CHEM 548: MATERIALS CHEMISTRY

LECTURE 3: SPACE GROUPS: LATTICES, GLIDES, AND SCREWS

Space groups: lattices and point groups, glide planes and screw axes, and reading Hermann–Mauguin symbols

Reading: Woodward, Karen, Evans, and Vogt, *Solid State Materials Chemistry* Ch. 1 §§1.1.4–1.1.7

LEARNING OBJECTIVES

Every structure you will look up, in a paper or a database, is filed under a symbol like $P2_1/c$, and this lecture teaches you how to read it.

Glide and screw	describe the two elements that add a fractional translation, and the operation each performs
Space group	build one from a Bravais lattice and a compatible point group, and account for all 230
Symmorphic split	distinguish symmorphic from non-symmorphic space groups
Symbol reading	read a Hermann–Mauguin space-group symbol position by position

FIVE ELEMENTS FIX A POINT, TWO DO NOT

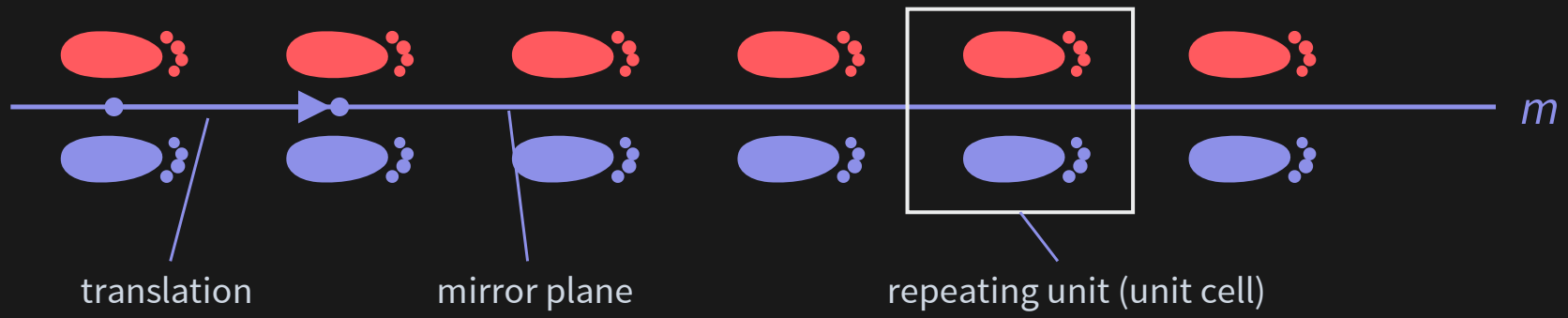
Symmetry Element	Symmetry Operation
1. Identity (1)	Nothing changes
2. Inversion center ($\bar{1}$)	Inversion through a point
3. Mirror plane (*m*)	Reflect through the plane
4. Proper rotation axis (N)	Rotate by 360/N degrees about the axis
5. Rotoinversion axis ($\bar{N}$)	Rotate by 360/N degrees about the axis, followed by inversion operation
6. Glide plane (*a*, *b*, *c*, *n*, *d*)	Reflect through a plane, then translate parallel to the plane
7. Screw axis (N_M)	Rotate by 360/N degrees about the axis, followed by a translation by M/N of the unit cell parallel to the axis

Everything above the line holds a point fixed; the last two rows add a translation.

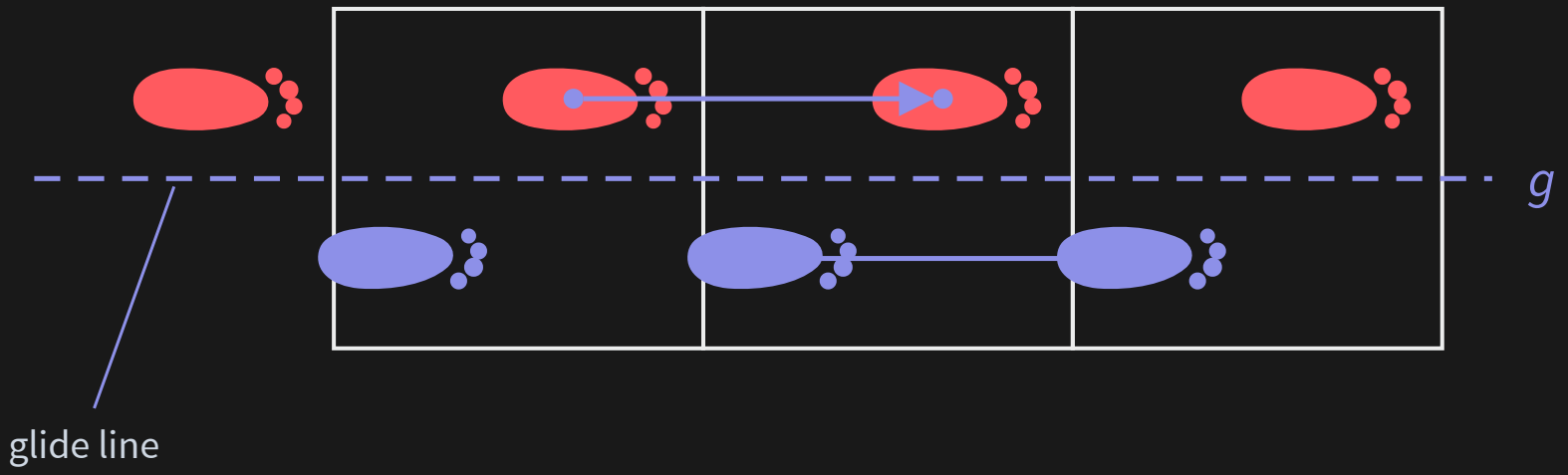
TRANSLATIONAL SYMMETRY

Slide the pattern by a whole unit-cell vector and every motif lands on an identical one — with one object per cell or a mirror-related pair, the translation repeats the contents whole cell by whole cell.



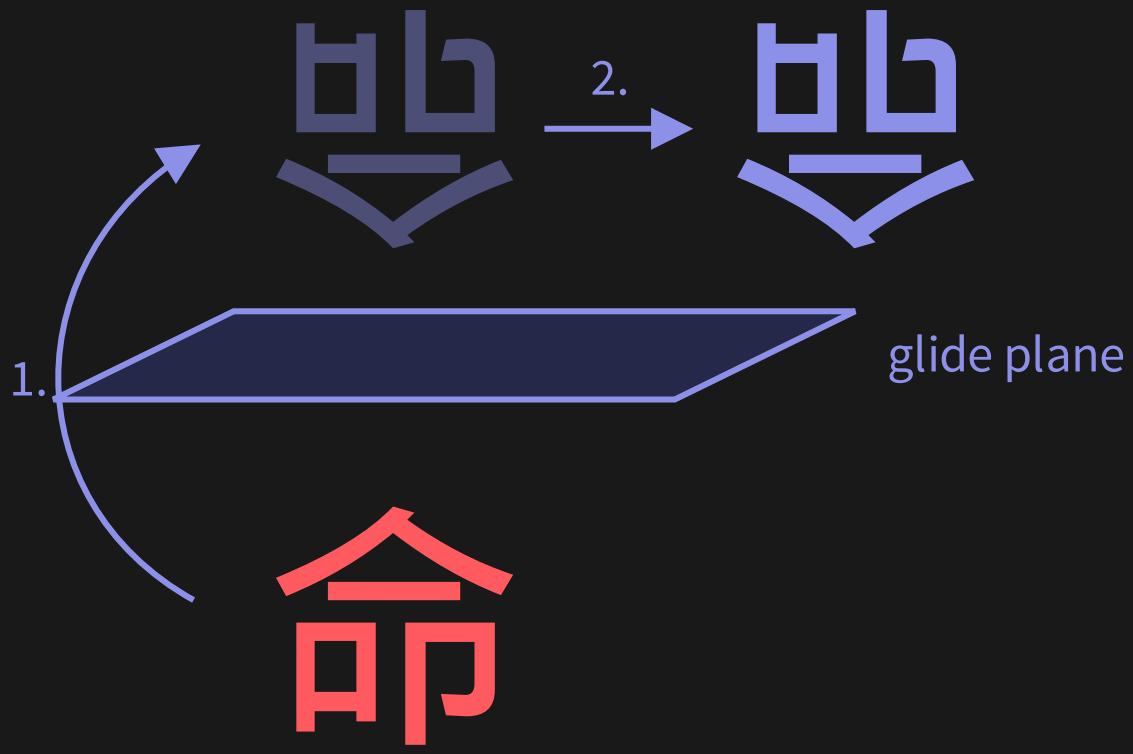


A GLIDE, ONE FOOTSTEP AT A TIME



glide reflection → (a) reflection at a plane / line
(b) translation (usually by ½ of the unit cell)

GLIDE PLANES



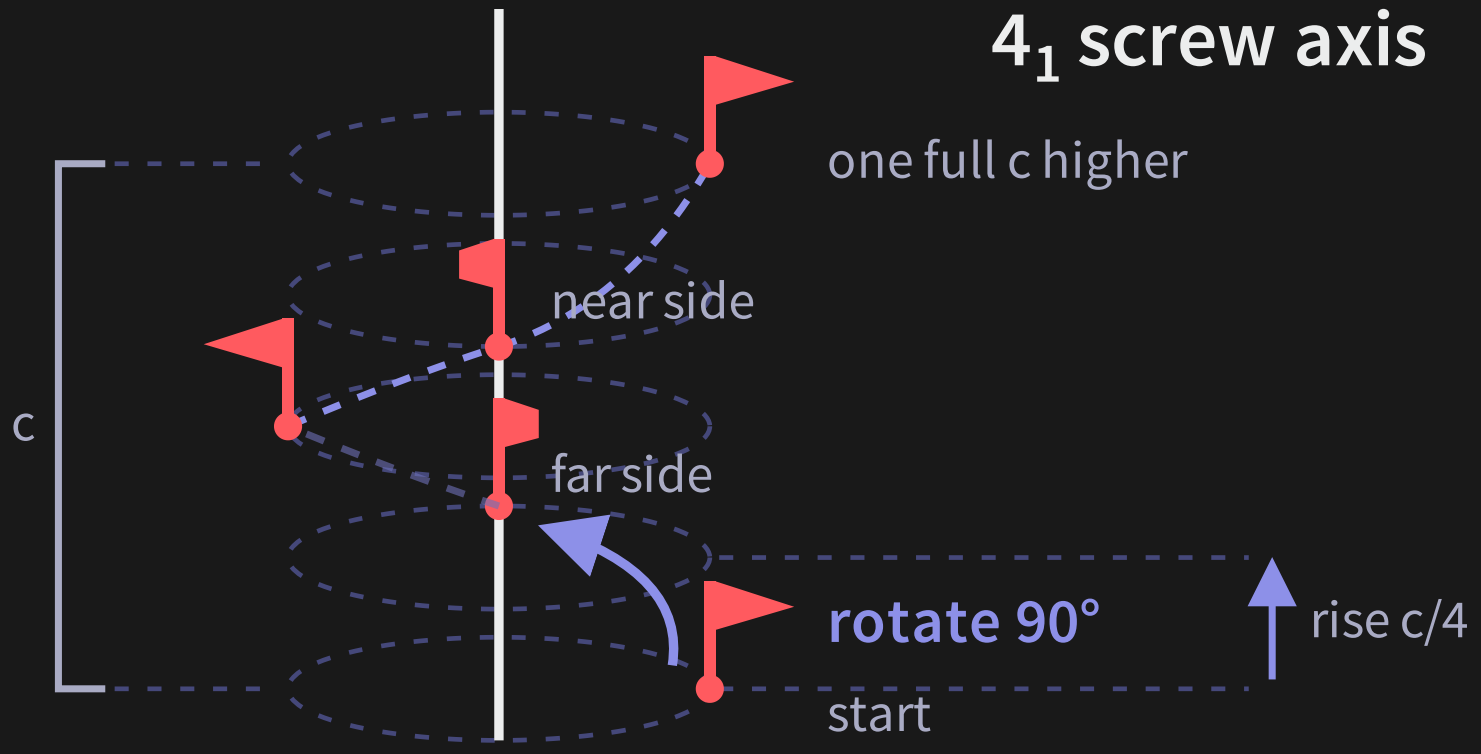
1. Reflect through the glide plane (just as with a mirror plane)

2. Translate parallel to the glide plane

TYPES OF GLIDE PLANES

Herman–Mauguin Symbol	Plane ⊥ to which axis	Translation vector
Axial Glides		
a	b or c	½ **a**
b	a or c	½ **b**
c	a or b	½ **c**
Diagonal glides, *n*	a	½ **b** + ½ **c**
	b	½ **a** + ½ **c**
	c	½ **a** + ½ **b**
Diamond glides, *d*	a	¼ **b** + ¼ **c**
	b	¼ **a** + ¼ **c**
	c	¼ **a** + ¼ **b**

N_M SCREW AXES



1. Rotate by 360/N (just as with a N-fold proper rotation axis)

2. Translate by M/N of a unit cell vector parallel to the screw axis

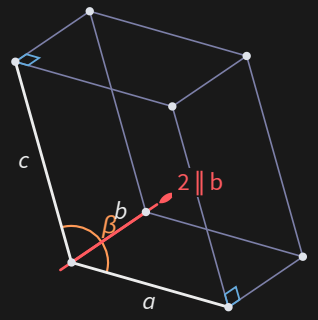
WHAT A SPACE GROUP IS

A point group holds one point fixed. A crystal also repeats by translation.

The space group is the complete symmetry of a crystal: the lattice translations, the point operations, and the glide and screw operations built from both.

There are exactly 230. Every crystal structure ever solved is filed under one of them.

FROM POINT GROUPS TO SPACE GROUPS



monoclinic: one twofold along b, β free

monoclinic P + 2 → P2

monoclinic C + 2/m → C2/m

lattice + **point group**

32 × 14 = 448 blind pairings

allowed pairings

the 14 Bravais lattices, grouped by crystal system

	triclinic	monoclinic	orthorhombic	tetragonal	rhombohedral	hexagonal	cubic
	P	P C	P C I F	P I	R	P	P I F
triclinic — 2 point groups	■						
monoclinic — 3 point groups		■					
orthorhombic — 3 point groups			■				
tetragonal — 7 point groups				■			
trigonal — 5 point groups					■	■	
hexagonal — 7 point groups						■	
cubic — 5 point groups							■

the 32 point groups, grouped by crystal system

P primitive · C base-centered · I body-centered · F face-centered · R rhombohedral

Per *Solid State Materials Chemistry*, §1.1.4.

SWAP IN A GLIDE OR A SCREW

P2 → $P2_1$	2 becomes 2_1	*the 2_1 screw is in no point group*
Pm → Pc	m becomes c glide	*the c glide is in no point group*

Symmorphic: built from a Bravais lattice and a point group alone.

Non-symmorphic: contains a glide plane or a screw axis.

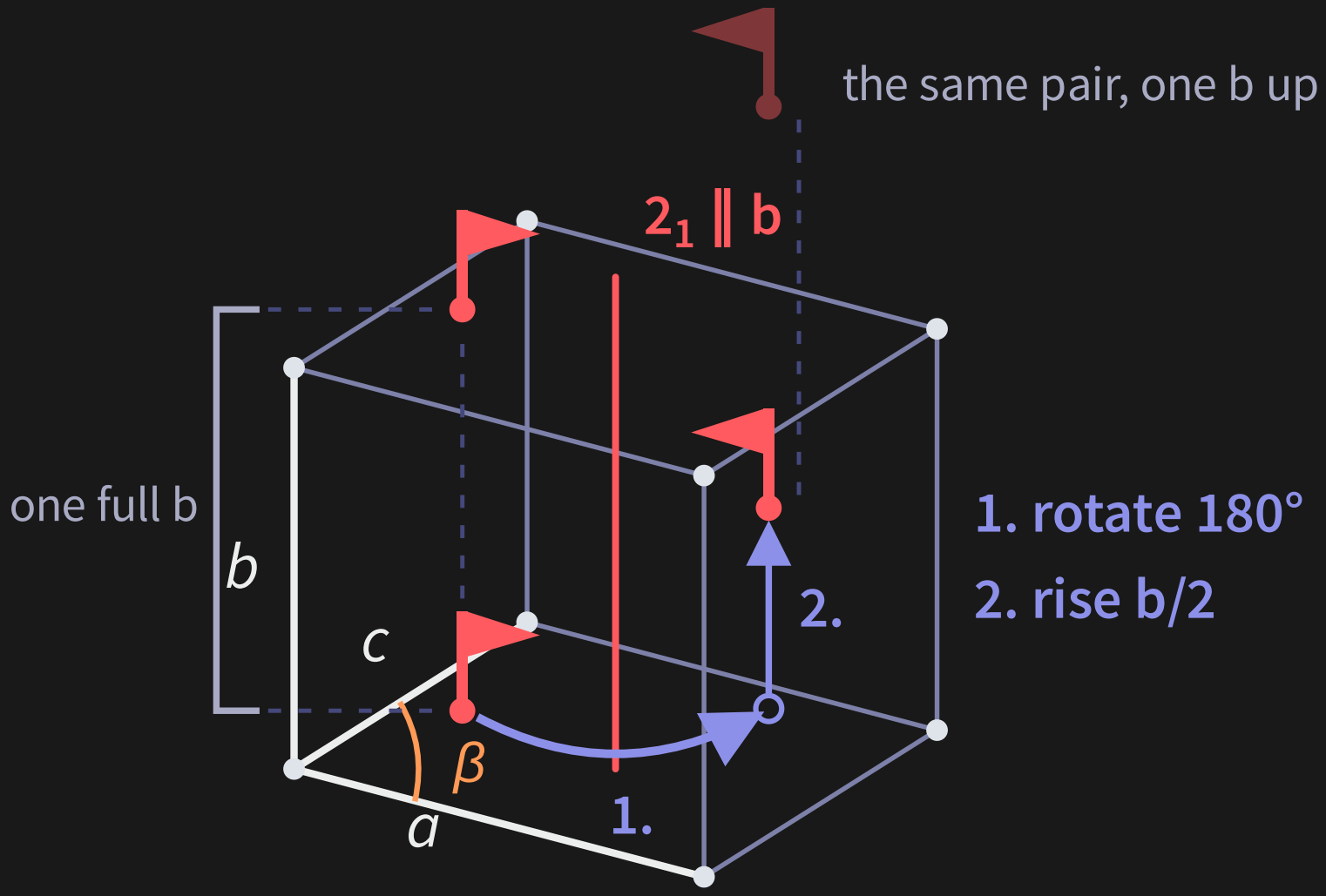


symmorphic — non-symmorphic

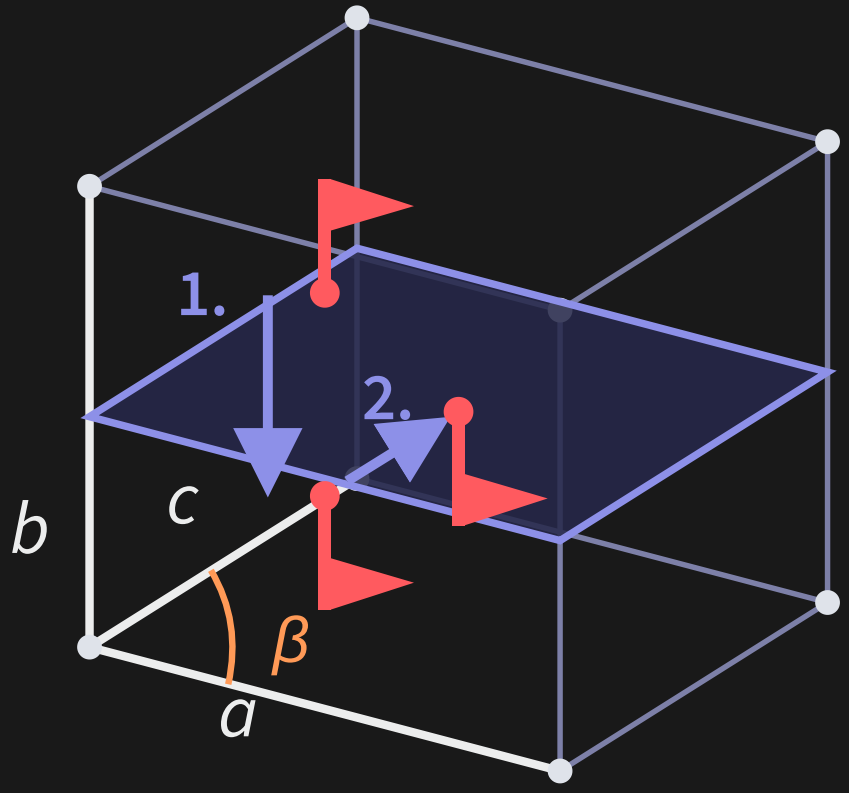
73 + 157 = **230** space groups

Per *Solid State Materials Chemistry*, §§1.1.5–1.1.7.

$P2_1$ IN THREE DIMENSIONS



PC IN THREE DIMENSIONS



c glide plane ⊥ b

1. reflect

2. slide by c/2

MONOCLINIC SPACE GROUPS BUILD STEP BY STEP

2 Bravais lattices: **P**, **C** · 3 point groups: **2**, **m**, **2/m**

SYMMORPHIC		NON-SYMMORPHIC		
P2	C2	$P2_1$	~~$C2_1$~~	≡ C2
Pm	Cm	Pc	Cc	
P2/m	C2/m	$P2_1/m$	~~$C2_1/m$~~	≡ C2/m
		P2/c	C2/c	
		$P2_1/c$	~~$C2_1/c$~~	≡ C2/c

2 lattices × 3 point groups = 6 symmorphic

swap in screws and glides: 10 more candidates

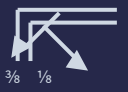
$C2_1$, $C2_1/m$, $C2_1/c$ duplicate C2, C2/m, C2/c → 16 − 3 = 13

INTERNATIONAL TABLES RECORD SPACE-GROUP SYMMETRY

International Tables for Crystallography Volume A

- This reference source contains the symmetry information for all 230 three-dimensional space groups (and more)
- You can access an online version of this reference at https://onlinelibrary.wiley.com/iucr/itc/Ac/

HOW THE INTERNATIONAL TABLES DRAW GLIDE PLANES

GLIDE PLANE	GLIDE VECTOR	NORMAL TO PROJECTION	PARALLEL TO PROJECTION
Axial: *a*, *b*, *c*	½ of one lattice vector		
Diagonal: *n*	½ of two lattice vectors, along a diagonal		
Diamond: *d*	¼ of two lattice vectors, centered cells only		

CONVENTIONAL DIRECTIONS FOR SPACE-GROUP NAMES

The same position in the symbol points along a different direction in each crystal system.

An **axis** runs **along** its position's direction; a **plane** lies **perpendicular** to it. In 2/m the axis and the plane share one position, so that mirror is perpendicular to the twofold, exactly what the slash meant last meeting.

Crystal system	What the positions mean, in order	Worked example
Monoclinic	one direction: **b**	$P2_1/c$: everything refers to b
Orthorhombic	**a**, then **b**, then **c**	Pnma: n ⊥ a, m ⊥ b, a glide ⊥ c
Tetragonal	**c**; then **a** and **b**; then the in-plane diagonals	$P4_12_12$: 4_1 ∥ c, 2_1 ∥ a and b, 2 ∥ diagonals
Trigonal & hexagonal	**c**; then the cell edges; then the in-plane diagonal	$P\bar{3}m1$: $\bar{3}$ ∥ c, m ⊥ edges, nothing on the diagonal
Cubic	the cell edges; then the body diagonals; then the face diagonals	$Pa\bar{3}$: a glide ⊥ edges, $\bar{3}$ ∥ body diagonals

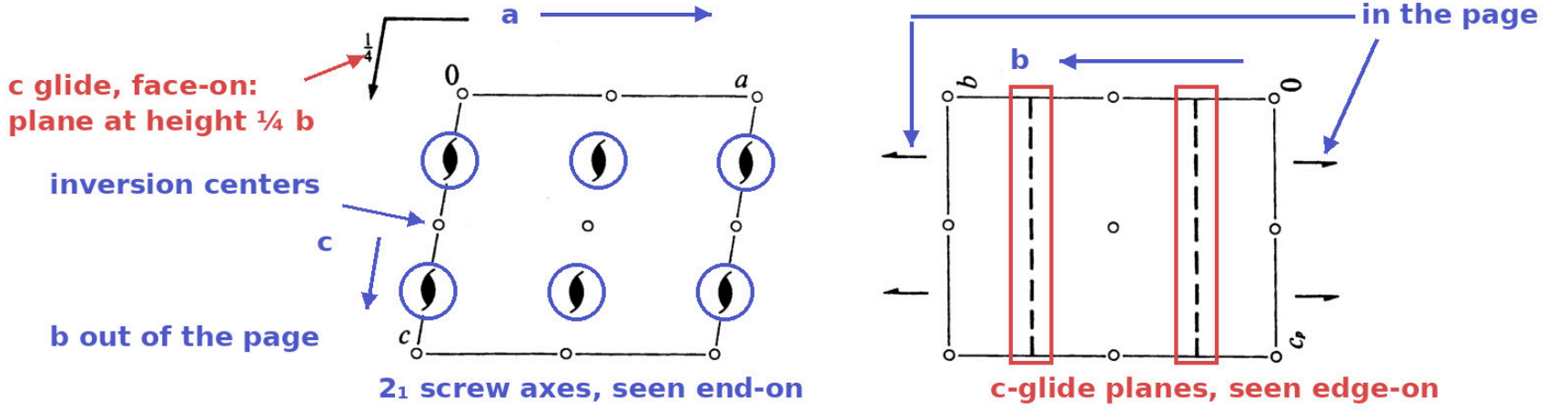
READING THE MONOCLINIC GROUP $P2_1/C$

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

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

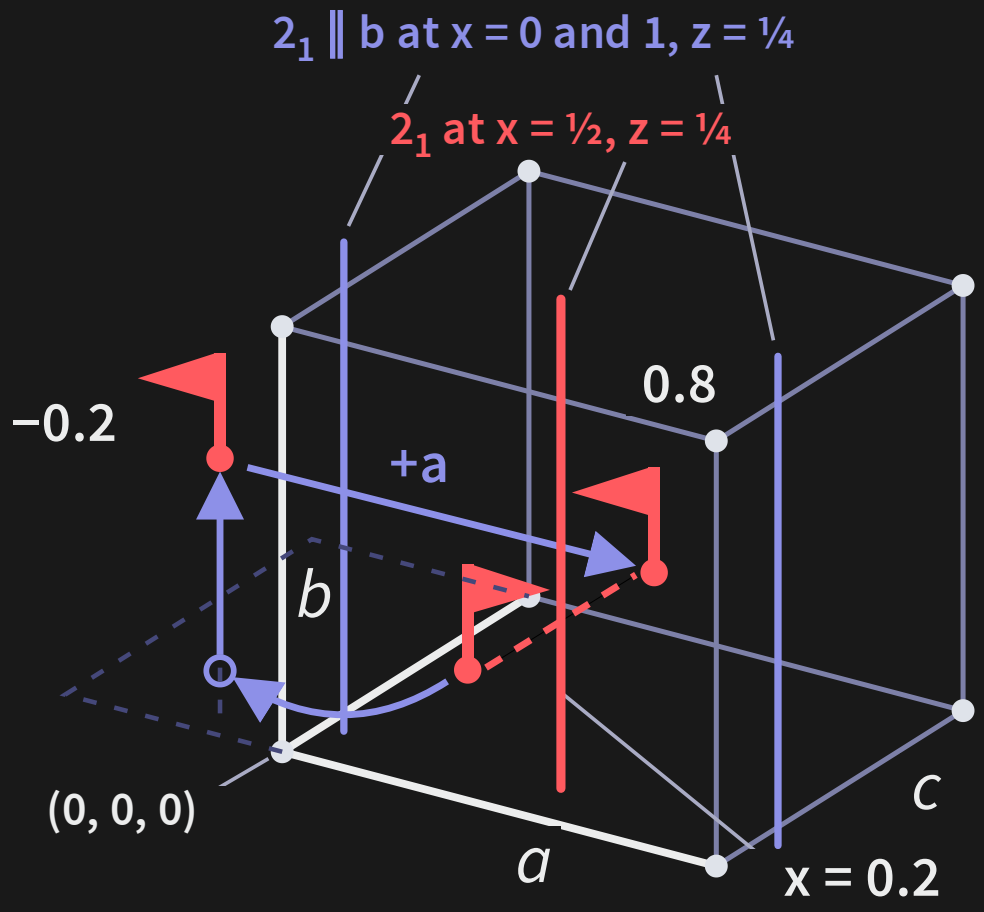
full symbol: a 1 in the empty a and c positions

UNIQUE AXIS b, CELL CHOICE 1



International Tables for Crystallography, Vol. A, entry No. 14.

WHERE THE EXTRA SCREWS COME FROM



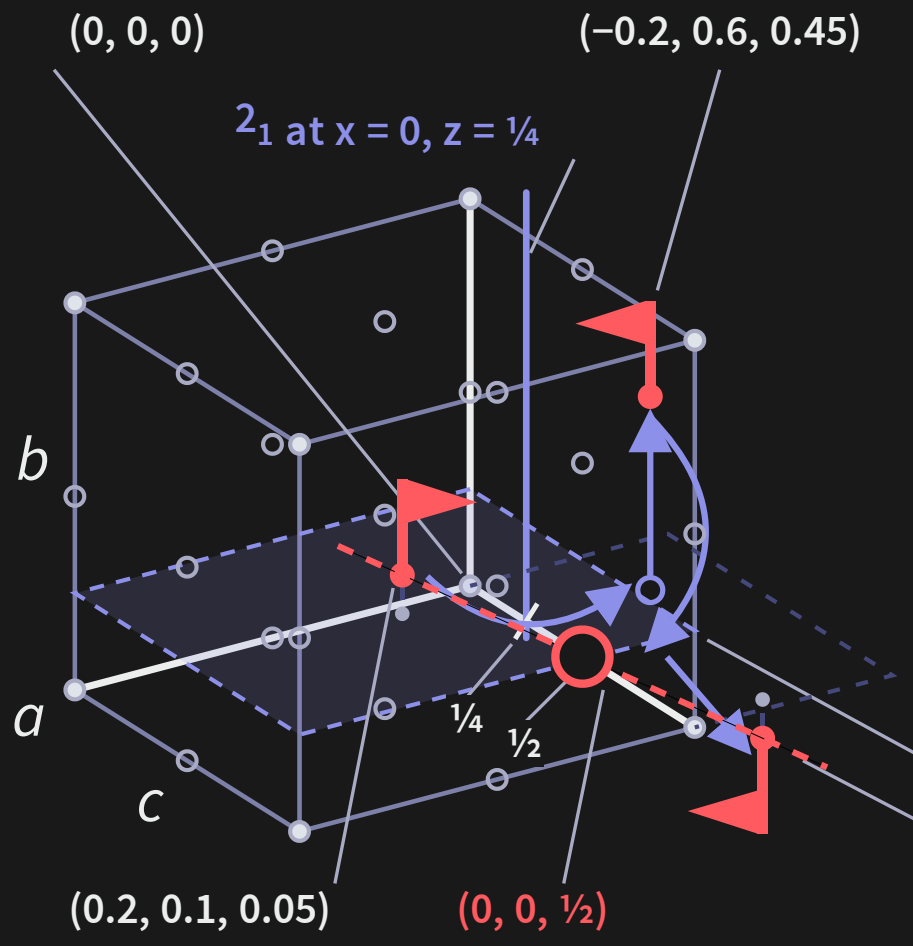
P at x = 0.2

2_1 at x = 0: x → −x, rise ½ b
0.2 → −0.2

+a: −0.2 → 0.8

net: 0.2 → 0.8, rise ½ b
= 2_1 at x = ½

WHERE THE INVERSION COMES FROM



	x	y	z
P	0.2	0.1	0.05
2_1	−x	y+½	−z+½
P after 2_1	−0.2	0.6	0.45
c	x	−y+½	z+½
after c	−0.2	−0.1	0.95
2_1 then c	−x	−y	1−z
= $\bar{1}$ at	0	0	½

$\bar{1}$ + lattice:
a center every ½ cell

c glide, ¼ b

$P2_1/C$: GENERATORS AND WYCKOFF POSITIONS

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

the 2_1 screw

the inversion

Positions

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

x ∥ a, y ∥ b, z ∥ c

unit-cell translations along a, b, and c

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

general position

(2) 2_1 screw

(3) inversion

(4) c glide

special positions

0,0,0 → 0,½,½

(screw and glide agree)

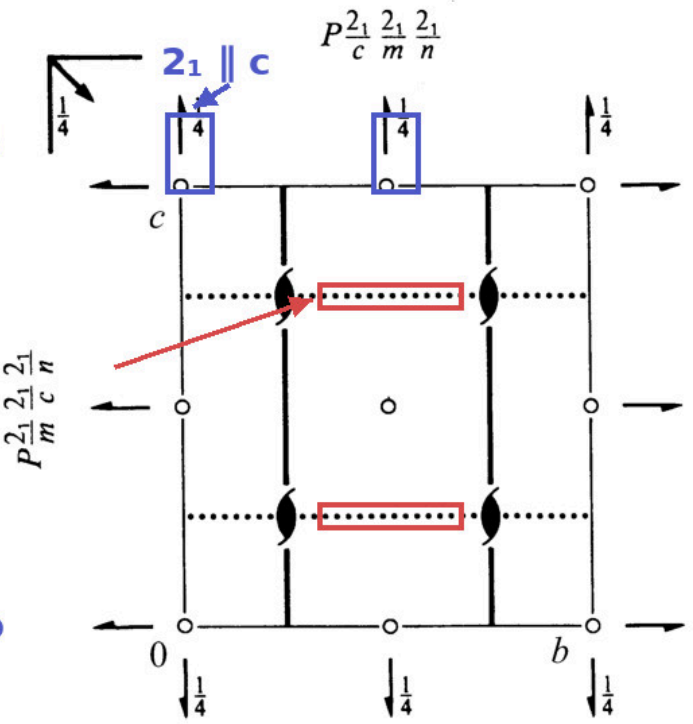
International Tables for Crystallography, Vol. A, entry No. 14.

PNMA: READING THE ENTRY

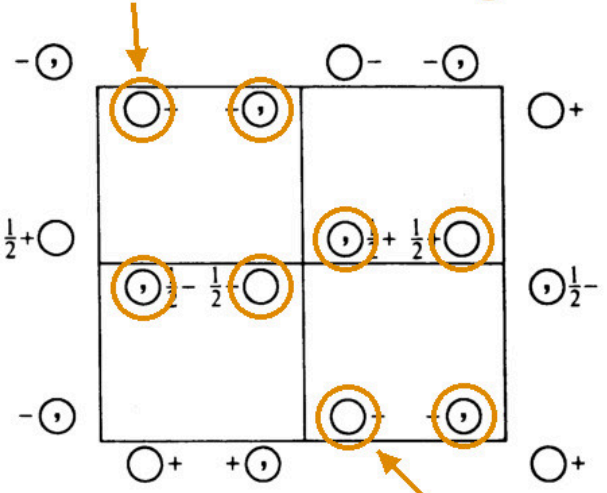
third drawing looks down a

same a glide, now dotted

b across, c up



eight copies here:
the multiplicity of 8d
a comma = mirror image



+ and − : z above or below the page
½+ : half a cell up c

International Tables for Crystallography, Vol. A, entry No. 62, p. 354.

PNMA: GENERATORS AND POSITIONS

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

the identity,
the three cell translations,
then (2), (3) and (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
			general position 8d: eight entries, four to a row, one per operation				General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
			site symbol: one slot per direction, a dot = no element there				Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+l,k=2n$

(2) the 2_1 screw along c
(5) the inversion
(6) the a glide ⊥ c
8 → 4

International Tables for Crystallography, Vol. A, entry No. 62, p. 355.

$P4_12_12$: READING THE ENTRY

International Tables for Crystallography (2016). Vol. A, Space group 92, p. 407.

Tetragonal

422 — point group

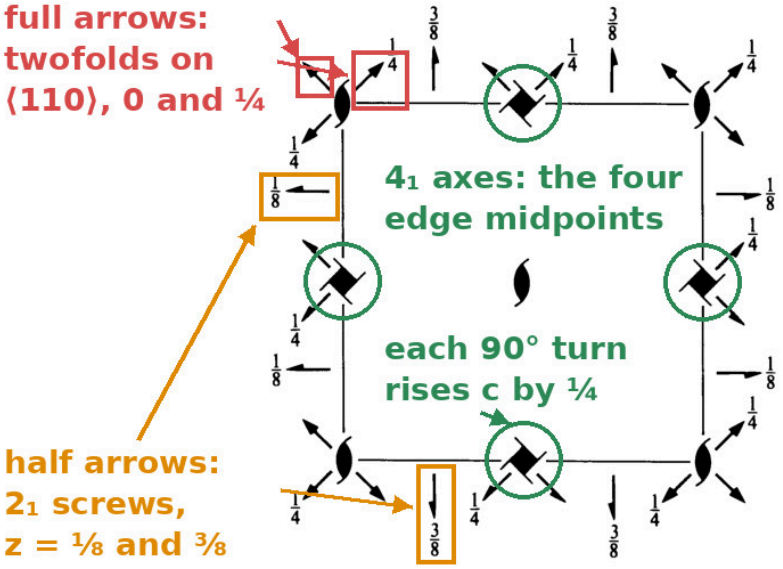
D_4^4 — Schoenflies symbol

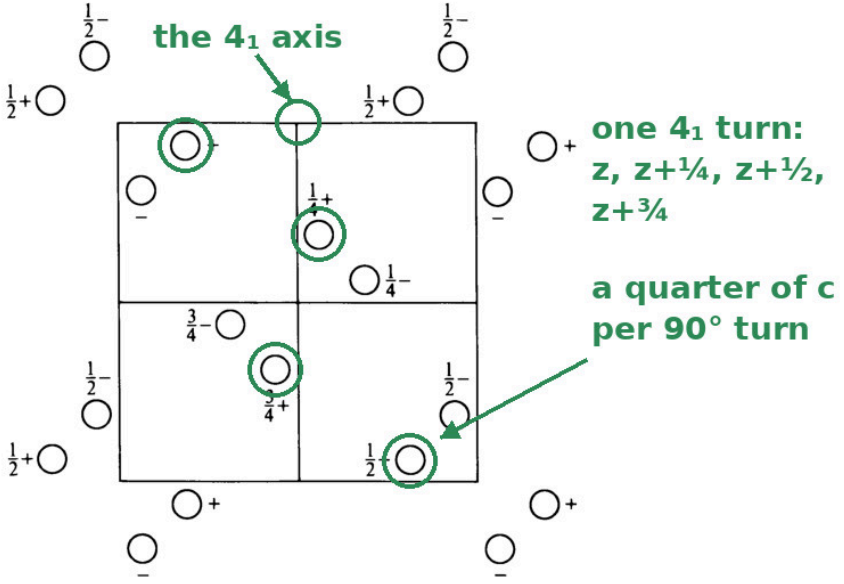
2: on ⟨110⟩
2_1: along a, b
4_1: along c

$P4_12_12$ — full symbol = short symbol

No. 92 — entry number

Patterson symmetry $P4/mmm$





International Tables for Crystallography, Vol. A, entry No. 92.

$P4_12_12$: POSITIONS AND HANDEDNESS

Symmetry operations

(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) $4^+(0,0,\frac{1}{4})$ $0,\frac{1}{2},z$ (4) $4^-(0,0,\frac{3}{4})$ $\frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)$ $\frac{1}{4},y,\frac{1}{8}$ (6) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{3}{8}$ (7) 2 $x,x,0$ (8) 2 $x,\bar{x},\frac{1}{4}$

every entry is a rotation or a screw

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

(2), (3), (5): the boxed ops above with the three cell translations

Positions

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

general position 8b: eight copies
(3) and (4) rise z by ¼ and ¾

no $\bar{1}$, no m, no glide: handedness never flips

site . . 2: the 2 in the third slot

4a lies on op (7): 2 at x,x,0

multiplicity 8 → 4

International Tables for Crystallography, Vol. A, entry No. 92.

P3̄M1: READING THE ENTRY

International Tables for Crystallography (2016). Vol. A, Space group 164, p. 534.

$P\bar{3}m1$ short symbol

D_{3d}^{3} Schoenflies

$\bar{3}m1$ point group

Trigonal

crystal system

No. 164 group number

$P\bar{3}2/m1$ full symbol

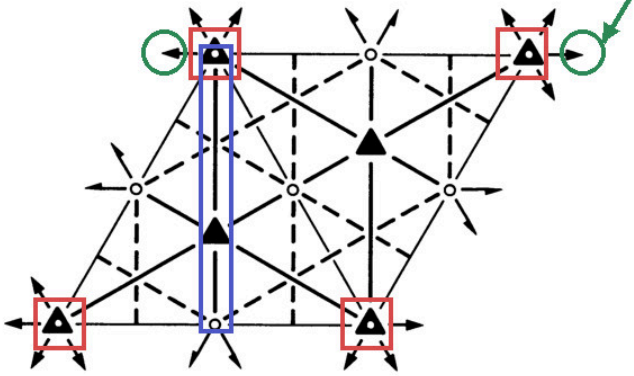
Patterson symmetry $P\bar{3}m1$

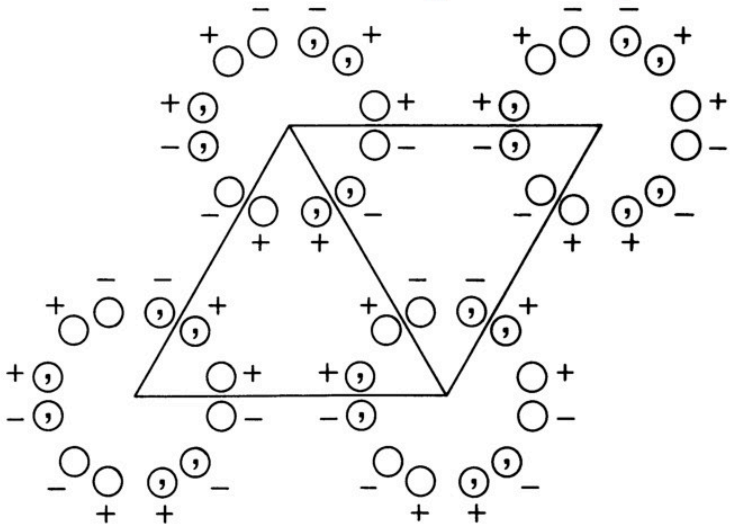
1st slot: c

2nd slot: the three cell edges

3rd slot: the diagonals, printed 1

the twofold arrows lie along the b edge





$\bar{3}$ at every cell corner

solid line: a mirror ⊥ the b edge, its trace a third-slot line

International Tables for Crystallography, Vol. A, entry No. 164.

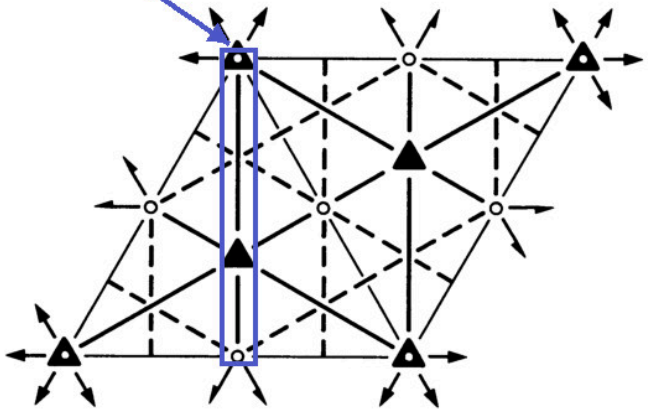
THE SAME M, ONE SLOT OVER: P3̄1M

$P\bar{3}m1$ D_{3d}^{3}

No. 164 $P\bar{3}2/m1$

No. 164: 2/m in the 2nd slot

mirror trace



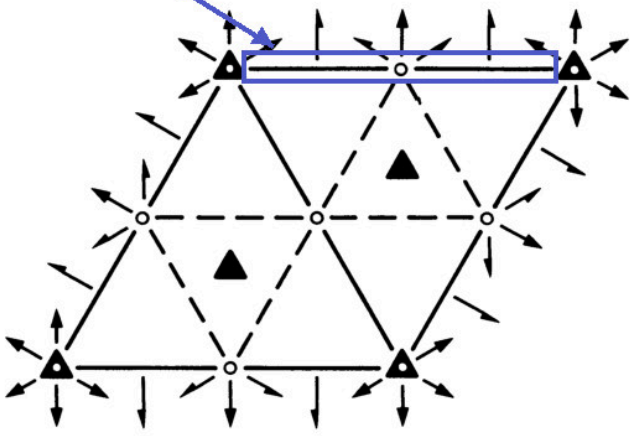
164: m ⊥ the b edge, (12) m 2x,x,z

$P\bar{3}1m$ D_{3d}^{1}

No. 162 $P\bar{3}12/m$

No. 162: 2/m in the 3rd slot

mirror trace



162: m ⊥ the diagonal, (12) m 0,y,z

same operations, one slot over: two different space groups

International Tables for Crystallography, Vol. A, entries No. 164 and No. 162.

P3̄M1: POSITIONS

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates			Reflection conditions
						General:
12	*j*	1	(1) x,y,z	(2) $\bar{y},x-y,z$	(3) $\bar{x}+y,\bar{x},z$	no conditions
			(4) $y,x,\bar{z}$	(5) $x-y,\bar{y},\bar{z}$	(6) $\bar{x},\bar{x}+y,\bar{z}$	
			(7) $\bar{x},\bar{y},\bar{z}$	(8) $y,\bar{x}+y,\bar{z}$	(9) $x-y,x,\bar{z}$	
			(10) $\bar{y},\bar{x},z$	(11) $\bar{x}+y,y,z$	(12) $x,x-y,z$	

12 j: the general position, one copy per numbered operation

Special: no extra conditions

6	*i*	. *m* .	$x,\bar{x},z$	$x,2x,z$	$2\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$2x,x,\bar{z}$	$\bar{x},2\bar{x},\bar{z}$
6	*h*	. 2 .	$x,0,\frac{1}{2}$	$0,x,\frac{1}{2}$	$\bar{x},\bar{x},\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,x,\frac{1}{2}$
6	*g*	. 2 .	$x,0,0$	$0,x,0$	$\bar{x},\bar{x},0$	$\bar{x},0,0$	$0,\bar{x},0$	$x,x,0$
3	*f*	. 2/*m* .	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			
3	*e*	. 2/*m* .	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},0$			
2	*d*	3 *m* .	$\frac{1}{3},\frac{2}{3},z$	$\frac{2}{3},\frac{1}{3},\bar{z}$				
2	*c*	3 *m* .	$0,0,z$	$0,0,\bar{z}$				
1	*b*	$\bar{3}$ *m* .	$0,0,\frac{1}{2}$					
1	*a*	$\bar{3}$ *m* .	$0,0,0$					

1 a at 0,0,0, site $\bar{3}$m .

← 12 operations, one atom

6: on a mirror or a twofold

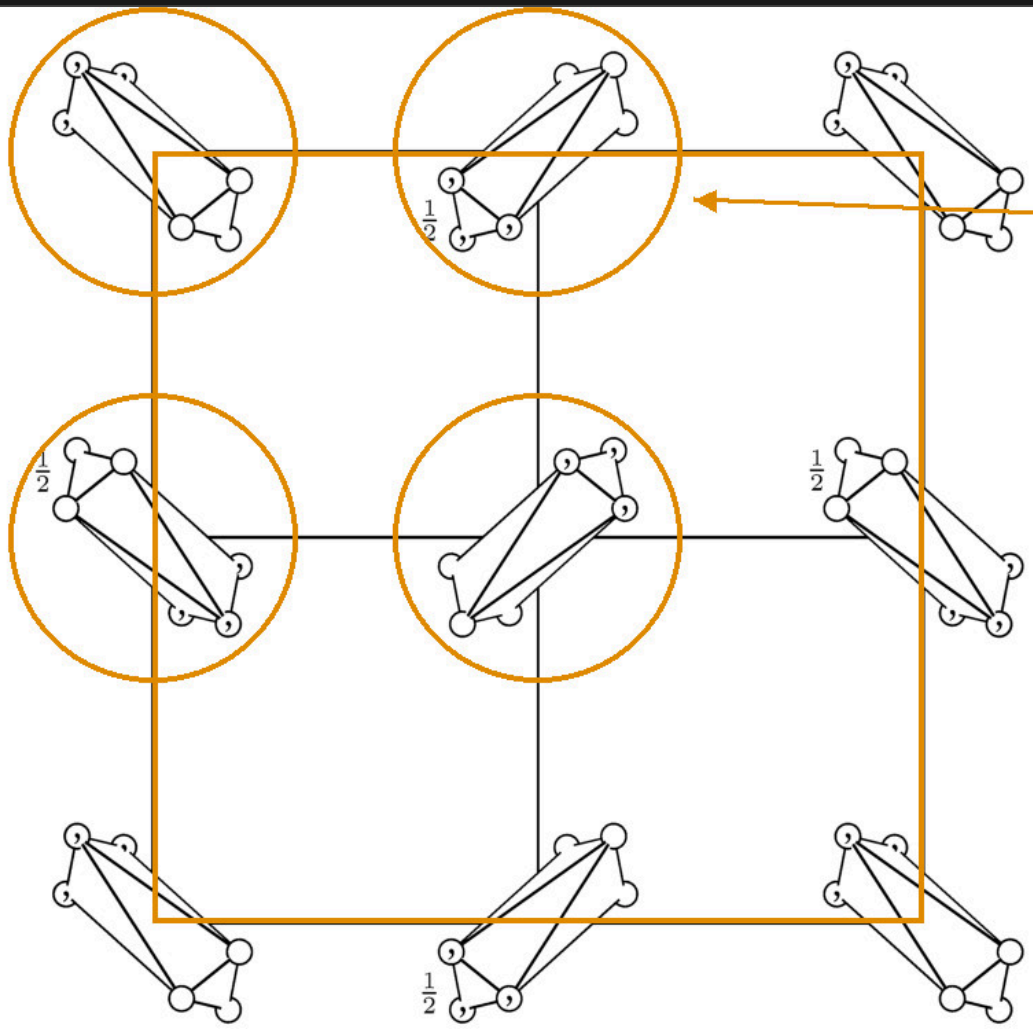
3: on a 2/m

2: on the threefold

1: on the $\bar{3}$m site

International Tables for Crystallography, Vol. A, entry No. 164.

PA3̄: READING THE ENTRY



four $\bar{3}$ sites in the cell
0,0,0 ½,0,½ 0,½,½ ½,½,0

six circles at each site:
three plain, three commas
4 × 6 = 24 general points

International Tables for Crystallography, Vol. A, entry No. 205, pp. 608–609.

PA3̄: POSITIONS

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

Reflection conditions

the general position: 24 points, the order of the point group m3̄

(1) identity, three cell translations, (2) (3) screws, (5) threefold, (13) inversion

			Coordinates				Reflection conditions
24	*d*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}$	h,k,l cyclically permutable General: $0kl$: $k=2n$ $h00$: $h=2n$
			(5) z,x,y	(6) $z+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{y}$	(7) $\bar{z}+\frac{1}{2},\bar{x},y+\frac{1}{2}$	(8) $\bar{z},x+\frac{1}{2},\bar{y}+\frac{1}{2}$	
			(9) y,z,x	(10) $\bar{y},z+\frac{1}{2},\bar{x}+\frac{1}{2}$	(11) $y+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{x}$	(12) $\bar{y}+\frac{1}{2},\bar{z},x+\frac{1}{2}$	
			(13) $\bar{x},\bar{y},\bar{z}$	(14) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(15) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(16) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	
			(17) $\bar{z},\bar{x},\bar{y}$	(18) $\bar{z}+\frac{1}{2},x+\frac{1}{2},y$	(19) $z+\frac{1}{2},x,\bar{y}+\frac{1}{2}$	(20) $z,\bar{x}+\frac{1}{2},y+\frac{1}{2}$	
			(21) $\bar{y},\bar{z},\bar{x}$	(22) $y,\bar{z}+\frac{1}{2},x+\frac{1}{2}$	(23) $\bar{y}+\frac{1}{2},z+\frac{1}{2},x$	(24) $y+\frac{1}{2},z,\bar{x}+\frac{1}{2}$	

4a: the point 0,0,0 sits on a 3̄, site symmetry of order 6: 24 ÷ 6 = 4

Special: as above, plus

8	*c*	. 3 .	x,x,x $\bar{x},\bar{x},\bar{x}$	$\bar{x}+\frac{1}{2},\bar{x},x+\frac{1}{2}$ $x+\frac{1}{2},x,\bar{x}+\frac{1}{2}$	$\bar{x},x+\frac{1}{2},\bar{x}+\frac{1}{2}$ $x,\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{x}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},x$	no extra conditions
4	*b*	. 3̄ .	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},0,0$	$0,0,\frac{1}{2}$	hkl: $h+k,h+l,k+l=2n$
4	*a*	. 3̄ .	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+k,h+l,k+l=2n$

site symmetry: one slot per direction: ⟨100⟩ ⟨111⟩ ⟨110⟩
a dot means nothing there
. 3 . is a 3 along ⟨111⟩

International Tables for Crystallography, Vol. A, entry No. 205, p. 609.

READING A SHORT SYMBOL

Crystal system	Shape	Its point groups	What the positions mean, in order
Triclinic	all skew	1, $1\bar{}$	no direction to name
Monoclinic	one lean	2, m, 2/m	one direction: **b**
Orthorhombic	a brick	222, mm2, mmm	**a**, then **b**, then **c**
Tetragonal	square column	4, $4\bar{}$, 4/m, 422, 4mm, $42\bar{}$m, 4/mmm	**c**; then **a** and **b**; then the in-plane diagonals
Trigonal & hexagonal	120° base	3, $3\bar{}$, 32, 3m, $3\bar{}$m; 6, $6\bar{}$, 6/m, 622, 6mm, $6\bar{}$m2, 6/mmm	**c**; then the cell edges; then the in-plane diagonal
Cubic	a die	23, m$3\bar{}$, 432, $4\bar{}$3m, m$3\bar{}$m	the cell edges; then the body diagonals; then the face diagonals

Per *Solid State Materials Chemistry*, §1.1.3, Table 1.1 and §1.1.7, Table 1.3.

1. Crystal system — write every glide as m and every screw as its rotation, then match what is left against a row above: **mma** becomes mmm, orthorhombic. A 3 in the first position is trigonal, in the second cubic

2. Bravais lattice — the leading letter is the centering, and system plus letter name the lattice; a trigonal group under **P** sits on the primitive hexagonal lattice, under **R** on the rhombohedral

3. Point group — the replaced symbol of step 1, without its lattice letter, is the point group

4. Symmorphic? — if you replaced anything in step 1, the symbol carries a glide or a screw and the group is non-symmorphic

YOUR TURN: PMMA AND P3M1

Short symbol	Crystal system	Bravais lattice	Point group
Pmma	orthorhombic	primitive orthorhombic	mmm
P3m1	trigonal	primitive hexagonal	3m, written 3m1

YOUR TURN: $I4_1/A$ AND $FD\bar{3}M$

Short symbol	Crystal system	Bravais lattice	Point group	Symmorphic?
$I4_1/a$	tetragonal	body-centered tetragonal	4/m	non-symmorphic
$Fd\bar{3}m$	cubic	face-centered cubic	$m\bar{3}m$	non-symmorphic

WHAT THE SPACE-GROUP FRAMEWORK CAPTURES

Operations	translation moves a whole repeat; a glide or a screw moves a fraction of one
230 groups	73 built from a Bravais lattice and a point group, 157 more from swapping in glides and screws
Symbols	centering first, then the operations in their conventional directions
Next meeting	start from fluorite in $Fm\bar{3}m$ and write a whole structure down compactly

PRACTICE QUESTIONS

Work the Lecture 3 practice questions before the next class.

Open the Lecture 3 practice questions

Every question carries a worked explanation, so you can check your reasoning as you go.