]$ $[\bar{1}\bar{1}1]$}	{$[1\bar{1}0]$ [110] $[01\bar{1}]$ [011] $[\bar{1}01]$ [101]}

1. 单斜晶系通常选***b***轴方向作为特征方向的唯一轴(图a)，群的全称为$P12_1m1$。和可以选***c***或***a***轴(图b)，全称为$P112_1m$或$P2_1m11$。互换后的结果见

2. 正交晶系的三个晶轴可以互换，结果见下表。

International Tables for Crystallography (2006). Vol. A, Chapter 2.2 p. 18

宏观对称要素

(不含平移操作的对称元素，没有衍射消光)

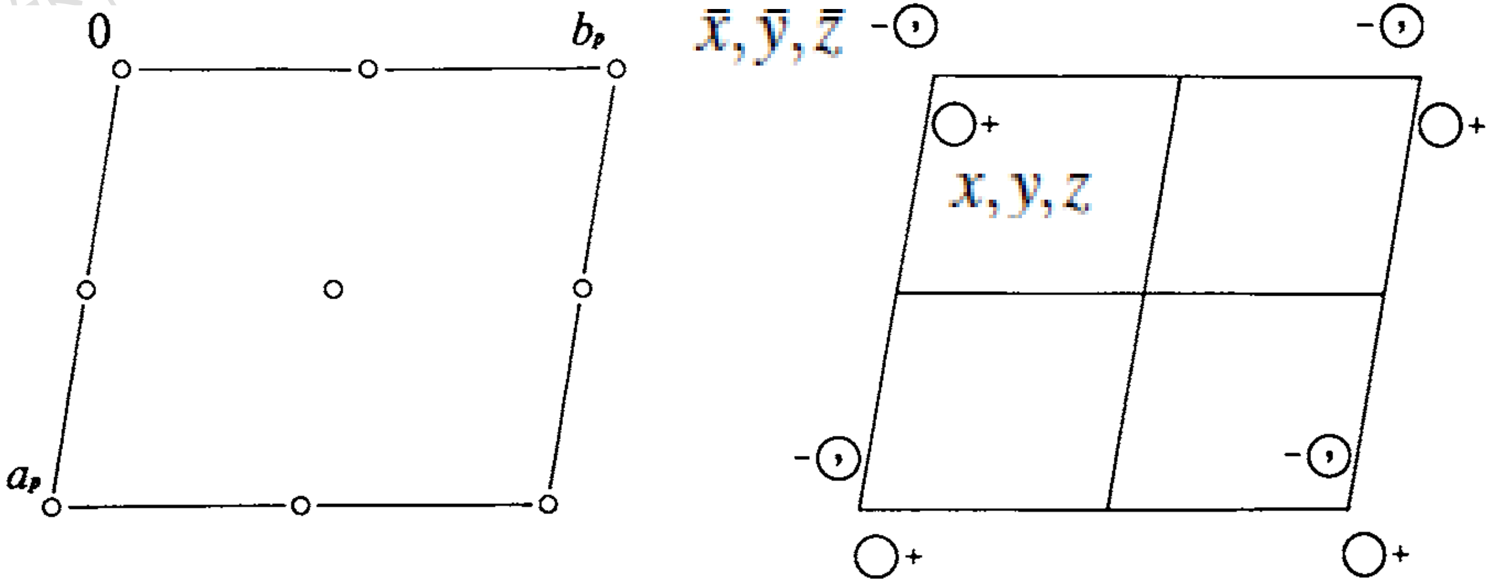
(1) 对称中心：i； (2) 对称面: m

(3) 旋转轴：1, 2, 3, 4, 6

(4) 反演旋转轴(旋转+反演)：$\bar{1}, \bar{3}, \bar{4}, \bar{6}$

$P\bar{1}$ (i)

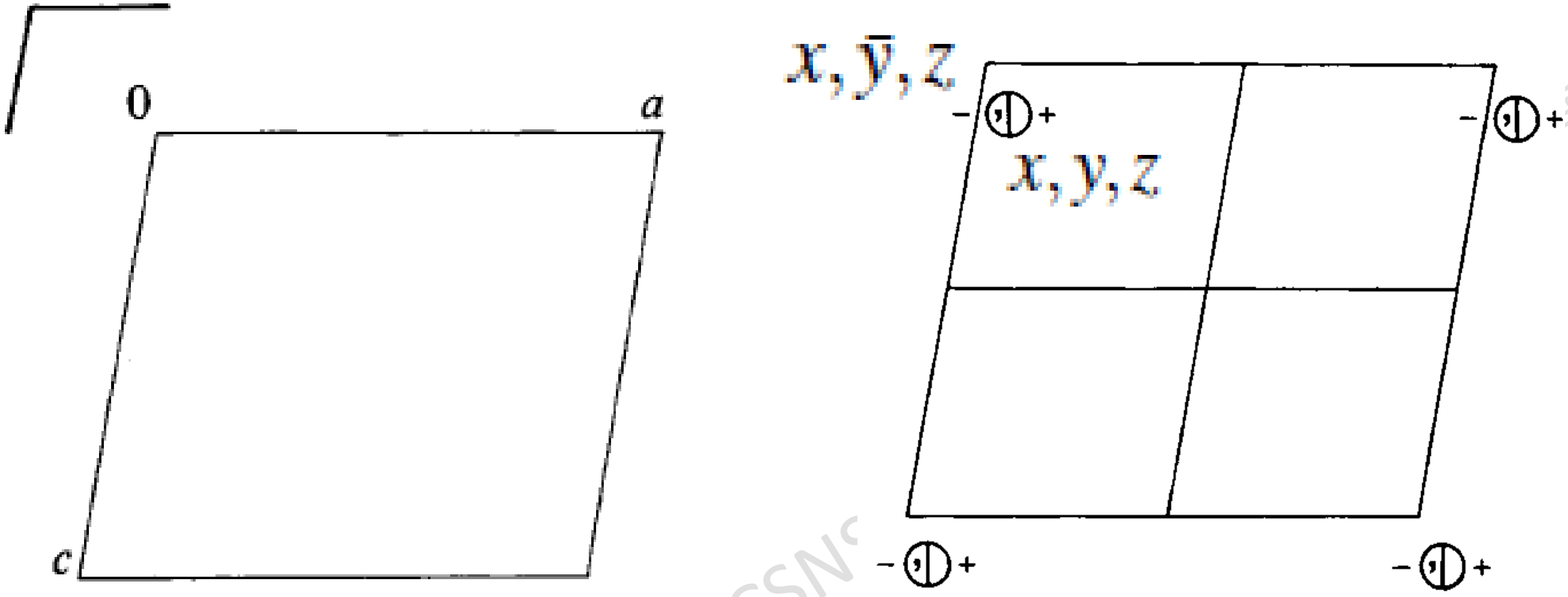
等效点数：2



Pm

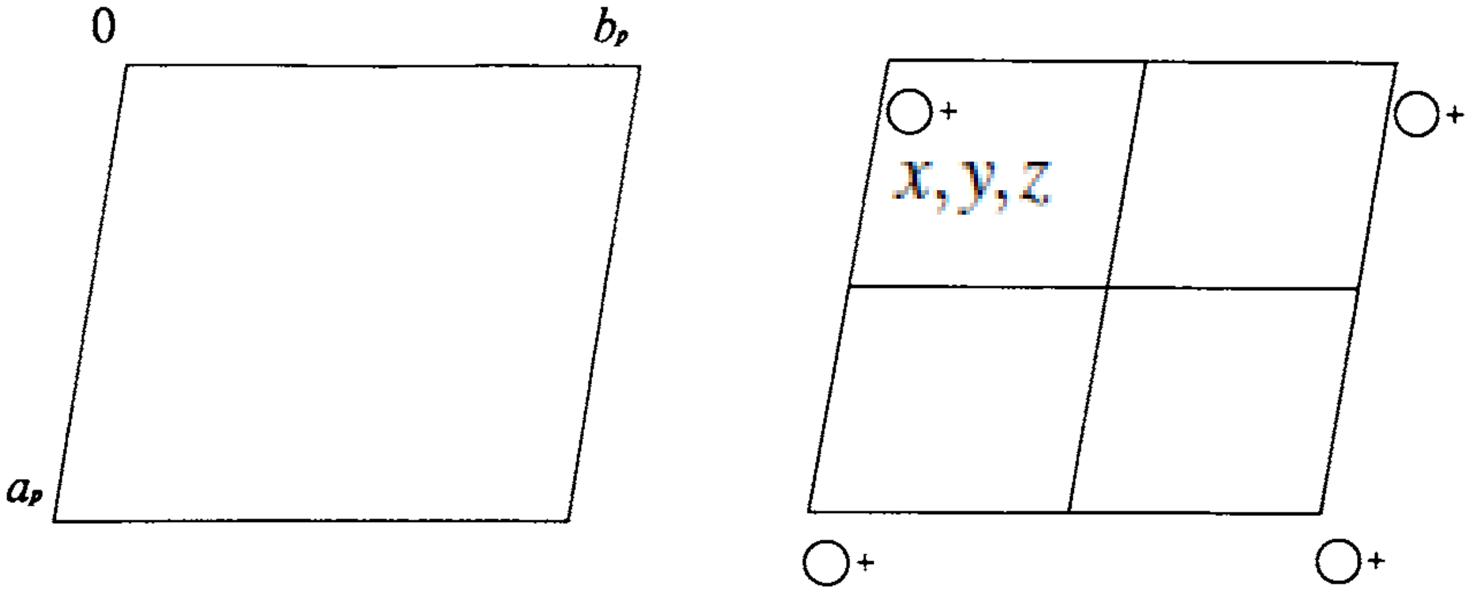
Unique axes b

等效点数：2



*P*1

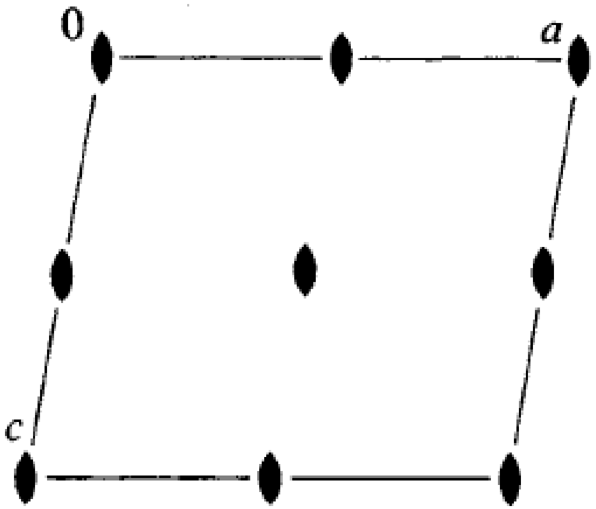
等效点数：1

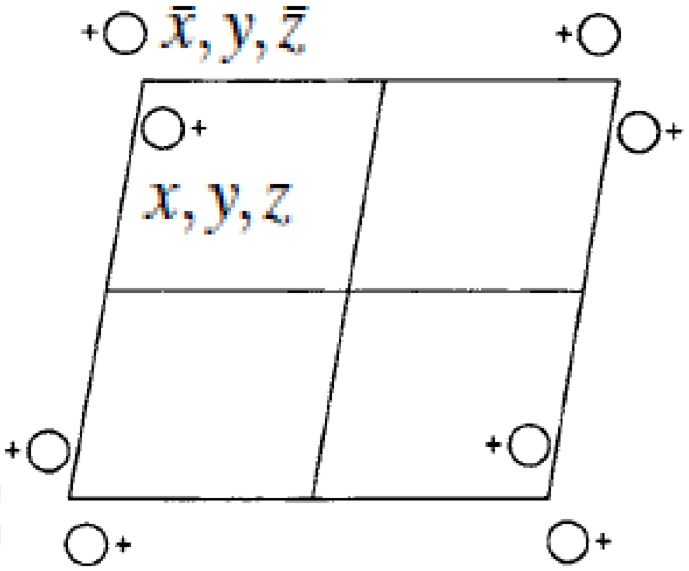


*P*2

Unique axes b

等效点数：2





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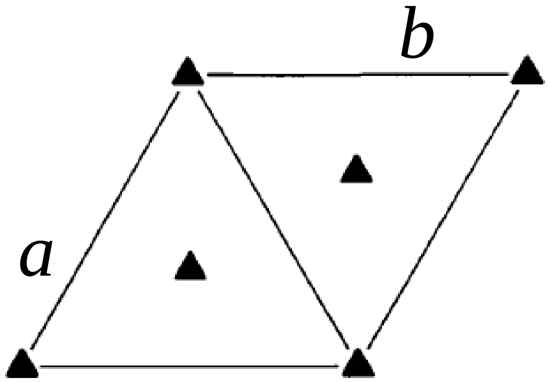
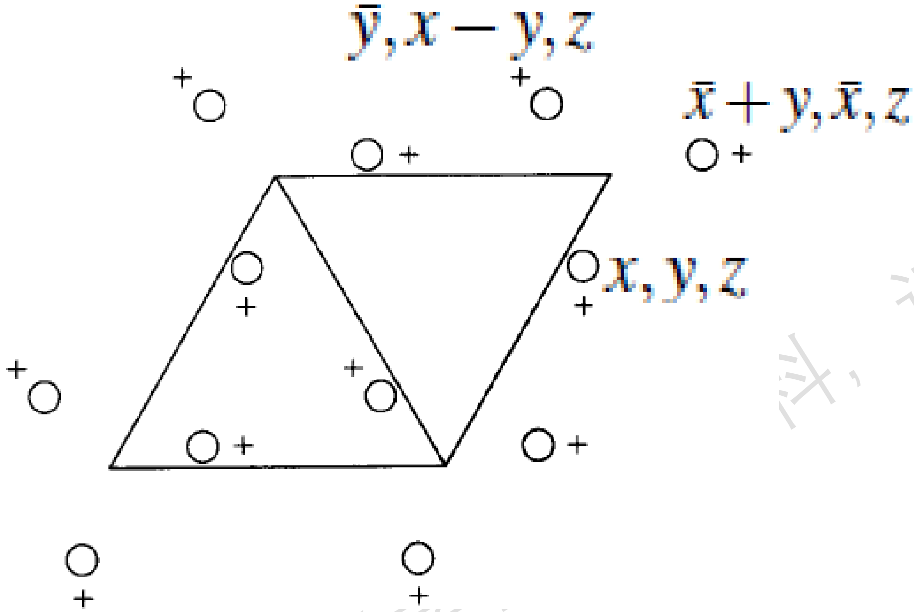
*P*3

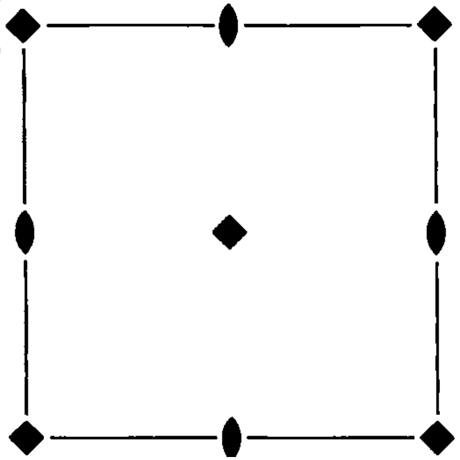
等效点数：3

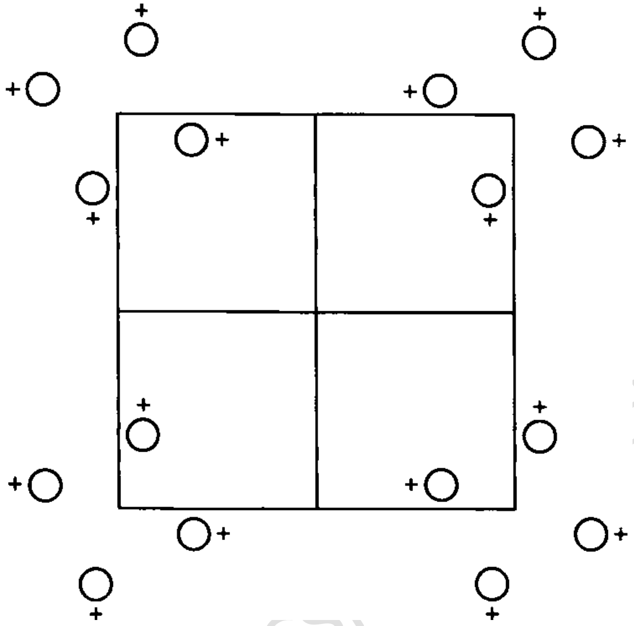




$P4$

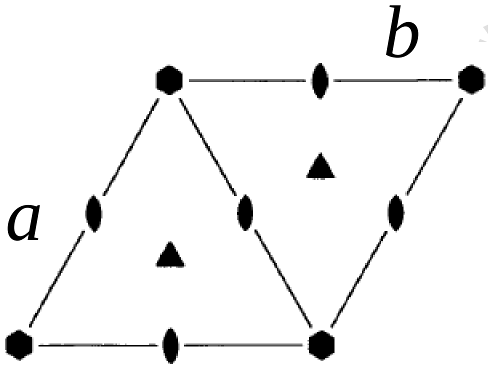
等效点数：4

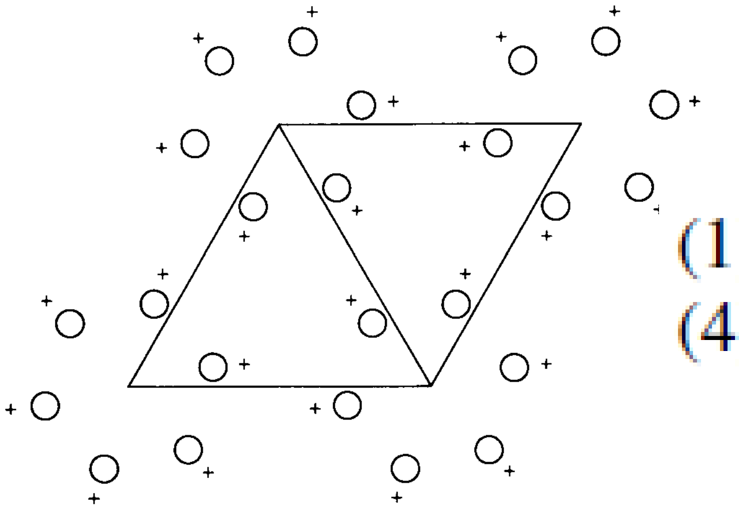




$(1)\ x,y,z$
$(2)\ \bar{x},\bar{y},z$
$(3)\ \bar{y},x,z$
$(4)\ y,\bar{x},z$

$P6$

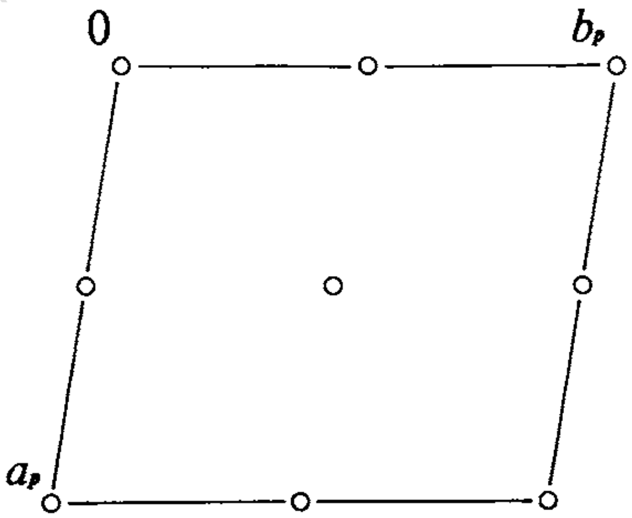


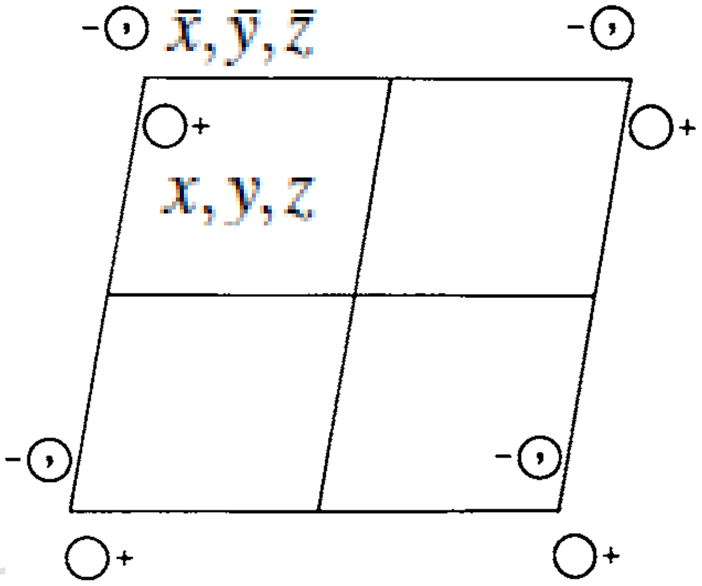


等效点数：6

$(1)\ x,y,z$ $(2)\ \bar{y},x-y,z$ $(3)\ \bar{x}+y,\bar{x},z$
$(4)\ \bar{x},\bar{y},z$ $(5)\ y,\bar{x}+y,z$ $(6)\ x-y,x,z$

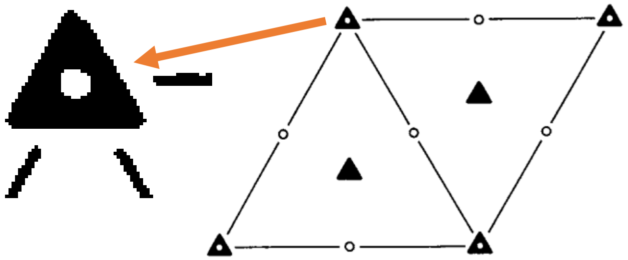
$P\bar{1}$ (*i*)

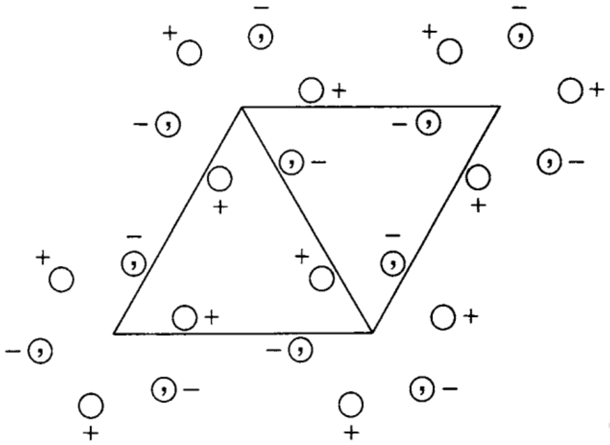




等效点数：2

$P\bar{3}$



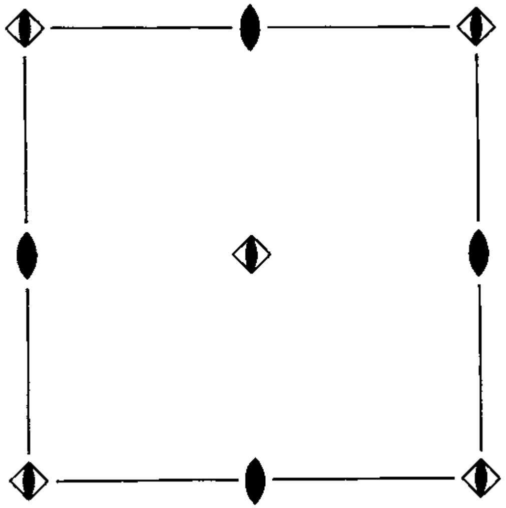


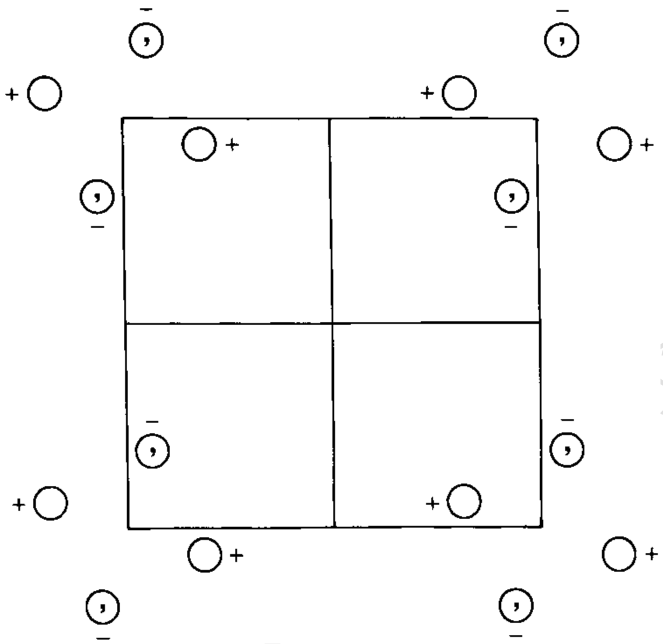
等效点数：6

(1) x,y,z
(2) $\bar{y},x-y,z$
(3) $\bar{x}+y,\bar{x},z$
(4) $\bar{x},\bar{y},\bar{z}$
(5) $y,\bar{x}+y,\bar{z}$
(6) $x-y,x,\bar{z}$

$P\bar{4}$

等效点数：4





(1) x,y,z

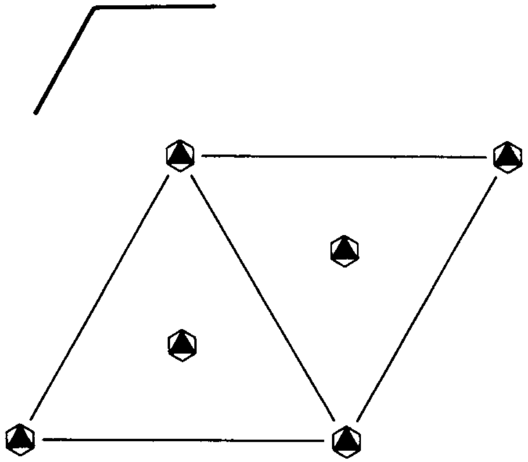
(2) $\bar{x},\bar{y},z$

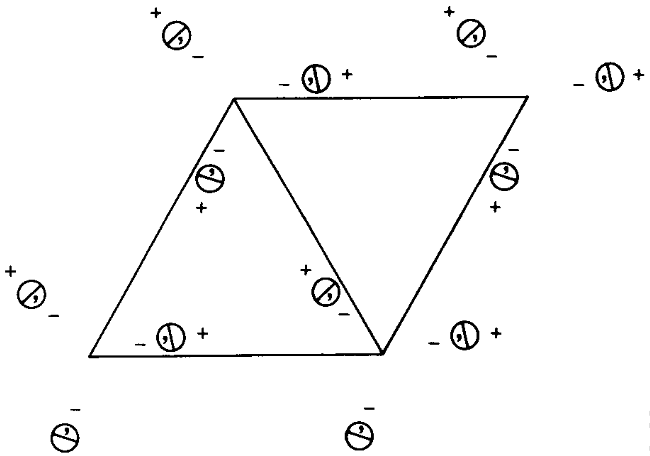
(3) $y,\bar{x},\bar{z}$

(4) $\bar{y},x,\bar{z}$

$P\bar{6}$

等效点数：6





(1) x,y,z (2) $\bar{y},x-y,z$ (3) $\bar{x}+y,\bar{x},z$

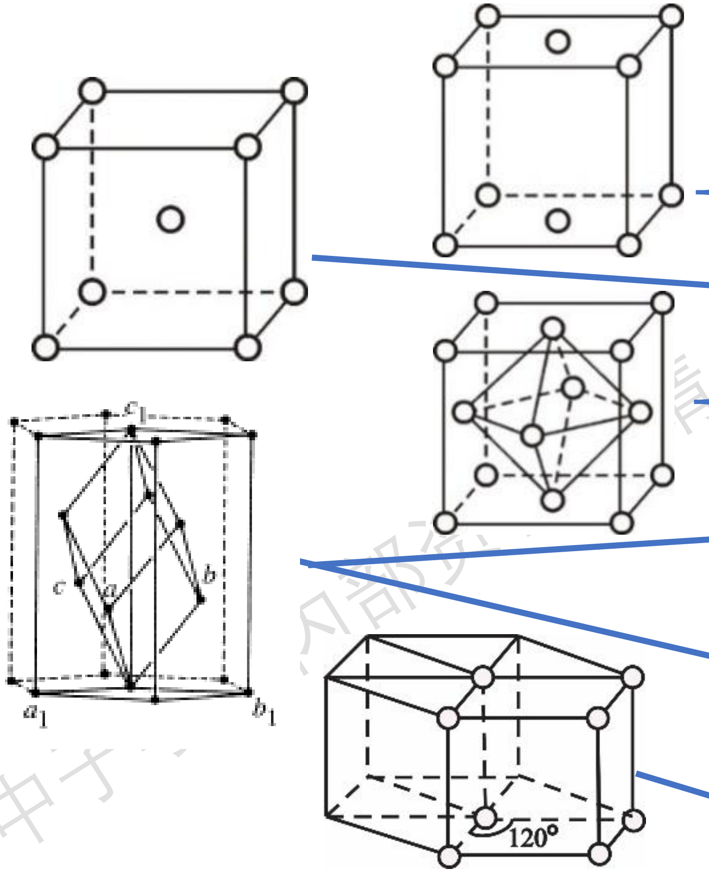
(4) $x,y,\bar{z}$ (5) $\bar{y},x-y,\bar{z}$ (6) $\bar{x}+y,\bar{x},\bar{z}$

Reflection Conditions (反射条件, 亦称消光规律)

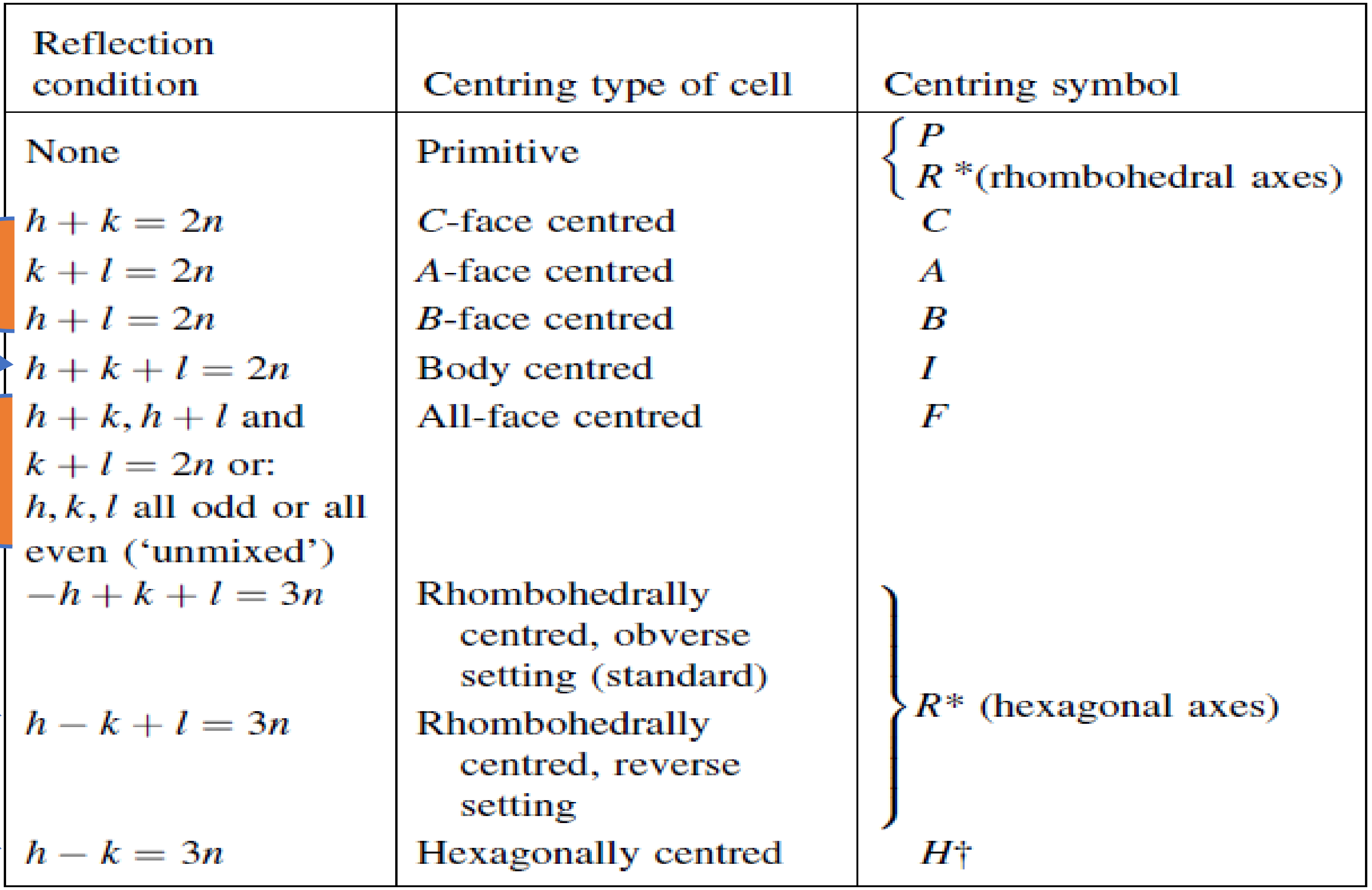
衍射强度 $I_{hkl} = CF^2_{hkl}$，结构因子 F_{hkl} 的大小表示一个晶胞对衍射能力的大小，当 $F_{hkl} \equiv 0$ 时称作结构消光，或系统消光。

材料的衍射消光规律是衍射分析中判断点阵类型，点阵阵点坐标，和确定空间群等的重要依据。

$$F^2_{hkl} = |\sum f_j (b_j, q_j f_{Mj}) \exp[2\pi i (h x + k y + l z)]|^2 e^{-2W}$$



Integral reflection conditions for centred lattice



Reflection condition	Centring type of cell	Centring symbol
None	Primitive	P R *(rhombohedral axes)
$h + k = 2n$	C-face centred	C
$k + l = 2n$	A-face centred	A
$h + l = 2n$	B-face centred	B
$h + k + l = 2n$	Body centred	I
$h + k, h + l$ and $k + l = 2n$ or: h, k, l all odd or all even ('unmixed')	All-face centred	F
$-h + k + l = 3n$	Rhombohedrally centred, obverse setting (standard)	R* (hexagonal axes)
$h - k + l = 3n$	Rhombohedrally centred, reverse setting	
$h - k = 3n$	Hexagonally centred	H†

*International tables for crystallography, Vol. A, 15 (1992).

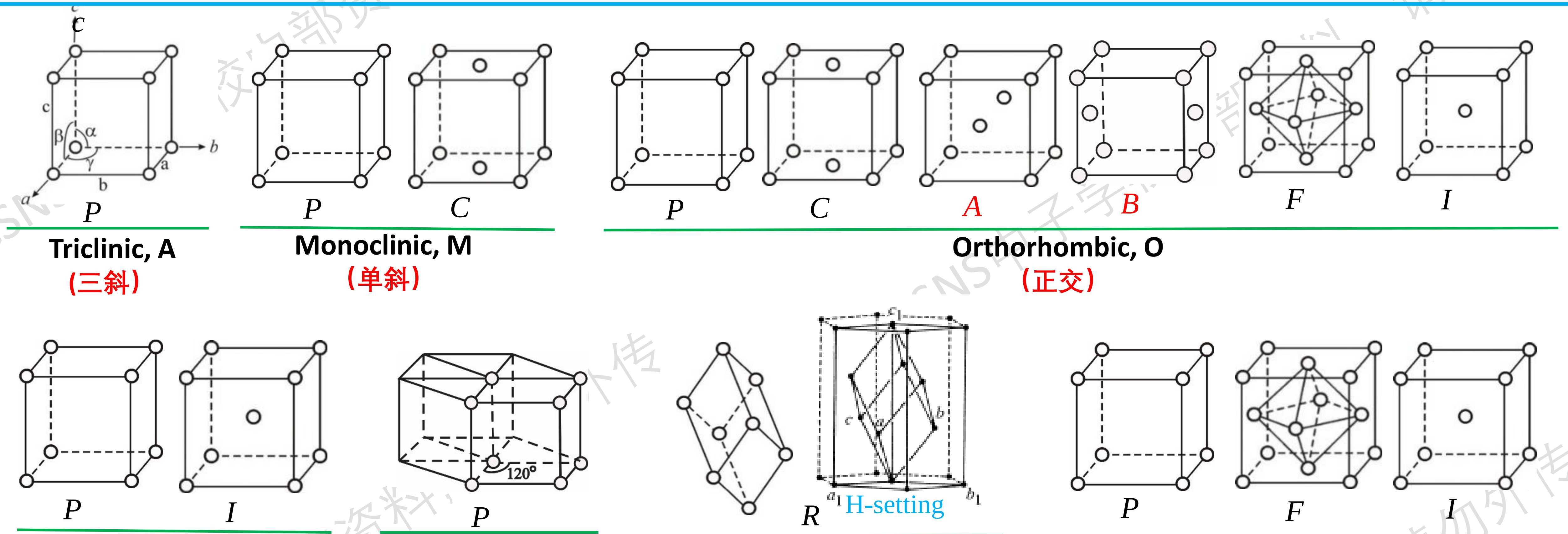
Lattice

The 14 crystal Bravais lattices

P （点阵类型）

$\boxed{P}bcn$ D_{2h}^{14} mmm Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$



Triclinic, A
（三斜）

Monoclinic, M
（单斜）

Orthorhombic, O
（正交）

Tetragonal, T
（四方）

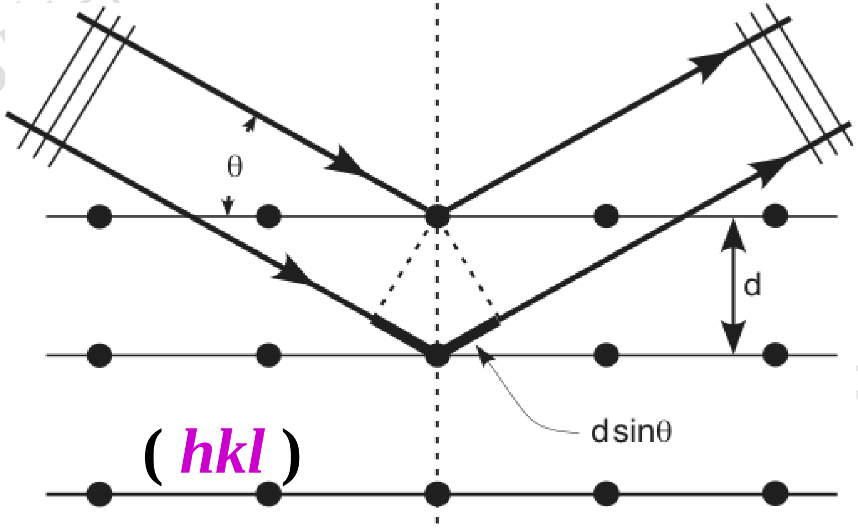
Hexagonal, H
（六方）

Trigonal, R
（三方）

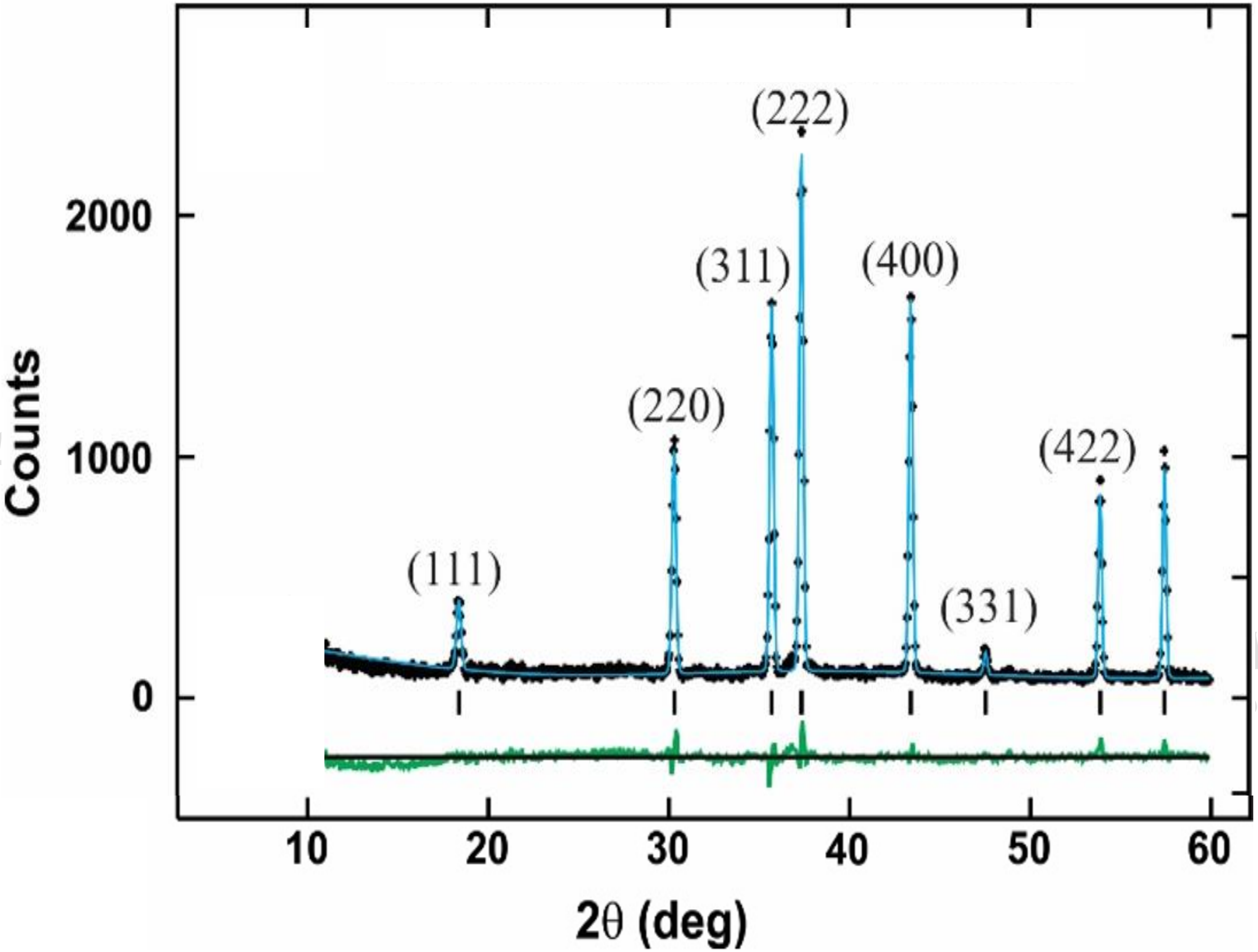
Cubic, C
（立方）

三维晶格中的14种Bravais点阵。由于七个晶系中对晶胞形状的定义不同，各个晶系中可能有的点阵类型也不一样。在三斜晶系中只可能有一种简单点阵*P*，而正交晶系中可能有 *P*, *C*, *F*, *I* 共4种点阵。

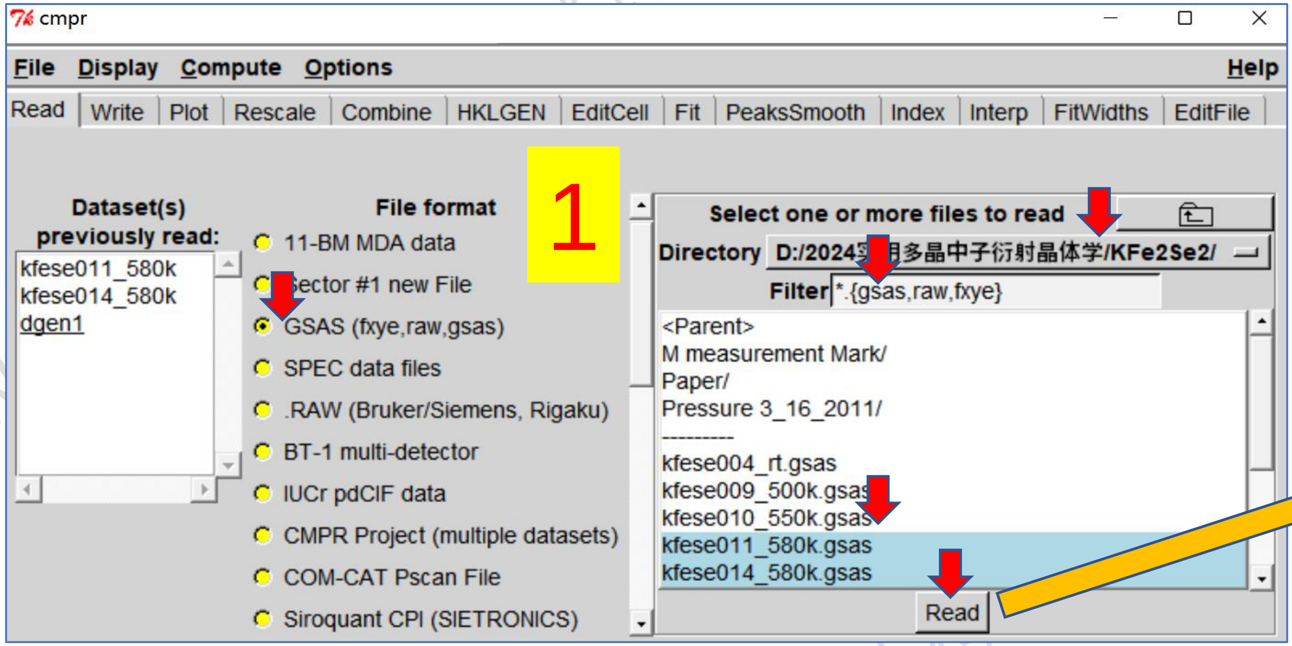
Bragg equation & reflection index



Bragg equation: $2d\sin\theta = n\lambda$



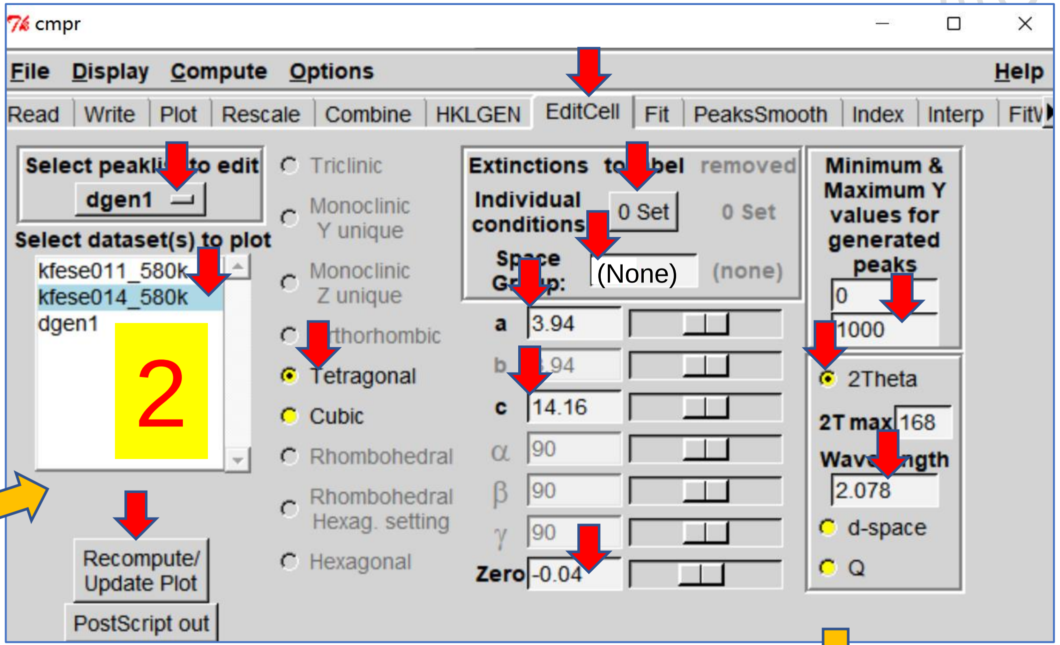
运用cmpr进行衍射峰指标化确定晶系和晶胞参数



Dataset(s) previously read:
kfese011_580k
kfese014_580k
dgen1

File format
○ 11-BM MDA data
○ Sector #1 new File
● GSAS (fxye,raw,gsas)
○ SPEC data files
○ .RAW (Bruker/Siemens, Rigaku)
○ BT-1 multi-detector
○ IUCr pdCIF data
○ CMPR Project (multiple datasets)
○ COM-CAT Pscan File
○ Siroquant CPI (SIETRONICS)

Select one or more files to read
Directory D:/2024 多晶中子衍射晶体学/KFe2Se2/
Filter *.{gsas,raw,fxye}
<Parent>
M measurement Mark/
Paper/
Pressure 3_16_2011/
----
kfese004_rt.gsas
kfese009_500k.gsas
kfese010_550k.gsas
kfese011_580k.gsas
kfese014_580k.gsas



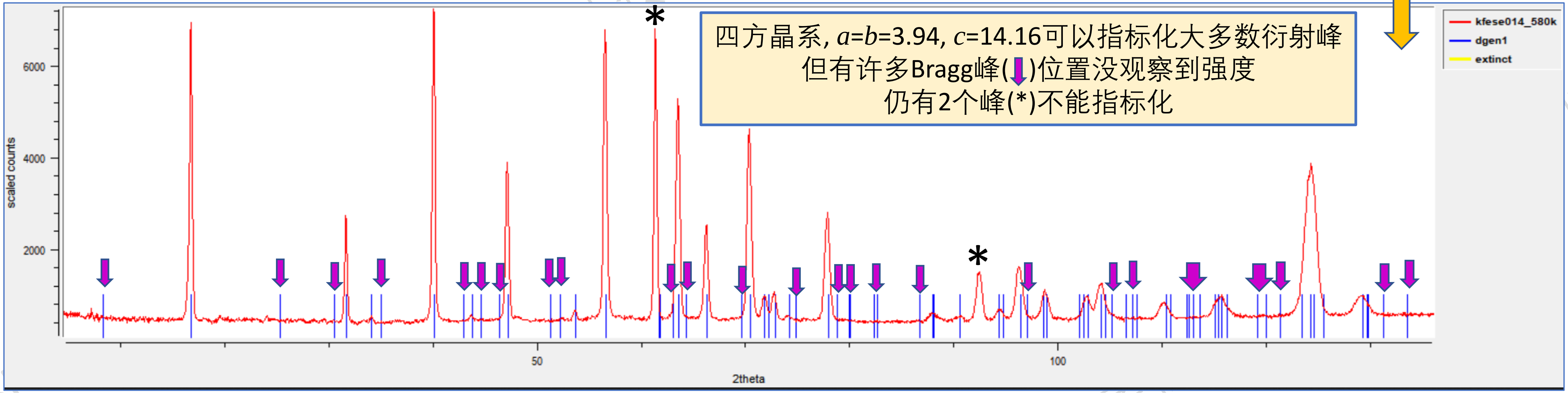
Select peaklist to edit: dgen1

Select dataset(s) to plot:
kfese011_580k
kfese014_580k
dgen1

○ Triclinic
○ Monoclinic Y unique
○ Monoclinic Z unique
○ Orthorhombic
● Tetragonal
○ Cubic
○ Rhombohedral
○ Rhombohedral Hexag. setting
○ Hexagonal

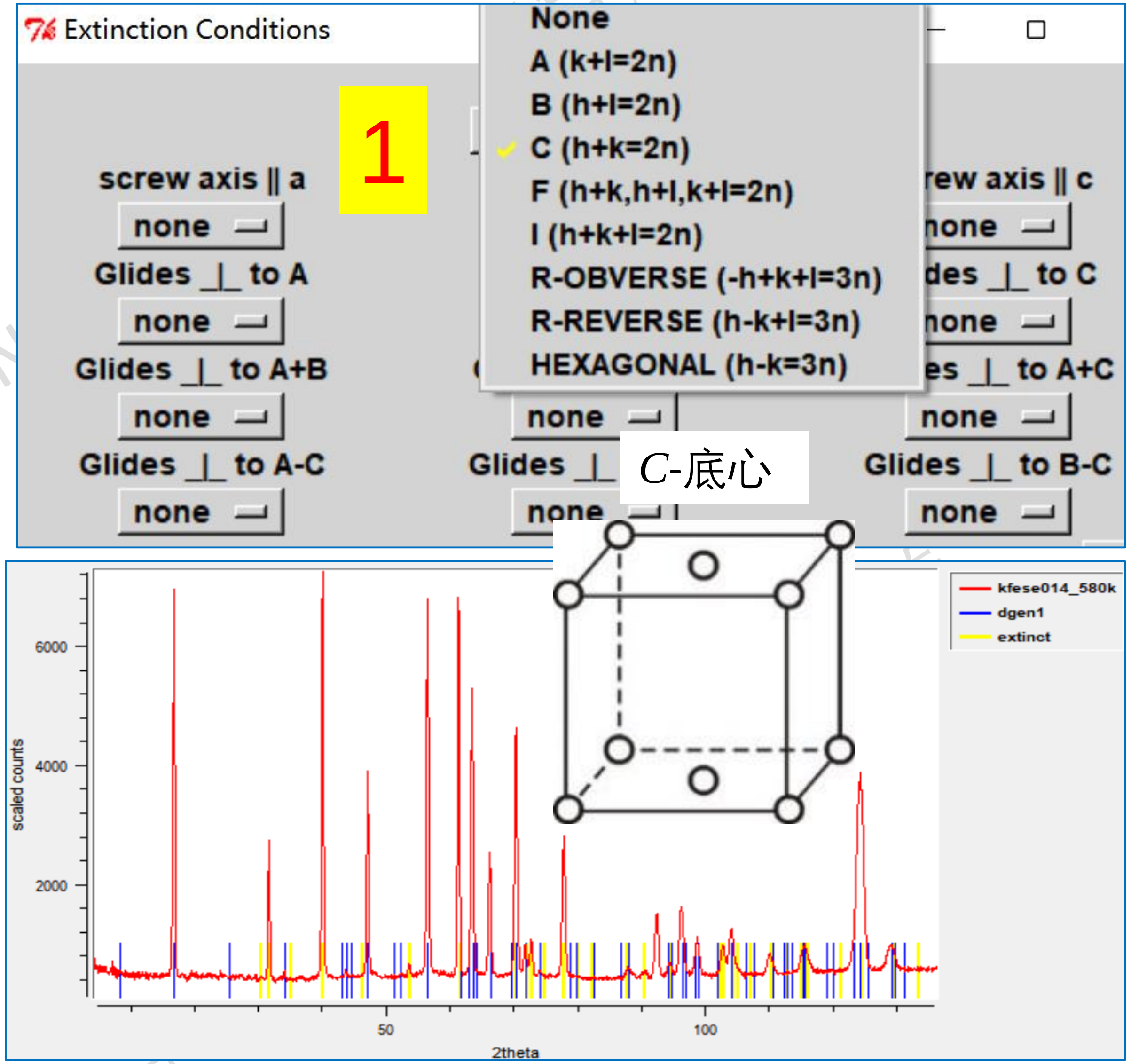
Extinctions to label removed
Individual conditions: 0 Set 0 Set
Space Group: (None) (none)
a 3.94
b 3.94
c 14.16
α 90
β 90
γ 90
Zero -0.04

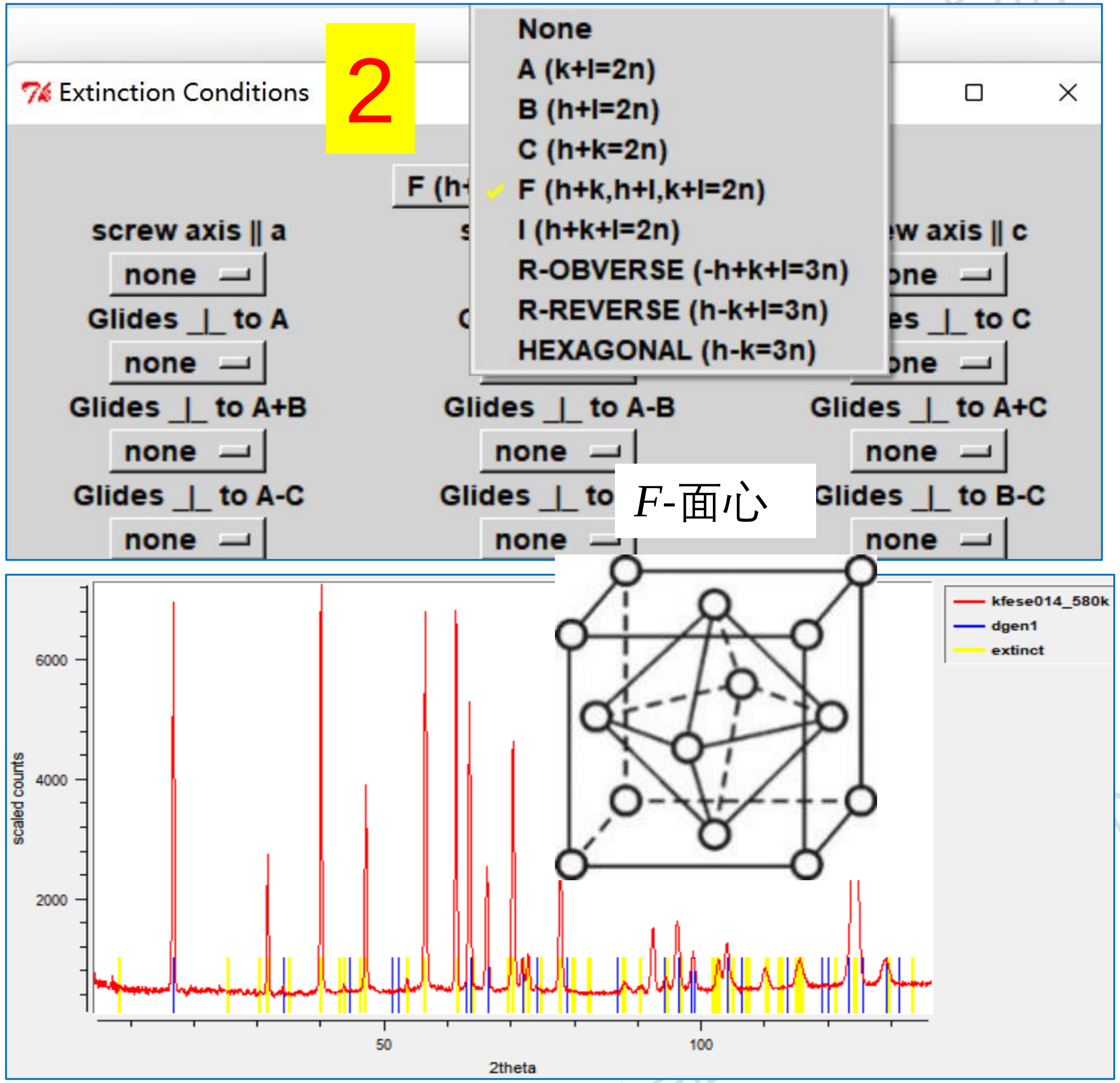
Minimum & Maximum Y values for generated peaks
0
1000
● 2Theta
2T max 168
Wavelength 2.078
○ d-space
○ Q



四方晶系, *a*=*b*=3.94, *c*=14.16可以指标化大多数衍射峰
但有许多Bragg峰(↓)位置没观察到强度
仍有2个峰(*)不能指标化

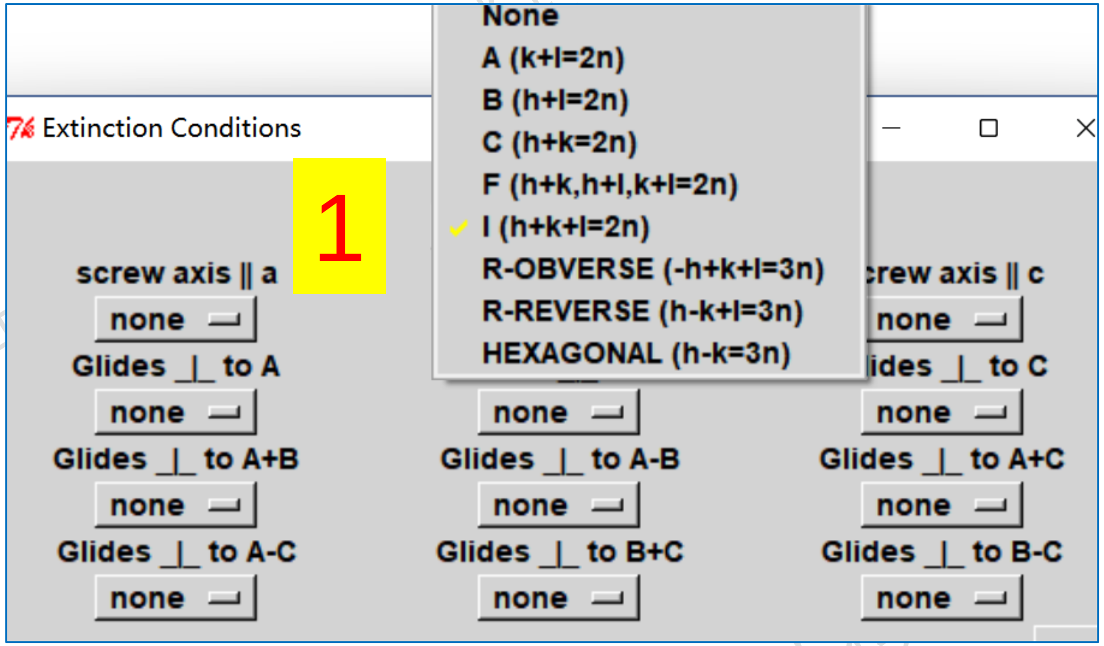
确定点阵





C-底心和*F*-面心点阵都不符合实验数据, 而且四方晶系不能有*C*-底心和*F*-面心点阵, 只能有简单(*P*)和体心(*I*)点阵.

体心(*I*)点阵圆满指标化实验数据



Extinction Conditions

1

screw axis || a: none

screw axis || c: none

Glides ⊥ to A: none

Glides ⊥ to C: none

Glides ⊥ to A+B: none

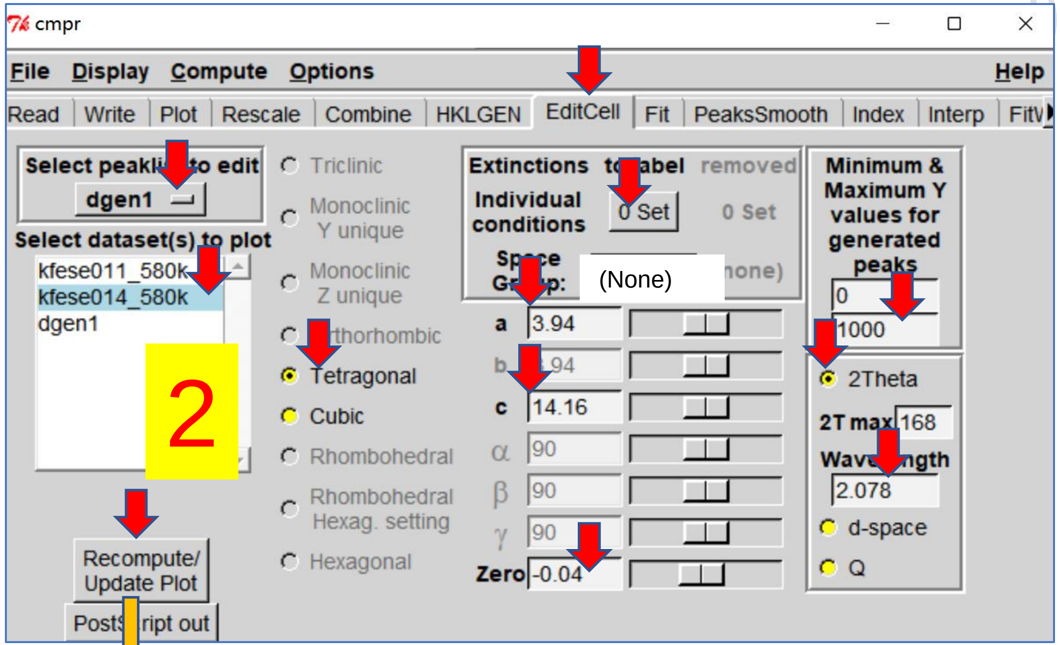
Glides ⊥ to A-B: none

Glides ⊥ to A+C: none

Glides ⊥ to A-C: none

Glides ⊥ to B+C: none

Glides ⊥ to B-C: none



cmpr

2

Select peaklist to edit: dgen1

Select dataset(s) to plot: kfese011_580k, kfese014_580k, dgen1

○ Triclinic
○ Monoclinic Y unique
○ Monoclinic Z unique
○ Orthorhombic
● Tetragonal
○ Cubic
○ Rhombohedral
○ Rhombohedral Hexag. setting
○ Hexagonal

Extinctions to label removed

Individual conditions: 0 Set 0 Set

Space Group: (None) (None)

a 3.94

b 3.94

c 14.16

α 90

β 90

γ 90

Zero -0.04

Minimum & Maximum Y values for generated peaks: 0 1000

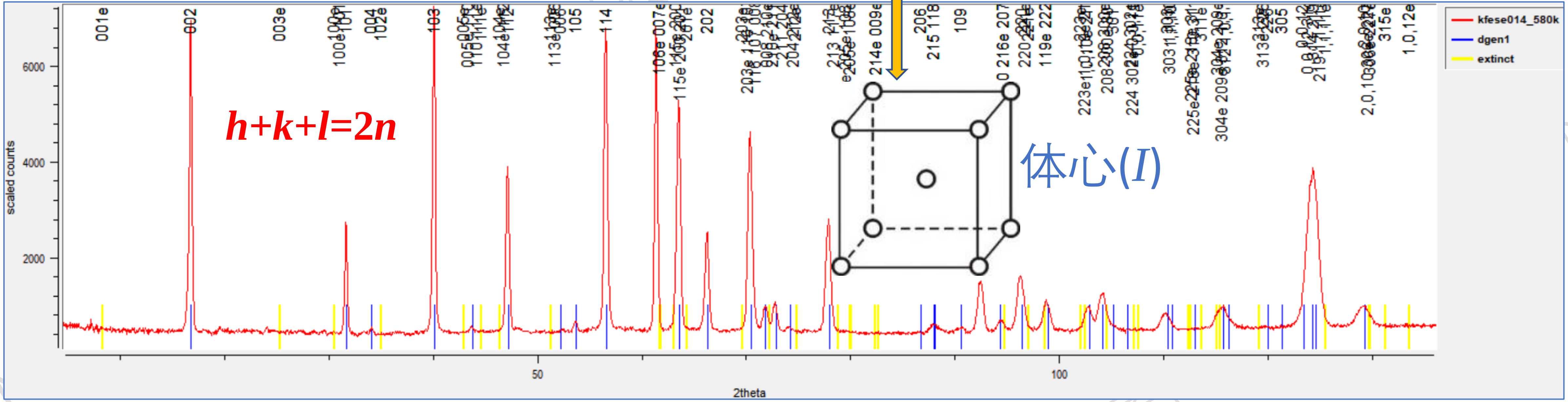
● 2Theta

2T max 168

Wavelength 2.078

○ d-space

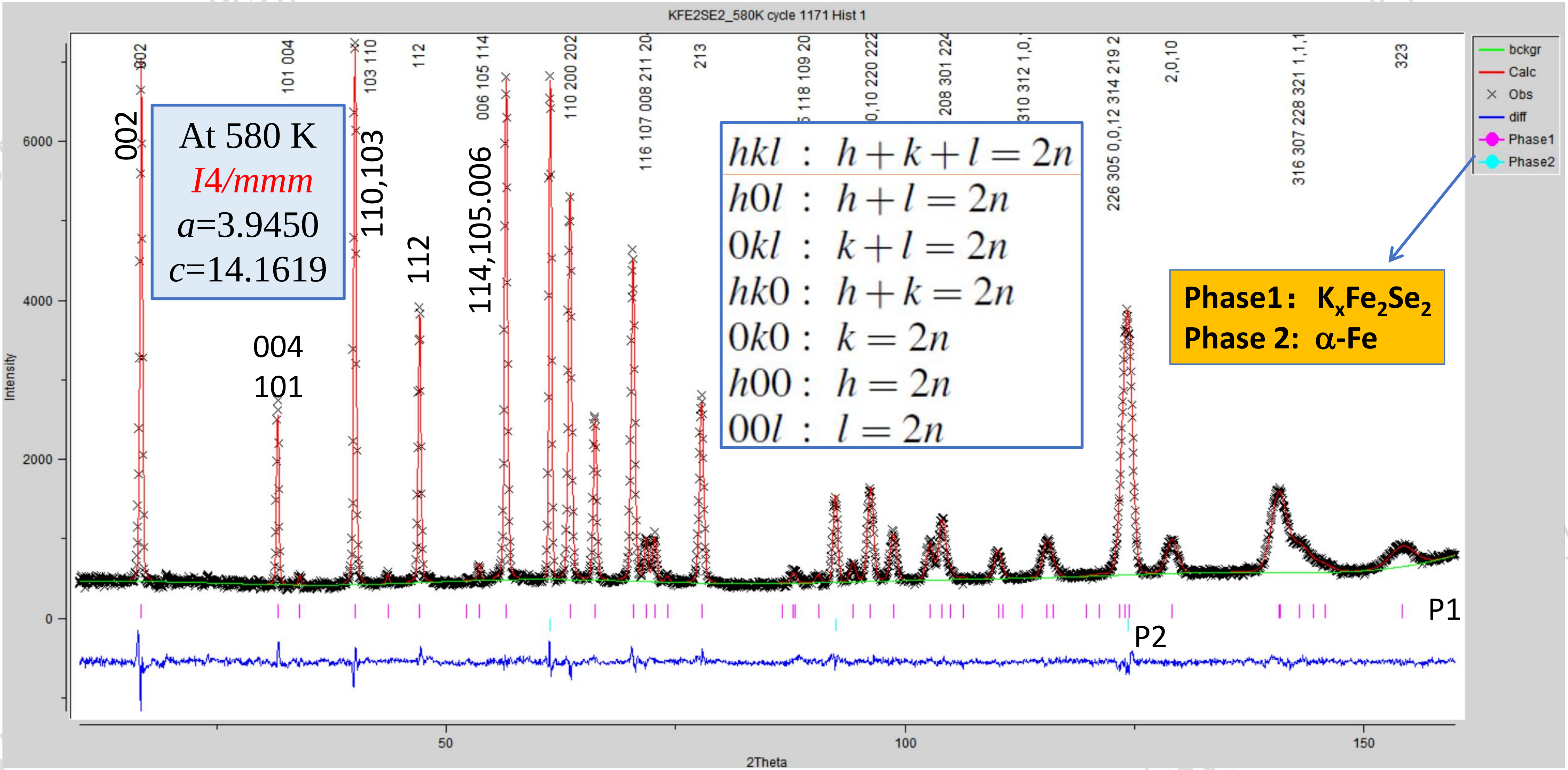
○ Q



h+k+l=2n

体心(*I*)

结构精化结果



At 580 K
I4/mmm
a=3.9450
c=14.1619

$hkl\ :\ h+k+l=2n$
$h0l\ :\ h+l=2n$
$0kl\ :\ k+l=2n$
$hk0\ :\ h+k=2n$
$0k0\ :\ k=2n$
$h00\ :\ h=2n$
$00l\ :\ l=2n$

Phase1： $K_xFe_2Se_2$
Phase 2: α-Fe

微观对称要素

（部分宏观对称元素+平移操作的对称元素，有衍射消光）

(1) 点阵：平移

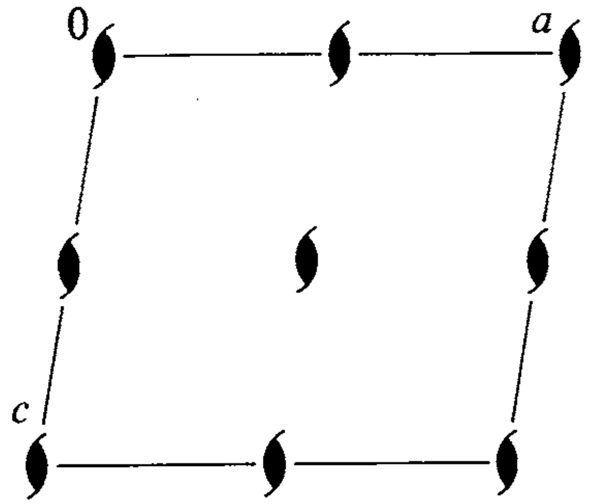
(2) 滑移面：*a*, *b*, *c*, *e*, *n*, *d*

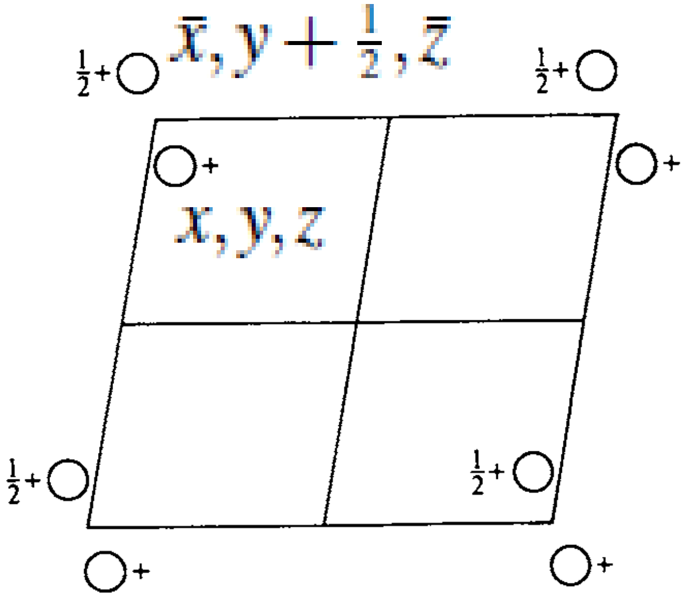
(3) 螺旋轴:2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5

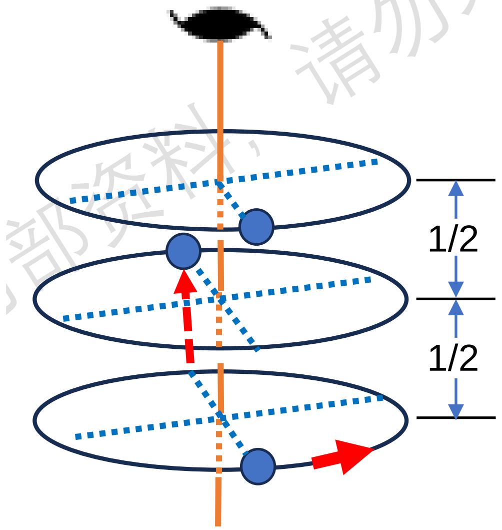
$P2_1$

Unique axes b

等效点数：2

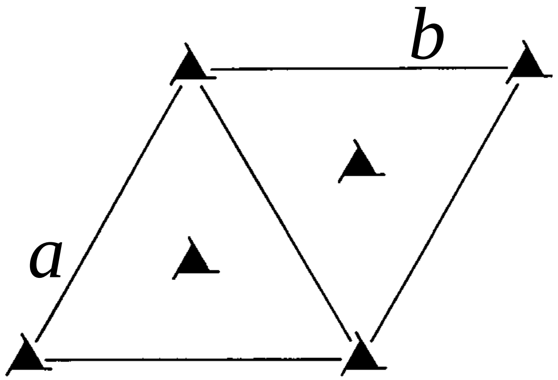


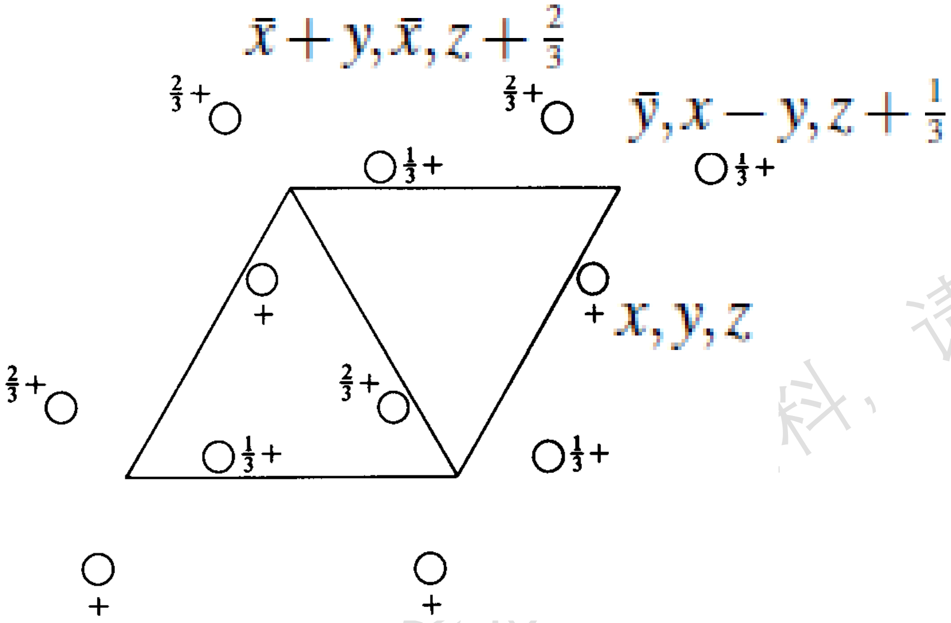




$P3_1$

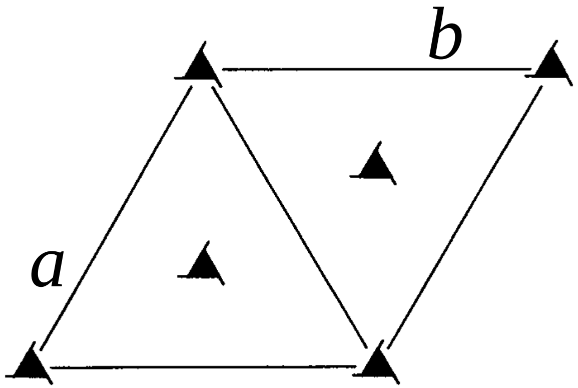
等效点数：3

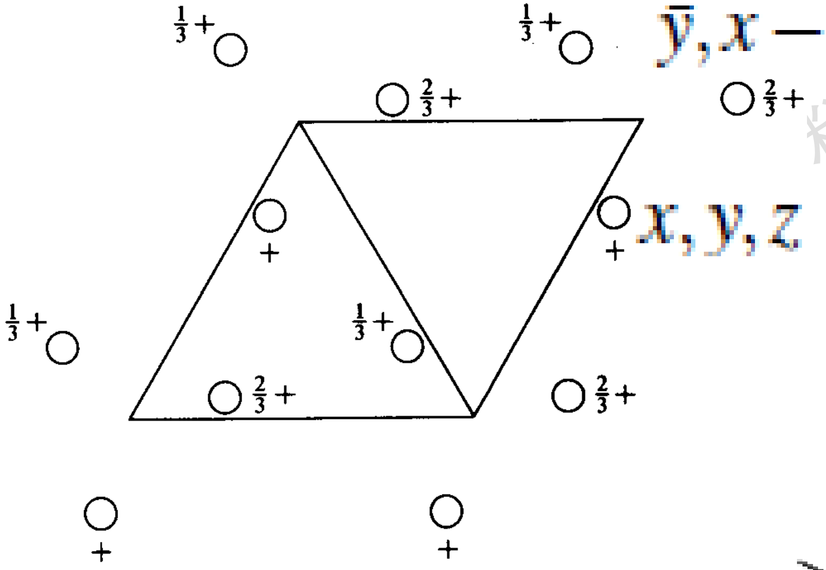




$P3_2$

等效点数：3





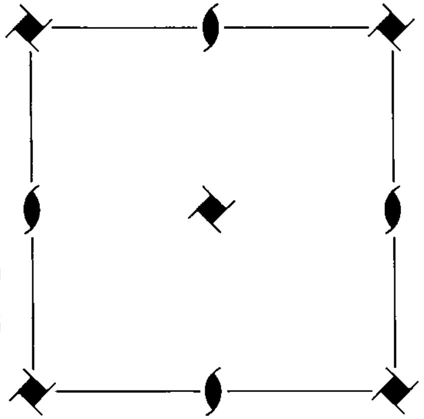
$\bar{x}+y, \bar{x}, z+\frac{1}{3}$

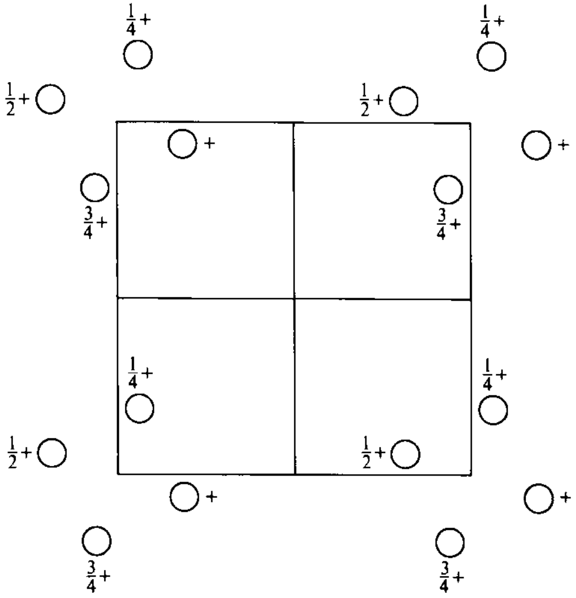
$\bar{y}, x-y, z+\frac{2}{3}$

x, y, z

$P4_1$

等效点数：4



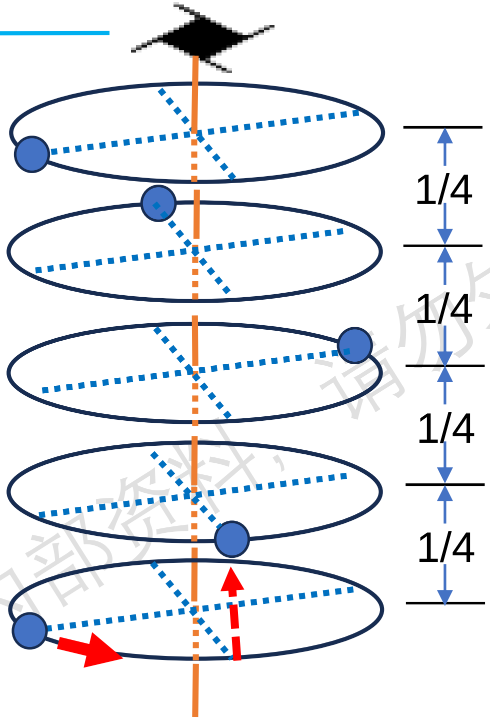


(1) x, y, z

(2) $\bar{x}, \bar{y}, z+\frac{1}{2}$

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

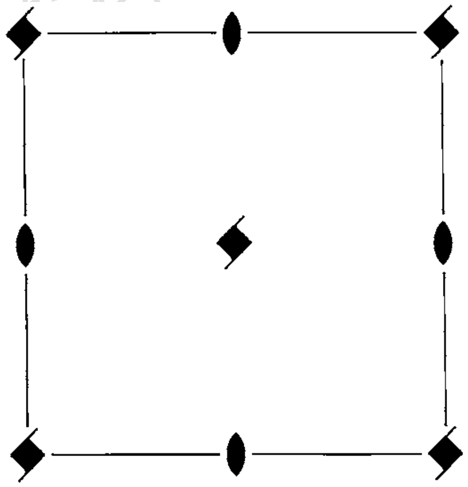
(4) $y, \bar{x}, z+\frac{3}{4}$

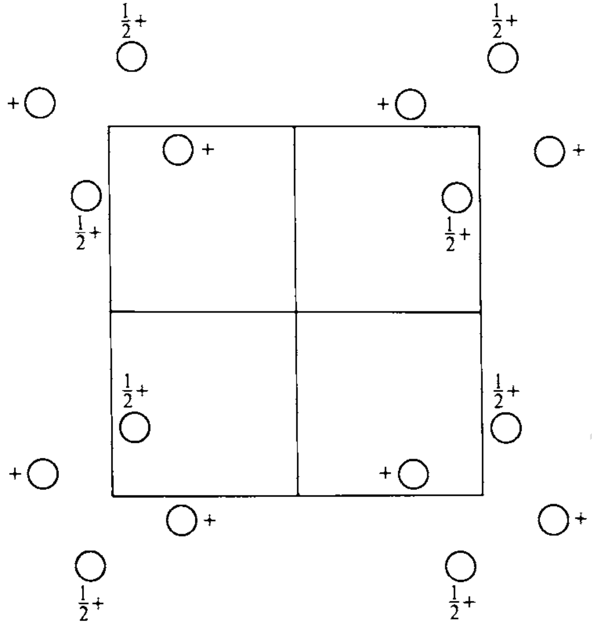


$P4_2$

等效点数：

4





(1) x, y, z

(2) $\bar{x}, \bar{y}, z$

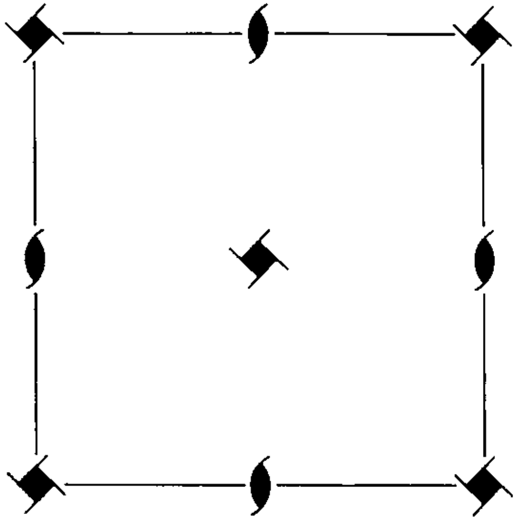
(3) $\bar{y}, x, z+\frac{1}{2}$

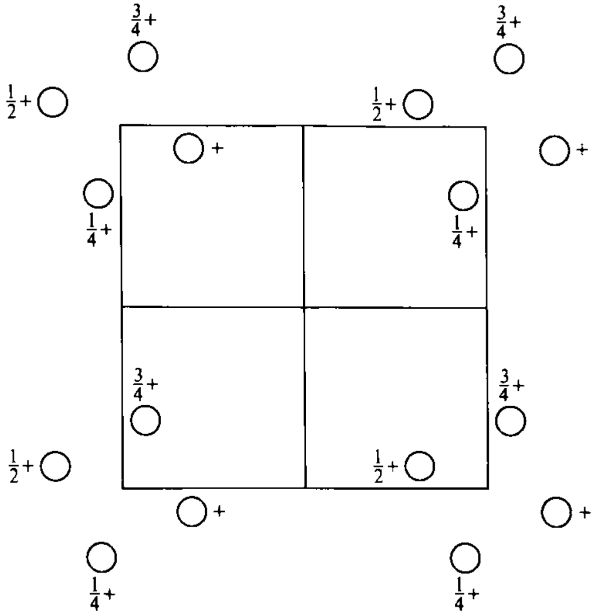
(4) $y, \bar{x}, z+\frac{1}{2}$

$P4_3$

等效点数：

4





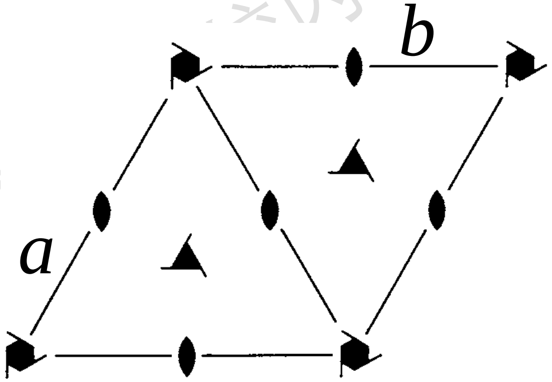
(1) x, y, z

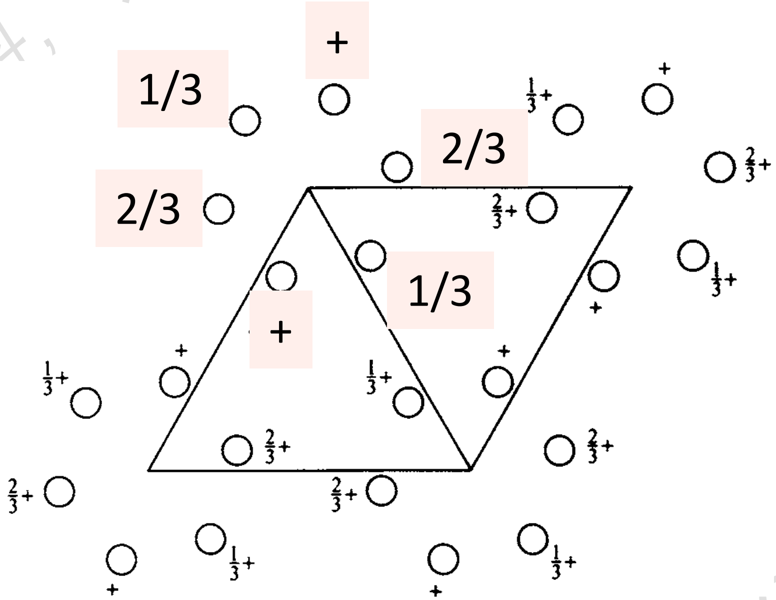
(2) $\bar{x}, \bar{y}, z+\frac{1}{2}$

(3) $\bar{y}, x, z+\frac{3}{4}$

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

$P6_2$





等效点数: 6

(1) x,y,z

(2) $\bar{y},x-y,z+\frac{2}{3}$

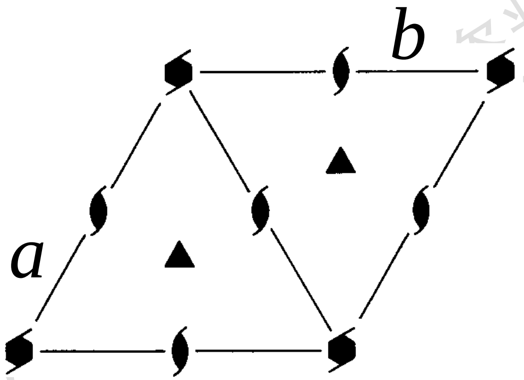
(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$

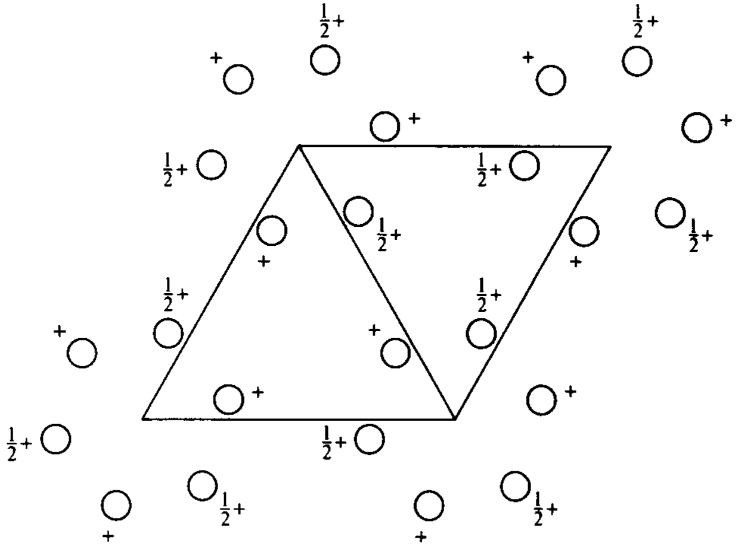
(4) $\bar{x},\bar{y},z$

(5) $y,\bar{x}+y,z+\frac{2}{3}$

(6) $x-y,x,z+\frac{1}{3}$

$P6_3$





等效点数: 6

(1) x,y,z

(2) $\bar{y},x-y,z$

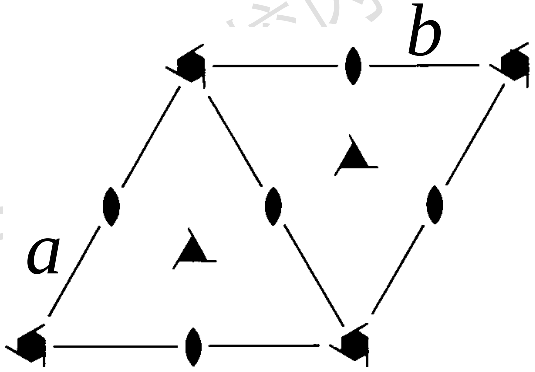
(3) $\bar{x}+y,\bar{x},z$

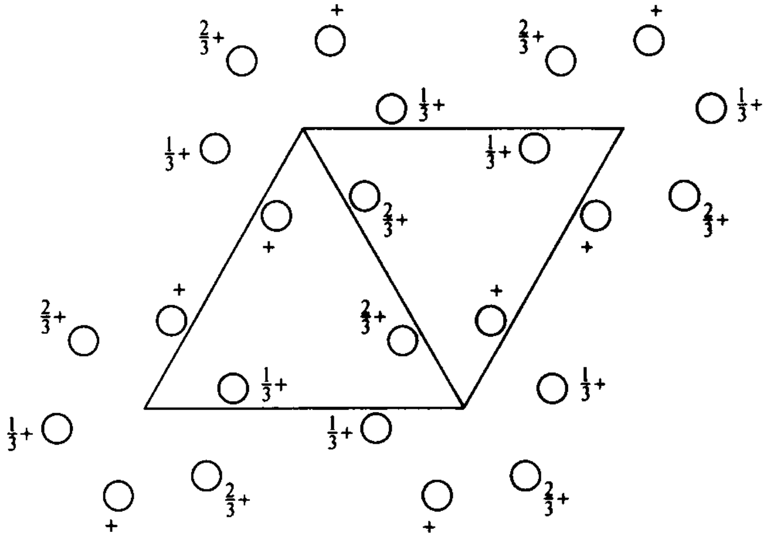
(4) $\bar{x},\bar{y},z+\frac{1}{2}$

(5) $y,\bar{x}+y,z+\frac{1}{2}$

(6) $x-y,x,z+\frac{1}{2}$

$P6_4$





等效点数: 6

(1) x,y,z

(2) $\bar{y},x-y,z+\frac{1}{3}$

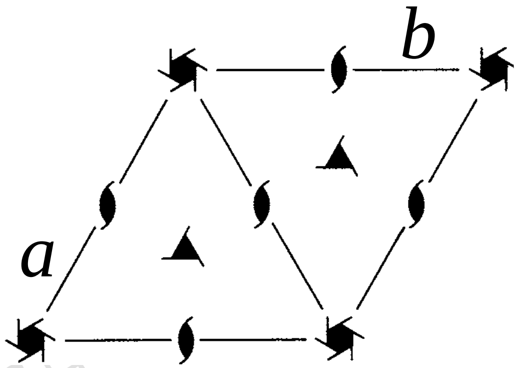
(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$

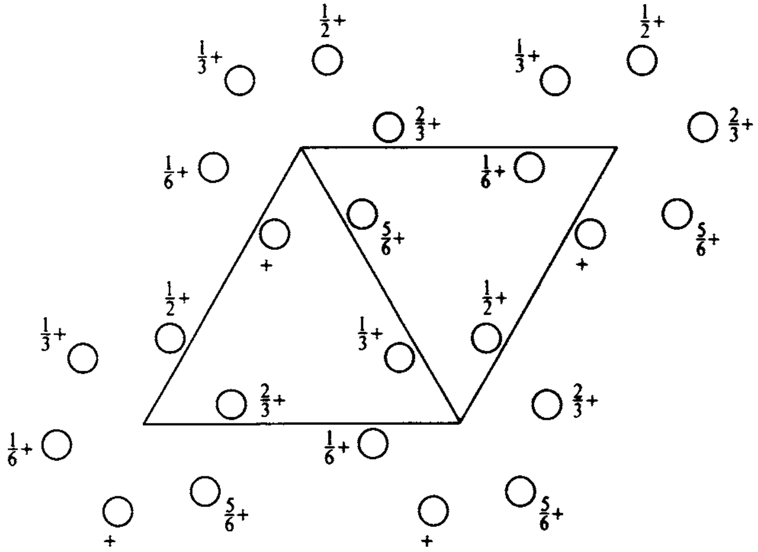
(4) $\bar{x},\bar{y},z$

(5) $y,\bar{x}+y,z+\frac{1}{3}$

(6) $x-y,x,z+\frac{2}{3}$

$P6_5$





等效点数: 6

(1) x,y,z

(2) $\bar{y},x-y,z+\frac{2}{3}$

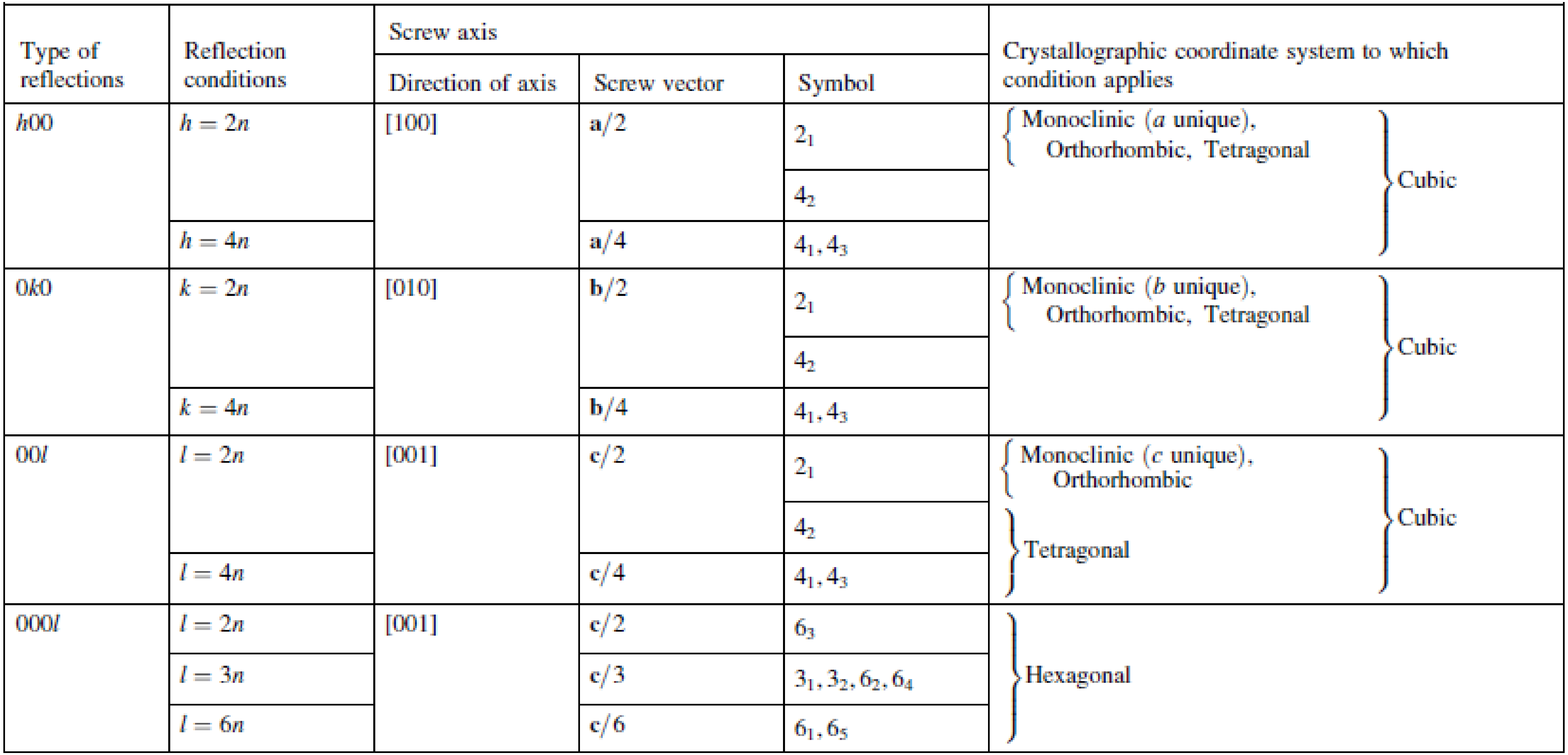
(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$

(4) $\bar{x},\bar{y},z+\frac{1}{2}$

(5) $y,\bar{x}+y,z+\frac{1}{6}$

(6) $x-y,x,z+\frac{5}{6}$

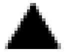
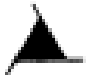
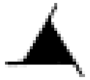
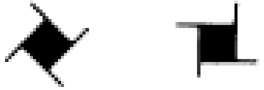
Zonal and serial reflection conditions for white screw axes



Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies	
		Direction of axis	Screw vector	Symbol		
$h00$	$h = 2n$	[100]	**a**/2	2_1	Monoclinic (*a* unique), Orthorhombic, Tetragonal	Cubic
				4_2		
	$h = 4n$		**a**/4	$4_1, 4_3$		
$0k0$	$k = 2n$	[010]	**b**/2	2_1	Monoclinic (*b* unique), Orthorhombic, Tetragonal	Cubic
				4_2		
	$k = 4n$		**b**/4	$4_1, 4_3$		
$00l$	$l = 2n$	[001]	**c**/2	2_1	Monoclinic (*c* unique), Orthorhombic	Cubic
				4_2	Tetragonal	
	$l = 4n$		**c**/4	$4_1, 4_3$		
$000l$	$l = 2n$	[001]	**c**/2	6_3	Hexagonal	
	$l = 3n$		**c**/3	$3_1, 3_2, 6_2, 6_4$		
	$l = 6n$		**c**/6	$6_1, 6_5$		

*International tables for crystallography, Vol. A, 29 (1992).

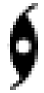
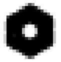
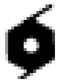
Symmetry axes normal to the plane of projection and symmetry points in the plane of the figure.

Symmetry axes or symmetry point	Graphical symbol	Translation	
Identity	None	None	1
Twofold rotation axis Twofold rotation point (two dimensions)		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Threefold rotation axis Threefold rotation point (two dimensions)		None	3
Threefold screw axis: '3 sub 1'		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'		$\frac{2}{3}$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)		None	4 (2)
Fourfold screw axis: '4 sub 1'		$\frac{1}{4}$	4_1 (2_1)
Fourfold screw axis: '4 sub 2'		$\frac{1}{2}$	4_2 (2)
Fourfold screw axis: '4 sub 3'		$\frac{3}{4}$	4_3 (2_1)

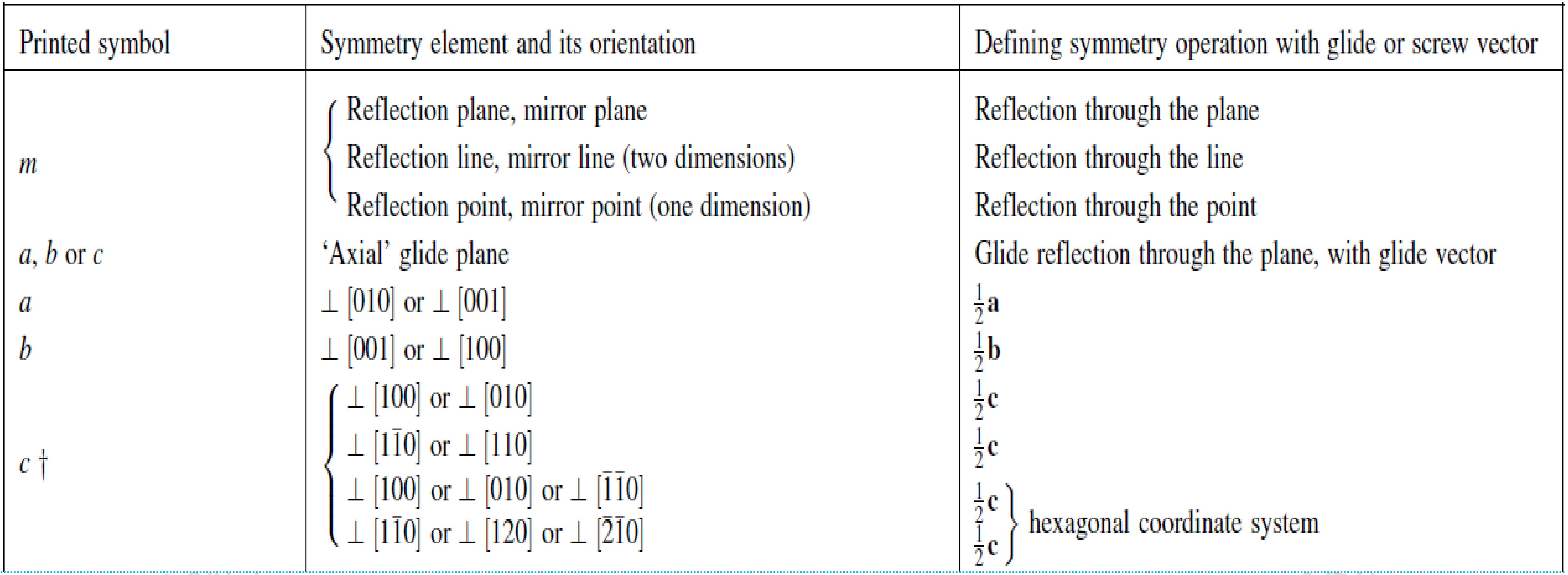
Symmetry axes normal to the plane of projection and symmetry points in the plane of the figure.

Symmetry axes or symmetry point	Graphical symbol	Translation	Symbol
Sixfold rotation axis Sixfold rotation point (two dimensions)	⬢	None	6 (3,2)
Sixfold screw axis: '6 sub 1'	⬢	$\frac{1}{6}$	6_1 $(3_1, 2_1)$
Sixfold screw axis: '6 sub 2'	⬢	$\frac{1}{3}$	6_2 $(3_2, 2)$
Sixfold screw axis: '6 sub 3'	⬢	$\frac{1}{2}$	6_3 $(3, 2_1)$
Sixfold screw axis: '6 sub 4'	⬢	$\frac{2}{3}$	6_4 $(3_1, 2)$
Sixfold screw axis: '6 sub 5'	⬢	$\frac{5}{6}$	6_5 $(3_2, 2_1)$
Centre of symmetry, inversion centre: '1 bar' Reflection point, mirror point (one dimension)	○	None	$\bar{1}$
Inversion axis: '3 bar'	▲	None	$\bar{3}$ $(3, \bar{1})$
Inversion axis: '4 bar'	◆ ◪	None	$\bar{4}$ (2)
Inversion axis: '6 bar'	▲	None	$\bar{6} \equiv 3/m$

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

Symmetry axes or symmetry point	Graphical symbol	Translation	Symbol
Twofold rotation axis with centre of symmetry		None	$2/m$ ($\bar{1}$)
Twofold screw axis with centre of symmetry		$\frac{1}{2}$	$2_1/m$ ($\bar{1}$)
Fourfold rotation axis with centre of symmetry		None	$4/m$ ($\bar{4}, 2, \bar{1}$)
'4 sub 2' screw axis with centre of symmetry		$\frac{1}{2}$	$4_2/m$ ($\bar{4}, 2, \bar{1}$)
Sixfold rotation axis with centre of symmetry		None	$6/m$ ($\bar{6}, \bar{3}, 3, 2, \bar{1}$)
'6 sub 3' screw axis with centre of symmetry		$\frac{1}{2}$	$6_3/m$ ($\bar{6}, \bar{3}, 3, 2_1, \bar{1}$)

1.3.1. Printed symbols for symmetry elements and for the corresponding symmetry operations in one, two and three dimensions.

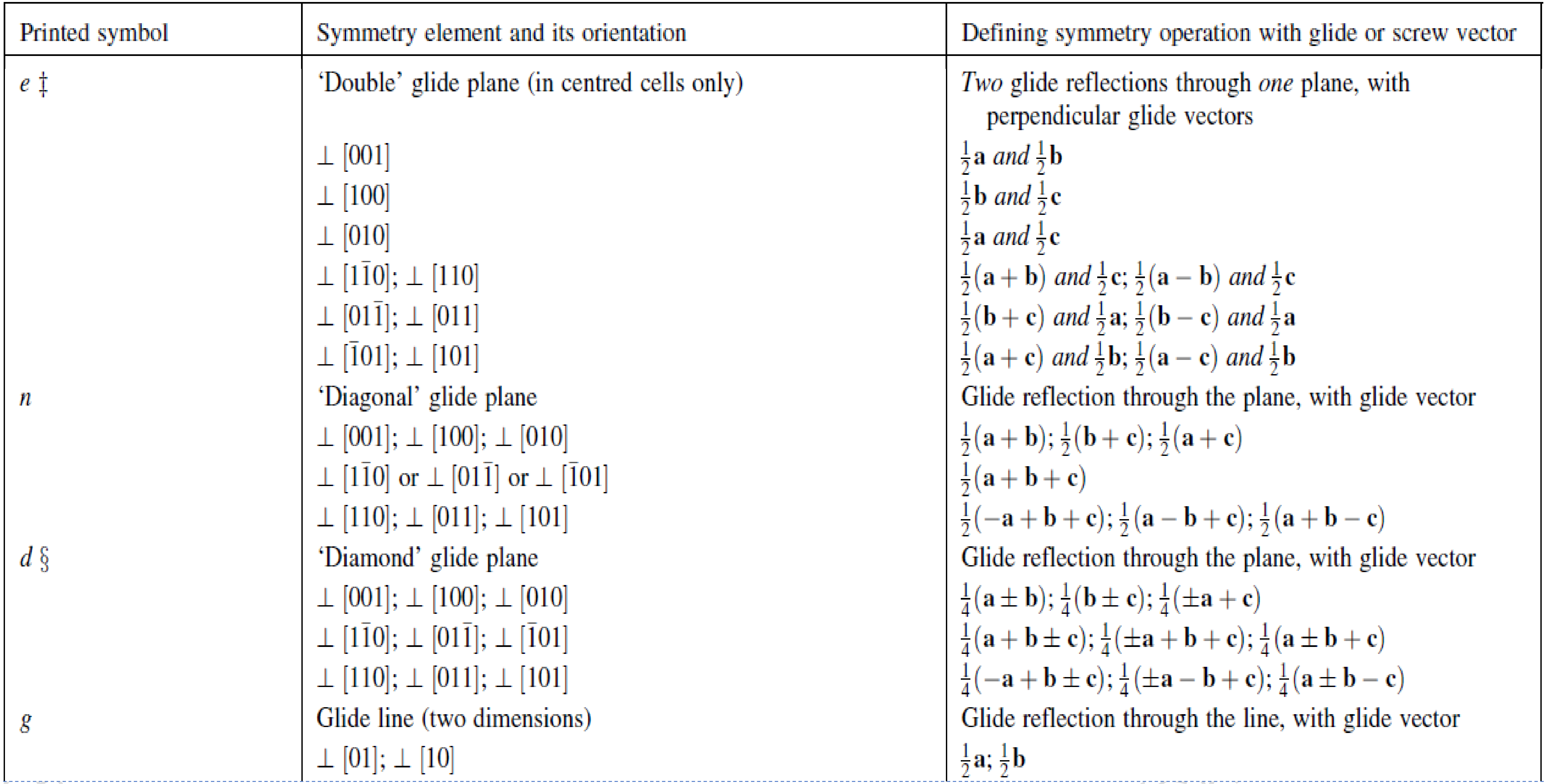


Printed symbol	Symmetry element and its orientation	Defining symmetry operation with glide or screw vector
m	Reflection plane, mirror plane Reflection line, mirror line (two dimensions) Reflection point, mirror point (one dimension)	Reflection through the plane Reflection through the line Reflection through the point
a, *b* or *c*	'Axial' glide plane	Glide reflection through the plane, with glide vector
a	$\perp [010]$ or $\perp [001]$	$\frac{1}{2}\mathbf{a}$
b	$\perp [001]$ or $\perp [100]$	$\frac{1}{2}\mathbf{b}$
c †	$\perp [100]$ or $\perp [010]$	$\frac{1}{2}\mathbf{c}$
	$\perp [1\bar{1}0]$ or $\perp [110]$	$\frac{1}{2}\mathbf{c}$
	$\perp [100]$ or $\perp [010]$ or $\perp [\bar{1}\bar{1}0]$	$\frac{1}{2}\mathbf{c}$ hexagonal coordinate system
	$\perp [1\bar{1}0]$ or $\perp [120]$ or $\perp [\bar{2}\bar{1}0]$	$\frac{1}{2}\mathbf{c}$

宏观对称元素： 对称面*m*和对称轴1, 2, 3, 4, 6, $\bar{1}$, $\bar{3}$, $\bar{4}$, $\bar{6}$， 即 没有平移操作的对称元素。

微观对称元素：滑移面*a, b, c, n, d* 和螺旋轴2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5等， 即宏“观对称元素+平移” 操作。

1.3.1 *continue*

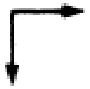
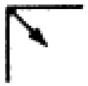
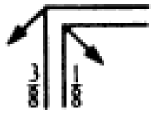


Printed symbol	Symmetry element and its orientation	Defining symmetry operation with glide or screw vector
e ‡	'Double' glide plane (in centred cells only)	*Two* glide reflections through *one* plane, with perpendicular glide vectors
	$\perp [001]$	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{b}$
	$\perp [100]$	$\frac{1}{2}\mathbf{b}$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp [010]$	$\frac{1}{2}\mathbf{a}$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp [1\bar{1}0]; \perp [110]$	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$; $\frac{1}{2}(\mathbf{a}-\mathbf{b})$ *and* $\frac{1}{2}\mathbf{c}$
	$\perp [01\bar{1}]; \perp [011]$	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$; $\frac{1}{2}(\mathbf{b}-\mathbf{c})$ *and* $\frac{1}{2}\mathbf{a}$
	$\perp [\bar{1}01]; \perp [101]$	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$; $\frac{1}{2}(\mathbf{a}-\mathbf{c})$ *and* $\frac{1}{2}\mathbf{b}$
n	'Diagonal' glide plane	Glide reflection through the plane, with glide vector
	$\perp [001]; \perp [100]; \perp [010]$	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$; $\frac{1}{2}(\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}+\mathbf{c})$
	$\perp [1\bar{1}0]$ or $\perp [01\bar{1}]$ or $\perp [\bar{1}01]$	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
	$\perp [110]; \perp [011]; \perp [101]$	$\frac{1}{2}(-\mathbf{a}+\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}-\mathbf{b}+\mathbf{c})$; $\frac{1}{2}(\mathbf{a}+\mathbf{b}-\mathbf{c})$
d §	'Diamond' glide plane	Glide reflection through the plane, with glide vector
	$\perp [001]; \perp [100]; \perp [010]$	$\frac{1}{4}(\mathbf{a}\pm\mathbf{b})$; $\frac{1}{4}(\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}+\mathbf{c})$
	$\perp [1\bar{1}0]; \perp [01\bar{1}]; \perp [\bar{1}01]$	$\frac{1}{4}(\mathbf{a}+\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}+\mathbf{b}+\mathbf{c})$; $\frac{1}{4}(\mathbf{a}\pm\mathbf{b}+\mathbf{c})$
	$\perp [110]; \perp [011]; \perp [101]$	$\frac{1}{4}(-\mathbf{a}+\mathbf{b}\pm\mathbf{c})$; $\frac{1}{4}(\pm\mathbf{a}-\mathbf{b}+\mathbf{c})$; $\frac{1}{4}(\mathbf{a}\pm\mathbf{b}-\mathbf{c})$
g	Glide line (two dimensions)	Glide reflection through the line, with glide vector
	$\perp [01]; \perp [10]$	$\frac{1}{2}\mathbf{a}$; $\frac{1}{2}\mathbf{b}$

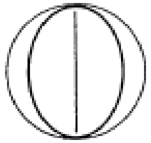
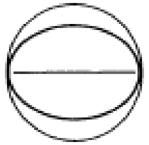
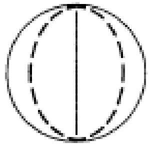
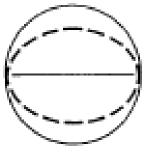
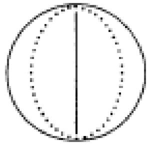
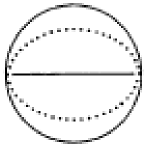
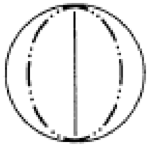
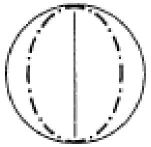
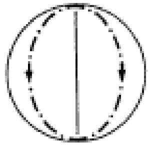
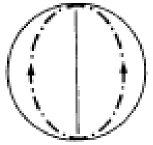
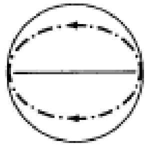
Symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)

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

Symmetry planes parallel to the plane of projection

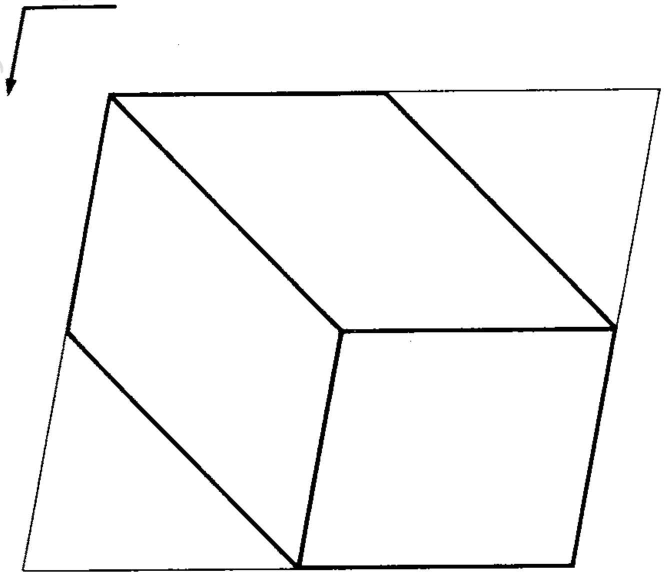
Symmetry plane	Graphical symbol*	Glide vector in units of lattice translation vectors parallel to the projection plane	Printed symbol
Reflection plane, mirror plane		None	*m*
'Axial' glide plane		$\frac{1}{2}$ lattice vector in the direction of the arrow	*a*, *b* or *c*
'Double' glide plane† (in centred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

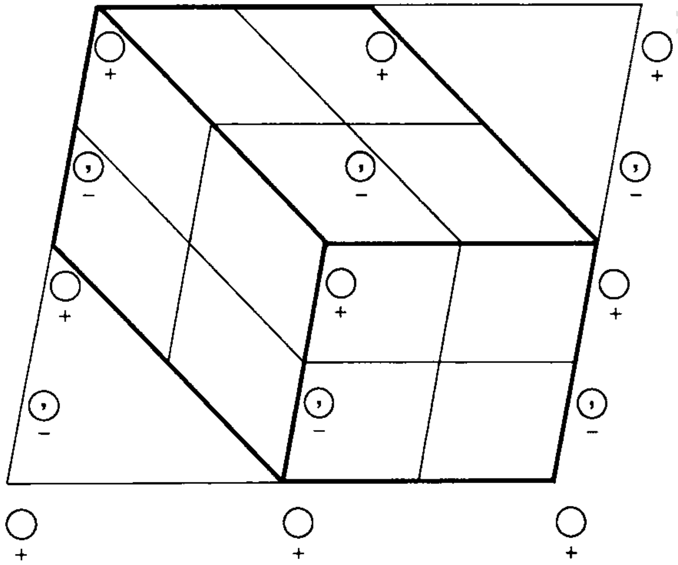
Symmetry planes inclined to the plane of projection (in cubic space groups of classes 43*m* and *m*3*m* only)

Symmetry plane	Graphical symbol* for planes normal to		Glide vector in units of lattice translation vectors for planes normal to		Printed symbol
	$[011]$ and $[01\bar{1}]$	$[101]$ and $[10\bar{1}]$	$[011]$ and $[01\bar{1}]$	$[101]$ and $[10\bar{1}]$	
Reflection plane, mirror plane			None	None	*m*
‘Axial’ glide plane			$\frac{1}{2}$ lattice vector along $[100]$	$\frac{1}{2}$ lattice vector along $[010]$	*a* or *b*
‘Axial’ glide plane			$\frac{1}{2}$ lattice vector along $[01\bar{1}]$ or along $[011]$	$\frac{1}{2}$ lattice vector along $[10\bar{1}]$ or along $[101]$	
‘Double’ glide plane† [in space groups $I\bar{4}3m$ (217) and $Im\bar{3}m$ (229) only]			*Two* glide vectors: $\frac{1}{2}$ along $[100]$ *and* $\frac{1}{2}$ along $[01\bar{1}]$ or $\frac{1}{2}$ along $[011]$	*Two* glide vectors: $\frac{1}{2}$ along $[010]$ *and* $\frac{1}{2}$ along $[10\bar{1}]$ or $\frac{1}{2}$ along $[101]$	*e*
‘Diagonal’ glide plane			*One* glide vector: $\frac{1}{2}$ along $[11\bar{1}]$ or along $[111]$‡	*One* glide vector: $\frac{1}{2}$ along $[11\bar{1}]$ or along $[111]$‡	*n*
‘Diamond’ glide plane¶ (pair of planes; in centred cells only)			$\frac{1}{2}$ along $[1\bar{1}1]$ or along $[111]$§	$\frac{1}{2}$ along $[\bar{1}11]$ or along $[111]$§	*d*
			$\frac{1}{2}$ along $[\bar{1}\bar{1}1]$ or along $[\bar{1}11]$§	$\frac{1}{2}$ along $[\bar{1}\bar{1}1]$ or along $[1\bar{1}1]$§	

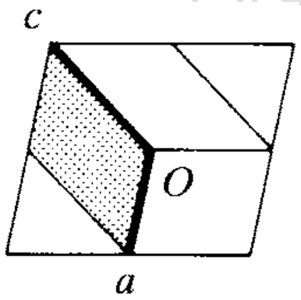
Pc

Unique axes b, Different cell choice



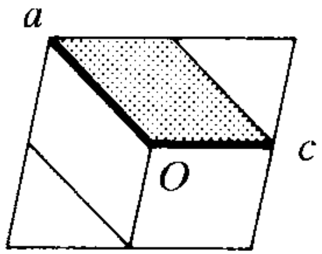


P 1 *a* 1



(1) x,y,z (2) $x+\frac{1}{2},\bar{y},z$

P 1 *n* 1

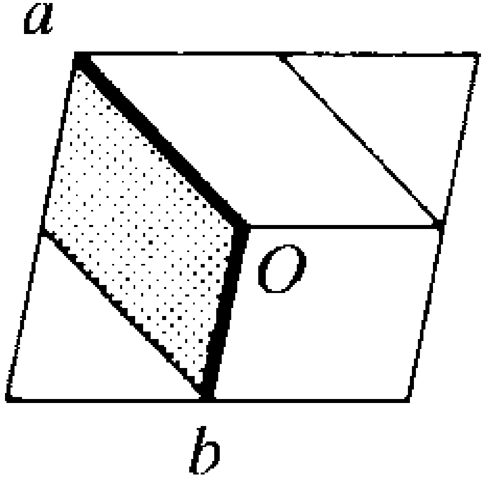


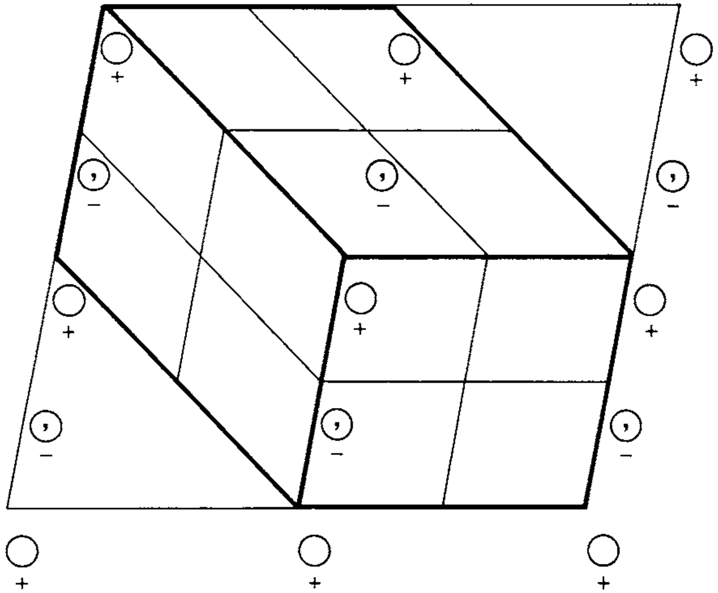
(1) x,y,z (2) $x+\frac{1}{2},\bar{y},z+\frac{1}{2}$

*P*11*b*

UNIQUE AXIS *c*

等效点数: 2





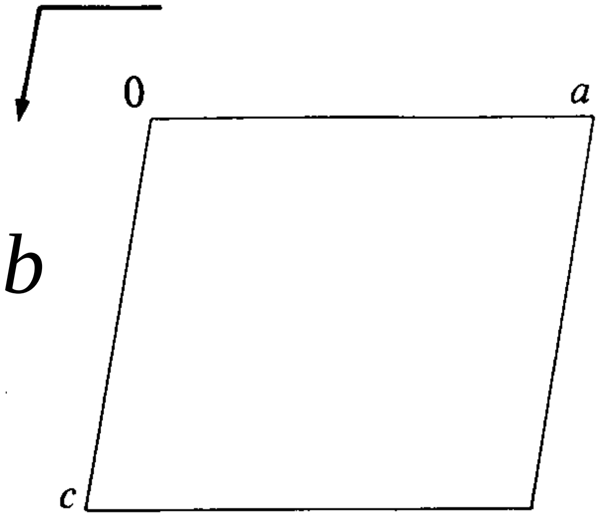
(1) x, y, z

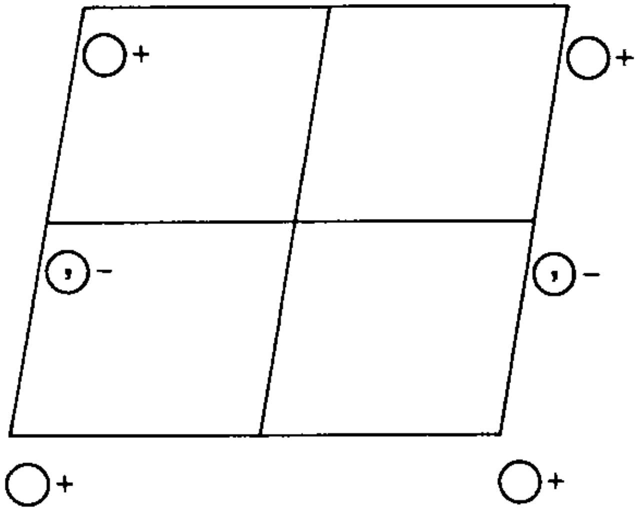
(2) $x, y+\frac{1}{2}, \bar{z}$

Pc

Unique axes b

等效点数: 2





(1) x, y, z

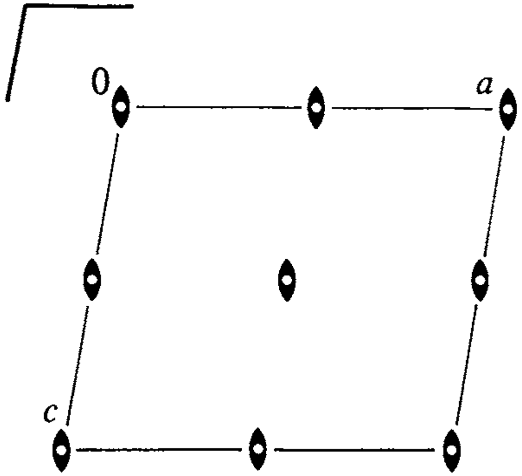
(2) $x, \bar{y}, z+\frac{1}{2}$

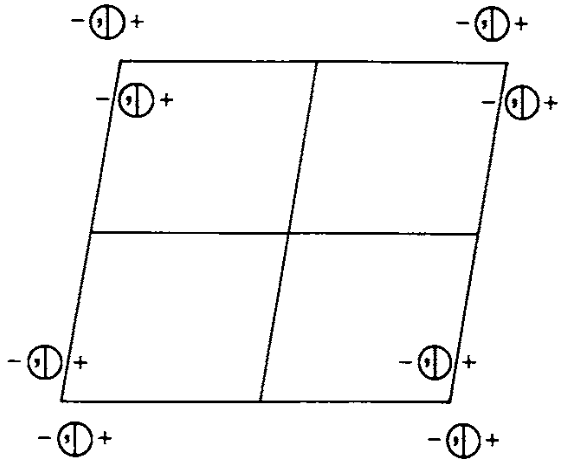
对称面（包括滑移面）与垂直的对称轴（包括螺旋轴）相交生成对称中心

$P2/m$

Unique axes b

等效点数: 4

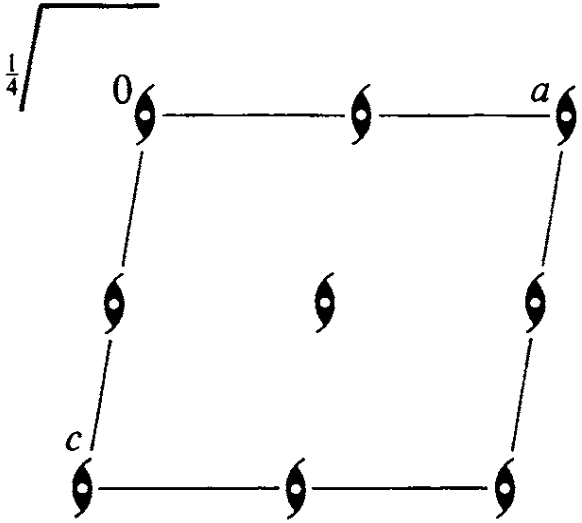


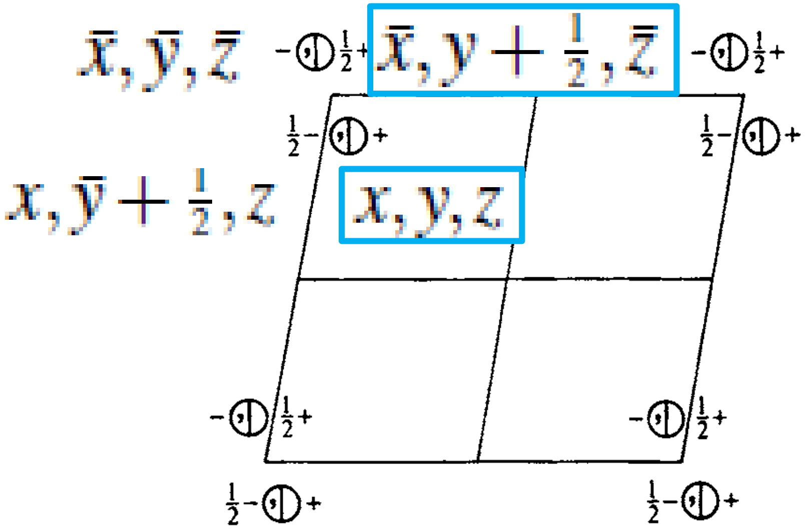


$P2_1/m$

Unique axes b

等效点数: 4

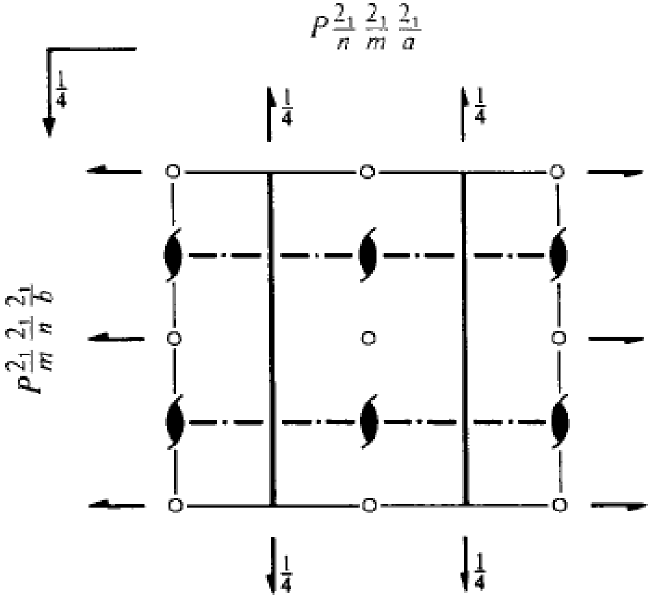


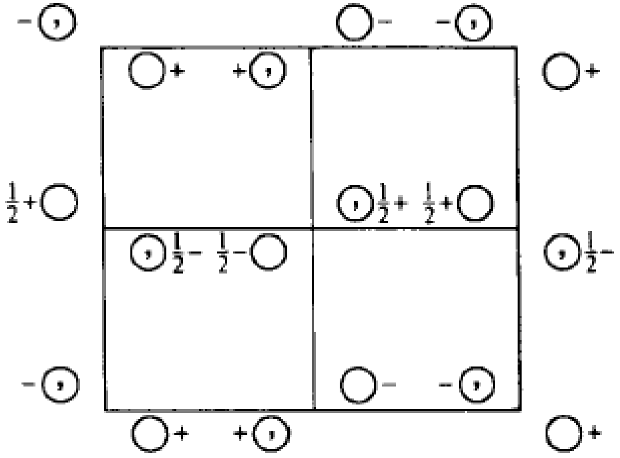


$Pnma$

$P\ 2_1/n\ 2_1/m\ 2_1/a$

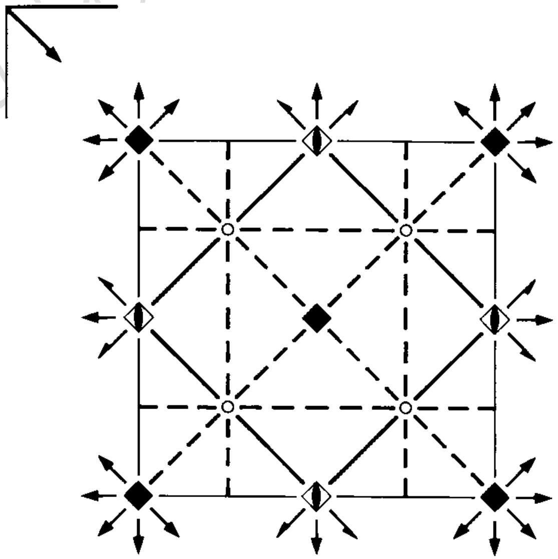
等效点数: 8

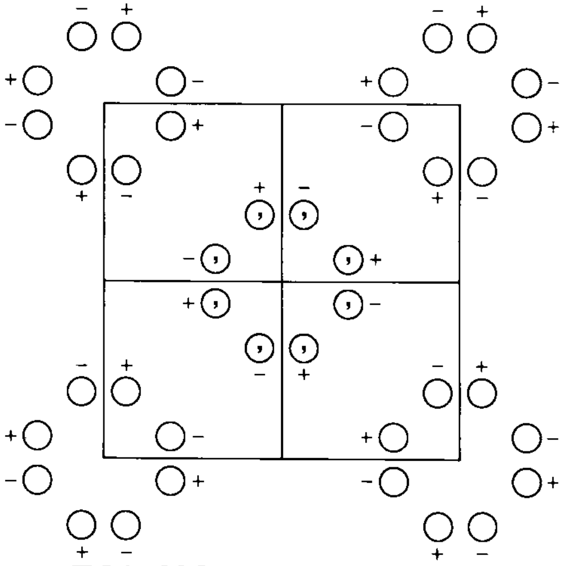




$P4/nbm$

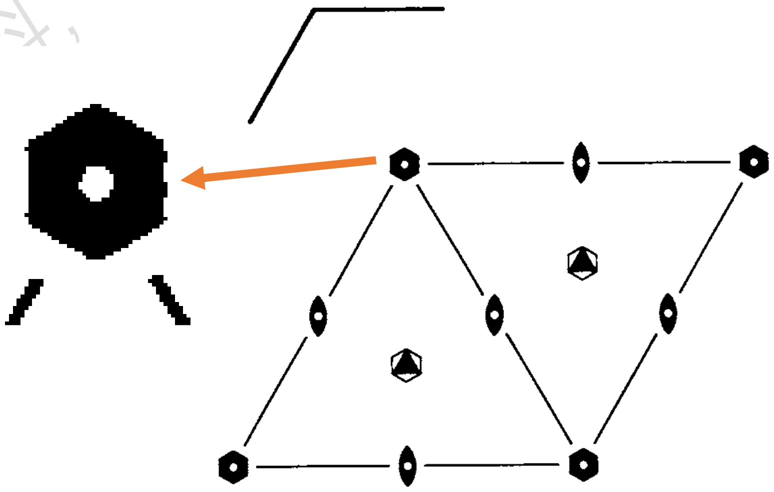
等效点数: 16

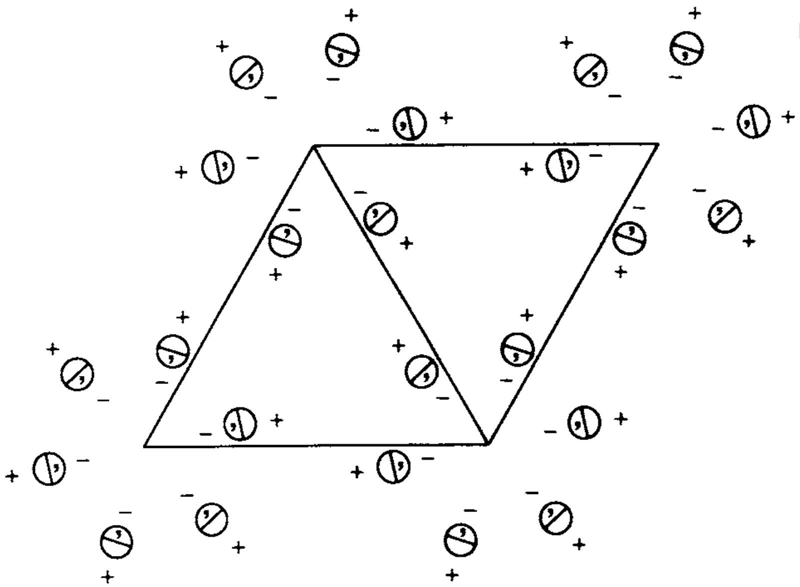




空间群-I
对称性部分

$P6/m$

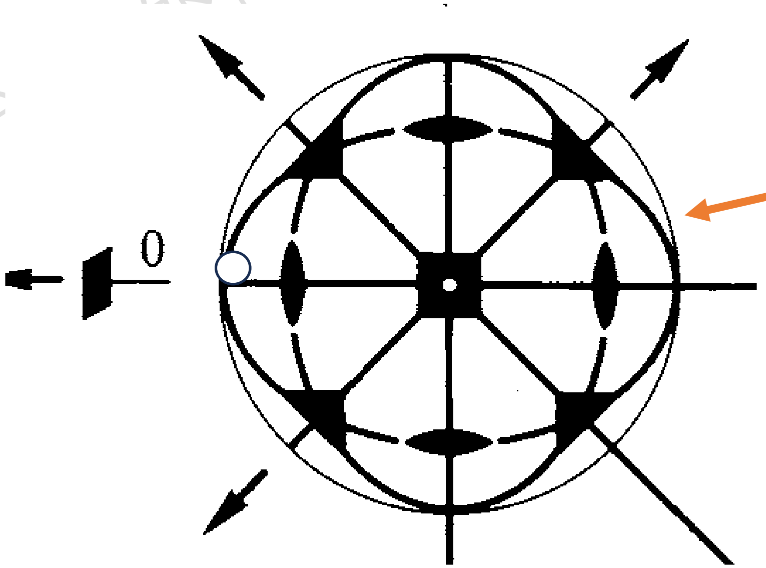




等效点数: **12**

$Pm\bar{3}m$

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



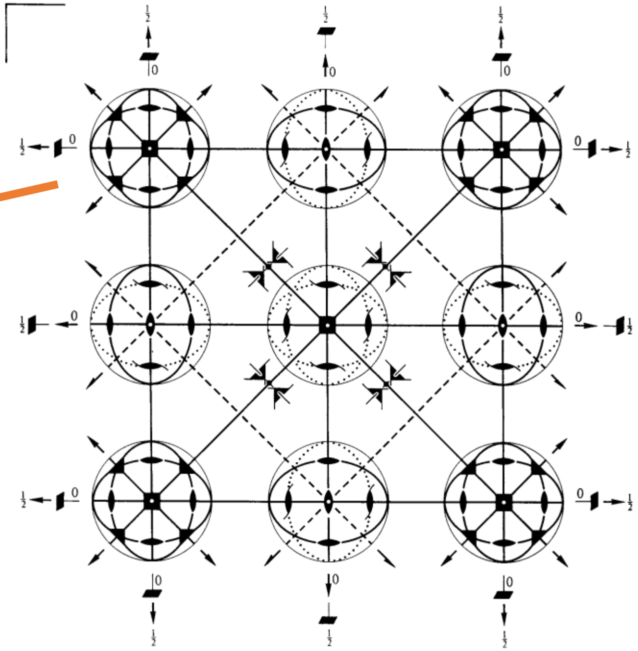


Table 2.2.13.2. *Zonal and serial reflection conditions for glide planes and screw axes (cf. Chapter 1.3)*

(*a*) Glide planes

Type of reflections	Reflection condition	Glide plane			Crystallographic coordinate system to which condition applies	
		Orientation of plane	Glide vector	Symbol		
$0kl$	$k = 2n$	(100)	$\mathbf{b}/2$	b	Monoclinic (*a* unique), Tetragonal	Orthorhombic, Cubic
	$l = 2n$		$\mathbf{c}/2$	c		
	$k + l = 2n$		$\mathbf{b}/2 + \mathbf{c}/2$	n		
	$k + l = 4n$ $(k, l = 2n)^*$		$\mathbf{b}/4 \pm \mathbf{c}/4$	d		
$h0l$	$l = 2n$	(010)	$\mathbf{c}/2$	c	Monoclinic (*b* unique), Tetragonal	Orthorhombic, Cubic
	$h = 2n$		$\mathbf{a}/2$	a		
	$l + h = 2n$		$\mathbf{c}/2 + \mathbf{a}/2$	n		
	$l + h = 4n$ $(l, h = 2n)^*$		$\mathbf{c}/4 \pm \mathbf{a}/4$	d		
$hk0$	$h = 2n$	(001)	$\mathbf{a}/2$	a	Monoclinic (*c* unique), Tetragonal	Orthorhombic, Cubic
	$k = 2n$		$\mathbf{b}/2$	b		
	$h + k = 2n$		$\mathbf{a}/2 + \mathbf{b}/2$	n		
	$h + k = 4n$ $(h, k = 2n)^*$		$\mathbf{a}/4 \pm \mathbf{b}/4$	d		

*International tables for crystallography, Vol. A, 28 (1992).

空间群-I
对称性部分

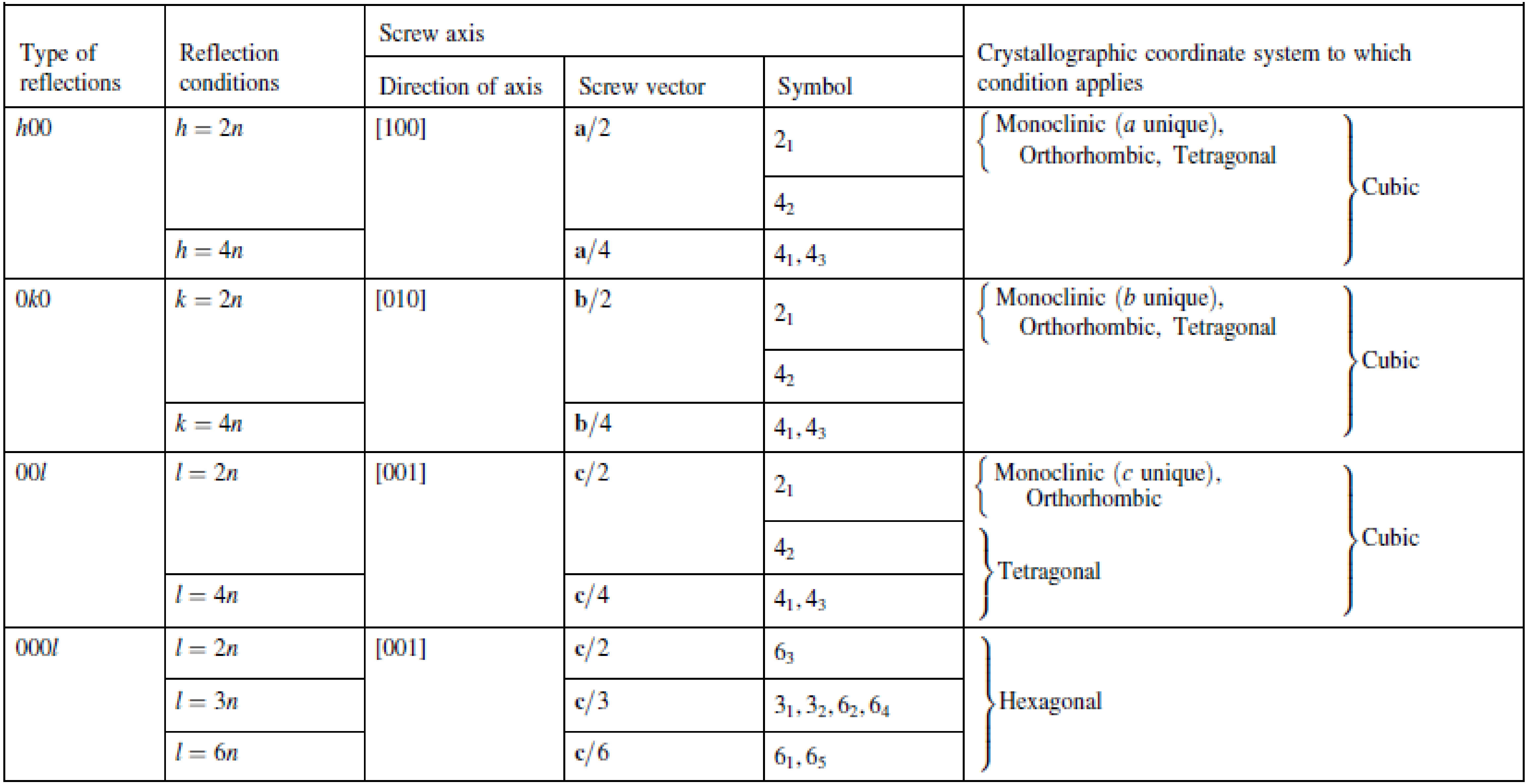
Table 2.2.13.2. *Zonal and serial reflection conditions for glide planes and screw axes (cf. Chapter 1.3)*

Glides planes continues

Type of reflections	Reflection condition	Glide plane			Crystallographic coordinate system to which condition applies
		Orientation of plane	Glide vector	Symbol	
$h\bar{h}0l$ $0k\bar{k}l$ $\bar{h}0hl$	$l = 2n$	$(11\bar{2}0)$ $(\bar{2}110)$ $(1\bar{2}10)$ $\{11\bar{2}0\}$	$\mathbf{c}/2$	c	Hexagonal
$hh.\overline{2h}.l$ $\overline{2h}.hhl$ $h.\overline{2h}.hl$	$l = 2n$	$(1\bar{1}00)$ $(01\bar{1}0)$ $(\bar{1}010)$ $\{1\bar{1}00\}$	$\mathbf{c}/2$	c	Hexagonal
hhl hkk hkh	$l = 2n$ $h = 2n$ $k = 2n$	$(1\bar{1}0)$ $(01\bar{1})$ $(\bar{1}01)$ $\{1\bar{1}0\}$	$\mathbf{c}/2$ $\mathbf{a}/2$ $\mathbf{b}/2$	c, n a, n b, n	Rhombohedral†
$hhl, h\bar{h}l$	$l = 2n$	$(1\bar{1}0), (110)$	$\mathbf{c}/2$	c, n	Tetragonal‡ Cubic§
	$2h + l = 4n$		$\mathbf{a}/4 \pm \mathbf{b}/4 \pm \mathbf{c}/4$	d	
$hkk, hk\bar{k}$	$h = 2n$	$(01\bar{1}), (011)$	$\mathbf{a}/2$	a, n	
	$2k + h = 4n$		$\pm\mathbf{a}/4 + \mathbf{b}/4 \pm \mathbf{c}/4$	d	
$hkh, \bar{h}kh$	$k = 2n$	$(\bar{1}01), (101)$	$\mathbf{b}/2$	b, n	
	$2h + k = 4n$		$\pm\mathbf{a}/4 \pm \mathbf{b}/4 + \mathbf{c}/4$	d	

**International tables for crystallography, Vol. A, 28 (1992).*

(b) Screw axes



Type of reflections	Reflection conditions	Screw axis			Crystallographic coordinate system to which condition applies
		Direction of axis	Screw vector	Symbol	
$h00$	$h = 2n$	[100]	$\mathbf{a}/2$	2_1	Monoclinic (a unique), Orthorhombic, Tetragonal Cubic
				4_2	
	$h = 4n$		$\mathbf{a}/4$	$4_1, 4_3$	
$0k0$	$k = 2n$	[010]	$\mathbf{b}/2$	2_1	Monoclinic (b unique), Orthorhombic, Tetragonal Cubic
				4_2	
	$k = 4n$		$\mathbf{b}/4$	$4_1, 4_3$	
$00l$	$l = 2n$	[001]	$\mathbf{c}/2$	2_1	Monoclinic (c unique), Orthorhombic Cubic
				4_2	Tetragonal
	$l = 4n$		$\mathbf{c}/4$	$4_1, 4_3$	
$000l$	$l = 2n$	[001]	$\mathbf{c}/2$	6_3	Hexagonal
	$l = 3n$		$\mathbf{c}/3$	$3_1, 3_2, 6_2, 6_4$	
	$l = 6n$		$\mathbf{c}/6$	$6_1, 6_5$	

**International tables for crystallography, Vol. A, 29 (1992).*

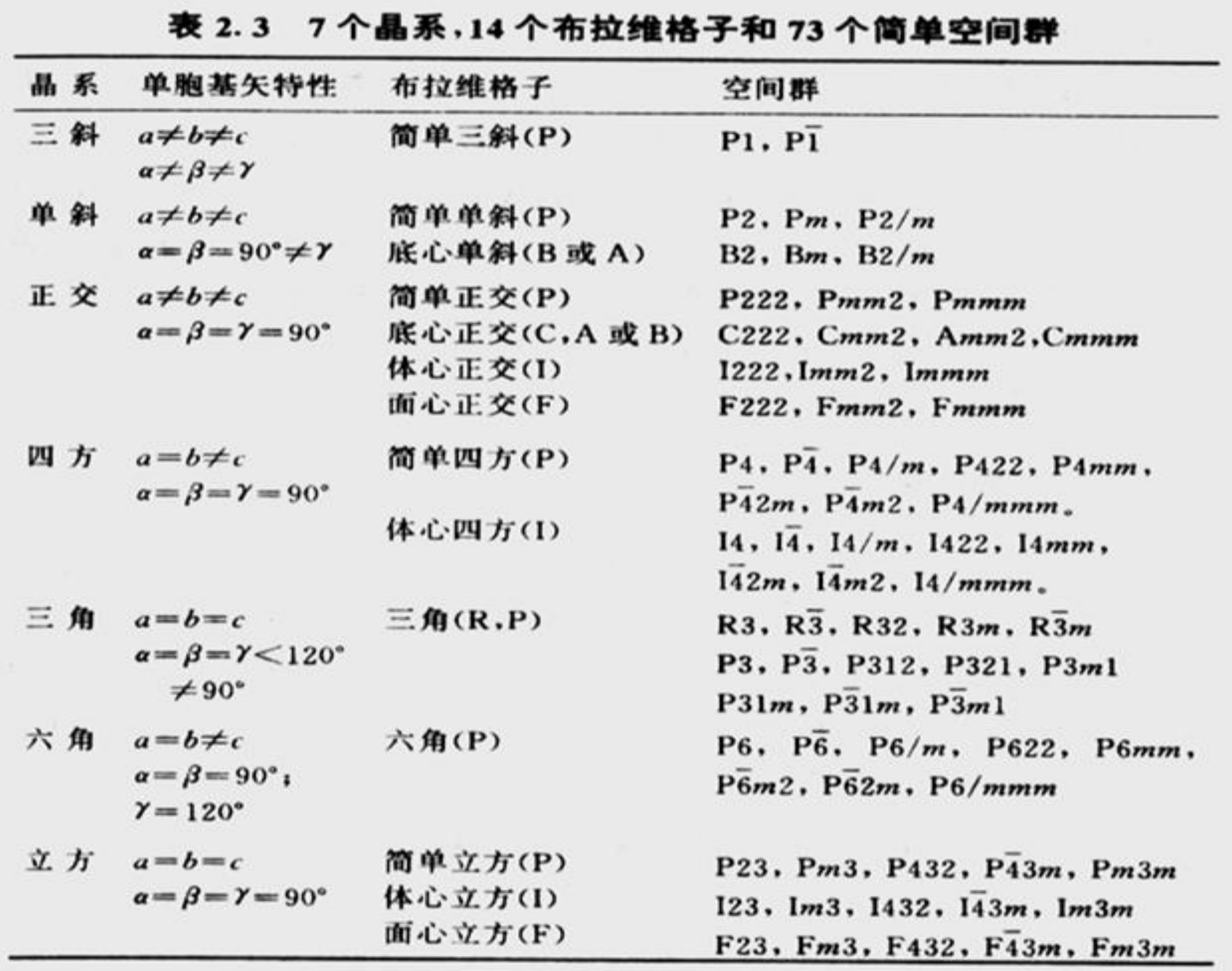


表 2.3　7 个晶系，14 个布拉维格子和 73 个简单空间群

晶系	单胞基矢特性	布拉维格子	空间群
三斜	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	简单三斜(P)	P1，$P\bar{1}$
单斜	$a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$	简单单斜(P) 底心单斜(B 或 A)	P2，Pm，$P2/m$ B2，Bm，$B2/m$
正交	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	简单正交(P) 底心正交(C，A 或 B) 体心正交(I) 面心正交(F)	P222，$Pmm2$，$Pmmm$ C222，$Cmm2$，$Amm2$，$Cmmm$ I222，$Imm2$，$Immm$ F222，$Fmm2$，$Fmmm$
四方	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	简单四方(P) 体心四方(I)	P4，$P\bar{4}$，$P4/m$，P422，$P4mm$，$P\bar{4}2m$，$P\bar{4}m2$，$P4/mmm$。 I4，$I\bar{4}$，$I4/m$，I422，$I4mm$，$I\bar{4}2m$，$I\bar{4}m2$，$I4/mmm$。
三角	$a = b = c$ $\alpha = \beta = \gamma < 120°$ $\neq 90°$	三角(R，P)	R3，$R\bar{3}$，R32，$R3m$，$R\bar{3}m$ P3，$P\bar{3}$，P312，P321，$P3m1$ $P31m$，$P\bar{3}1m$，$P\bar{3}m1$
六角	$a = b \neq c$ $\alpha = \beta = 90°$； $\gamma = 120°$	六角(P)	P6，$P\bar{6}$，$P6/m$，P622，$P6mm$， $P\bar{6}m2$，$P\bar{6}2m$，$P6/mmm$
立方	$a = b = c$ $\alpha = \beta = \gamma = 90°$	简单立方(P) 体心立方(I) 面心立方(F)	P23，$Pm3$，P432，$P\bar{4}3m$，$Pm3m$ I23，$Im3$，I432，$I\bar{4}3m$，$Im3m$ F23，$Fm3$，F432，$F\bar{4}3m$，$Fm3m$

* 不含平移和微观对称要素的空间群

* 此类空间群在衍射中只有点阵有消光可以确定

Symmetry combinations

$Pbcn$ D_{2h}^{14} mmm Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$

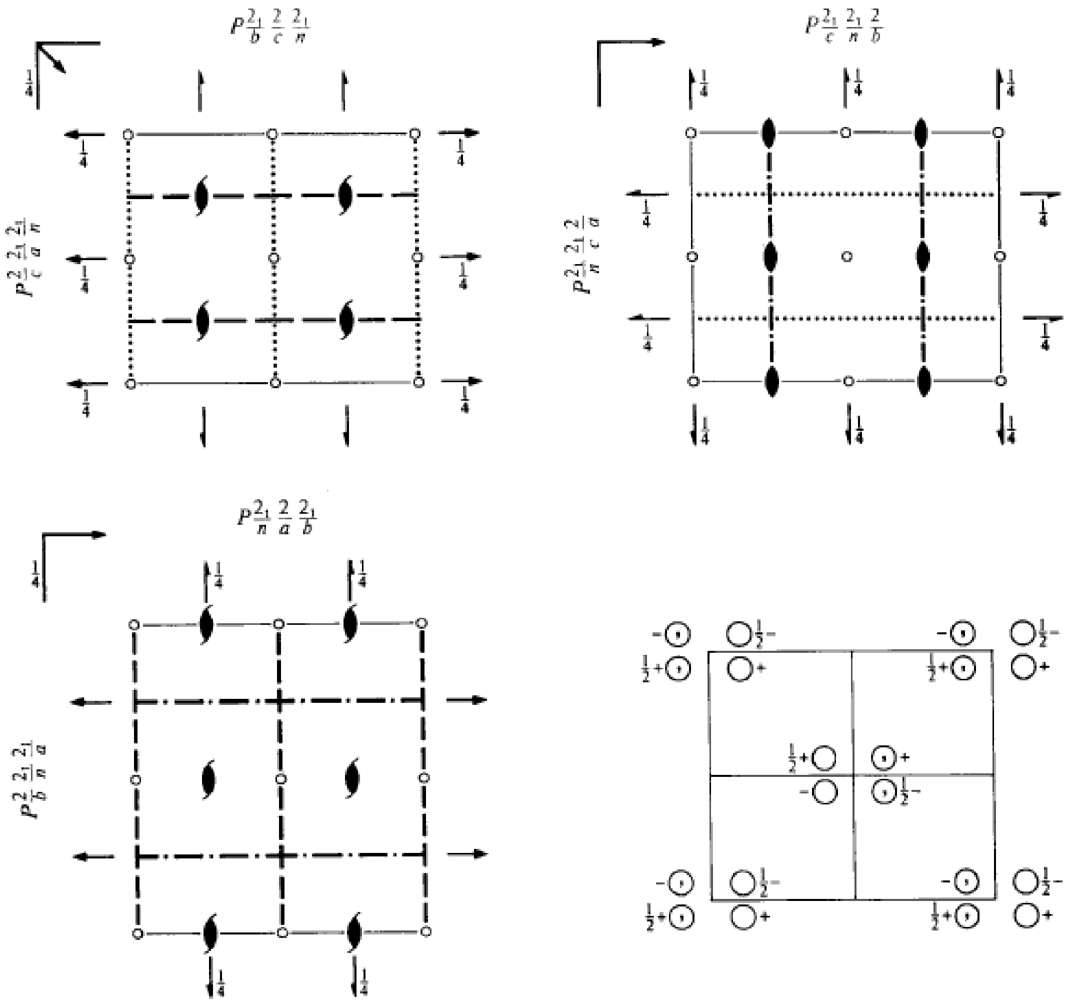
$P\ 2_1/b\ 2/c\ 2_1/n$

Origin at $\bar{1}$ on $1c1$

Asymmetric unit

$$0 \leq x \leq \tfrac{1}{2};$$
$$0 \leq y \leq \tfrac{1}{2};$$
$$0 \leq z \leq \tfrac{1}{2}$$

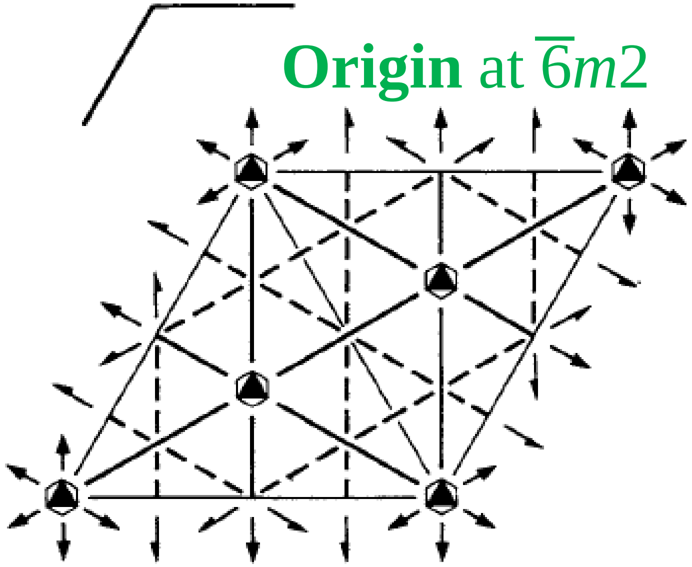
For single crystal diffraction data collecting



Choice of a suitable origin

(1) All centrosymmetric space groups are described with an inversion centre as origin.

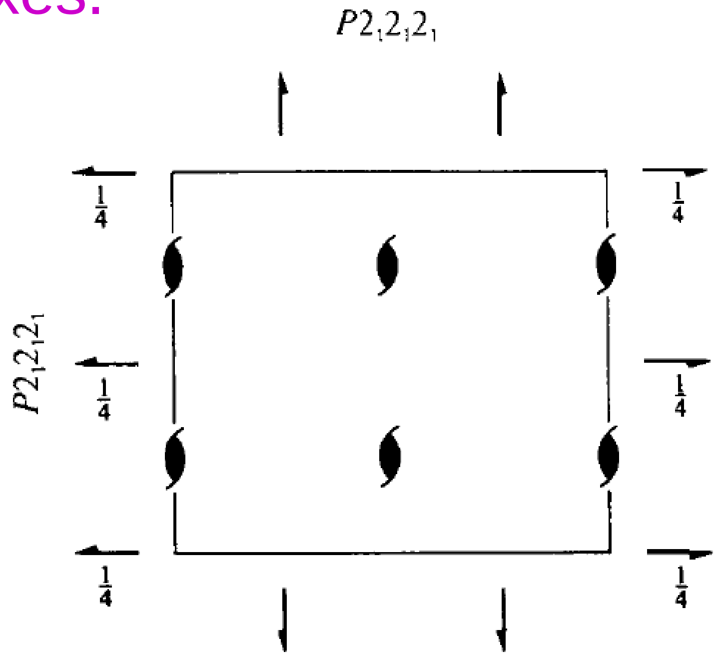
(2) For noncentrosymmetric space groups, as in $P\bar{6}m2$ (187), the origin is at a point of highest site symmetry.



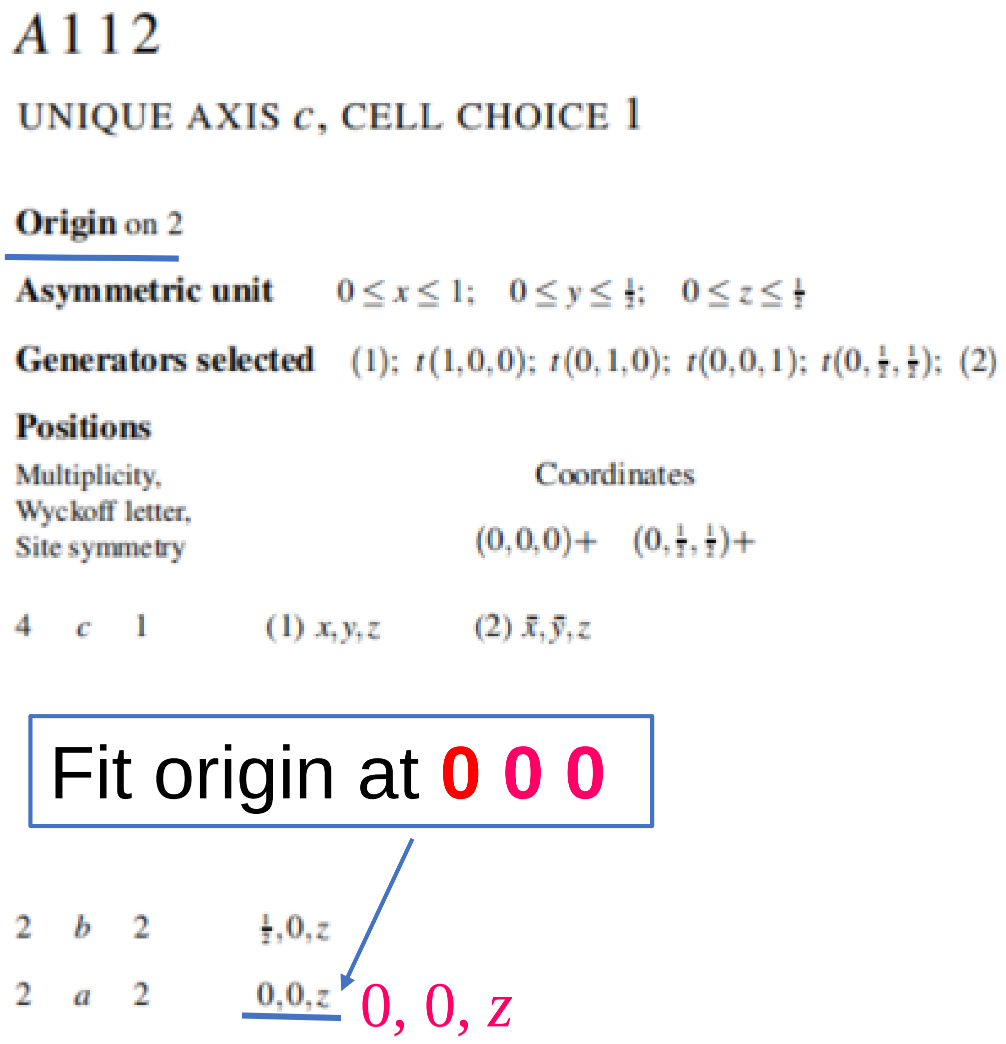
Origin at $\bar{6}m2$

(3) In space group $P2_12_12_1$ (19), the origin is chosen in such a way that it is surrounded symmetrically by three pairs of 2_1 axes.

Origin at midpoint of three non-intersecting pairs of parallel 2_1 axes



Fit origin



$A\,1\,1\,2$

UNIQUE AXIS c, CELL CHOICE 1

Origin on 2

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

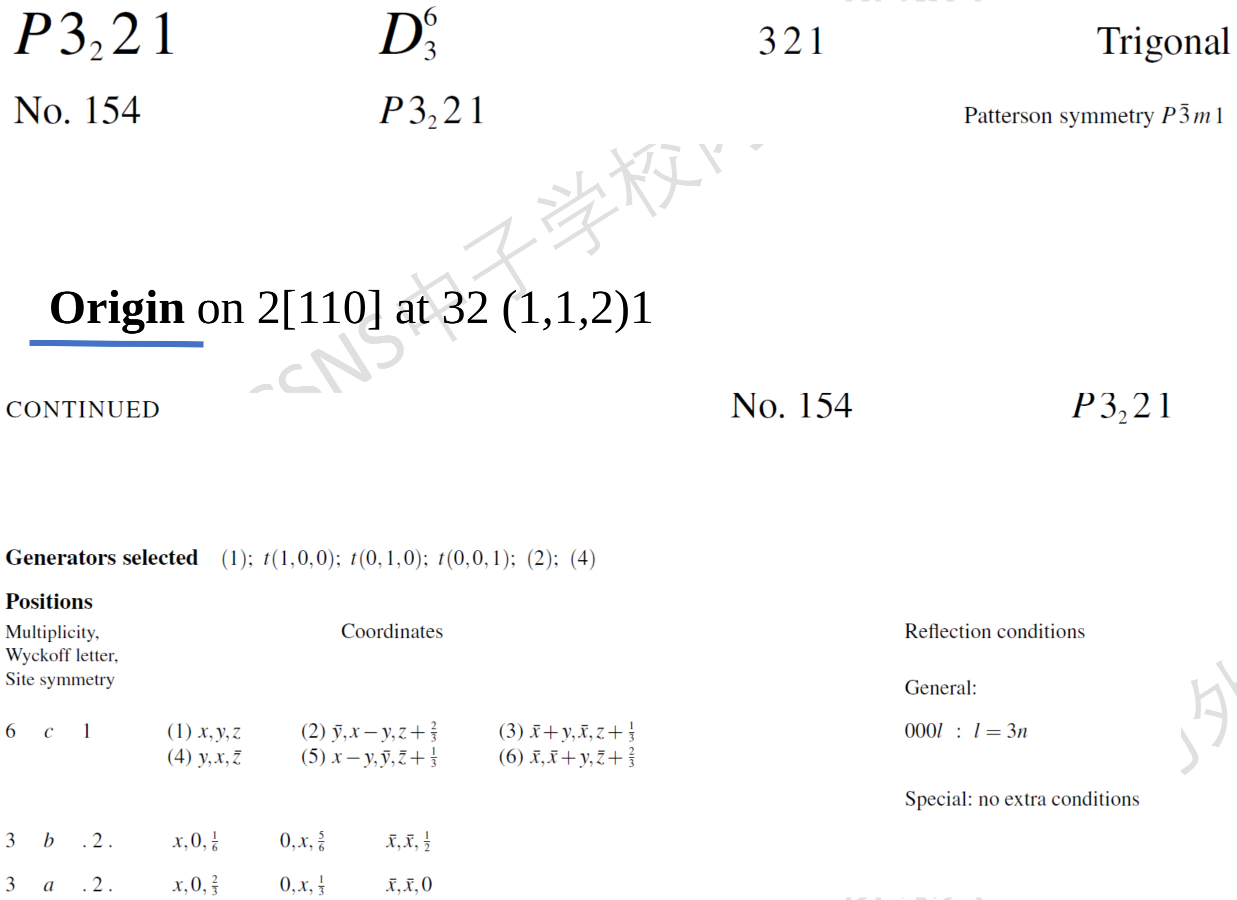
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; (2)

Positions

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

Fit origin at **0 0 0**

$0,\ 0,\ z$



$P\,3_2\,2\,1$	D_3^6	$3\,2\,1$	Trigonal
No. 154	$P\,3_2\,2\,1$		Patterson symmetry $P\,\bar{3}\,m\,1$

Origin on 2[110] at 32 (1,1,2)1

CONTINUED No. 154 $P\,3_2\,2\,1$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
6	c	1	(1) x,y,z (4) $y,x,\bar{z}$	(2) $\bar{y},x-y,z+\frac{2}{3}$ (5) $x-y,\bar{y},\bar{z}+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{1}{3}$ (6) $\bar{x},\bar{x}+y,\bar{z}+\frac{2}{3}$	$000l$: $l=3n$
						Special: no extra conditions
3	b	$.\,2\,.$	$x,0,\frac{1}{6}$	$0,x,\frac{5}{6}$	$\bar{x},\bar{x},\frac{1}{2}$	
3	a	$.\,2\,.$	$x,0,\frac{2}{3}$	$0,x,\frac{1}{3}$	$\bar{x},\bar{x},0$	

$x,\ 0,\ 2/3$

Fit origin at ***x*, 0, 2/3**

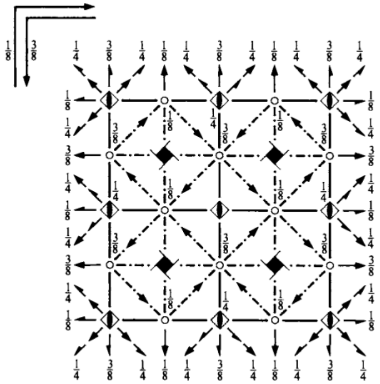
No. 141 and 142 have two origin choices

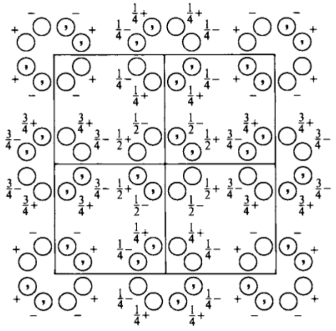
International Tables for Crystallography (2006). Vol. A, Space group 141, pp. 482–485.

$I4_1/amd$ D_{4h}^{19} $4/mmm$ Tetragonal

No. 141 $I\ 4_1/a\ 2/m\ 2/d$ Patterson symmetry $I4/mmm$

Origin choice 1





Origin at $\bar{4}m2$, at $0, \frac{1}{4}, -\frac{1}{8}$ from centre $(2/m)$

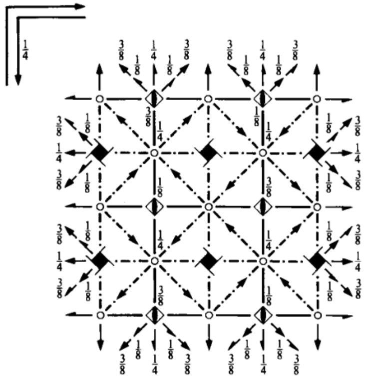
Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{8}$

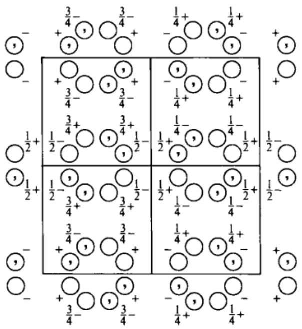
8	*e*	$2mm.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$
8	*d*	$.2/m.$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$
8	*c*	$.2/m.$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$
4	*b*	$\bar{4}m2$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$		
4	*a*	$\bar{4}m2$	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$		

$I4_1/amd$ D_{4h}^{19} $4/mmm$ Tetragonal

No. 141 $I\ 4_1/a\ 2/m\ 2/d$ Patterson symmetry $I4/mmm$

Origin choice 2



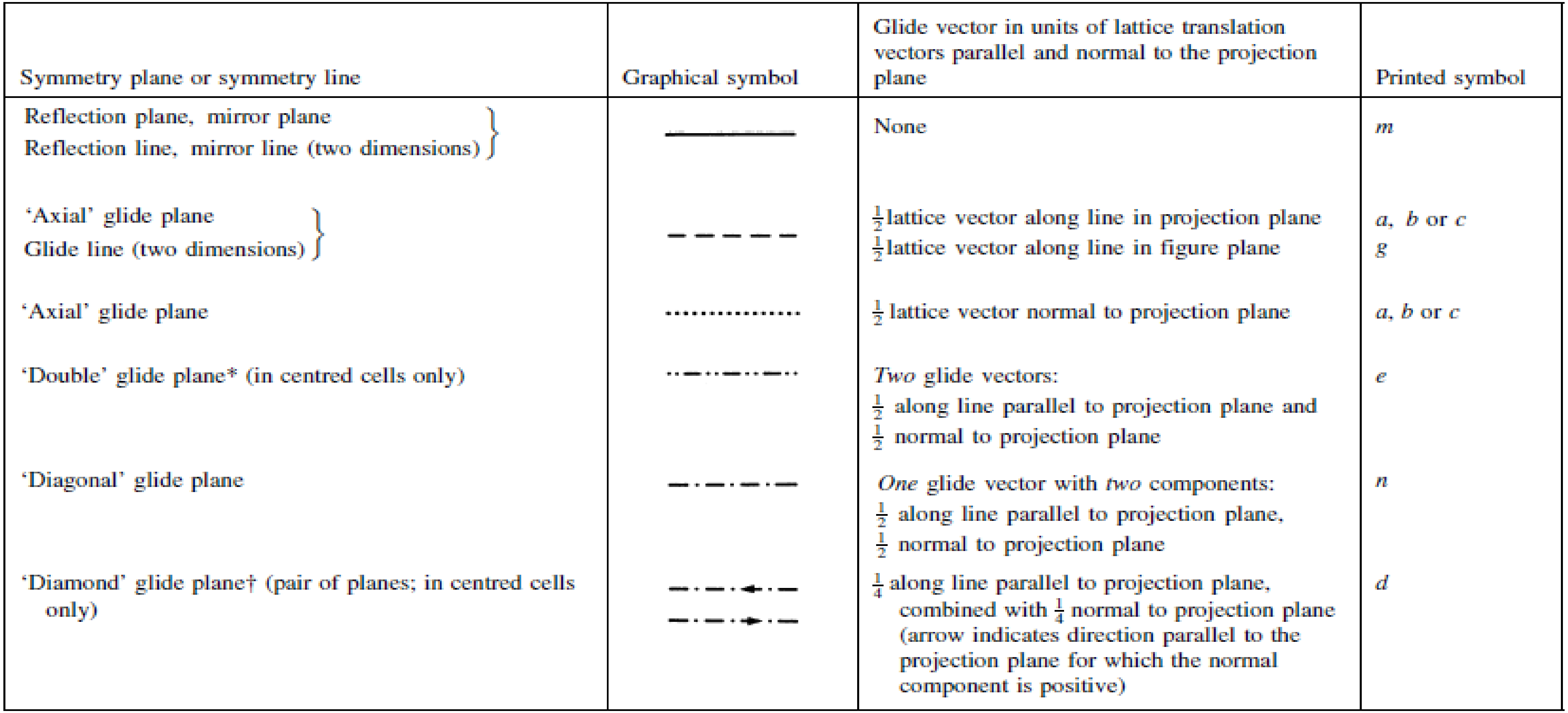


Origin at centre $(2/m)$ at $b\,(2/m, 2_1/n)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad -\frac{1}{4} \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{8}$

8	*e*	$2mm.$	$0,\frac{1}{4},z$	$0,\frac{3}{4},z+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{1}{4}$
8	*d*	$.2/m.$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$
8	*c*	$.2/m.$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$
4	*b*	$\bar{4}m2$	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{5}{8}$		
4	*a*	$\bar{4}m2$	$0,\frac{3}{4},\frac{1}{8}$	$\frac{1}{2},\frac{3}{4},\frac{3}{8}$		

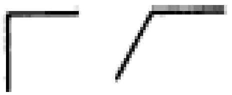
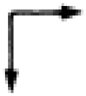
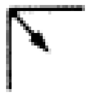
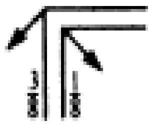
Symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)



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

**International tables for crystallography, Vol. A, 7 (1992).*

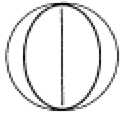
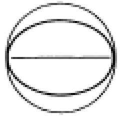
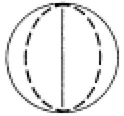
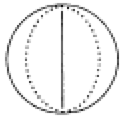
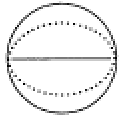
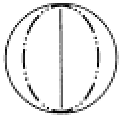
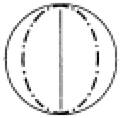
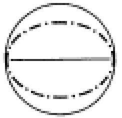
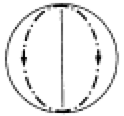
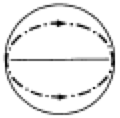
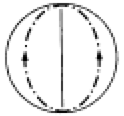
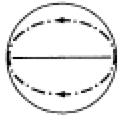
Symmetry planes parallel to the plane of projection

Symmetry plane	Graphical symbol*	Glide vector in units of lattice translation vectors parallel to the projection plane	Printed symbol
Reflection plane, mirror plane		None	*m*
'Axial' glide plane		$\frac{1}{2}$ lattice vector in the direction of the arrow	*a*, *b* or *c*
'Double' glide plane† (in centred cells only)		*Two* glide vectors: $\frac{1}{2}$ in either of the directions of the two arrows	*e*
'Diagonal' glide plane		*One* glide vector with *two* components $\frac{1}{2}$ in the direction of the arrow	*n*
'Diamond' glide plane‡ (pair of planes; in centred cells only)		$\frac{1}{4}$ in the direction of the arrow; the glide vector is always half of a centring vector, *i.e.* one quarter of a diagonal of the conventional face-centred cell	*d*

* The symbols are given at the upper left corner of the space-group diagrams. A fraction h attached to a symbol indicates two symmetry planes with 'heights' h and $h+\frac{1}{2}$ above the plane of projection; *e.g.* $\frac{1}{8}$ stands for $h=\frac{1}{8}$ and $\frac{5}{8}$. No fraction means $h=0$ and $\frac{1}{2}$ (*cf.* Section 2.2.6).

**International tables for crystallography, Vol. A, 8 (1992).*

Symmetry planes inclined to the plane of projection (in cubic space groups of classes $\bar{4}3m$ and $m\bar{3}m$ only)

Symmetry plane	Graphical symbol* for planes normal to		Glide vector in units of lattice translation vectors for planes normal to		Printed symbol
	$[011]$ and $[01\bar{1}]$	$[101]$ and $[10\bar{1}]$	$[011]$ and $[01\bar{1}]$	$[101]$ and $[10\bar{1}]$	
Reflection plane, mirror plane			None	None	m
‘Axial’ glide plane			$\frac{1}{2}$ lattice vector along $[100]$	$\frac{1}{2}$ lattice vector along $[010]$	a or b
‘Axial’ glide plane			$\frac{1}{2}$ lattice vector along $[01\bar{1}]$ or along $[011]$	$\frac{1}{2}$ lattice vector along $[10\bar{1}]$ or along $[101]$	
‘Double’ glide plane† [in space groups $I\bar{4}3m$ (217) and $Im\bar{3}m$ (229) only]			*Two* glide vectors: $\frac{1}{2}$ along $[100]$ *and* $\frac{1}{2}$ along $[01\bar{1}]$ or $\frac{1}{2}$ along $[011]$	*Two* glide vectors: $\frac{1}{2}$ along $[010]$ *and* $\frac{1}{2}$ along $[10\bar{1}]$ or $\frac{1}{2}$ along $[101]$	e
‘Diagonal’ glide plane			*One* glide vector: $\frac{1}{2}$ along $[11\bar{1}]$ or along $[111]$‡	*One* glide vector: $\frac{1}{2}$ along $[11\bar{1}]$ or along $[111]$‡	n
‘Diamond’ glide plane¶ (pair of planes; in centred cells only)			$\frac{1}{2}$ along $[1\bar{1}1]$ or along $[111]$§	$\frac{1}{2}$ along $[\bar{1}11]$ or along $[111]$§	d
			$\frac{1}{2}$ along $[\bar{1}\bar{1}1]$ or along $[\bar{1}11]$§	$\frac{1}{2}$ along $[\bar{1}\bar{1}1]$ or along $[1\bar{1}1]$§	

* The symbols represent orthographic projections. In the cubic space-group diagrams, complete orthographic projections of the symmetry elements around high-symmetry points, such as $0,0,0; \frac{1}{2},0,0; \frac{1}{4},\frac{1}{4},0$, are given as ‘inserts’.

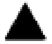
† For further explanations of the ‘double’ glide plane e see Note (iv) below and Note (x) in Section 1.3.2.

‡ In the space groups $F\bar{4}3m$ (216), $Fm\bar{3}m$ (225) and $Fd\bar{3}m$ (227), the shortest lattice translation vectors in the glide directions are $\mathbf{t}(1,\frac{1}{2},\frac{\bar{1}}{2})$ or $\mathbf{t}(1,\frac{1}{2},\frac{1}{2})$ and $\mathbf{t}(\frac{1}{2},1,\frac{\bar{1}}{2})$ or $\mathbf{t}(\frac{1}{2},1,\frac{1}{2})$, respectively.

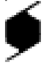
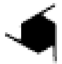
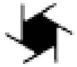
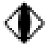
§ The glide vector is half of a centring vector, *i.e.* one quarter of the diagonal of the conventional body-centred cell in space groups $I\bar{4}3d$ (220) and $Ia\bar{3}d$ (230).

**International tables for crystallography, Vol. A, 8 (1992).*

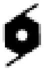
1.4.5. Symmetry axes normal to the plane of projection and symmetry points in the plane of the figure

Symmetry axis or symmetry point	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Identity	None	None	1
Twofold rotation axis Twofold rotation point (two dimensions)		None	2
Twofold screw axis: ‘2 sub 1’		$\frac{1}{2}$	2_1
Threefold rotation axis Threefold rotation point (two dimensions)		None	3
Threefold screw axis: ‘3 sub 1’		$\frac{1}{3}$	3_1
Threefold screw axis: ‘3 sub 2’		$\frac{2}{3}$	3_2
Fourfold rotation axis Fourfold rotation point (two dimensions)		None	4 (2)
Fourfold screw axis: ‘4 sub 1’		$\frac{1}{4}$	4_1 (2_1)
Fourfold screw axis: ‘4 sub 2’		$\frac{1}{2}$	4_2 (2)
Fourfold screw axis: ‘4 sub 3’		$\frac{3}{4}$	4_3 (2_1)

1.4.5. *Continue*

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

1.4.5. *Continue*

Symmetry axis or symmetry point	Graphical symbol*	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol (partial elements in parentheses)
Fourfold rotation axis with centre of symmetry		None	$4/m\ (\bar{4}, 2, \bar{1})$
'4 sub 2' screw axis with centre of symmetry		$\frac{1}{2}$	$4_2/m\ (\bar{4}, 2, \bar{1})$
Sixfold rotation axis with centre of symmetry		None	$6/m\ (\bar{6}, \bar{3}, 3, 2, \bar{1})$
'6 sub 3' screw axis with centre of symmetry		$\frac{1}{2}$	$6_3/m\ (\bar{6}, \bar{3}, 3, 2_1, \bar{1})$

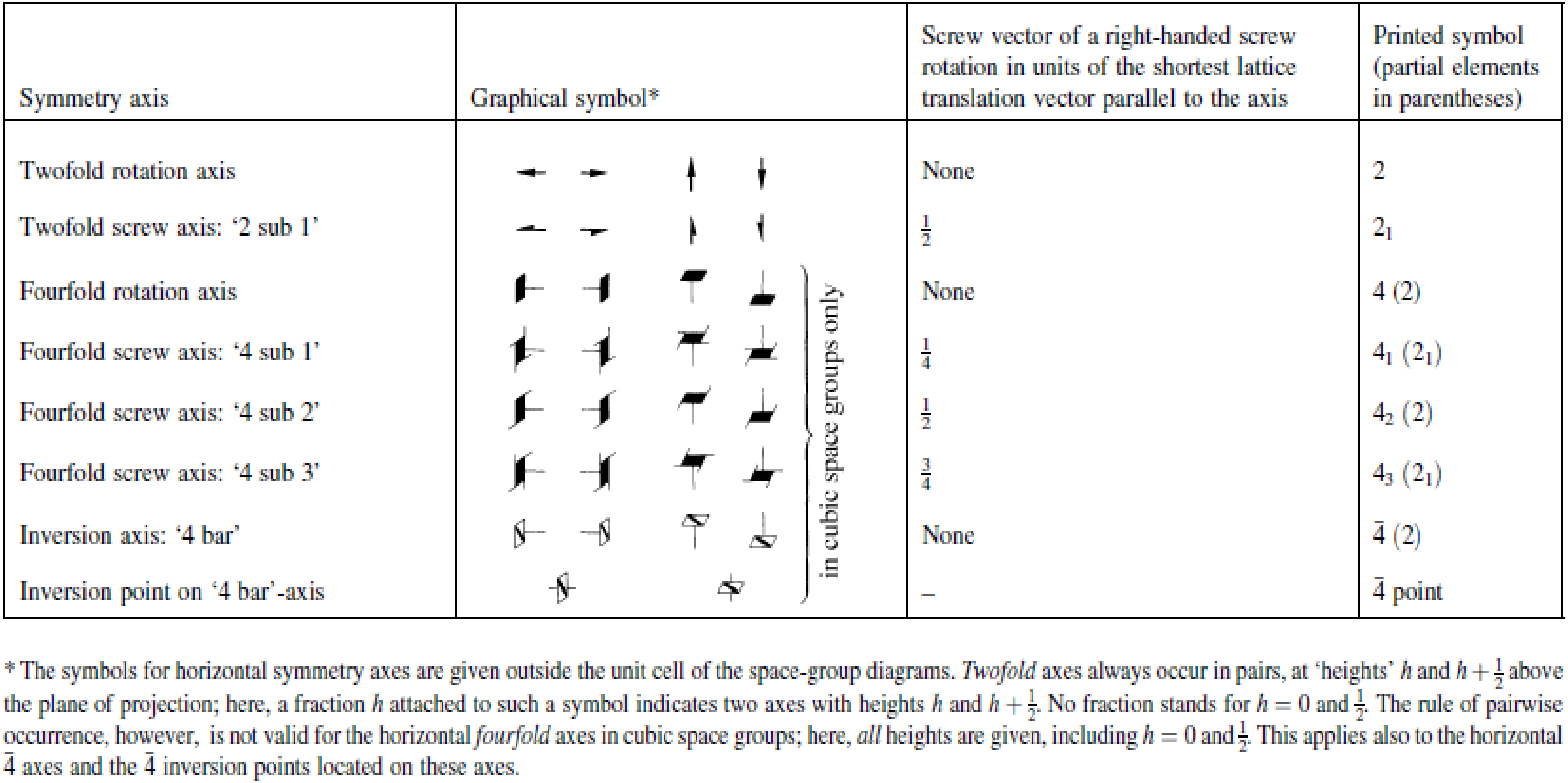
* Notes on the 'heights' *h* of symmetry points $\bar{1}$, $\bar{3}$, $\bar{4}$ and $\bar{6}$:

(1) Centres of symmetry $\bar{1}$ and $\bar{3}$, as well as inversion points $\bar{4}$ and $\bar{6}$ on $\bar{4}$ and 6 axes parallel to [001], occur in pairs at 'heights' *h* and *h*+1/2. In the space-group diagrams, only one fraction *h* is given, *e.g.* ¼ stands for *h*=1/4 and 3/4. No fraction means *h*=0 and 1/2. In *cubic* space groups, however, because of their complexity, *both* fractions are given for vertical 4 axes, including *h*=0 and ½.

(2) Symmetries 4/*m* and 6/*m* contain vertical $\bar{4}$ and $\bar{6}$ axes; their $\bar{4}$ and $\bar{6}$ inversion points coincide with the centres of symmetry. This is not indicated in the space-group diagrams.

(3) Symmetries $4_2/m$ and $6_3/m$ also contain vertical $\bar{4}$ and $\bar{6}$ axes, but their $\bar{4}$ and $\bar{6}$ inversion points alternate with the centres of symmetry; *i.e.* $\bar{1}$ points at *h* and *h*=1/2 interleave with $\bar{4}$ or $\bar{6}$ points at *h*=1/4 and *h*=3/4. In the tetragonal and hexagonal space-group diagrams, only *one* fraction for $\bar{1}$ and one for $\bar{4}$ or $\bar{6}$ is given. In the cubic diagrams, *all four* fractions are listed for $4_2/m$; *e.g.* $Pm\bar{3}n$ (No. 223): $\bar{1}$: 0, ½; $\bar{4}$: 1/4,3/4.

Symmetry axes parallel to the plane of projection



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

* The symbols for horizontal symmetry axes are given outside the unit cell of the space-group diagrams. *Twofold* axes always occur in pairs, at 'heights' h and $h+\frac{1}{2}$ above the plane of projection; here, a fraction h attached to such a symbol indicates two axes with heights h and $h+\frac{1}{2}$. No fraction stands for $h=0$ and $\frac{1}{2}$. The rule of pairwise occurrence, however, is not valid for the horizontal *fourfold* axes in cubic space groups; here, *all* heights are given, including $h=0$ and $\frac{1}{2}$. This applies also to the horizontal $\bar{4}$ axes and the $\bar{4}$ inversion points located on these axes.

**International tables for crystallography, Vol. A, 10 (1992).*

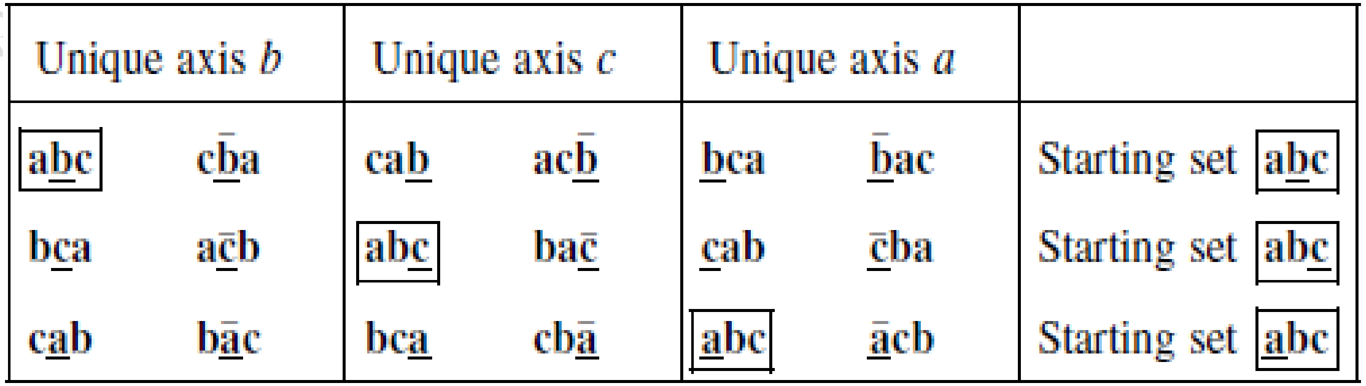
Symmetry axes inclined to the plane of projection (in cubic space group only)

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

* The dots mark the intersection points of axes with the plane at $h = 0$. In some cases, the intersection points are obscured by symbols of symmetry elements with height $h \geq 0$; examples: $Fd\bar{3}$ (203), origin choice 2; $Pn\bar{3}n$ (222), origin choice 2; $Pm\bar{3}n$ (223); $Im\bar{3}m$ (229); $Ia\bar{3}d$ (230).

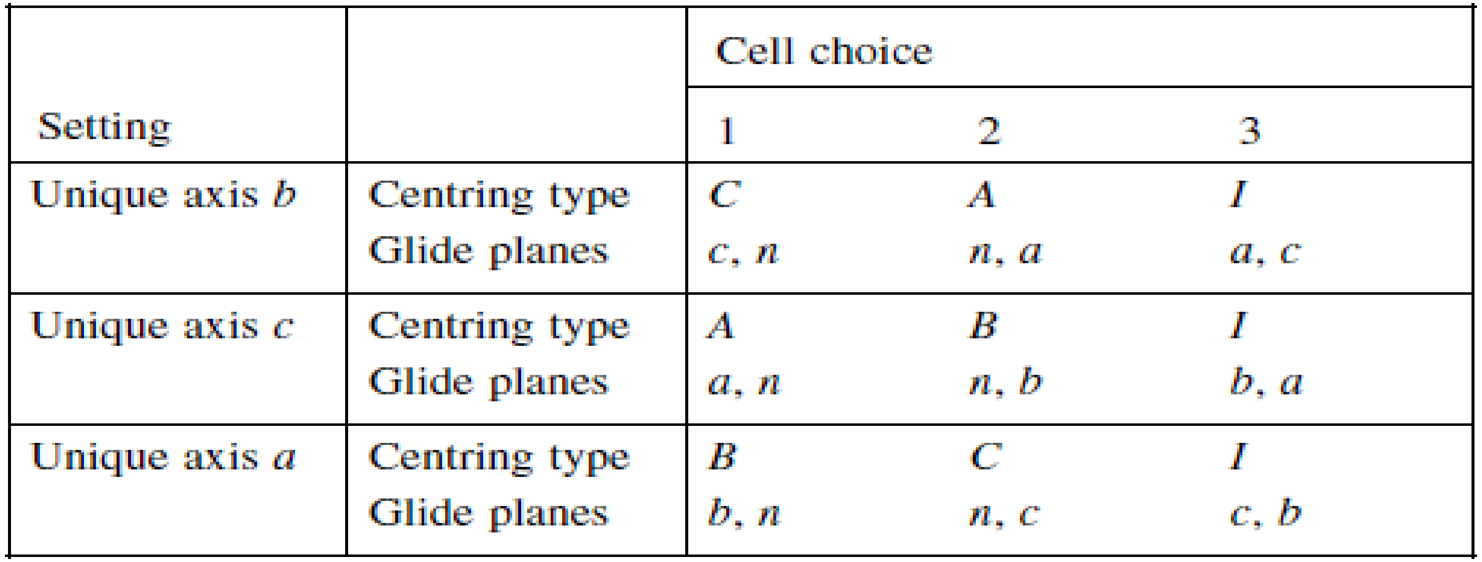
**International tables for crystallography, Vol. A, 10 (1992).*

Table 2.2.16.1. *Monoclinic setting symbols (unique axis is underlined)*



Unique axis b		Unique axis c		Unique axis a		
$\boxed{a\underline{b}c}$	$c\underline{\bar{b}}a$	$ca\underline{b}$	$ac\underline{\bar{b}}$	$\underline{b}ca$	$\underline{\bar{b}}ac$	Starting set $\boxed{a\underline{b}c}$
$b\underline{c}a$	$a\underline{\bar{c}}b$	$\boxed{ab\underline{c}}$	$ba\underline{\bar{c}}$	$\underline{c}ab$	$\underline{\bar{c}}ba$	Starting set $\boxed{ab\underline{c}}$
$c\underline{a}b$	$b\underline{\bar{a}}c$	$bc\underline{a}$	$cb\underline{\bar{a}}$	$\boxed{\underline{a}bc}$	$\underline{\bar{a}}cb$	Starting set $\boxed{\underline{a}bc}$

Table 2.2.16.2. *Symbols for centring types and glide planes of monoclinic space groups*



		Cell choice		
Setting		1	2	3
Unique axis b	Centring type Glide planes	C c, n	A n, a	I a, c
Unique axis c	Centring type Glide planes	A a, n	B n, b	I b, a
Unique axis a	Centring type Glide planes	B b, n	C n, c	I c, b

Note: An interchange of two axes involves a change of the handedness of the coordinate system. In order to keep the system right-handed, one sign reversal is necessary.

Table 4.3.2.1. Index of symbols for space groups for various settings and cells

MONOCLINIC SYSTEM

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						Unique axis *b* Unique axis *c* Unique axis *a*
			$\mathbf{a\underline{b}c}$	$\mathbf{c\underline{\bar{b}}a}$	$\mathbf{ab\underline{c}}$	$\mathbf{ba\underline{\bar{c}}}$	$\mathbf{\underline{a}bc}$	$\mathbf{\underline{\bar{a}}cb}$	
3	C_2^1	$P2$	$P121$	$P121$	$P112$	$P112$	$P211$	$P211$	
4	C_2^2	$P2_1$	$P12_11$	$P12_11$	$P112_1$	$P112_1$	$P2_111$	$P2_111$	
5	C_2^3	$C2$	$C121$ 2_1	$A121$ 2_1	$A112$ 2_1	$B112$ 2_1	$B211$ 2_1	$C211$ 2_1	Cell choice 1
			$A121$ 2_1	$C121$ 2_1	$B112$ 2_1	$A112$ 2_1	$C211$ 2_1	$B211$ 2_1	Cell choice 2
			$I121$ 2_1	$I121$ 2_1	$I112$ 2_1	$I112$ 2_1	$I211$ 2_1	$I211$ 2_1	Cell choice 3
6	C_s^1	Pm	$P1m1$	$P1m1$	$P11m$	$P11m$	$Pm11$	$Pm11$	
7	C_s^2	Pc	$P1c1$	$P1a1$	$P11a$	$P11b$	$Pb11$	$Pc11$	Cell choice 1
			$P1n1$	$P1n1$	$P11n$	$P11n$	$Pn11$	$Pn11$	Cell choice 2
			$P1a1$	$P1c1$	$P11b$	$P11a$	$Pc11$	$Pb11$	Cell choice 3
8	C_s^3	Cm	$C1m1$ a	$A1m1$ c	$A11m$ b	$B11m$ a	$Bm11$ c	$Cm11$ b	Cell choice 1
			$A1m1$ c	$C1m1$ a	$B11m$ a	$A11m$ b	$Cm11$ b	$Bm11$ c	Cell choice 2
			$I1m1$ n	$I1m1$ n	$I11m$ n	$I11m$ n	$Im11$ n	$Im11$ n	Cell choice 3
9	C_s^4	Cc	$C1c1$ n	$A1a1$ n	$A11a$ n	$B11b$ n	$Bb11$ n	$Cc11$ n	Cell choice 1
			$A1n1$ a	$C1n1$ c	$B11n$ b	$A11n$ a	$Cn11$ c	$Bn11$ b	Cell choice 2
			$I1a1$ c	$I1c1$ a	$I11b$ a	$I11a$ b	$Ic11$ b	$Ib11$ c	Cell choice 3

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Monoclinic system (*cont.*)

No. of space group	Schoenflies symbol	Standard short Hermann–Mauguin symbol	Extended Hermann–Mauguin symbols for various settings and cell choices						
			$a\underline{b}c$	$c\underline{\bar{b}}a$	$ab\underline{c}$	$ba\underline{\bar{c}}$	$\underline{a}bc$	$\underline{\bar{a}}cb$	Unique axis *b* Unique axis *c* Unique axis *a*
10	C_{2h}^1	$P2/m$	$P1\frac{2}{m}1$	$P1\frac{2}{m}1$	$P11\frac{2}{m}$	$P11\frac{2}{m}$	$P\frac{2}{m}11$	$P\frac{2}{m}11$	
11	C_{2h}^2	$P2_1/m$	$P1\frac{2_1}{m}1$	$P1\frac{2_1}{m}1$	$P11\frac{2_1}{m}$	$P11\frac{2_1}{m}$	$P\frac{2_1}{m}11$	$P\frac{2_1}{m}11$	
12	C_{2h}^3	$C2/m$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$	$A1\frac{2}{m}1$ $\frac{2_1}{c}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$	$B11\frac{2}{m}$ $\frac{2_1}{a}$	$B\frac{2}{m}11$ $\frac{2_1}{c}$	$C\frac{2}{m}11$ $\frac{2_1}{b}$	Cell choice 1
			$A1\frac{2}{m}1$ $\frac{2_1}{c}$	$C1\frac{2}{m}1$ $\frac{2_1}{a}$	$B11\frac{2}{m}$ $\frac{2_1}{a}$	$A11\frac{2}{m}$ $\frac{2_1}{b}$	$C\frac{2}{m}11$ $\frac{2_1}{b}$	$B\frac{2}{m}11$ $\frac{2_1}{c}$	Cell choice 2
			$I1\frac{2}{m}1$ $\frac{2_1}{n}$	$I1\frac{2}{m}1$ $\frac{2_1}{n}$	$I11\frac{2}{m}$ $\frac{2_1}{n}$	$I11\frac{2}{m}$ $\frac{2_1}{n}$	$I\frac{2}{m}11$ $\frac{2_1}{n}$	$I\frac{2}{m}11$ $\frac{2_1}{n}$	Cell choice 3
13	C_{2h}^4	$P2/c$	$P1\frac{2}{c}1$	$P1\frac{2}{a}1$	$P11\frac{2}{a}$	$P11\frac{2}{b}$	$P\frac{2}{b}11$	$P\frac{2}{c}11$	Cell choice 1
			$P1\frac{2}{n}1$	$P1\frac{2}{n}1$	$P11\frac{2}{n}$	$P11\frac{2}{n}$	$P\frac{2}{n}11$	$P\frac{2}{n}11$	Cell choice 2
			$P1\frac{2}{a}1$	$P1\frac{2}{c}1$	$P11\frac{2}{b}$	$P11\frac{2}{a}$	$P\frac{2}{c}11$	$P\frac{2}{b}11$	Cell choice 3

ORTHORHOMBIC SYSTEM

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol abc	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**bac̄**	**cab**	**c̄ba**	**bca**	**ac̄b**
16	D_2^1	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$	$P222$
17	D_2^2	$P222_1$	$P222_1$	$P222_1$	$P2_122$	$P2_122$	$P22_12$	$P22_12$
18	D_2^3	$P2_12_12$	$P2_12_12$	$P2_12_12$	$P22_12_1$	$P22_12_1$	$P2_122_1$	$P2_122_1$
19	D_2^4	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
20	D_2^5	$C222_1$	$C222_1$ $2_12_12_1$	$C222_1$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$A2_122$ $2_12_12_1$	$B22_12$ $2_12_12_1$	$B22_12$ $2_12_12_1$
21	D_2^6	$C222$	$C222$ 2_12_12	$C222$ 2_12_12	$A222$ 22_12_1	$A222$ 22_12_1	$B222$ 2_122_1	$B222$ 2_122_1
22	D_2^7	$F222$	$F222$ 2_12_12 22_12_1 2_122_1	$F222$ 2_12_12 2_122_1 22_12_1	$F222$ 22_12_1 2_122_1 2_12_12	$F222$ 22_12_1 2_12_12 2_122_1	$F222$ 2_122_1 2_12_12 22_12_1	$F222$ 2_122_1 22_12_1 2_12_12
23	D_2^8	$I222$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$	$I222$ $2_12_12_1$
24	D_2^9	$I2_12_12_1$	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222	$I2_12_12_1$ 222
25	C_{2v}^1	$Pmm2$	$Pmm2$	$Pmm2$	$P2mm$	$P2mm$	$Pm2m$	$Pm2m$
26	C_{2v}^2	$Pmc2_1$	$Pmc2_1$	$Pcm2_1$	$P2_1ma$	$P2_1am$	$Pb2_1m$	$Pm2_1b$
27	C_{2v}^3	$Pcc2$	$Pcc2$	$Pcc2$	$P2aa$	$P2aa$	$Pb2b$	$Pb2b$
28	C_{2v}^4	$Pma2$	$Pma2$	$Pbm2$	$P2mb$	$P2cm$	$Pc2m$	$Pm2a$
29	C_{2v}^5	$Pca2_1$	$Pca2_1$	$Pbc2_1$	$P2_1ab$	$P2_1ca$	$Pc2_1b$	$Pb2_1a$
30	C_{2v}^6	$Pnc2$	$Pnc2$	$Pcn2$	$P2na$	$P2an$	$Pb2n$	$Pn2b$
31	C_{2v}^7	$Pmn2_1$	$Pmn2_1$	$Pnm2_1$	$P2_1mn$	$P2_1nm$	$Pn2_1m$	$Pm2_1n$
32	C_{2v}^8	$Pba2$	$Pba2$	$Pba2$	$P2cb$	$P2cb$	$Pc2a$	$Pc2a$
33	C_{2v}^9	$Pna2_1$	$Pna2_1$	$Pbn2_1$	$P2_1nb$	$P2_1cn$	$Pc2_1n$	$Pn2_1a$
34	C_{2v}^{10}	$Pnn2$	$Pnn2$	$Pnn2$	$P2nn$	$P2nn$	$Pn2n$	$Pn2n$

ORTHORHOMBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**ba$\bar{c}$**	**cab**	**$\bar{c}$ba**	**bca**	**a$\bar{c}$b**
35	C_{2v}^{11}	$Cmm2$	$Cmm2$ $ba2$	$Cmm2$ $ba2$	$A2mm$ $2cb$	$A2mm$ $2cb$	$Bm2m$ $c2a$	$Bm2m$ $c2a$
36	C_{2v}^{12}	$Cmc2_1$	$Cmc2_1$ $bn2_1$	$Ccm2_1$ $na2_1$	$A2_1ma$ 2_1cn	$A2_1am$ 2_1nb	$Bb2_1m$ $n2_1a$	$Bm2_1b$ $c2_1n$
37	C_{2v}^{13}	$Ccc2$	$Ccc2$ $nn2$	$Ccc2$ $nn2$	$A2aa$ $2nn$	$A2aa$ $2nn$	$Bb2b$ $n2n$	$Bb2b$ $n2n$
38	C_{2v}^{14}	$Amm2$	$Amm2$ $nc2_1$	$Bmm2$ $cn2_1$	$B2mm$ 2_1na	$C2mm$ 2_1an	$Cm2m$ $b2_1n$	$Am2m$ $n2_1b$
39*	C_{2v}^{15}	$Aem2$	$Aem2$ $ec2_1$	$Bme2$ $ce2_1$	$B2em$ 2_1ea	$C2me$ 2_1ae	$Cm2e$ $b2_1e$	$Ae2m$ $e2_1b$
40	C_{2v}^{16}	$Ama2$	$Ama2$ $nn2_1$	$Bbm2$ $nn2_1$	$B2mb$ 2_1nn	$C2cm$ 2_1nn	$Cc2m$ $n2_1n$	$Am2a$ $n2_1n$
41*	C_{2v}^{17}	$Aea2$	$Aea2$ $en2_1$	$Bbe2$ $ne2_1$	$B2eb$ 2_1en	$C2ce$ 2_1ne	$Cc2e$ $n2_1e$	$Ae2a$ $e2_1n$
42	C_{2v}^{18}	$Fmm2$	$Fmm2$ $ba2$ $nc2_1$ $cn2_1$	$Fmm2$ $ba2$ $cn2_1$ $nc2_1$	$F2mm$ $2cb$ 2_1na 2_1an	$F2mm$ $2cb$ 2_1an 2_1na	$Fm2m$ $c2a$ $b2_1n$ $n2_1b$	$Fm2m$ $c2a$ $n2_1b$ $b2_1n$
43	C_{2v}^{19}	$Fdd2$	$Fdd2$ $dd2_1$	$Fdd2$ $dd2_1$	$F2dd$ 2_1dd	$F2dd$ 2_1dd	$Fd2d$ $d2_1d$	$Fd2d$ $d2_1d$
44	C_{2v}^{20}	$Imm2$	$Imm2$ $nn2_1$	$Imm2$ $nn2_1$	$I2mm$ 2_1nn	$I2mm$ 2_1nn	$Im2m$ $n2_1n$	$Im2m$ $n2_1n$
45	C_{2v}^{21}	$Iba2$	$Iba2$ $cc2_1$	$Iba2$ $cc2_1$	$I2cb$ 2_1aa	$I2cb$ 2_1aa	$Ic2a$ $b2_1b$	$Ic2a$ $b2_1b$
46	C_{2v}^{22}	$Ima2$	$Ima2$ $nc2_1$	$Ibm2$ $cn2_1$	$I2mb$ 2_1na	$I2cm$ 2_1an	$Ic2m$ $b2_1n$	$Im2a$ $n2_1b$

ORTHORHOMBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**ba$\bar{c}$**	**cab**	**$\bar{c}$ba**	**bca**	**a$\bar{c}$b**
47	D_{2h}^{1}	$P\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*	*Pmmm*
48	D_{2h}^{2}	$P\frac{2}{n}\frac{2}{n}\frac{2}{n}$	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*	*Pnnn*
49	D_{2h}^{3}	$P\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Pccm*	*Pccm*	*Pmaa*	*Pmaa*	*Pbmb*	*Pbmb*
50	D_{2h}^{4}	$P\frac{2}{b}\frac{2}{a}\frac{2}{n}$	*Pban*	*Pban*	*Pncb*	*Pncb*	*Pcna*	*Pcna*
51	D_{2h}^{5}	$P\frac{2_1}{m}\frac{2}{m}\frac{2}{a}$	*Pmma*	*Pmmb*	*Pbmm*	*Pcmm*	*Pmcm*	*Pmam*
52	D_{2h}^{6}	$P\frac{2}{n}\frac{2_1}{n}\frac{2}{a}$	*Pnna*	*Pnnb*	*Pbnn*	*Pcnn*	*Pncn*	*Pnan*
53	D_{2h}^{7}	$P\frac{2}{m}\frac{2}{n}\frac{2_1}{a}$	*Pmna*	*Pnmb*	*Pbmn*	*Pcnm*	*Pncm*	*Pman*
54	D_{2h}^{8}	$P\frac{2_1}{c}\frac{2}{c}\frac{2}{a}$	*Pcca*	*Pccb*	*Pbaa*	*Pcaa*	*Pbcb*	*Pbab*
55	D_{2h}^{9}	$P\frac{2_1}{b}\frac{2_1}{a}\frac{2}{m}$	*Pbam*	*Pbam*	*Pmcb*	*Pmcb*	*Pcma*	*Pcma*
56	D_{2h}^{10}	$P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}$	*Pccn*	*Pccn*	*Pnaa*	*Pnaa*	*Pbnb*	*Pbnb*
57	D_{2h}^{11}	$P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}$	*Pbcm*	*Pcam*	*Pmca*	*Pmab*	*Pbma*	*Pcmb*
58	D_{2h}^{12}	$P\frac{2_1}{n}\frac{2_1}{n}\frac{2}{m}$	*Pnnm*	*Pnnm*	*Pmnn*	*Pmnn*	*Pnmn*	*Pnmn*
59	D_{2h}^{13}	$P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}$	*Pmmn*	*Pmmn*	*Pnmm*	*Pnmm*	*Pmnm*	*Pmnm*
60	D_{2h}^{14}	$P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$	*Pbcn*	*Pcan*	*Pnca*	*Pnab*	*Pbna*	*Pcnb*
61	D_{2h}^{15}	$P\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*Pbca*	*Pcab*	*Pbca*	*Pcab*	*Pbca*	*Pcab*

ORTHORHOMBIC SYSTEM (*cont.*)

No. of space group	Schoenflies symbol	Standard full Hermann–Mauguin symbol **abc**	Extended Hermann–Mauguin symbols for the six settings of the same unit cell					
			abc (standard)	**ba$\bar{\mathbf{c}}$**	**cab**	**$\bar{\mathbf{c}}$ba**	**bca**	**a$\bar{\mathbf{c}}$b**
62	D_{2h}^{16}	$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	*Pnma*	*Pmnb*	*Pbnm*	*Pcmn*	*Pmcn*	*Pnam*
63	D_{2h}^{17}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{m}$	*Cmcm* *bnn*	*Ccmm* *nan*	*Amma* *ncn*	*Amam* *nnb*	*Bbmm* *nna*	*Bmmb* *cnn*
64*†	D_{2h}^{18}	$C\frac{2}{m}\frac{2}{c}\frac{2_1}{e}$	*Cmce* *bne*	*Ccme* *nae*	*Aema* *ecn*	*Aeam* *enb*	*Bbem* *nea*	*Bmeb* *cen*
65	D_{2h}^{19}	$C\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Cmmm* *ban*	*Cmmm* *ban*	*Ammm* *ncb*	*Ammm* *ncb*	*Bmmm* *cna*	*Bmmm* *cna*
66	D_{2h}^{20}	$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$	*Cccm* *nnn*	*Cccm* *nnn*	*Amaa* *nnn*	*Amaa* *nnn*	*Bbmb* *nnn*	*Bbmb* *nnn*
67*†	D_{2h}^{21}	$C\frac{2}{m}\frac{2}{m}\frac{2}{e}$	*Cmme* *bae*	*Cmme* *bae*	*Aemm* *ecb*	*Aemm* *ecb*	*Bmem* *cea*	*Bmem* *cea*
68*	D_{2h}^{22}	$C\frac{2}{c}\frac{2}{c}\frac{2}{e}$	*Ccce* *nne*	*Ccce* *nne*	*Aeaa* *enn*	*Aeaa* *enn*	*Bbeb* *nen*	*Bbeb* *nen*
69	D_{2h}^{23}	$F\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*Fmmm* *ban* *ncb* *cna*	*Fmmm* *ban* *cna* *ncb*	*Fmmm* *ncb* *cna* *ban*	*Fmmm* *ncb* *ban* *cna*	*Fmmm* *cna* *ban* *ncb*	*Fmmm* *cna* *ncb* *ban*
70	D_{2h}^{24}	$F\frac{2}{d}\frac{2}{d}\frac{2}{d}$	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*
71	D_{2h}^{25}	$I\frac{2}{m}\frac{2}{m}\frac{2}{m}$	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*	*I mmm* *nnn*
72	D_{2h}^{26}	$I\frac{2}{b}\frac{2}{a}\frac{2}{m}$	*I bam* *ccn*	*I bam* *ccn*	*I mcb* *naa*	*I mcb* *naa*	*I cma* *bnb*	*I cma* *bnb*
73	D_{2h}^{27}	$I\frac{2_1}{b}\frac{2_1}{c}\frac{2_1}{a}$	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*	*I bca* *cab*	*I cab* *bca*
74†	D_{2h}^{28}	$I\frac{2_1}{m}\frac{2_1}{m}\frac{2_1}{a}$	*I mma* *nnb*	*I mmb* *nna*	*I bmm* *cnn*	*I cmm* *bnn*	*I mcm* *nan*	*I mam* *ncn*

* For the five space groups *Aem*2 (39), *Aea*2 (41), *Cmce* (64), *Cmme* (67) and *Ccce* (68), the ‘new’ space-group symbols, containing the symbol ‘*e*’ for the ‘double’ glide plane, are given for all settings. These symbols were first introduced in the Fourth Edition of this volume (*IT* 1995); *cf. Foreword to the Fourth Edition*. For further explanations, see Section 1.3.2, Note (x) and the space-group diagrams.

† For space groups *Cmca* (64), *Cmma* (67) and *Imma* (74), the first lines of the extended symbols, as tabulated here, correspond with the symbols for the six settings in the diagrams of these space groups (Part 7). An alternative formulation which corresponds with the coordinate triplets is given in Section 4.3.3.

空间群-II

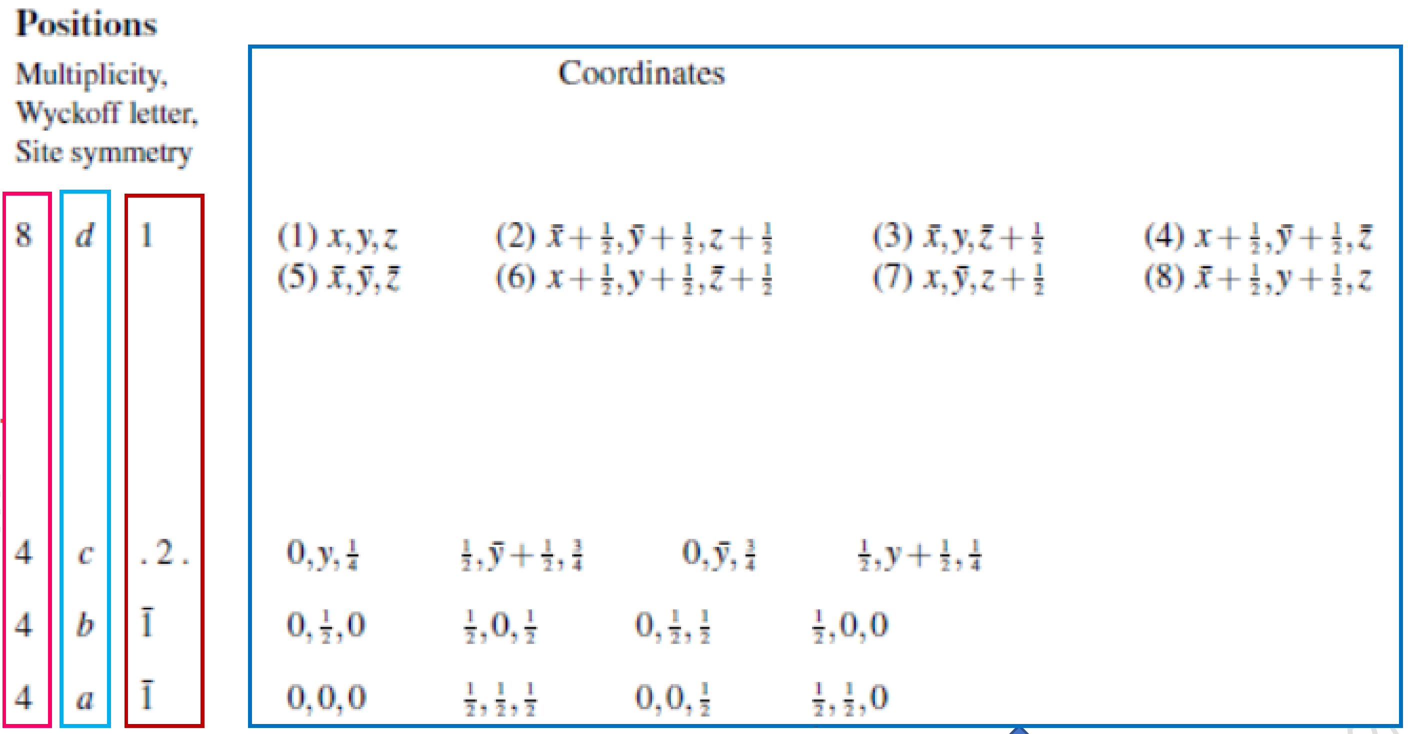
结构参数与衍射条件

结构参数

$Pbcn$ D_{2h}^{14} mmm Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry $Pmmm$

多重性(multiplicity): 告诉我们如果安置一个特定原子在该位置，经过空间群的所有对称性操后总共会产生原子数目，称等效点数目。有一般和特殊等效点系。一般等效点系是经过空间群的全部对称元素操作得到的全部点。等效点位置的对称性最低（1次轴），数目最多。该空间群的一般等效点数目为“8”。特殊等效点系的点处于特殊位置，处于等效元素上得到的一组点，数目比一般等效点数目少。



Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
8	d	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$
4	c	. 2 .	$0,y,\frac{1}{4}$	$\frac{1}{2},\bar{y}+\frac{1}{2},\frac{3}{4}$	$0,\bar{y},\frac{3}{4}$	$\frac{1}{2},y+\frac{1}{2},\frac{1}{4}$
4	b	$\bar{1}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$

Wychoff 等效点系记号，从高对称性开始按英文字母顺序指定的位置标记。如在此空间群中“*c*” 表示该等效点数目“4”，等效点系位于*b*方向的“2”次轴上，以及对应的等效点坐标。在描述结构表中以“4*c*”表示。

对称元素(symmetry): 等效点所处位置的对称元素。

等效点系的全部位置的坐标： 等效点是指如4*a*的等效点处于对称中心位置，通过空间群的所有对称操作后会产生4个等效位置：0,0,0; ½, ½, ½; 0,0, ½; ½, ½,0。

$C1m1$

C-*center* : lattice

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},0)+$

Reflection conditions

General:

4 b 1 (1) x,y,z (2) $x,\bar{y},z$

hkl : $h+k=2n$ Independent

$h0l$: $h=2n$

$0kl$: $k=2n$

$hk0$: $h+k=2n$

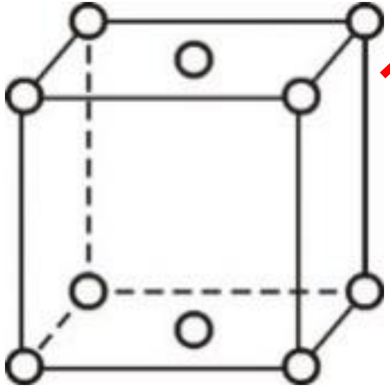
$0k0$: $k=2n$

$h00$: $h=2n$

Dependent

Special: no extra conditions

2 a m $x,0,z$



C-face center

$A1m1$

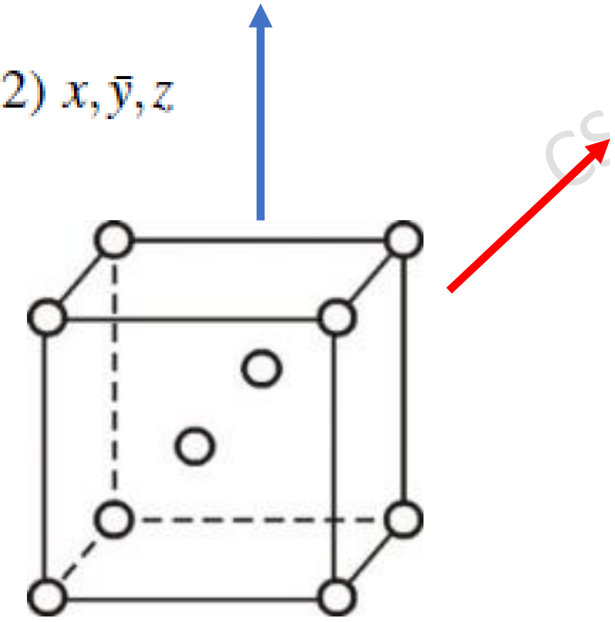
Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+ \quad (0,\tfrac{1}{2},\tfrac{1}{2})+$

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



A-face center

Reflection conditions

General:

hkl : $k+l=2n$ Independent

$h0l$: $l=2n$
$0kl$: $k+l=2n$
$hk0$: $k=2n$
$0k0$: $k=2n$
$00l$: $l=2n$

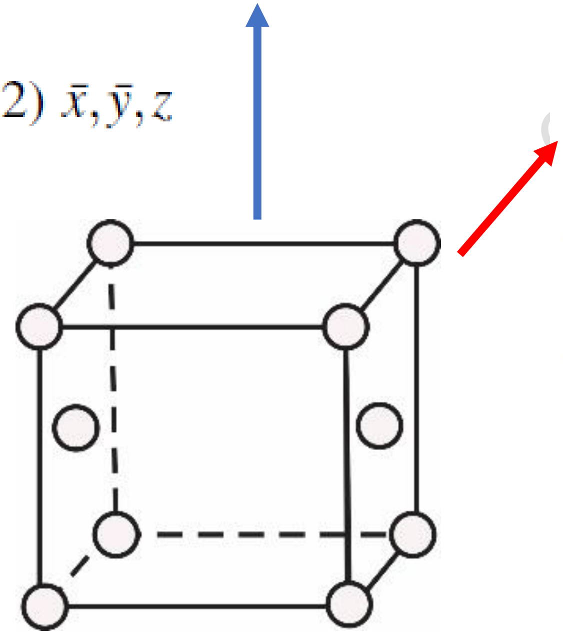
Dependent

Special: no extra conditions

$B112$

Positions

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



B-face center

Reflection conditions

General:

hkl : $h+l=2n$ Independent

$hk0$: $h=2n$

$0kl$: $l=2n$

$h0l$: $h+l=2n$

$00l$: $l=2n$

$h00$: $h=2n$

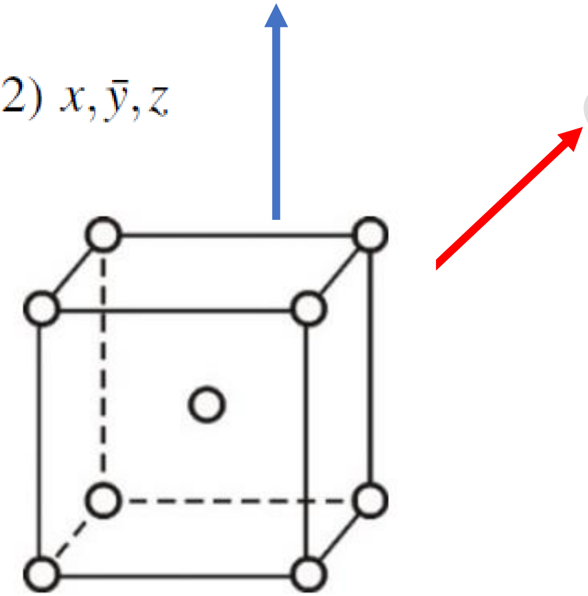
Dependent

Special: no extra conditions

$I\,1m1$

Positions

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



Body center

Reflection conditions

General:

$$hkl : h+k+l=2n \quad \text{Independent}$$

$$\left.\begin{array}{l} h0l : h+l=2n \\ 0kl : k+l=2n \\ hk0 : h+k=2n \\ 0k0 : k=2n \\ h00 : h=2n \\ 00l : l=2n \end{array}\right\} \text{Dependent}$$

Special: no extra conditions

Fmmm

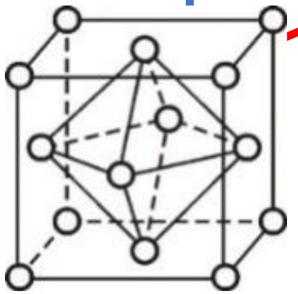
Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$	General:
32	*p*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	hkl : $h+k,h+l,k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$	$0kl$: $k,l=2n$
							$h0l$: $h,l=2n$
							$hk0$: $h,k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
16	*o*	. . *m*	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	no extra conditions

Independent

Dependent

All-face center

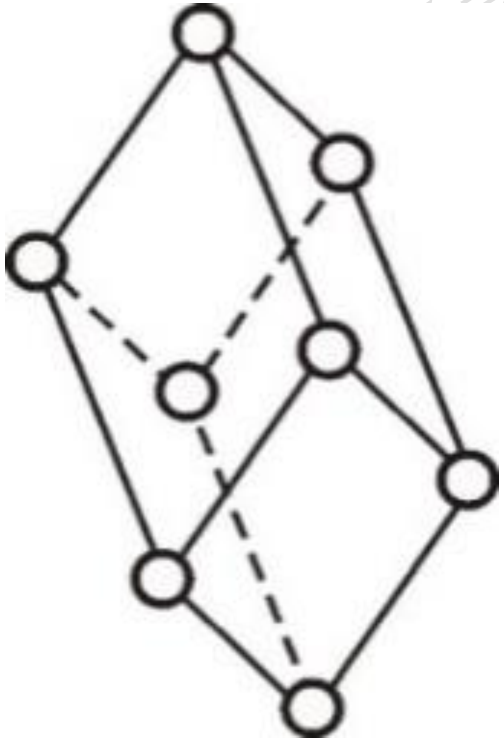


No. 160 *R*3*m*

RHOMBOHEDRAL AXES

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
6	*c*	1	(1) x,y,z (4) z,y,x	(2) z,x,y (5) y,x,z	(3) y,z,x (6) x,z,y
3	*b*	$.m$	x,x,z	z,x,x	x,z,x
1	*a*	$3m$	x,x,x		



Reflection conditions

General:

no conditions

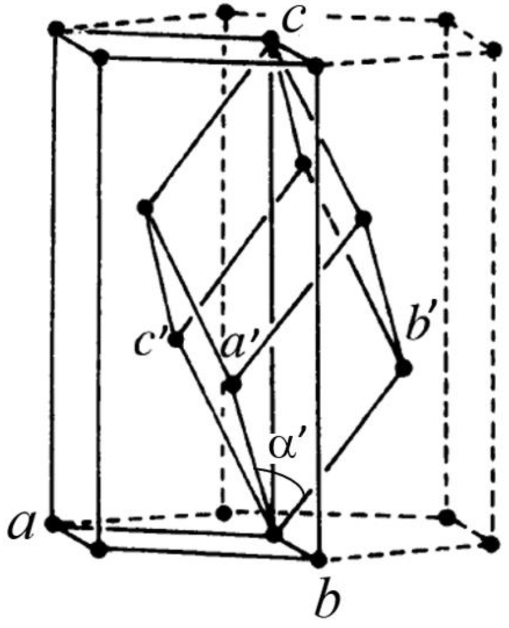
Special: no extra conditions

No. 160 *R*3*m*

HEXAGONAL AXES

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates		
			$(0,0,0)+$	$(\frac{2}{3},\frac{1}{3},\frac{1}{3})+$	$(\frac{1}{3},\frac{2}{3},\frac{2}{3})+$
18	*c*	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$
			(4) $\bar{y},\bar{x},z$	(5) $\bar{x}+y,y,z$	(6) $x,x-y,z$
9	*b*	$.m$	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$
3	*a*	$3m$	$0,0,z$		



Reflection conditions

General:

Independent

$hkil$: $-h+k+l=3n$

$hki0$: $-h+k=3n$
$hh\bar{2h}l$: $l=3n$
$h\bar{h}0l$: $h+l=3n$
$000l$: $l=3n$
$h\bar{h}00$: $h=3n$

Dependent

Special: no extra conditions

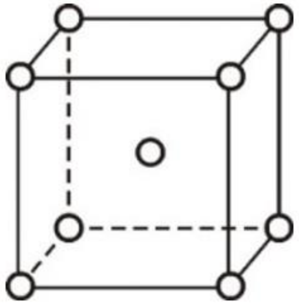
Ibca

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			$(0,0,0)+ \quad (\frac{1}{2},\frac{1}{2},\frac{1}{2})+$				General:
16	*f*	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	hkl : $h+k+l=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h,k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	*e*	. . 2	$0,\frac{1}{4},z$	$0,\frac{3}{4},\bar{z}+\frac{1}{2}$	$0,\frac{3}{4},\bar{z}$	$0,\frac{1}{4},z+\frac{1}{2}$	hkl : $l=2n$
8	*d*	. 2 .	$\frac{1}{4},y,0$	$\frac{1}{4},\bar{y},\frac{1}{2}$	$\frac{3}{4},\bar{y},0$	$\frac{3}{4},y,\frac{1}{2}$	hkl : $k=2n$
8	*c*	2 . .	$x,0,\frac{1}{4}$	$\bar{x}+\frac{1}{2},0,\frac{3}{4}$	$\bar{x},0,\frac{3}{4}$	$x+\frac{1}{2},0,\frac{1}{4}$	hkl : $h=2n$
8	*b*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	hkl : $k,l=2n$
8	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $k,l=2n$

Body-centred

independent



Dependent

特殊位置

Pbcn D_{2h}^{14} *mmm* Orthorhombic

No. 60 $P\ 2_1/b\ 2/c\ 2_1/n$ Patterson symmetry *Pmmm*

P *mmm* 劳埃群

Paterson群

Table 2.2.5.1. *Patterson symmetries for three dimensions*

Laue class	Lattice type					Patterson symmetry (with space-group number)				
$\bar{1}$	*P*					$P\bar{1}$ (2)				
$2/m$	*P*	*C*				$P2/m$ (10)	$C2/m$ (12)			
mmm	*P*	*C*	*I*	*F*		*Pmmm* (47)	*Cmmm* (65)	*Immm* (71)	*Fmmm* (69)	
$4/m$	*P*		*I*			$P4/m$ (83)		$I4/m$ (87)		
$4/mmm$	*P*		*I*			$P4/mmm$ (123)		$I4/mmm$ (139)		
$\bar{3}$	*P*				*R*	$P\bar{3}$ (147)				$R\bar{3}$ (148)
$\bar{3}m1$	*P*				*R*	$P\bar{3}m1$ (164)				$R\bar{3}m$ (166)
$\bar{3}1m$	*P*					$P\bar{3}1m$ (162)				
$6/m$	*P*					$P6/m$ (175)				
$6/mmm$	*P*					$P6/mmm$ (191)				
$m\bar{3}$	*P*		*I*	*F*		$Pm\bar{3}$ (200)		$Im\bar{3}$ (204)	$Fm\bar{3}$ (202)	
$m\bar{3}m$	*P*		*I*	*F*		$Pm\bar{3}m$ (221)		$Im\bar{3}m$ (229)	$Fm\bar{3}m$ (225)	

$$P(x,y,z)=\frac{1}{V}\sum_h\sum_k\sum_l |F(hkl)|^2\cos 2\pi(hx+ky+lz).$$

The symbol for the Patterson space group of a crystal structure can be deduced from that of its space group in two steps:
(i) Glide planes and screw axes have to be replaced by the corresponding mirror planes and rotation axes, resulting in a symmorphic space group.
(ii) If this symmorphic space group is not centrosymmetric, inversions have to be added.

三斜晶系：只有一次轴

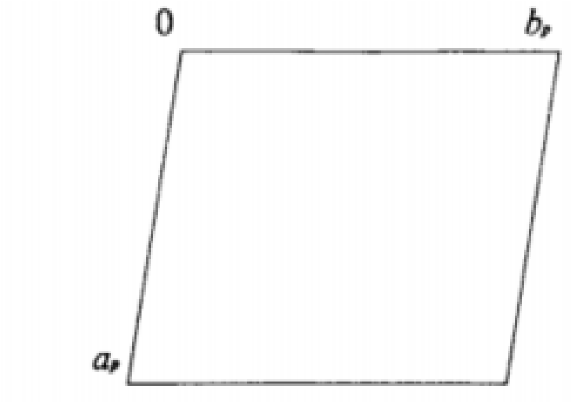
点阵符号后是1或 -1 （如：*P*1， *P*$\bar{1}$）

$P1$ C_1^1

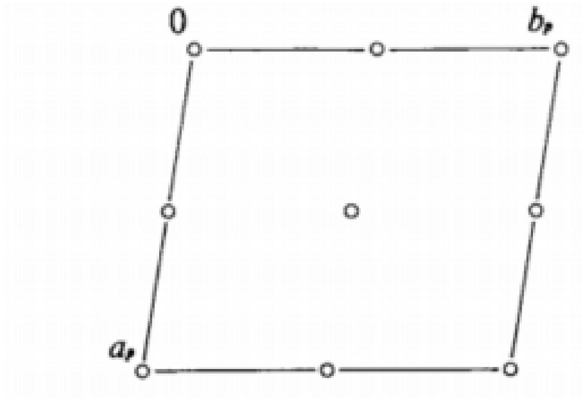
No. 1 $P1$

$P\bar{1}$ C_i^1

No. 2 $P\bar{1}$



Origin arbitrary



Origin at $\bar{1}$

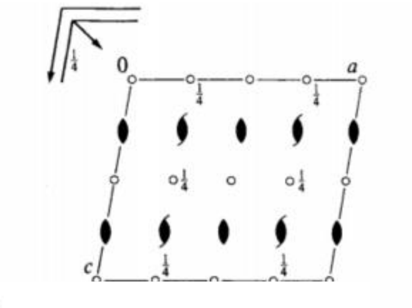
单斜晶系：只有一个二次轴

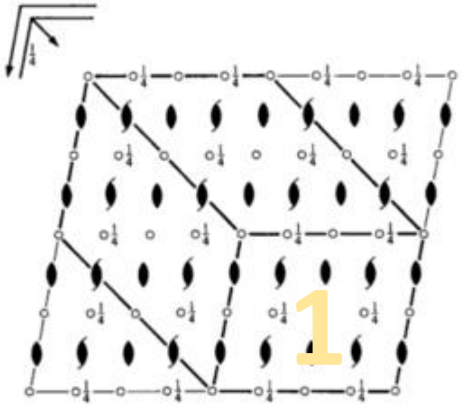
点阵符号后有：唯一的镜面，滑移面，2次旋转轴或者2次螺旋轴，或者轴/平面符号（即：*Cc*，*P*2， *P*2_1/*n*)

$C2/c$　　C_{2h}^6

No. 15　　$C12/c1$

UNIQUE AXIS *b*, CELL CHOICE 1





Origin at $\bar{1}$ on glide plane *c*

$A112/a$　**Origin** at $\bar{1}$ on glide plane *a*

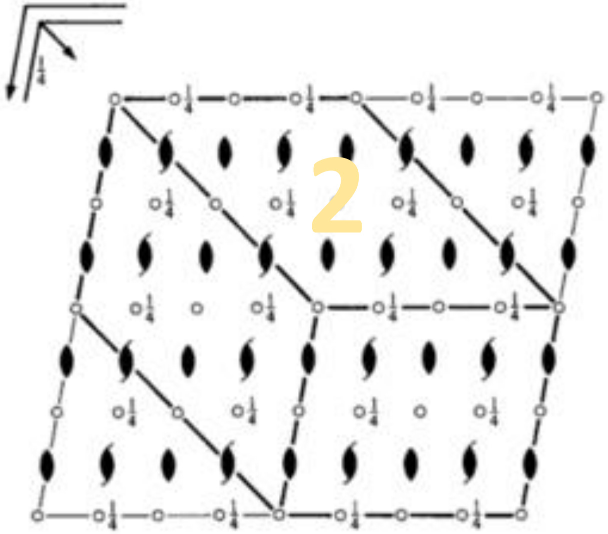
UNIQUE AXIS *c*, CELL CHOICE 1

$A12/n1$

UNIQUE AXIS *b*, CELL CHOICE 2

$B112/n$

UNIQUE AXIS *c*, CELL CHOICE 2



Origin at $\bar{1}$ on glide plane *n*

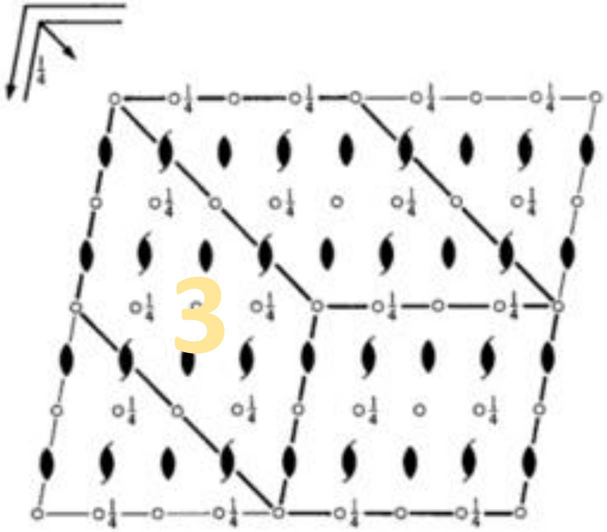
Origin at $\bar{1}$ on glide plane *n*

$I12/a1$

UNIQUE AXIS *b*, CELL CHOICE 3

$I112/b$

UNIQUE AXIS *c*, CELL CHOICE 3



Origin at $\bar{1}$ on glide plane *a*

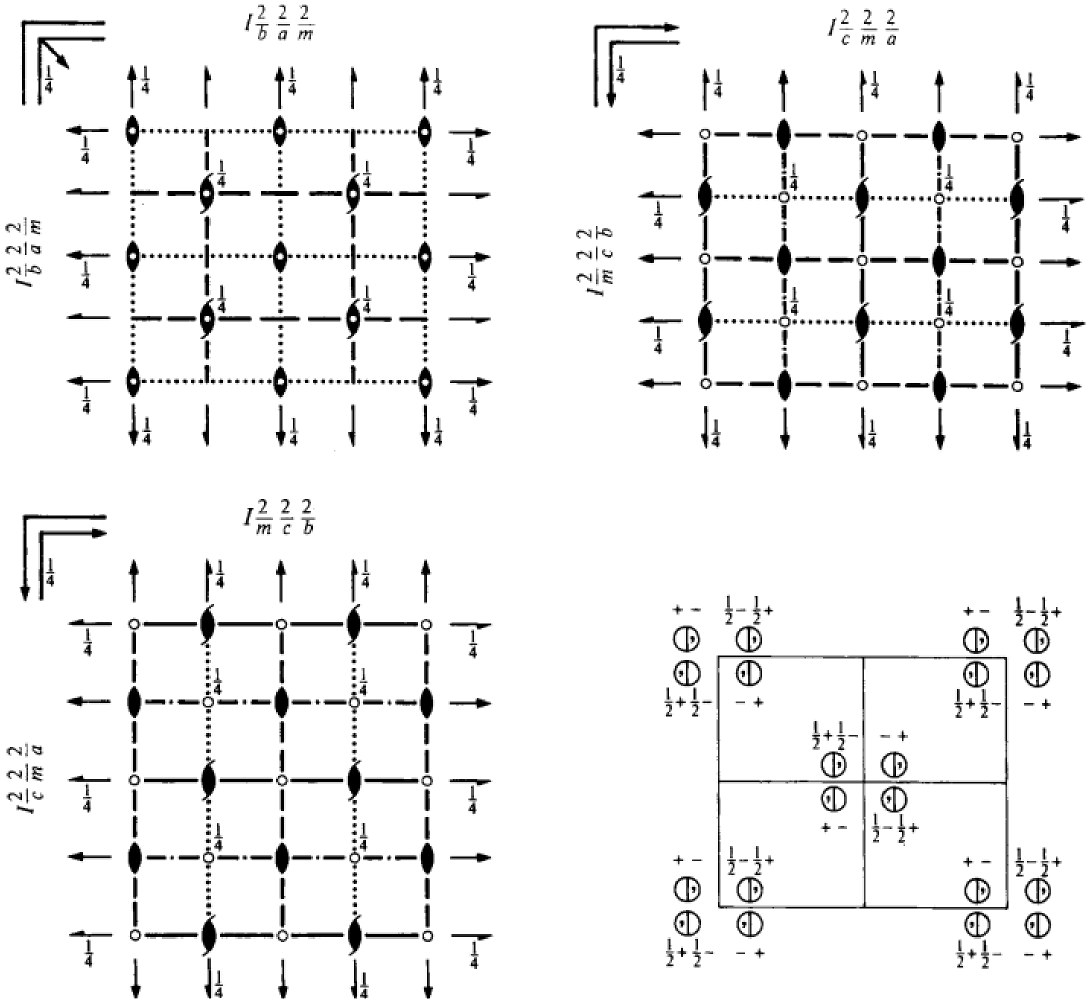
Origin at $\bar{1}$ on glide plane *b*

Ibam D_{2h}^{26} *mmm* Orthorhombic

No. 72 $I\ 2/b\ 2/a\ 2/m$ Patterson symmetry *Immm*

正交：有三个互相垂直的二次轴

点阵符号后的：全部三个符号是镜面，滑移面，2次旋转轴或2次螺旋轴（即：*Pnma*, *Cmc*2_1, *Pnc*2)



Origin at centre $(2/m)$ at $cc2/m$

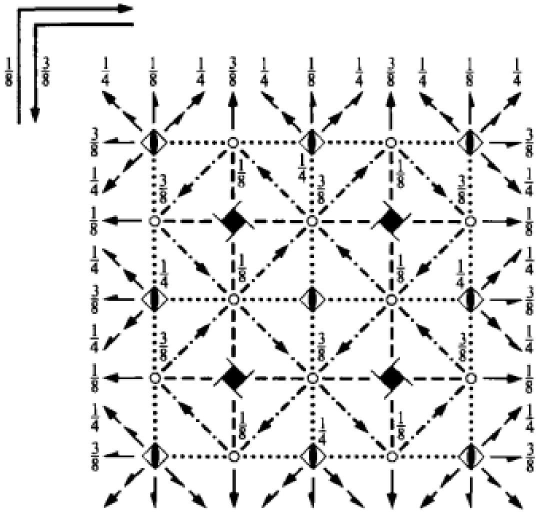
四方晶系：唯一的高次轴是四次轴

第一个对称符号：4, $\bar{4}$, 4_1, 4_2或4_3（如：$P\bar{4}$，$P4_12_12$, $I4/m$, $P4/mcc$)

$I4_1/acd$ D_{4h}^{20}

No. 142 $I\ 4_1/a\ 2/c\ 2/d$

ORIGIN CHOICE 1



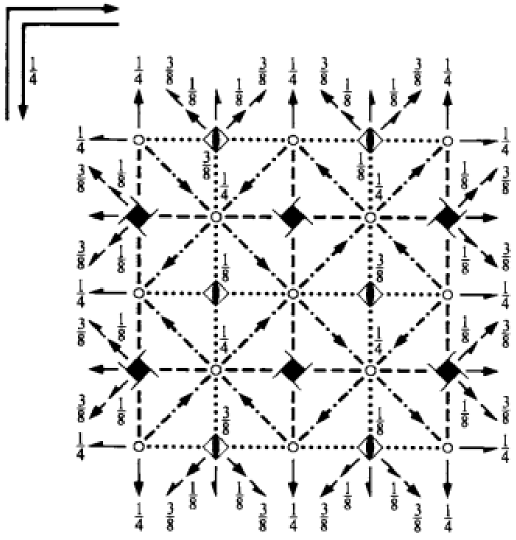
Origin at $\bar{4}c2_1$, at $0, \frac{1}{4}, -\frac{1}{8}$ from $\bar{1}$

8	*a*	$\bar{4}$..	0,0,0	$0,\frac{1}{2},\frac{1}{4}$	$\frac{1}{2},0,\frac{1}{4}$	$\frac{1}{2},\frac{1}{2},0$

$I4_1/acd$ D_{4h}^{20}

No. 142 $I\ 4_1/a\ 2/c\ 2/d$

ORIGIN CHOICE 2



Origin at $\bar{1}$ at $b(c,a)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}$

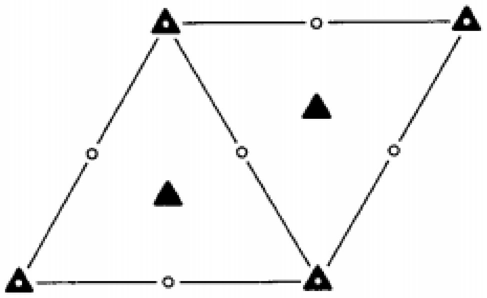
8	*a*	$\bar{4}$..	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{3}{4},\frac{3}{8}$

三方晶系：唯一的高次轴是三次轴

第一个对称符号：3, $\bar{3}$, 3_1, 或3_2（如：$P3_1m$, $R3$, $R\bar{3}c$, $P312$)

$P\bar{3}$ C_{3i}^{1}

No. 147 $P\bar{3}$

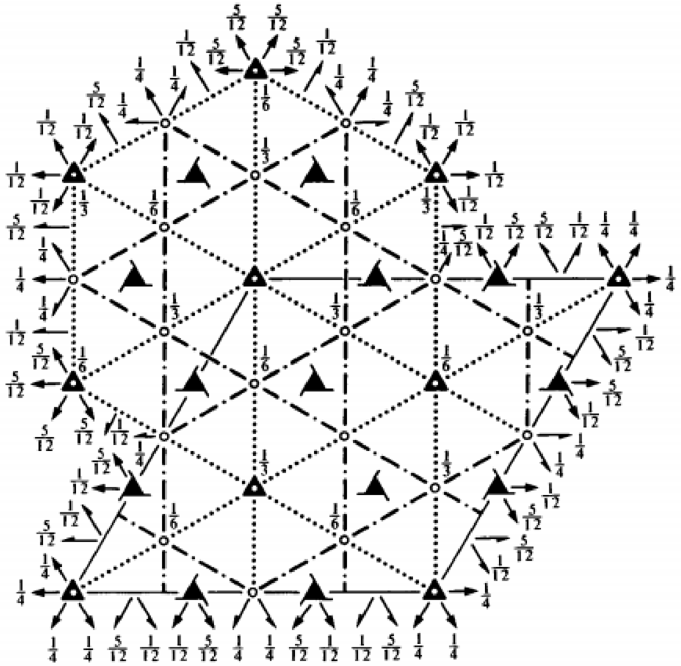


Origin at centre ($\bar{3}$)

$R\bar{3}c$ D_{3d}^{6} $\bar{3}m$

No. 167 $R\bar{3}2/c$

HEXAGONAL AXES



Origin at centre ($\bar{3}$) at $\bar{3}c$

三方晶系的***R***点阵可以选择

Rhombohedral axes setting或Hexagonal axes setting

六方晶系：唯一的高次轴是六次轴

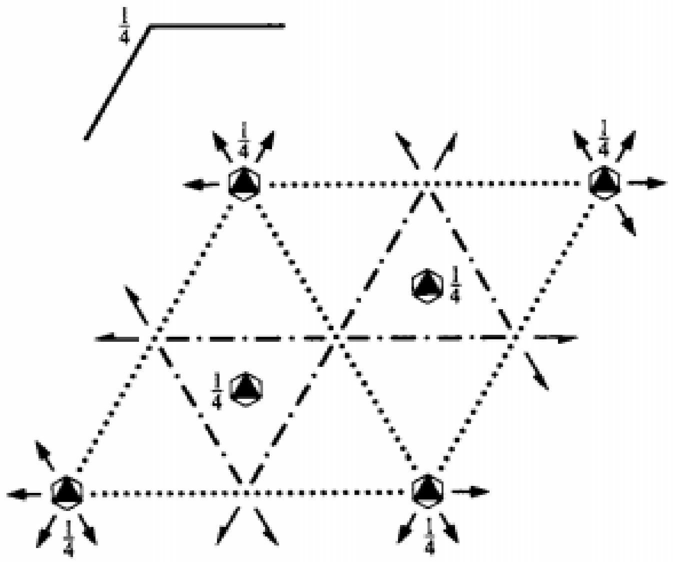
第一个对称符号：6，$\bar{6}$，6_1，6_2，6_3，6_4，6_5（如：*P6mm*，*P$\bar{6}$*，*P6_3/mcm*）

$P\bar{6}2c$ D_{3h}^{4}

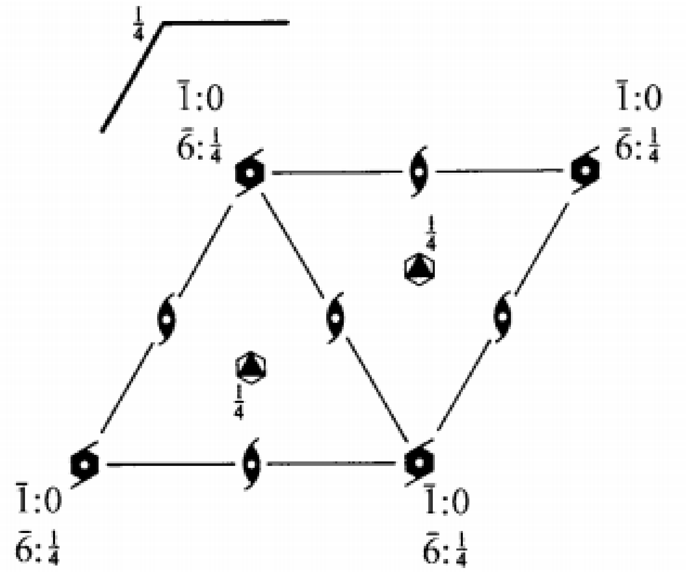
No. 190 $P\bar{6}2c$

$P6_3/m$ C_{6h}^{2}

No. 176 $P6_3/m$



Origin at 32c



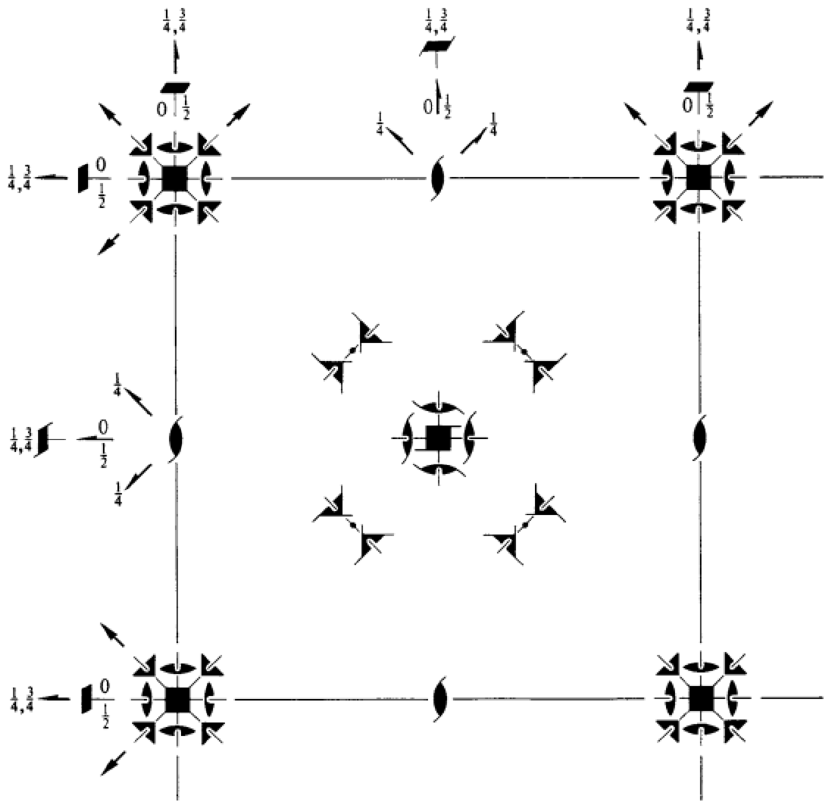
Origin at centre ($\bar{3}$) on 6_3

立方晶系：有四个三次轴

第二个对称符号：3或 $\bar{3}$（如：$Ia3$，$Pm\bar{3}m$, $Fd\bar{3}m$)

$F432$ O^3 432

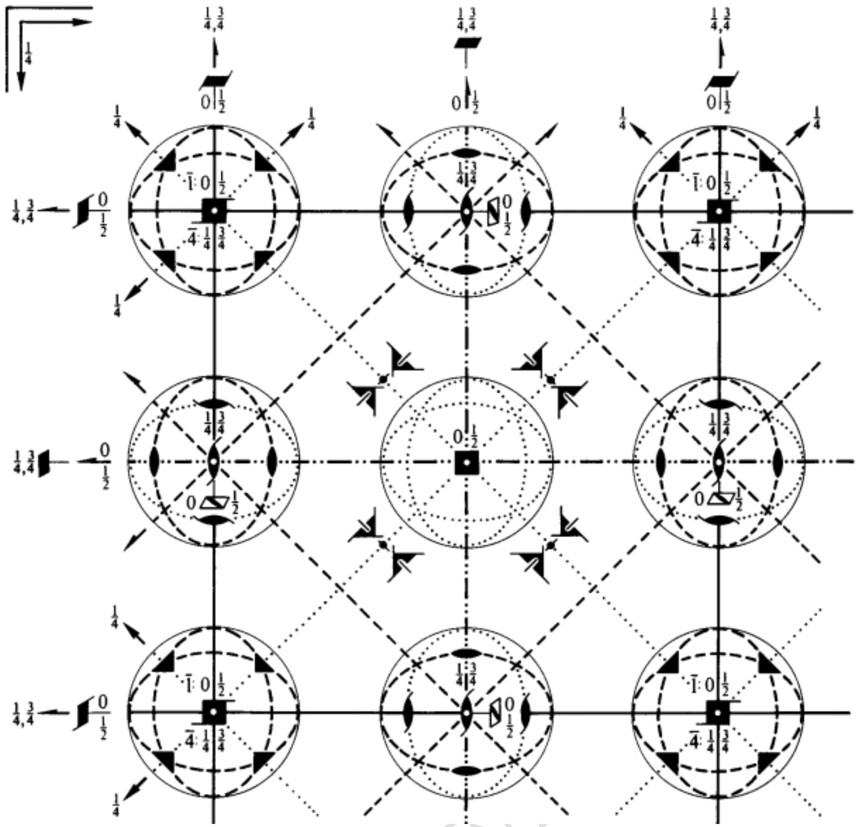
No. 209 $F432$ Patters



Origin at 432

$Fm\bar{3}c$ O_h^6 $m\bar{3}m$

No. 226 $F\ 4/m\ \bar{3}\ 2/c$ Patterson sy



Origin at centre ($m\bar{3}$ **)**

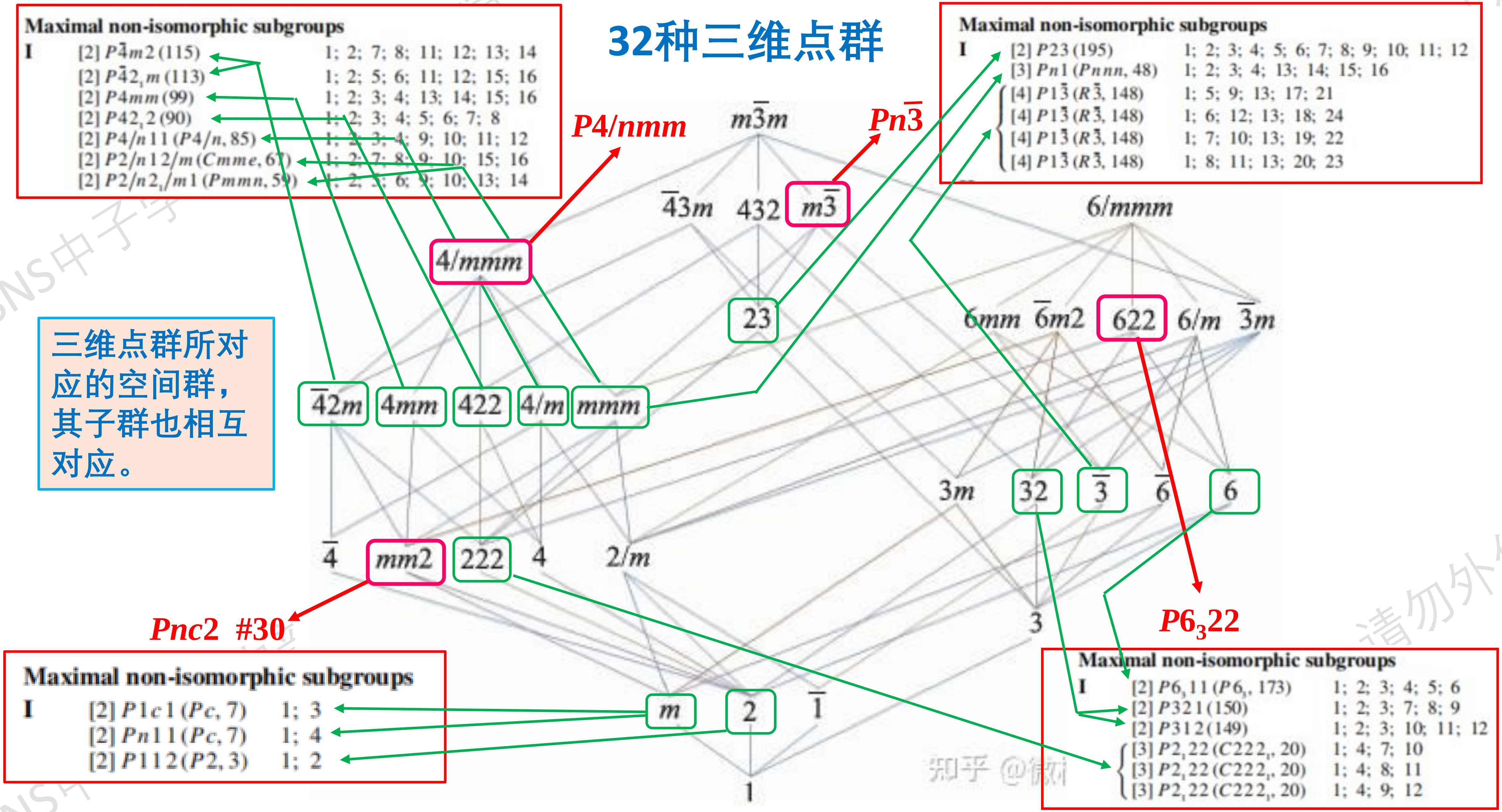
辨别晶系的简单方法

Symbol	从对称性辨认晶系	从空间群符号辨认晶系
Triclinic	只有一次轴或一次反演轴	点阵符号后是1或 $\bar{1}$（如：$P\bar{1}$， P1）
Monoclinic	最高对称元素是：1个二次轴或镜面	点阵符号后有：唯一的镜面，滑移面，2次旋转轴或者2次螺旋轴，或者轴/平面符号（即：*Cc*，*P2*， $P2_1/n$)
Orthorhombic	最高对称元素是：2个以上的二次轴或镜面	点阵符号后的：全部三个符号是镜面，滑移面，2次旋转轴或2次螺旋轴（即：*P222*，*Pnma*, $Cmc2_1$, *Pnc2*)
Tetragonal	最高对称元素是：唯一的高次轴是四次轴或四次螺旋轴或反演轴	第一个对称符号：$\bar{4}$, 4, 4_1, 4_2或4_3（如：¯ *P4*，$P4_12_12$, *I4/m*, *P4/mcc*)
Trigonal **Rhombohedral**	最高对称元素具有：唯一的高次轴是三次轴或三次螺旋轴或反演轴	第一个对称符号：3, $\bar{3}$, 3_1, 或3_2（如：$P3_1m$, $R\bar{3}$, *R3c*, *P312*)
Hexagonal	最高对称元素具：有唯一的高次轴是六次轴或六次螺旋轴或反演轴	第一个对称符号：6，$\bar{6}$，6_1，6_2，6_3，6_4，6_5（如：*P6mm*，$P\bar{6}$，$P6_3/mcm$)
Cubic	具有：四个三次轴	第二个对称符号：3或 $\bar{3}$（如：*Ia*3，$Pm\bar{3}m$, $Fd\bar{3}m$)

空间群-III

子群和超群

32种三维点群



Maximal non-isomorphic subgroups

I	[2] $P\bar{4}m2$ (115)	1; 2; 7; 8; 11; 12; 13; 14
	[2] $P\bar{4}2_1m$ (113)	1; 2; 5; 6; 11; 12; 15; 16
	[2] $P4mm$ (99)	1; 2; 3; 4; 13; 14; 15; 16
	[2] $P42_12$ (90)	1; 2; 3; 4; 5; 6; 7; 8
	[2] $P4/n11$ ($P4/n$, 85)	1; 2; 3; 4; 9; 10; 11; 12
	[2] $P2/n12/m$ ($Cmme$, 67)	1; 2; 7; 8; 9; 10; 15; 16
	[2] $P2/n2_1/m1$ ($Pmmn$, 59)	1; 2; 5; 6; 9; 10; 13; 14

Maximal non-isomorphic subgroups

I	[2] $P23$ (195)	1; 2; 3; 4; 5; 6; 7; 8; 9; 10; 11; 12
	[3] $Pn1$ ($Pnnn$, 48)	1; 2; 3; 4; 13; 14; 15; 16
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 5; 9; 13; 17; 21
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 6; 12; 13; 18; 24
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 7; 10; 13; 19; 22
	[4] $P1\bar{3}$ ($R\bar{3}$, 148)	1; 8; 11; 13; 20; 23

三维点群所对应的空间群，其子群也相互对应。

Maximal non-isomorphic subgroups

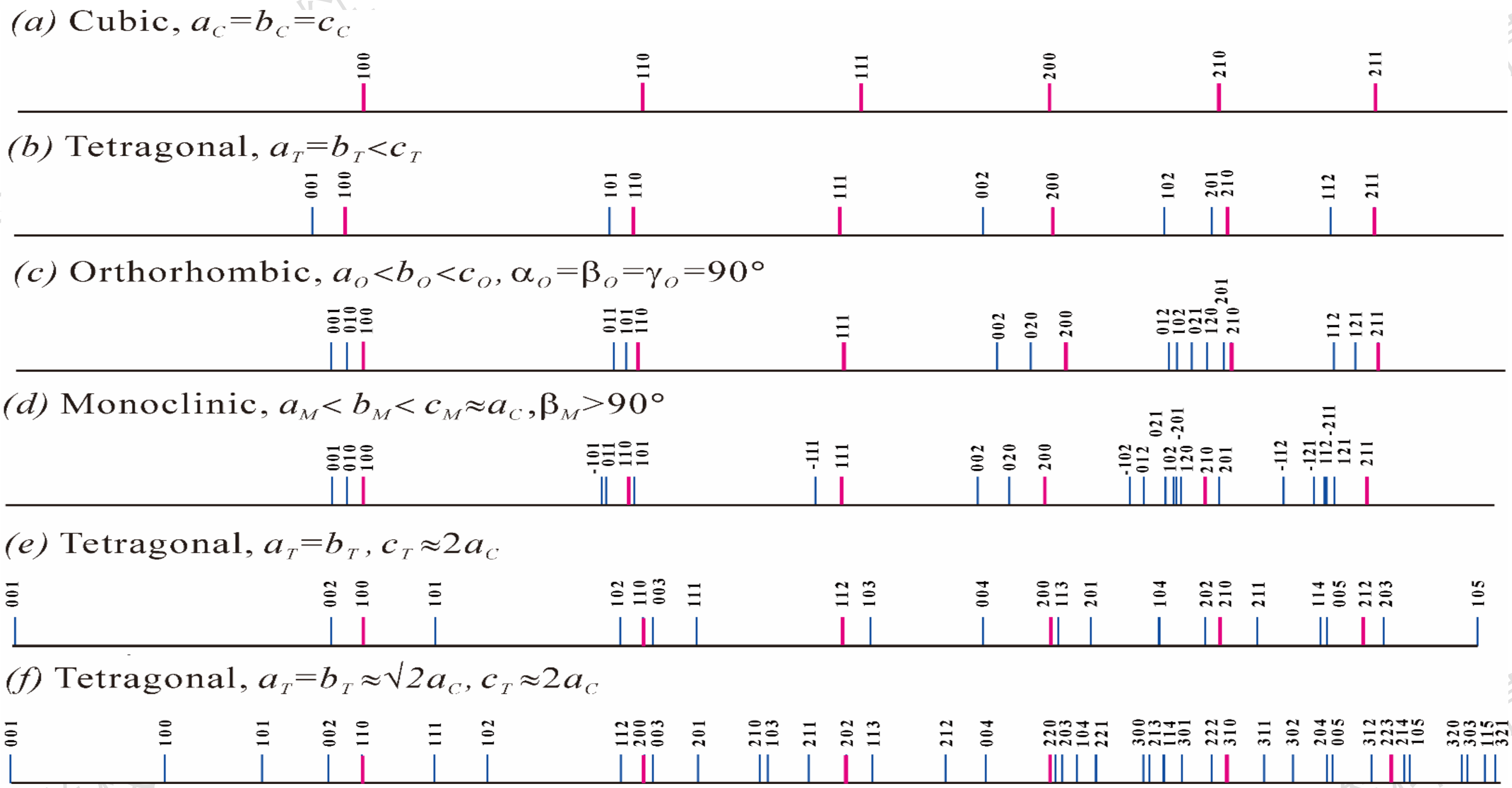
I	[2] $P1c1$ (Pc, 7)	1; 3
	[2] $Pn11$ (Pc, 7)	1; 4
	[2] $P112$ ($P2_1$, 3)	1; 2

Maximal non-isomorphic subgroups

I	[2] $P6_311$ ($P6_3$, 173)	1; 2; 3; 4; 5; 6
	[2] $P321$ (150)	1; 2; 3; 7; 8; 9
	[2] $P312$ (149)	1; 2; 3; 10; 11; 12
	[3] $P2_122$ ($C222_1$, 20)	1; 4; 7; 10
	[3] $P2_122$ ($C222_1$, 20)	1; 4; 8; 11
	[3] $P2_122$ ($C222_1$, 20)	1; 4; 9; 12

32 种三维空间点群的关系(此处使用的是Hermann—Mauguin记号)

Examples of possible diffraction peak position with consideration of the primary lattice



(a) Cubic, $a_C=b_C=c_C$

(b) Tetragonal, $a_T=b_T<c_T$

(c) Orthorhombic, $a_O<b_O<c_O, \alpha_O=\beta_O=\gamma_O=90°$

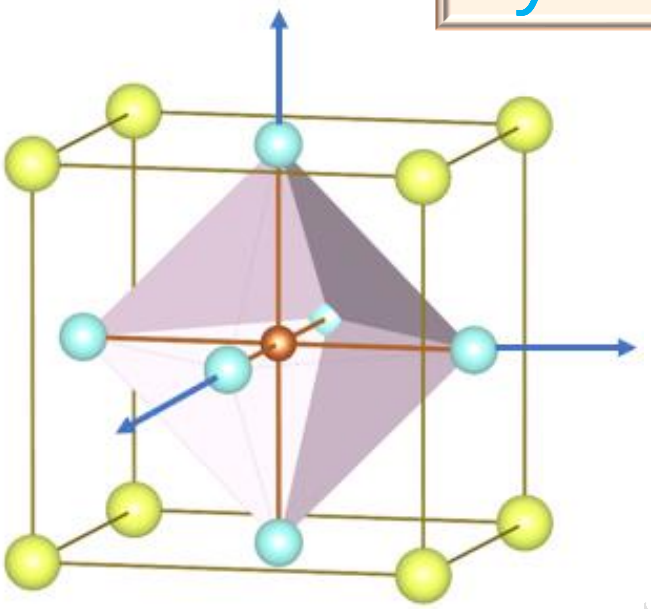
(d) Monoclinic, $a_M< b_M< c_M\approx a_C, \beta_M>90°$

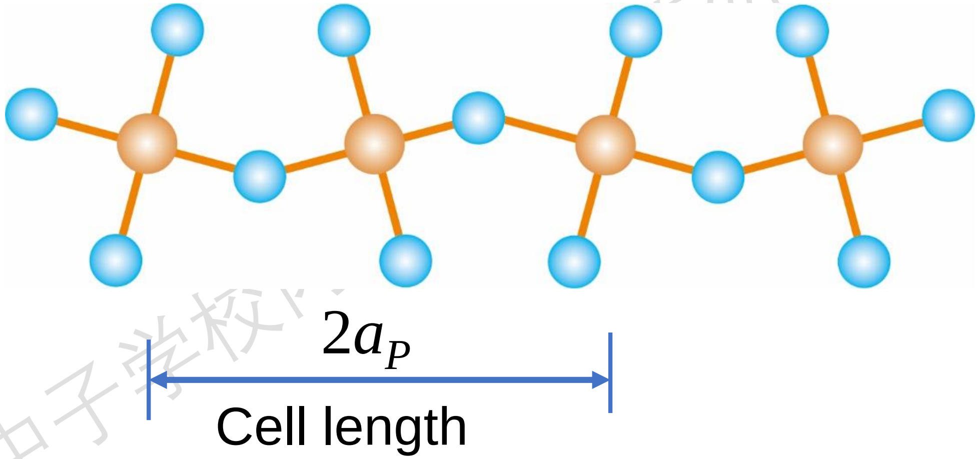
(e) Tetragonal, $a_T=b_T, c_T\approx 2a_C$

(f) Tetragonal, $a_T=b_T\approx\sqrt{2}a_C, c_T\approx 2a_C$

Schematic plot of the possible diffraction peaks with consideration of the primary lattice only. The red thick lines are the reflections corresponding to a cubic lattice, and the blue thin lines are the reflections due to the peak lattice splitting or the superlattice peaks. *(a)* Reflections from a simple cubic lattice; *(b), (c), and (d)* reflections from tetragonal, orthorhombic, and monoclinic lattices, respectively. Due to the lattice distortion, a cubic peak may be split into two or more peaks; *(e) and (f)* reflections show the presence of peak splitting and also superpeaks (such as the peaks of *hkl* with *l*=odd) from the superlattice.

Symmetry with Octahedral Tilting





Octahedra tilting

3 tilts	$a^+b^+c^+$	$a^+b^+c^-$	$a^+b^-c^-$	$a^-b^-c^-$
2 tilts	$a^0b^+c^+$	$a^0b^+c^-$	$a^0b^-c^-$	
1 tilt	$a^0b^0c^+$	$a^0b^0c^-$		
No tilt	$a^0b^0c^0$			

Glazer, A. M. “The Classification of Tilted Octahedra in Perovskites” *Acta Cryst.* **B28**. 3385, 1972, and “Simple Ways of Determining Perovskite structures”. *Acta Cryst.* **A31**. 756, 1975.

Octahedra tilting and symmetry in proveskites

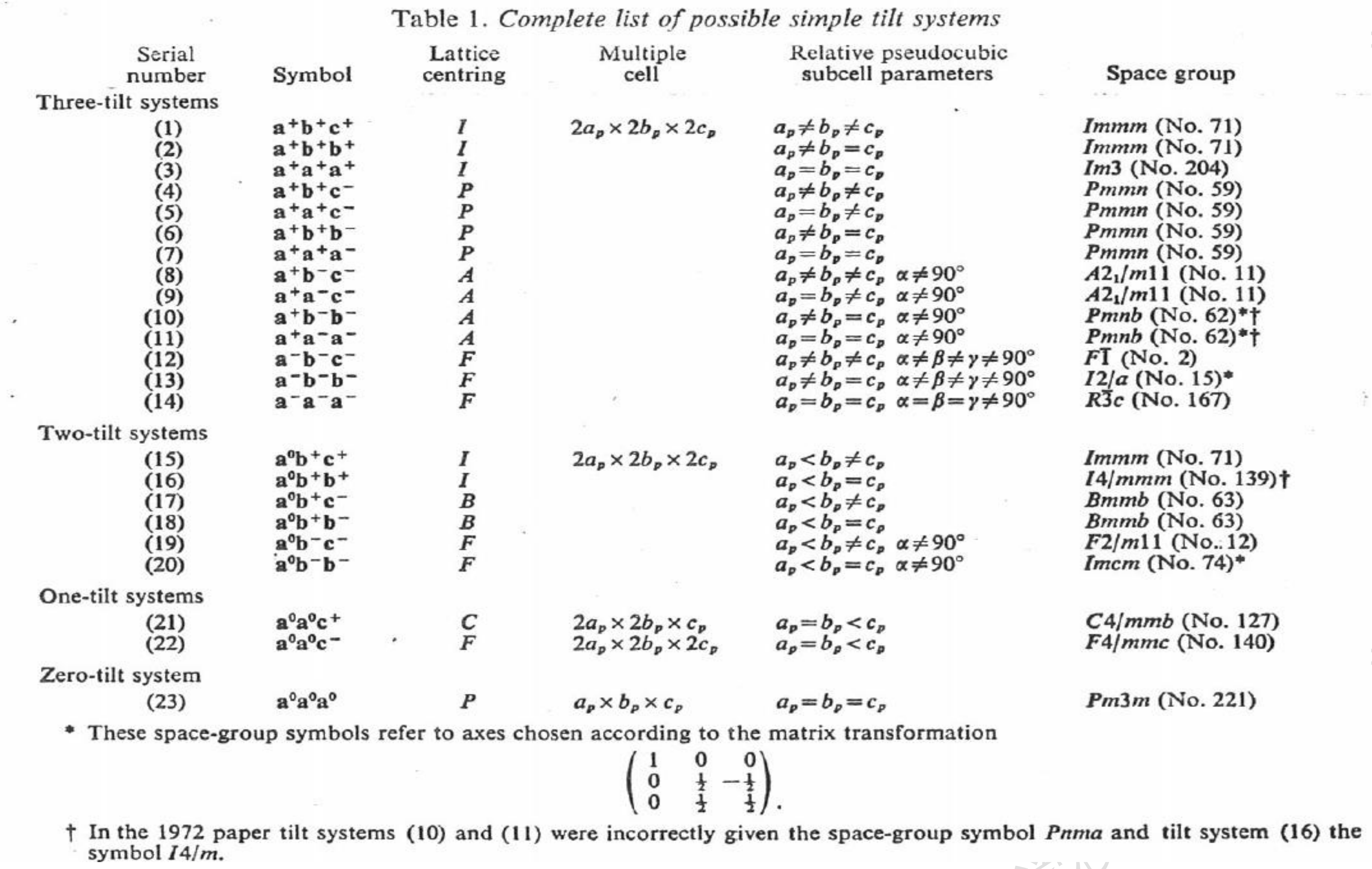


Table 1. *Complete list of possible simple tilt systems*

Serial number	Symbol	Lattice centring	Multiple cell	Relative pseudocubic subcell parameters	Space group
Three-tilt systems					
(1)	$a^+b^+c^+$	*I*	$2a_p \times 2b_p \times 2c_p$	$a_p \neq b_p \neq c_p$	*Immm* (No. 71)
(2)	$a^+b^+b^+$	*I*		$a_p \neq b_p = c_p$	*Immm* (No. 71)
(3)	$a^+a^+a^+$	*I*		$a_p = b_p = c_p$	*Im*3 (No. 204)
(4)	$a^+b^+c^-$	*P*		$a_p \neq b_p \neq c_p$	*Pmmn* (No. 59)
(5)	$a^+a^+c^-$	*P*		$a_p = b_p \neq c_p$	*Pmmn* (No. 59)
(6)	$a^+b^+b^-$	*P*		$a_p \neq b_p = c_p$	*Pmmn* (No. 59)
(7)	$a^+a^+a^-$	*P*		$a_p = b_p = c_p$	*Pmmn* (No. 59)
(8)	$a^+b^-c^-$	*A*		$a_p \neq b_p \neq c_p \quad \alpha \neq 90°$	$A2_1/m11$ (No. 11)
(9)	$a^+a^-c^-$	*A*		$a_p = b_p \neq c_p \quad \alpha \neq 90°$	$A2_1/m11$ (No. 11)
(10)	$a^+b^-b^-$	*A*		$a_p \neq b_p = c_p \quad \alpha \neq 90°$	*Pmnb* (No. 62)*†
(11)	$a^+a^-a^-$	*A*		$a_p = b_p = c_p \quad \alpha \neq 90°$	*Pmnb* (No. 62)*†
(12)	$a^-b^-c^-$	*F*		$a_p \neq b_p \neq c_p \quad \alpha \neq \beta \neq \gamma \neq 90°$	$F\bar{1}$ (No. 2)
(13)	$a^-b^-b^-$	*F*		$a_p \neq b_p = c_p \quad \alpha \neq \beta \neq \gamma \neq 90°$	*I*2/*a* (No. 15)*
(14)	$a^-a^-a^-$	*F*		$a_p = b_p = c_p \quad \alpha = \beta = \gamma \neq 90°$	$R\bar{3}c$ (No. 167)
Two-tilt systems					
(15)	$a^0b^+c^+$	*I*	$2a_p \times 2b_p \times 2c_p$	$a_p < b_p \neq c_p$	*Immm* (No. 71)
(16)	$a^0b^+b^+$	*I*		$a_p < b_p = c_p$	*I*4/*mmm* (No. 139)†
(17)	$a^0b^+c^-$	*B*		$a_p < b_p \neq c_p$	*Bmmb* (No. 63)
(18)	$a^0b^+b^-$	*B*		$a_p < b_p = c_p$	*Bmmb* (No. 63)
(19)	$a^0b^-c^-$	*F*		$a_p < b_p \neq c_p \quad \alpha \neq 90°$	*F*2/*m*11 (No. 12)
(20)	$a^0b^-b^-$	*F*		$a_p < b_p = c_p \quad \alpha \neq 90°$	*Imcm* (No. 74)*
One-tilt systems					
(21)	$a^0a^0c^+$	*C*	$2a_p \times 2b_p \times c_p$	$a_p = b_p < c_p$	*C*4/*mmb* (No. 127)
(22)	$a^0a^0c^-$	*F*	$2a_p \times 2b_p \times 2c_p$	$a_p = b_p < c_p$	*F*4/*mmc* (No. 140)
Zero-tilt system					
(23)	$a^0a^0a^0$	*P*	$a_p \times b_p \times c_p$	$a_p = b_p = c_p$	*Pm*3*m* (No. 221)

* These space-group symbols refer to axes chosen according to the matrix transformation

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

† In the 1972 paper tilt systems (10) and (11) were incorrectly given the space-group symbol *Pnma* and tilt system (16) the symbol *I*4/*m*.

$Pbcn$	D_{2h}^{14}	mmm	Orthorhombic
No. 60	$P\ 2_1/b\ 2/c\ 2_1/n$		Patterson symmetry $Pmmm$

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

当空间群从$Pbcn$ 降到$P2_12_12$时， $Pbcn$ 的一般等效点系8d位置有8个等效点，而$P2_12_12$的一般等效点系4c只有4个等效点，因此需另加一个4c位置（虚线框）。

8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$

Maximal non-isomorphic subgroups

I	[2] $P2_1cn$ ($Pna2_1$, 33)	1; 4; 6; 7
	[2] $Pb2n$ ($Pnc2$, 30)	1; 3; 6; 8
	[2] $Pbc2_1$ ($Pca2_1$, 29)	1; 2; 7; 8
	[2] $P2_122_1$ ($P2_12_12$, 18)	1; 2; 3; 4
	[2] $P112_1/n$ ($P2_1/c$, 14)	1; 2; 5; 6
	[2] $P2_1/b11$ ($P2_1/c$, 14)	1; 4; 5; 8
	[2] $P12/c1$ ($P2/c$, 13)	1; 3; 5; 7

Positions

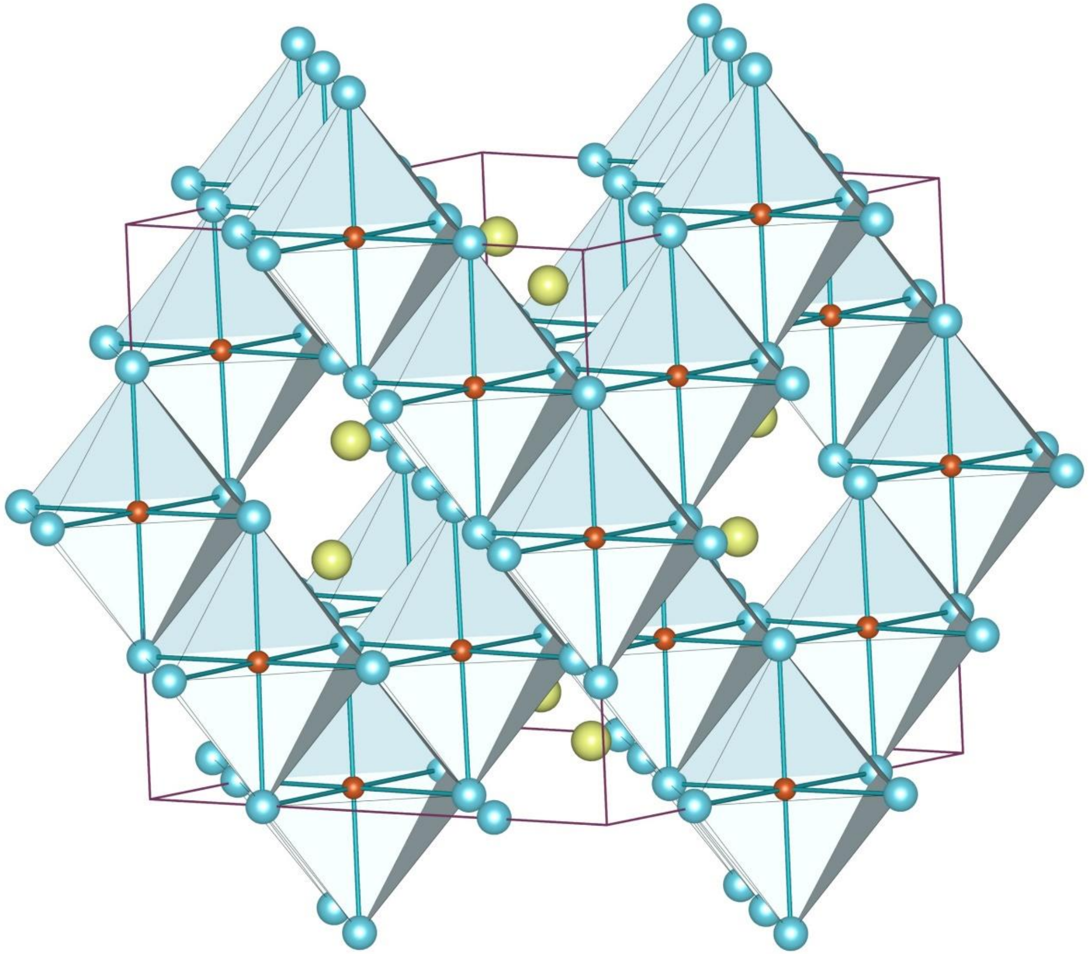
$P2_12_12$

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

4	c	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$
4	c	1	(5) $\bar{x},\bar{y},\bar{z}$	(6) $x\cancel{+\frac{1}{2}},y\cancel{+\frac{1}{2}},\bar{z}\cancel{+\frac{1}{2}}$	(7) $x,\bar{y},z\cancel{+\frac{1}{2}}$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$
2	b	..2	$0,\frac{1}{2},z$	$\frac{1}{2},0,\bar{z}$		
2	a	..2	$0,0,z$	$\frac{1}{2},\frac{1}{2},\bar{z}$		

Structure Transition and Magnetic properties in Spinel Antiferromagnet $GeCo_2O_4$ and Relative Compounds.

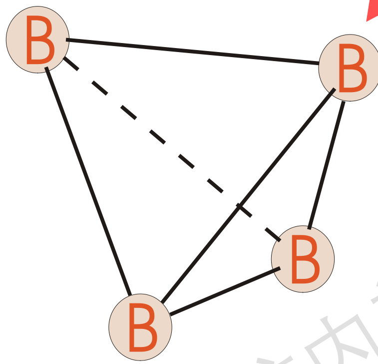


Spinal, Cubic-*Fd*3*m* symmetry

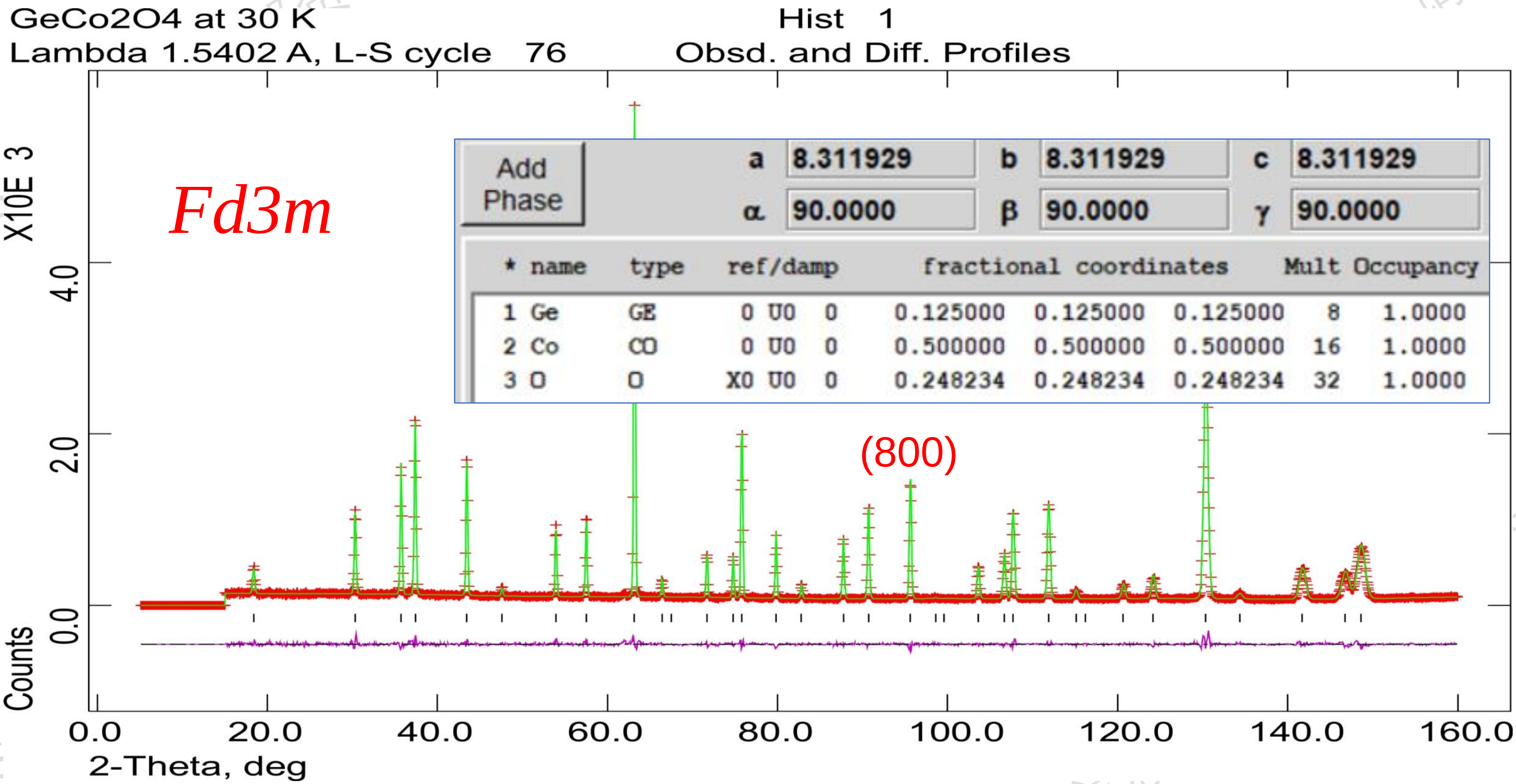
AB_2O_4

T-site, AO_4

O-site, BO_6



Frustrated coupling

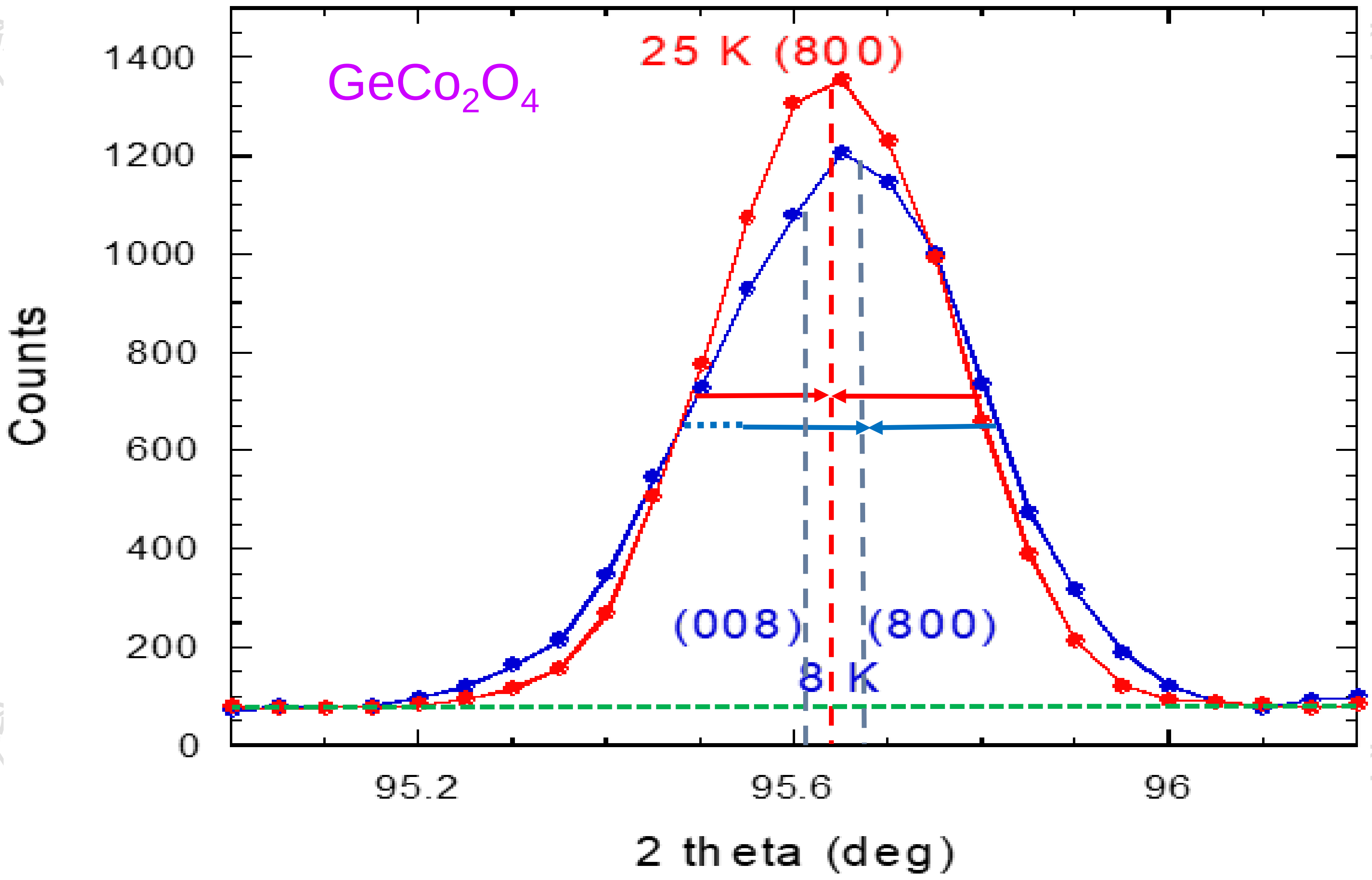


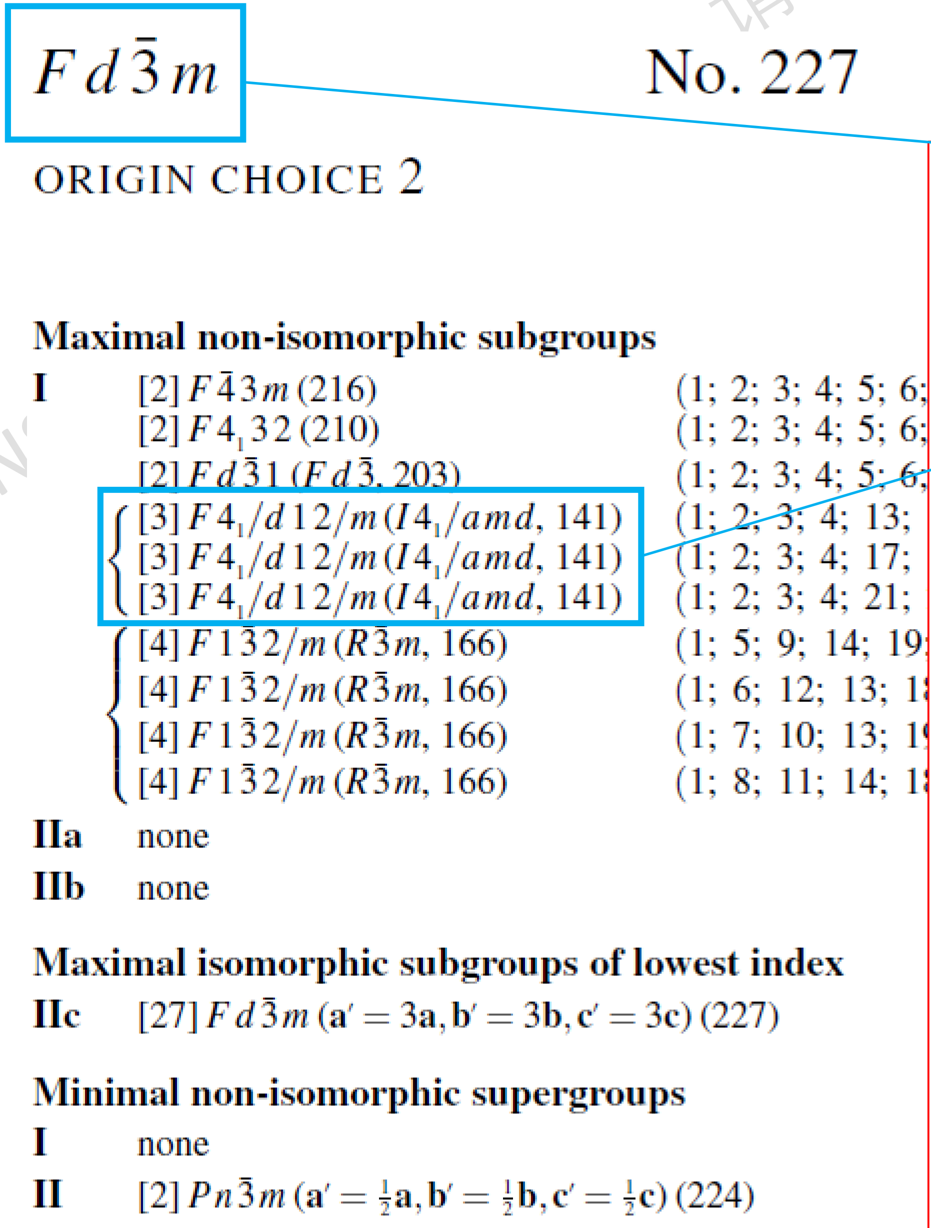
a 8.311929 b 8.311929 c 8.311929

α 90.0000 β 90.0000 γ 90.0000

*	name	type	ref/damp	fractional coordinates			Mult	Occupancy
1	Ge	GE	0 U0 0	0.125000	0.125000	0.125000	8	1.0000
2	Co	CO	0 U0 0	0.500000	0.500000	0.500000	16	1.0000
3	O	O	X0 U0 0	0.248234	0.248234	0.248234	32	1.0000

A structural transition from cubic to tetragonal





$Fd\bar{3}m$

No. 227

CONTINUED

ORIGIN CHOICE 2

Maximal non-isomorphic subgroups

I [2] $F\bar{4}3m$ (216) (1; 2; 3; 4; 5; 6;
[2] $F4_132$ (210) (1; 2; 3; 4; 5; 6;
[2] $Fd\bar{3}1$ ($Fd\bar{3}$, 203) (1; 2; 3; 4; 5; 6;
[3] $F4_1/d12/m$ ($I4_1/amd$, 141) (1; 2; 3; 4; 13;
[3] $F4_1/d12/m$ ($I4_1/amd$, 141) (1; 2; 3; 4; 17;
[3] $F4_1/d12/m$ ($I4_1/amd$, 141) (1; 2; 3; 4; 21;
[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166) (1; 5; 9; 14; 19;
[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166) (1; 6; 12; 13;
[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166) (1; 7; 10; 13;
[4] $F1\bar{3}2/m$ ($R\bar{3}m$, 166) (1; 8; 11; 14;

IIa none

IIb none

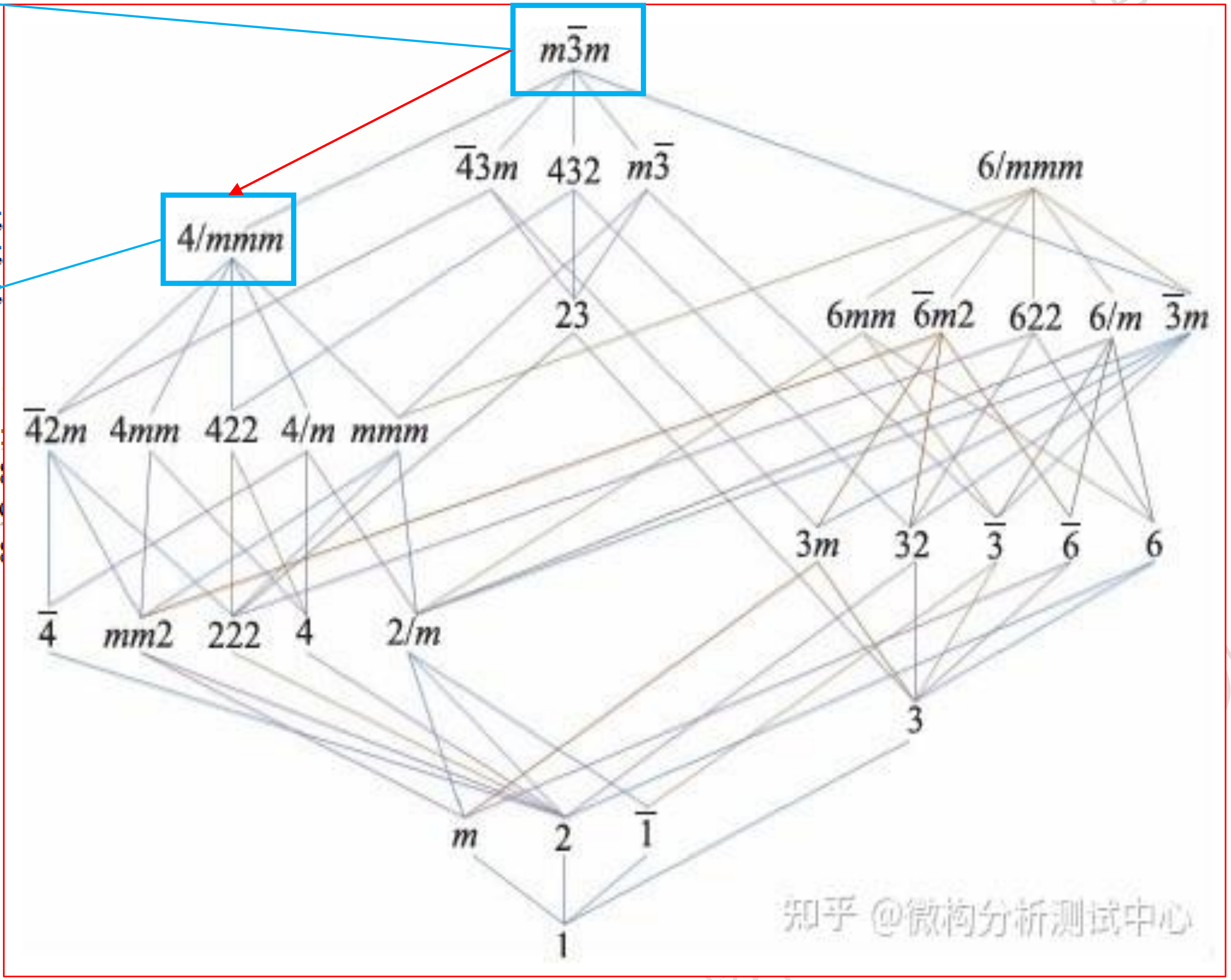
Maximal isomorphic subgroups of lowest index

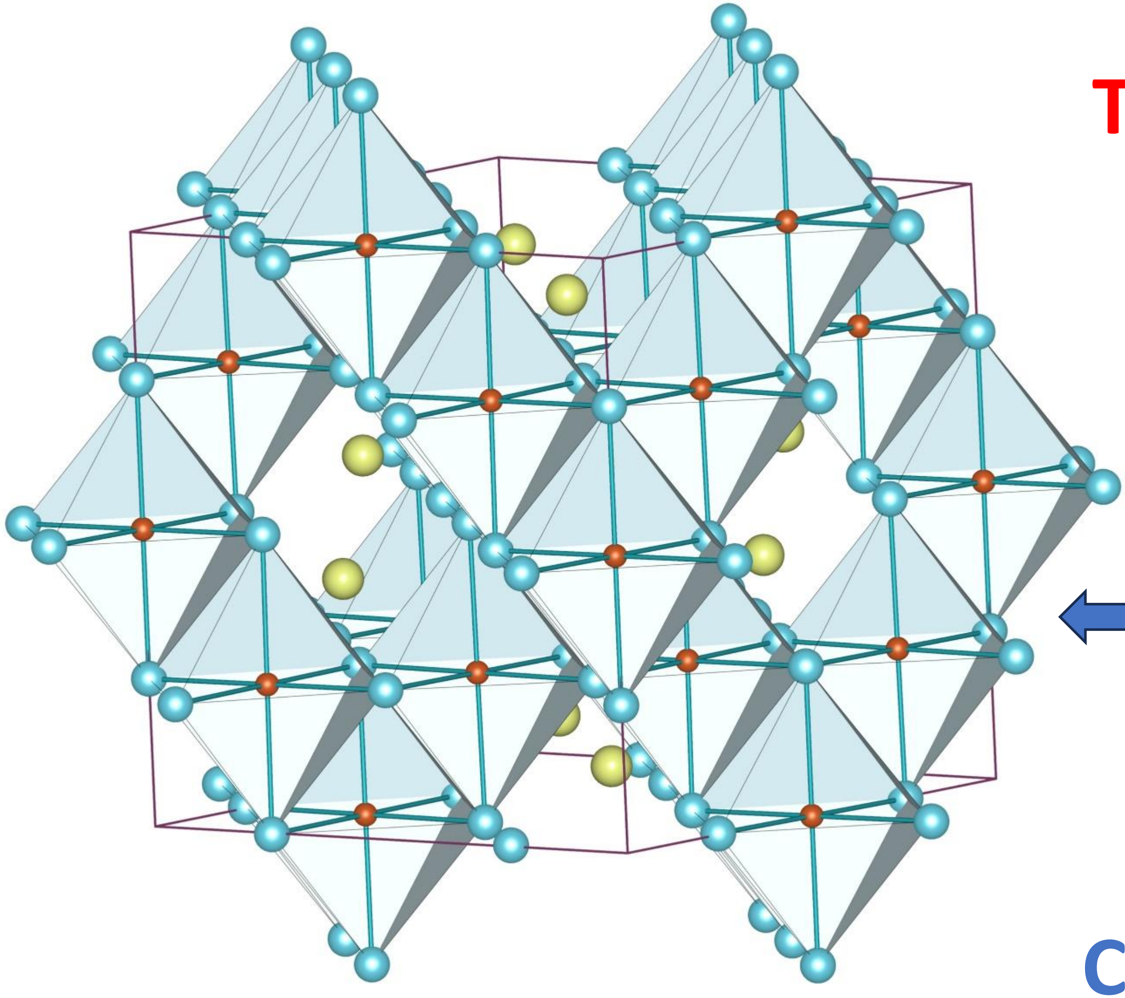
IIc [27] $Fd\bar{3}m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}, \mathbf{c}' = 3\mathbf{c}$) (227)

Minimal non-isomorphic supergroups

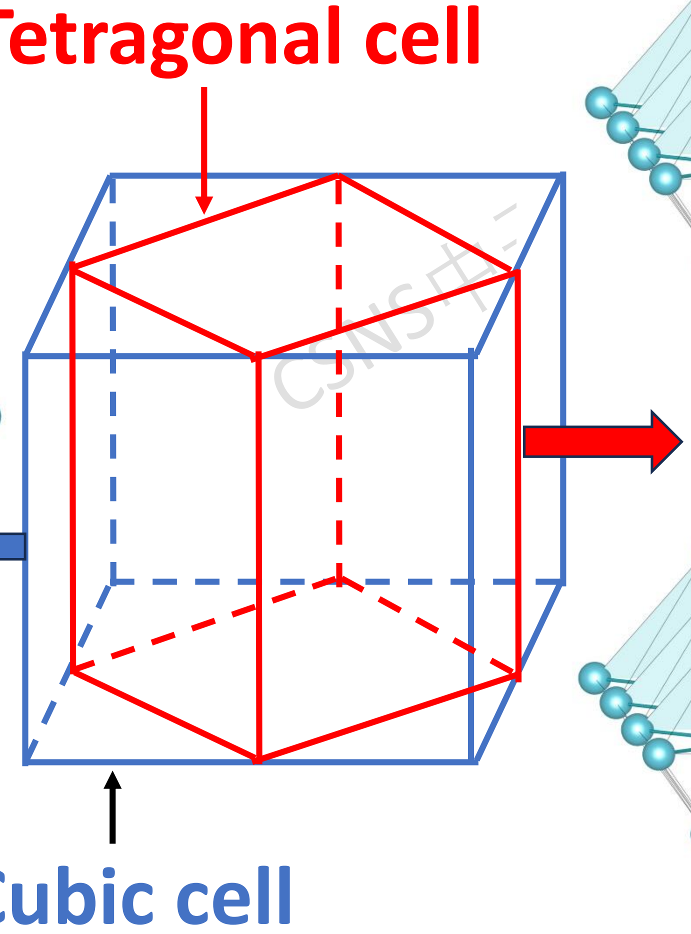
I none

II [2] $Pn\bar{3}m$ ($\mathbf{a}' = \frac{1}{2}\mathbf{a}, \mathbf{b}' = \frac{1}{2}\mathbf{b}, \mathbf{c}' = \frac{1}{2}\mathbf{c}$) (224)



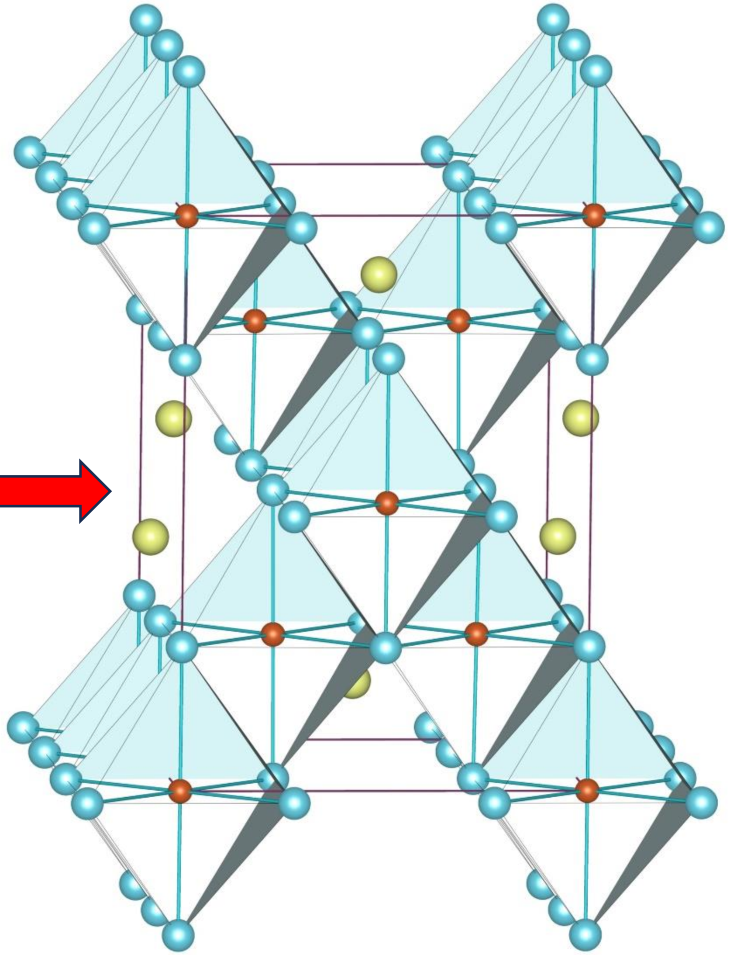


#227-Fd3m



Tetragonal cell

Cubic cell



#141-I4$_1$/amd

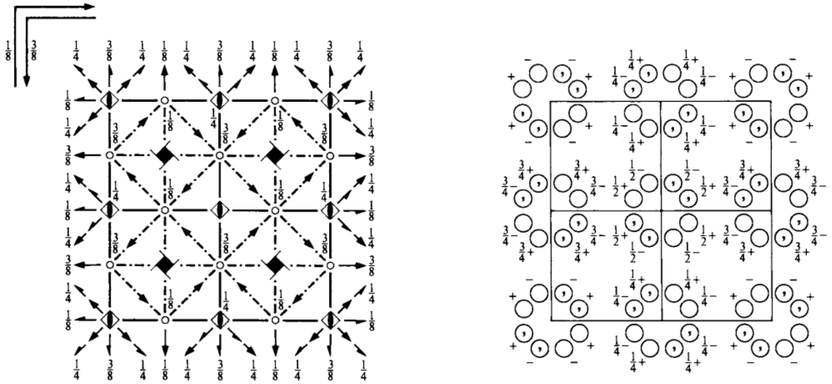
No. 141 and 142 have two origin choices

International Tables for Crystallography (2006). Vol. A, Space group 141, pp. 482–485.

$I4_1/amd$ D_{4h}^{19} $4/mmm$ Tetragonal

No. 141 $I\ 4_1/a\ 2/m\ 2/d$ Patterson symmetry $I4/mmm$

Origin choice 1



Origin at $\bar{4}m2$, at $0, \frac{1}{4}, -\frac{1}{8}$ from centre $(2/m)$

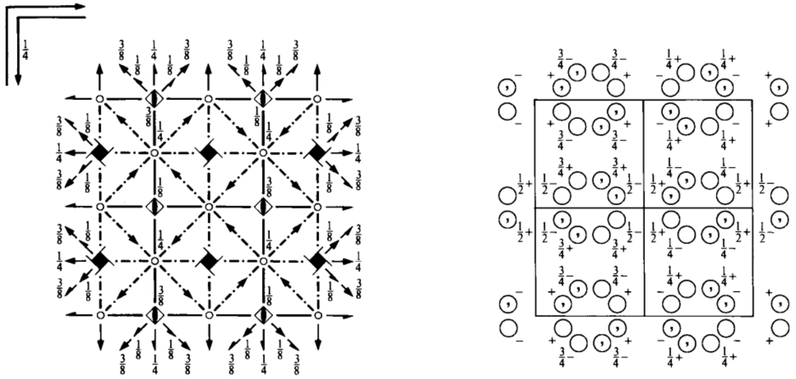
Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{2};\quad 0 \le z \le \frac{1}{8}$

8	e	$2mm.$	$0,0,z$	$0,\frac{1}{2},z+\frac{1}{4}$	$\frac{1}{2},0,\bar{z}+\frac{3}{4}$	$\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$
8	d	$.2/m.$	$0,\frac{1}{4},\frac{5}{8}$	$\frac{1}{2},\frac{1}{4},\frac{1}{8}$	$\frac{3}{4},\frac{1}{2},\frac{7}{8}$	$\frac{3}{4},0,\frac{3}{8}$
8	c	$.2/m.$	$0,\frac{1}{4},\frac{1}{8}$	$\frac{1}{2},\frac{1}{4},\frac{5}{8}$	$\frac{3}{4},\frac{1}{2},\frac{3}{8}$	$\frac{3}{4},0,\frac{7}{8}$
4	b	$\bar{4}m2$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},\frac{3}{4}$		
4	a	$\bar{4}m2$	$0,0,0$	$0,\frac{1}{2},\frac{1}{4}$		

$I4_1/amd$ D_{4h}^{19} $4/mmm$ Tetragonal

No. 141 $I\ 4_1/a\ 2/m\ 2/d$ Patterson symmetry $I4/mmm$

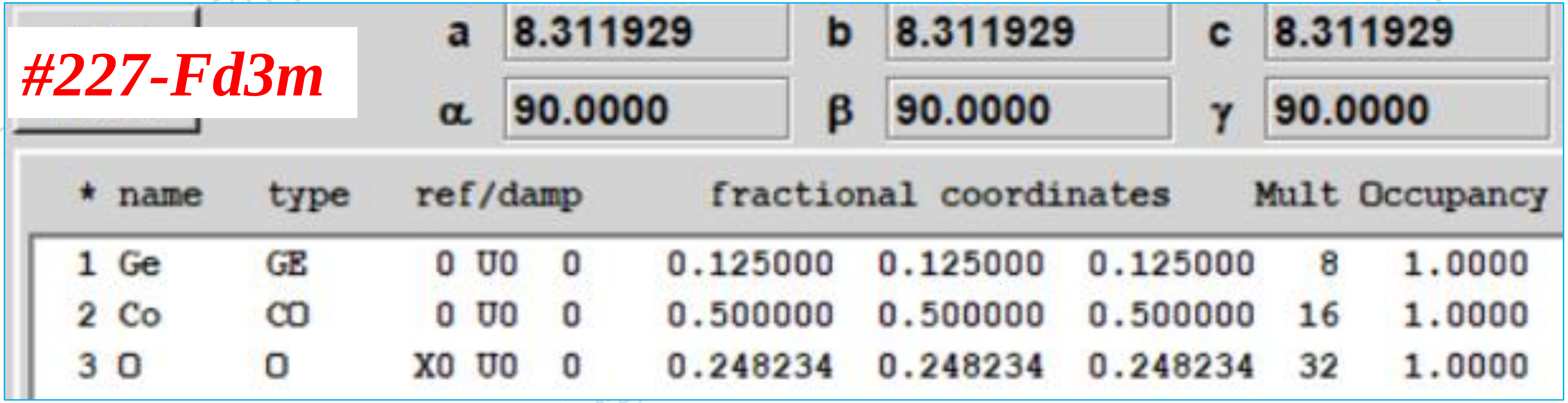
Origin choice 2



Origin at centre $(2/m)$ at $b(2/m,2_1/n)d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}m2$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad -\frac{1}{4} \le y \le \frac{1}{4};\quad 0 \le z \le \frac{1}{8}$

8	e	$2mm.$	$0,\frac{1}{4},z$	$0,\frac{3}{4},z+\frac{1}{4}$	$\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{1}{2},\frac{3}{4},\bar{z}+\frac{1}{4}$
8	d	$.2/m.$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$
8	c	$.2/m.$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$
4	b	$\bar{4}m2$	$0,\frac{1}{4},\frac{3}{8}$	$0,\frac{3}{4},\frac{5}{8}$		
4	a	$\bar{4}m2$	$0,\frac{3}{4},\frac{1}{8}$	$\frac{1}{2},\frac{3}{4},\frac{3}{8}$		

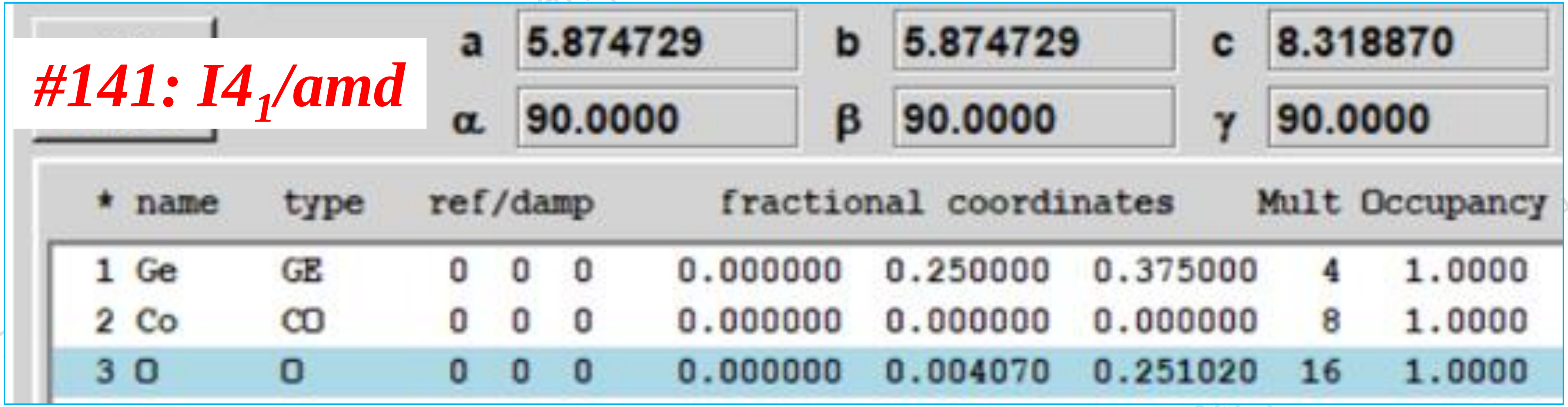


#227-Fd3m

a 8.311929 b 8.311929 c 8.311929

α 90.0000 β 90.0000 γ 90.0000

*	name	type	ref/damp			fractional coordinates			Mult	Occupancy
1	Ge	GE	0	U0	0	0.125000	0.125000	0.125000	8	1.0000
2	Co	CO	0	U0	0	0.500000	0.500000	0.500000	16	1.0000
3	O	O	X0	U0	0	0.248234	0.248234	0.248234	32	1.0000



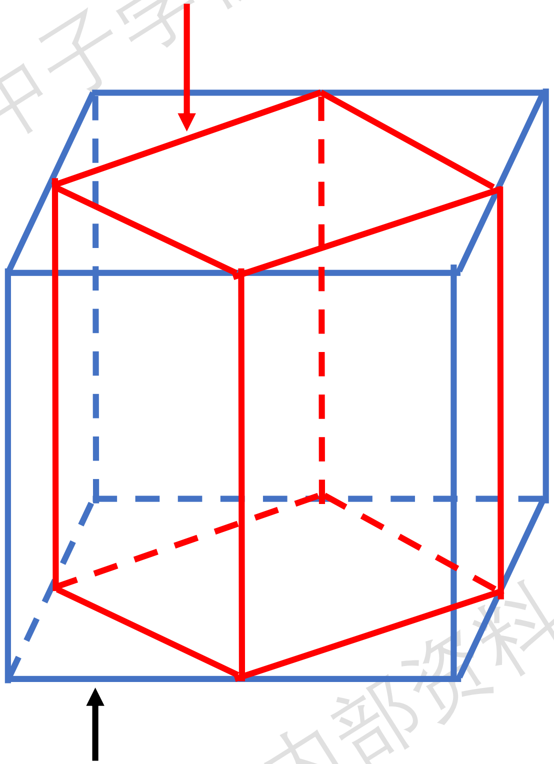
#141: $I4_1/amd$

a 5.874729 b 5.874729 c 8.318870

α 90.0000 β 90.0000 γ 90.0000

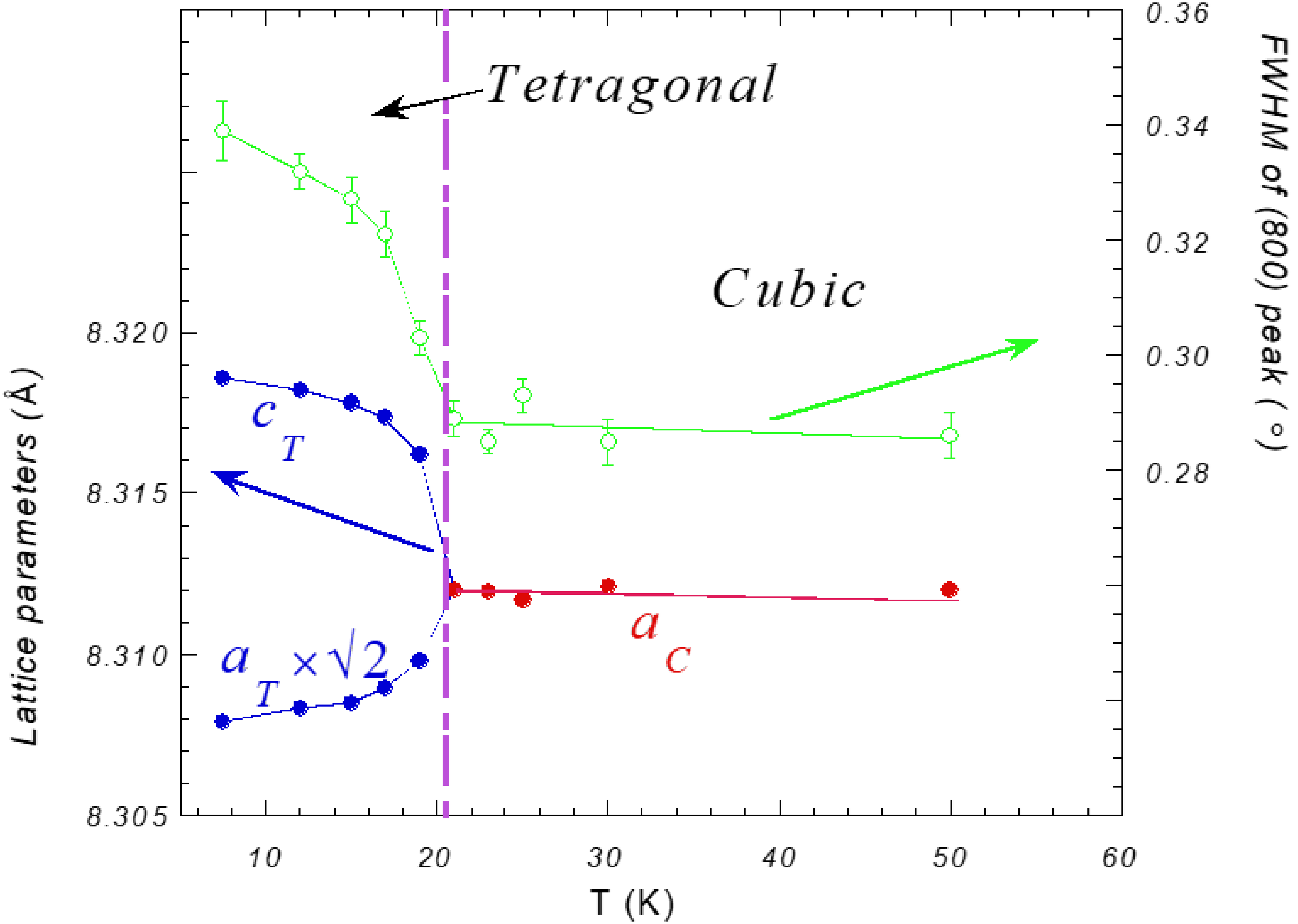
*	name	type	ref/damp			fractional coordinates			Mult	Occupancy
1	Ge	GE	0	0	0	0.000000	0.250000	0.375000	4	1.0000
2	Co	CO	0	0	0	0.000000	0.000000	0.000000	8	1.0000
3	O	O	0	0	0	0.000000	0.004070	0.251020	16	1.0000

Structural transition of $GeCo_2O_4$ occurs at ~21K

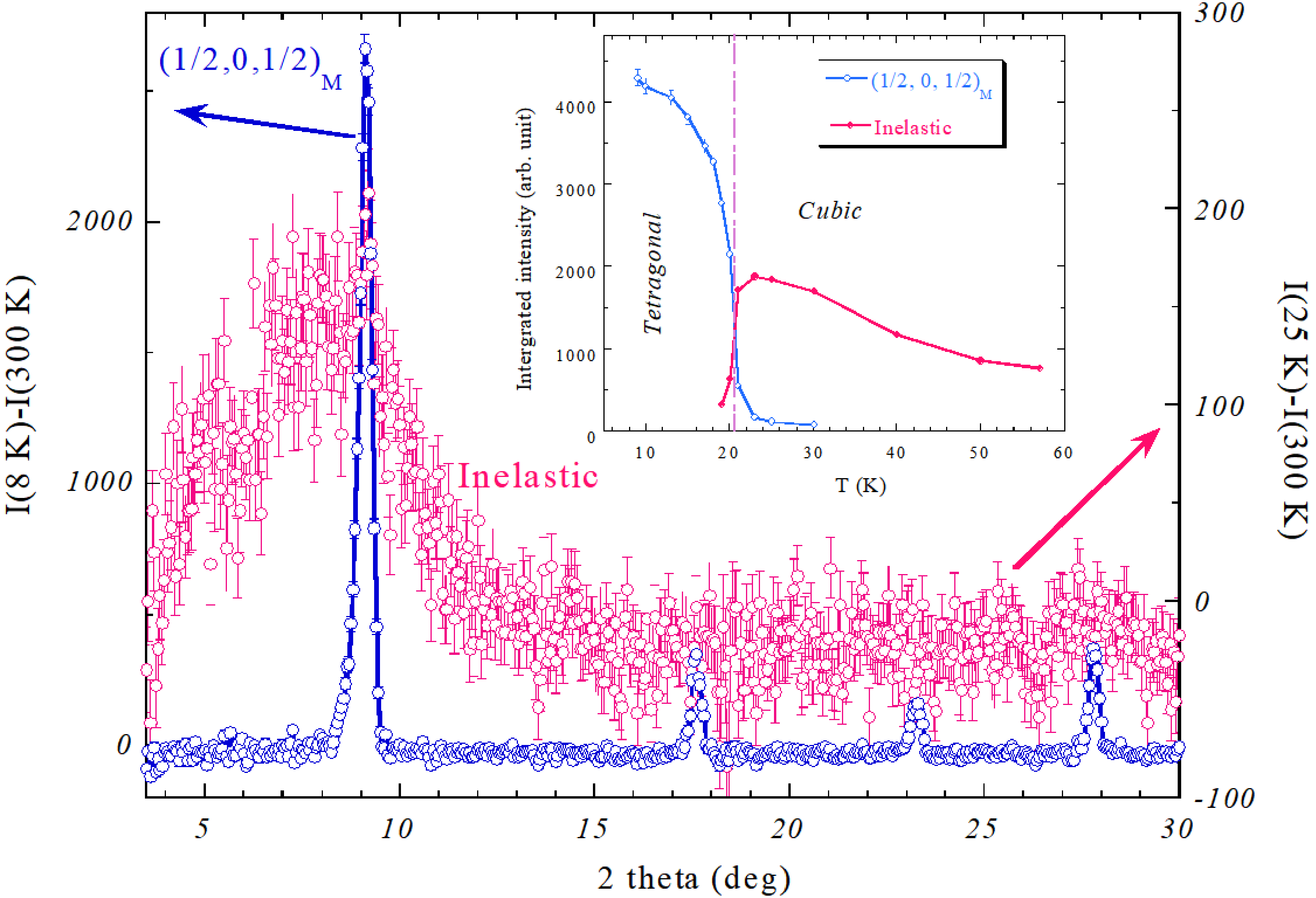


Tetragonal cell

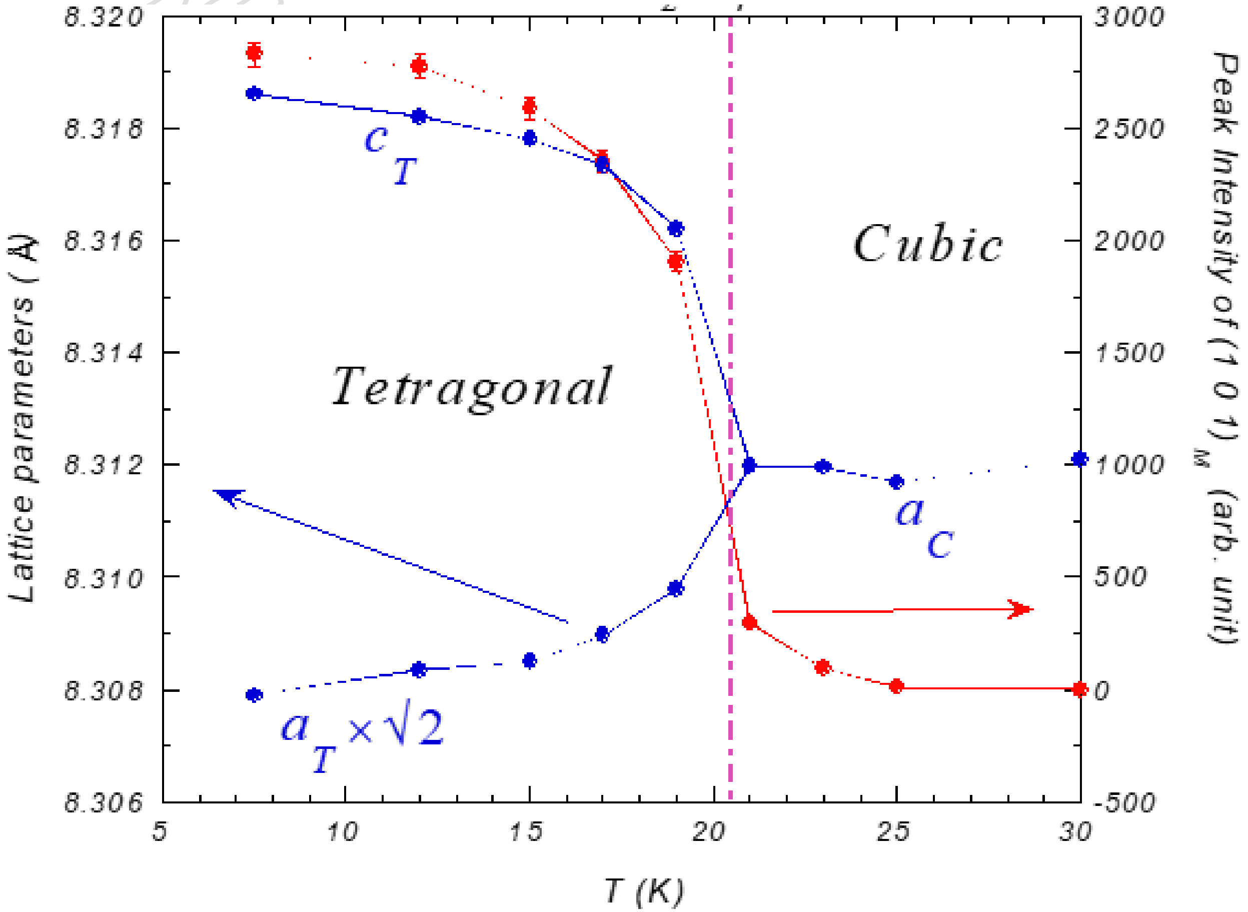
Cubic cell

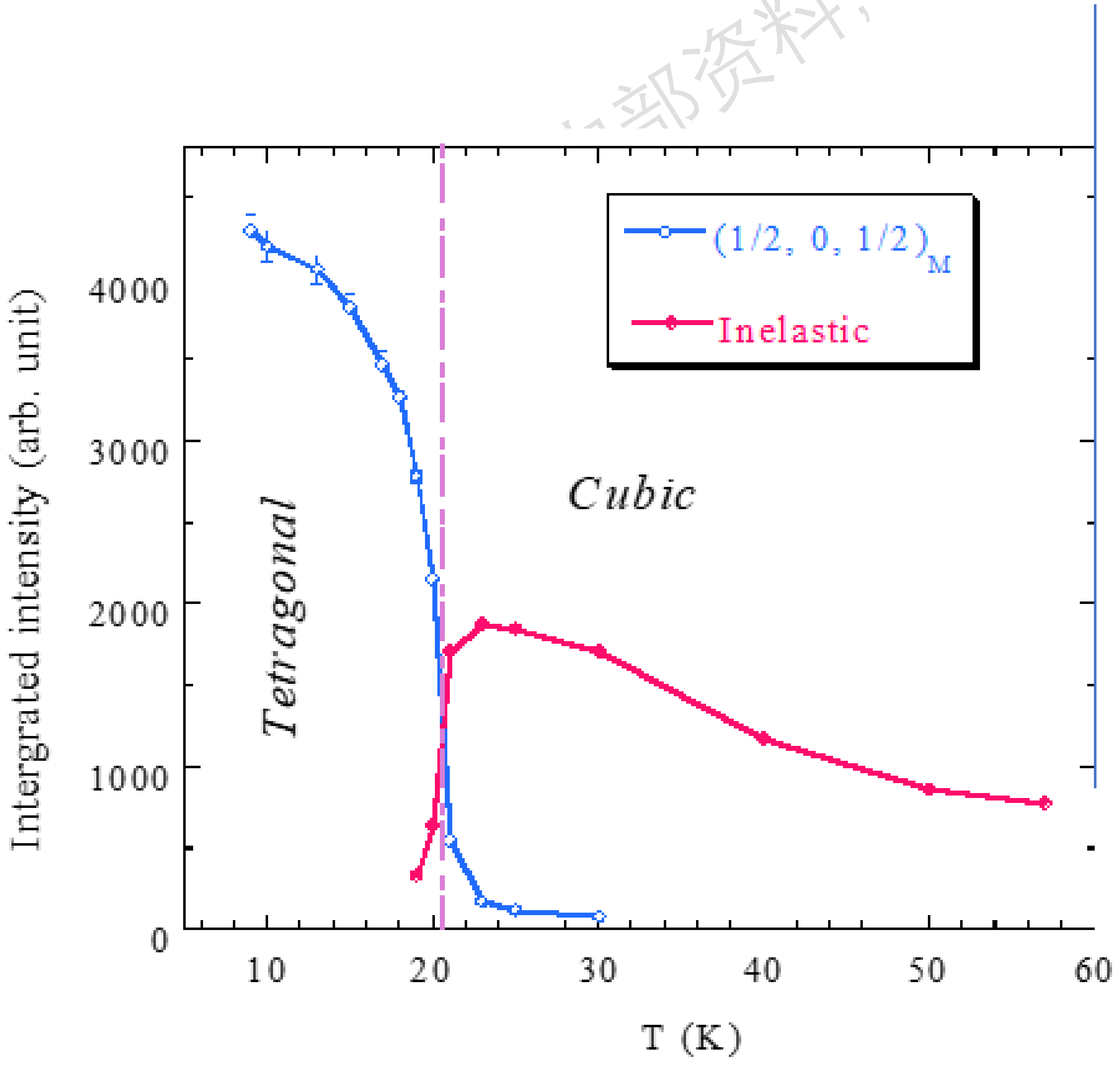


$GeCo_2O_4$


(1/2,0,1/2)M
Inelastic
I(8 K)-I(300 K)
0
1000
2000
I(25 K)-I(300 K)
-100
0
100
200
300
2 theta (deg)
5
10
15
20
25
30
Intergrated intensity (arb. unit)
0
1000
2000
3000
4000
T (K)
10
20
30
40
50
60
(1/2, 0, 1/2)M
Inelastic
Tetragonal
Cubic

Nuclear and Magnetic Structure Transitions at ~21 K





Thanks!