

# Symmetry

“A body is said to be symmetrical when it can be divided into parts that are related to each other in certain ways. The operation of transferring one part to the position of a symmetrically related part is termed a *symmetry operation*, the result of which is to leave the final state of the body indistinguishable from its original state. In general, successive application of the symmetry operation must ultimately bring the body actually into its original state again.”

From: Lipson/Cochran, *The Determination of Crystal Structures*

Lipson, H., and W. Cochran. *The Determination of Crystal Structures*. Ithaca, NY: Cornell University Press, 1966. ISBN: 080140276X.

# Symmetry Operations

In two dimensions there are (besides identity): **mirror**, rotation, and glide

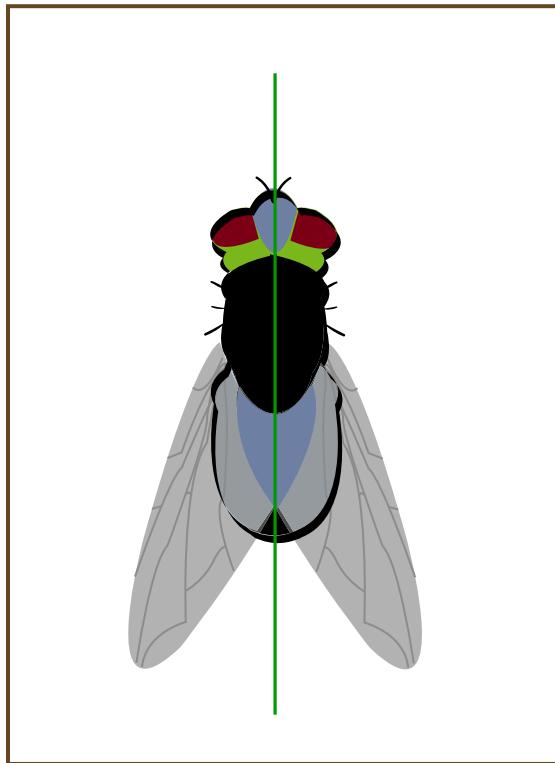


Figure by MIT OpenCourseWare.

The symbol for the mirror is a solid line.

# Symmetry Operations

In two dimensions there are (besides identity): mirror, **rotation**, and glide

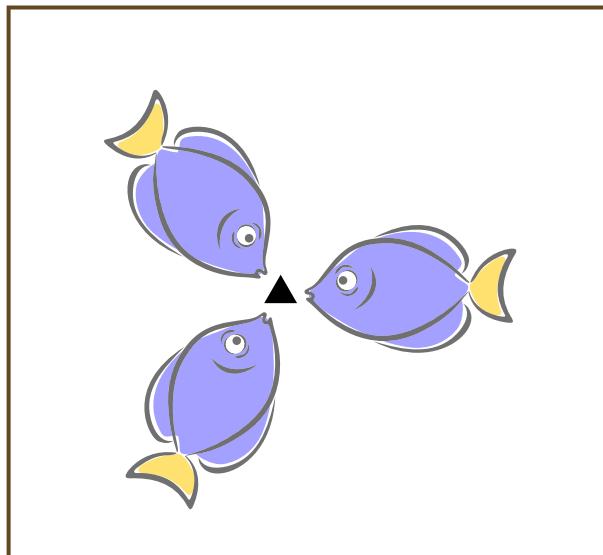


Figure by MIT OpenCourseWare.

The symbol for the threefold is a triangle: ▲ (120° rotation)

Twofold: ●  
180° rotation

Fourfold: ◆  
90° rotation

Sixfold: ◆◆  
60° rotation

# Symmetry Operations

In two dimensions there are (besides identity): mirror, rotation, and **glide**

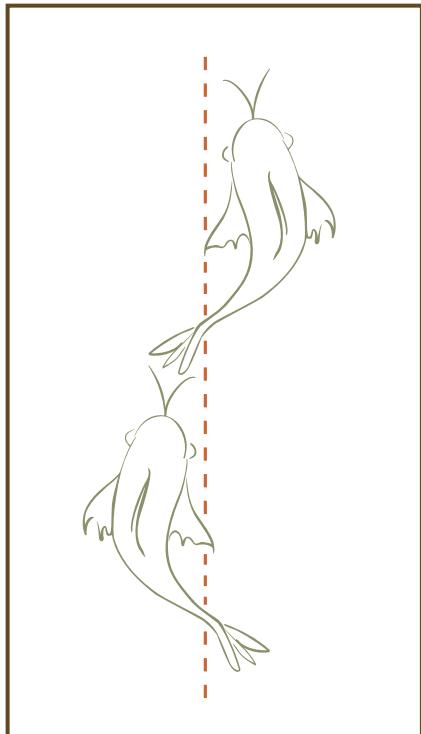


Figure by MIT OpenCourseWare.

The symbol for the glide is a dashed line.

## Symmetry plus Translation

“In a two-dimensional design, such as that of a wall-paper, a unit of pattern is repeated at regular intervals. Let us chose some representative point in the unit of pattern, and mark the position of similar points in all the other units. If these points be considered alone, the pattern being for the moment disregarded, it will be seen that they form a regular network. By drawing lines through them, the area can be divided into a series of cells each of which contains a unit of the pattern. It is immaterial which point of the design is chosen as representative, for a similar network of points will always be obtained.”

Bragg, Sir Lawrence, et al. *The Crystalline State, Volumes I-IV*. Ithaca, NY: Cornell University Press, 1965.

# Symmetry plus Translation

Removed due to copyright restrictions.

Please see:

Schattschneider, Doris. *Visions of Symmetry: Notebooks, Periodic Drawings, and Related Work of M. C. Escher*. New York, NY: W. H. Freeman & Co., 1999, pp. 297. ISBN: 0716721260.

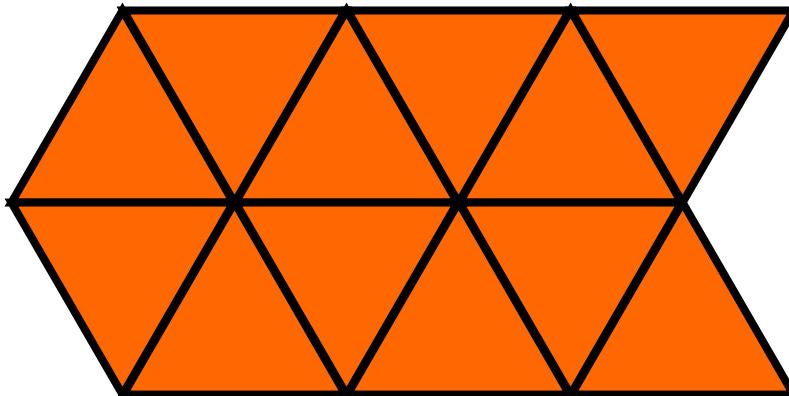
Escher No. 47 [Two Birds].

# Symmetry Operations

Some symmetry operations are compatible with translation, some are not.

Compatible are:

- mirror
- glide
- twofold rotation
- threefold rotation
- fourfold rotation
- sixfold rotation

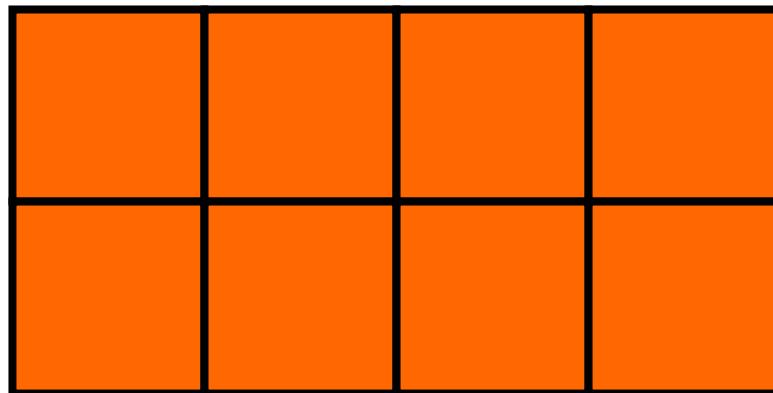


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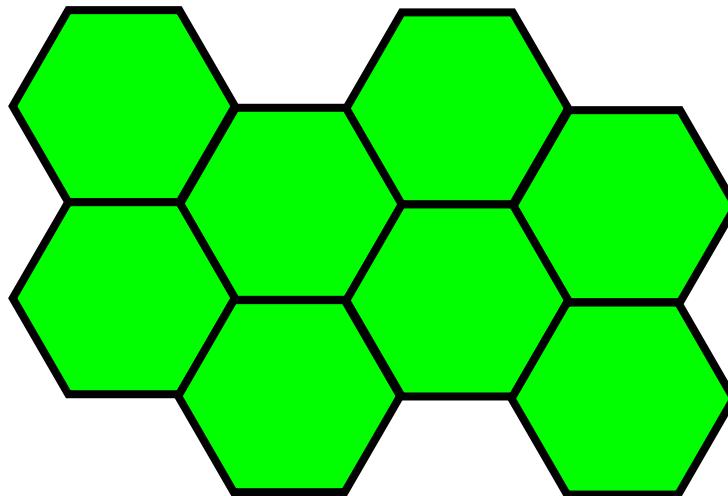


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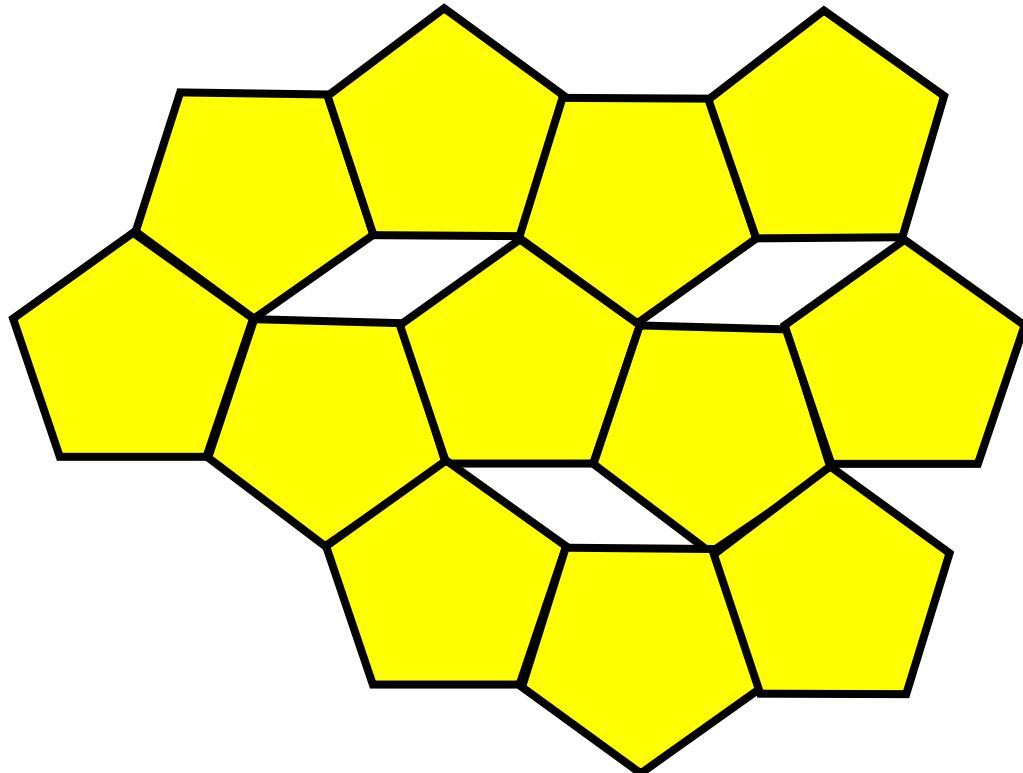


# Symmetry Operations

Some symmetry operations are compatible with translation, some are not.

Compatible are:

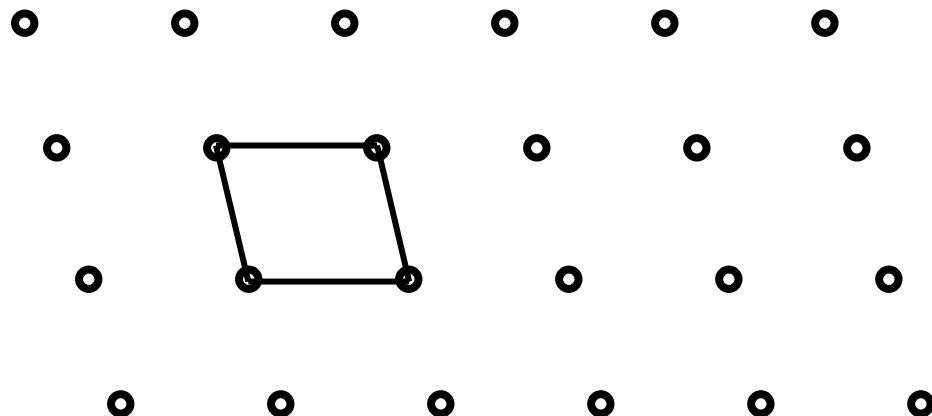
- mirror
- glide
- twofold rotation
- threefold rotation
- fourfold rotation
- sixfold rotation



# Combining Symmetry Operations

There are 17 possible combinations of the symmetry elements mentioned plus periodic translation: the 17 plane groups.

We have five different lattice types: **oblique** (parallelogram) ( $a \neq b, \neq 90^\circ$ )

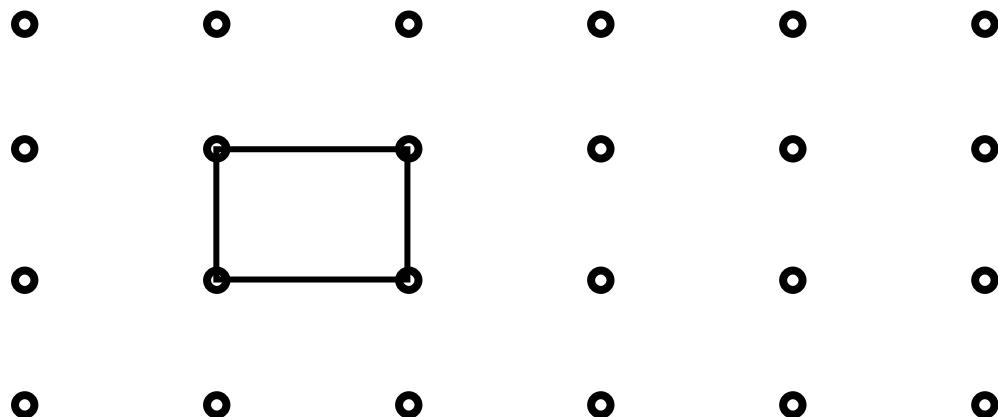


Plane groups:  $p1$  and  $p2$

# Combining Symmetry Operations

There are 17 possible combinations of the symmetry elements mentioned plus periodic translation: the 17 plane groups.

We have five different lattice types: **rectangular** ( $a \neq b$ ,  $90^\circ$ )

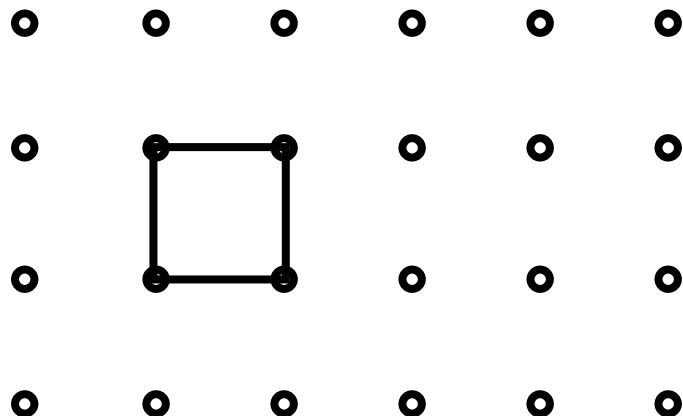


Plane groups: *pm*, *pg*, *p2mg*, *p2mm* and *p2gg*

# Combining Symmetry Operations

There are 17 possible combinations of the symmetry elements mentioned plus periodic translation: the 17 plane groups.

We have five different lattice types: **square** ( $a = b$ ,  $90^\circ$ )

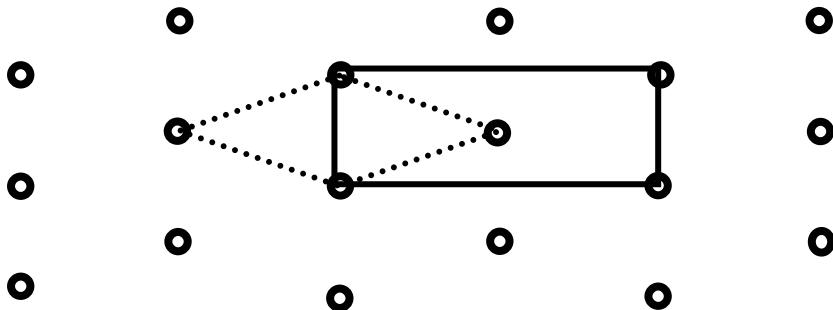


Plane groups:  $p4$ ,  $p4mm$  and  $p4gm$

# Combining Symmetry Operations

There are 17 possible combinations of the symmetry elements mentioned plus periodic translation: the 17 plane groups.

We have five different lattice types: **centered rectangular** ( $a = b$ ,  $90^\circ$ )

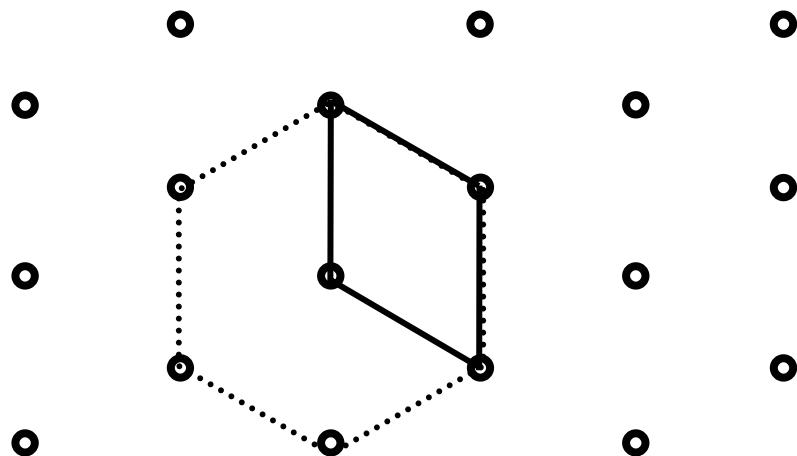


Plane groups: cm and c2mm

# Combining Symmetry Operations

There are 17 possible combinations of the symmetry elements mentioned plus periodic translation: the 17 plane groups.

We have five different lattice types: and **rhombic** or hexagonal ( $a = b$ ,  $120^\circ$ )



Plane groups:  $p3$ ,  $p31m$ ,  $p3m1$ ,  $p6$  and  $p6mm$

# Finding the Plane Group

Removed due to copyright restrictions.

Please see:

Schattschneider, Doris. *Visions of Symmetry: Notebooks, Periodic Drawings, and Related Work of M. C. Escher*. New York, NY: W. H. Freeman & Co., 1999, pp. 297. ISBN: 0716721260.

Escher No. 47 [Two Birds].

No symmetry besides translation: The lattice type is **oblique**, plane group ***p1***. Each unit mesh (unit cell) contains 1 white bird and 1 blue bird.

# Finding the Plane Group

Removed due to copyright restrictions.

Please see:

Schattschneider, Doris. *Visions of Symmetry: Notebooks, Periodic Drawings, and Related Work of M. C. Escher*. New York, NY: W. H. Freeman & Co., 1999, pp. 185. ISBN: 0716721260.

86. System  $VIII^0$  and  $IX^0$ .

## Going 3D

In three dimensions we have additional symmetry operators: inversion centers and screw axes. In addition, the mirror becomes a mirror plane, and the glides become glide planes.

The inversion center can be understood as the intersection of a mirror and a twofold axis.

Screw axes are like spiral staircases. The rotation is combined with a translation in a defined crystallographic direction by a defined step (half a unit cell for twofold screw axes, a third of a unit cell for threefold screw axes, etc.

# Going 3D

## Symbols for symmetry elements in three dimensions:

\* in plane  
perpendicular  
to plane

Removed due to copyright restrictions.

Please see:

Massa, Werner. *Crystal Structure Determination*. 2nd ed. Translated into English by R. O. Gould. New York, NY: Springer, 2004, pp. 51. ISBN: 3540206442.

Table 6.2

# Screw Axes on a Left Hand (For Biologists)

Removed due to copyright restrictions.

Please see:

Glusker, Jenny Pickworth, and Kenneth N. Trueblood. *Crystal Structure Analysis: A Primer*. 2nd ed. New York, NY: Oxford University Press, 1985, pp. 93-95. ISBN: 0195035437.

Fig. 7.1

# And Now: The Version For Chemists

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Please see:

Massa, Werner. *Crystal Structure Determination*. 2nd ed. Translated into English by R. O. Gould. New York, NY: Springer, 2004, pp. 49-50. ISBN: 3540206442.

Fig. 6.8

# Metric Symmetry of the Crystal Lattice

The metric symmetry is the symmetry of the crystal lattice without taking into account the arrangement of the atoms in the unit cell. In reciprocal space, this is equivalent to looking at the **positions** of the reflections without taking into account their relative **intensities**.

There are 7 so called **crystal systems** (triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal, and cubic). The rhombohedral system can be understood as a special case of the trigonal system, but some crystallographer count it as a separate crystal system.

Taking into account possible lattice centerings, there are 14 so called **Bravais lattices**.

# The 14 Bravais Lattices

Triclinic:

$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$

Lattice: P

Monoclinic:

$a \neq b \neq c, \alpha = \gamma = 90^\circ \neq \beta$

Lattice: P, C

Orthorhombic:

$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$

Lattice: P, C, I, F

Tetragonal:

$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$

Lattice: P, I

Trigonal/Hexagonal:

$a = b \neq c, \alpha = 90^\circ, \gamma = 120^\circ$

Lattice: P, R

Cubic:

$a = b = c, \alpha = \beta = \gamma = 90^\circ$

Lattice: P, I, F

## Laue Symmetry

The **Laue symmetry** is the symmetry in reciprocal space (taking into account the reflex intensities). Friedel's law is assumed to be true.

The Laue symmetry can be lower than the highest metric symmetry (e.g. monoclinic with  $\beta = 90^\circ$ ), but never higher.

# Laue Symmetry

Crystal System	Laue Group	Point Group
Triclinic	-1	1, -1
Monoclinic	2/m	2, m, 2/m
Orthorhombic	mmm	222, mm2, mmm
Tetragonal	4/m	4, -4, 4/m
	4/mmm	422, 4mm, -42m, 4/mmm
Trigonal/ Rhombohedral	-3	3, -3
	-3/m	32, 3m, -3m
Hexagonal	6/m	6, -6, 6/m
	6/mmm	622, 6mm, -6m2, 6/mmm
Cubic	m3	23, m3
	m3m	432, -43m, m3m

# Space Groups

Instead of 17 in two dimensions, in 3D there are 230 different ways of combining symmetry elements with translation and lattice centering: the 230 space groups.

# Space Group No 10

Removed due to copyright restrictions.

Please see:

Hahn, Theo, ed. *International Tables for Crystallography, Volume A: Space-Group Symmetry*. 2nd revised ed. Dordrecht, Holland: D. Reidel Publishing Company, 1987.

# Space Group No 14

Removed due to copyright restrictions.

Please see:

Hahn, Theo, ed. *International Tables for Crystallography, Volume A: Space-Group Symmetry*. 2nd revised ed.

# Space Group No 230

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Please see:

Hahn, Theo, ed. *International Tables for Crystallography, Volume A: Space-Group Symmetry*. 2nd revised ed.

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5.069 Crystal Structure Analysis  
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