

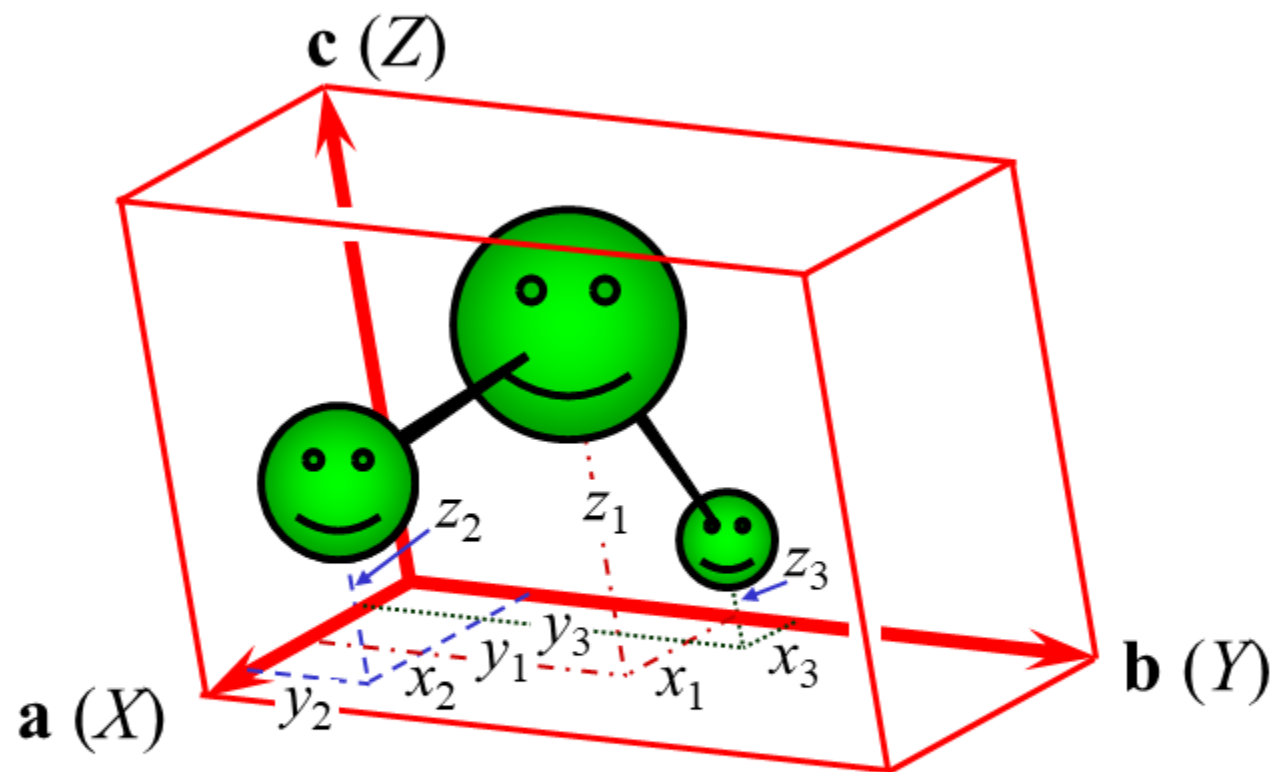
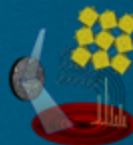


Figure 2.1. Illustration of the content of the unit cell. The coordinates of the center of gravity of each atom are given as triplets, i.e. x_1, y_1, z_1 ; x_2, y_2, z_2 and x_3, y_3, z_3 .

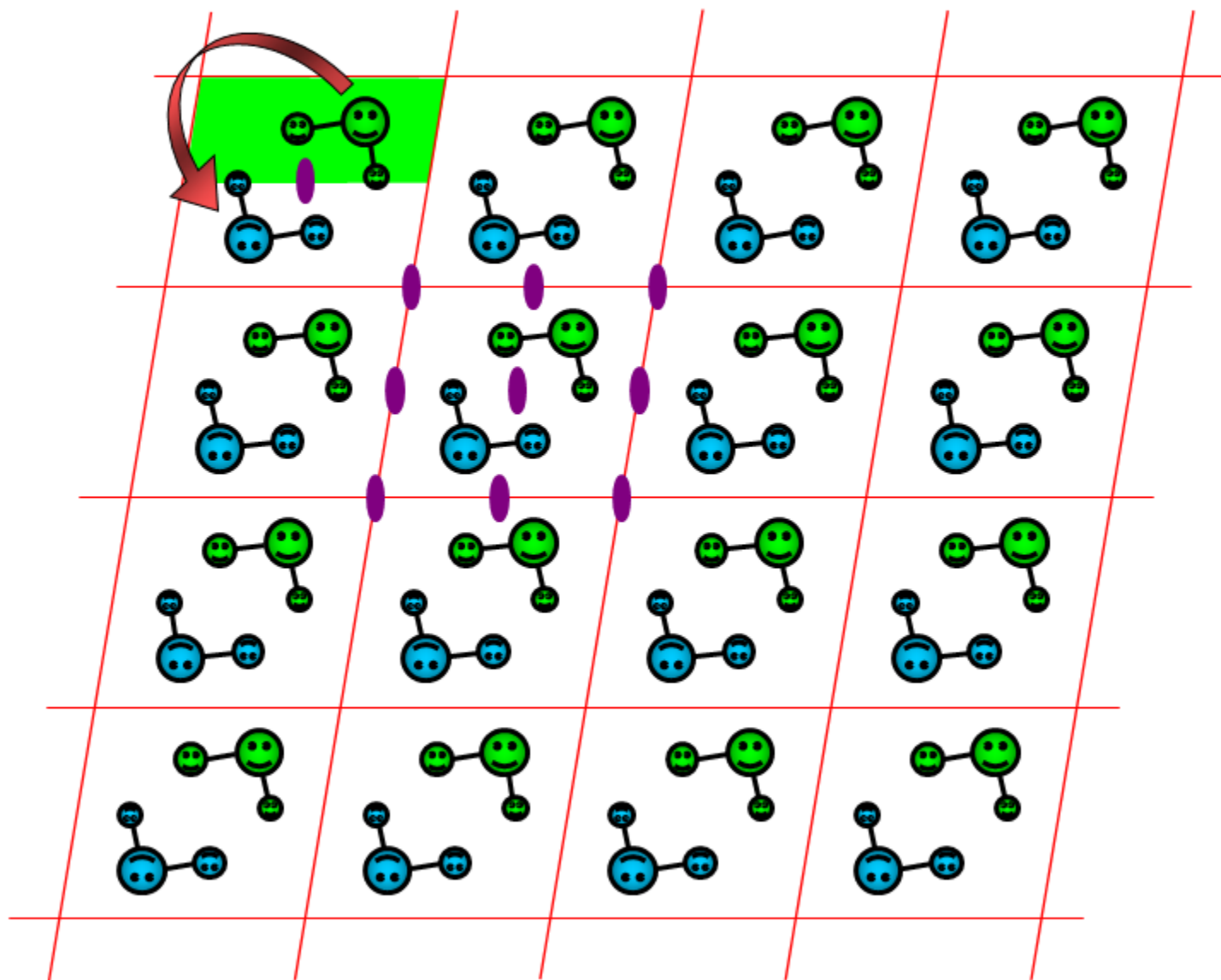
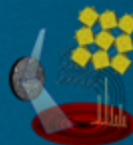


Figure 2.2. Asymmetric unit (*green parallelogram*) contains an independent molecule, which is green as well. *Blue* molecules are related to *green* molecules in each unit cell via rotation by 180° around the lines perpendicular to the plane of the projection at the center of each unit cell. The difference in color is used only to highlight symmetrical relationships since all molecules are indeed identical. All rotation axes intersecting every unit cell are shown in a neighboring cell.

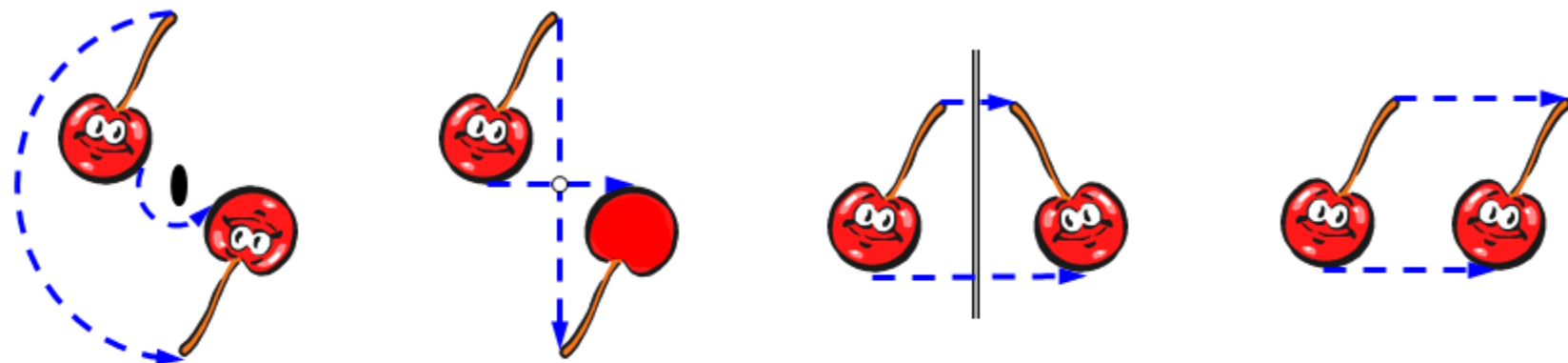
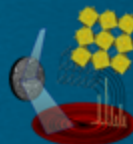


Figure 2.3. Simple symmetry operations. From *left to right*: rotation, inversion, reflection and translation.

Symmetry operation	Geometrical representation	Symmetry element
Rotation	Line (axis)	Rotation axis
Inversion	Point (center)	Center of inversion
Reflection	Plane	Mirror plane
Translation	Vector	Translation vector

Table 2.1. Simple symmetry operations and conforming symmetry elements.



Symmetry operation	Rotation	Inversion	Reflection	Translation
Rotation	-	Roto-inversion axis ^a	No ^b	Screw axis
Inversion	-	-	No ^b	No ^b
Reflection	-	-	-	Glide plane
Translation	-	-	-	-

Table 2.2. Derivation of complex symmetry elements.

Rotation angle, φ	Rotation axes		Roto-inversion axes	
	International symbol	Graphical symbol ^a	International symbol	Graphical symbol ^a
360°	1	none	$\bar{1}$	
180°	2		$\bar{2} = m^c$	
120°	3		$\bar{3} = 3 + \bar{1}$	
90°	4		$\bar{4}$	
60°	6		$\bar{6} = 3 + m \perp 3$	

Table 2.3. Symbols of finite crystallographic symmetry elements.

Eq. 2.1. $\varphi = \frac{360^\circ}{N}$

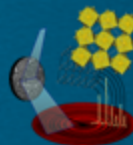


Figure 2.4. From *left to right*: horizontal twofold rotation axis (*top*) and its alternative symbol (*bottom*), diagonal threefold inversion axis inclined to the plane of the projection, horizontal fourfold rotation axis, and horizontal and diagonal mirror planes. *Horizontal* or *vertical lines* are commonly used to indicate axes located in the plane of the projection, and *diagonal lines* are used to indicate axes, which form an angle other than the right angle or zero with the plane of the projection.

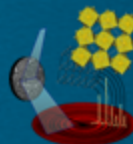


Figure 2.5. Trigonal pyramid with its apex up (*left*) and down (*right*) relative to the plane of the paper. Different shades of blue are used to emphasize enantiomorphous objects.

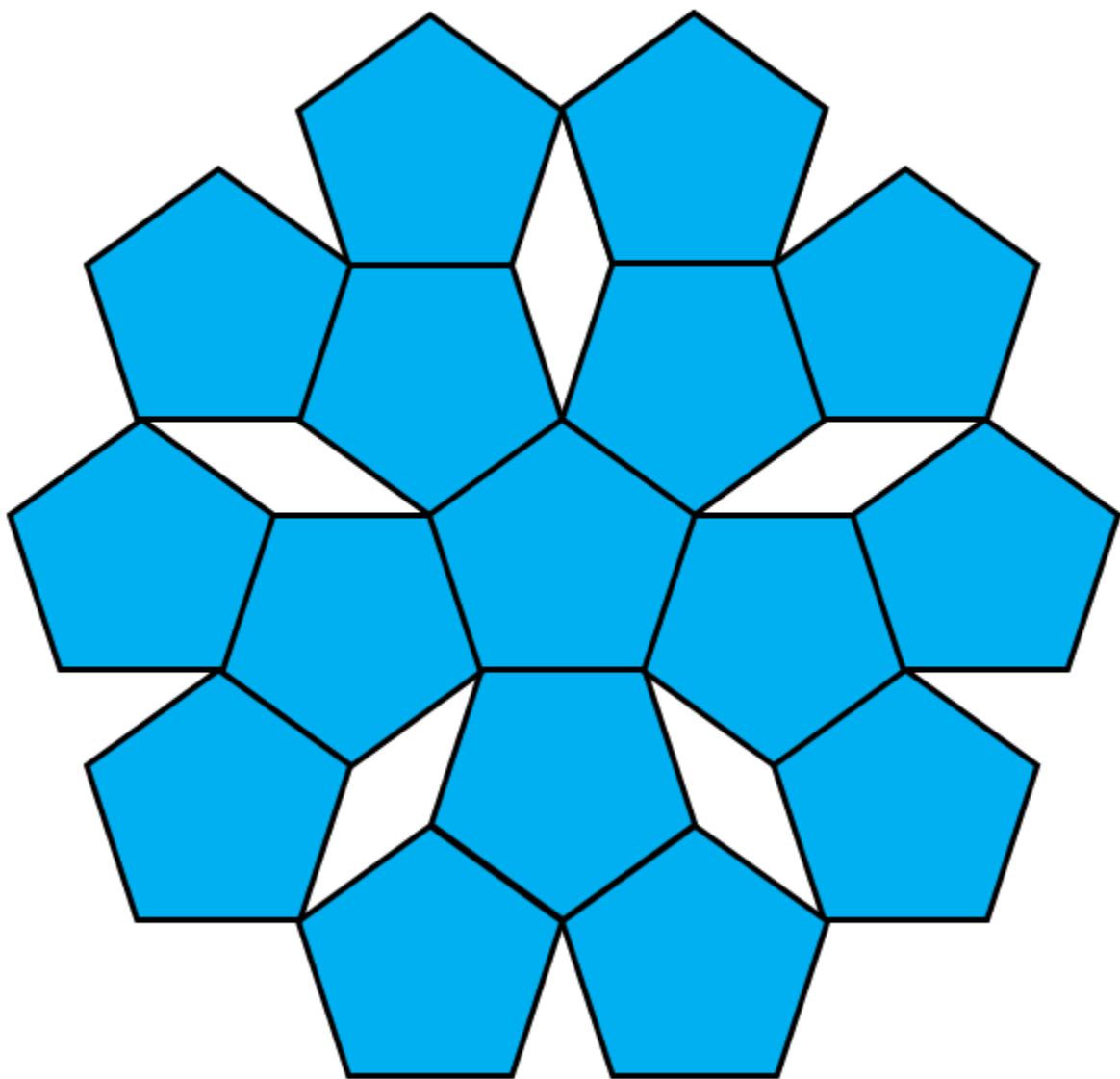
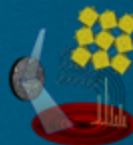


Figure 2.6. Filling the area with *blue pentagons*. *White parallelograms* represent voids in the two-dimensional pattern of pentagons.

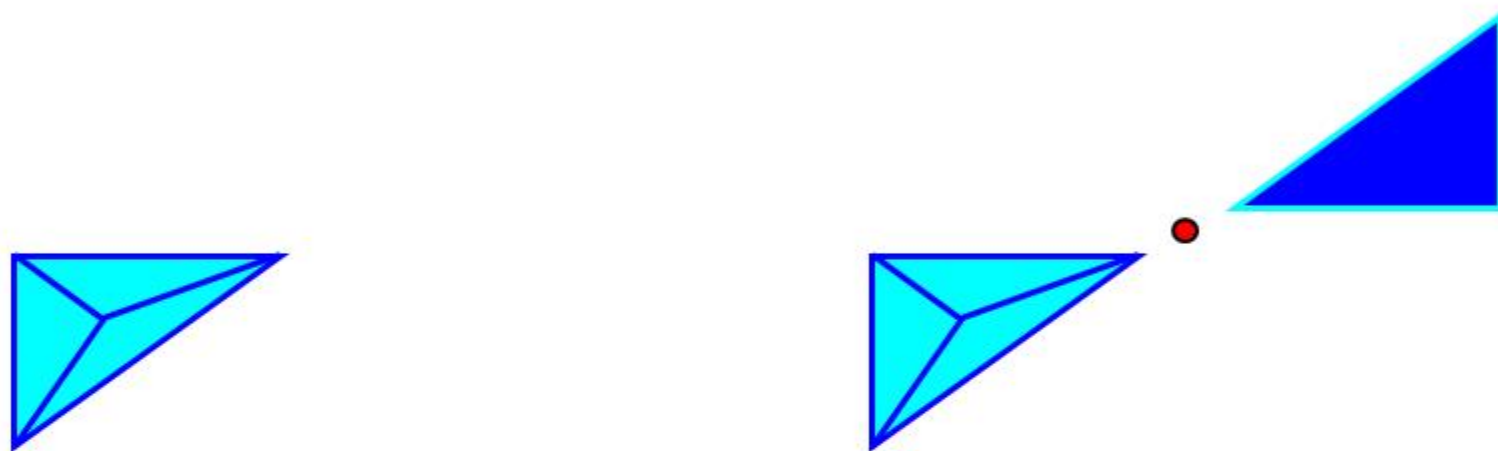


Figure 2.7. Onefold rotation axis (*left*, unmarked since it can be located anywhere) and center of inversion (*right*).

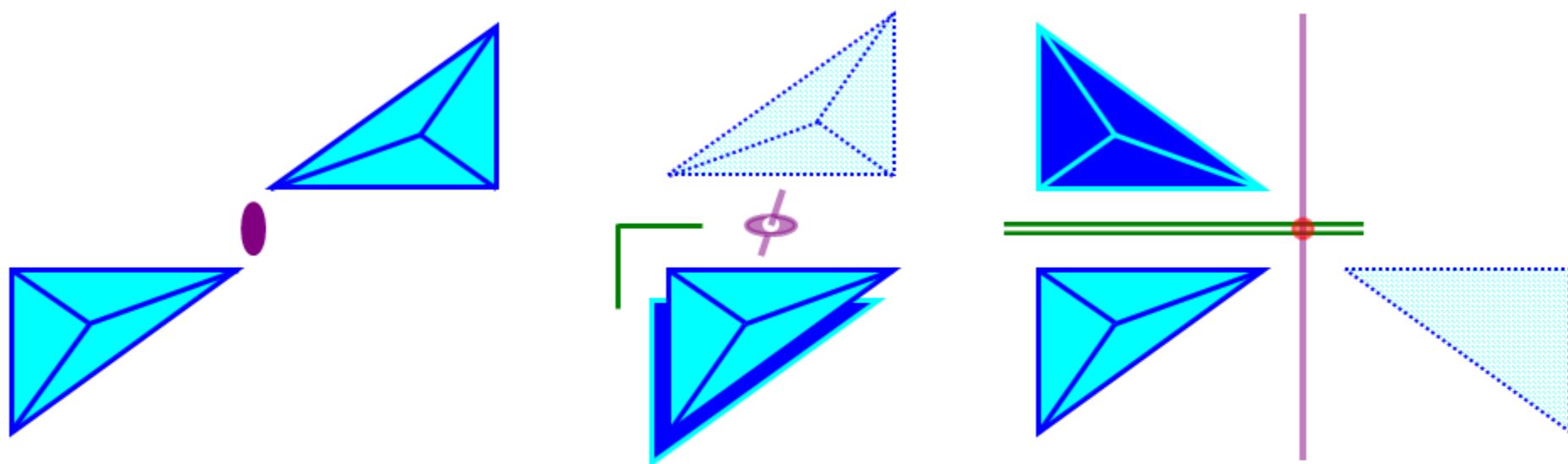
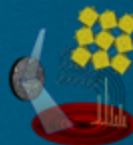


Figure 2.8. Two-fold rotation axis perpendicular to the plane of the projection (*left*), and mirror planes (*middle* and *right*). In the middle – the mirror plane nearly coincides with the plane of the projection (the equivalent twofold inversion axis is tilted by a few degrees away from the vertical) for clarity. On the right – the mirror plane is perpendicular to the plane of the projection. Also shown in the middle and on the right is how the twofold inversion axis, which is perpendicular to the mirror plane, yields the same result as the mirror plane.

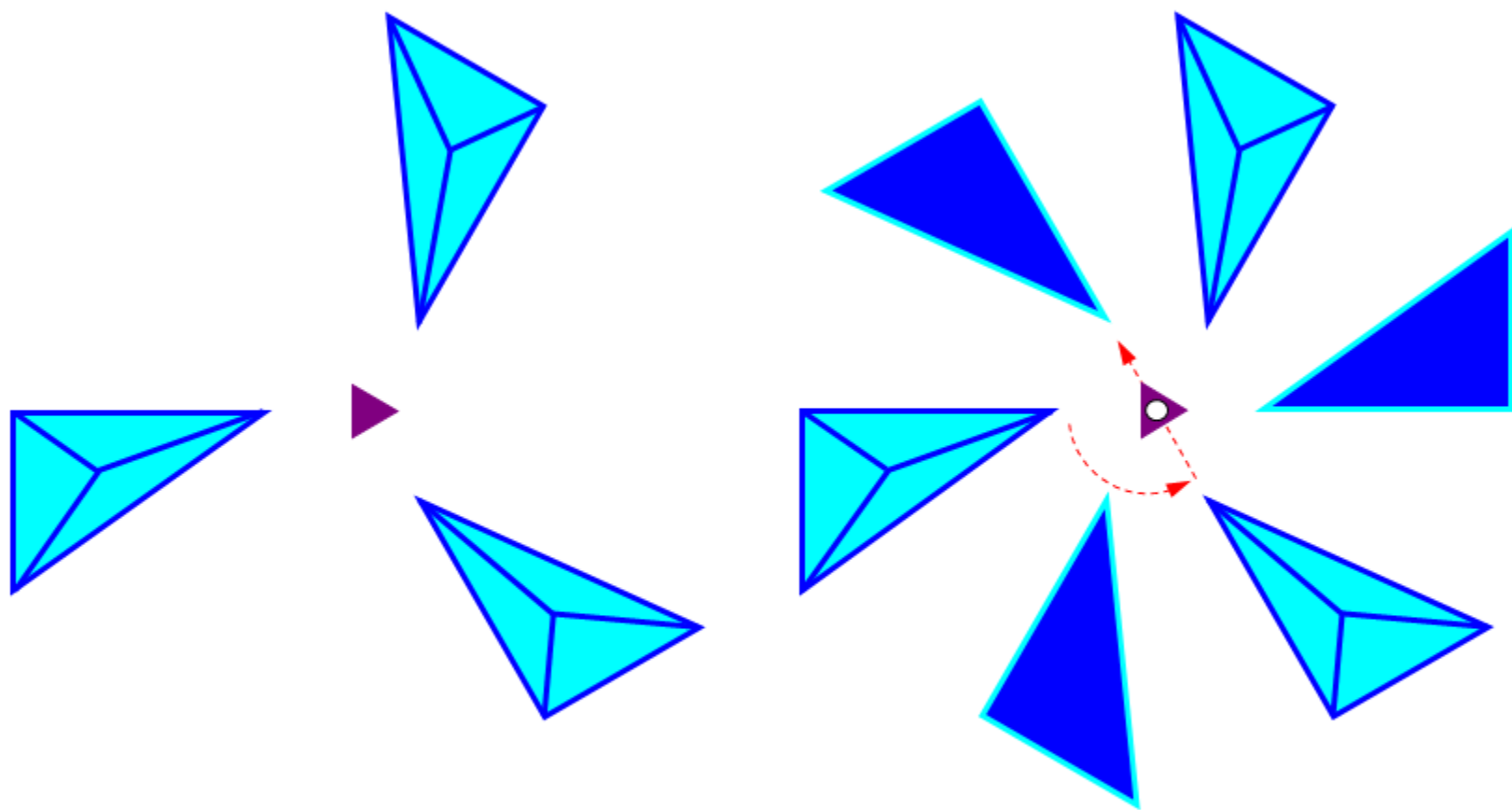
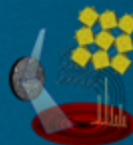


Figure 2.9. Threefold rotation (*left*) and threefold inversion (*right*) axes perpendicular to the plane of the projection. The *dashed arrows* on the right schematically show the counterclockwise rotation by 120° and a simultaneous inversion through the center of symmetry located on the axis.

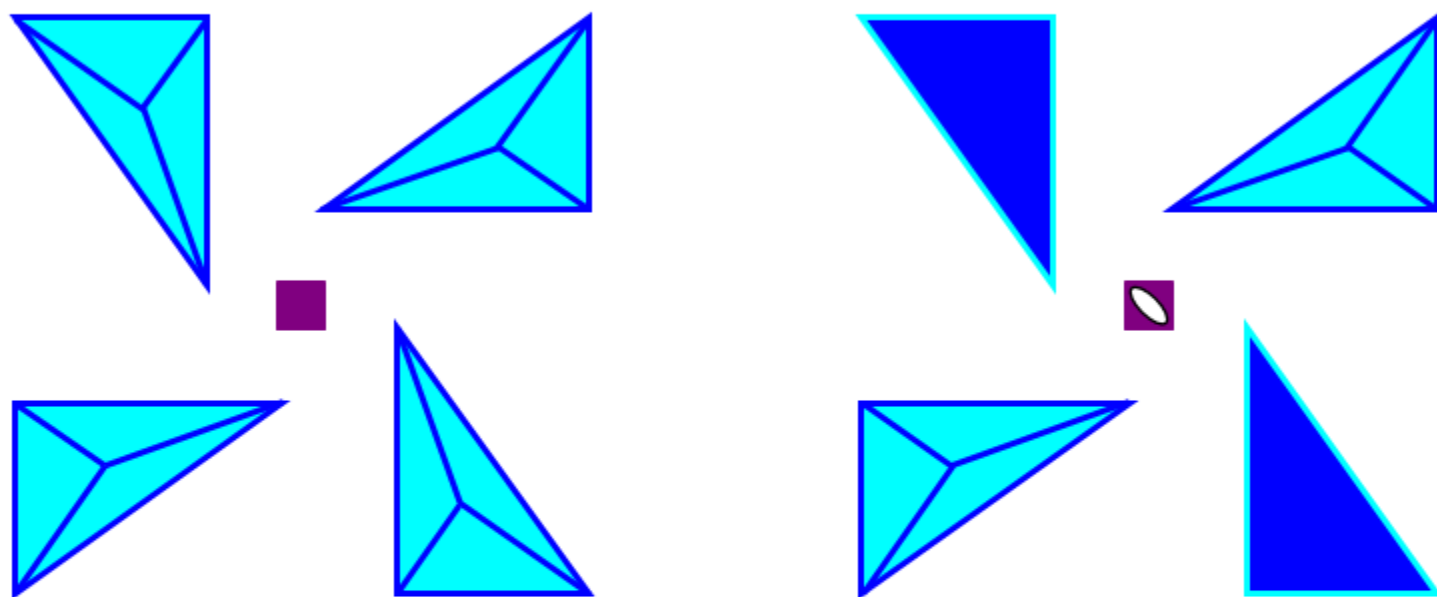
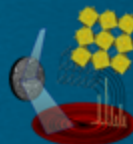


Figure 2.10. Fourfold rotation (*left*) and fourfold inversion (*right*) axes perpendicular to the plane of the projection.

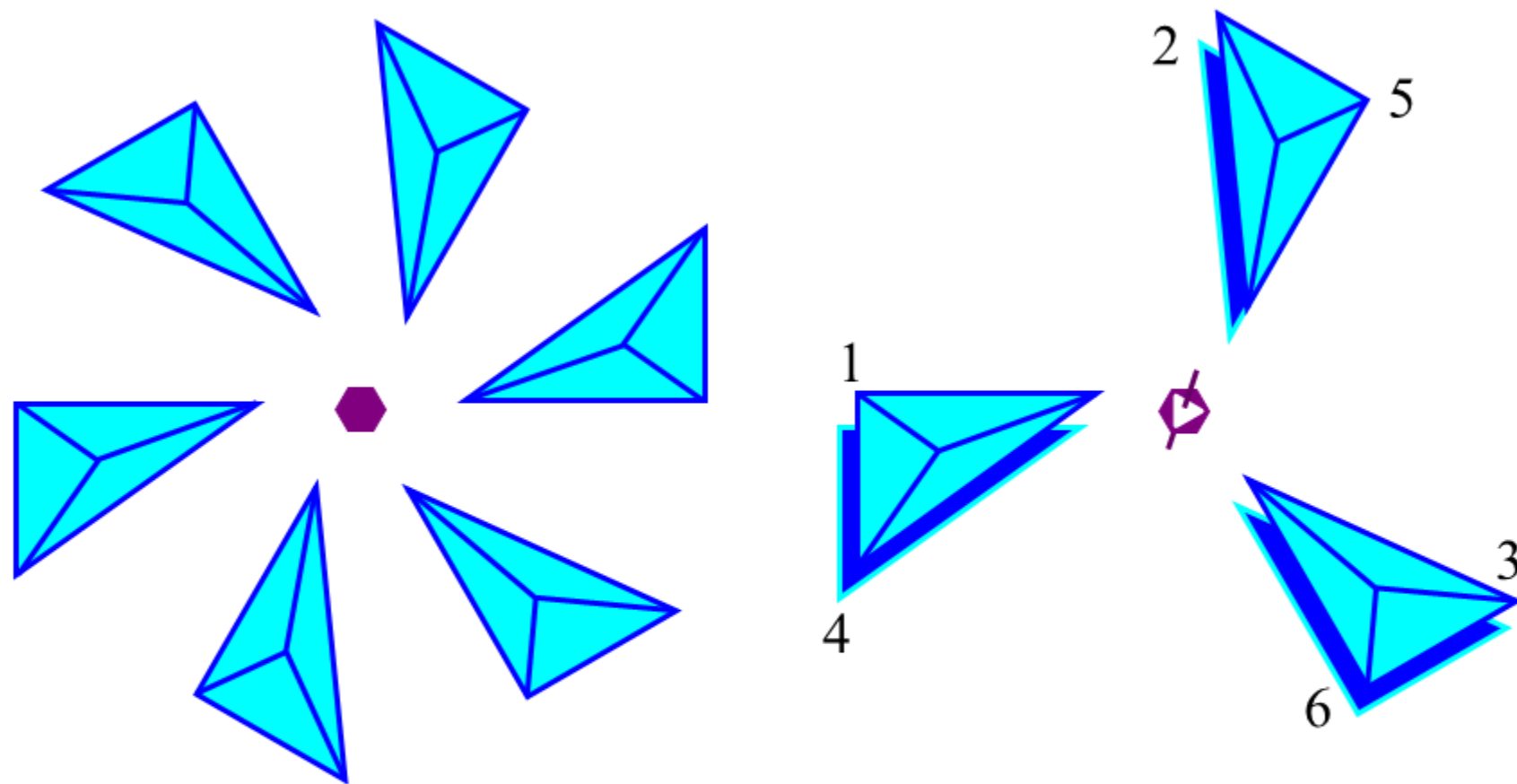
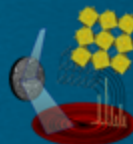


Figure 2.11. Sixfold rotation (*left*) and sixfold inversion (*right*) axes. The sixfold inversion axis is tilted by a few degrees away from the vertical to visualize all six symmetrically equivalent pyramids. The numbers next to the pyramids represent the original object (1), the first generated object (2), and so on. The odd numbers are for the pyramids with their apexes up.

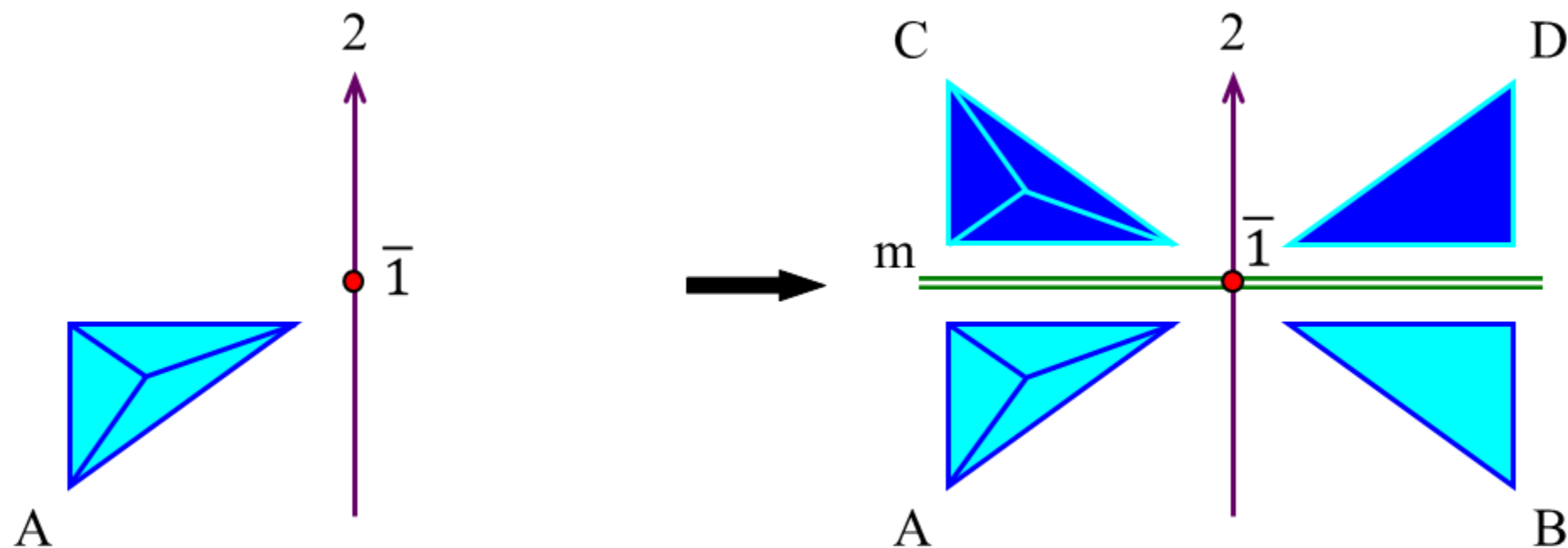
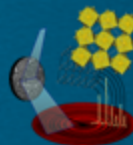


Figure 2.12. Schematic illustrating the interaction of symmetry elements. A twofold rotation axis (2) and a center of inversion (1) located on the axis (*left*) result in a mirror plane perpendicular to the axis intersecting it at the center of inversion (*right*). The important difference from Figure 2.8 (*middle* and *right*), where neither the two-fold axis nor the center of inversion is present independently, the combination of four pyramids (A, B, C, and D) here includes both of these symmetry elements.

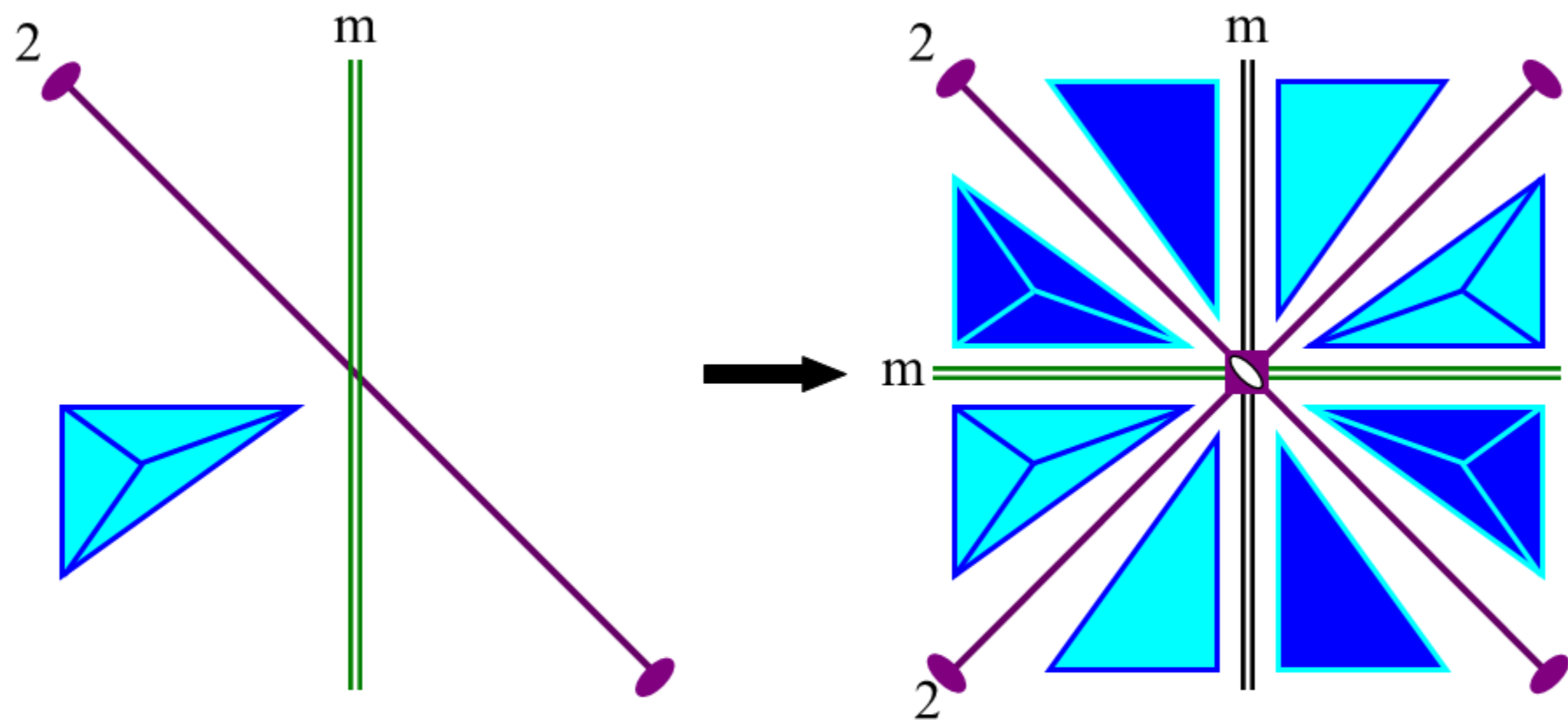
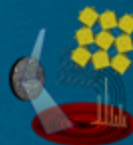


Figure 2.13. Mirror plane (m) and twofold rotation axis (2) intersecting at 45° (*left*) result in additional symmetry elements: two mirror planes, twofold rotation axis and fourfold inversion axis (*right*).

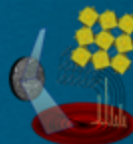


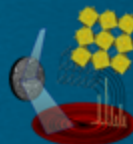
Table 2.4. Typical interactions between finite symmetry elements.

First element	Second element	Derived element (major)	Comments, examples
$\bar{1}$	N-fold axis	m for even N	$\bar{2} = m$
		N-fold inversion axis for odd N	$\bar{3}$
2	2 at $\phi = 30, 45, 60,$ or 90°	N-fold rotation axis, $N = 180/\phi$	6, 4, 3, or 2 perpendicular to 1 st and 2 nd axes
m	m at $\phi = 30, 45, 60,$ or 90°	same as above	6, 4, 3, or 2 along the common line
m	2 at 90°	center of inversion	$\bar{1}$ where m and 2 intersect
m	2 at $\phi = 30, 45, 60^\circ$	N-fold inversion axis, $N = 180/(90-\phi)$	$\bar{3}, \bar{4}$ or $\bar{6}$ in m and perpendicular to 2
3 or $\bar{3}$	2, 4, or $\bar{4}$ at 54.74° ; 3 or $\bar{2}$ at 70.53°	four intersecting 3 or $\bar{3}$ plus other symmetry elements	symmetry of a cube or tetrahedron



Table 2.5. Symmetry elements resulting from all possible combinations of 1 , $\bar{1}$, 2 , and m when 2 is perpendicular to m and $\bar{1}$ is located at the intersection of 2 and m .

Symmetry operation	1	$\bar{1}$	2	m
1	1	$\bar{1}$	2	m
$\bar{1}$	$\bar{1}$	1	m	2
2	2	m	1	$\bar{1}$
m	m	2	$\bar{1}$	1



The four properties of a group:

1. *Closure* — $G_i \times G_j = G_k$
2. *Associability* — $(G_i \times G_j) \times G_k = G_i \times (G_j \times G_k)$
3. *Identity* — $E \times G_i = G_i \times E = G_i$
4. *Inversion* — $G_i^{-1} \times G_i = G_i \times G_i^{-1} = E.$

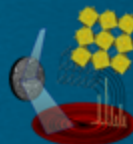


Table 2.6. Seven crystal systems and the corresponding characteristic symmetry elements.

Crystal system	Characteristic symmetry element or combination of symmetry elements
<i>Triclinic</i>	No axes other than onefold rotation or onefold inversion
<i>Monoclinic</i>	Unique twofold axis and/or single mirror plane
<i>Orthorhombic</i>	Three mutually perpendicular twofold axes, either rotation or inversion
<i>Trigonal</i>	Unique threefold axis, either rotation or inversion
<i>Tetragonal</i>	Unique fourfold axis, either rotation or inversion
<i>Hexagonal</i>	Unique sixfold axis, either rotation or inversion
<i>Cubic</i>	Four threefold axes, either rotation or inversion, along four body diagonals of a cube

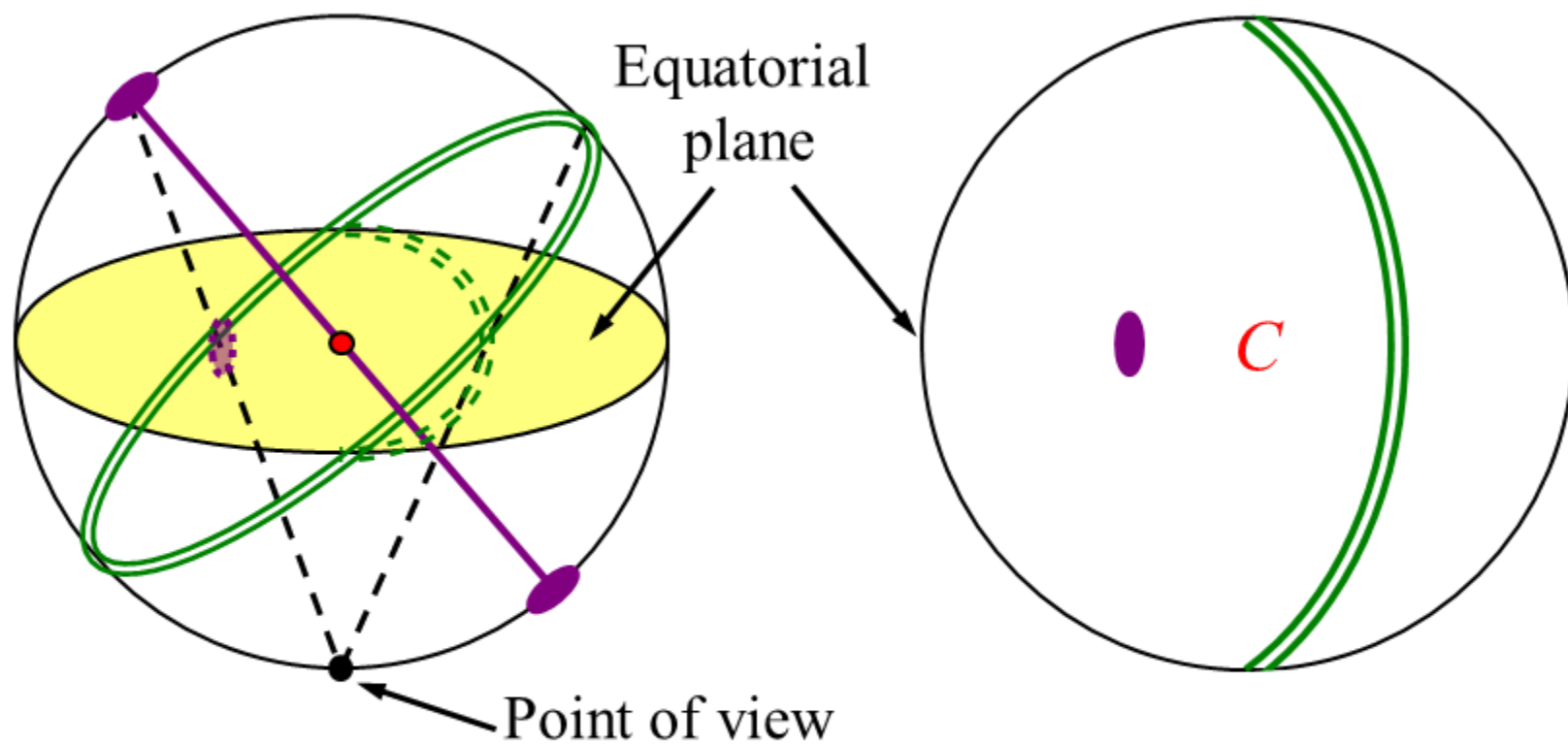
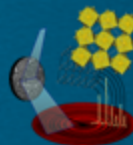


Figure 2.14. The schematic of how to construct a stereographic projection. The location of the center of inversion is indicated using letter *C* in the middle of the stereographic projection.

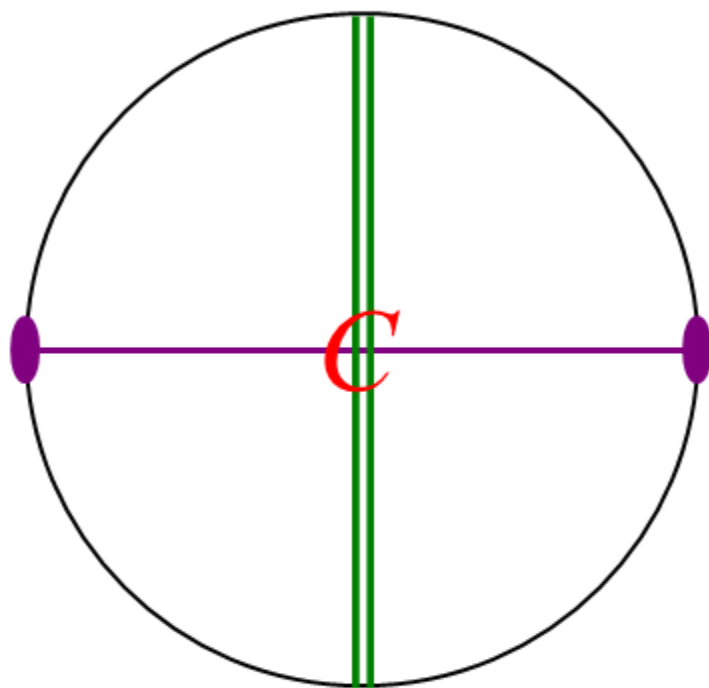
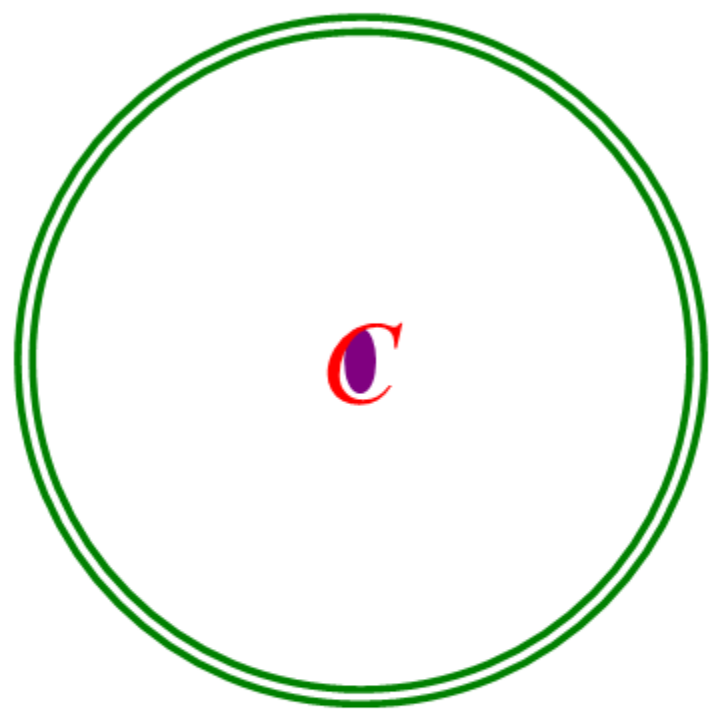
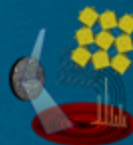


Figure 2.15. The two conventional stereographic projections of the point-group symmetry containing a twofold axis, a mirror plane and a center of inversion. The onefold rotation is not shown.

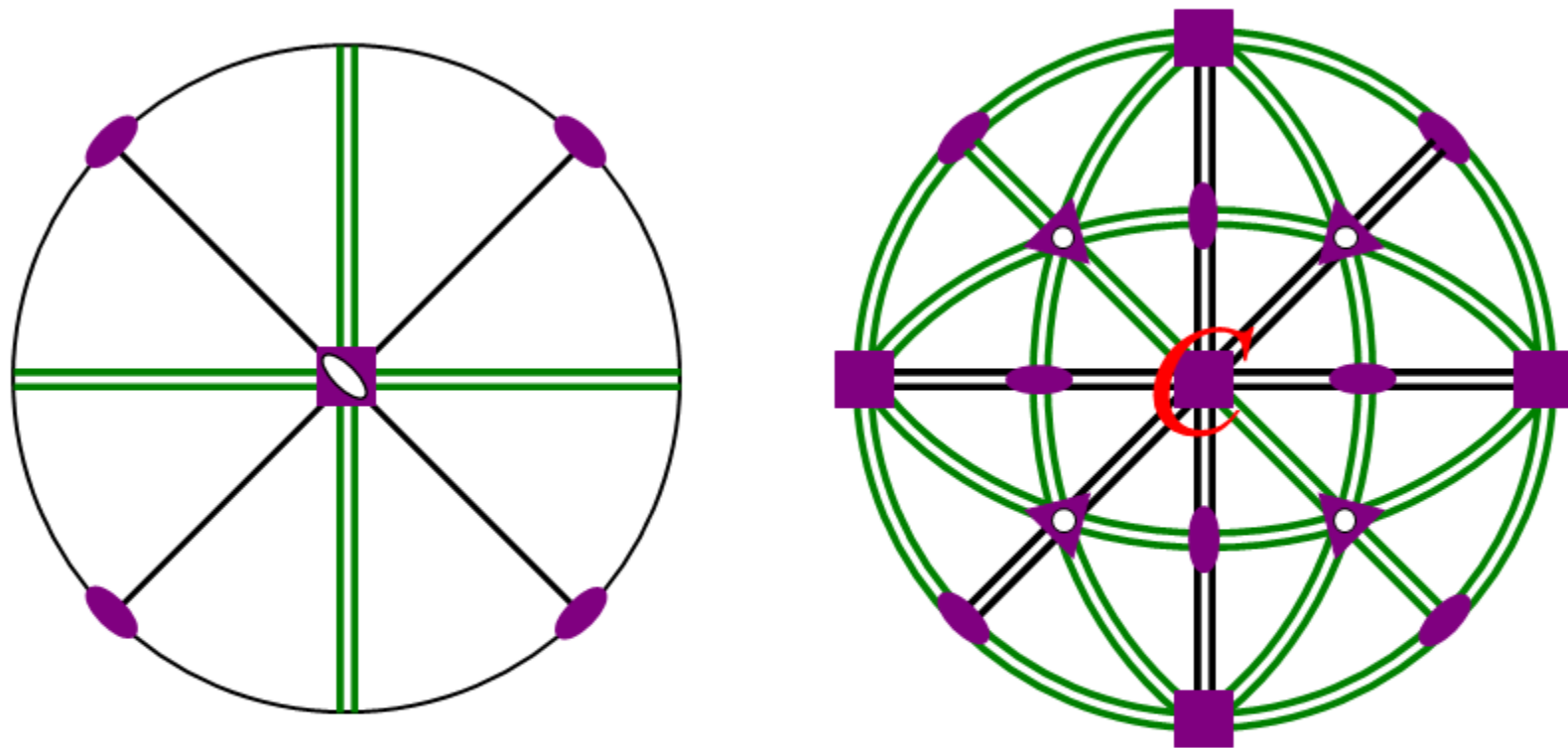
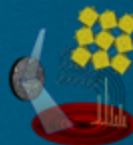


Figure 2.16. Examples of the stereographic projections with tetragonal (*left*) and cubic (*right*) symmetry.

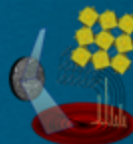


Table 2.7. Symbols of crystallographic point groups.

Crystal system	First position		Second position		Third position		Point group
	element	direction	element	direction	element	direction	
<i>Triclinic</i>	1 or $\bar{1}$	N/A	none		none		1, $\bar{1}$
<i>Monoclinic</i>	2, m or 2/m	Y	none		none		2, m, 2/m
<i>Orthorhombic</i>	2 or m	X	2 or m	Y	2 or m	X	222, mm2, mmm
<i>Tetragonal</i>	4, $\bar{4}$ or 4/m	Z	none or 2 or m	X	none or 2 or m	base diagonal	4, $\bar{4}$, 4/m, 422, 4mm, $\bar{4}2m$, 4/mmm
<i>Trigonal</i>	3 or $\bar{3}$	Z	none or 2 or m	X	none		3, $\bar{3}$, 32, 3m, $\bar{3}m$
<i>Hexagonal</i>	6, $\bar{6}$ or 6/m	Z	none or 2 or m	X	none or 2 or m	base diagonal	6, $\bar{6}$, 6/m, 622, 6mm, $\bar{6}2m$, 6/mmm
<i>Cubic</i>	2, m, 4 or $\bar{4}$	X	3 or $\bar{4}$	body diagonal	none or 2 or m	face diagonal	23, m3, 432, $\bar{4}3m$, $m\bar{3}m$

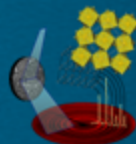


Table 2.9. The 11 Laue classes and six “powder” Laue classes.

Crystal system	Laue class	‘Powder’ Laue class	Point groups
<i>Triclinic</i>	$\bar{1}$	$\bar{1}$	1, $\bar{1}$
<i>Monoclinic</i>	2/m	2/m	2, m, 2/m
<i>Orthorhombic</i>	mmm	mmm	222, mm2, mmm
<i>Tetragonal</i>	4/m	4/mmm	4, $\bar{4}$, 4/m
	4/mmm	4/mmm	422, 4mm, $\bar{4}m2$, 4/mmm
<i>Trigonal</i>	$\bar{3}$	6/mmm	3, $\bar{3}$
	$\bar{3}m$	6/mmm	32, 3m, $\bar{3}m$
<i>Hexagonal</i>	6/m	6/mmm	6, $\bar{6}$, 6/m
	6/mmm	6/mmm	622, 6mm, $\bar{6}m2$, 6/mmm
<i>Cubic</i>	$m\bar{3}$	$m\bar{3}m$	23, $m\bar{3}$
	$m\bar{3}m$	$m\bar{3}m$	432, $\bar{4}3m$, $m\bar{3}m$

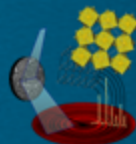


Table 2.10. Lattice symmetry and unit cell shapes.

Crystal family	Unit cell symmetry	Unit cell shape/parameters
<i>Triclinic</i>	$\bar{1}$	$a \neq b \neq c; \alpha \neq \beta \neq \gamma \neq 90^\circ$
<i>Monoclinic</i>	$2/m$	$a \neq b \neq c; \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$
<i>Orthorhombic</i>	mmm	$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$
<i>Tetragonal</i>	$4/mmm$	$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$
<i>Hexagonal and Trigonal</i>	$6/mmm$	$a = b \neq c; \alpha = \beta = 90^\circ, \gamma = 120^\circ$
<i>Cubic</i>	$m\bar{3}m$	$a = b = c; \alpha = \beta = \gamma = 90^\circ$

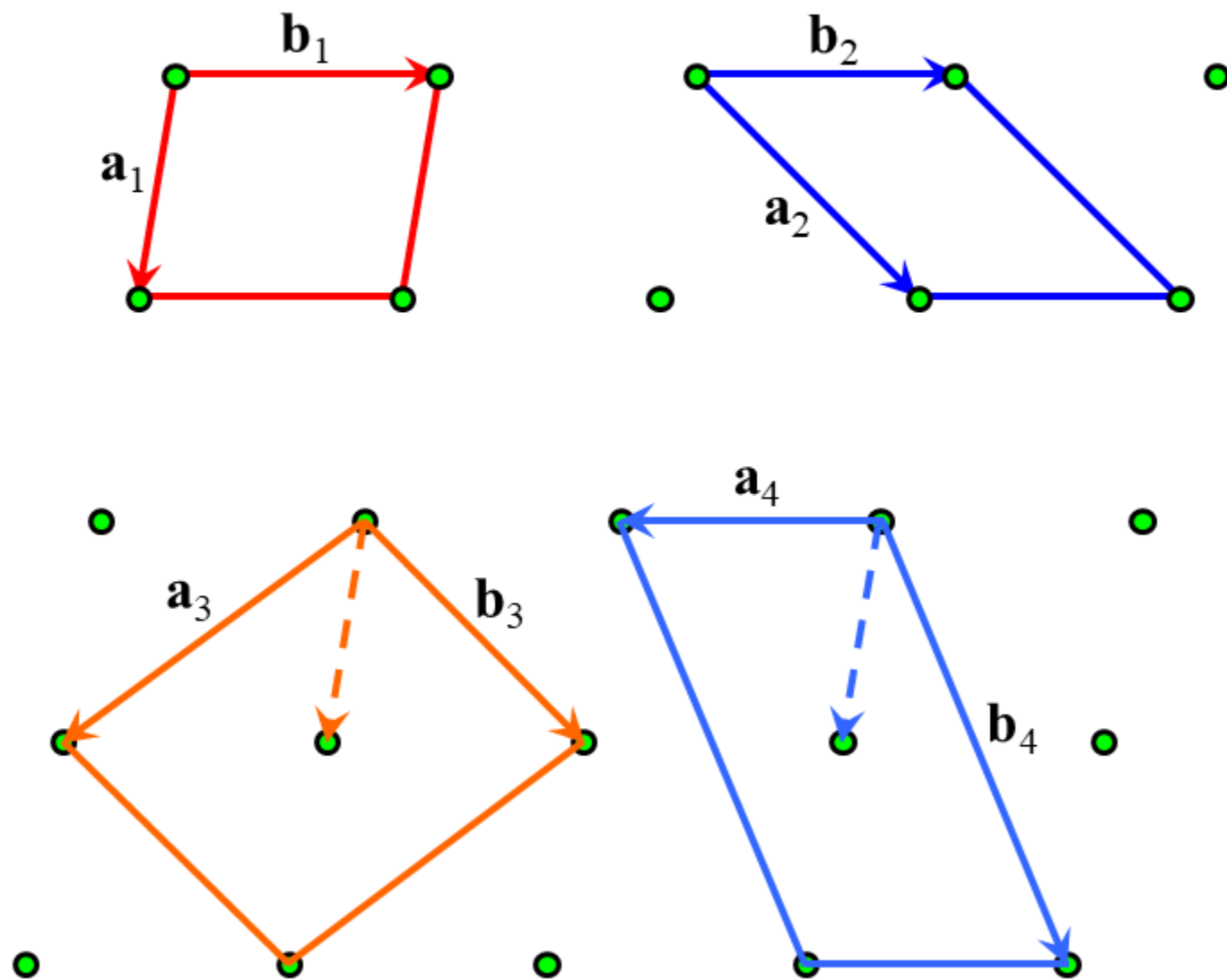
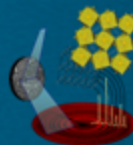


Figure 2.17. Illustration of different ways to select a unit cell in the same two-dimensional lattice.

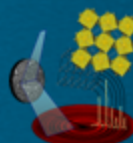


Table 2.11. Rules for selecting the unit cell in different crystal systems.

Crystal family	Standard unit cell choice	Alternative unit cell choice
<i>Triclinic</i>	Angles as close to 90° as possible (<i>Niggli</i>)	All angle(s) are $\geq 90^\circ$ (<i>Delaunay</i>)
<i>Monoclinic</i>	Y-axis is $\parallel$ to 2-fold rotation axis (or perpendicular to mirror plane) and $\beta \geq 90^\circ$	Same as the standard choice, but Z-axis in place of Y, and angle γ in place of β are allowed
<i>Orthorhombic</i>	Axes are chosen $\parallel$ to the 3 mutually perpendicular 2-fold rotation axes (or perpendicular to mirror planes)	None
<i>Tetragonal</i>	Z-axis $\parallel$ to the unique 4-fold rotation (inversion) axis. All axes are mutually perpendicular with each other	None
<i>Hexagonal and Trigonal</i>	Z-axis is $\parallel$ to 3- or 6-fold rotation (inversion) axis. X- and Y-axes form a 90° angle with the Z-axis and a 120° angle with each other	In a trigonal symmetry, ^a threefold axis is chosen along the body diagonal of the primitive unit cell, then $a = b = c$ and $\alpha = \beta = \gamma \neq 90^\circ$
<i>Cubic</i>	Axes are always $\parallel$ to the 3 mutually perpendicular two- or fourfold rotation axes, while the 4 threefold rotation (inversion) axes are $\parallel$ to 3 body diagonals of a cube	None

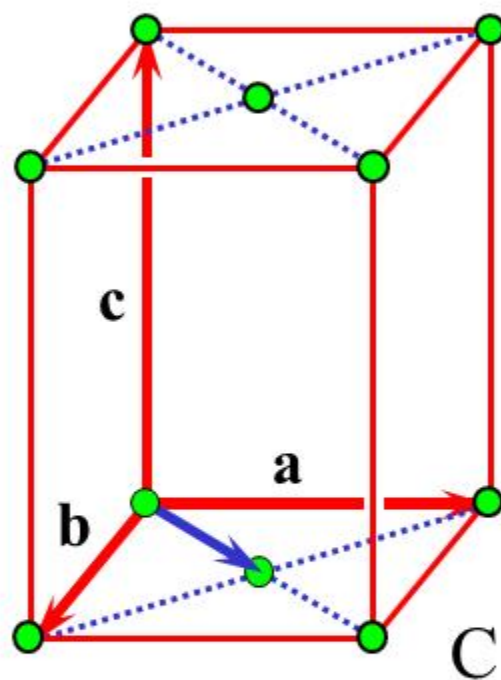
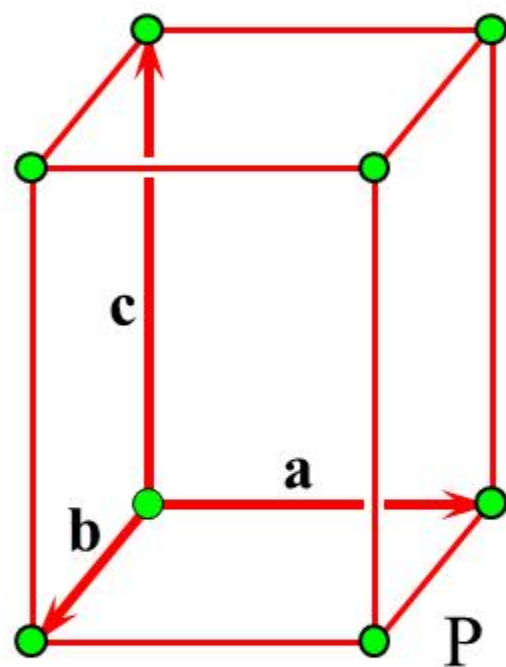


Figure 2.18. Primitive unit cell (*left*) and base-centered unit cell (*right*).

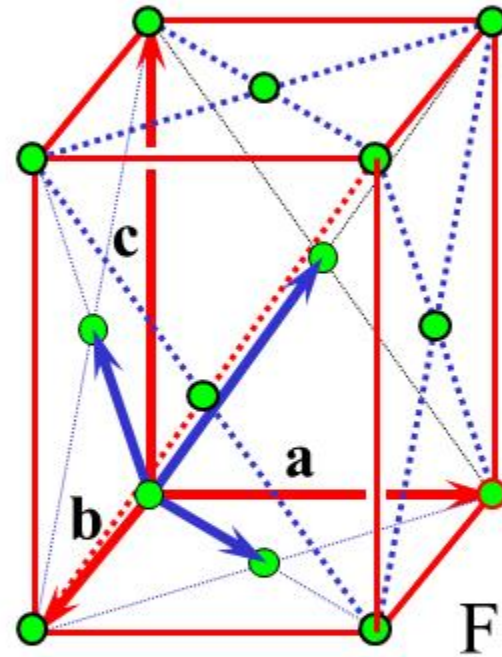
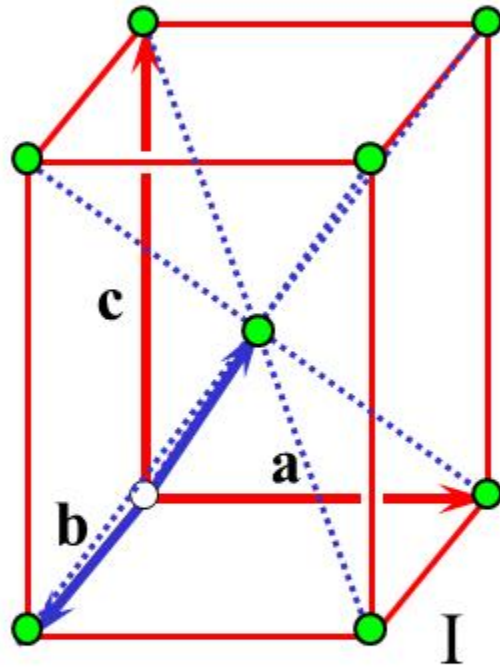


Figure 2.19. Body-centered unit cell (*left*) and face centered unit cell (*right*).

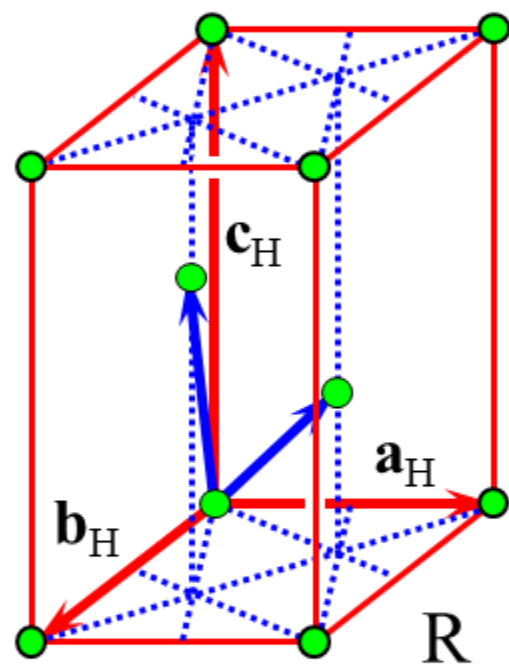
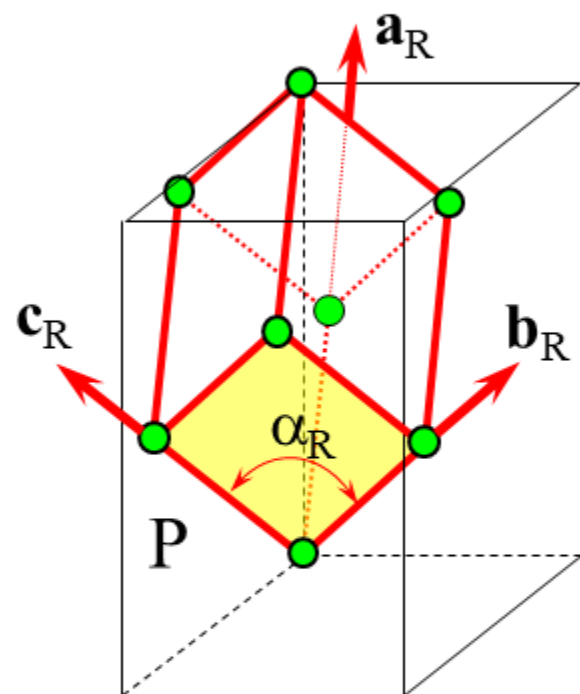
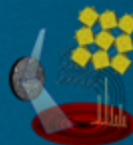
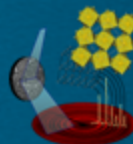


Figure 2.20. Primitive (*left*) and hexagonal rhombohedral (*right*) unit cells.



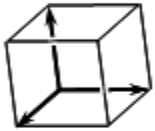
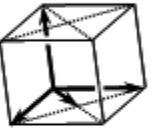
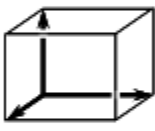
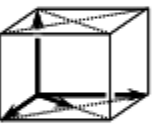
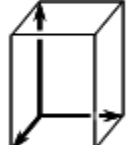
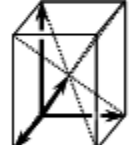
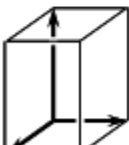
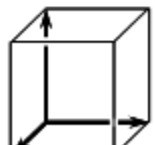
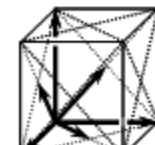
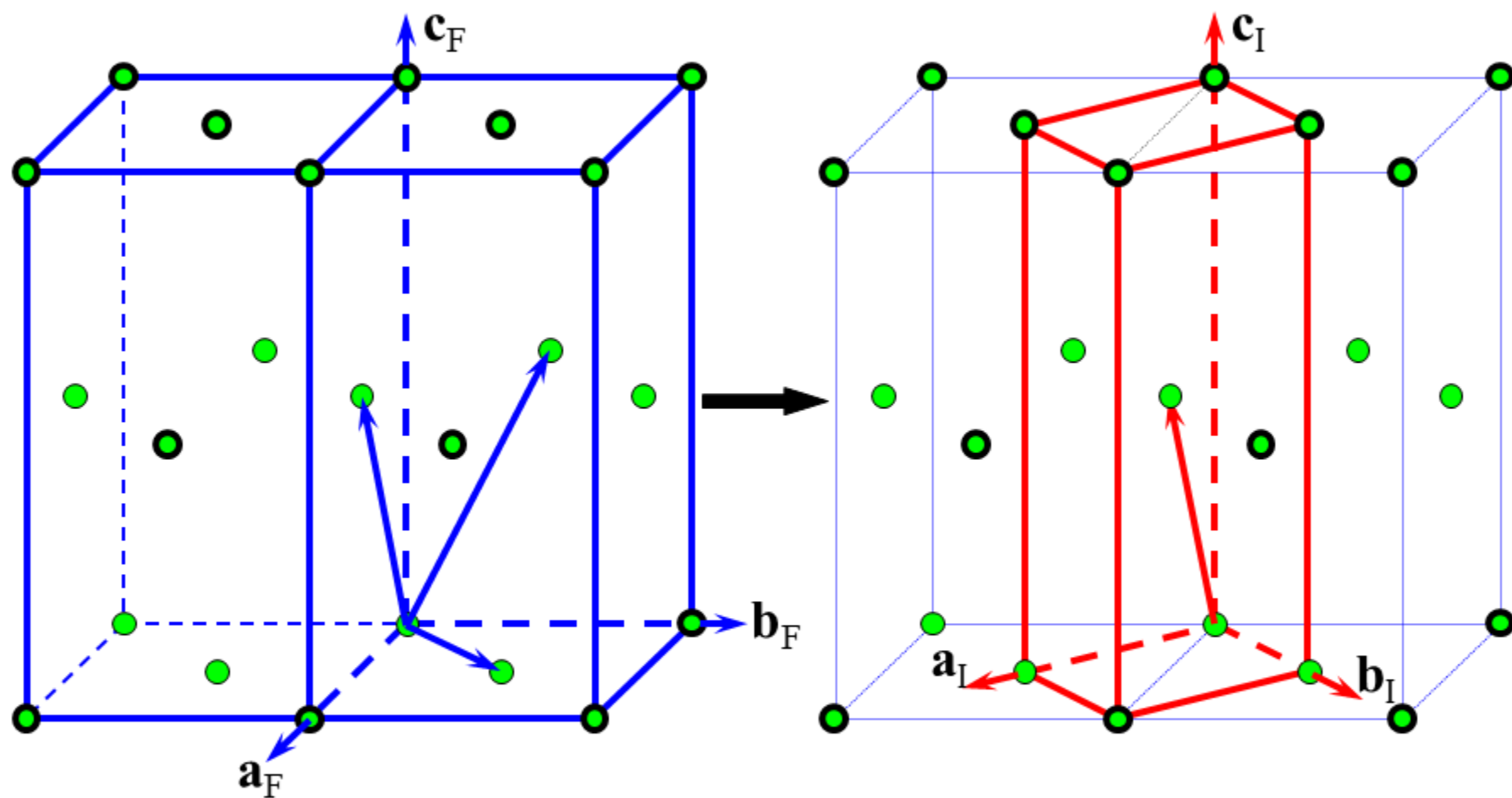
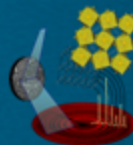
Crystal system	P	C	I	F	R
<i>Triclinic</i>					
<i>Monoclinic</i>					
<i>Orthorhombic</i>					
<i>Tetragonal</i>					
<i>Hexagonal</i> <i>Trigonal</i>					
<i>Cubic</i>					

Table 2.13.
The 14 Bravais lattices



Eqs. 2.5, 2.6, and 2.7

$$\mathbf{a}_I = \frac{1}{2}(\mathbf{a}_F - \mathbf{b}_F)$$

$$\mathbf{b}_I = \frac{1}{2}(\mathbf{a}_F + \mathbf{b}_F)$$

$$\mathbf{c}_I = \mathbf{c}_F$$

Eq. 2.9. $V_I = V_F/2$

Figure 2.21. The reduction of the tetragonal face-centered lattice (*left*) to the tetragonal body-centered lattice with half the volume of the unit cell (*right*). Small green circles indicate lattice points.