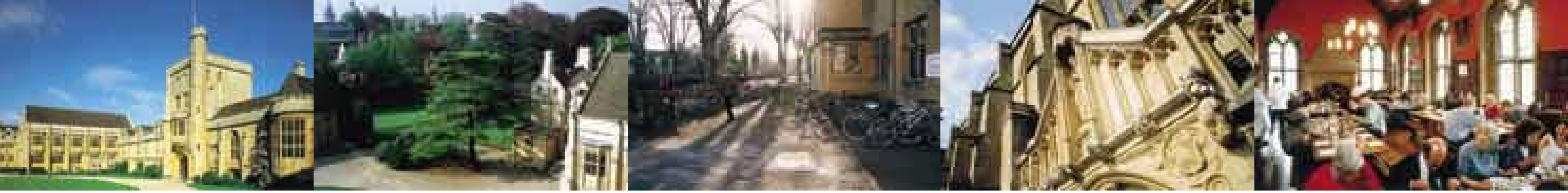


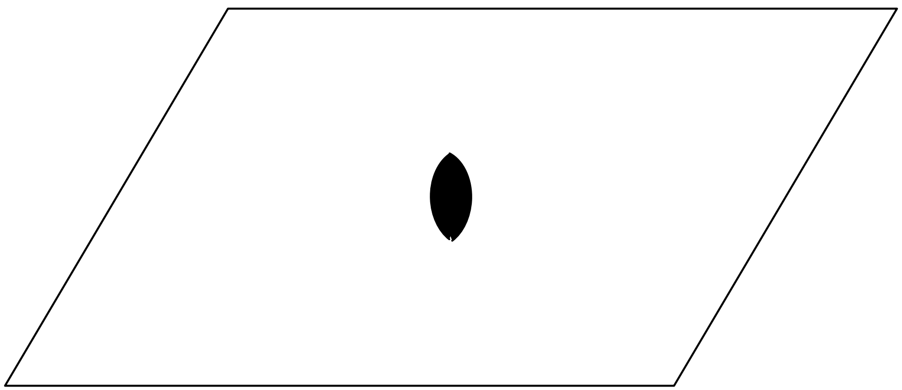
Symmetry, space groups, reciprocal space

P.G. Radaelli

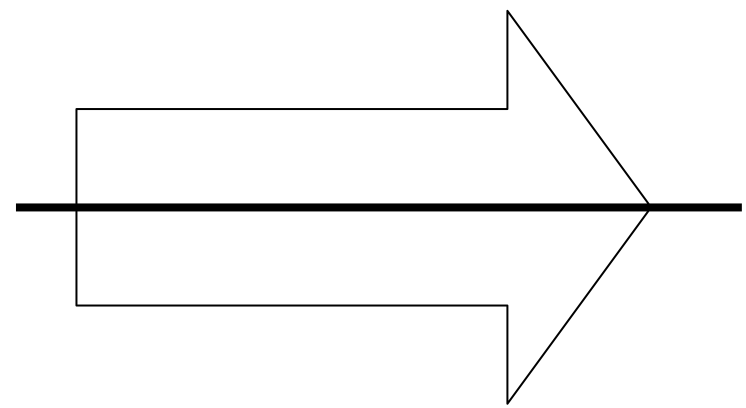
ISIS Facility - RAL

ftp://ftp.nd.rl.ac.uk/scratch/UCL_Teaching_2007/

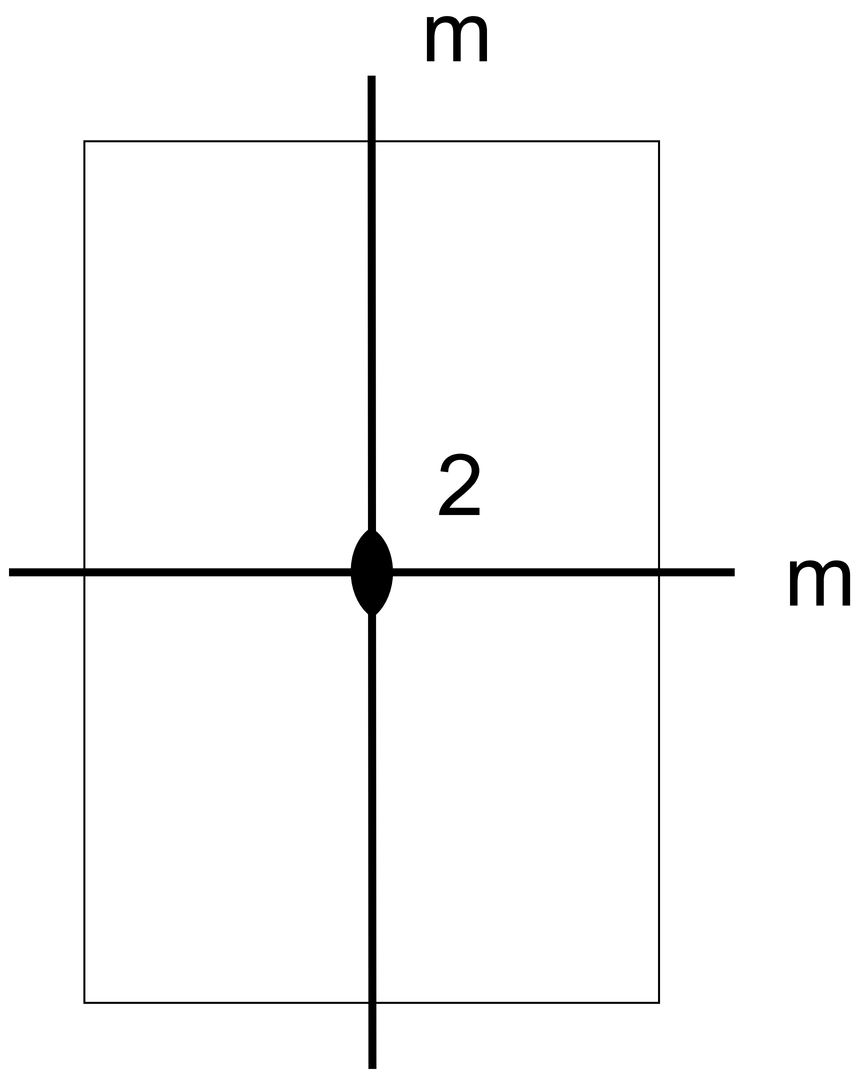
Science & Technology Facilities Council

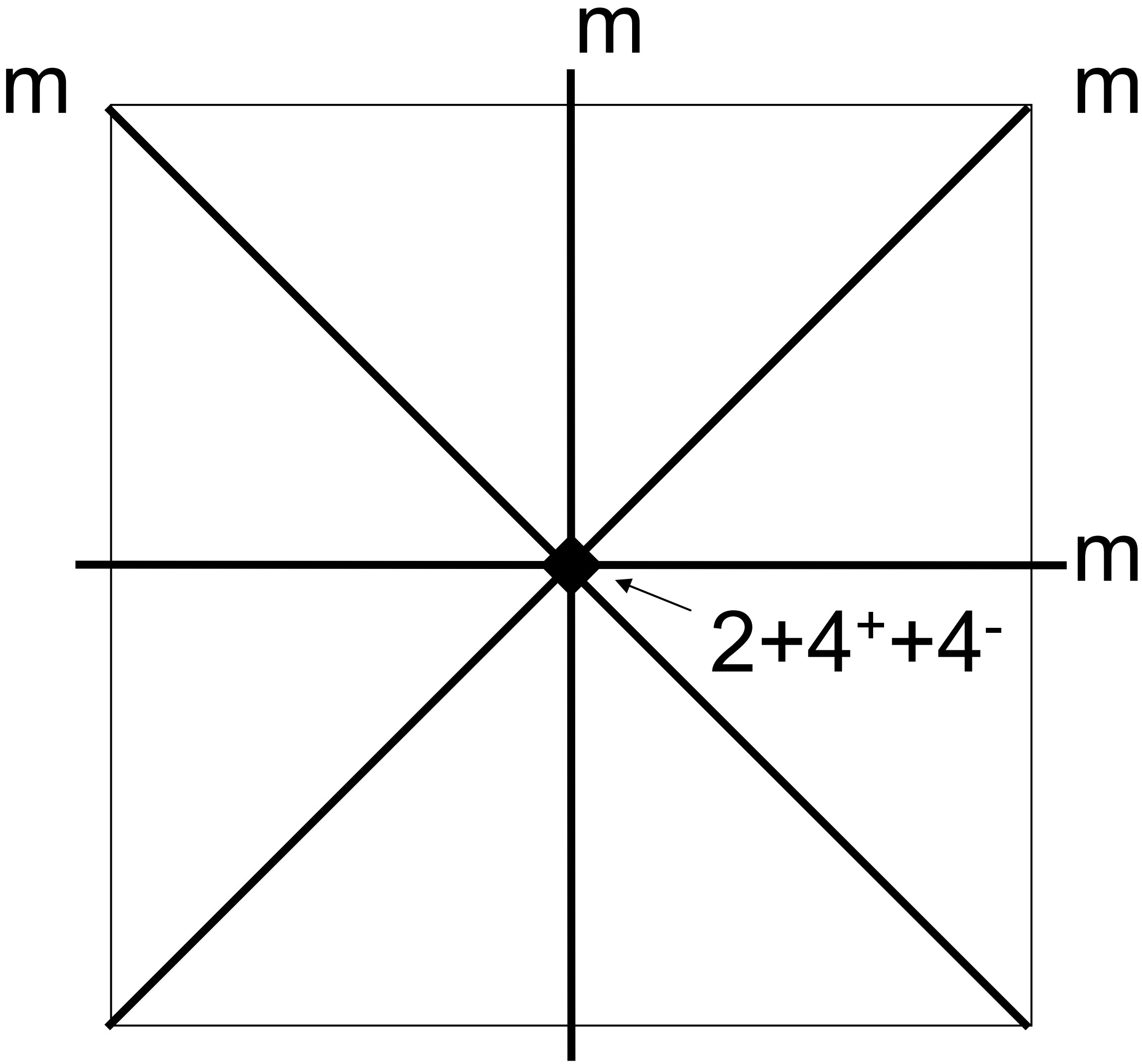


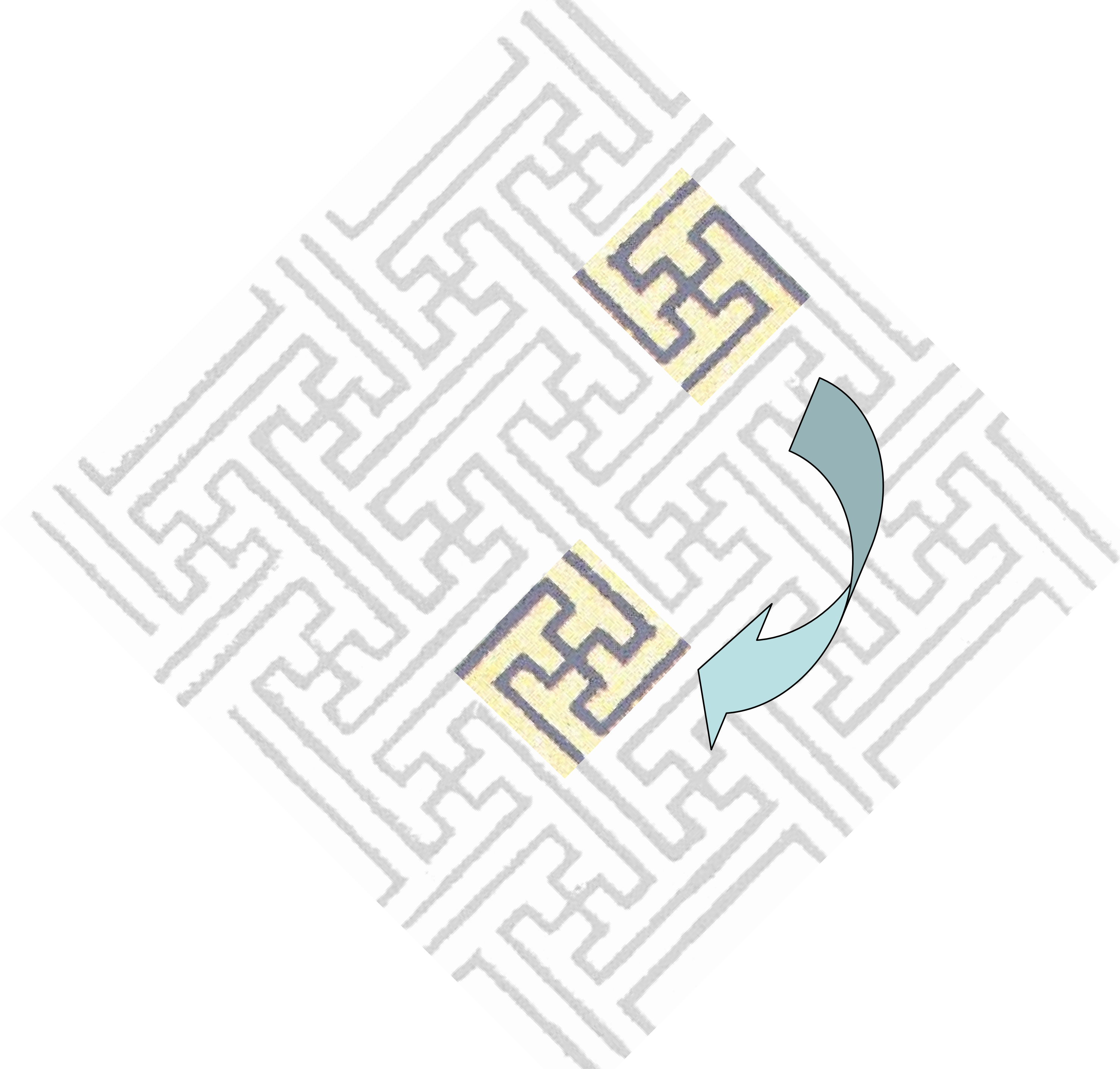
2



m

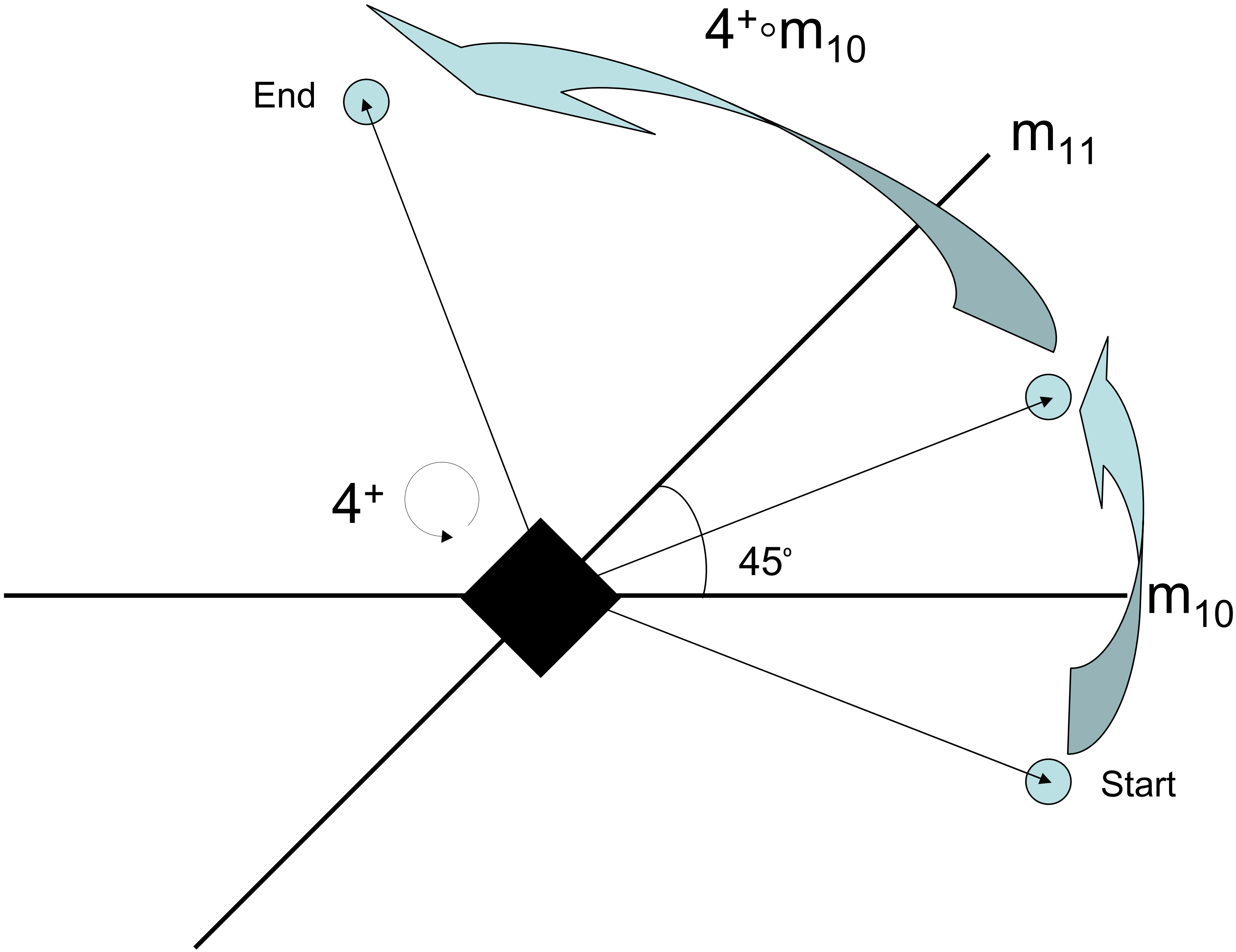

m
2
m


m
m
m
m
2+4⁺+4⁻



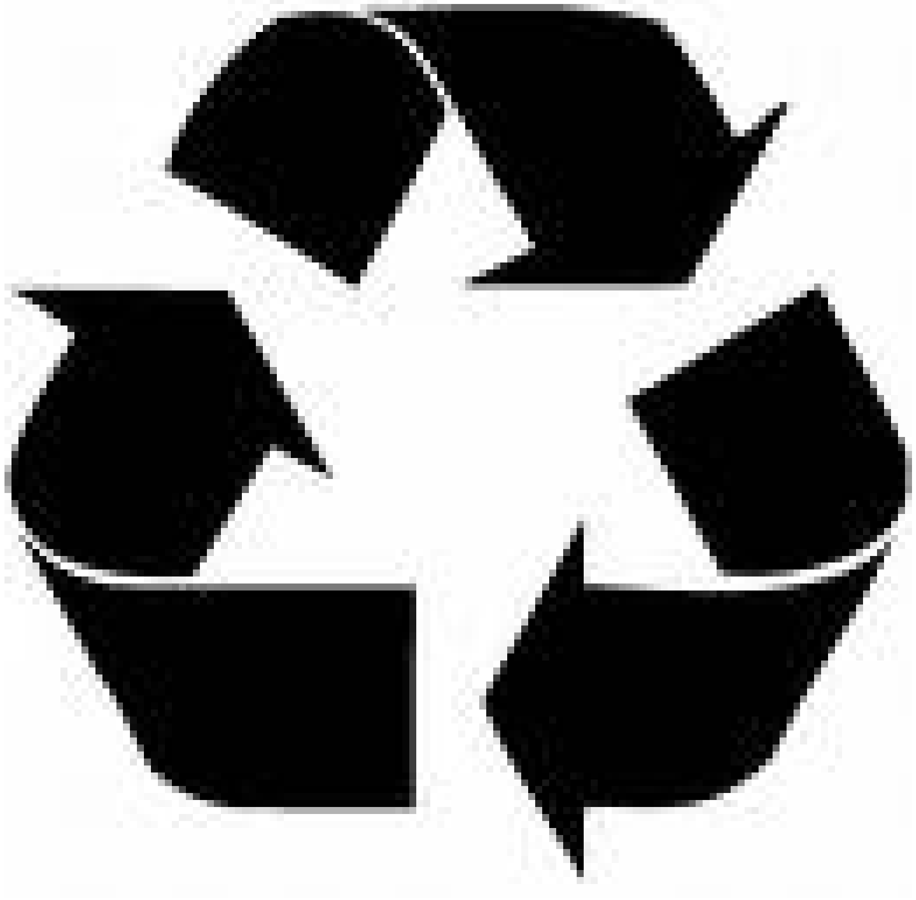
Parallelogram and arrow groups

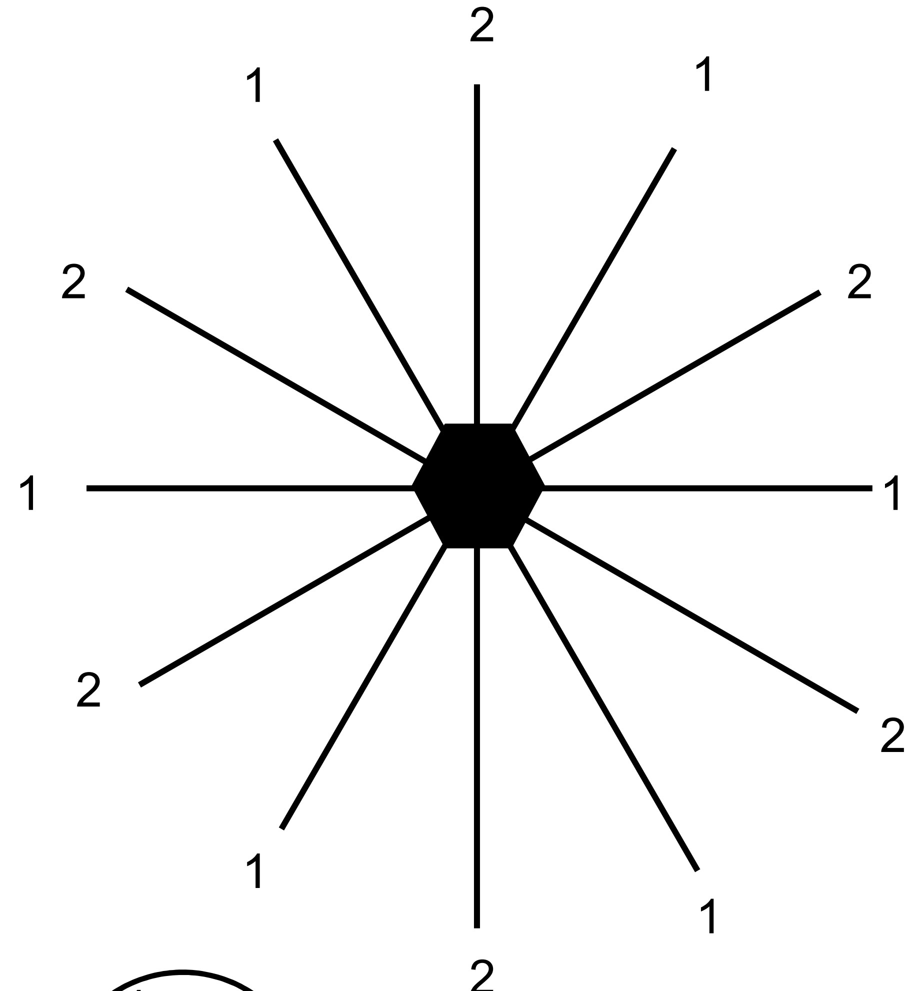
	E	2 or m
E	E	2 or m
2 or m	2 or m	E


$4^+ \circ m_{10}$
End
m_{11}
4^+
45°
m_{10}
Start

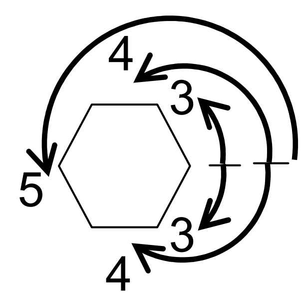
Graph Symmetry (conjugation)

$$g \cdot [h] = [g \circ h \circ g^{-1}]$$

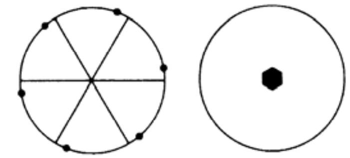
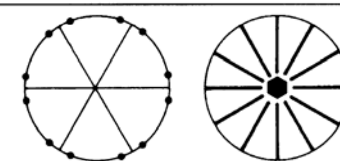


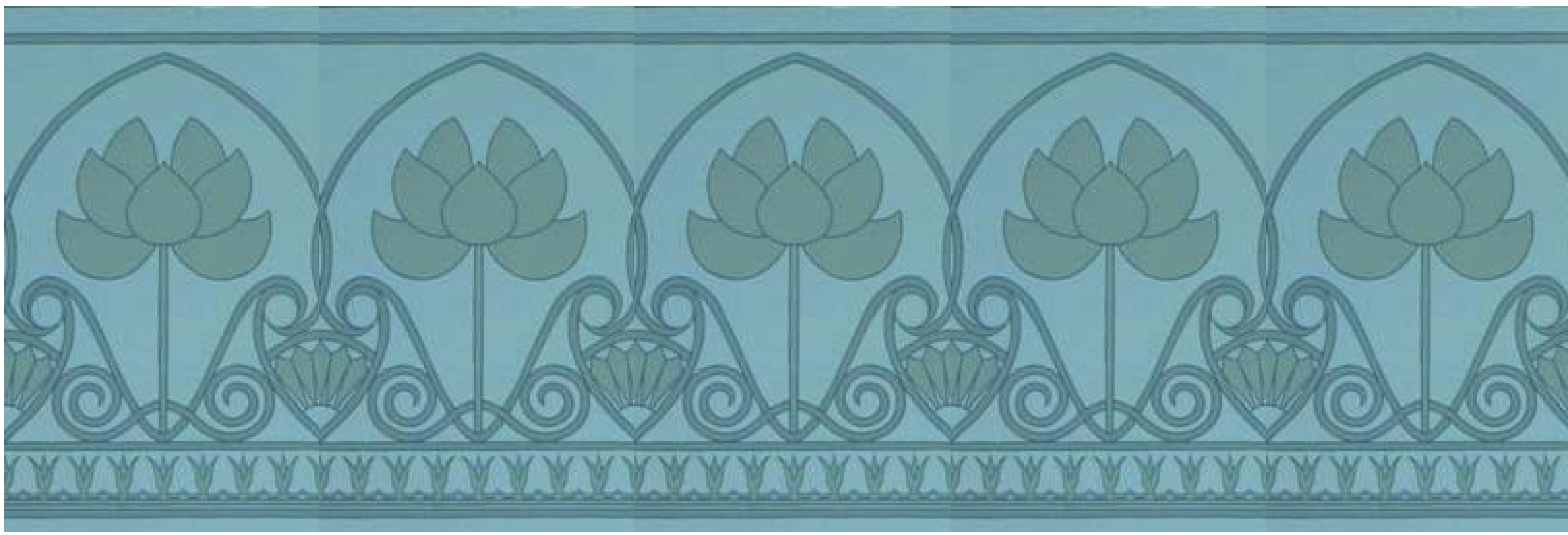


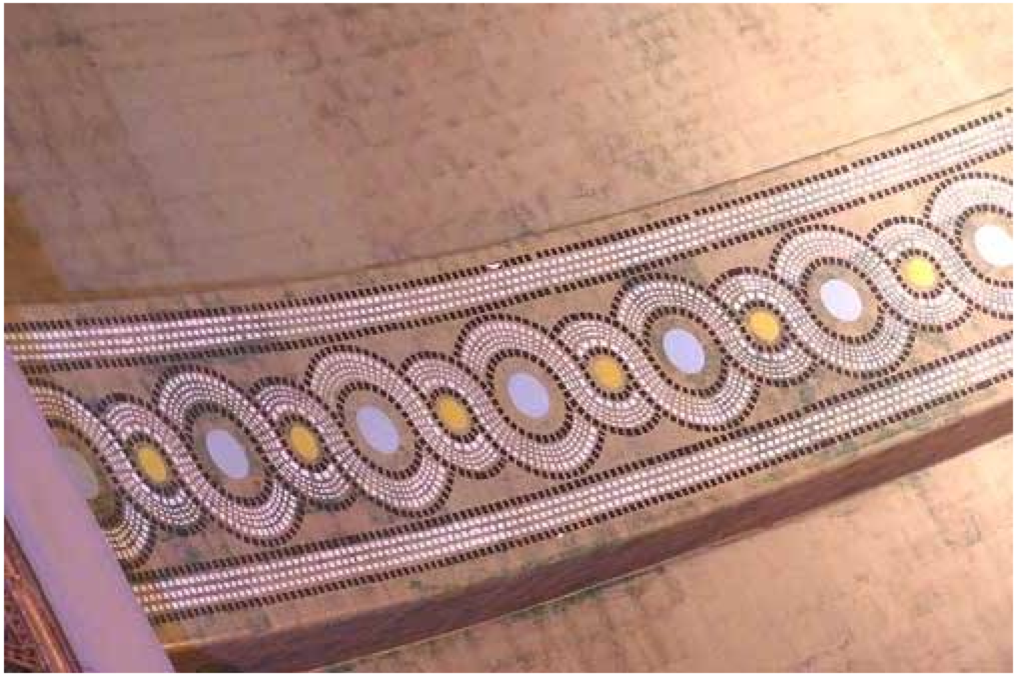
2
1
1
2
2
1
1
2
2
1
1
2

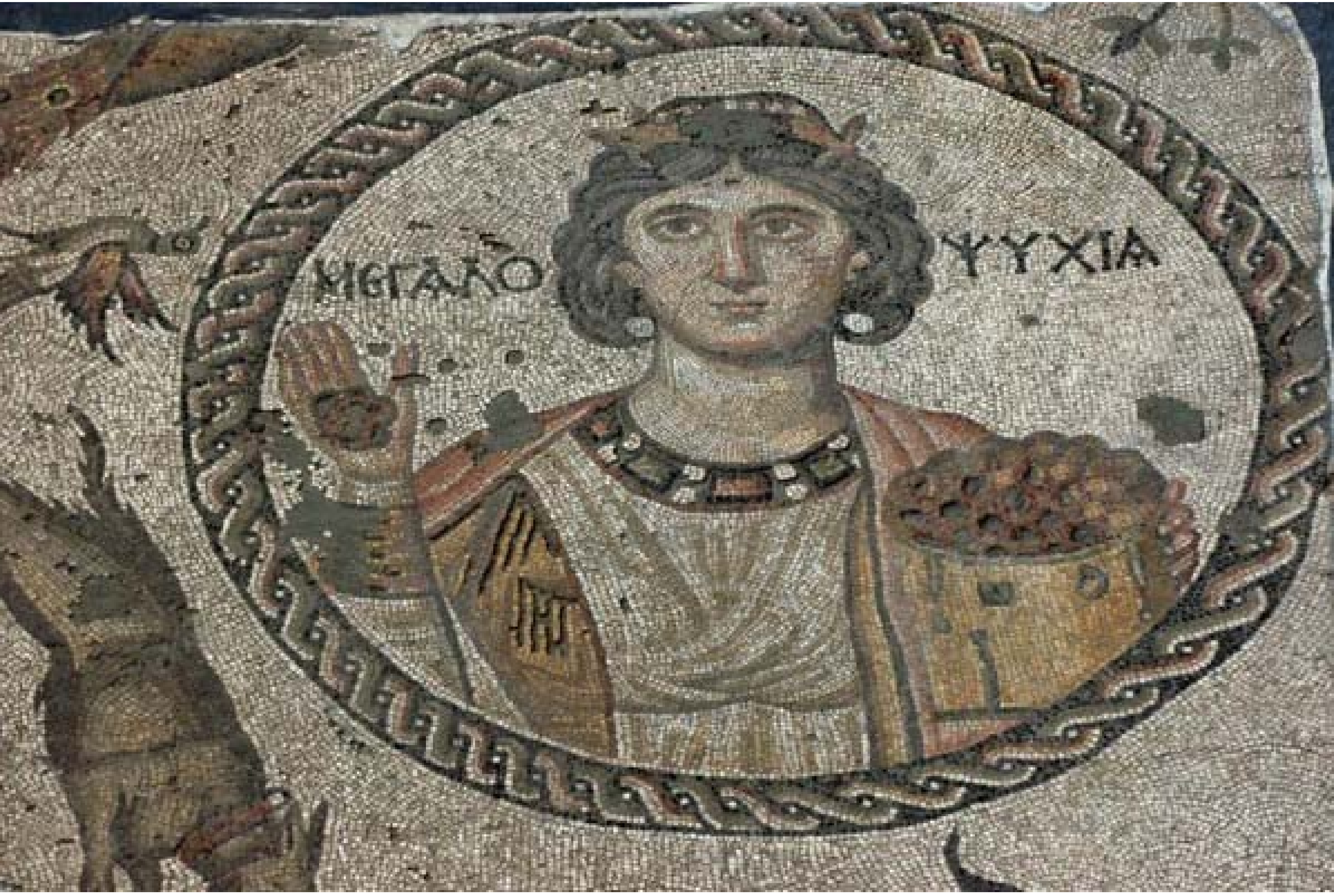


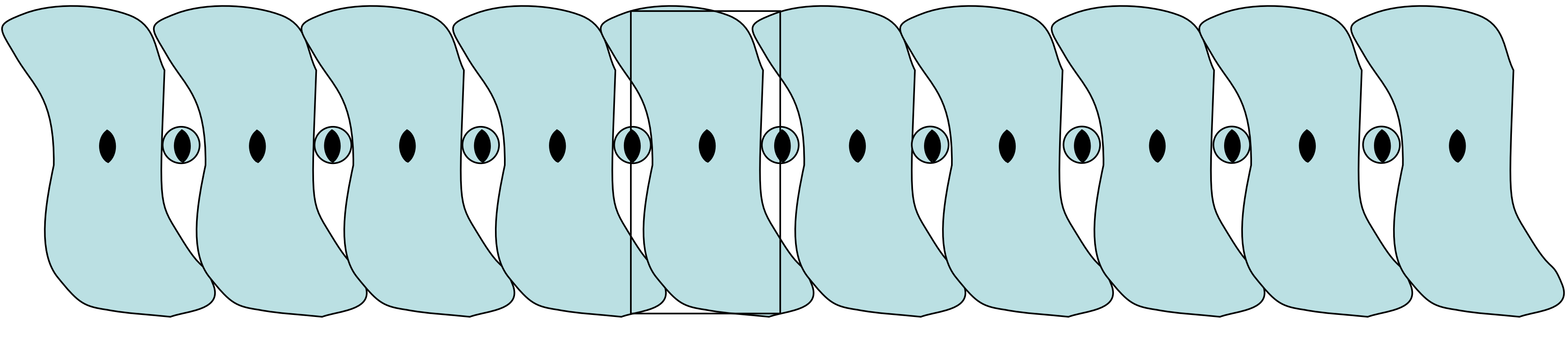
4
3
5
3
4

6				
6	*a*	1	Hexagon *Hexagon* (*d*)	(hki) (ihk) (kih) $(\bar{h}\bar{k}\bar{i})$ $(\bar{i}\bar{h}\bar{k})$ $(\bar{k}\bar{i}\bar{h})$
6*mm*				
12	*c*	1	Dihexagon *Truncated hexagon* (*f*)	(hki) (ihk) (kih) $(\bar{h}\bar{k}\bar{i})$ $(\bar{i}\bar{h}\bar{k})$ $(\bar{k}\bar{i}\bar{h})$ $(\bar{k}\bar{h}\bar{i})$ $(\bar{i}\bar{k}\bar{h})$ $(\bar{h}\bar{i}\bar{k})$ (khi) (ikh) (hik)
6	*b*	*.m.*	Hexagon *Hexagon* (*e*)	$(10\bar{1})$ $(\bar{1}10)$ $(0\bar{1}1)$ $(\bar{1}01)$ $(1\bar{1}0)$ $(01\bar{1})$
6	*a*	*..m*	Hexagon *Hexagon* (*d*)	$(11\bar{2})$ $(\bar{2}11)$ $(1\bar{2}1)$ $(\bar{1}\bar{1}2)$ $(2\bar{1}\bar{1})$ $(\bar{1}2\bar{1})$



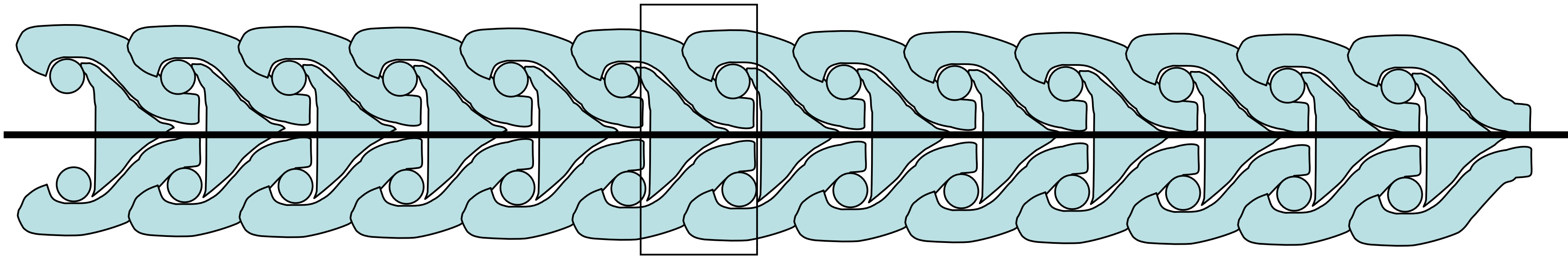



ΜΕΓΑΛΟ
ΨΥΧΙΑ

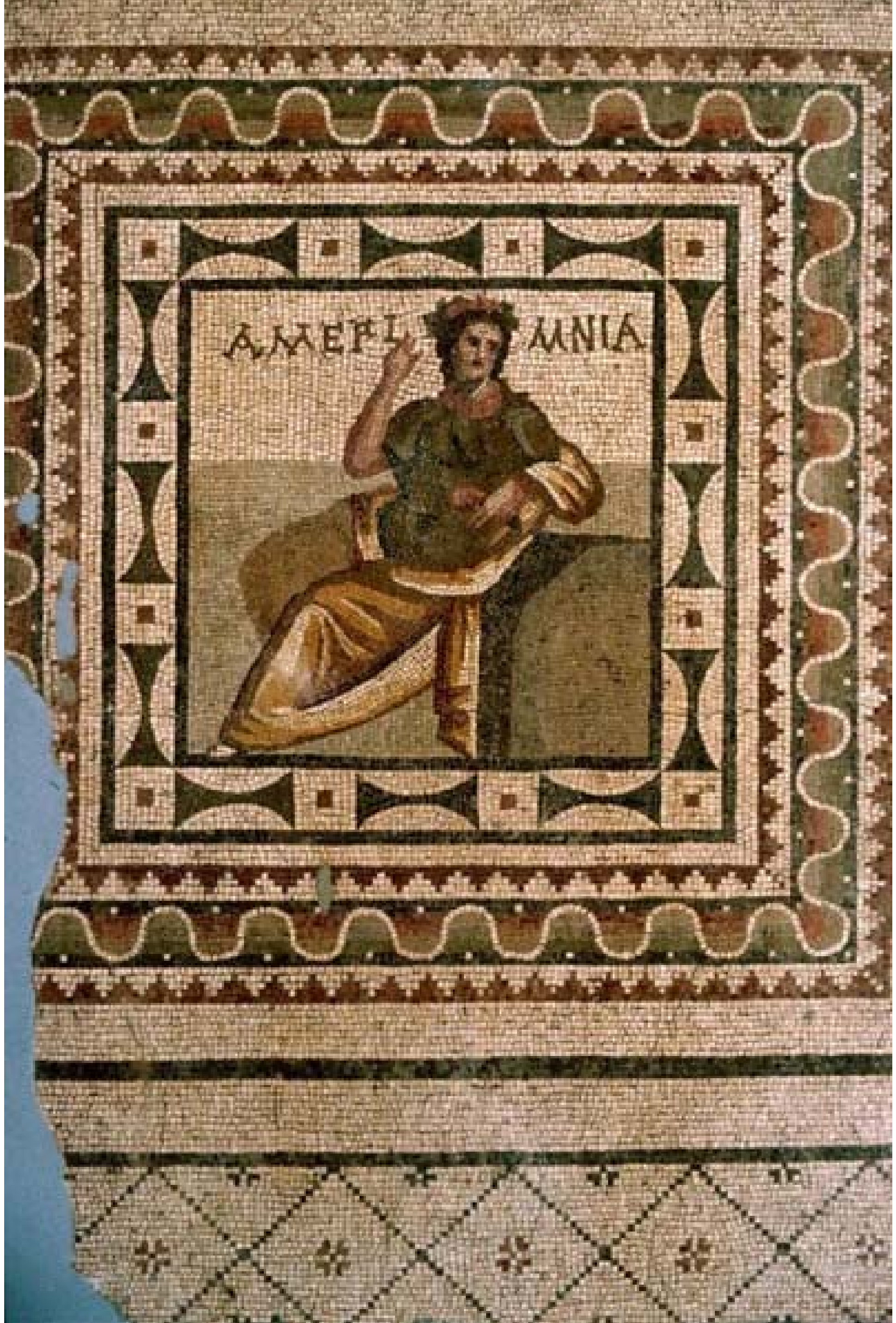


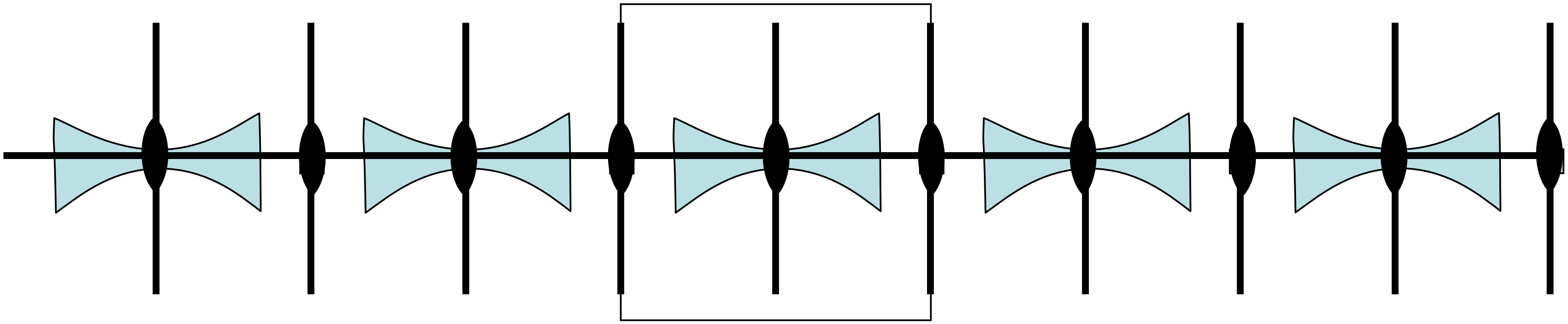
p211


ΤΟ ΟΛΥΜΠΙΑΚΟΝ

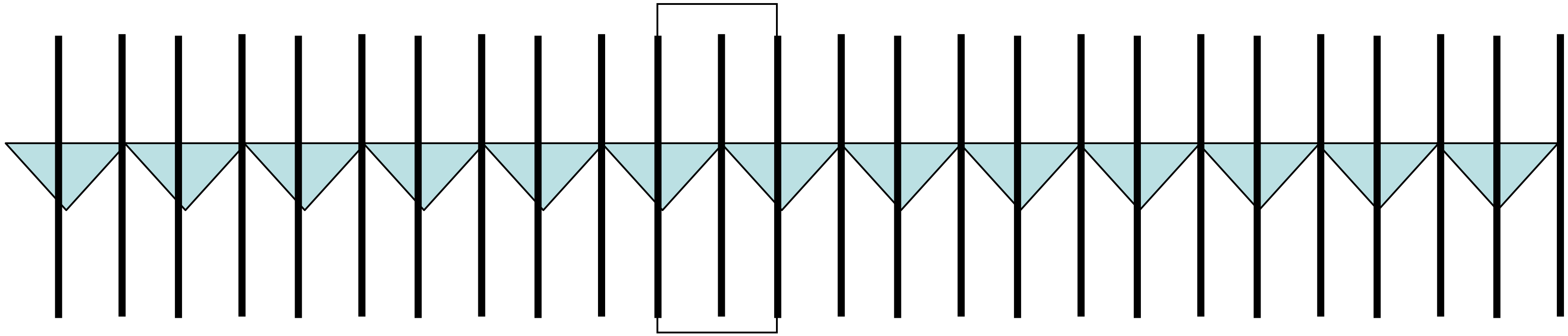


p11m

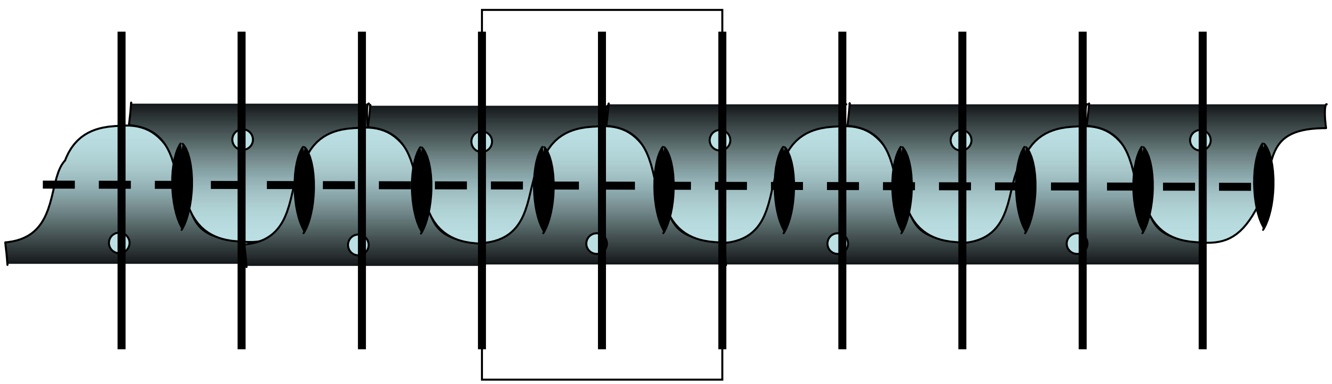

ΑΜΕΡΙ
ΜΝΙΑ



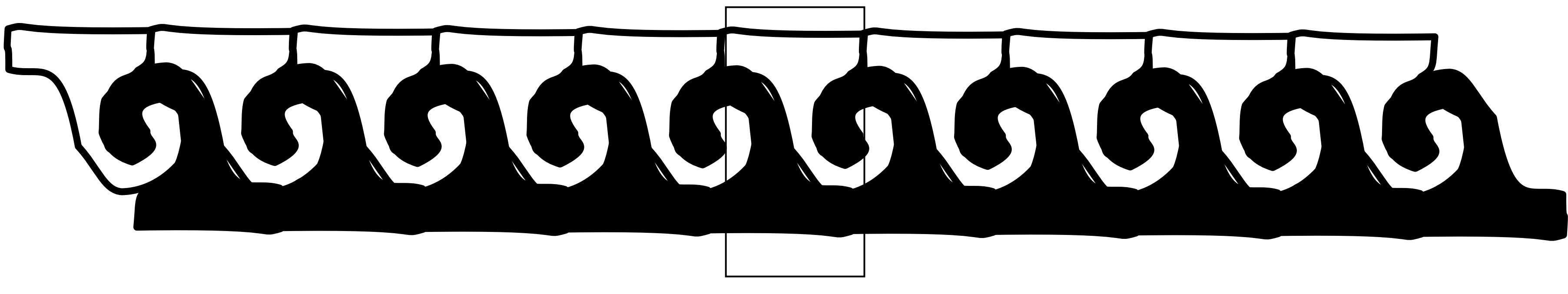
p2mm



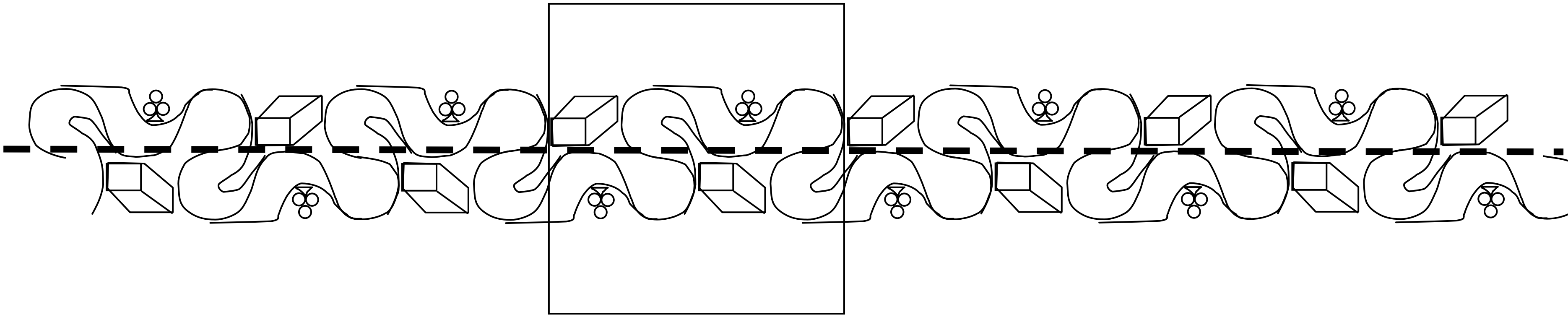
p1m1



p2mg

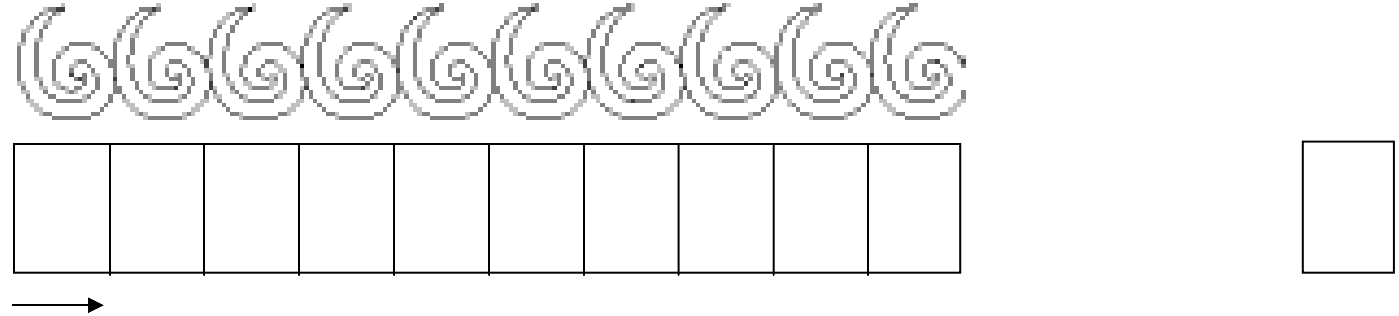


p1



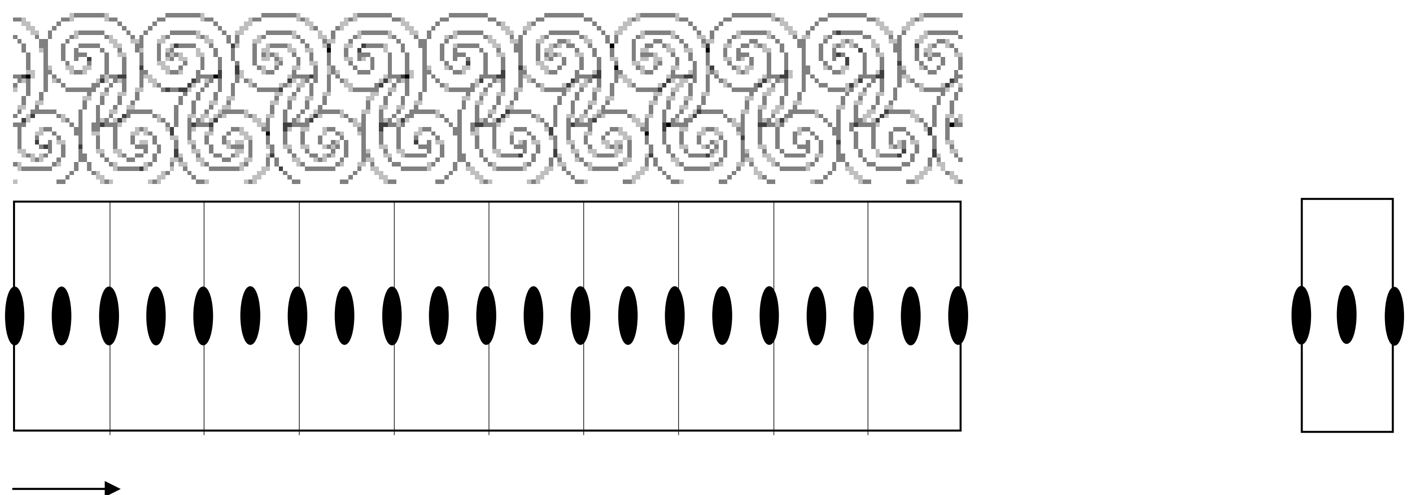
p11g

1



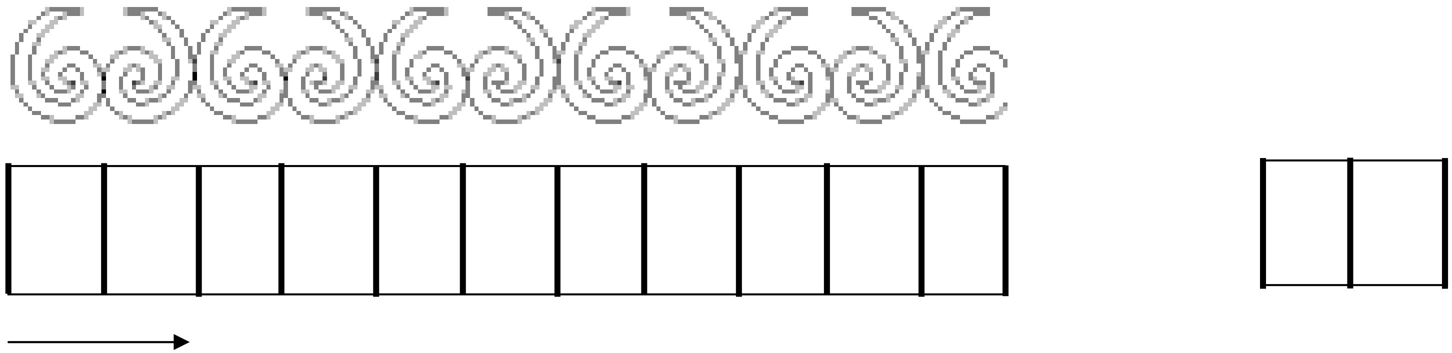
p1

2



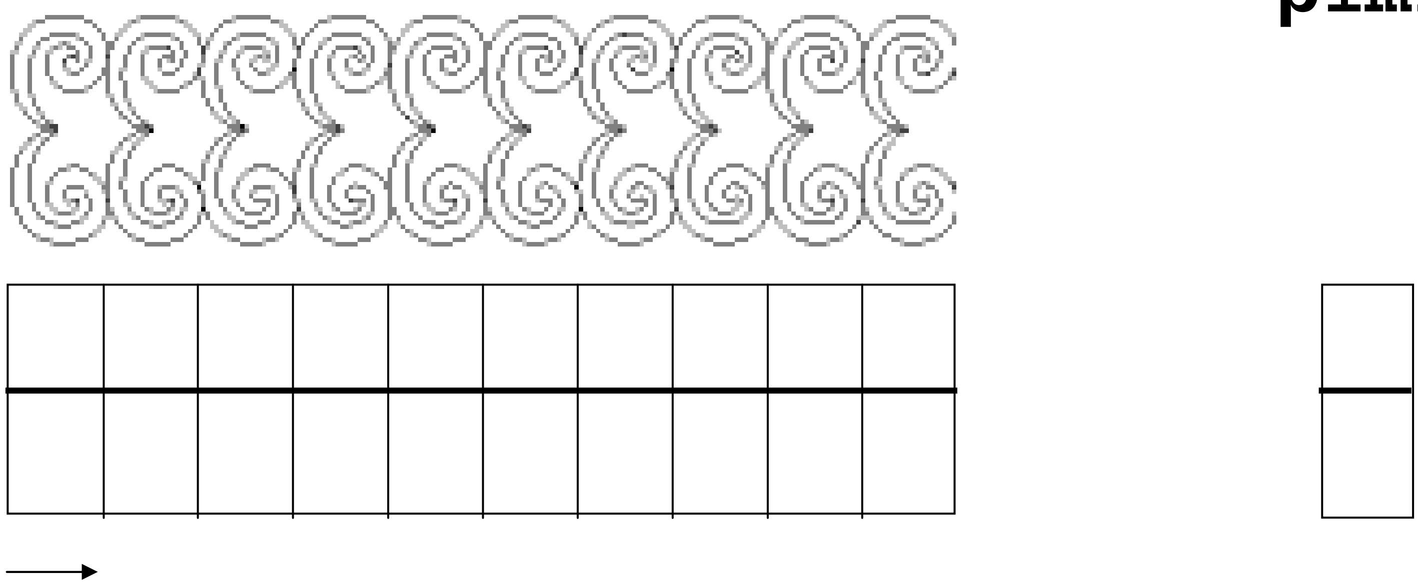
p211

3



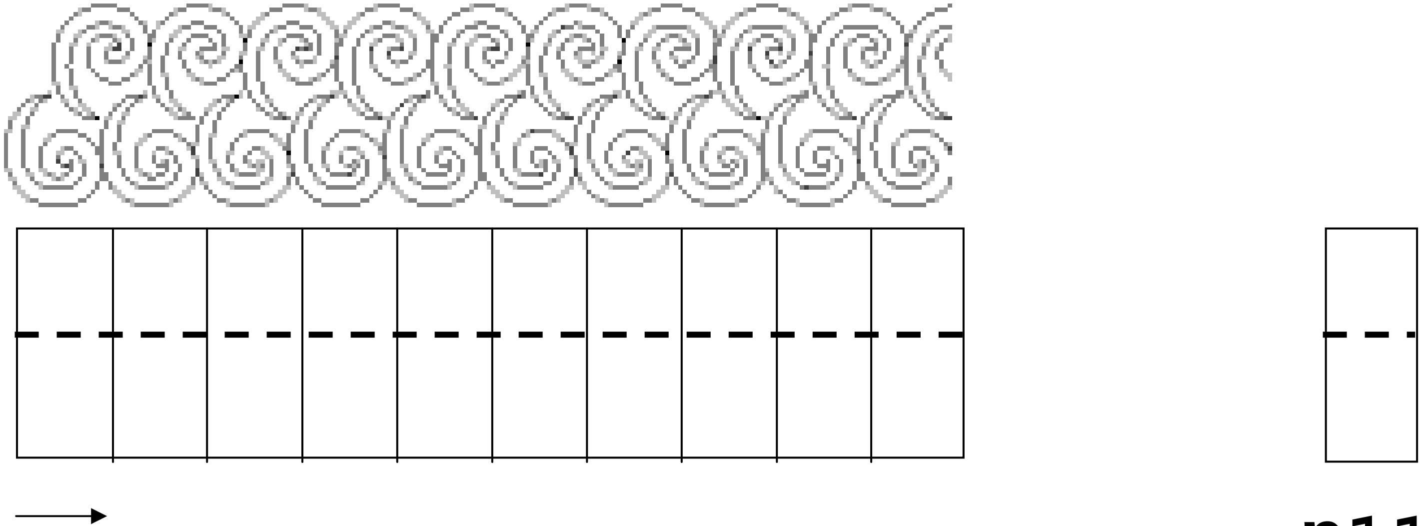
p1m1

4



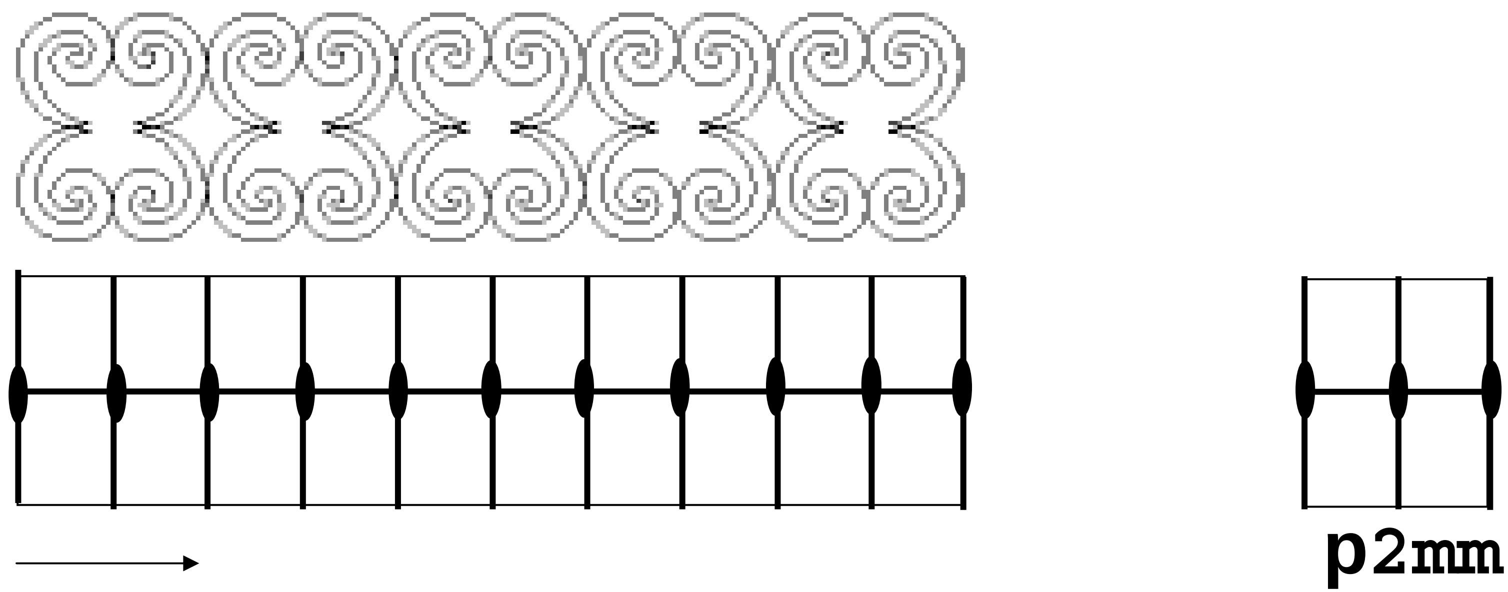
p11m

5



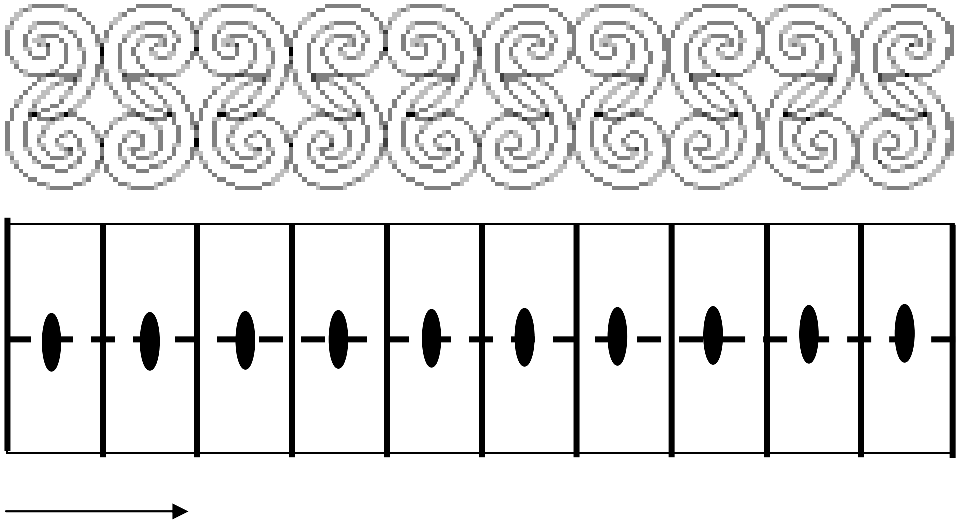
p11g

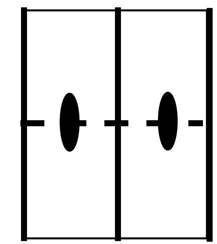
6



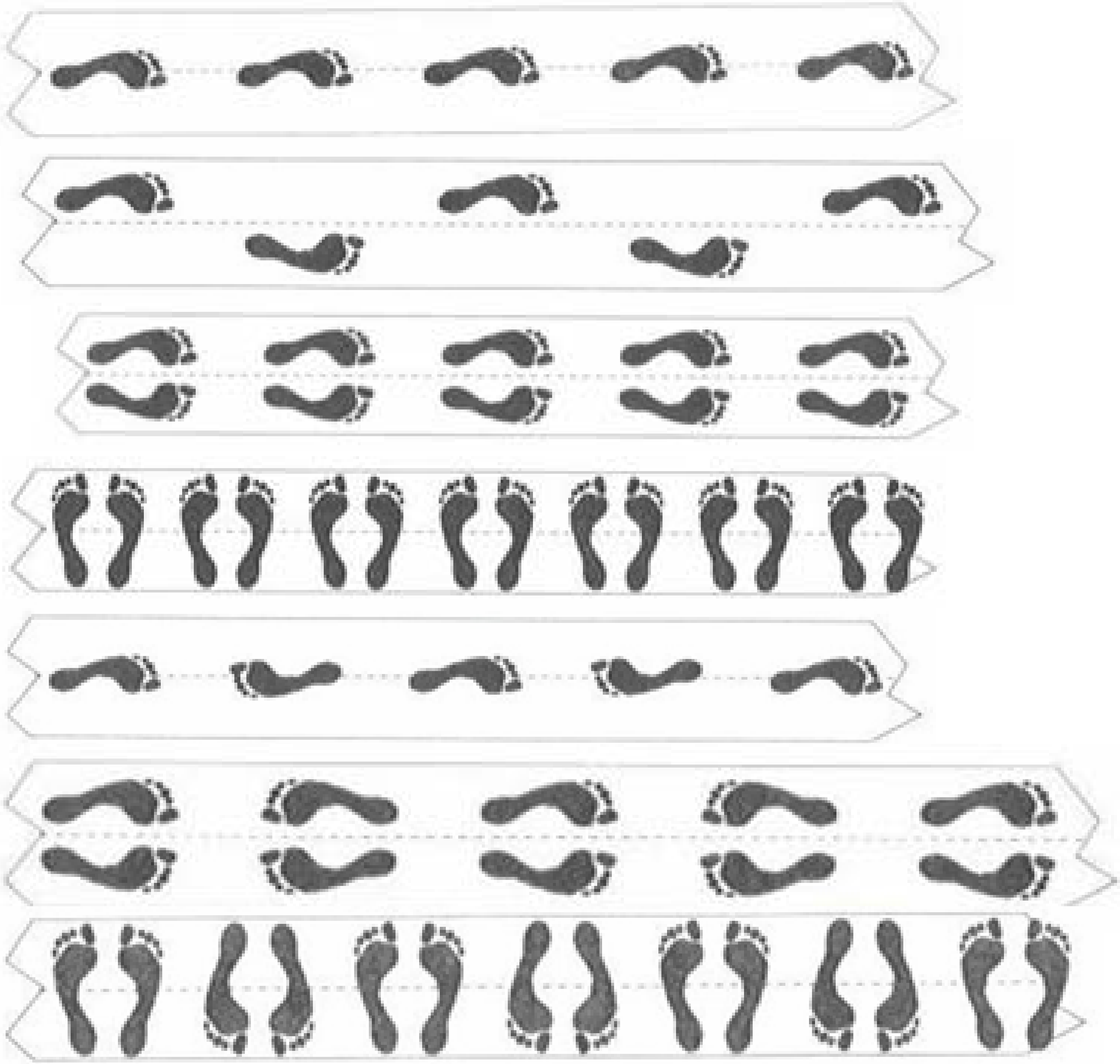
p2mm

7

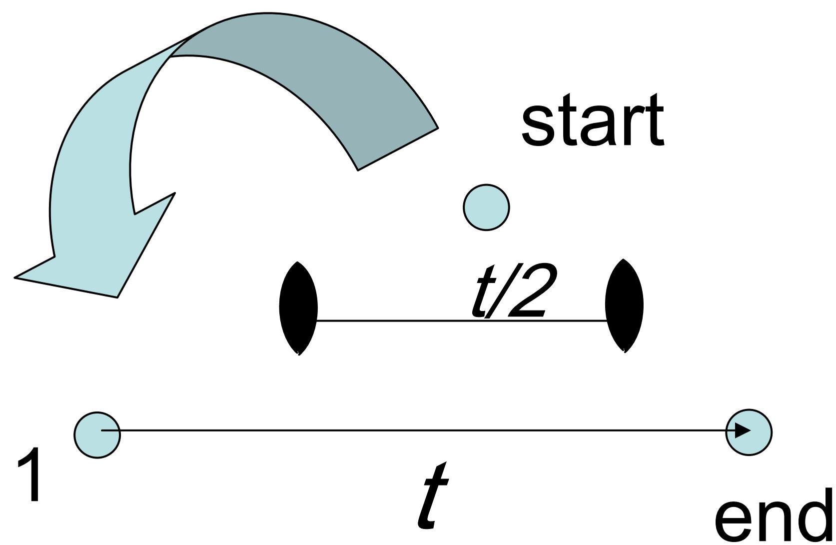




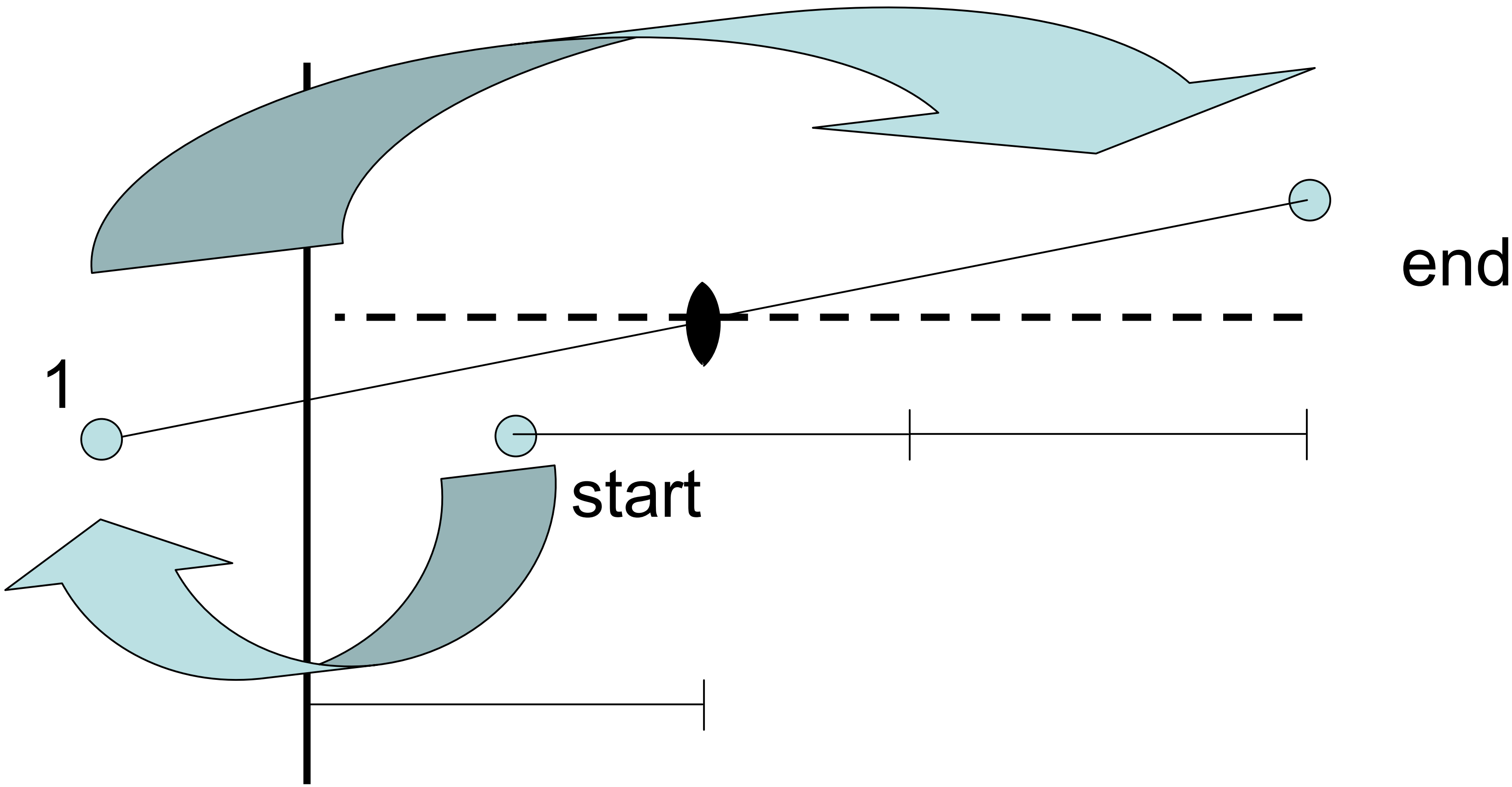
p2mg



$t \circ 2$

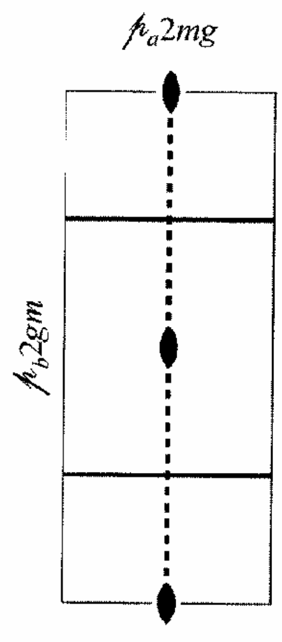


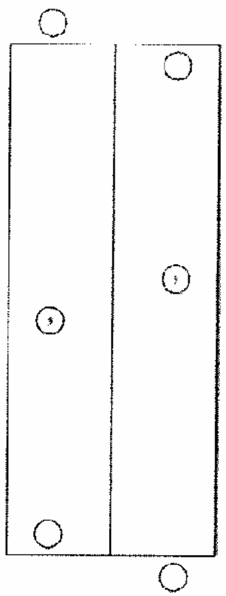
$2 \circ m$



$p2mg$ $2mm$ Rectangular

No. 7 $p2mg$ Patterson symmetry $p2mm$





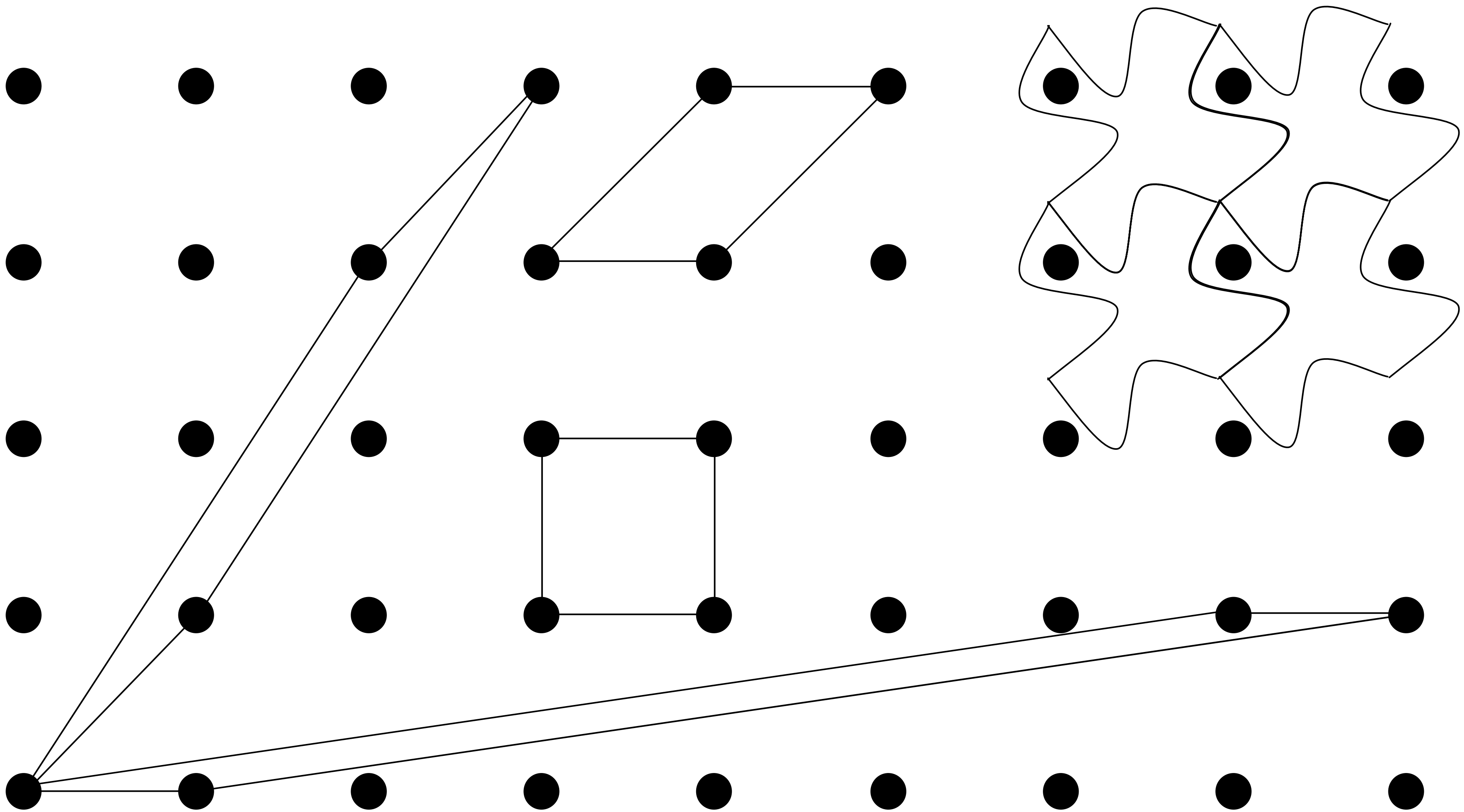
Origin at $21g$

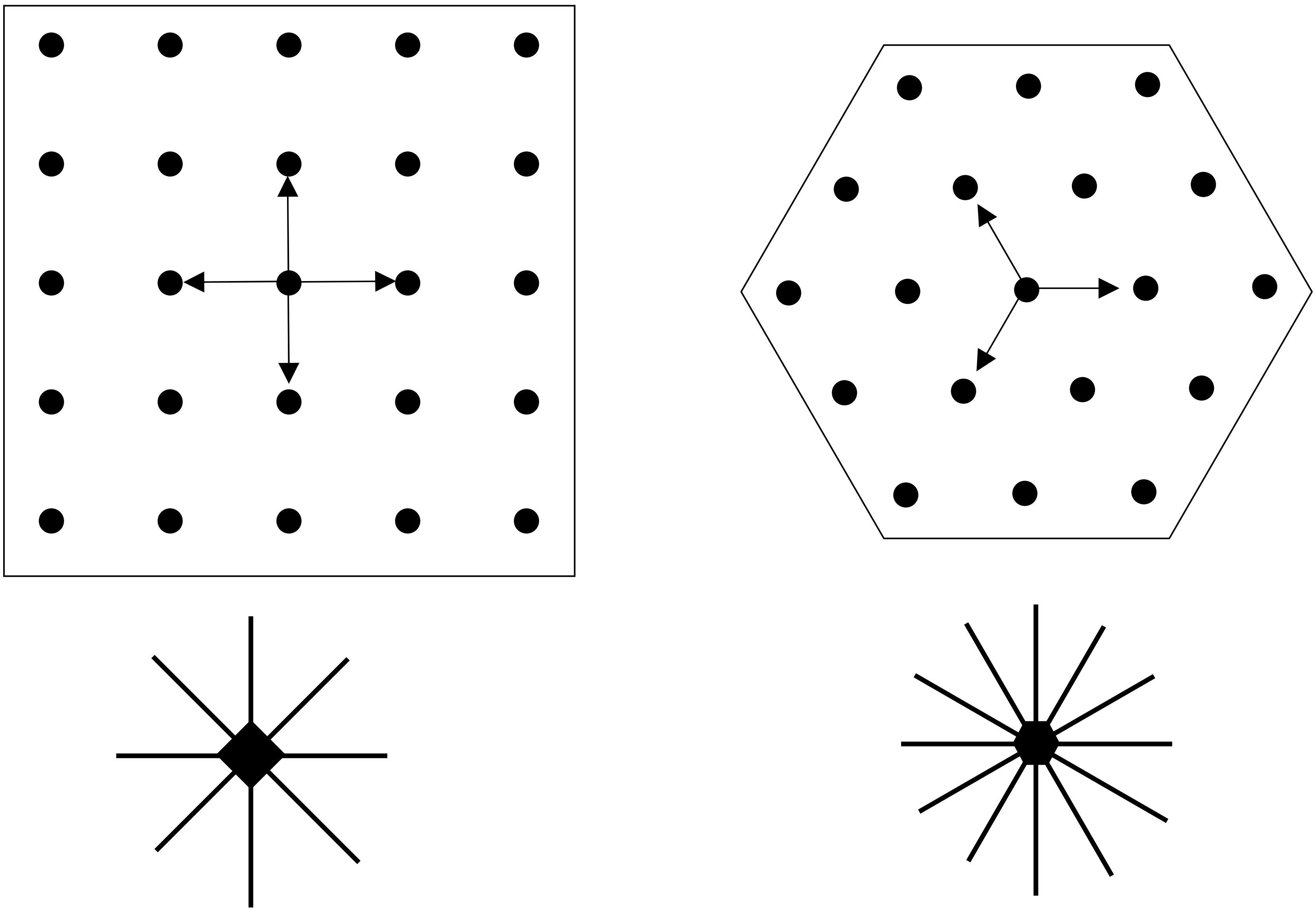
Asymmetric unit $0 \leq x \leq \frac{1}{4}$

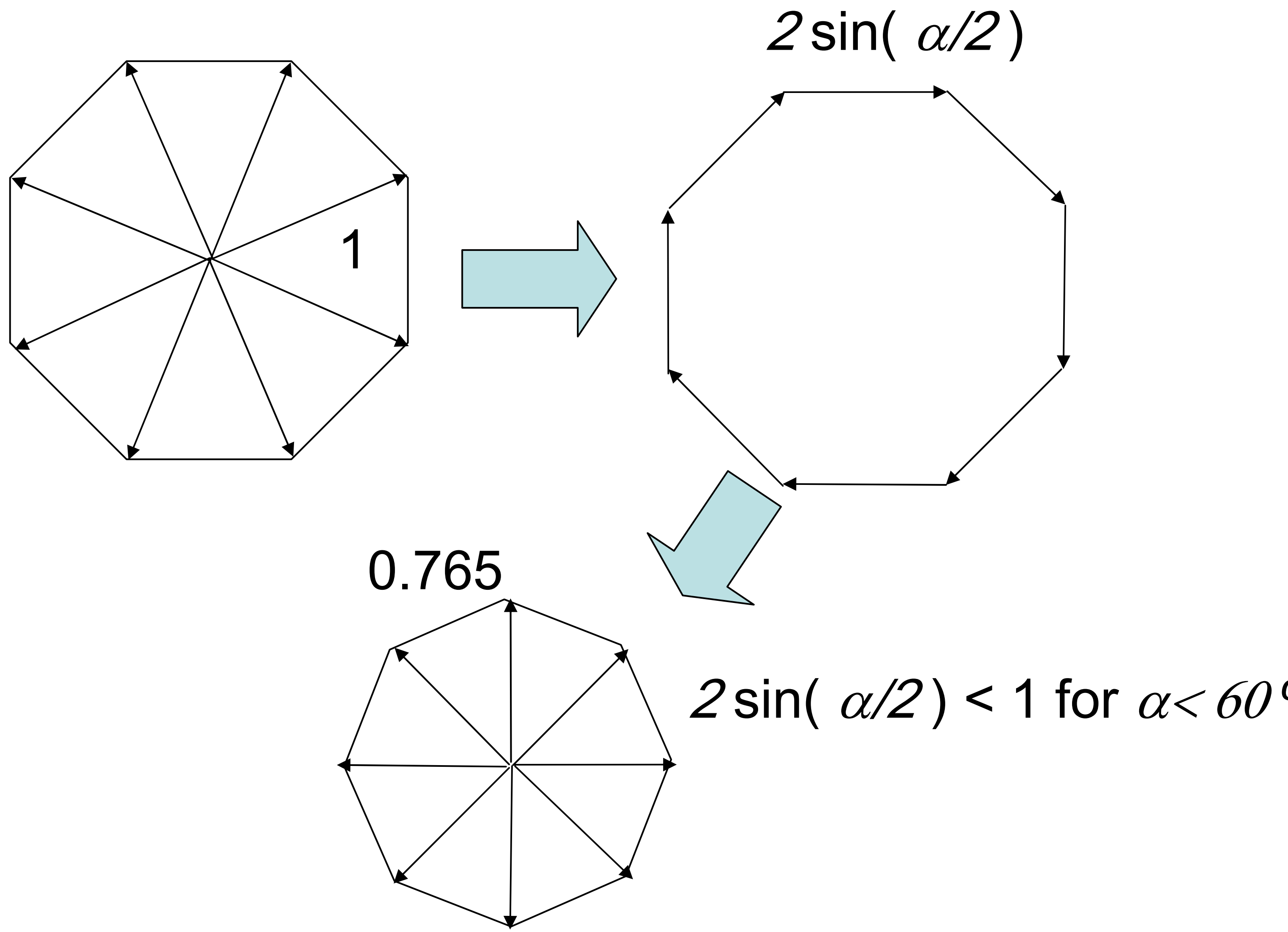
Symmetry operations

(1) 1 (2) 2 $0,0$ (3) m $\frac{1}{4},y$ (4) g $x,0$

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

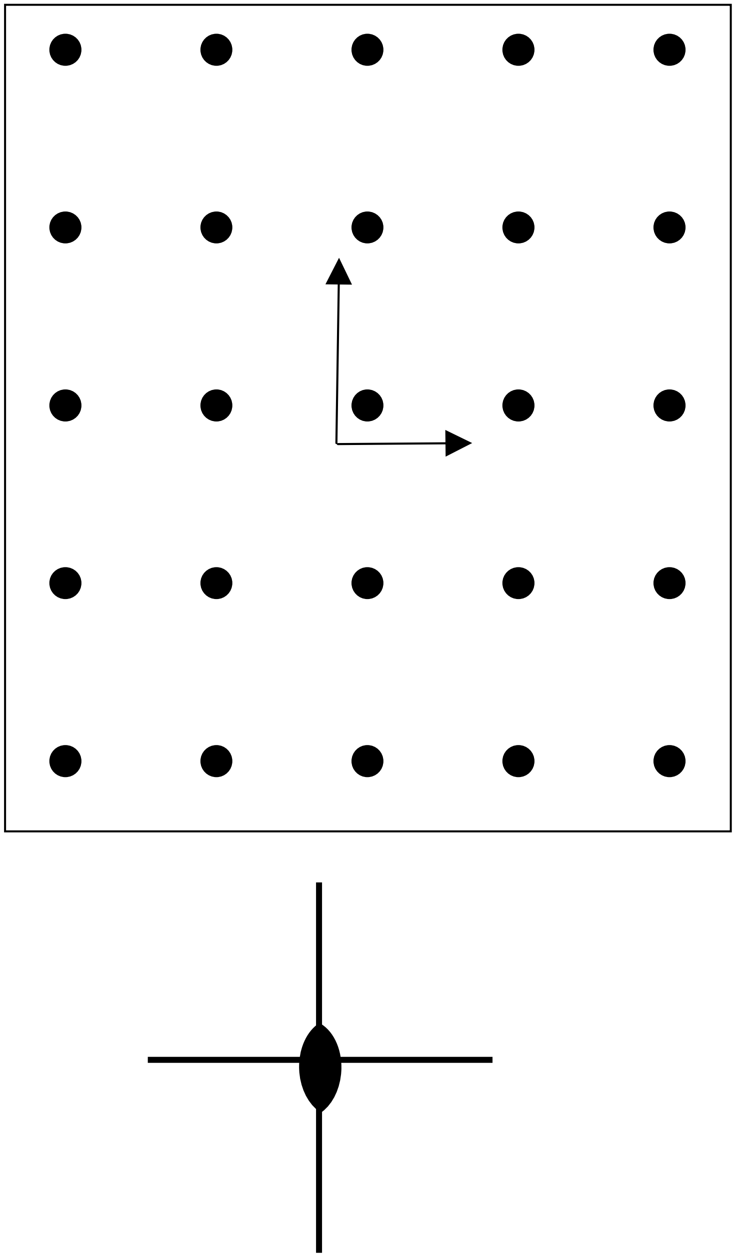




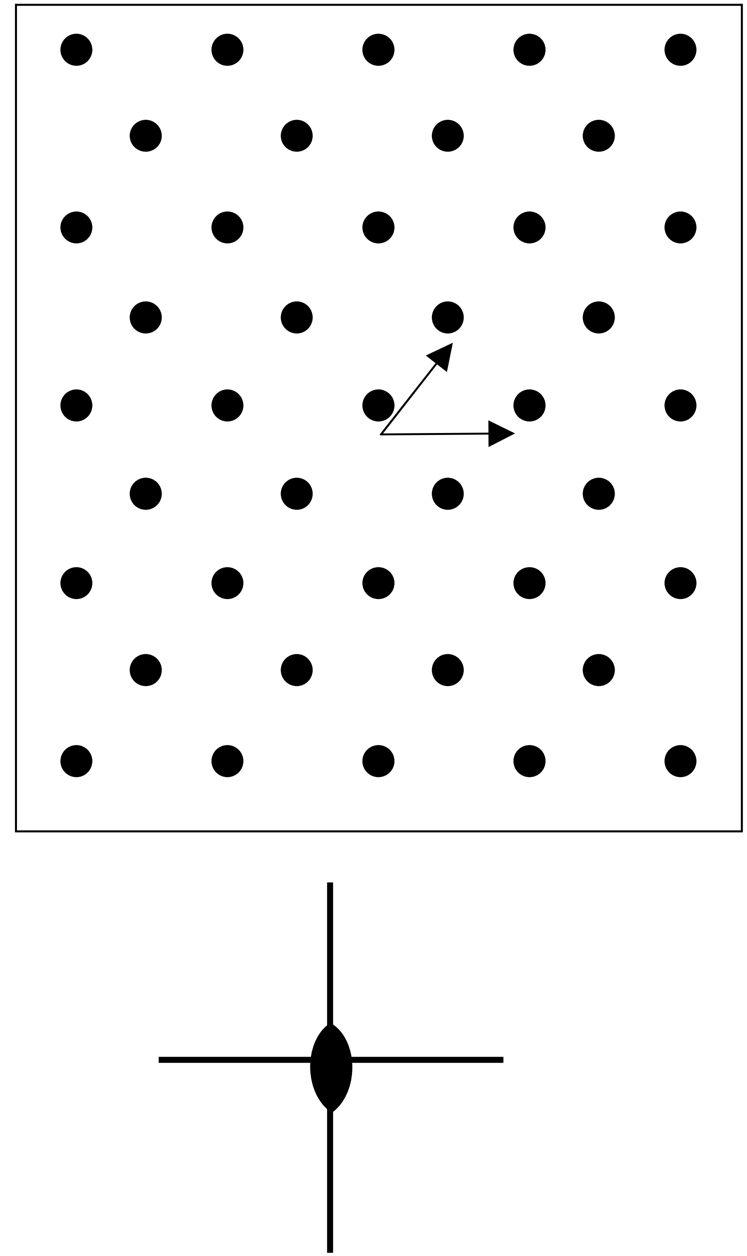


$2\sin(\alpha/2)$
1
0.765
$2\sin(\alpha/2) < 1$ for $\alpha < 60^o$

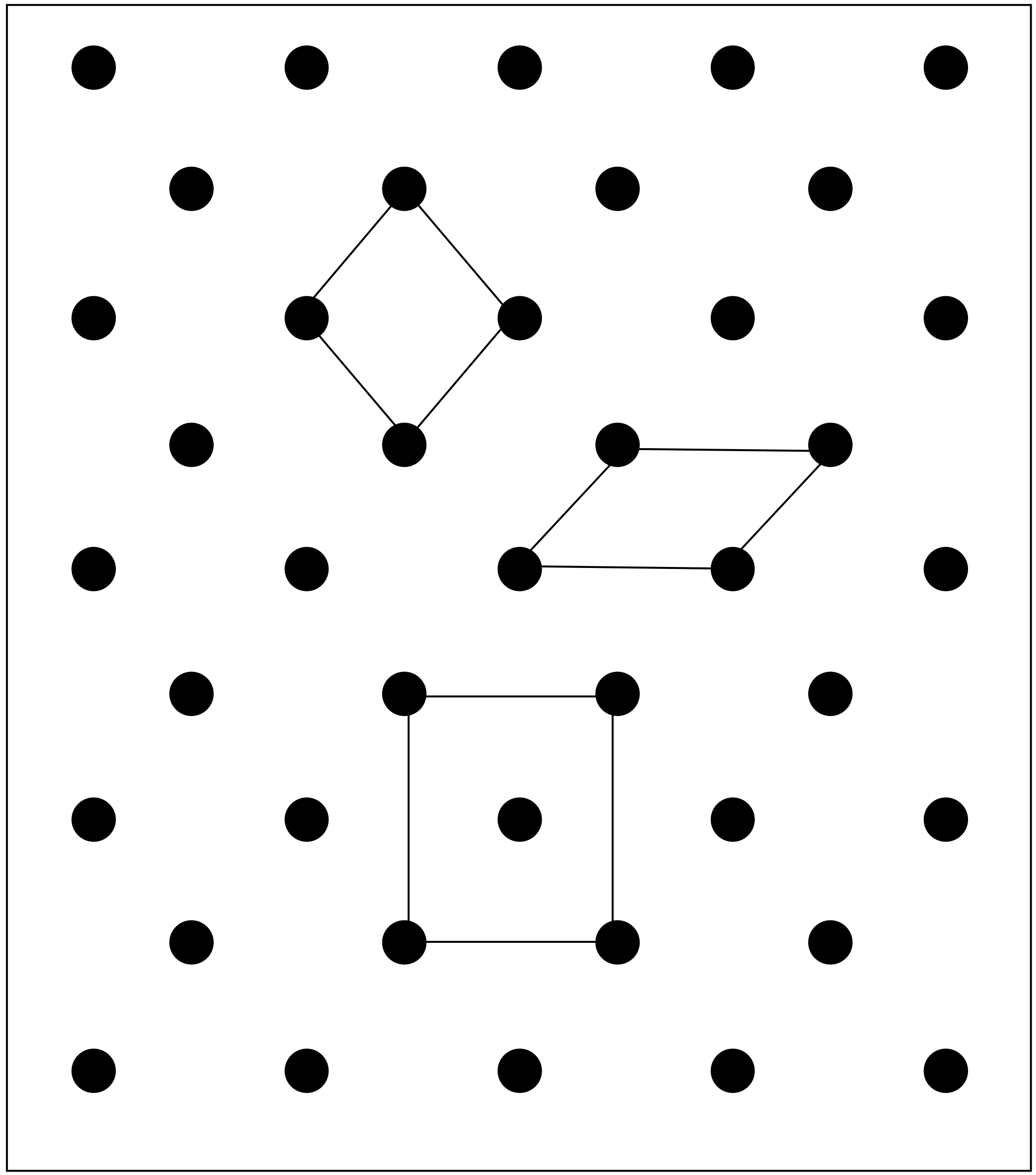
“*p*”



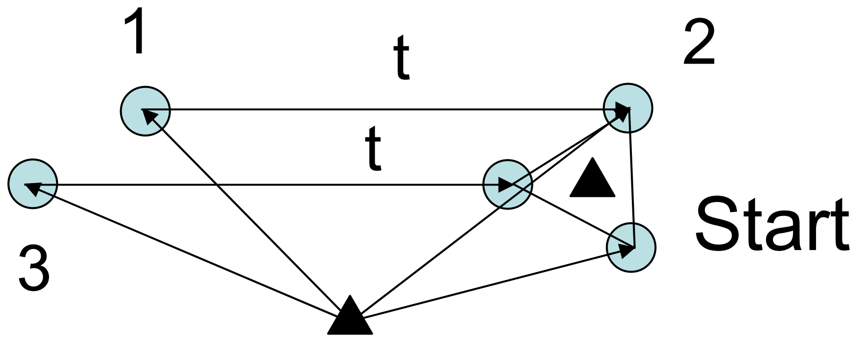
“*c*”

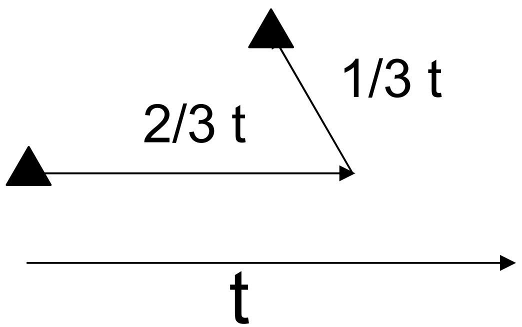


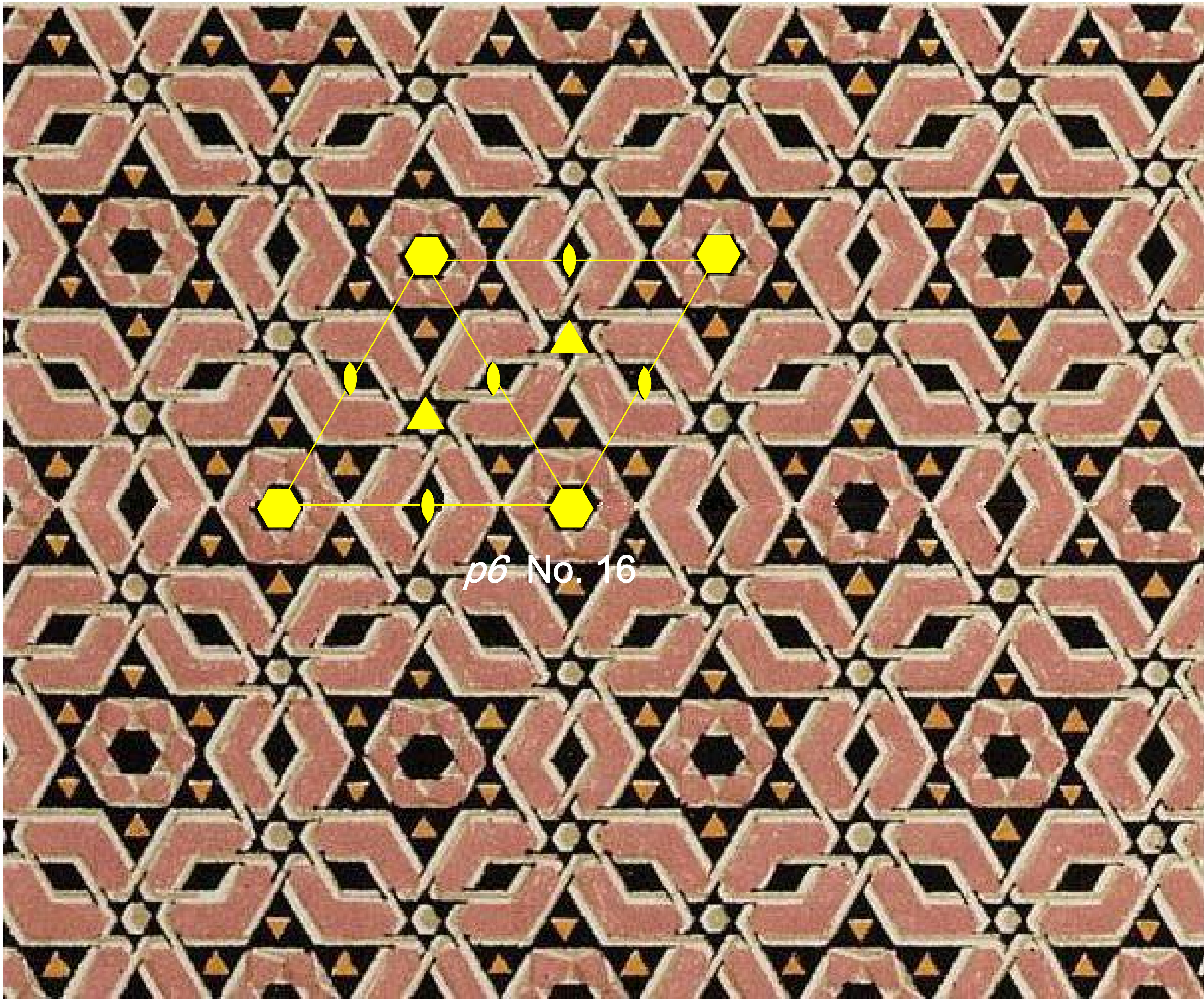
“c”

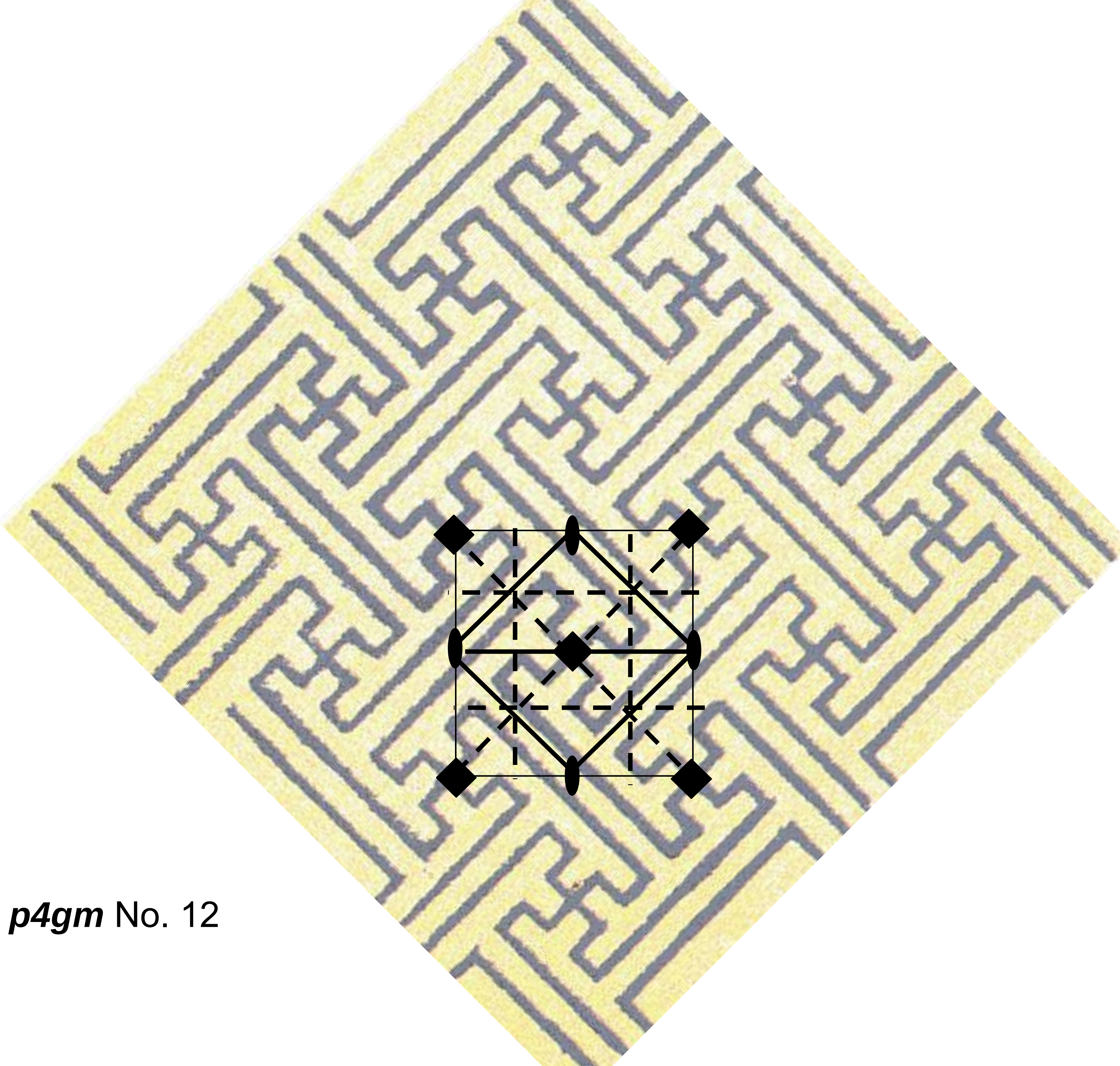


Geometrical construction for [t∘3]

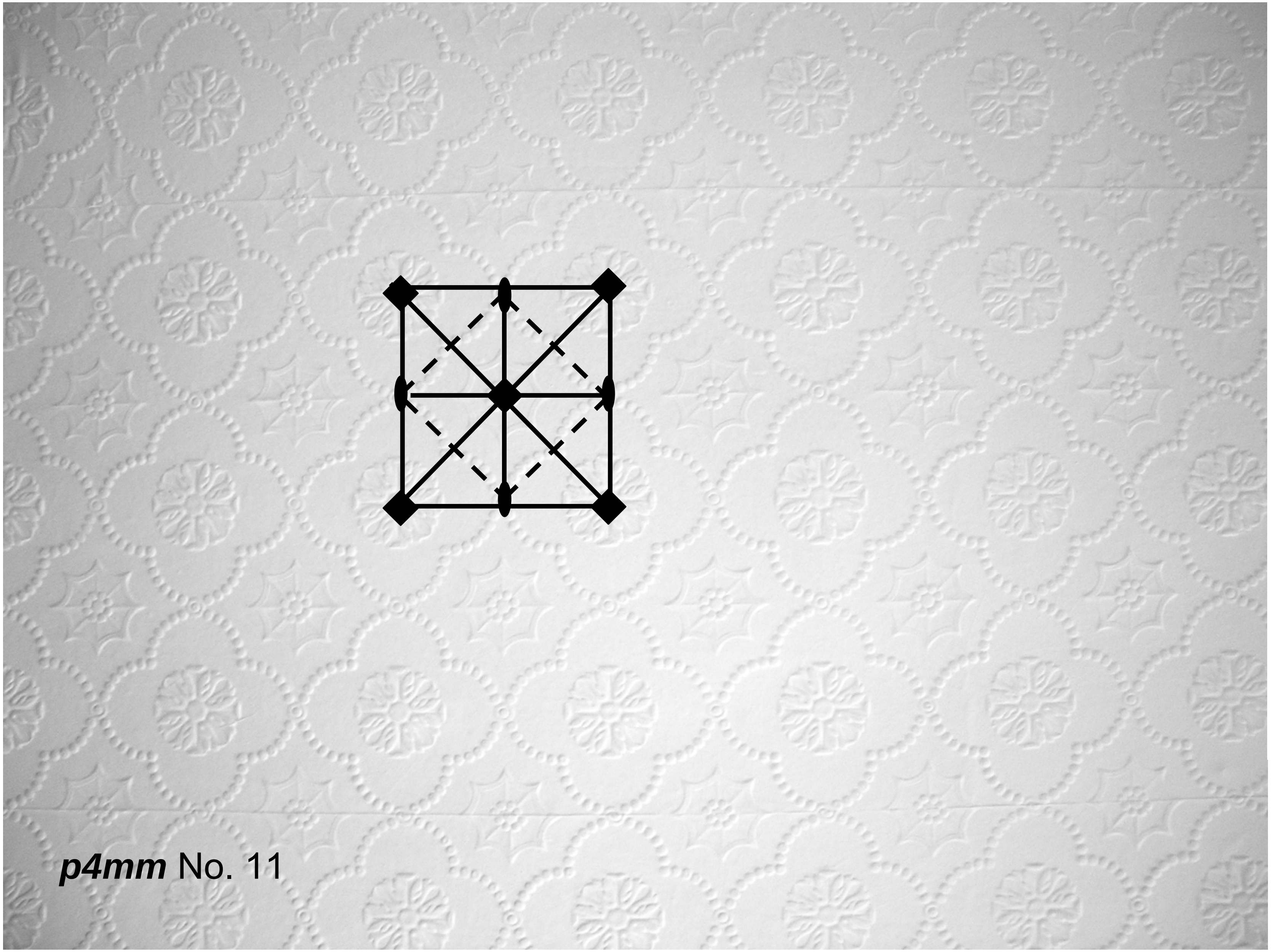


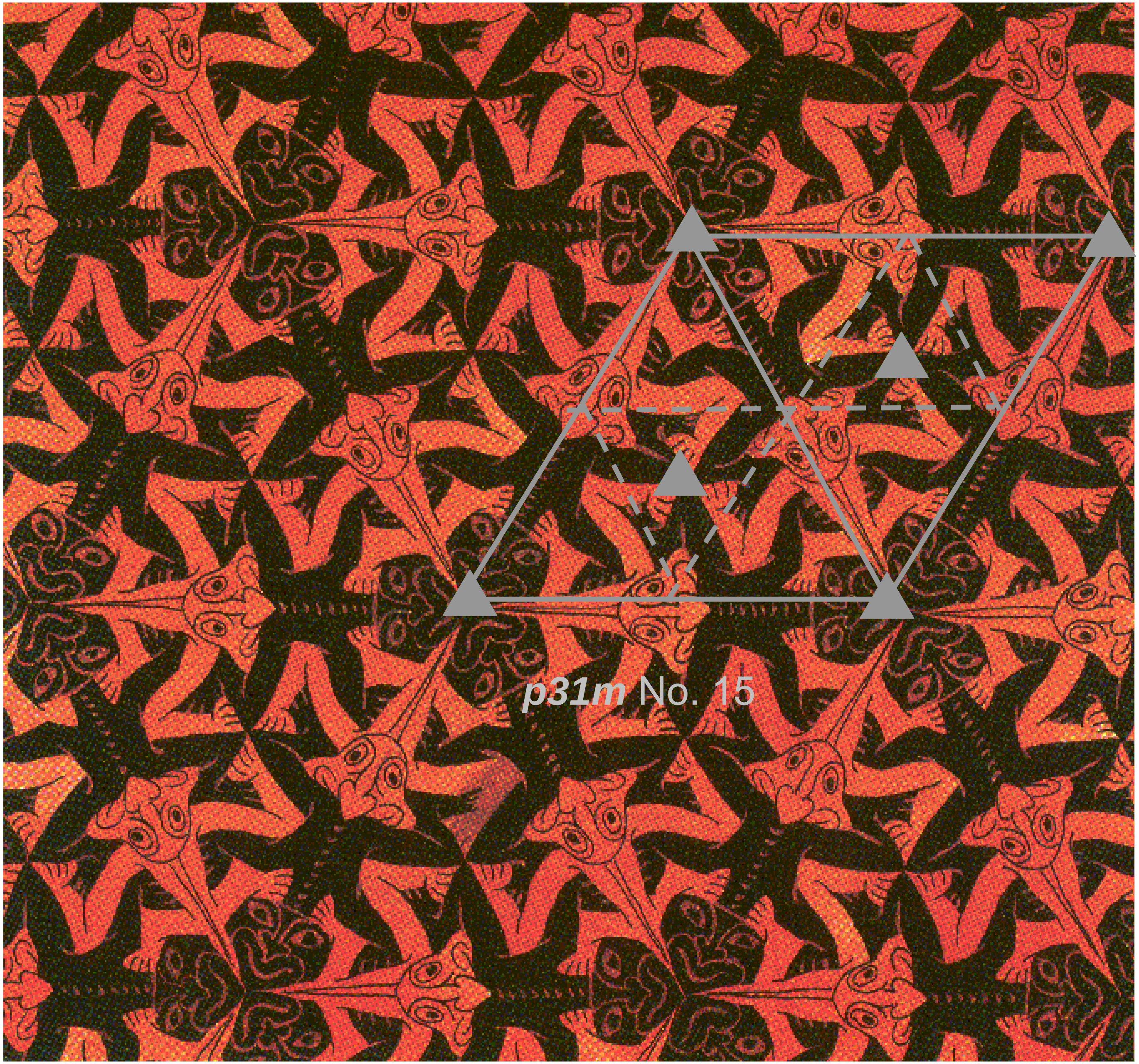



p6 No. 16



p4gm No. 12

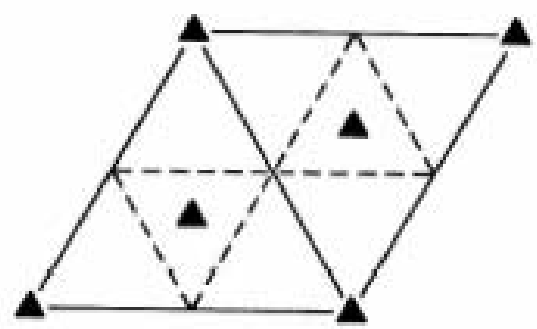

p4mm No. 11

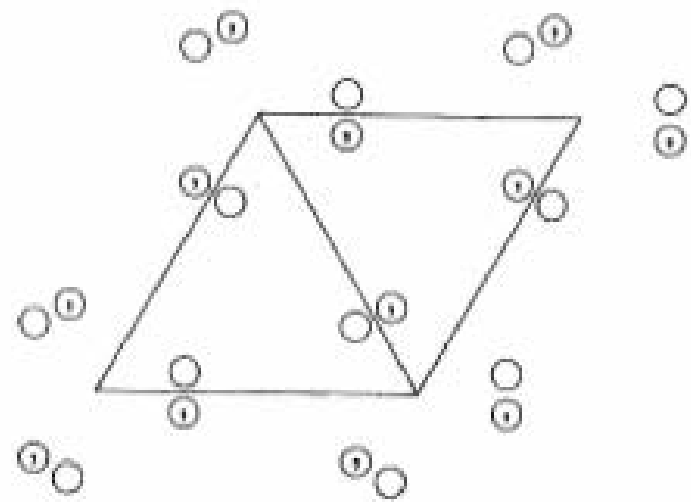

p31m No. 15

$p31m$ | $3m$ | Hexagonal

No. 15 | $p31m$

Patterson symmetry $p6mm$





Origin at $31m$

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

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

Symmetry operations

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

(4) m x,x (5) m $x,0$ (6) m $0,y$

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

Positions

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

Maximal non-isomorphic subgroups

I [2] $p311$ ($p3$, 13) 1; 2; 3
[3] $p11m$ (cm, 5) 1; 4
[3] $p11m$ (cm, 5) 1; 5
[3] $p11m$ (cm, 5) 1; 6

IIa none

IIb [3] $h31m$ ($\mathbf{a}' = 3\mathbf{a}, \mathbf{b}' = 3\mathbf{b}$) ($p3m1$, 14)

Maximal isomorphic subgroups of lowest index

IIc [4] $p31m$ ($\mathbf{a}' = 2\mathbf{a}, \mathbf{b}' = 2\mathbf{b}$) (15)

Minimal non-isomorphic supergroups

I [2] $p6mm$ (17)

II [3] $h31m$ ($p3m1$, 14)

Generic roto-translation

Cartesian Coordinates

$$\begin{bmatrix} x_2 \\ y_2 \\ z_2 \end{bmatrix} = \begin{bmatrix} t_x \\ t_y \\ t_z \end{bmatrix} + \boldsymbol{R} \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix} \tag{5.5}$$

Rotations around coordinate axes

Cartesian Coordinates

$$\boldsymbol{R}_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}$$

$$\boldsymbol{R}_y = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}$$

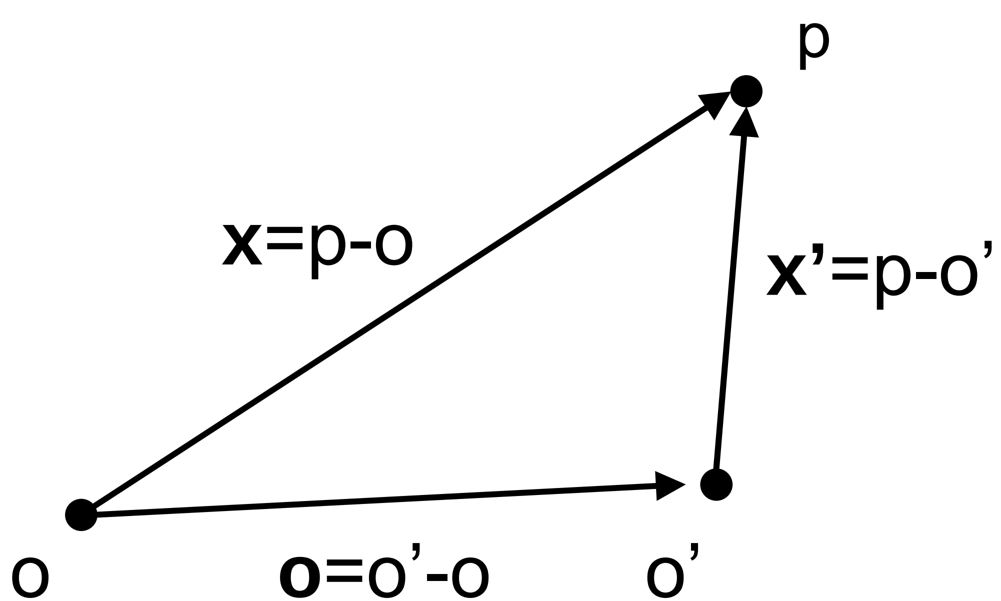
$$\boldsymbol{R}_z = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotations around generic axis

Cartesian Coordinates

$$\mathcal{M}(\hat{\mathbf{v}},\theta) = \begin{bmatrix} \cos\theta + (1-\cos\theta)x^2 & (1-\cos\theta)xy - (\sin\theta)z & (1-\cos\theta)xz + (\sin\theta)y \\ (1-\cos\theta)yx + (\sin\theta)z & \cos\theta + (1-\cos\theta)y^2 & (1-\cos\theta)yz - (\sin\theta)x \\ (1-\cos\theta)zx - (\sin\theta)y & (1-\cos\theta)zy + (\sin\theta)x & \cos\theta + (1-\cos\theta)z^2 \end{bmatrix} \tag{5.8}$$

Coordinate systems on an affine space



$\mathbf{x}' = \mathbf{x} - \mathbf{o}$

Basis vector transformations (*covariant*)

$$
\begin{aligned}
[\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3] &= [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3]\boldsymbol{P} \\
&= [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3] \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{bmatrix}
\end{aligned}
$$

Component transformations (*contravariant*)

$$
\begin{aligned}
\begin{bmatrix} v'^1 \\ v'^2 \\ v'^3 \end{bmatrix} &= \boldsymbol{Q} \begin{bmatrix} v^1 \\ v^2 \\ v^3 \end{bmatrix} \\
&= \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{bmatrix} \begin{bmatrix} v^1 \\ v^2 \\ v^3 \end{bmatrix}
\end{aligned}
$$

$$\mathbf{v} = \mathbf{a}_i v^i = \mathbf{a}'_j v'^j = \mathbf{a}_i P^i_j Q^j_k v^k \tag{5.18}$$

$$P^i_j Q^j_k = \delta^i_k \rightarrow \boldsymbol{Q} = \boldsymbol{P}^{-1} \tag{5.19}$$

Coordinate transformations

x'=x-o

$$x'^i = Q^i_j x^j - o'^i = Q^i_j (x^j - o^j)$$

$$x^i = (Q^{-1})^i_j (x'^j + o'^j) = (Q^{-1})^i_j x'^j + o^j$$

Dual basis

$$\mathbf{b}^i = 2\pi \mathbf{a}_k (G^{-1})^{ki} \qquad (5.34)$$

$$\mathbf{a}_i \cdot \mathbf{b}^j = \mathbf{a}_i \cdot \mathbf{a}_k (G^{-1})^{kj} = G_{ik} (G^{-1})^{kj} = 2\pi \delta_i^j$$

$$\mathbf{q} = q_i \mathbf{b}^i$$

$$\mathbf{q} \cdot \mathbf{v} = 2\pi q_i v^i$$

Dual basis in 3D

$$\begin{aligned}
\mathbf{b}_1 &= 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\
\mathbf{b}_2 &= 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\
\mathbf{b}_3 &= 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}
\end{aligned}$$

$$q_i = \frac{1}{2\pi} \mathbf{q} \cdot \mathbf{a}_i$$

Reciprocal Lattice

$$o + h_i \mathbf{b}^i;$$

$$h_i = h, k, l = \text{integers}$$

Reciprocal Lattice

Alternative definition

$$o + \mathbf{q}; \quad \text{such that}$$

$$\mathbf{q} \cdot \mathbf{v} = 2\pi n$$

For every symmetry translation vector **v**

$$q_i = \frac{1}{2\pi} \mathbf{q} \cdot \mathbf{a}_i \quad \Rightarrow \quad q_i \text{ are integers}$$

The reverse is not always true!

$$\mathbf{q} \cdot \mathbf{v} = 2\pi q_i v^i$$

is an integral multiple of 2π *only* if all the v^i *are* integers, which is not the case for *conventional centred bases.*

Primitive RL

$$o + h_i \mathbf{b}^i;$$

$$h_i = h, k, l = \text{integers}$$

Where $\mathbf{b}^i$ is a *dual primitive basis.*

$$o + \mathbf{q}; \quad \text{such that}$$

$$\mathbf{q} \cdot \mathbf{v} = 2\pi n$$

Conventional *RL*

Will have "extra" **q** vectors for which.

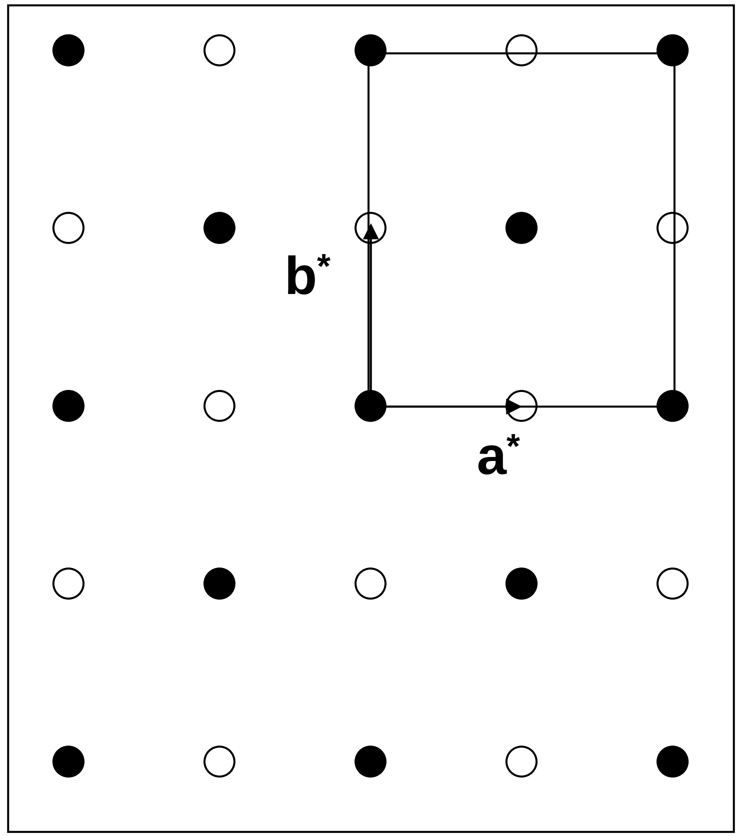
$$\mathbf{q} \cdot \mathbf{v}_c \neq 2\pi n$$

These **q** vectors are said to be extinct by centering. Conversely

$$\mathbf{q} \cdot \mathbf{v}_c = 2\pi n$$

is said to be a *reflection condition*.

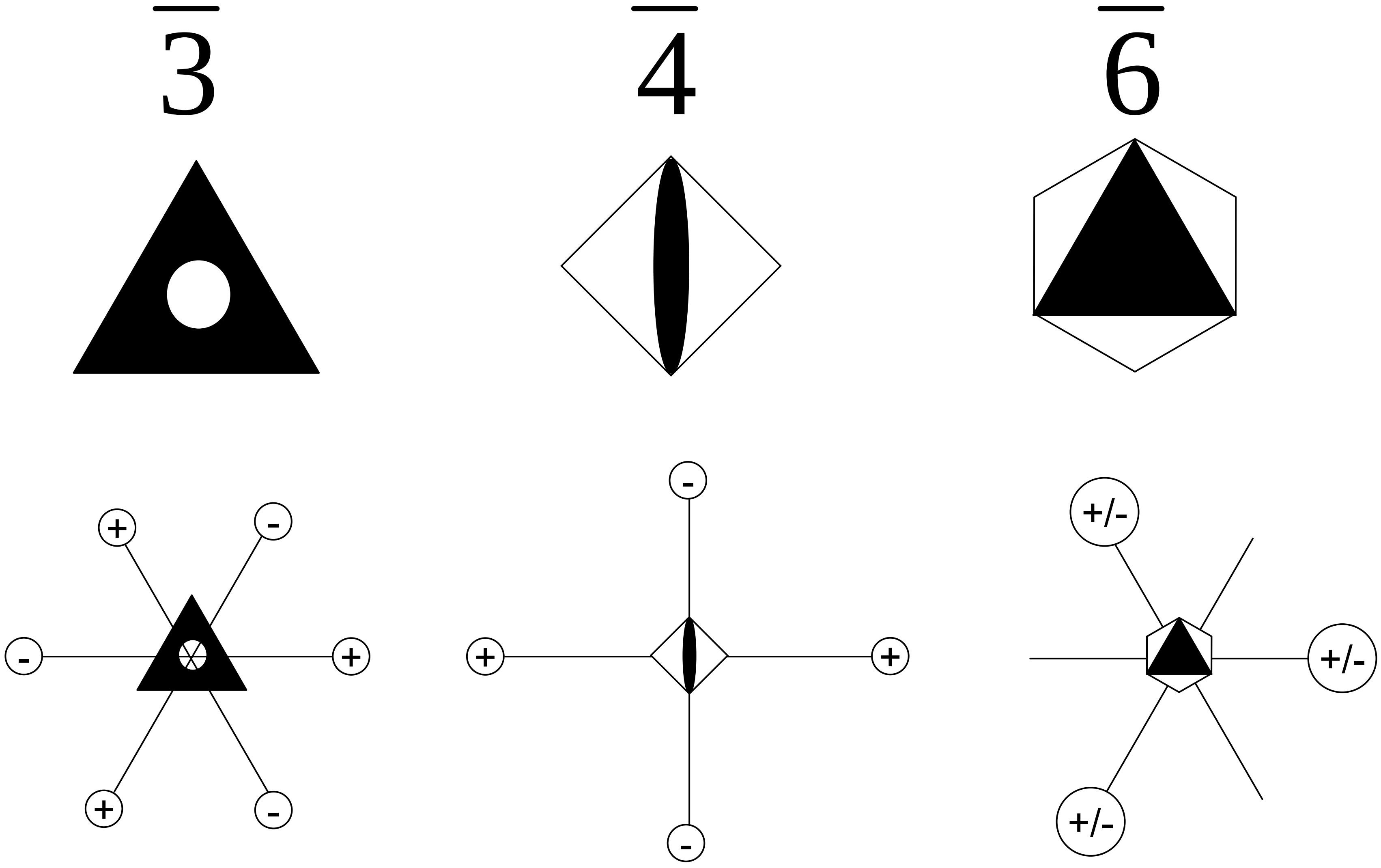
l even or odd



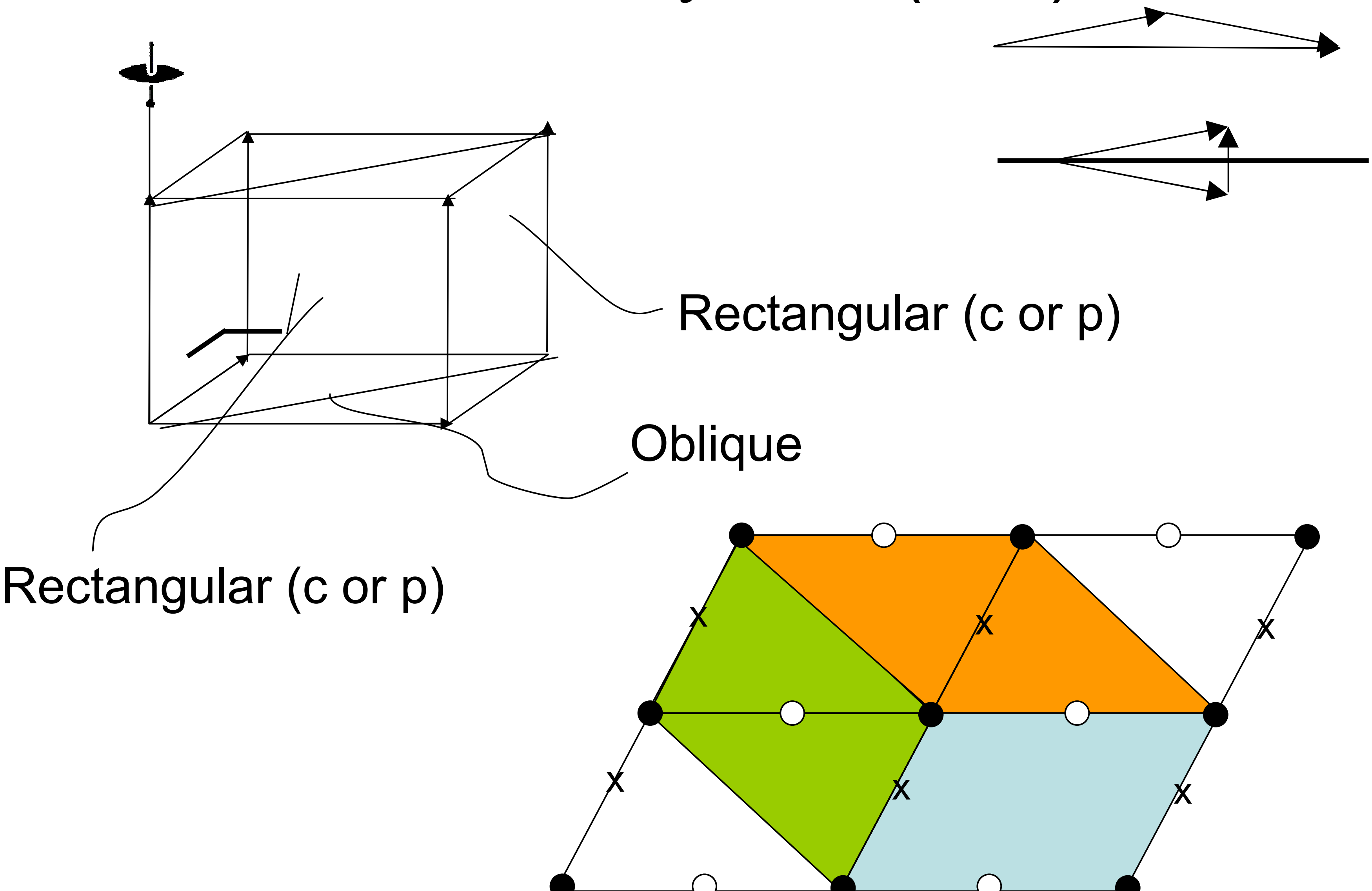
$$2\pi\frac{1}{2}(h+k)$$

“C” centered cell

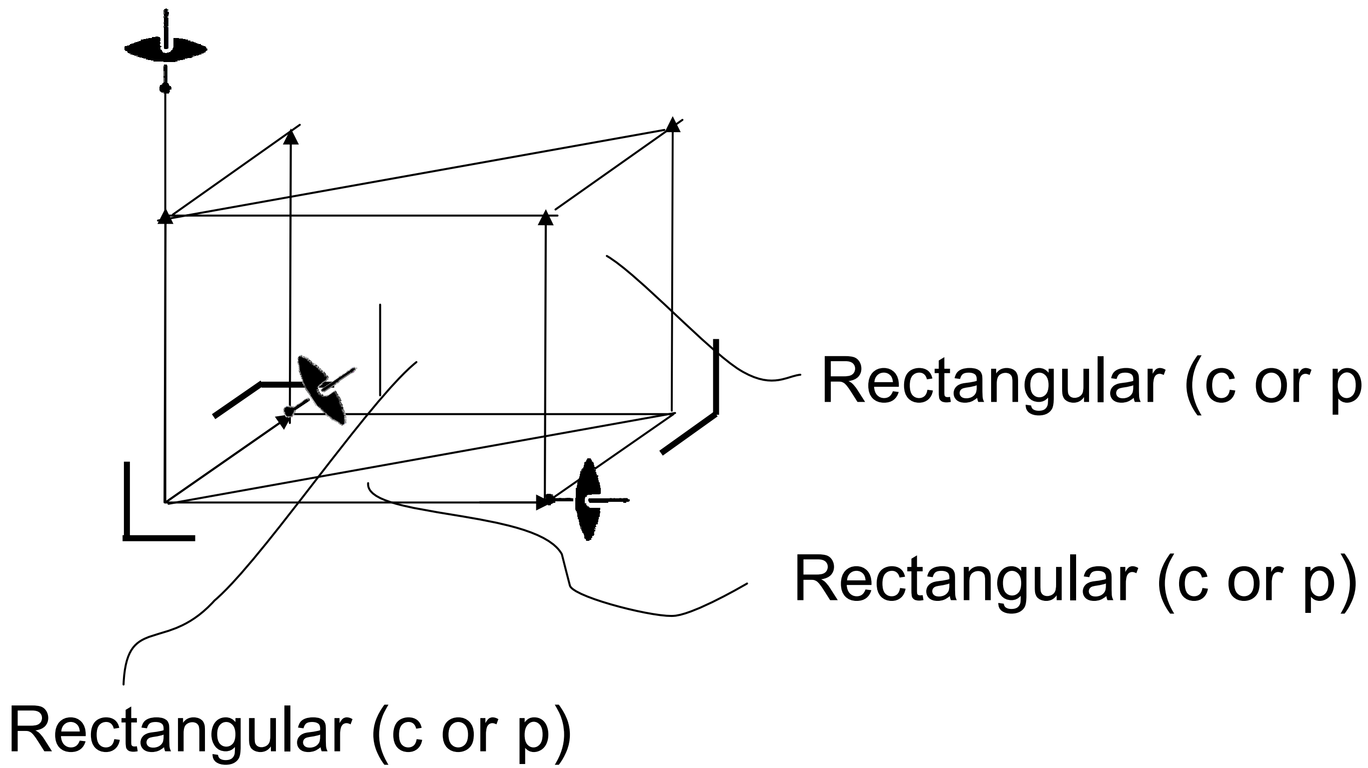
Roto-inversion operators



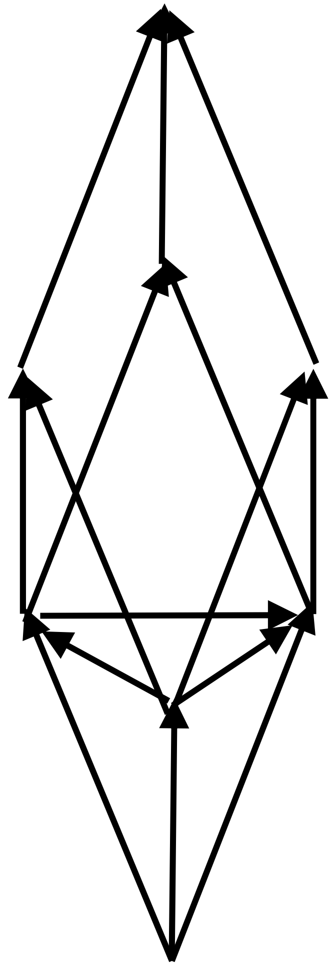
Monoclinic system (*2/m*)

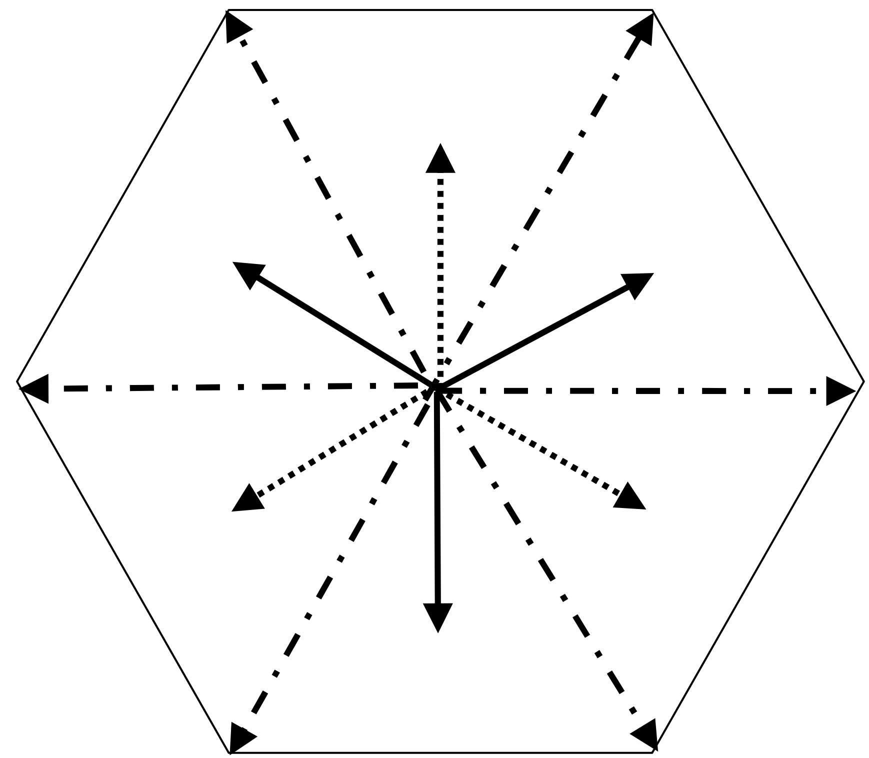


Orthorhombic system (*mmm*)

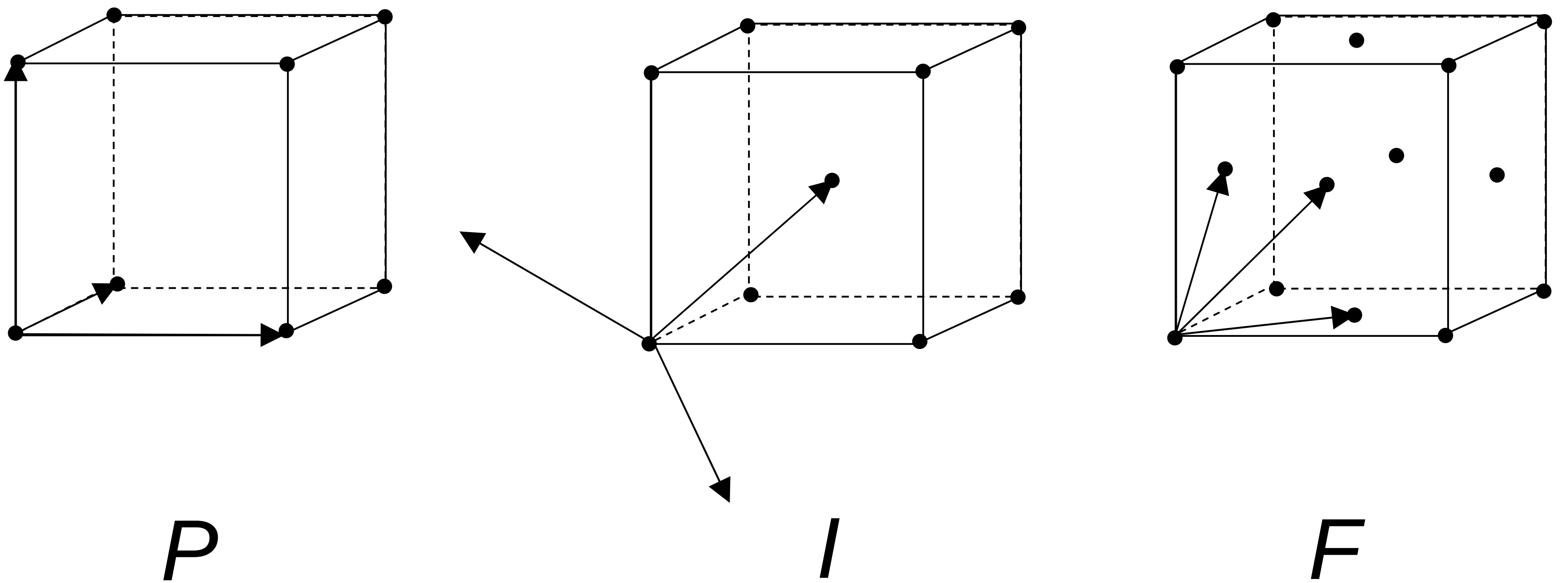


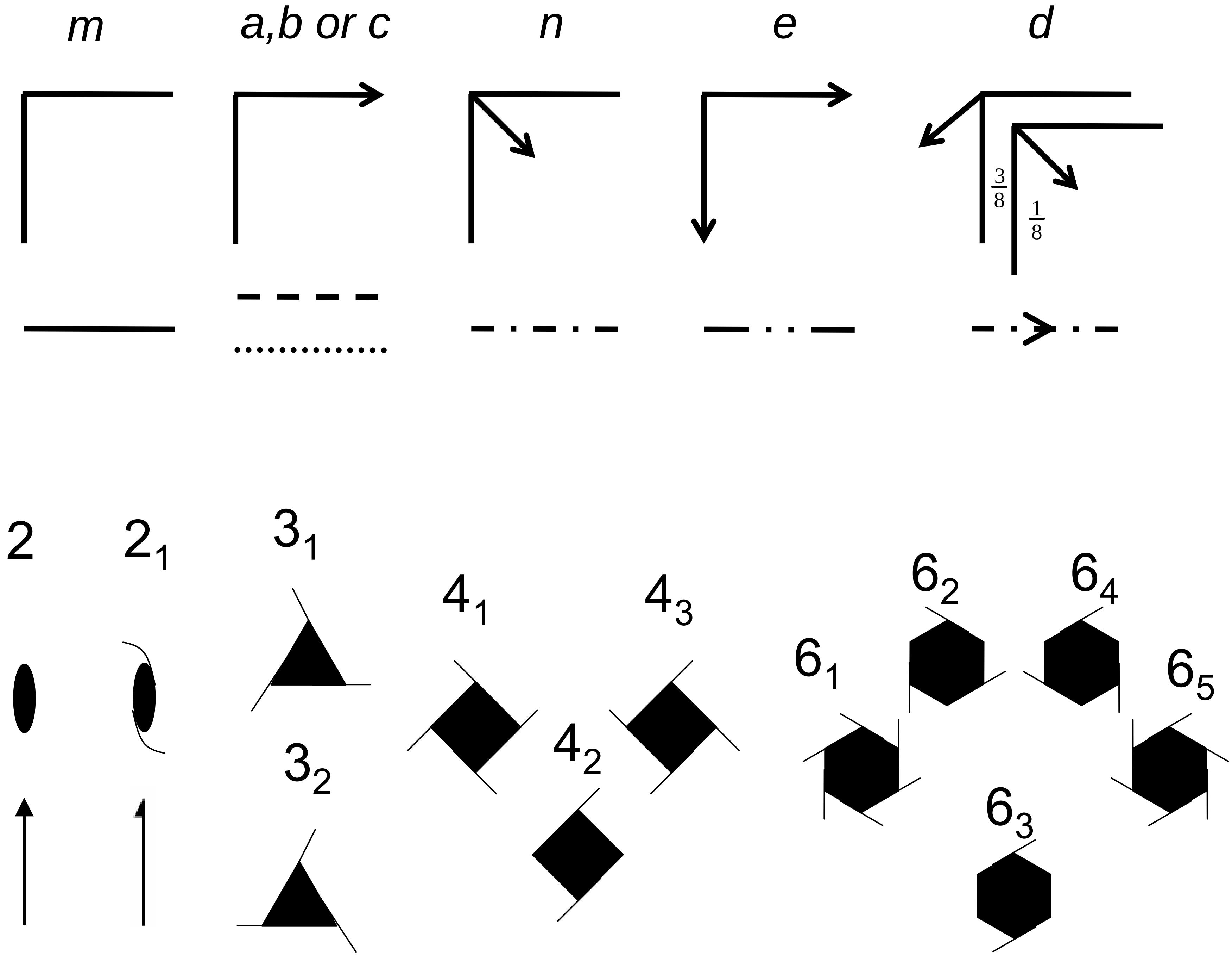
R- centered trigonal lattice





Cubic lattices




m
a,b or c
n
e
d
3/8
1/8
2
2₁
3₁
3₂
4₁
4₂
4₃
6₁
6₂
6₃
6₄
6₅