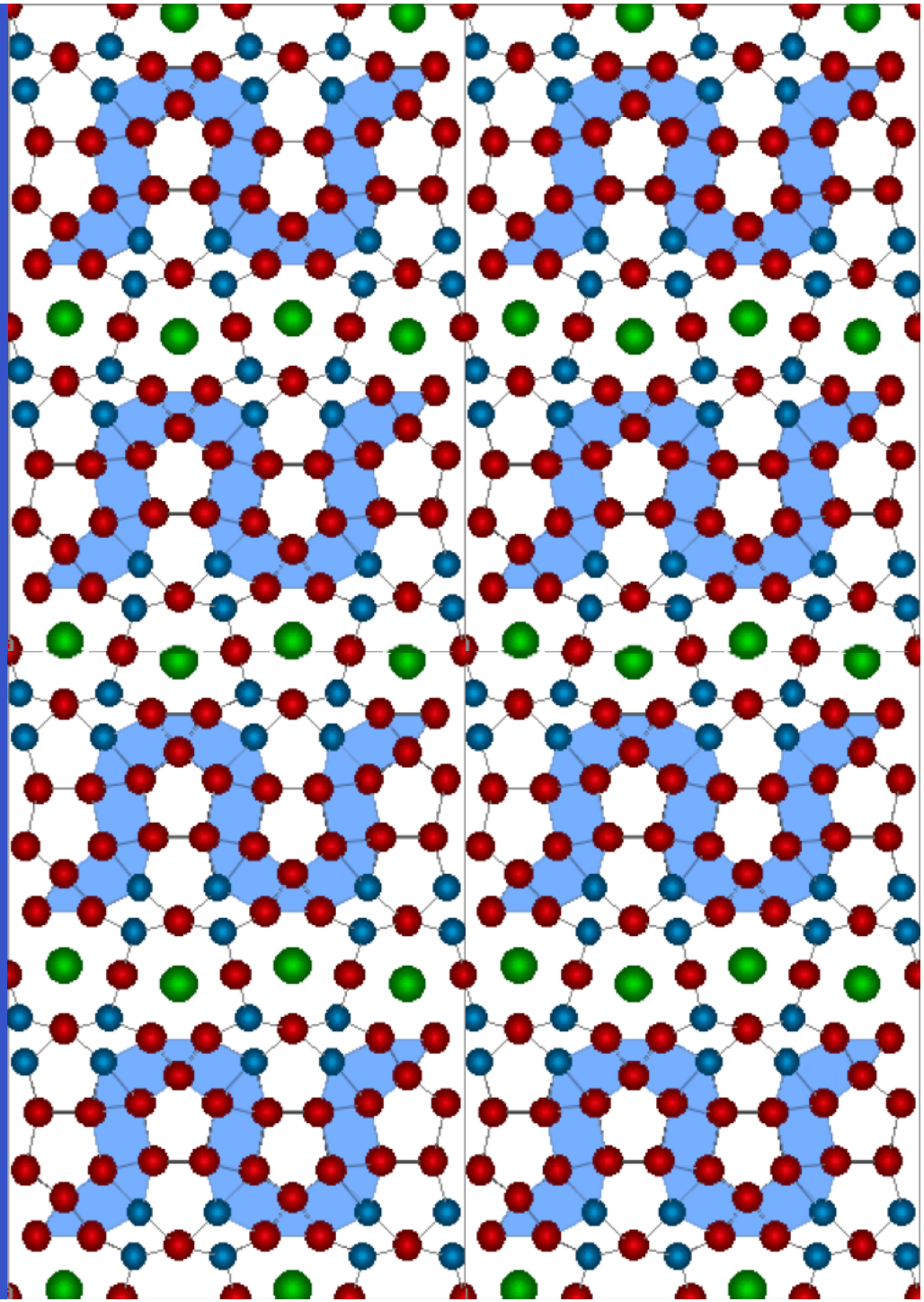
crystallography III



230 space groups

Combine 32 point groups (rotational symmetry) with

a. 14 Bravais lattices (translational symmetry)

b. glide planes (rotational + translational symmetry) - a, b, c, n, d

c. screw axes (rotational + translational symmetry) - 2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5

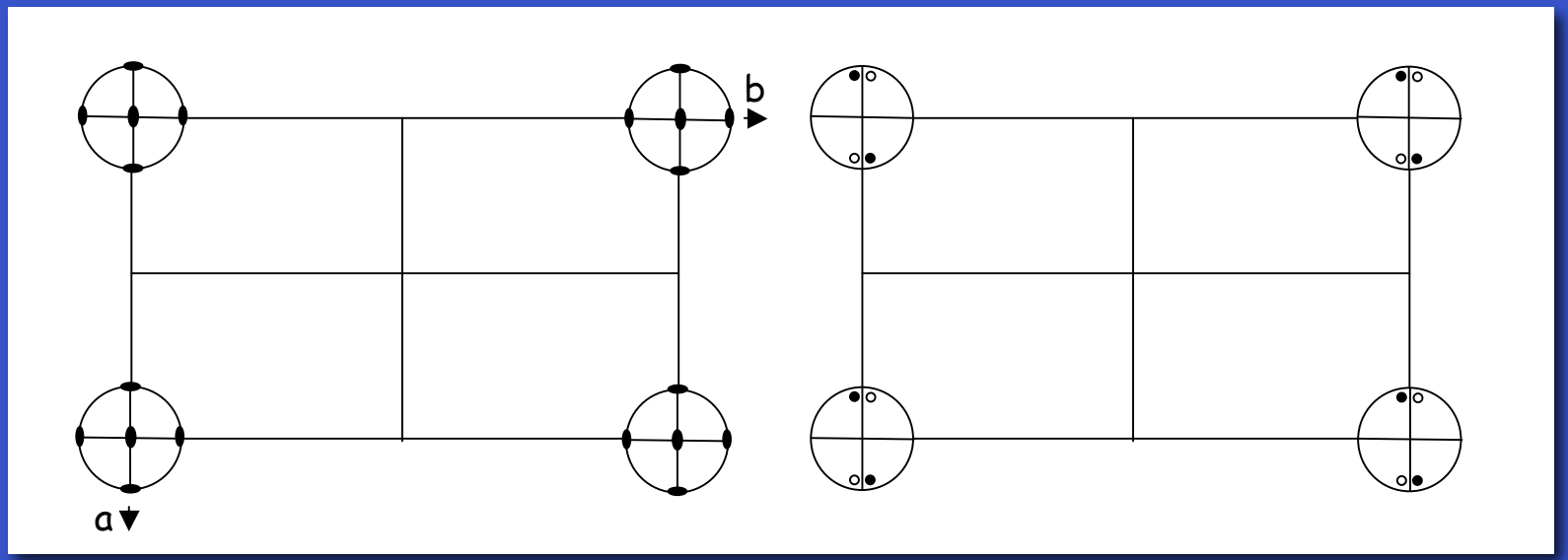
Examples:

Ccc2, P1, I 4_1/a 2/c 2/d, F 4/m $\bar{3}$ 2/m, P 6_3/m 2/m 2/c

lattice centering screw axis glide plane

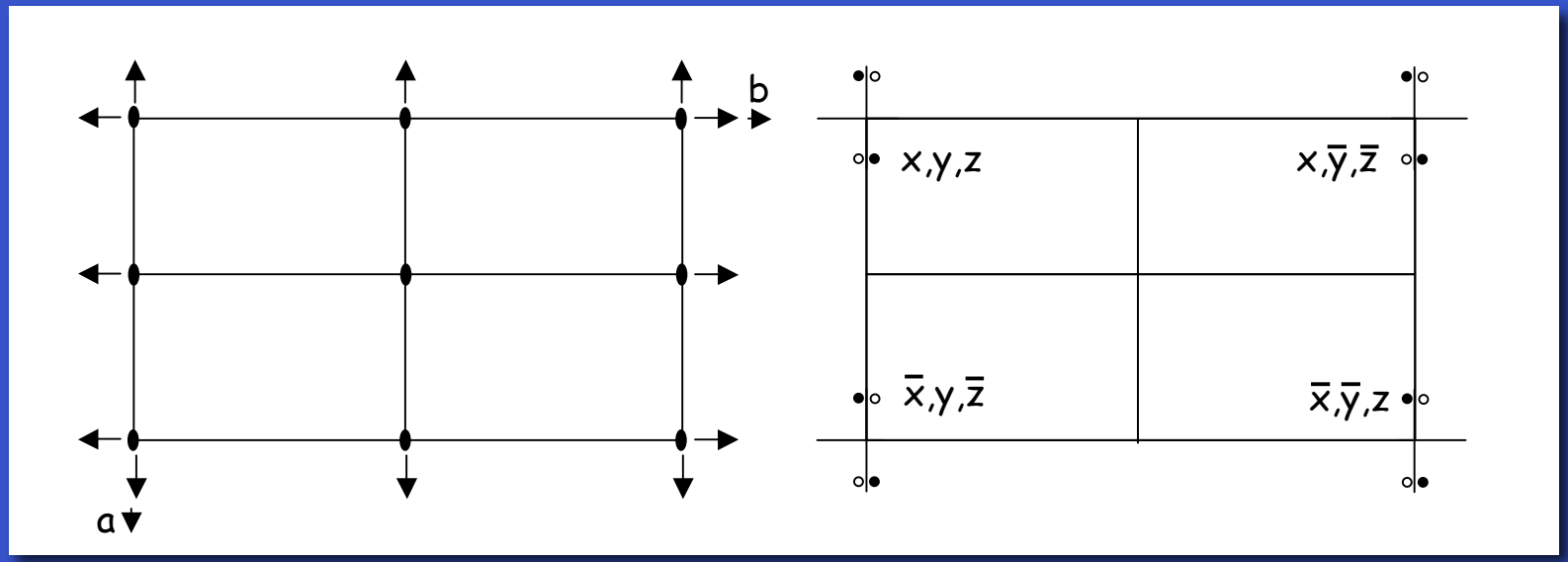
Space group diagrams

Example: P222



Space group diagrams

Example: P222



General equipoint: 4u (x,y,z) $(\bar{x},y,\bar{z})$ $(x,\bar{y},\bar{z})$ $(\bar{x},\bar{y},z)$

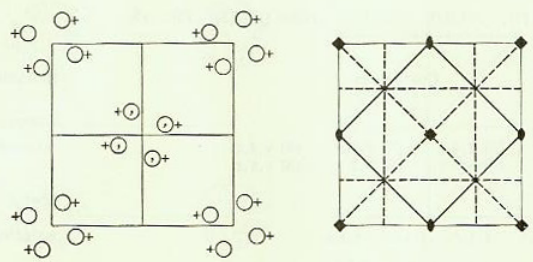
Special equipoints: 1a (0,0,0); 1b (1/2,0,0); … 2i $(x,0,0)$, $(\bar{x},0,0)$; 2j $(x,0,1/2)$, $(\bar{x},0,1/2)$; … 2m $(0,y,z)$ $(0,\bar{y},0)$; …

Space group tables

International Tables for Crystallography, Vol. A

$P\,4\,b\,m$ $\quad C_{4v}^{2}$ $\quad 4\,m\,m$ $\quad$ Tetragonal

No. 100 $\quad P\,4\,b\,m$ $\quad$ Patterson symmetry $P\,4/m\,m\,m$



Origin on $4\,1\,g$

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

Symmetry operations

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

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$	$0kl$: $k=2n$
			(5) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z$	(6) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z$	(7) $\bar{y}+\frac{1}{2},\bar{x}+\frac{1}{2},z$	(8) $y+\frac{1}{2},x+\frac{1}{2},z$	$h00$: $h=2n$
							Special: as above, plus
4	c	$..m$	$x,x+\frac{1}{2},z$	$\bar{x},\bar{x}+\frac{1}{2},z$	$\bar{x}+\frac{1}{2},x,z$	$x+\frac{1}{2},\bar{x},z$	no extra conditions
2	b	$2.mm$	$\frac{1}{2},0,z$	$0,\frac{1}{2},z$			hkl : $h+k=2n$
2	a	$4..$	$0,0,z$	$\frac{1}{2},\frac{1}{2},z$			hkl : $h+k=2n$

Symmetry of special projections

Along [001] $p\,4\,g\,m$
$\mathbf{a}'=\mathbf{a}$ $\quad \mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

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

Along [110] $p\,1\,m\,1$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\quad \mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

Maximal non-isomorphic subgroups

I	[2]$P\,4\,1\,1\,(P\,4)$	1; 2; 3; 4
	[2]$P\,2\,b\,1\,(P\,b\,a\,2)$	1; 2; 5; 6
	[2]$P\,2\,1\,m\,(C\,m\,m\,2)$	1; 2; 7; 8
IIa	none	
IIb	[2]$P\,4_2\,b\,c\,(\mathbf{c}'=2\mathbf{c})$; [2]$P\,4_2\,n\,m\,(\mathbf{c}'=2\mathbf{c})$; [2]$P\,4\,n\,c\,(\mathbf{c}'=2\mathbf{c})$	

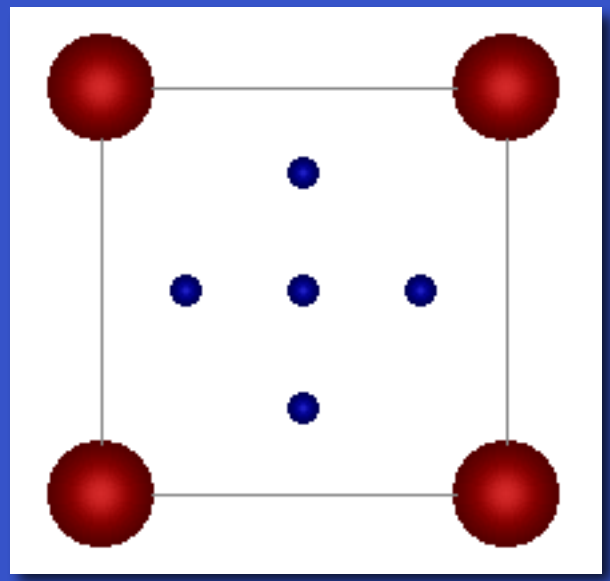
Describing crystal structures

Need:

lattice parameters
space group
equipoints occupied
positional parameters

Example:

LaB_6 a = 4.1566 Å
P 4/m $\bar{3}$ 2/m
La in 1a, B in 6f
x = 0.207

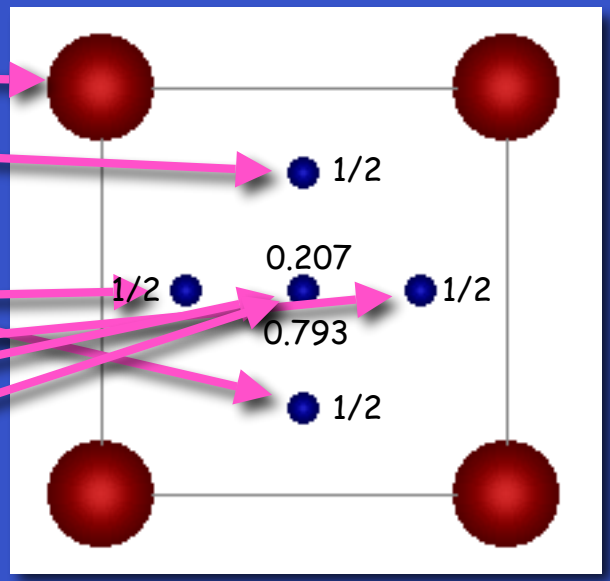


Describing crystal structures

LaB_6 a = 4.1566 Å
P 4/m $\bar{3}$ 2/m
La in 1a, B in 6f
x = 0.207

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

1a - (0,0,0)
6f - (x,1/2,1/2)
6f - ($\bar{x}$,1/2,1/2)
6f - (1/2,x,1/2)
6f - (1/2,$\bar{x}$,1/2)
6f - (1/2,1/2,x)
6f - (1/2,1/2,$\bar{x}$)



Exercises

1. C

   a = 3.500Å

   F $4_1/d\ \bar{3}\ 2/m$

   C in 8a

   F (0,0,0)+ (1/2,1/2,0)+ (1/2 ,0,1/2)+ (0,1/2,1/2)+

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

   projection down [001]

2. $CaCu_5$

   a = 5.082, c = 4.078Å

   P6/mmm

   Ca in 1a, Cu in 2c, 3g

   2c: (1/3,2/3,0) (2/3,1/3,0)

   3g: (1/2,0,1/2) (0,1/2,1/2) (1/2,1/2,1/2)

   projection down [001]