Space Group - 1

Read

Ott Chapter 10 (exclude 10.1)

Hammond Chapter 4.6

Krawitz Chapter 1.6~1.8

Sherwood & Cooper Chapter 3.7~3.8

Hammond Chapter 2.1 ~ 2.5

Krawitz Chapter 1.1~1.5

Space group

- 32 point groups - symmetry groups of many molecules and of all crystals so long as morphology is considered

- space group - symmetry of crystal lattices and crystal structures
  - ✓ 14 Bravais lattice
  - ✓ centered lattices - new symmetry operations
  - ✓ reflection + translation
  - ✓ rotation + translation

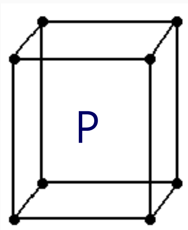
Space group

- If translation operations are included with rotation and inversion → We have 230 three-dim. space groups
- Translation operations
  - ✓ Unit cell translations
  - ✓ Centering operations (Lattices) (***A, B, C, I, F, R***)
  - ✓ Glide planes (reflection + translation) (*a, b, c, n, d*)
  - ✓ Screw axes (rotation + translation) (2_1, 3_1, 3_2)
- Hermann-Mauguin symbols (4 positions)
  - ✓ First position is Lattice type (P, A, B, C, I, F or R)
  - ✓ Second, third and fourth positions as with point groups

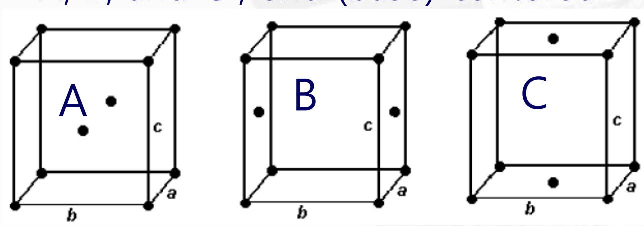
$Cmm2$ (35) $\qquad P\frac{4}{m}\bar{3}\frac{2}{m}$ (225) $\qquad F\bar{4}3m$ (No.216)

Lattice types – P I F C R

P ; primitive

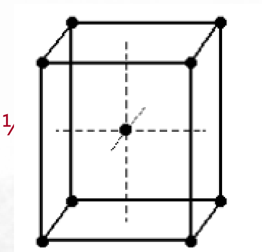


A, B, and C ; end (base)-centered



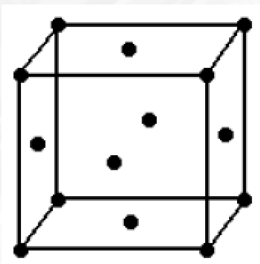
I ; body-centered

- ✓ Point @ ½, ½, ½
- ✓ Multiplicity = 2



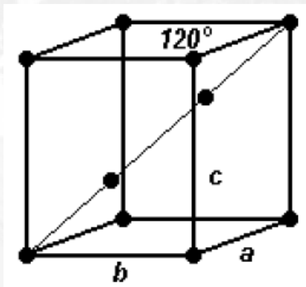
F ; face-centered

- ✓½, ½, 0
- ✓½, 0, ½
- ✓0, ½, ½
- ✓Multiplicity = 4



R ; rhombohedral

- ✓2/3, 1/3, 1/3
- ✓1/3, 2/3, 2/3
- ✓Multiplicity = 3
- ✓Trigonal system



Space lattice

➢ 14 Bravais lattice

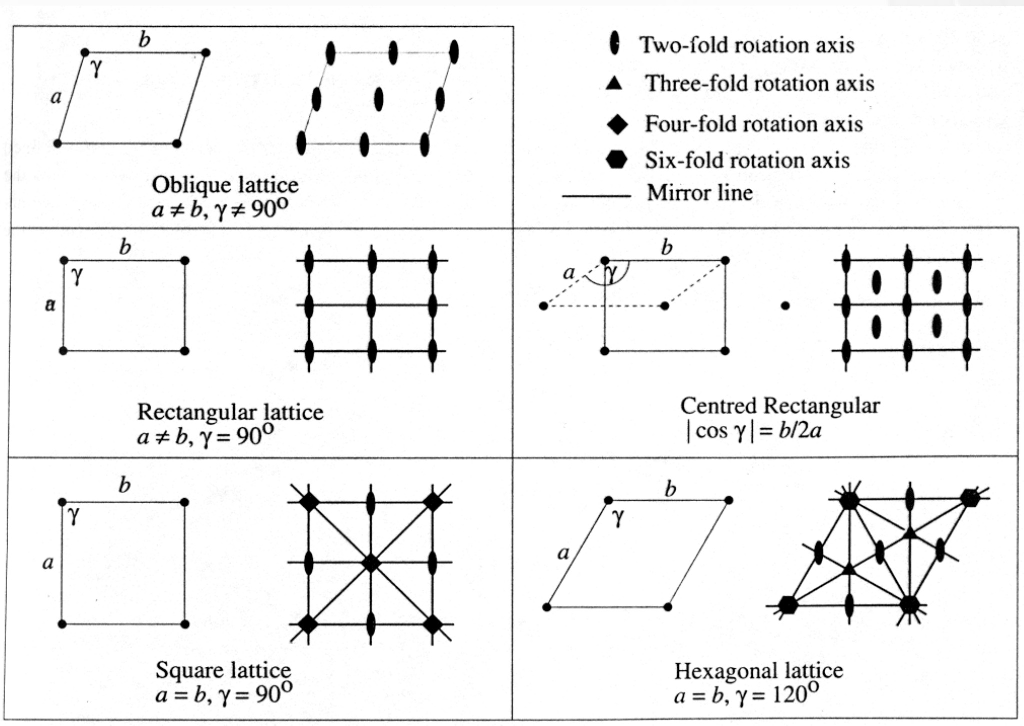
	P	C	I	F
Triclinic	P$\bar{1}$			
Monoclinic	P 2/m	C 2/m		
Orthorhombic	P 2/m 2/m 2/m	C 2/m 2/m 2/m	I 2/m 2/m 2/m	F 2/m 2/m 2/m
Tetragonal	P 4/m 2/m 2/m		I 4/m 2/m 2/m	
Trigonal	P 6/m 2/m 2/m	R $\bar{3}$ 2/m		
Hexagonal				
Cubic	P 4/m $\bar{3}$ 2/m		I 4/m $\bar{3}$ 2/m	F 4/m $\bar{3}$ 2/m

The 14 Bravais lattice represent the 14 and only way in which it is possible to fill space by a 3D periodic array of points.

Ott Chap 7

5 plane lattices

➢ 5 plane lattices + 10 plane point groups + glide line → 17 plane groups



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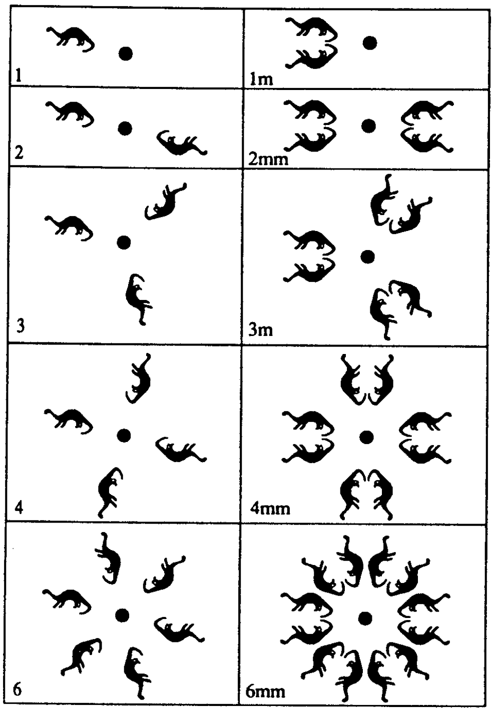
17 plane groups

10 plane point groups



5 plane lattices — 10 plane point groups — 17 plane groups

Crystal system	Point groups compatible with crystal system	Lattices in system	Space groups compatible with lattice
Oblique $a \neq b, \gamma \neq 90°$	1, 2	p (primitive)	p1, p2
Rectangular $a \neq b, \gamma = 90°$	1m, 2mm	p (primitive)	pm, p2mm, pg, p2mg p2gg
		c (centred)	cm, c2mm
Square $a = b, \gamma = 90°$	4, 4mm	p (primitive)	p4, p4mm, p4gm
Hexagonal $a = b, \gamma = 120°$	3, 3m, 6, 6mm	p (primitive)	p3, p31m, p3m1 p6, p6mm

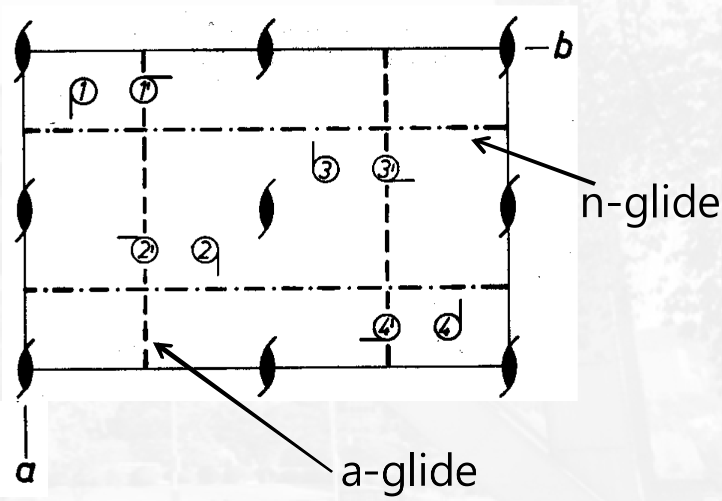
Space group notation

- $Pna2_1$: orthorhombic

n-glide normal to a-axis

a-glide normal to b-axis

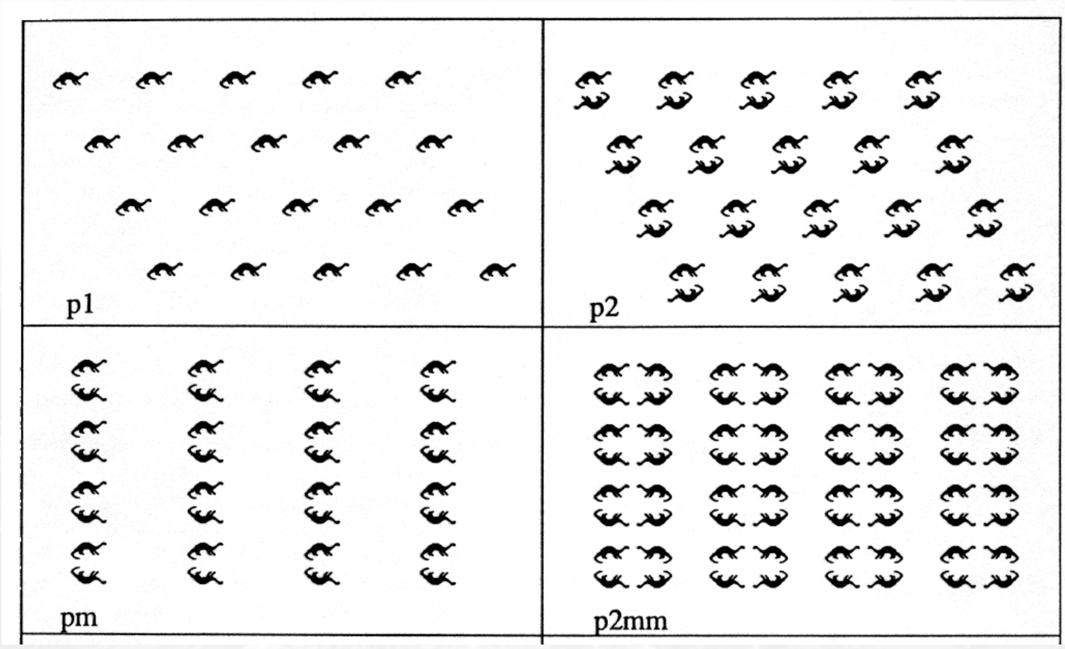
2_1 screw axis along c-axis



a b c
Symmetry directions
of orthorhombic

17 plane groups (1/5)

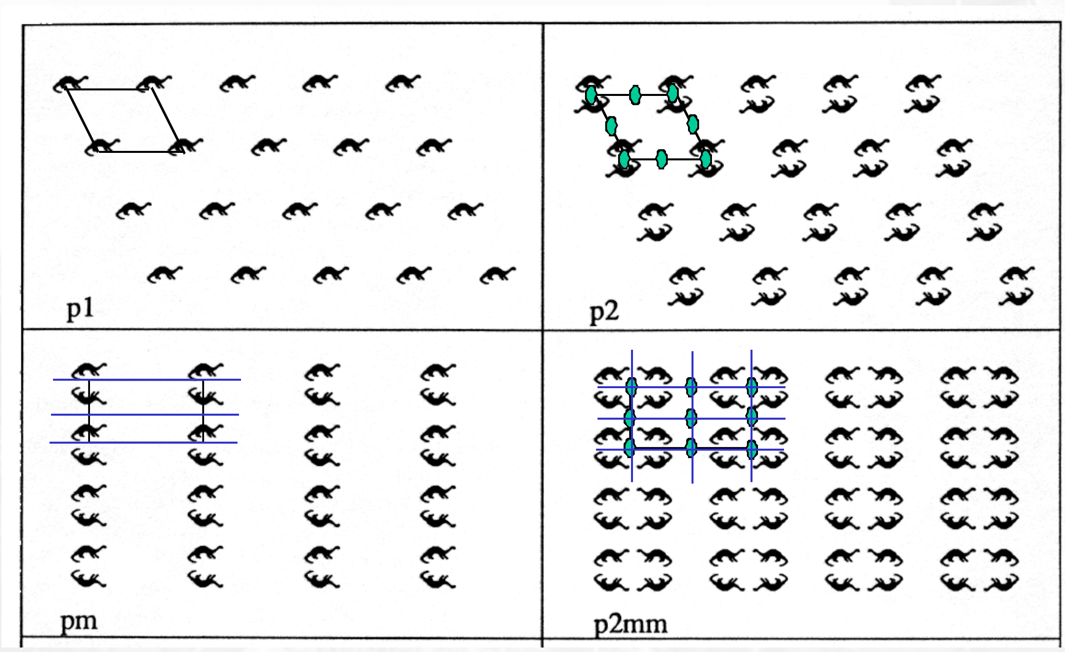
How to recognize motifs, symmetry elements, and lattice types



For 17 plane groups, see Hammond 2.1 ~ 2.5, figure 2.6, 2.7, 2.8

17 plane groups (1/5)

How to recognize motifs, symmetry elements, and lattice types



For 17 plane groups, see Hammond 2.1 ~ 2.5, figure 2.6, 2.7, 2.8

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]}

Symmetry directions

- Letters for the centering types of cells
  - ✓ Lower-case for 2-D (plane groups)
  - ✓ Capital letters for 3-D (space group)
- Lattice symmetry directions that carry no symmetry elements for the space group are represented by the symbol "1"

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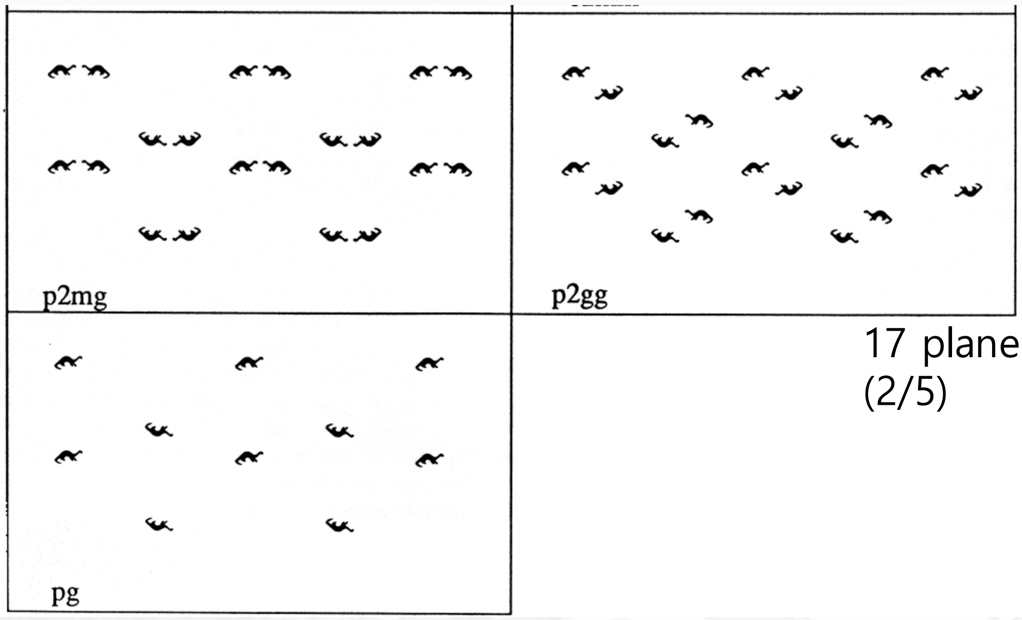
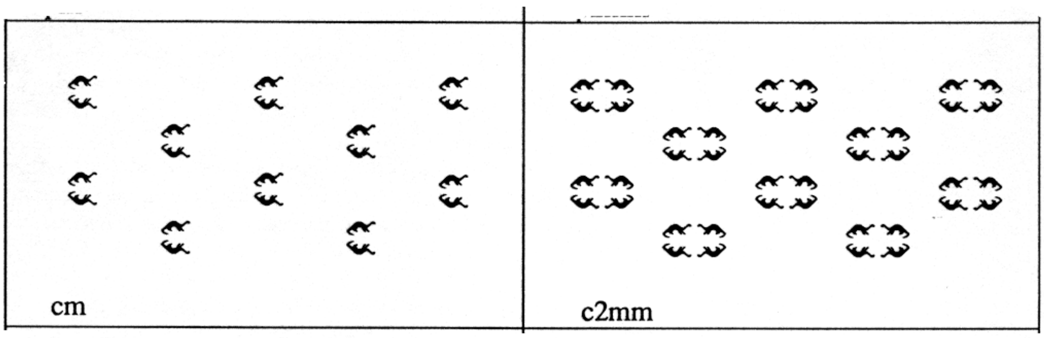
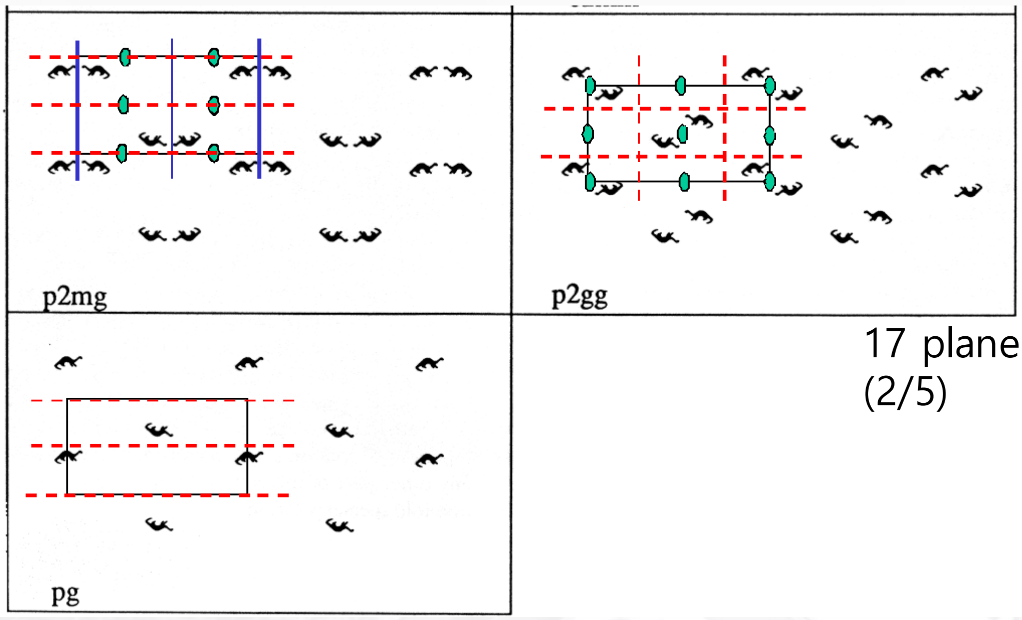
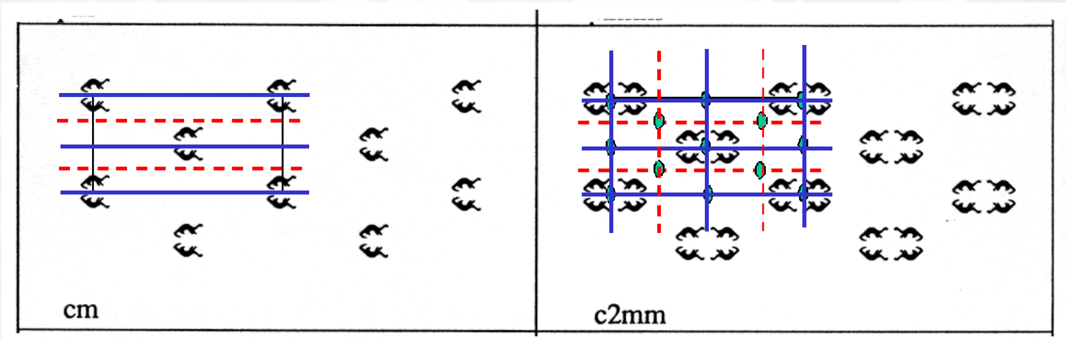


17 plane groups (2/5)

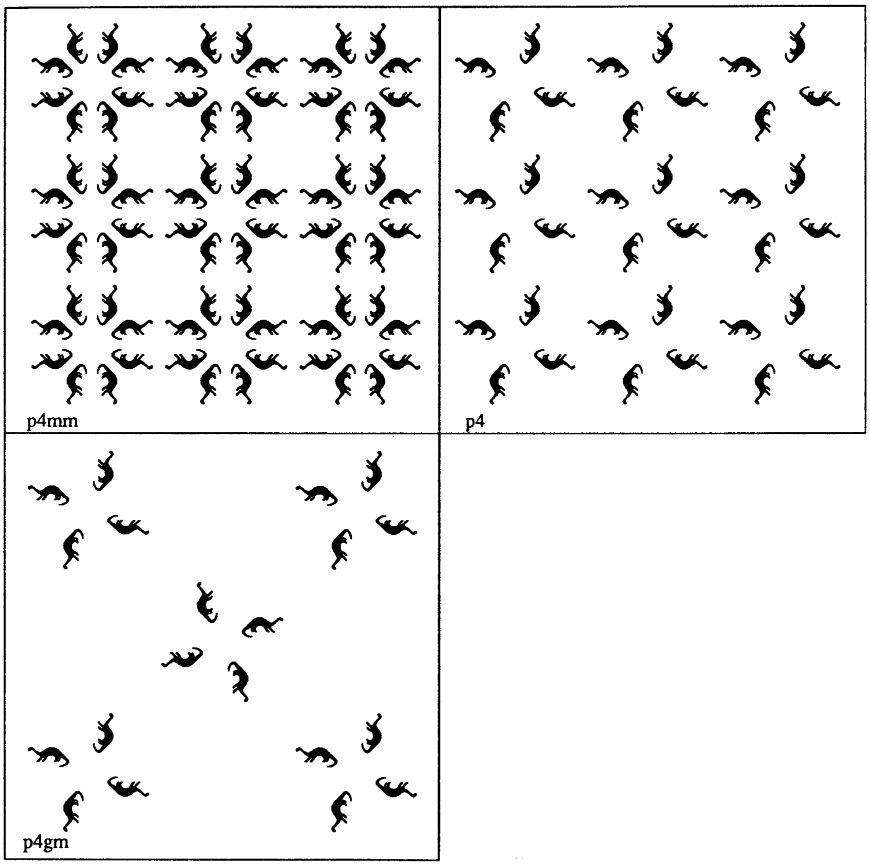




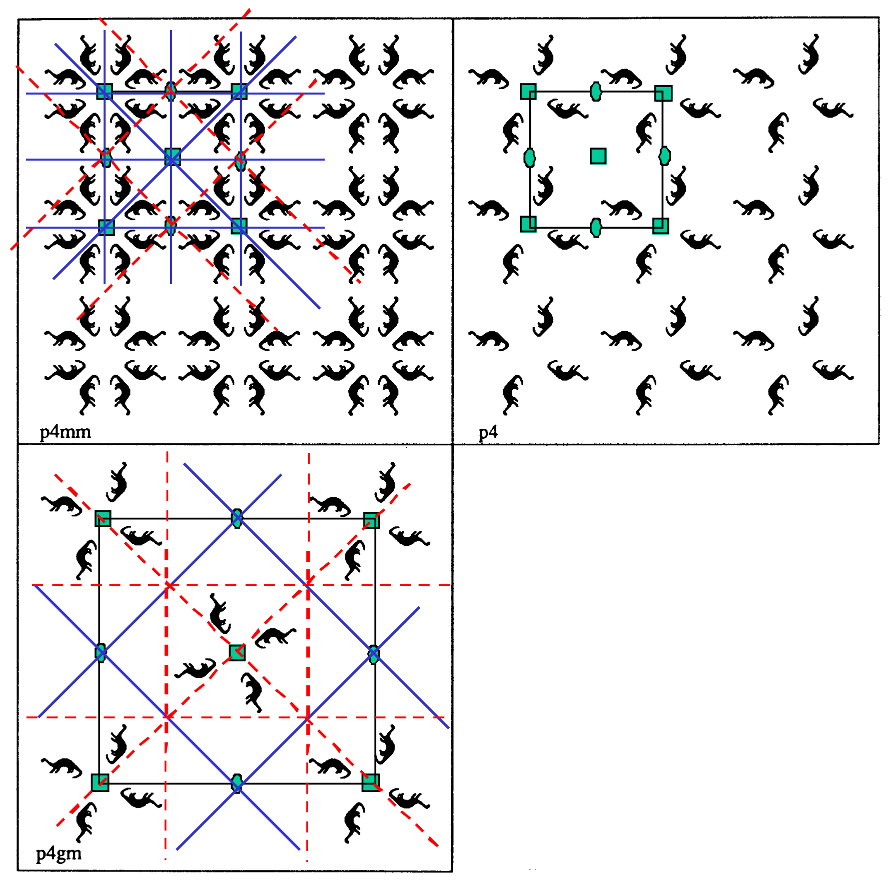
17 plane groups (2/5)



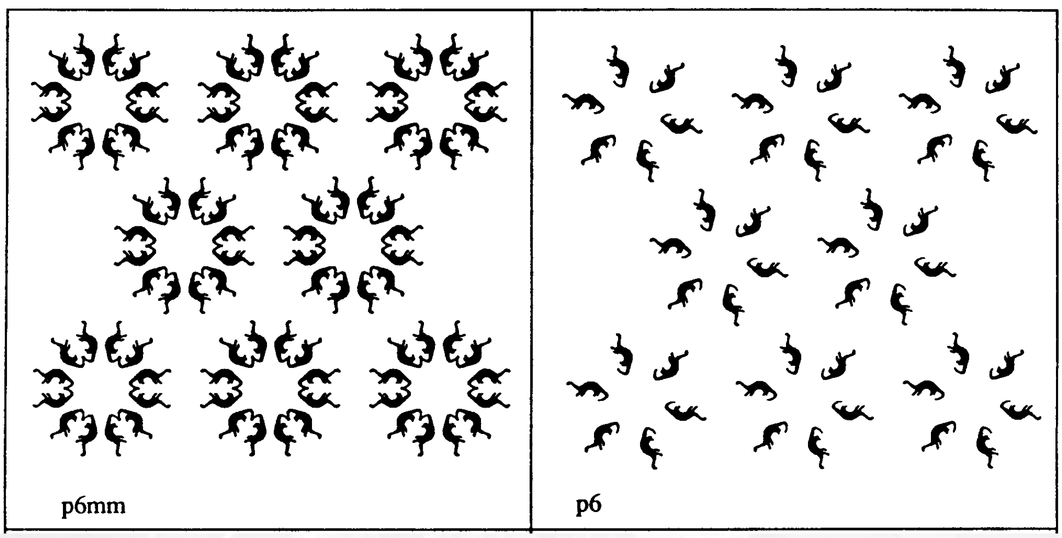
17 plane groups (3/5)

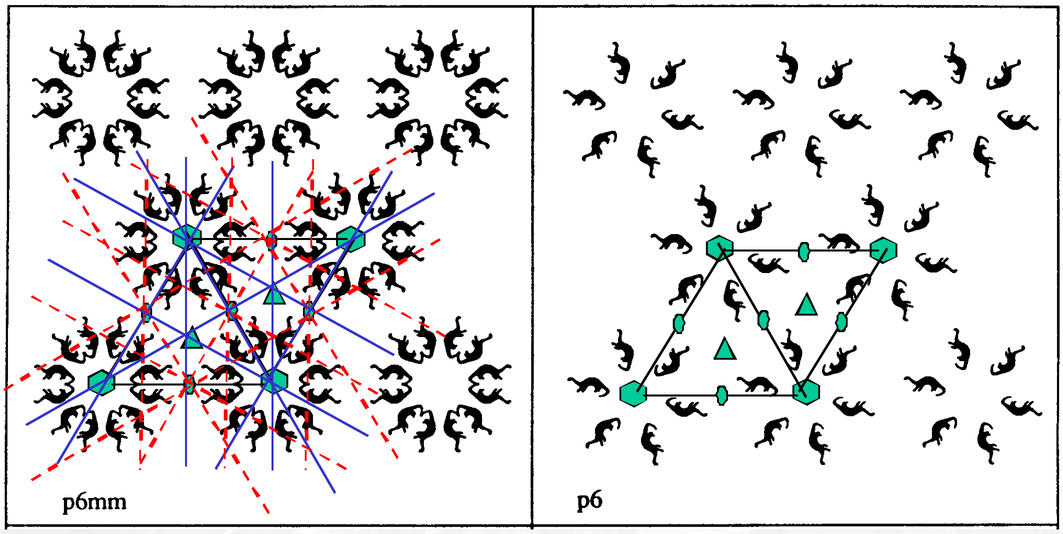


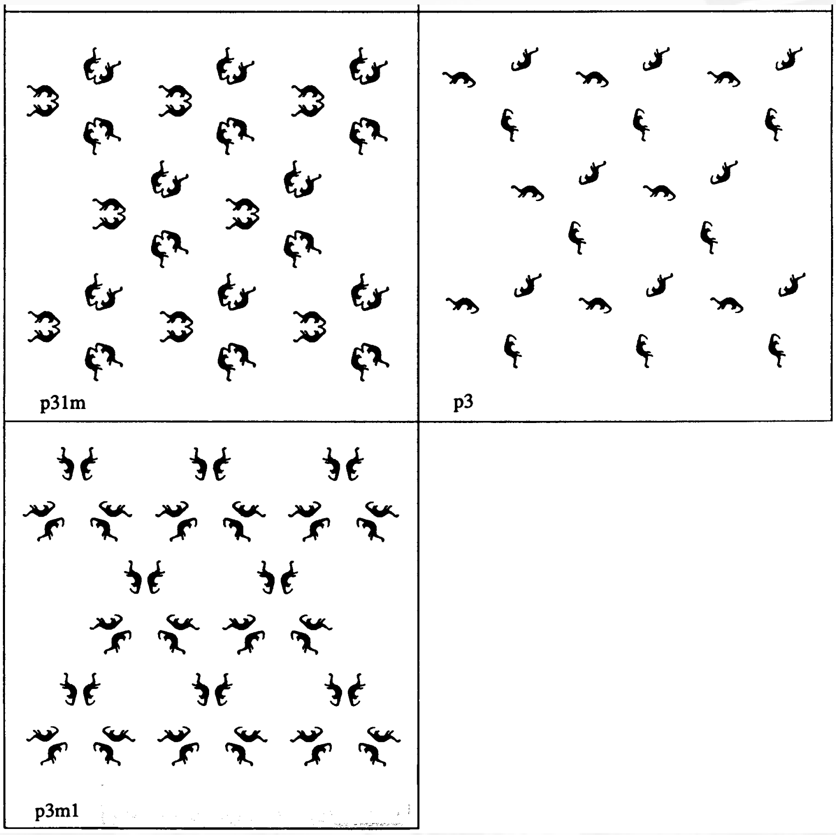
17 plane groups (3/5)



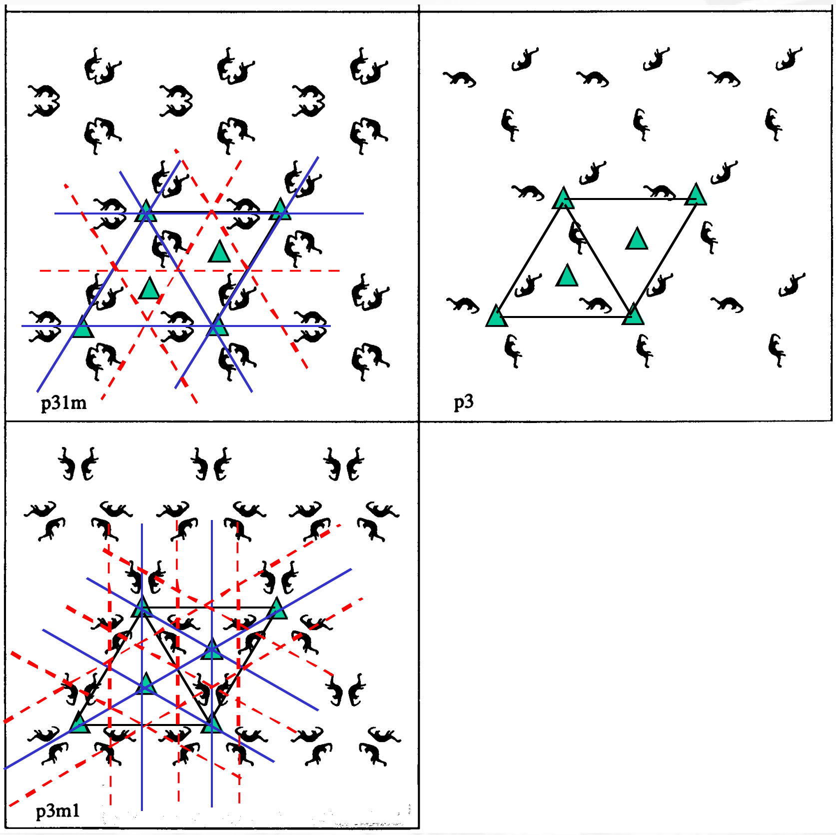
17 plane groups (4/5)




p6mm
p6


p31m
p3
p3m1

17 plane groups (5/5)



Symmetry directions

Lattice	Symmetry direction (position in Hermann–Mauguin symbol) Primary	Secondary	Tertiary
Two dimensions			
Oblique	Rotation point in plane		
Rectangular	Rotation point in plane	[10]	[01]
Square	Rotation point in plane	$\left\{\begin{matrix}[10]\\ [01]\end{matrix}\right\}$	$\left\{\begin{matrix}[1\bar{1}]\\ [11]\end{matrix}\right\}$
Hexagonal	Rotation point in plane	$\left\{\begin{matrix}[10]\\ [01]\\ [\bar{1}\bar{1}]\end{matrix}\right\}$	$\left\{\begin{matrix}[1\bar{1}]\\ [12]\\ [\bar{2}\bar{1}]\end{matrix}\right\}$
Three dimensions			
Triclinic	None		
Monoclinic*	[010] ('unique axis *b*') [001] ('unique axis *c*')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	$\left\{\begin{matrix}[100]\\ [010]\end{matrix}\right\}$	$\left\{\begin{matrix}[1\bar{1}0]\\ [110]\end{matrix}\right\}$
Hexagonal	[001]	$\left\{\begin{matrix}[100]\\ [010]\\ [\bar{1}\bar{1}0]\end{matrix}\right\}$	$\left\{\begin{matrix}[1\bar{1}0]\\ [120]\\ [\bar{2}\bar{1}0]\end{matrix}\right\}$
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Rhombohedral (rhombohedral axes)	[111]	$\left\{\begin{matrix}[1\bar{1}0]\\ [01\bar{1}]\\ [\bar{1}01]\end{matrix}\right\}$	
Cubic	$\left\{\begin{matrix}[100]\\ [010]\\ [001]\end{matrix}\right\}$	$\left\{\begin{matrix}[111]\\ [1\bar{1}\bar{1}]\\ [\bar{1}1\bar{1}]\\ [\bar{1}\bar{1}1]\end{matrix}\right\}$	$\left\{\begin{matrix}[1\bar{1}0] & [110]\\ [01\bar{1}] & [011]\\ [\bar{1}01] & [101]\end{matrix}\right\}$

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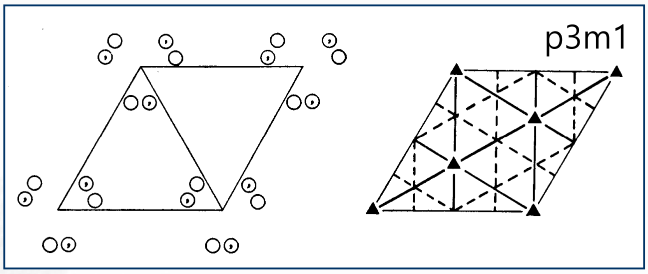
p31m vs. p3m1 (plane group)



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]}
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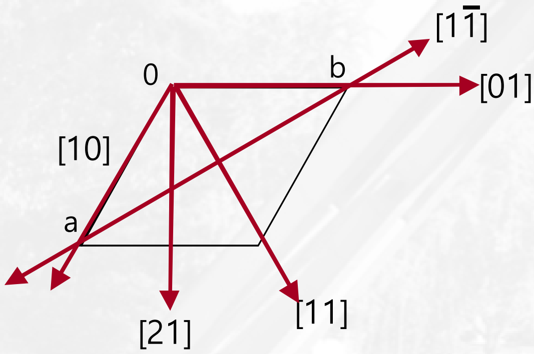
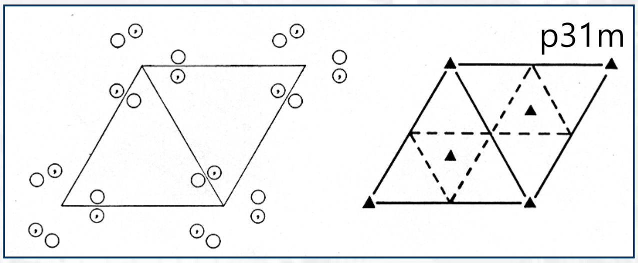
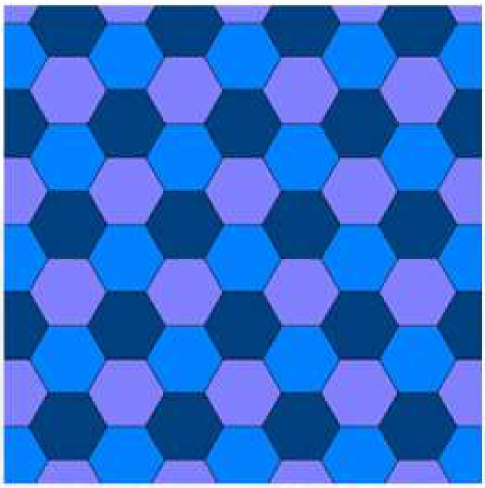




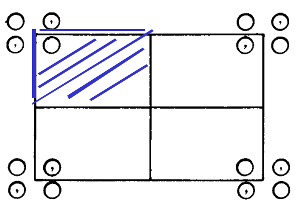


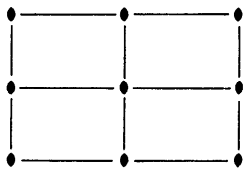
Which is *p*3*m*1?

③ Rectangular ② $2mm$ ① $p2mm$

⑥ Patterson symmetry $p2mm$ ⑤ $p2mm$ ④ No. 6

⑦





Origin at $2mm$

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

Symmetry operations

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

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

① short Hermann-Mauguin symbol of the plane group

② short Hermann-Mauguin symbol of the point group

③ crystal system

④ sequential number of plane group

⑤ full international (Hermann-Mauguin) symbol for the plane group

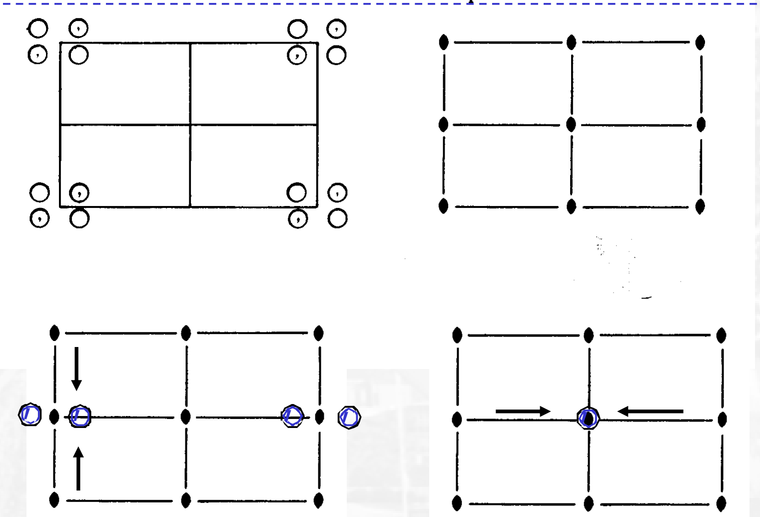
⑥ patterson symmetry

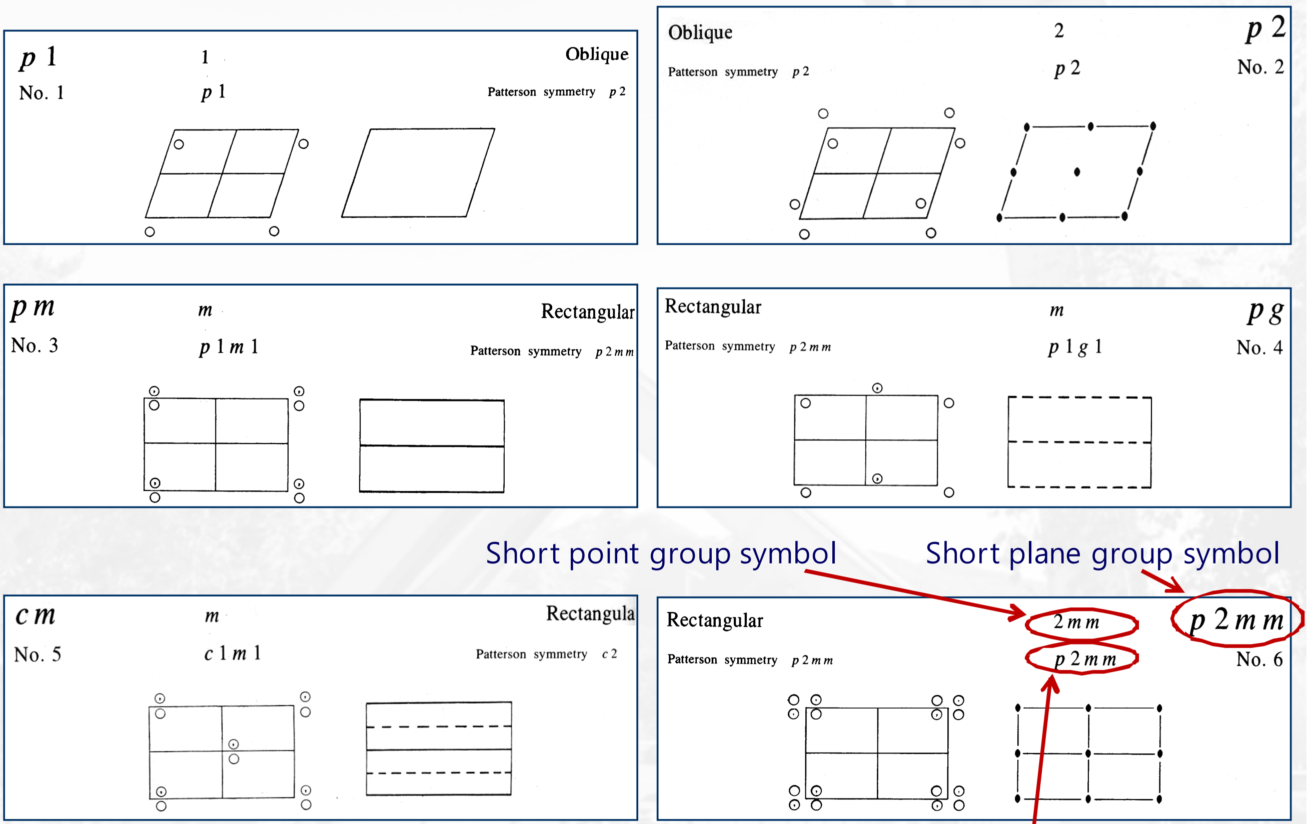
⑦ diagram for the symmetry elements and the general position

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General: no conditions
4	i	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x},y$	(4) $x,\bar{y}$	
							Special: no extra conditions
2	h	$.m.$	$\frac{1}{2},y$	$\frac{1}{2},\bar{y}$			
2	g	$.m.$	$0,y$	$0,\bar{y}$			
2	f	$..m$	$x,\frac{1}{2}$	$\bar{x},\frac{1}{2}$			
2	e	$..m$	$x,0$	$\bar{x},0$			
1	d	$2mm$	$\frac{1}{2},\frac{1}{2}$				
1	c	$2mm$	$\frac{1}{2},0$				
1	b	$2mm$	$0,\frac{1}{2}$				
1	a	$2mm$	$0,0$				

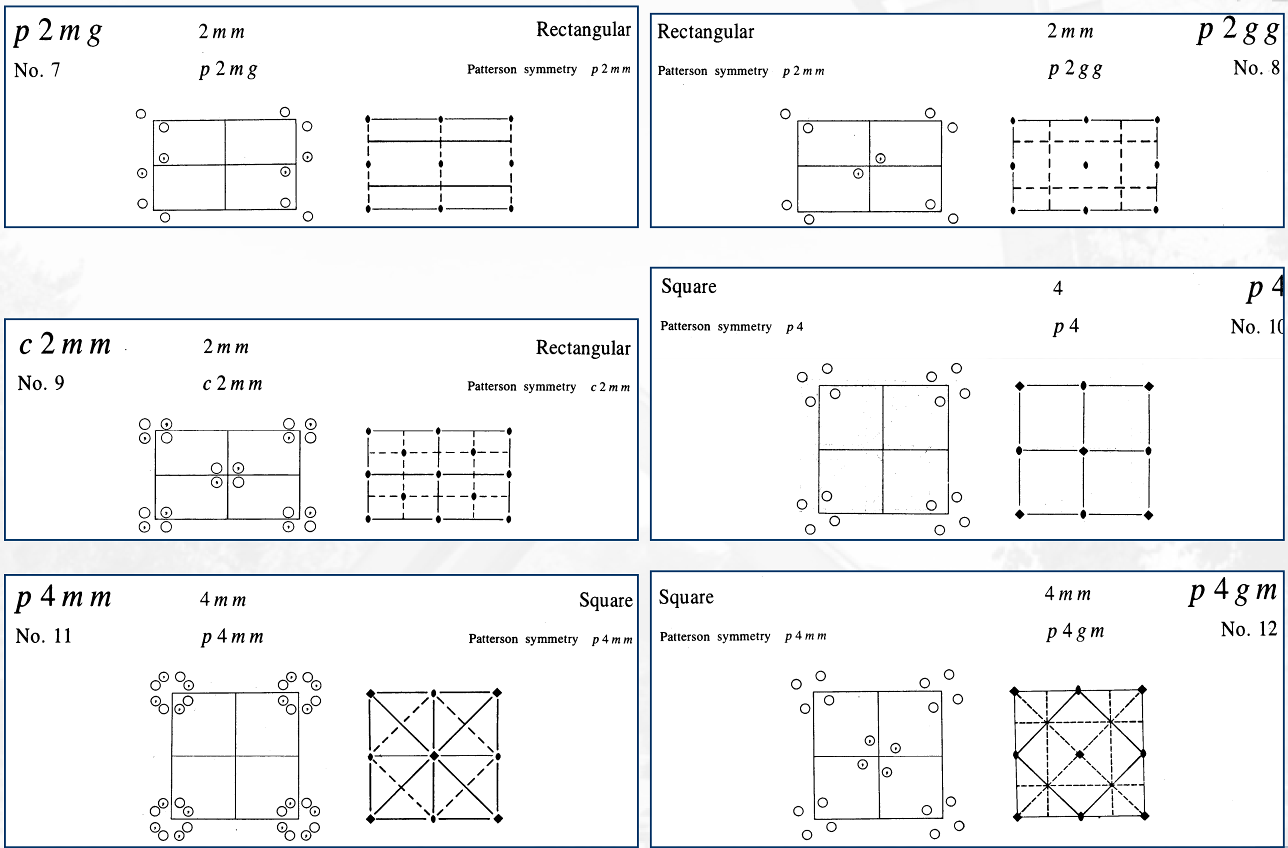




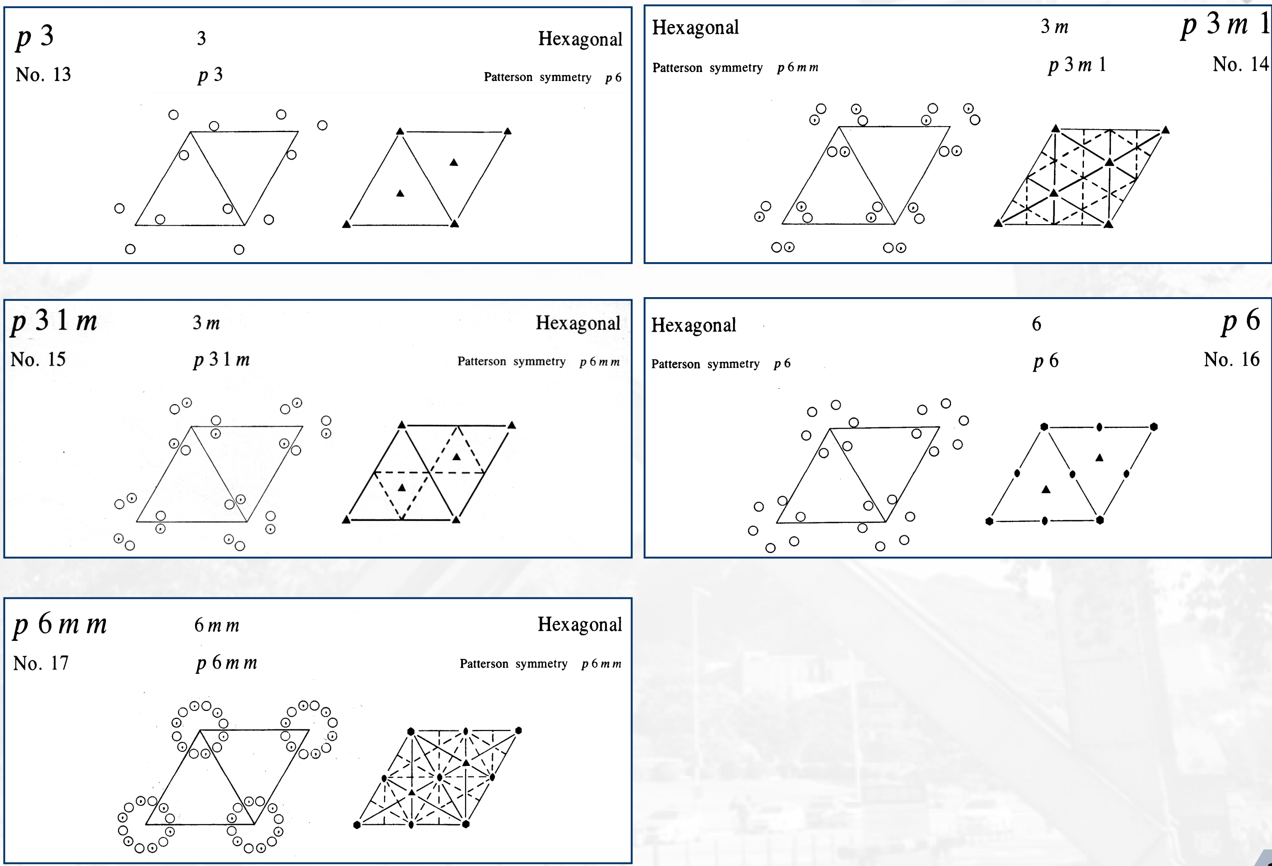
Short point group symbol

Short plane group symbol

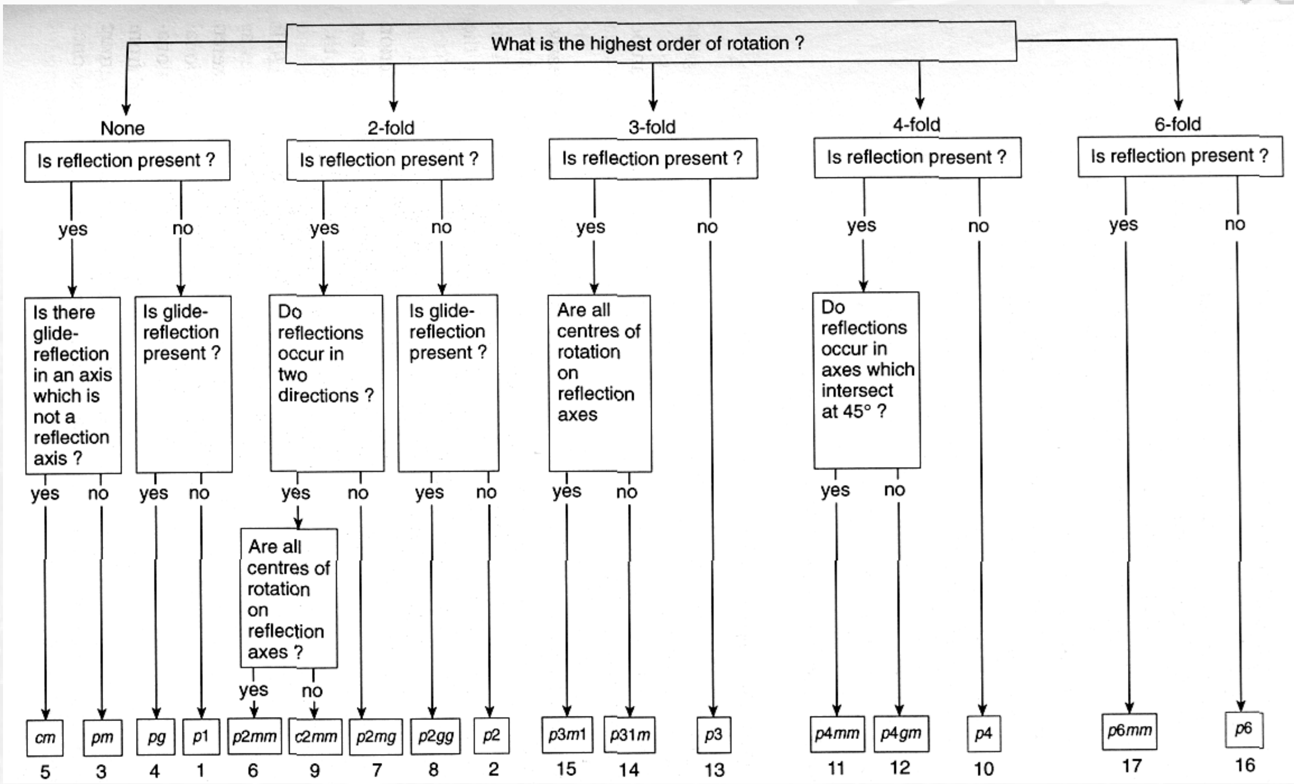
full plane group symbol



International Tables for X-ray Crystallography > plane group

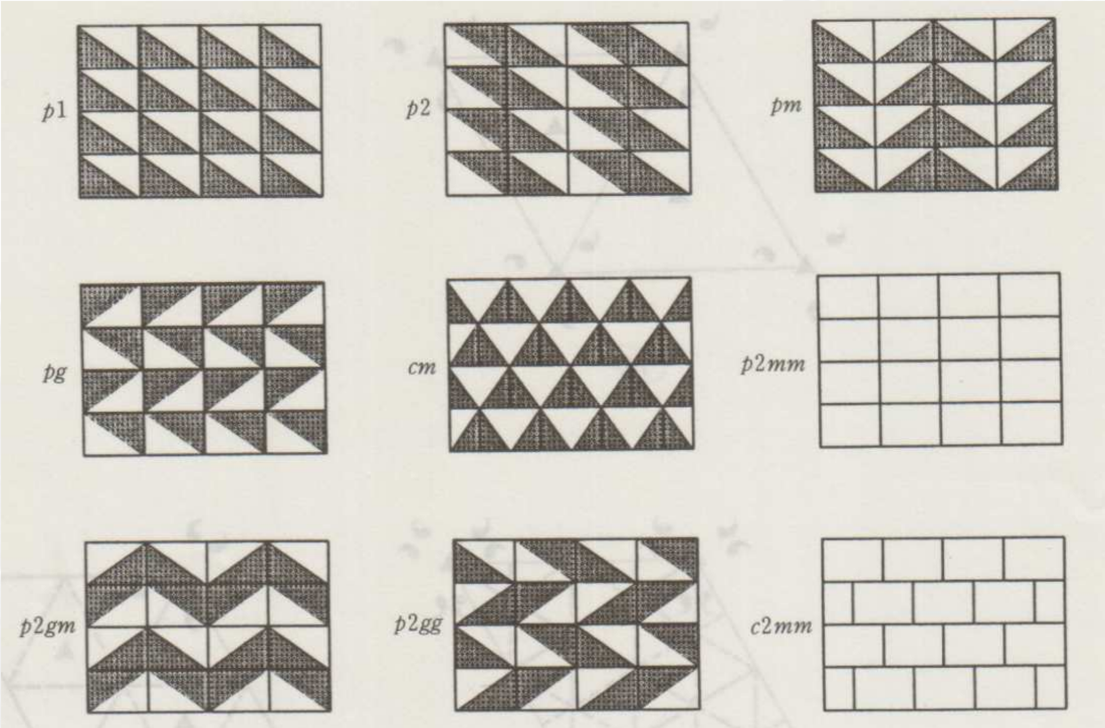


Flow diagram for identifying plane groups

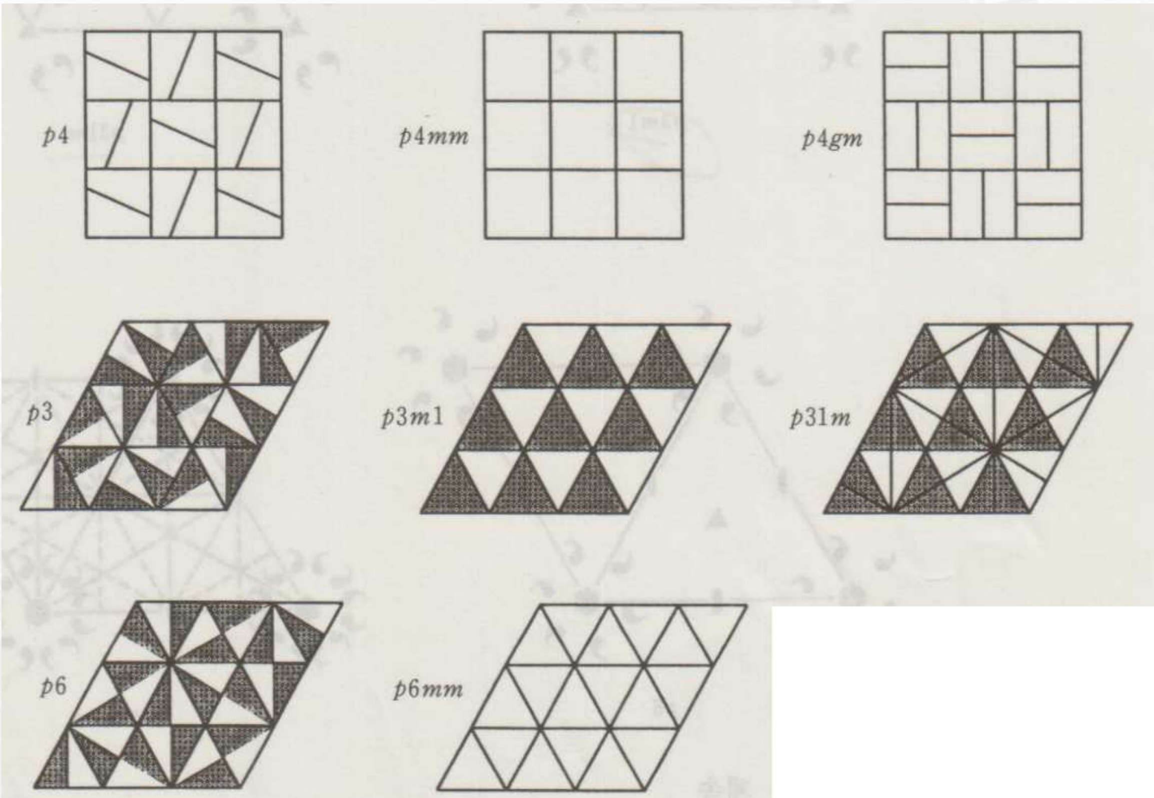


Hammond Chap 2

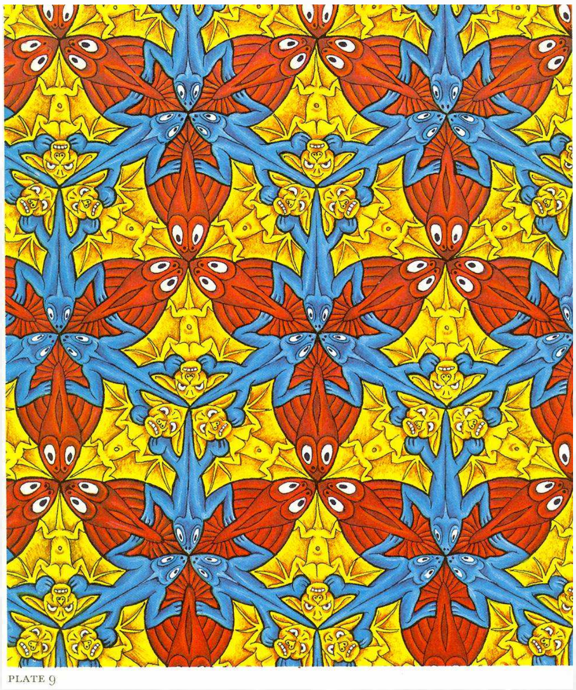
Examples of 17 plane groups

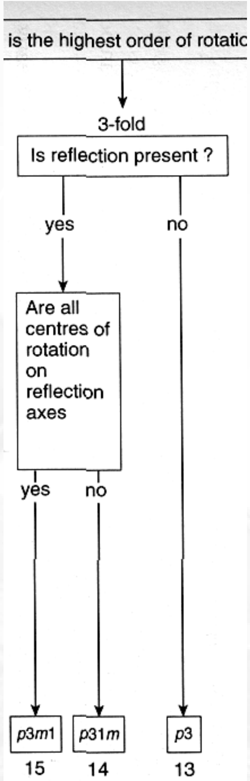


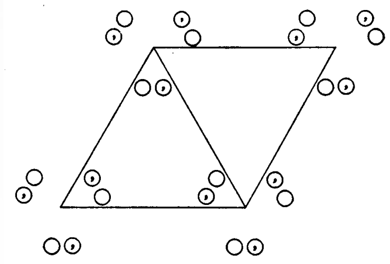
Examples of 17 plane groups

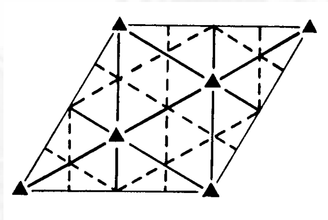


Example 1









p3m1

Example 2

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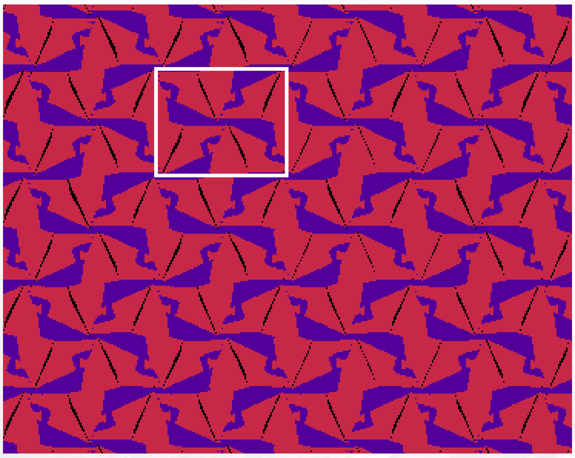
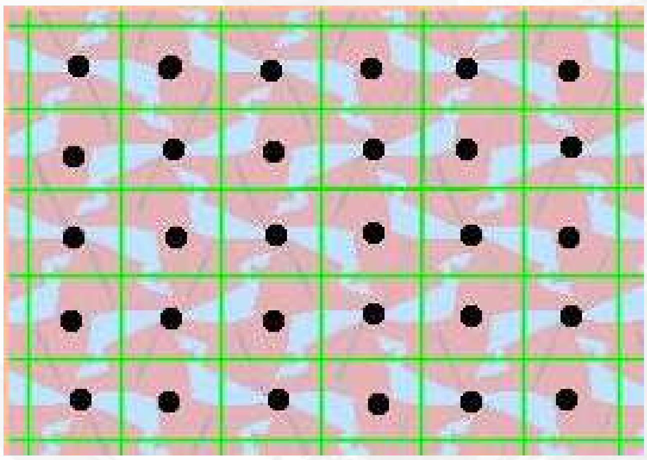
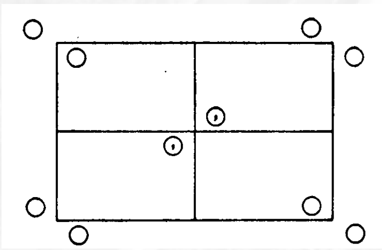
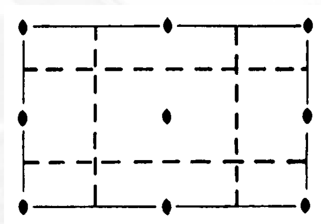




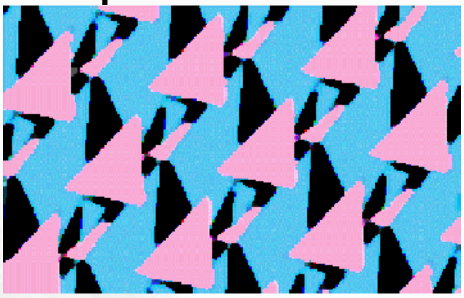




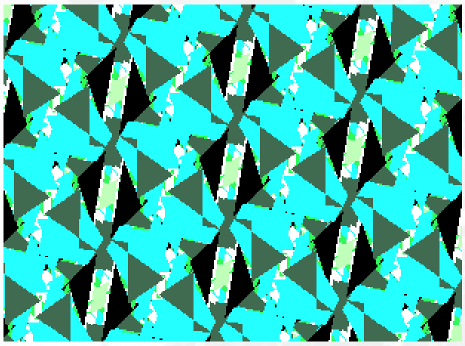
p2gg

Example 3

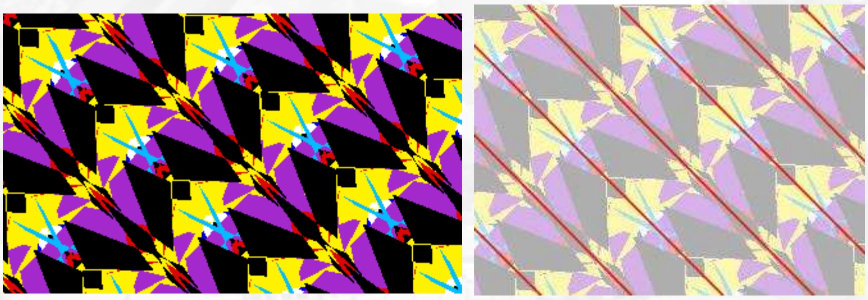
p1



p2

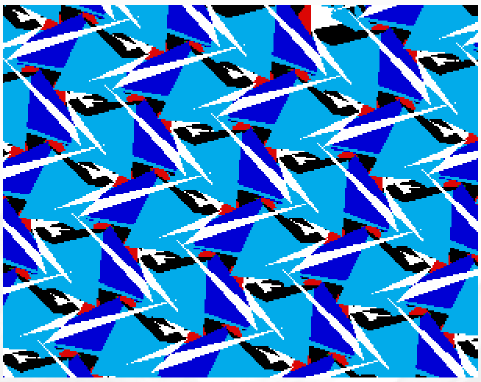


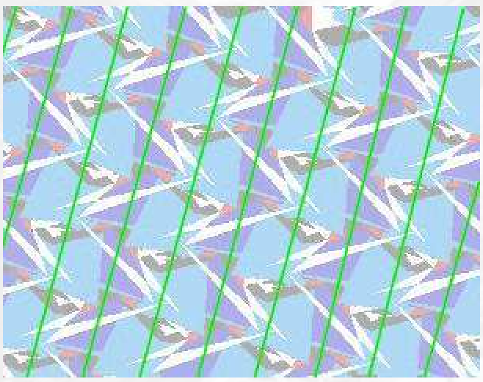
pm

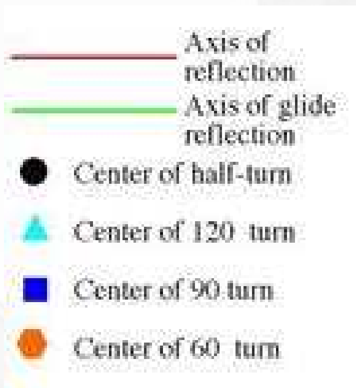


Example 4

Pg

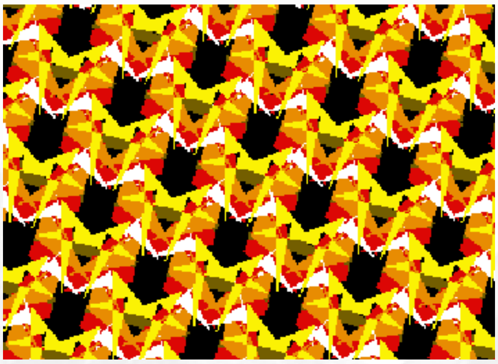


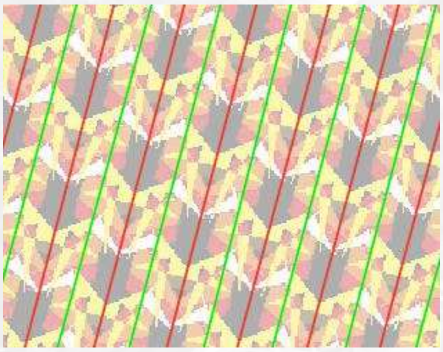




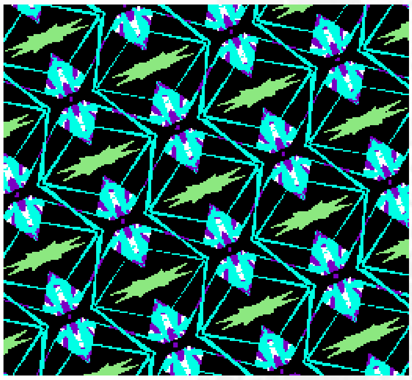
Example 5

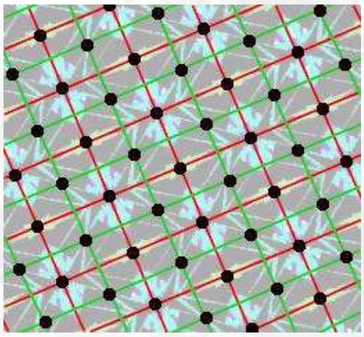
cm





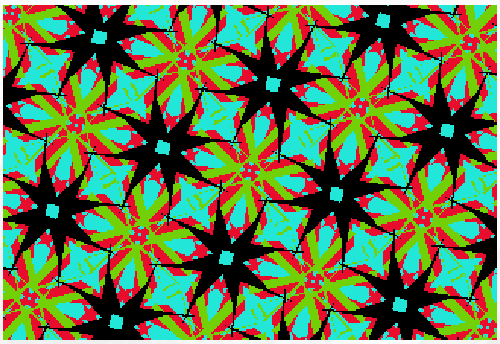
c2mm

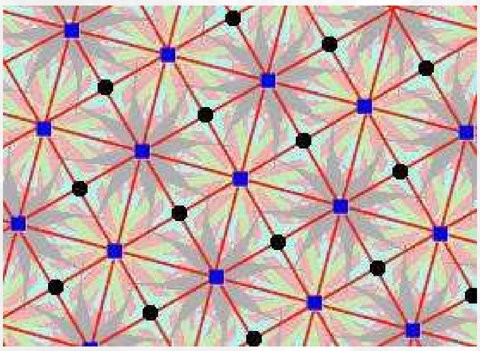




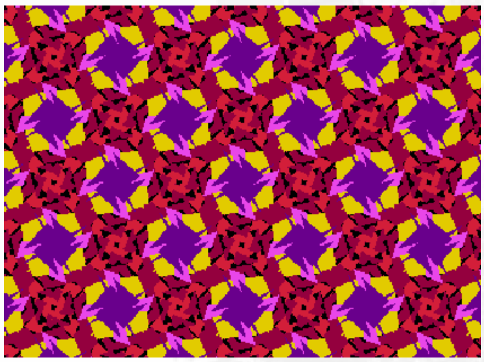
Example 6

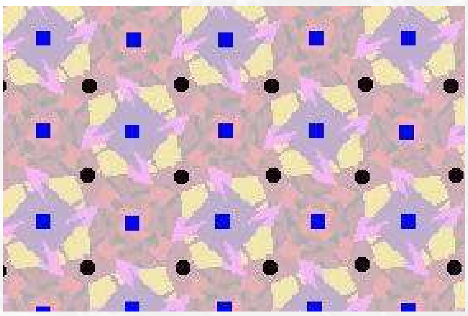
p4mm





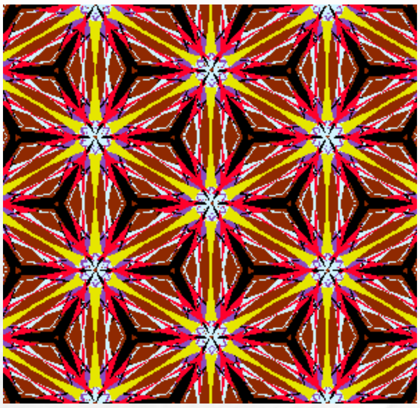
p4

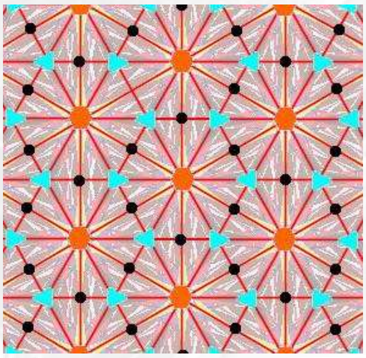




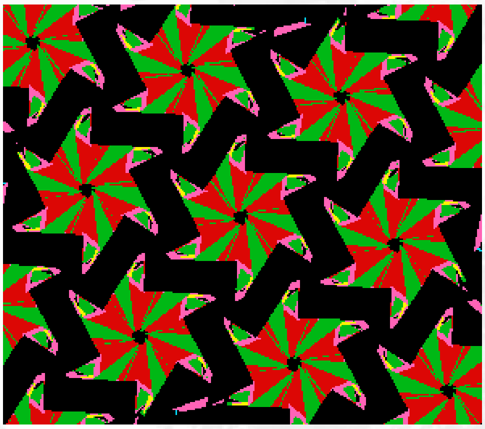
Example 7

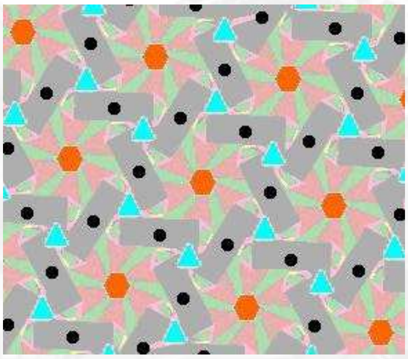
p6mm





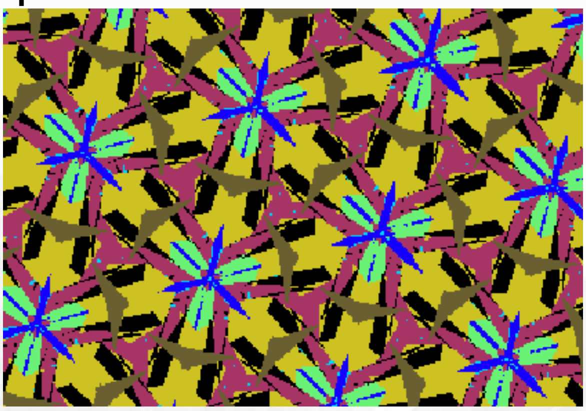
p6

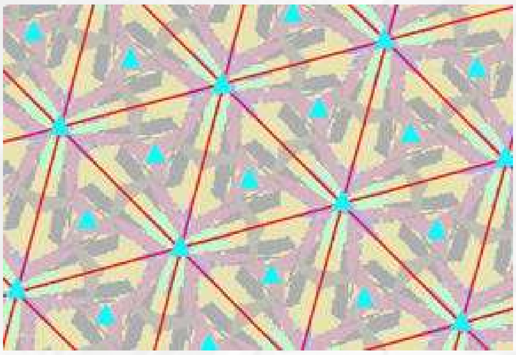




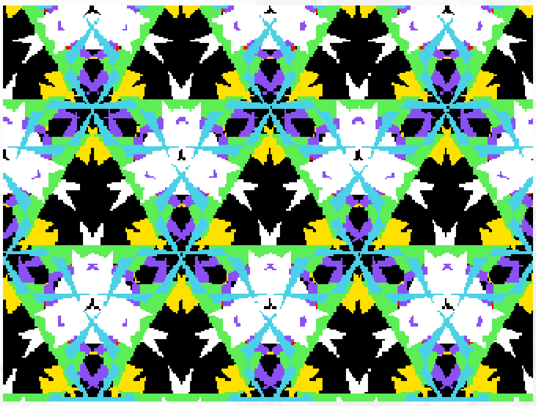
Example 8

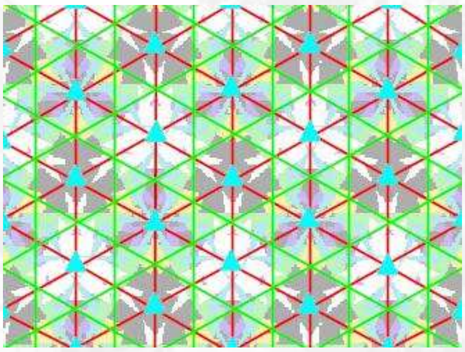
p31m





p3m1





todos

- Read
  - ✓ Ott Chapter 10
  - ✓ Hammond Chapter 4.6
  - ✓ Krawitz Chapter 1.6~1.8
  - ✓ Sherwood & Cooper Chapter 3.7~3.8
  - ✓ Hammond Chapter 2.1 ~ 2.5
  - ✓ Krawitz Chapter 1.1~1.5

- Space Group-1 HW (due in 1 week)
  - ✓ Ott chapter 10 --- 1, 3
  - ✓ Hammond chapter 2 --- 2, 3, 4