Symmetry in the unit cell: 4-fold rotation

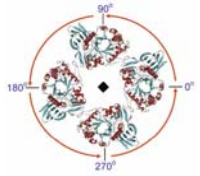


Figure 5-11 Rotation around a 4-fold rotation axis. The tetragonal unit cell is generated by rotation of the molecular motif around a 4-fold axis, depicted by the tetrad symbol (◆). Note that the 4-fold operation has generated a molecular assembly with a distinct solvent channel in the center in the direction of the 4-fold axis.

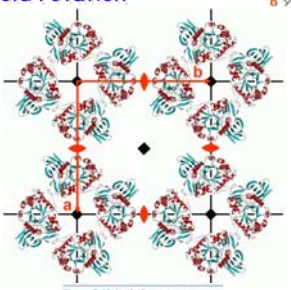


Figure 5-12 A p4 plane structure. Additional new 2-fold (◆) and 4-fold (◆) rotation axes are created by the unit cell translations. The structure has extensive solvent channels, quite typical for crystal structures with high order rotation axes.

The asymmetric unit suffices to reconstruct the unit cell

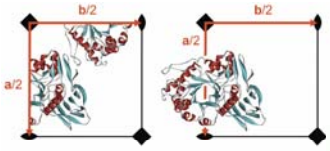
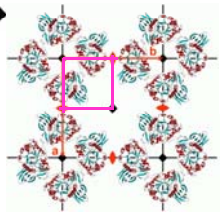


Figure 5-13 Asymmetric unit of the p4 structure. The asymmetric unit of p4 covers one fourth of the unit cell. The asymmetric unit to the left would be ideal for producing a tile (or in crystallographic computations of the unit cell contents), but the representation to the right is much better suited for displaying the molecule.
Biomolecular Crystallography B Rupp (2010)

The asymmetric unit contents together with the unit cell symmetry allows to reconstruct the entire unit cell (and the entire crystal structure).



Trigonal or hexagonal cell?

Figure 5-14 The hexagonal plane lattice. A hexagonal tile can be cut up into three equivalent rhombic pieces. Depending on the internal symmetry, the hexagonal lattice can form a hexagonal or trigonal unit cell.

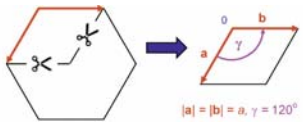
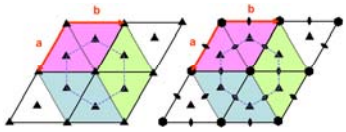


Figure 5-15 Trigonal and hexagonal plane system. A hexagon can be created from three trigonal or hexagonal unit cells, rotated by 120° and 240°, respectively (the three equivalent unit cells are indicated by the three colors). In a unit cell with hexagonal internal symmetry, additional 2-fold axes are created on the cell edges and in the center of the hexagonal unit cell. These relations are the same in 3-dimensional crystals, where the drawing is identical to a projection down the perpendicular third axis, **c**, pointing upward from the paper plane.



3- and 6-fold rotations

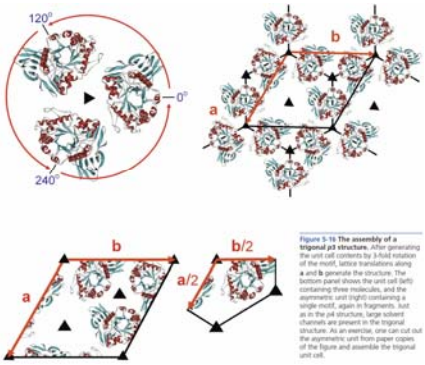


Figure 5-16 The assembly of a trigonal p3 structure. After generating the unit cell contents by 3-fold rotation of the motif, lattice translations along **a** and **b** generate the structure. The bottom panel shows the unit cell (left) containing three molecules, and the asymmetric unit (right) containing a single motif, again in fragments. Just as in the p4 structure, large solvent channels are present in the trigonal structure. As an exercise, one can cut out the asymmetric unit from paper copies of the figure and assemble the trigonal unit cell.

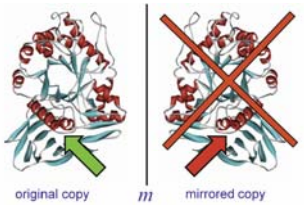
Only 5 chiral plane groups exist

Lattice properties	Minimum internal symmetry	Two-dimensional crystal system	Cell centering	Plane groups
$a \neq b$, $\gamma \neq 90°$	None	Oblique	*p*	***p1***, ***p2***
$a \neq b$, $\gamma = 90°$	2-fold rotation axis	Rectangular	*p*	*pm*, *pg*, *p2mm* *p2mg*, *p2gg*
			c	*cm*, *c2mm*
$a = b$, $\gamma = 90°$	4-fold rotation axis	Square	*p*	***p4***, *p4mm*, *p4gm*
$a = b$, $\gamma = 120°$	3-fold rotation axis	Trigonal	*p*	***p3***, *p3m1*, *p31m*
	6-fold rotation axis	Hexagonal	*p*	***p6***, *p6mm*

Table 5-1 The 17 plane groups. The groups listed in bold type are the only five plane groups allowed for asymmetric, chiral motifs. Note that whether a crystal system (hence unit cell) is trigonal or hexagonal depends on the internal symmetry (3-fold or 6-fold axis) of the crystal lattice and cannot be decided from the lattice dimensions or unit cell parameters alone. This is also true for the 3-dimensional case. Note that plane groups that contain mirror operations (m) or glide planes (g) are not possible for asymmetric motifs, because they change the handedness of the chiral motif. This limitation also holds in the 3-dimensional case.

Mirror operations change handedness

Figure 5-17 Mirror operations change the handedness of the motif. A mirror operation applied to a chiral structure produces a copy with opposite handedness and is thus not allowed. The change of handedness can be most easily seen by following the sense of direction of the helices pointed out by the colored arrows. The left, original molecule properly has right-handed α-helices, while the mirrored copy has left-handed helices (see also Figure 5-31).



As a rule, a symmetry operation must not change the motif (group closure requirement). This also holds for 3-d space, as we will show.