Handout 3: Crystallographic Plane & Space Groups

Chem 4850/6850/8850
X-ray Crystallography
Department of Chemistry & Biochemistry

cora.lind@utoledo.edu

THE UNIVERSITY OF TOLEDO

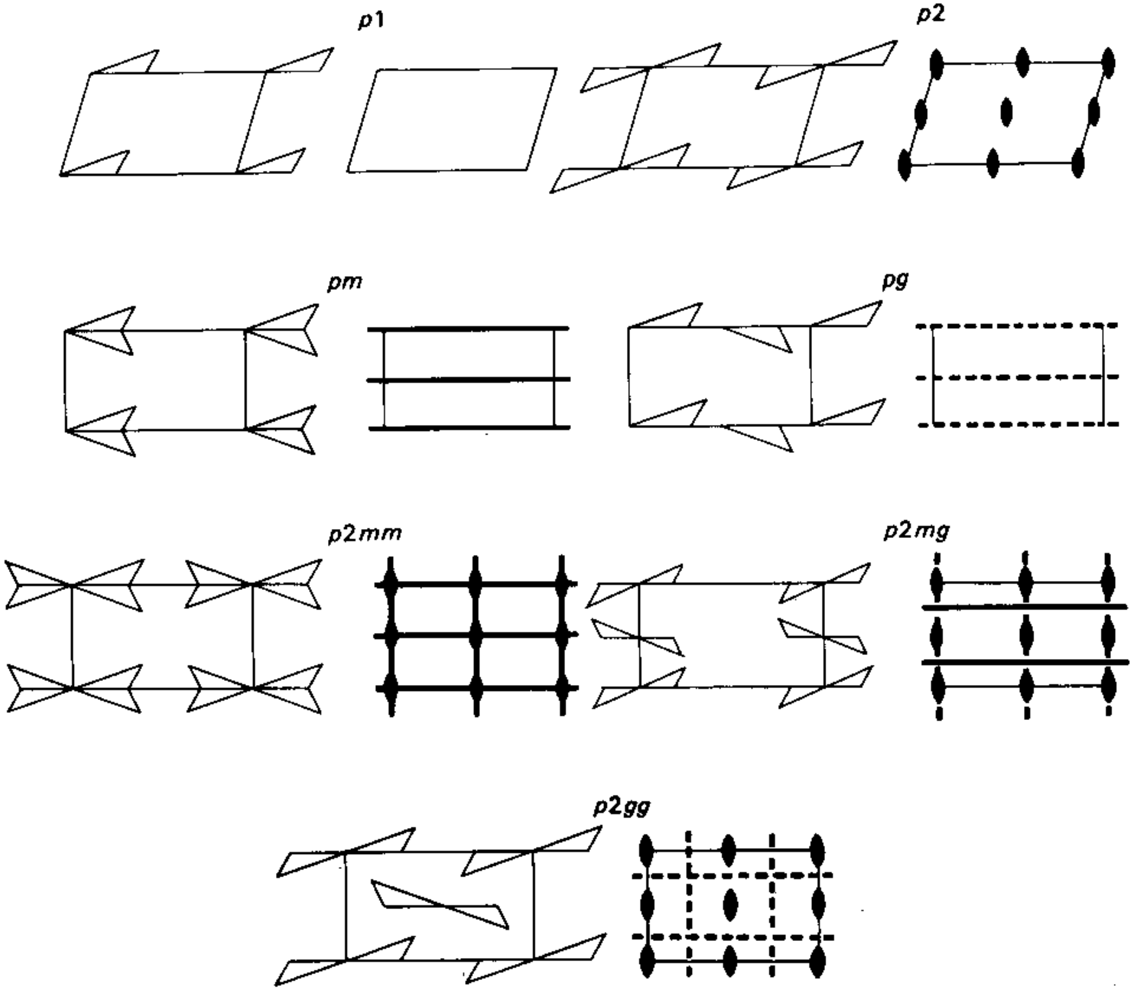
Crystallographic symmetry

- **Key points to remember:**
  - Crystallographic symmetry involves long range order and must produce space filling
    - Only 2, 3, 4, 6-fold rotations
  - Internal symmetry must be compatible with unit cell symmetry, e.g., edges must be mapped onto each other through symmetry operations
  - We need to consider translational (unit cell, centering, glides, screws) and point (rotations, mirrors, inversions, roto-inversions) symmetry
  - Any combinations of symmetry elements must still fulfill these conditions
    - 32 crystallographic point groups that give rise to periodicity in 3D (10 in 2D)
    - 230 crystallographic space groups in 3D (17 plane groups in 2D)

Interpretation of space group symbols

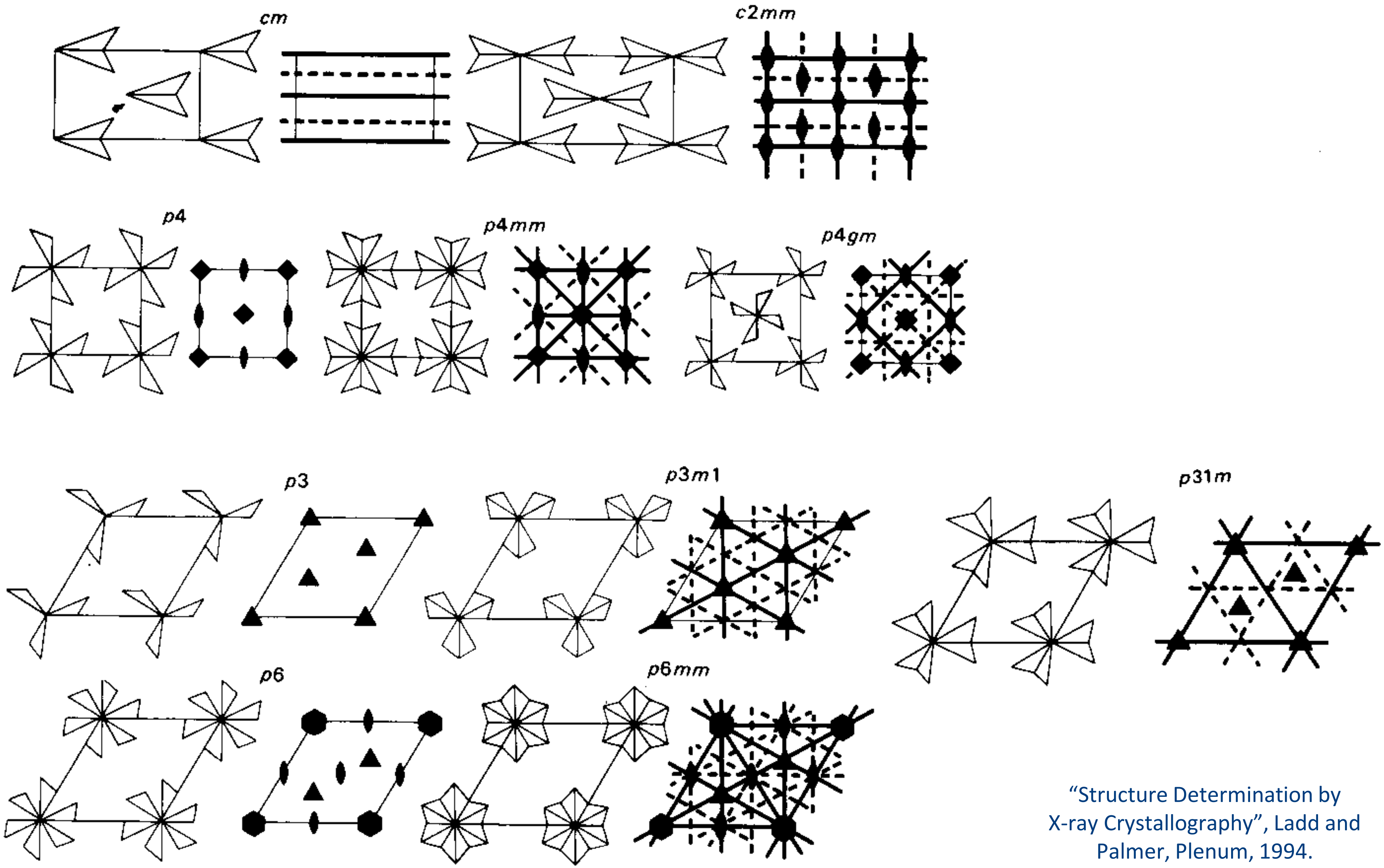
- **All space group symbols start with a capital letter corresponding to the lattice centering, followed by a collection of symbols for symmetry operations in the three lattice directions (plane groups use lower case letter for centering, p or c)**
- **There are sometimes short notations for space group symbols**
  - P 1 2 1 is usually written as P 2
    - primitive monoclinic cell that has a two-fold rotation along the b axis
  - P 2_1 2_1 2_1 (cannot be abbreviated)
    - primitive orthorhombic cell that has a 21 screw along each axis
  - C m m a (full symbol: C 2/m 2/m 2/a)
    - C-centered orthorhombic cell with a mirror plane perpendicular to a and b and an a glide plane perpendicular to c
    - also has implied symmetry elements (e.g., the 2-fold rotations)

The 17 plane groups (1)



"Structure Determination by X-ray Crystallography", Ladd and Palmer, Plenum, 1994.

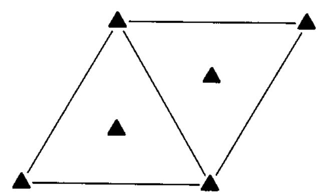
The 17 plane groups (2)

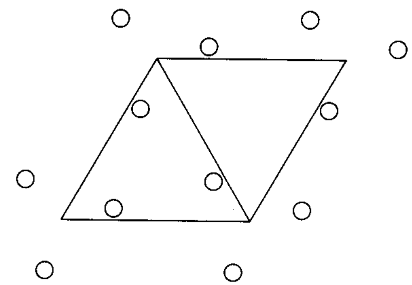


“Structure Determination by X-ray Crystallography”, Ladd and Palmer, Plenum, 1994.

No. 13 $p3$

Patterson symmetry $p6$





All pages following in this handout are from
"International Tables for Crystallography, Vol. A", Kluwer, 1993.

Origin at 3

Asymmetric unit $0 \le x \le \frac{2}{3}$; $0 \le y \le \frac{2}{3}$; $x \le (1+y)/2$; $y \le \min(1-x,(1+x)/2)$

Vertices $0,0$ $\frac{1}{2},0$ $\frac{2}{3},\frac{1}{3}$ $\frac{1}{3},\frac{2}{3}$ $0,\frac{1}{2}$

Symmetry operations

(1) 1 (2) 3^{+} 0,0 (3) 3^{-} 0,0

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
3	d	1	(1) x,y (2) $\bar{y},x-y$ (3) $\bar{x}+y,\bar{x}$	no conditions
				Special: no extra conditions
1	c	3 . .	$\frac{2}{3},\frac{1}{3}$	
1	b	3 . .	$\frac{1}{3},\frac{2}{3}$	
1	a	3 . .	0,0	

Maximal non-isomorphic subgroups

I [3]p 1 1

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3]h 3 ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}$) ($p3$)

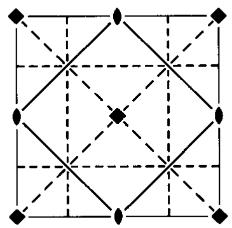
Minimal non-isomorphic supergroups

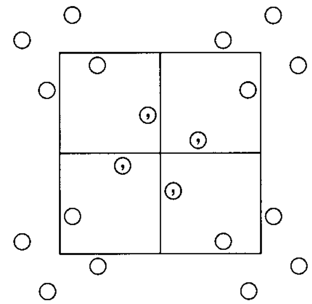
I [2]p 3m 1; [2]p 3 1m; [2]p 6

II none

Square $4mm$ ***p*4*gm***

Patterson symmetry $p4mm$ $p4gm$ **No. 12**





Origin at $41g$

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

Symmetry operations

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates				Reflection conditions
					General:
8 d 1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{y},x$	(4) $y,\bar{x}$	$h0$: $h=2n$
	(5) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(6) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$	(7) $y+\frac{1}{2},x+\frac{1}{2}$	(8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$0k$: $k=2n$
					Special: as above, plus
4 c $..m$	$x,x+\frac{1}{2}$	$\bar{x},\bar{x}+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x$	$x+\frac{1}{2},\bar{x}$	no extra conditions
2 b $2.mm$	$\frac{1}{2},0$	$0,\frac{1}{2}$			hk: $h+k=2n$
2 a $4..$	$0,0$	$\frac{1}{2},\frac{1}{2}$			hk: $h+k=2n$

Maximal non-isomorphic subgroups

I [2]$p411$ ($p4$) 1; 2; 3; 4
[2]$p2g1$ ($p2gg$) 1; 2; 5; 6
[2]$p21m$ ($c2mm$) 1; 2; 7; 8

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [9]$p4gm$ ($\mathbf{a}'=3\mathbf{a}$, $\mathbf{b}'=3\mathbf{b}$)

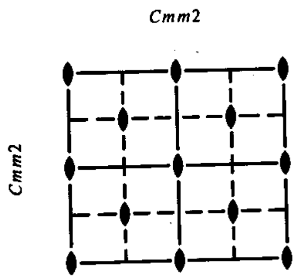
Minimal non-isomorphic supergroups

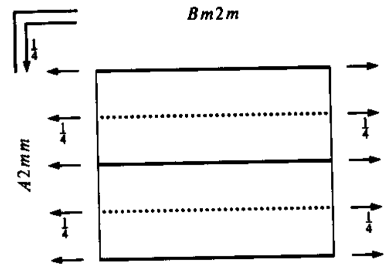
I none

II [2]$c4gm$ ($p4mm$)

① $Cmm2$ C_{2v}^{11} $mm2$ Orthorhombic

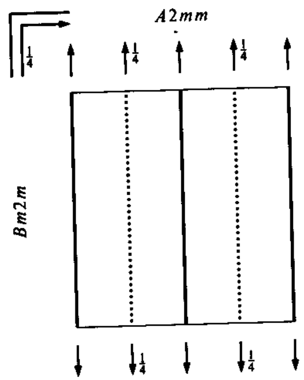
② No. 35 $Cmm2$ Patterson symmetry $Cmmm$

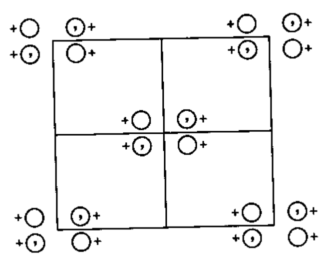




All pages following in this handout are from "International Tables for Crystallography, Vol. A", Kluwer, 1993.

③





Short explanation of the space-group data (*cf*. *Section* 2.2)

① *Headline*: Section 2.3.

Short Hermann–Mauguin symbol (Sections 2.4 and 12.2)	Schoenflies symbol (Sections 12.1 and 12.2)	Crystal class (Point group) (Sections 10.1 and 12.1)	Crystal system (Section 2.1)

② Number of space group [Same as in *IT*(1952)] — Full Hermann–Mauguin symbol (Sections 2.4 and 12.3) — Patterson symmetry (Section 2.5)

③ *Space-group diagrams*, consisting of one or several projections of the symmetry elements and one illustration of a set of equivalent points in general position. The numbers and types of the diagrams depend on the crystal system. The diagrams and their axes are described in Section 2.6; the graphical symbols of symmetry elements are listed in Section 1.4.
For monoclinic space groups see Section 2.16; for orthorhombic settings see Section 2.6(iv).

Table 2.4.1. *Lattice symmetry directions for two and three dimensions*

Directions which 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.

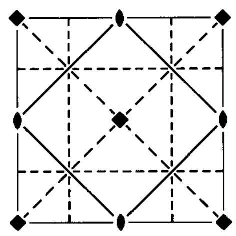
Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Two dimensions Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		$\{[10], [01]\}$	$\{[1\bar{1}], [11]\}$
Hexagonal		$\{[10], [01], [\bar{1}\bar{1}]\}$	$\{[1\bar{1}], [12], [\bar{2}\bar{1}]\}$
Three dimensions Triclinic	None		
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	$\{[100], [010], [001]\}$	$\{[111], [1\bar{1}\bar{1}], [\bar{1}1\bar{1}], [\bar{1}\bar{1}1]\}$	$\{[1\bar{1}0], [110], [01\bar{1}], [011], [\bar{1}01], [101]\}$

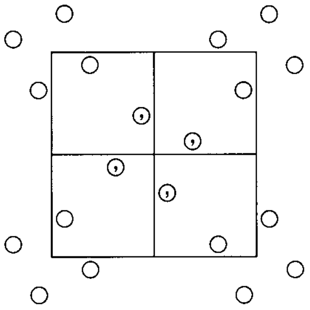
*For the full Hermann–Mauguin symbols see text.

- Hermann-Mauguin symbols consist of
  - letter indicating centering of the cell (P, R, I, F, C)
  - set of characters indicating symmetry elements
- Use lower case letters for plane group centering, capital letters for space group centering
- The one, two or three entries after the centering letter refer to one, two or three kinds of symmetry directions of the lattice as outlined in Table 2.4.1
  - Can be singular directions (monoclinic and orthorhombic) or sets of equivalent directions
- Symmetry planes are represented by their normals
  - If a symmetry axis and a symmetry plane normal are parallel, the two characters are separated by a slash, e.g., P2/m ("P 2 over m")
- The symbol 1 is used for lattice directions that carry no symmetry elements
  - may be omitted if no misinterpretation is possible, e.g., P6 instead of P611 etc.
  - May be written to distinguish standard settings (e.g., monoclinic, unique axis b) from non-standard settings (unique axis a or c)
  - For high symmetry space groups, symmetry axes are often suppressed in the short symbol (e.g., Pnma vs. P 2_1/n 2_1/m 2_1/a)

Square $4mm$ $p4gm$

Patterson symmetry $p4mm$ $p4gm$ No. 12





All pages following in this handout are from "International Tables for Crystallography, Vol. A", Kluwer, 1993.

Origin at $41g$

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

Symmetry operations

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
8 d 1	(1) x,y (2) $\bar{x},\bar{y}$ (3) $\bar{y},x$ (4) $y,\bar{x}$ (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2}$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2}$ (7) $y+\frac{1}{2},x+\frac{1}{2}$ (8) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2}$	$h0$: $h=2n$ $0k$: $k=2n$
		Special: as above, plus
4 c $..m$	$x,x+\frac{1}{2}$ $\bar{x},\bar{x}+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x$ $x+\frac{1}{2},\bar{x}$	no extra conditions
2 b $2.mm$	$\frac{1}{2},0$ $0,\frac{1}{2}$	hk: $h+k=2n$
2 a $4..$	$0,0$ $\frac{1}{2},\frac{1}{2}$	hk: $h+k=2n$

Maximal non-isomorphic subgroups

I [2]$p411$ ($p4$) 1; 2; 3; 4
[2]$p2g1$ ($p2gg$) 1; 2; 5; 6
[2]$p21m$ ($c2mm$) 1; 2; 7; 8

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [9]$p4gm$ ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}$)

Minimal non-isomorphic supergroups

I none

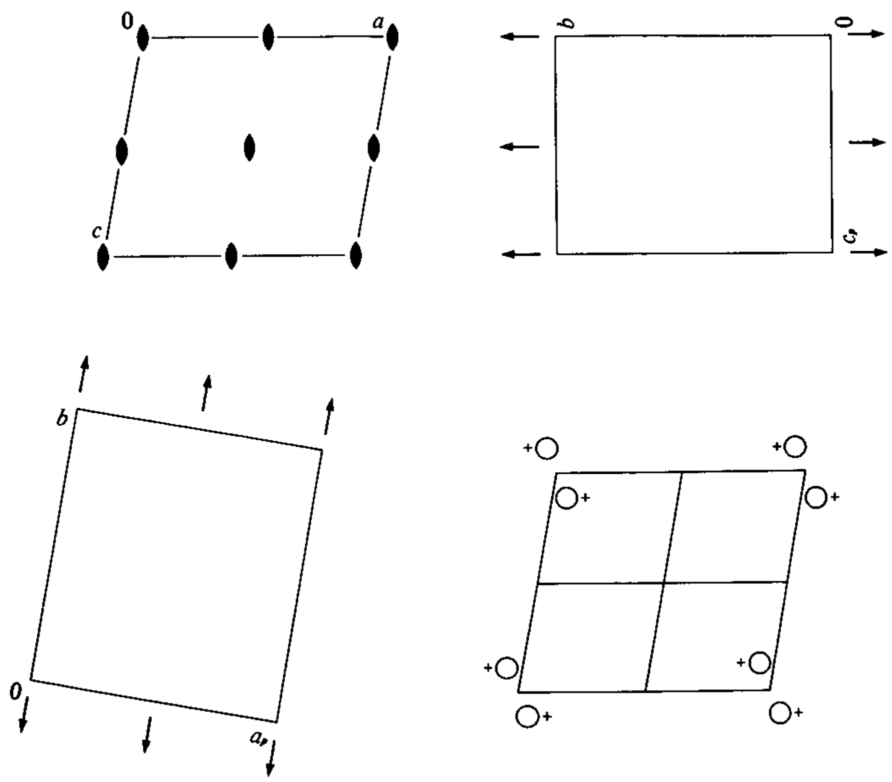
II [2]$c4gm$ ($p4mm$)

$P2$ $\quad C_2^1$ $\quad 2$ $\quad$ Monoclinic

No. 3 $\quad P121$ $\quad$ **Patterson symmetry** $P\,1\,2/m\,1$

UNIQUE AXIS b

All pages following in this handout are from "International Tables for Crystallography, Vol. A", Kluwer, 1993.



Origin on 2

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

Symmetry operations

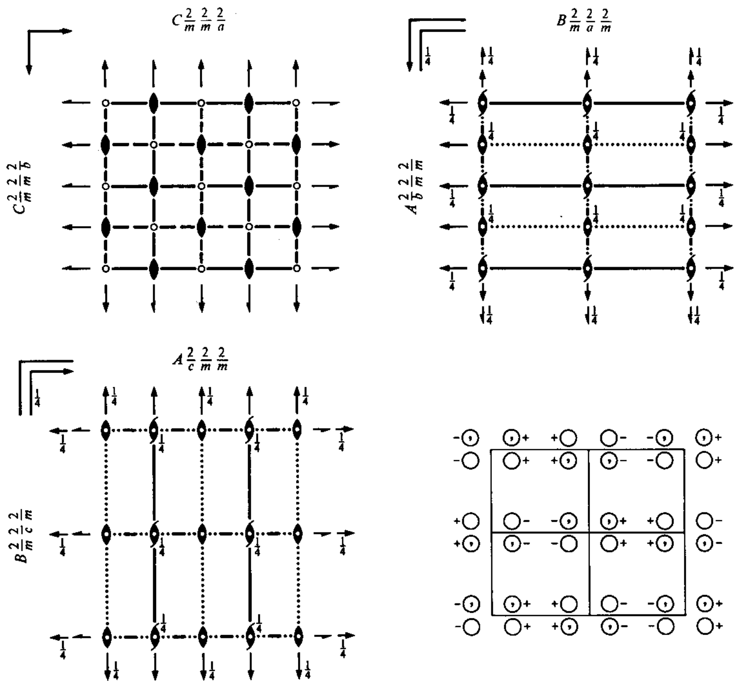
(1) 1 $\qquad$ (2) 2 $\;0,y,0$

THE UNIVERSITY OF TOLEDO

$Cmma$ D_{2h}^{21} mmm **Orthorhombic**

No. 67 $C\,2/m\,2/m\,2/a$ Patterson symmetry $Cmmm$

New space-group symbol $Cmme$; *cf.* Section 1.3



All pages following in this handout are from "International Tables for Crystallography, Vol. A", Kluwer, 1993.

Origin at centre ($2/m$) at $2/m\,2_1/a\,e$

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

Symmetry operations

For (0,0,0)+ set

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

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

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

Maximal isomorphic subgroups of lowest index

IIc [3]$Cmma$ ($\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b}$); [2]$Cmma$ ($\mathbf{c}'=2\mathbf{c}$)

Minimal non-isomorphic supergroups

I [2]$P4/nbm$; [2]$P4/nmm$; [2]$P4_2/nnm$; [2]$P4_2/ncm$

II [2]$Fmmm$; [2]$Pmmm$ ($2\mathbf{a}'=\mathbf{a}, 2\mathbf{b}'=\mathbf{b}$)

Space group diagrams

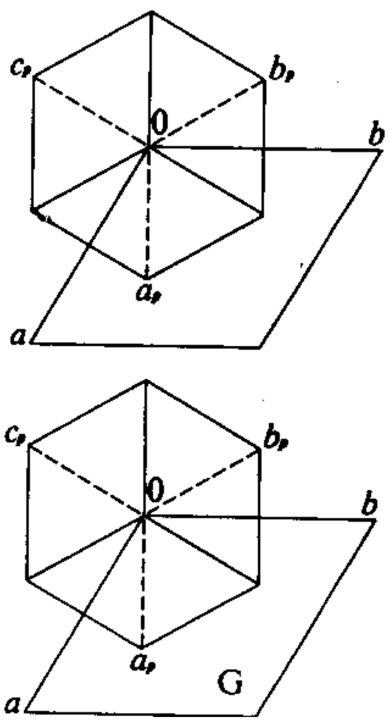


Fig. 2.6.9. Rhombohedral R space groups. Obverse triple hexagonal cell with 'hexagonal axes' a, b and primitive rhombohedral cell with projections of 'rhombohedral axes' a_p, b_p, c_p. Note: In the actual space-group diagrams only the upper edges (full lines), not the lower edges (dashed lines) of the primitive rhombohedral cell are shown (G = General-position diagram).

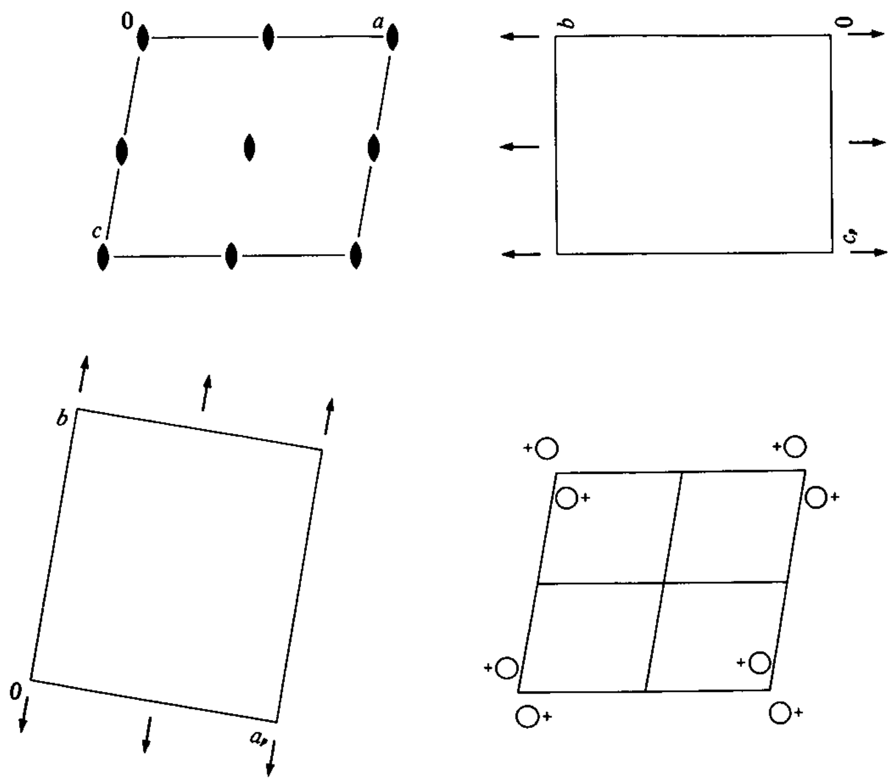
- Show the relative locations and orientations of the symmetry elements
  - Depending on how complex the space group symmetry is, one or several drawings can be used
- Illustrate the arrangement of a set of symmetry equivalent points of a general position
  - A "general position" is any point in the unit cell that does not coincide with any symmetry elements
  - Maximum number of atoms generated
- Except for representations with rhombohedral axes, all projection directions are along a cell axis
  - In rhombohedral, triclinic and monoclinic cells, this can result in the other axes not being parallel to the plane of projection and is indicated by a subscript *p*
- Symmetry elements that lie above the plane of projection are designated by the height *h* above the plane. *h* is given as a fraction along the lattice direction of projection
- For rhombohedral space groups, two settings are given, one with rhombohedral and one with hexagonal axes

$P\,2$ $\quad C_2^1$ $\quad 2$ $\quad$ Monoclinic

No. 3 $\quad P\,1\,2\,1$ $\quad$ **Patterson symmetry** $P\,1\,2/m\,1$

UNIQUE AXIS b

All pages following in this handout are from
“International Tables for Crystallography, Vol. A”, Kluwer, 1993.



Origin on 2

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

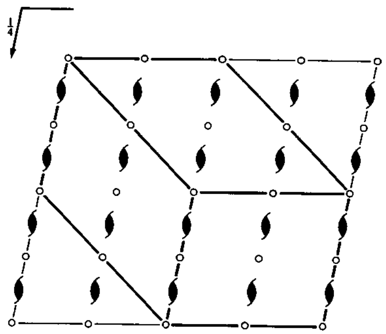
Symmetry operations

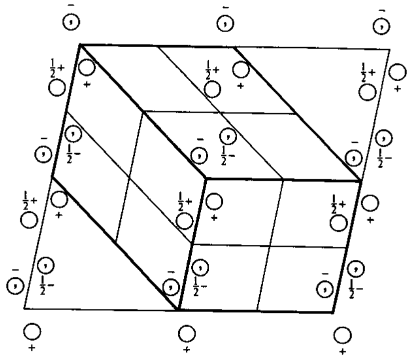
(1) 1 $\qquad$ (2) 2 $\;0,y,0$

$P\,2_1/c$ $\quad C_{2h}^5$ $\quad 2/m$ $\quad$ Monoclinic

No. 14

UNIQUE AXIS b, DIFFERENT CELL CHOICES

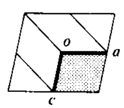




All pages following in this handout are from “International Tables for Crystallography, Vol. A”, Kluwer, 1993.

$P\,1\,2_1/c\,1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

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

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

Positions

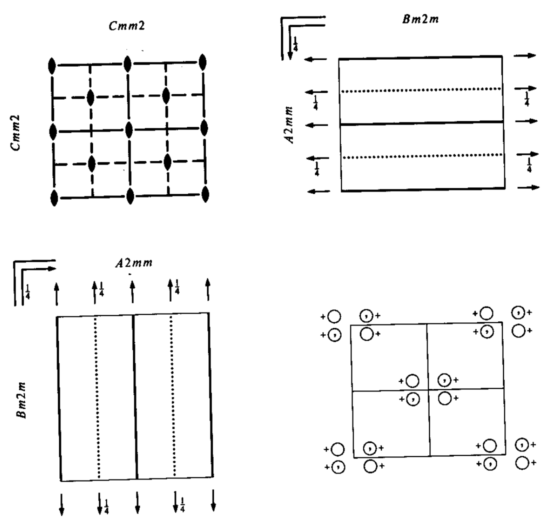
Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above,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

THE UNIVERSITY OF TOLEDO

① $Cmm2$ $\quad C_{2v}^{11}$ $\quad mm2$ $\quad$ Orthorhombic

② No. 35 $\quad Cmm2$ $\quad$ Patterson symmetry $Cmmm$

③



④ **Origin** on $mm2$

⑤ **Asymmetric unit** $\quad 0\le x\le \frac{1}{4};\quad 0\le y\le \frac{1}{2};\quad 0\le z\le 1$

⑥ **Symmetry operations**

For (0,0,0)+ set

(1) 1 $\quad$ (2) 2 $\;0,0,z$ $\quad$ (3) $m\;\; x,0,z$ $\quad$ (4) $m\;\; 0,y,z$

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

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $\quad$ (2) 2 $\;\frac{1}{4},\frac{1}{4},z$ $\quad$ (3) $a\;\; x,\frac{1}{4},z$ $\quad$ (4) $b\;\; \frac{1}{4},y,z$

④ **Origin** on $mm2$

⑤ **Asymmetric unit** $\quad 0\le x\le \frac{1}{4};\quad 0\le y\le \frac{1}{2};\quad 0\le z\le 1$

⑥ **Symmetry operations**

For (0,0,0)+ set

(1) 1 $\quad$ (2) 2 $\;0,0,z$ $\quad$ (3) $m\;\; x,0,z$ $\quad$ (4) $m\;\; 0,y,z$

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

(1) $t(\frac{1}{2},\frac{1}{2},0)$ $\quad$ (2) 2 $\;\frac{1}{4},\frac{1}{4},z$ $\quad$ (3) $a\;\; x,\frac{1}{4},z$ $\quad$ (4) $b\;\; \frac{1}{4},y,z$

④ *Origin* of the unit cell: Section 2.7. The site symmetry of the origin and its location with respect to the symmetry elements are given.

⑤ *Asymmetric unit*: Section 2.8. One choice of asymmetric unit is given.

⑥ *Symmetry operations:* Sections 2.9 and 11. For each point $\tilde{x},\tilde{y},\tilde{z}$ of the general position that symmetry operation is listed which transforms the initial point x,y,z into the point under consideration. The symbol describes the nature of the operation, its glide or screw component (given between parentheses), if present, and the location of the corresponding symmetry element.
The symmetry operations are numbered in the same way as the corresponding coordinate triplets of the general position. For centred space groups the same numbering system is applied in each block, *e.g.* under 'For $(\frac{1}{2},\frac{1}{2},0)+$ set'.

Choice of origin

- In all centrosymmetric space groups, the origin is chosen on an inversion center
  - A second origin choice can be given if there are other high symmetry sites
- In all non-centrosymmetric space groups, the origin is at the point of highest symmetry
  - Usually, the highest rotation axis
  - Screw axes are used if no simple rotation axes are present
  - If no rotation or screw axes are present, the intersection of mirror and glide planes is chosen as origin
  - Exceptions: In $P2_12_12_1$ and related supergroups, the origin is chosen so that it is surrounded symmetrically by three pairs of 2_1 axes

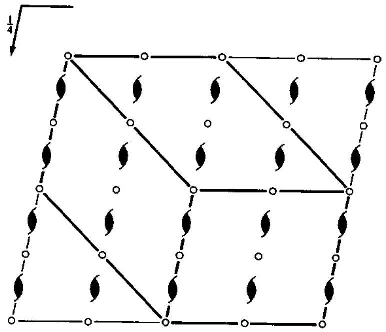
Asymmetric unit

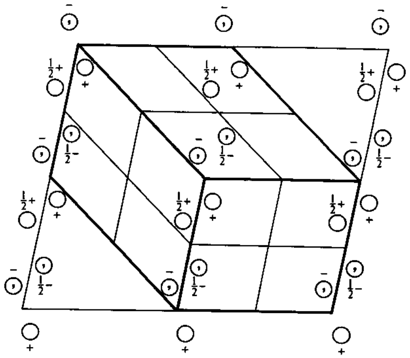
- The smallest part of space from which the whole of space can be filled exactly by application of all symmetry operations
  - Mirror planes and rotation axes must form boundary planes and edges
  - Centers of inversion must be on vertices or at the midpoints of boundary planes or edges
- For higher symmetry unit cells, the shape of the asymmetric unit can be rather complicated

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

No. 14

UNIQUE AXIS *b*, DIFFERENT CELL CHOICES

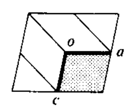




All pages following in this handout are from “International Tables for Crystallography, Vol. A”, Kluwer, 1993.

$P\,1\,2_1/c\,1$

UNIQUE AXIS *b*, CELL CHOICE 1



Origin at $\bar{1}$

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

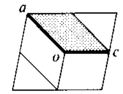
Generators selected $\quad$ (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
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) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	*d*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	*c*	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	*b*	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	*a*	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

$P\,1\,2_1/n\,1$

UNIQUE AXIS b, CELL CHOICE 2



Origin at $\bar{1}$

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

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

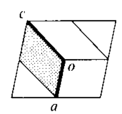
Positions

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

All pages following in this handout are from "International Tables for Crystallography, Vol. A", Kluwer, 1993.

$P\,1\,2_1/a\,1$

UNIQUE AXIS b, CELL CHOICE 3



Origin at $\bar{1}$

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

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

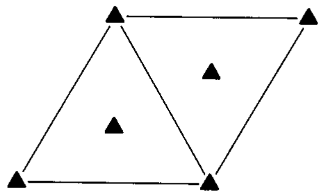
Positions

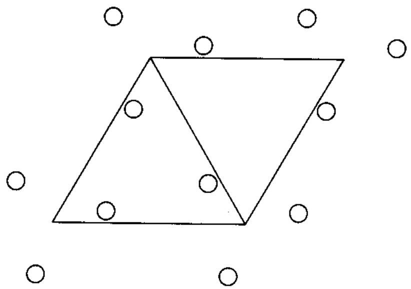
Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
4 e 1	(1) x,y,z (2) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	$h0l$: $h=2n$ $0k0$: $k=2n$ $h00$: $h=2n$
		Special: as above, plus
2 d $\bar{1}$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

THE UNIVERSITY OF TOLEDO

$p\,3$

Patterson symmetry $p\,6$





All pages following in this handout are from
"International Tables for Crystallography, Vol. A", Kluwer, 1993.

Origin at 3

Asymmetric unit $\quad 0\le x\le \frac{2}{3};\quad 0\le y\le \frac{2}{3};\quad x\le(1+y)/2;\quad y\le \min(1-x,(1+x)/2)$

Vertices $\quad 0,0 \quad \frac{1}{3},0 \quad \frac{2}{3},\frac{1}{3} \quad \frac{1}{3},\frac{2}{3} \quad 0,\frac{1}{3}$

Symmetry operations

(1) 1 $\qquad$ (2) 3^{+} 0,0 $\qquad$ (3) 3^{-} 0,0

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

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates	Reflection conditions
		General:
3 d 1	(1) x,y $\quad$ (2) $\bar{y},x-y$ $\quad$ (3) $\bar{x}+y,\bar{x}$	no conditions
		Special: no extra conditions
1 c 3 . .	$\frac{2}{3},\frac{1}{3}$	
1 b 3 . .	$\frac{1}{3},\frac{2}{3}$	
1 a 3 . .	0,0	

Maximal non-isomorphic subgroups

I $\quad$ [3] $p\,1$ $\quad$ 1

IIa $\quad$ none

IIb $\quad$ none

Maximal isomorphic subgroups of lowest index

IIc $\quad$ [3] $h\,3$ ($\mathbf{a}'=3\mathbf{a}, \mathbf{b}'=3\mathbf{b}$) ($p3$)

Minimal non-isomorphic supergroups

I $\quad$ [2] $p\,3m\,1$; [2] $p\,3\,1m$; [2] $p\,6$

II $\quad$ none

② Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3)

③ Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	f	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl: $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	e	$m..$	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	d	$.m.$	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	c	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl: $h=2n$
2	b	$mm2$	$0,\frac{1}{2},z$				no extra conditions
2	a	$mm2$	$0,0,z$				no extra conditions

④ Symmetry of special projections

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

Along [100] $p1m1$
$\mathbf{a}'=\frac{1}{2}\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,0,0$

Along [010] $p11m$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\frac{1}{2}\mathbf{a}$
Origin at $0,y,0$

⑥ Symmetry operations

For $(0,0,0)+$ set

(1) 1 (2) 2 $0,0,z$ (3) m $x,0,z$ (4) m $0,y,z$

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

(1) $t(\frac{1}{2},\frac{1}{2},0)$ (2) 2 $\frac{1}{4},\frac{1}{4},z$ (3) a $x,\frac{1}{4},z$ (4) b $\frac{1}{4},y,z$

Short explanation of the space-group data (*continued*)

① *Headline* in abbreviated form.

② *Generators selected*: Sections 2.10 and 8.3.5. A set of generators, as selected for these *Tables*, is listed in the form of translations and numbers of general-position coordinates. The generators determine the sequence of the coordinate triplets in the general position and of the corresponding symmetry operations.

③ *Positions*: Sections 2.11 and 8.3.2. The general Wyckoff position is given at the top, followed downwards by the various special Wyckoff positions with decreasing multiplicity and increasing site symmetry. For each general and special position its multiplicity, Wyckoff letter, oriented site-symmetry symbol, as well as the appropriate coordinate triplets and the reflection conditions, are listed. The coordinate triplets of the general position are numbered sequentially; *cf. Symmetry operations*.

Oriented site-symmetry symbol (third column): Section 2.12. The site symmetry at the points of a special position is given in oriented form.

Reflection conditions (right-most column): Section 2.13.

[*Lattice complexes* are described in Section 14; Tables 14.1 and 14.2 show the assignment of Wyckoff positions to Wyckoff sets and to lattice complexes.]

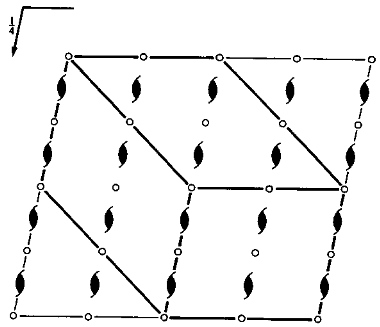
④ *Symmetry of special projections*: Section 2.14. For each space group, orthographic projections along three (symmetry) directions are listed. Given are the projection direction, the plane group of the projection, as well as the axes and the origin of the projected cell.

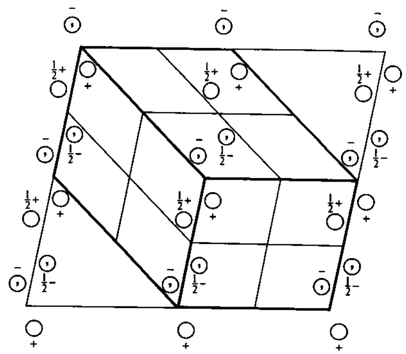
2023-2024

$P\,2_1/c$ $\quad C_{2h}^5$ $\quad 2/m$ $\quad$ Monoclinic

No. 14

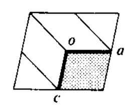
UNIQUE AXIS b, DIFFERENT CELL CHOICES





$P\,1\,2_1/c\,1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $\quad 0 \le x \le 1;\quad 0 \le y \le \tfrac{1}{4};\quad 0 \le z \le 1$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\tfrac{1}{2},\bar{z}+\tfrac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\tfrac{1}{2},z+\tfrac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\tfrac{1}{2},0,\tfrac{1}{2}$	$\tfrac{1}{2},\tfrac{1}{2},0$			hkl: $k+l=2n$
2	c	$\bar{1}$	$0,0,\tfrac{1}{2}$	$0,\tfrac{1}{2},0$			hkl: $k+l=2n$
2	b	$\bar{1}$	$\tfrac{1}{2},0,0$	$\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}$			hkl: $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\tfrac{1}{2},\tfrac{1}{2}$			hkl: $k+l=2n$

⑤ Maximal non-isomorphic subgroups

I	$[2]C\,1\,1\,2\,(P\,2)$	$(1;2)+$
	$[2]C\,1\,m\,1\,(C\,m)$	$(1;3)+$
	$[2]C\,m\,1\,1\,(C\,m)$	$(1;4)+$
IIa	$[2]P\,m\,m\,2$	$1;2;3;4$
	$[2]P\,b\,a\,2$	$1;2;(3;4)+(\frac{1}{2},\frac{1}{2},0)$
	$[2]P\,b\,m\,2\,(P\,m\,a\,2)$	$1;3;(2;4)+(\frac{1}{2},\frac{1}{2},0)$
	$[2]P\,m\,a\,2$	$1;4;(2;3)+(\frac{1}{2},\frac{1}{2},0)$

IIb $[2]C\,c\,c\,2\,(\mathbf{c}'=2\mathbf{c})$; $[2]C\,m\,c\,2_1\,(\mathbf{c}'=2\mathbf{c})$; $[2]C\,c\,m\,2_1\,(\mathbf{c}'=2\mathbf{c})(C\,m\,c\,2_1)$; $[2]I\,m\,m\,2\,(\mathbf{c}'=2\mathbf{c})$; $[2]I\,b\,a\,2\,(\mathbf{c}'=2\mathbf{c})$; $[2]I\,b\,m\,2\,(\mathbf{c}'=2\mathbf{c})(I\,m\,a\,2)$; $[2]I\,m\,a\,2\,(\mathbf{c}'=2\mathbf{c})$

⑥ Maximal isomorphic subgroups of lowest index

IIc $[3]C\,m\,m\,2\,(\mathbf{a}'=3\mathbf{a}$ or $\mathbf{b}'=3\mathbf{b})$; $[2]C\,m\,m\,2\,(\mathbf{c}'=2\mathbf{c})$

⑦ Minimal non-isomorphic supergroups

I $[2]C\,m\,m\,m$; $[2]C\,m\,m\,a$; $[2]P\,4\,m\,m$; $[2]P\,4\,b\,m$; $[2]P\,4_2\,c\,m$; $[2]P\,4_2\,n\,m$; $[2]P\,\bar{4}\,2\,m$; $[2]P\,\bar{4}\,2_1\,m$; $[3]P\,6\,m\,m$

II $[2]F\,m\,m\,2$; $[2]P\,m\,m\,2\,(2\mathbf{a}'=\mathbf{a},2\mathbf{b}'=\mathbf{b})$

⑤ *Maximal non-isomorphic subgroups*: Sections 2.15 and 8.3.3.
Type **I**: *translationengleiche* or *t* subgroups
Type **IIa**: *klassengleiche* or *k* subgroups, obtained by 'decentring' the conventional cell; applies only to space groups with centred cells;
Type **IIb**: *klassengleiche* or *k* subgroups, obtained by enlarging the conventional cell.
Given are: For types **I** and **IIa**: Index [between brackets]; 'unconventional' Hermann–Mauguin symbol of the subgroup; 'conventional' Hermann–Mauguin symbol of the subgroup, if different (between parentheses); coordinate triplets retained in subgroup.
For type **IIb**: Index [between brackets]; 'unconventional' Hermann–Mauguin symbol of the subgroup; basis-vector relations between group and subgroup (between parentheses); 'conventional' Hermann–Mauguin symbol of the subgroup, if different (between parentheses).

⑥ *Maximal isomorphic subgroups of lowest index*: Sections 2.15, 8.3.3, and 13.1.
Type **IIc**: *klassengleiche* or *k* subgroups of lowest index which are of the same type as the group, *i.e.* have the same standard Hermann–Mauguin symbol. Data as for subgroups of type **IIb**.

⑦ *Minimal non-isomorphic supergroups*: Sections 2.15 and 8.3.3.
The list contains the reverse relations of the subgroup tables; only types **I** (*t* supergroups) and **II** (*k* supergroups) are distinguished. Data as for subgroups of type **IIb**.

Sub- and supergroups

- Can be used to describe symmetry related space groups
- Subgroups contain a set of symmetry operations that also belongs to the space group being discussed
  - The set of symmetry operations must also form a space group
  - If it is possible to take symmetry elements away "step by step", an "order" of space groups can be established with decreasing symmetry: G > M > H
  - A subgroup H is called a *maximal subgroup* if there is no subgroup of higher symmetry between H and G (example: $P2_1/c$ has $P2_1$, Pc and P-1 as maximal subgroups, while P1 is a non-maximal subgroup)
  - All subgroups can be listed as *chains* of maximal subgroups (e.g., $P2_1/c$ > P-1 > P1)
- Symmetry can be reduced by several means
  - Removal of point symmetry elements: *translationsgleiche* or *t* subgroups (translation equivalent)
  - "Thinning out" of symmetry operations, e.g., doubling of a cell axis in the same space group, which is equivalent to loss of translational symmetry, or by replacing rotation axes by screw axes: *klassengleiche* or *k* subgroups (same class/point group)
- Supergroups are the opposite of subgroups, so if a space group *X* is listed as a subgroup of another space group *Y*, then *Y* must be listed as a supergroup of *X*