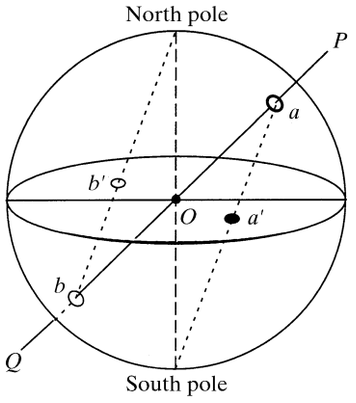

Fig. 2.1.3.1. How to construct a stereographic projection. Imagine a sphere around the crystal with O as the centre. O is also the origin of the coordinate system of the crystal. Symmetry elements of the point groups pass through O. Line OP is normal to a crystal plane. It cuts through the sphere at point a. This point a is projected onto the horizontal plane through O in the following way: a vertical dashed line is drawn through O normal to the projection plane and connecting a north and a south pole. Point a is connected to the pole on the other side of the projection plane, the south pole, and is projected onto the horizontal plane at a'. For a normal OQ intersecting the lower part of the sphere, the point of intersection b is connected to the north pole and projected at b'. For the symmetry elements, their points of intersection with the sphere are projected onto the horizontal plane.

morphic space groups. (Enantiomorphic means the structure is not superimposable on its mirror image.) Apparently, some of these space groups supply more favourable packing conditions for proteins than others. The most favoured space group is $P2_12_12_1$ (Table 2.1.2.1). A consequence of symmetry is that multiple copies of particles exist in the unit cell. For instance, in space group $P2_1$ (space group No. 4), one can always expect two exactly identical entities in the unit cell, and one half of the unit cell uniquely represents the structure. This unique part of the structure is called the asymmetric unit. Of course, the asymmetric unit does not necessarily contain one protein molecule. Sometimes the unit cell contains fewer molecules than anticipated from the number of asymmetric units. This happens when the molecules occupy a position on a crystallographic axis. This is called a special position.

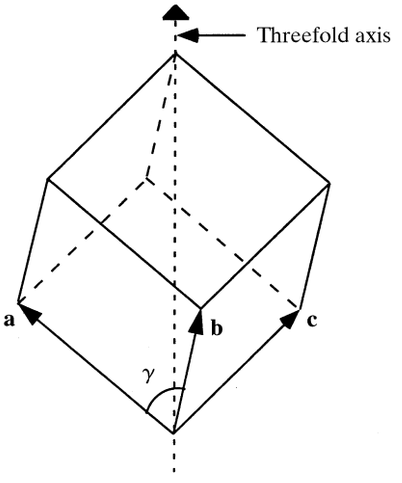

Fig. 2.1.3.2. A rhombohedral unit cell.

In this situation, the molecule itself obeys the axial symmetry. Otherwise, the molecules in an asymmetric unit are on general positions. There may also be two, three or more equal or nearly equal molecules in the asymmetric unit related by noncrystallographic symmetry.

2.1.3. Point groups and crystal systems

If symmetry can be recognised in the external shape of a body, like a crystal or a virus molecule, corresponding symmetry elements have no translations, because internal translations (if they exist) do not show up in macroscopic properties. Moreover, they pass through one point, and this point is not affected by the symmetry operations (point-group symmetry). For idealized crystal shapes, the symmetry axes are limited to one-, two-, three-, four- and sixfold rotation axes because of the space-filling requirement for crystals. With the addition of mirror planes and inversion centres, there are a total of 32 possible crystallographic point groups.

Not all combinations of axes are allowed. For instance, a combination of two twofold axes at an arbitrary angle with respect to each other would multiply to an infinite number of twofold axes. A twofold axis can only be combined with another twofold axis at 90°. A third twofold axis is then automatically produced perpendicular to the first two (point group 222). In the same way, a threefold axis can only be combined with three twofold axes perpendicular to the threefold axis (point group 32).

For crystals of biological macromolecules, point groups with mirrors or inversion centres are not allowed, because these molecules are chiral. This restricts the number of crystallographic point groups for biological macromolecules to 11; these are the enantiomorphic point groups and are presented in Table 2.1.3.1.

Although the crystals of asymmetric molecules can only belong to one of the 11 enantiomorphic point groups, it is nevertheless important to be aware of the other point groups, especially the 11 centrosymmetric ones (Table 2.1.3.2). This is because if anomalous scattering can be neglected, the X-ray diffraction pattern of a crystal is always centrosymmetric, even if the crystal itself is asymmetric (see Sections 2.1.7 and 2.1.8).

The protein capsids of spherical virus molecules have their subunits packed in a sphere with icosahedral symmetry (532). This is the symmetry of a noncrystallographic point group (Table 2.1.3.3). A fivefold axis is allowed because translation symmetry does not apply to a virus molecule. Application of the 532 symmetry leads to 60 identical subunits in the sphere. This is the simplest type of spherical virus (triangulation number $T = 1$). Larger numbers of subunits can also be incorporated in this icosahedral surface lattice, but then the subunits lie in quasi-equivalent environments and T assumes values of 3, 4 or 7. For instance, for $T = 3$ particles there are 180 identical subunits in quasi-identical environments.

On the basis of their symmetry, the point groups are subdivided into crystal systems as follows. For each of the point groups, a set of axes can be chosen displaying the external symmetry of the crystal as clearly as possible, and, in this way, the seven crystal systems of Table 2.1.3.4 are obtained. If no other symmetry is present apart from translational symmetry, the crystal belongs to the triclinic system. With one twofold axis or screw axis, it is monoclinic. The convention in the monoclinic system is to choose the b axis along the twofold axis. The orthorhombic system has three mutually perpendicular twofold (screw) axes. Another convention is that in tetragonal, trigonal and hexagonal crystals, the axis of highest symmetry is labelled c. These conventions can deviate from the guide rules for unit-cell choice given in Section 2.1.1.

The seven crystal systems are based on the point-group symmetry. Except for the triclinic unit cell, all other cells can

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Table 2.1.3.1. *The 11 enantiomorphic point groups*

The point groups are presented as two stereographic projections (see Fig. 2.1.3.1). On the right is a projection of the symmetry elements, and on the left a projection of the general faces. They are arranged according to the crystal system to which they belong: triclinic, monoclinic *etc*. Different point groups are separated by full horizontal rules. The monoclinic point groups are given in two settings: in the conventional setting with the twofold axis along **b** (unique axis *b*), and the other setting with unique axis *c*. The *b* axis is horizontal in the projection plane, and the *c* axis is normal to the plane. Three-, four- and sixfold axes are always set along the *c* axis, normal to the plane. A special case is the trigonal system; either hexagonal axes or rhombohedral axes can be chosen. In the hexagonal case, the threefold axis is along the *c* axis. The other two axes are chosen along or between the twofold axes, which include an angle of 120°. In the rhombohedral setting, the threefold axis is along the body diagonal of the unit cell, and the unit cell vectors **a**, **b** and **c** are the shortest non-coplanar lattice vectors symmetrically equivalent with respect to the threefold axis (Fig. 2.1.3.2). Symbols:

- ● General face above the plane
- ○ General face below the plane
- ⬮ Twofold rotation axis
- ▲ Threefold rotation axis
- ■ Fourfold rotation axis
- ⬢ Sixfold rotation axis

Adapted with permission from *IT* A (1995), Table 10.2.2. Copyright (1995) International Union of Crystallography.

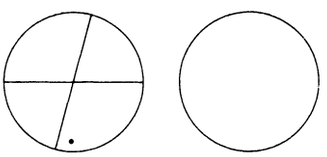
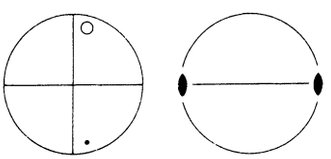
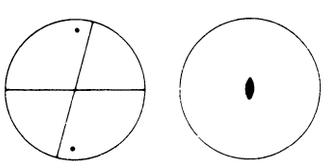
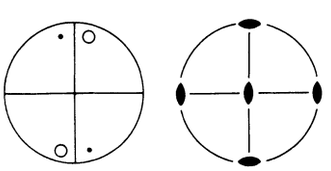
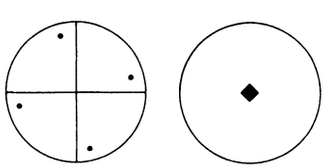
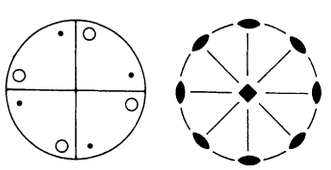
TRICLINIC	1	
MONOCLINIC	2	 Unique axis *b*  Unique axis *c*
ORTHORHOMBIC	222	
TETRAGONAL	4	
TETRAGONAL	422	

Table 2.1.3.1. *The 11 enantiomorphic point groups* (*cont.*)

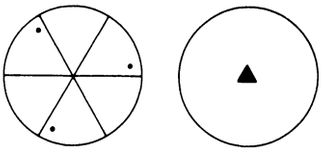
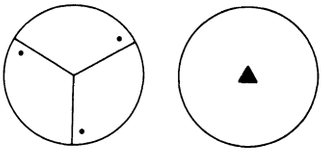
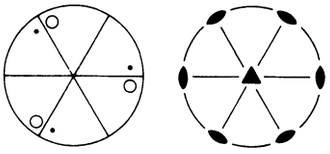
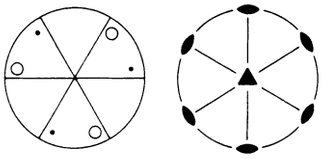
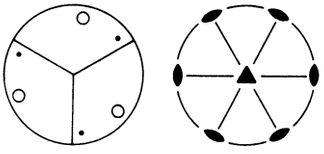
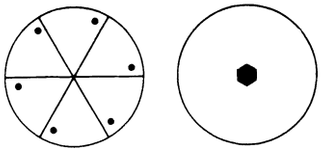
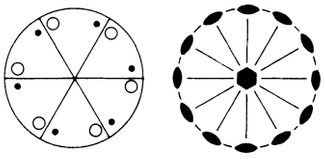
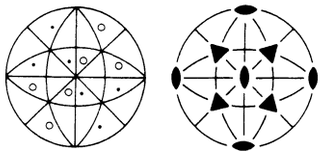
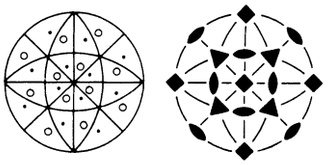
TRIGONAL Hexagonal axes	3	
TRIGONAL Rhombohedral axes	3	
TRIGONAL Hexagonal axes	321	
TRIGONAL Hexagonal axes	312	
TRIGONAL Rhombohedral axes	32	
HEXAGONAL	6	
HEXAGONAL	622	
CUBIC	23	
CUBIC	432	

Table 2.1.3.2. *The 11 point groups with a centre of symmetry*

For details see Table 2.1.3.1. Projections of mirror planes are indicated by a bold line or circle. The inversion centre $(\bar{1})$ is indicated by a small circle at the origin. Adapted with permission from *IT* A (1995), Table 10.2.2. Copyright (1995) International Union of Crystallography.

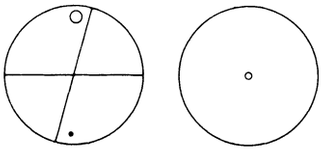
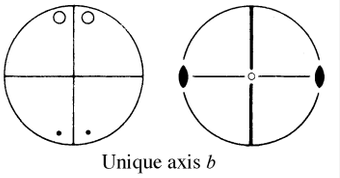
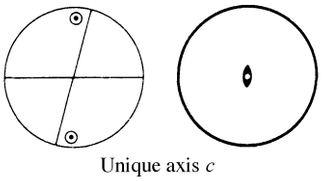
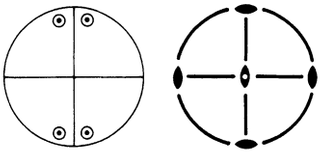
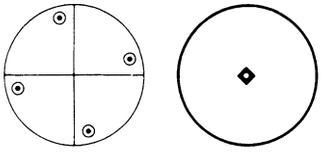
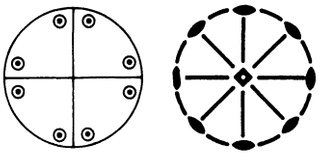
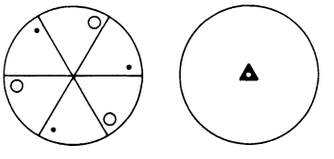
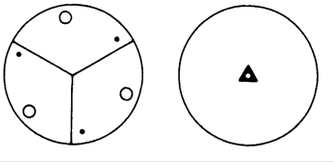
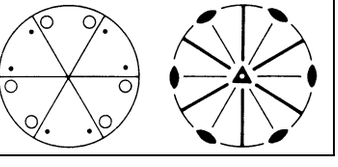
TRICLINIC	$\bar{1}$	
MONOCLINIC	$2/m$	 Unique axis b  Unique axis c
ORTHORHOMBIC	mmm or $\frac{2}{m}\frac{2}{m}\frac{2}{m}$	
TETRAGONAL	$4/m$	
TETRAGONAL	$4/mmm$ or $\frac{4}{m}\frac{2}{m}\frac{2}{m}$	
TRIGONAL Hexagonal axes	$\bar{3}$	
TRIGONAL Rhombohedral axes	$\bar{3}$	
TRIGONAL Hexagonal axes	$\bar{3}m1$ or $\bar{3}\frac{2}{m}1$	

Table 2.1.3.2. *The 11 point groups with a centre of symmetry* (*cont.*)

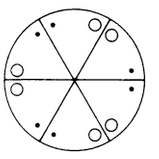
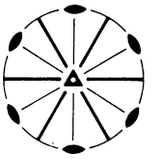
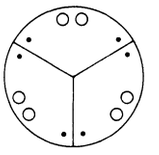
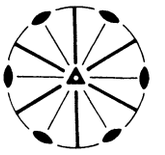
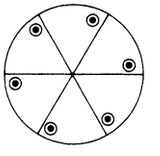
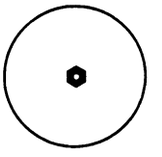
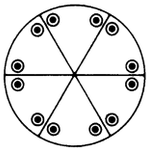
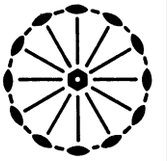
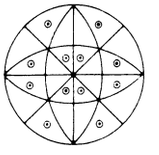
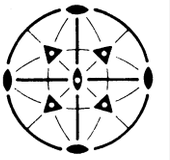
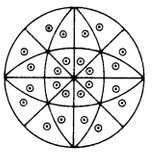
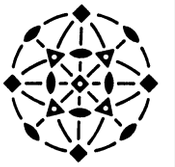
TRIGONAL Hexagonal axes	$\bar{3}1m$ or $\bar{3}1\frac{2}{m}$		
TRIGONAL Rhombohedral axes	$\bar{3}m$ or $\bar{3}\frac{2}{m}$		
HEXAGONAL	$6/m$		
HEXAGONAL	$6/mmm$ or $\frac{6}{m}\frac{2}{m}\frac{2}{m}$		
CUBIC	$m\bar{3}$ or $\frac{2}{m}\bar{3}$		
CUBIC	$m\bar{3}m$ or $\frac{4}{m}\bar{3}\frac{2}{m}$		

Table 2.1.3.3. *The icosahedral point group 532*

For details see Table 2.1.3.1. Adapted with permission from *IT* A (1995), Table 10.4.3. Copyright (1995) International Union of Crystallography.

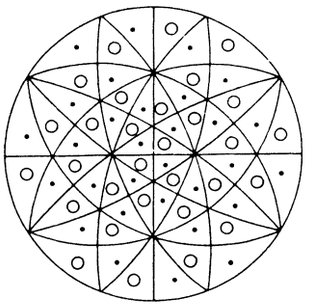
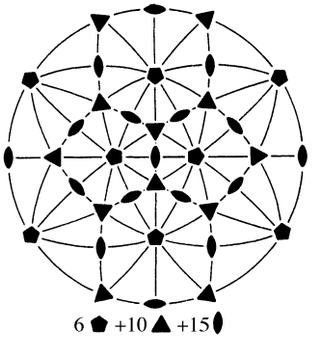
ICOSAHEDRAL	532		

Table 2.1.3.4. *The seven crystal systems*

Crystal system	Conditions imposed on cell geometry	Minimum point-group symmetry
Triclinic	None	1
Monoclinic	Unique axis b: $\alpha = \gamma = 90°$	2
Orthorhombic	$\alpha = \beta = \gamma = 90°$	222
Tetragonal	$a = b$; $\alpha = \beta = \gamma = 90°$	4
Trigonal	Hexagonal axes: $a = b$; $\alpha = \beta = 90°$; $\gamma = 120°$	3
	Rhombohedral axes: $a = b = c$; $\alpha = \beta = \gamma$ *	
Hexagonal	$a = b$; $\alpha = \beta = 90°$; $\gamma = 120°$	6
Cubic	$a = b = c$; $\alpha = \beta = \gamma = 90°$	23

* A rhombohedral unit cell can be regarded as a cube extended or compressed along the body diagonal (the threefold axis) (see Fig. 2.1.3.2).

occur either as primitive unit cells or as centred unit cells (Section 2.1.1). A total of 14 different types of unit cell exist, depicted in Fig. 2.1.3.3. Their corresponding crystal lattices are commonly called Bravais lattices.

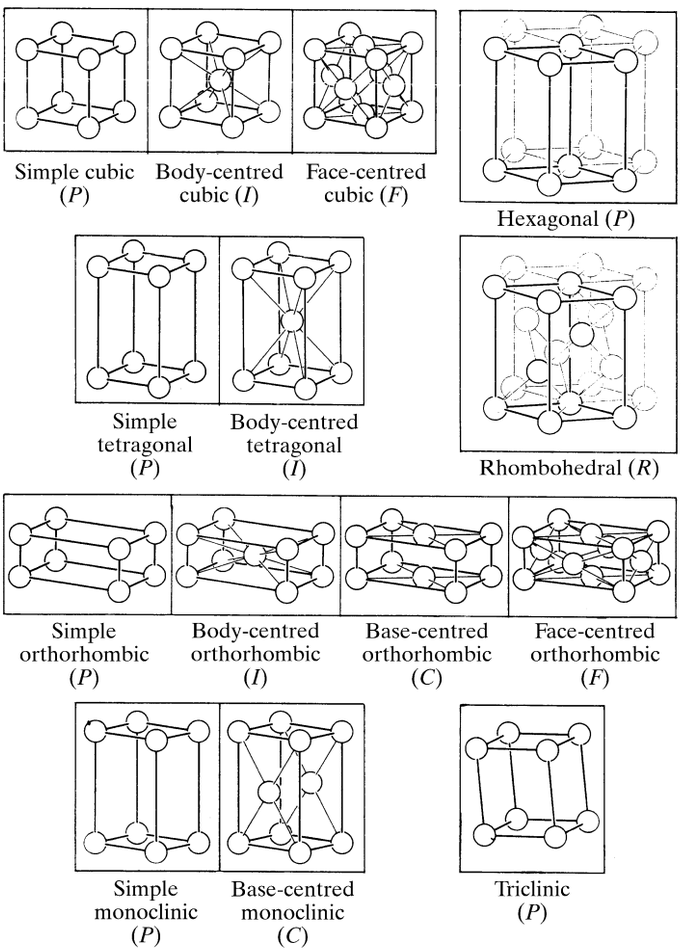


Fig. 2.1.3.3. The 14 Bravais lattices. Reproduced with permission from Burzlaff & Zimmermann (1995). Copyright (1995) International Union of Crystallography.

2.1.4. Basic diffraction physics

2.1.4.1. *Diffraction by one electron*

The scattering of an X-ray beam by a crystal results from interaction between the electric component of the beam and the electrons in the crystal. The magnetic component has hardly any effect and can be disregarded.

If a monochromatic polarized beam hits an electron, the electron starts to oscillate in the direction of the electric vector of the incident beam (Fig. 2.1.4.1). This oscillating electron acts as the aerial of a transmitter and radiates X-rays with the same or lower frequency as the incident beam. The frequency change is due to the Compton effect: the photons of the incident beam collide with the electron and lose part of their energy. This is inelastic scattering, and the scattered radiation is incoherent with the incident beam. Compton scattering contributes to the background in a diffraction experiment. In elastic scattering, the scattered radiation has the same wavelength as the incident radiation, and this is the radiation responsible for the interference effects in diffraction. It was shown by Thomson that if the electron is completely free the following hold:

(1) The phase difference between the incident and the scattered beam is π, because the scattered radiation is proportional to the displacement of the electron, which differs by π in phase with its acceleration imposed by the electric vector.

(2) The amplitude of the electric component of the scattered wave at a distance r which is large in comparison with the wavelength of the radiation is

$$E_{\rm el} = E_o \frac{1}{r} \frac{e^2}{mc^2} \sin\varphi,$$

where E_o is the amplitude of the electric vector of the incident beam, e is the electron charge, m is its mass, c is the speed of light and φ is the angle between the oscillation direction of the electron and the scattering direction (Fig. 2.1.4.1). Note that $E_o \sin\varphi$ is the component of E_o perpendicular to the scattering direction.

In terms of energy,

$$I_{\rm el} = I_o \frac{1}{r^2} \left(\frac{e^2}{mc^2}\right)^2 \sin^2\varphi. \qquad (2.1.4.1a)$$

The scattered energy per unit solid angle is

references