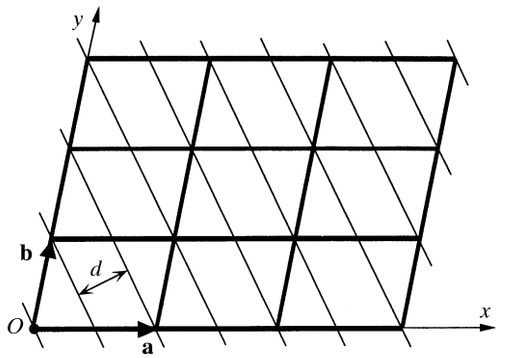
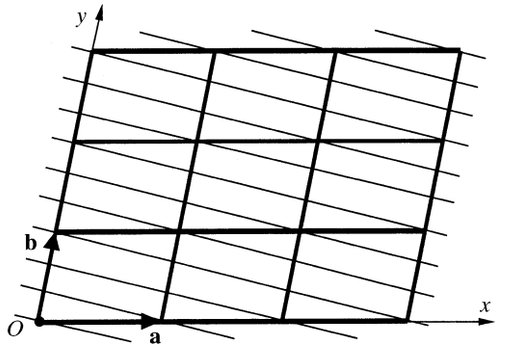
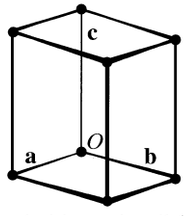


(*a*)

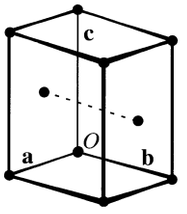


(*b*)

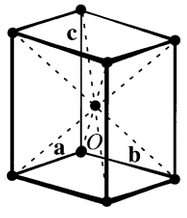
Fig. 2.1.1.3. A two-dimensional lattice with 3 × 3 unit cells. In both (*a*) and (*b*), a set of equidistant parallel lattice planes is drawn. They pass through all lattice points. Lattice planes always divide the unit-cell axes into a whole number of equal parts – 1, 2, 3 *etc*. For instance, in (*a*), the vector **a** of the unit cell is cut into two parts, and the vector **b** into only one part. This set of planes is then given the indices $h = 2$ and $k = 1$. In three dimensions, there would be a third index, *l*. In (*b*), the set of lattice planes has the indices $h = 1$ and $k = 3$. In general, lattice planes have the indices (*hkl*), known as Miller indices. If a set of lattice planes is parallel to an axis, the corresponding index is 0. For instance, (001) is the set of planes parallel to the unit-cell vectors **a** and **b**. Note that the projection of **a**/*h* on the line normal to the lattice plane is equal to the lattice-plane distance *d*. This is also true for **b**/*k*. Reproduced with permission from Drenth (1999). Copyright (1999) Springer-Verlag.



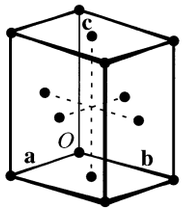
A primitive unit cell (*P*)



A unit cell centred in the (010) planes (*B*)



A body-centred unit cell (*I*)



A face-centred unit cell (*F*)

Fig. 2.1.1.4. Non-centred and centred unit cells. Reproduced with permission from Drenth (1999). Copyright (1999) Springer-Verlag.

(6) Of those not lying in the *ab* plane, none is shorter than **c**.

(7) The three angles between the basis vectors **a**, **b** and **c** are either all acute ($<90°$) or all obtuse ($\geq 90°$).

It should be noted that the rules for choosing **a**, **b** and **c** are not always obeyed, because of other conventions (see Section 2.1.3). Condition (3) sometimes leads to a centred unit cell instead of a primitive cell. Primitive cells have only one lattice point per unit cell, whereas non-primitive cells contain two or more lattice points. They are designated *A*, *B* or *C* if opposite faces of the cell are centred: *A* for *bc* centring, *B* for *ac* centring and *C* for *ab* centring. If all faces are centred, the designation is *F*, and if the cell is body-centred, it is *I* (Fig. 2.1.1.4).

2.1.2. Symmetry

A symmetry operation can be defined as an operation which, when applied, results in a structure indistinguishable from the original one. According to this definition, the periodic repetition along **a**, **b** and **c** represents translational symmetry.

In addition, rotational symmetry exists, but only rotational angles of 60, 90, 120, 180 and 360° are allowed (*i.e*. rotation over 360/*n* degrees, where *n* is an integer). These correspond to *n*-fold rotation axes, with $n = 6, 4, 3, 2$ and 1 (identity), respectively. Rotation axes with $n = 5$ or $n > 6$ are not found as crystallographic symmetry axes, because translations of unit cells containing these axes do not completely fill three-dimensional space. Another type of rotational symmetry axis is the screw axis. It combines a rotation with a translation. For a twofold screw axis, the translation is over 1/2 of the unit-cell length in the direction of the axis; for a threefold screw axis, it is 1/3 or 2/3 *etc*. In this way, the translational symmetry operators can be obeyed. The requirement that translations are 1/2, 1/3, 2/3 *etc*. of the unit-cell length does not exist for individual objects that are not related by crystallographic translational symmetry operators. For instance, an α-helix has 3.6 residues per turn.

Besides translational and rotational symmetry operators, mirror symmetry and inversion symmetry exist. Mathematically, it can be proven that not all combinations of symmetry elements are allowed, but that 230 different combinations can occur. They are the space groups which are discussed extensively in *IT* A (1995). The graphical and printed symbols for the symmetry elements are also found in *IT* A (pp. 9–10).

Biological macromolecules consist of building blocks such as amino acids or sugars. In general, these building-block structures are not symmetrical and the mirror images of the macromolecules do not exist in nature. Space groups with mirror planes and/or inversion centres are not allowed for crystals of these molecules, because these symmetry operations interchange right and left hands. Biological macromolecules crystallize in one of the 65 enantio-

Table 2.1.2.1. *The most common space groups for protein crystals*

Situation as of April 1997; data extracted from the Protein Data Bank and supplied by Rob Hooft, EMBL Heidelberg.

Space group	Occurrence (%)
$P2_12_12_1$	23
$P2_1$	11
$P3_221$	8
$P2_12_12$	6
$C2$	6

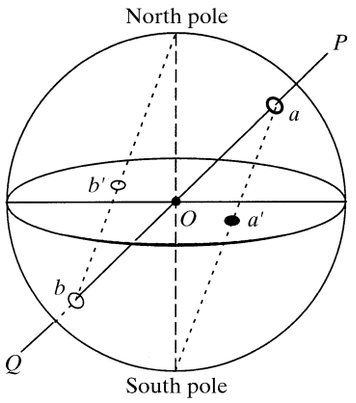


Fig. 2.1.3.1. How to construct a stereographic projection. Imagine a sphere around the crystal with O as the centre. O is also the origin of the coordinate system of the crystal. Symmetry elements of the point groups pass through O. Line OP is normal to a crystal plane. It cuts through the sphere at 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.

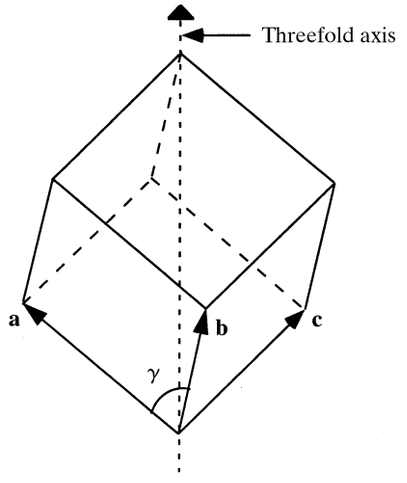


Fig. 2.1.3.2. A rhombohedral unit cell.

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

references