

How to read (and understand) Volume A of *International Tables for Crystallography*: an introduction for nonspecialists

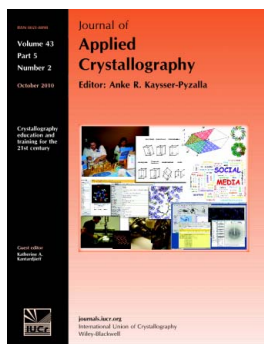
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How to read (and understand) Volume A of *International Tables for Crystallography*: an introduction for nonspecialists

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Since fewer and fewer students get proper crystallographic education at the undergraduate level, the responsibility to promote and propagate this knowledge must be directed to alternative channels. It is not a marginal issue, because the language of crystallography is rather hermetic and, without proper support, it might disappear from the collective scientific knowledge, so that in the next generation there would be no-one able to use it properly, to say nothing about advancing the field. Black-box crystallography might be useful in some situations, but it cannot replace well informed, conscious scientific pursuits by properly trained specialists. Without sufficient understanding of crystallographic terms and principles, the now thriving branch of structural research would wither, and this could have particularly lamentable consequences for structural biology. The purpose of this article is to teach non-initiated persons, primarily structural biologists, how to interpret the information contained in the fundamental Volume A of *International Tables for Crystallography* (ITA). An excellent and comprehensive overview of many issues concerning crystal symmetry is presented in a book by Burns & Glazer (*Space Groups for Solid State Scientists*, 2nd ed. New York: Academic Press, 1990), also explaining the contents of ITA, but this text is unfortunately not popular among structural biologists. There are several superb handbooks explaining the foundations of structural crystallography but they usually do it without direct reference to ITA. There is also a comprehensive introduction included in ITA, but it is written in rather hermetic language and is, therefore, not suitable for nonspecialists with no training in exact sciences. This article, which uses simple language to explain all the terms encountered on the space-group pages of ITA, is meant to bridge this growing gap in crystallographic instruction. The explanations are illustrated with actual examples taken directly from the pages of ITA.

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1. Introduction

Crystallography is a peculiar science, at the same time interdisciplinary – it overlaps with the principal natural sciences of physics, chemistry and biology – and yet rather hermetic. The language of crystallography is not really difficult, but it is very exact and must be learned. By tradition of individual countries, crystallography has been taught in the schools of physics, chemistry, or even biology or earth sciences: or perhaps we should say ‘was taught’ as, because of changing fashions, it appears that teaching basic sciences is no longer trendy. On the wave of these seasonal moods, crystallography has vanished from most university curricula and there is a very real danger that, as a result of this regrettable policy, no one in the next generation of scientists will be capable of under-

standing (let alone speaking) the language of crystallography. This would be a true catastrophe because a thriving science would essentially wither and die within one generation. Although this scenario seems almost inconceivable, we might be drifting toward a day when opening Volume A of *International Tables for Crystallography* (ITA), the fundamental compendium of crystallographic space-group symmetry, would be equivalent to opening a book of hieroglyphs. The current volume of ITA (2005) is very large and presents many detailed issues related to various aspects of space-group symmetry. Its predecessor, the ‘red’ Volume I of *International Tables for X-ray Crystallography* (1952), was leaner because it contained only more basic, yet usually sufficient, information for the interpretation of each space-group symmetry. The text below refers to the most recent ‘blue’ or ‘white-green’

volumes of ITA and the online version available at <http://it.iucr.org>.

We have been approached many times, by physicists, chemists and especially structural biologists, asking for help with the interpretation of the information contained in that volume or in publications on crystal structures referring to symmetry information. Since we expect that demand for such advice will not subside but, on the contrary, will grow and become more pressing, we have decided to summarize our educational experience in this area in the form of an extended article. We hope that the material presented herein is (still) intelligible and useful. In essence, we are presenting a simplified and very basic introduction to the use of ITA. This article is not intended to replace, in any way, the excellent handbooks written for protein crystallographers (*e.g.* Rupp, 2009) or for a more general audience (*e.g.* Burns & Glazer, 1990; Giacovazzo, 2002). Instead, it can be treated as a bridge between those handbooks and ITA, prepared with the structural biologist in mind.

Fig. 1 shows a copy of two pages from ITA, dedicated to one of the space groups, $P4_32_12$. On the following pages we will explain the various symbols in as simple terms as possible. In fact, the first part of ITA contains such explanations, but they are written in a rather scholarly fashion, sometimes difficult to understand for people not used to the language of crystallography. Below is a short summary of all the items present on those pages; detailed explanations will follow.

The left-hand page contains the following information:

- (a) Crystal system (Tetragonal)
- (b) Point-group symbol (422)
- (c) Space-group symbol in international or Hermann–Mauguin notation ($P4_32_12$)
- (d) Space-group symbol in Schönflies notation (D_4^8)
- (e) Space-group number (96)
- (f) Corresponding Patterson symmetry ($P4/mmm$)
- (g) Diagram of symmetry operations (left diagram)
- (h) Diagram of equivalent positions (right diagram)

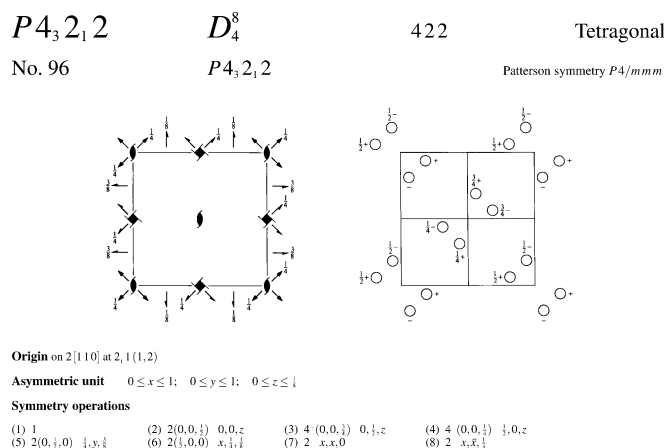


Figure 1
Two pages from ITA, presenting the information relevant for space group $P4_32_12$.

- (i) Position of the unit-cell origin relative to symmetry operators
- (j) Possible choice of asymmetric unit
- (k) Positions of symmetry operators relative to the unit-cell origin

The right-hand page contains the following information:

- (a) Repeated space-group number and symbol (96, $P4_32_12$)
- (b) List of equivalent general-position points in algebraic notation (uppermost entry under ‘Positions’)
- (c) Lists of special positions (all other ‘Positions’)
- (d) Symmetry of two-dimensional projections
- (e) List of subgroups and supergroups
- (f) List of symmetry operations generating the group (at the top of the page)
- (g) Conditions for presence (and absence) of diffracted reflections expressed as index rules

2. Interpretation and explanation of individual items

2.1. Crystal systems

In idealized theory, a crystal is built from identical blocks (parallelepipeds), called unit cells, which are repeated one next to another in three dimensions an infinite number of times, thus forming a three-dimensional lattice. This is a rather good approximation for structural crystallographers, since, because of the small size of the individual unit cells, usually tens to hundreds of ångströms ($1 \text{ \AA} = 10^{-8} \text{ cm}$), the number of unit cells inside even a small (10–100 μm across) crystal is several orders of magnitude larger than the number of unit cells at the surface, so that surface effects can be reasonably neglected (*e.g.* in a diffraction experiment). Depending on the shape and symmetry of the unit cell, crystals are classified into seven symmetry systems, called crystal systems, with specific conditions, as defined in Table 1, imposed on the lengths (a, b, c) of the unit-cell edges and on the angles (α, β, γ) between them. The ‘inequality’ conditions in Table 1 should be inter-

| | | |
|--|---|--|
| CONTINUED | No. 96 | $P4_32_12$ |
| Generators selected (1); $r(1, 0, 0)$; $r(0, 1, 0)$; $r(0, 0, 1)$; (2); (3); (5) | | |
| Positions | | |
| Multiplicity | Coordinates | Reflection conditions |
| Wyckoff letter | | General: |
| Site symmetry | | 00 l : $l = 4n$ |
| 8 | 4 1 (1) x, y, z (2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ | $h00$: $h = 2n$ |
| | (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, z + \frac{1}{2}$ (7) y, x, z (8) $\bar{y}, \bar{x}, z + \frac{1}{2}$ | Special: as above, plus |
| 4 | a $\dots 2$ $x, x, 0$ $\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ | $0kl$: $l = 2n + 1$ or $2k + l = 4n$ |
| Symmetry of special projections | | |
| Along $[001]$ $p4gm$ | Along $[100]$ $p2gg$ | Along $[110]$ $p2gm$ |
| $a' = a$ $b' = b$ | $a' = b$ $b' = c$ | $a' = \frac{1}{2}(-a + b)$ $b' = c$ |
| Origin at $0, \frac{1}{2}, z$ | Origin at $x, \frac{1}{2}, \frac{1}{2}$ | Origin at $x, x, 0$ |
| Maximal non-isomorphic subgroups | | |
| I | [2] $P4_1, 1$ ($P4_1, 78$) | 1; 2; 3; 4 |
| | [2] $P2_1, 2$ ($C222, 20$) | 1; 2; 7; 8 |
| | [2] $P2_1, 2, 1$ ($P2_1, 2, 2, 19$) | 1; 2; 5; 6 |
| IIa | none | |
| IIb | none | |
| Maximal isomorphic subgroups of lowest index | | |
| IIc | [3] $P4_3, 2, 2$ ($c' = 3c$) (92); [5] $P4_3, 2, 2$ ($c' = 5c$) (96); [9] $P4_3, 2, 2$ ($a' = 3a, b' = 3b$) (96) | |
| Minimal non-isomorphic supergroups | | |
| I | [3] $P4_3, 32$ (212) | |
| II | [2] $C4_2, 22$ ($P4_2, 22, 95$); [2] $I4_2, 22$ (98); [2] $P4_3, 2, 2$ ($c' = \frac{1}{3}c$) (94) | |

Table 1

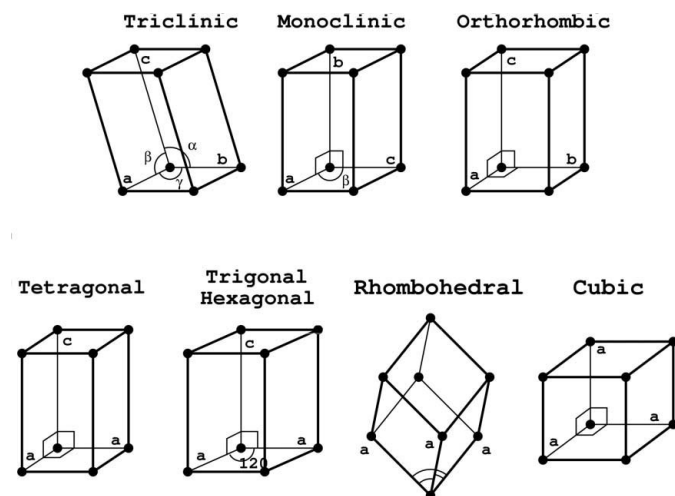
The seven crystal systems, with their characteristic symmetry and restrictions on unit-cell geometry.

| System | Unit-cell dimensions | Unit-cell angles (°) | Characteristic symmetry |
|--------------|----------------------|---|---|
| Triclinic | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma \neq 90$ | Only inversion center possible |
| Monoclinic | $a \neq b \neq c$ | $\alpha = \gamma = 90, \beta \neq 90$ | Single twofold axis or/and mirror |
| Orthorhombic | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90$ | Three perpendicular twofold axes or/and mirrors |
| Tetragonal | $a = b \neq c$ | $\alpha = \beta = \gamma = 90$ | One fourfold axis |
| Trigonal | $a = b \neq c$ | $\alpha = \beta = 90, \gamma = 120$ | One threefold axis |
| | $a = b = c$ | $\alpha = \beta = \gamma \neq 90$ | |
| Hexagonal | $a = b \neq c$ | $\alpha = \beta = 90, \gamma = 120$ | One sixfold axis |
| Cubic | $a = b = c$ | $\alpha = \beta = \gamma = 90$ | Four threefold axes |

preted as 'do not have to be equal' rather than 'have to be different'. For example, $\alpha \neq \beta \neq \gamma \neq 90^\circ$ means that α , β and γ do not have to be equal to each other and do not have to equal 90° . Nevertheless, it may happen by chance that a crystal with all cell dimensions equal and all cell angles of 90° may not have four threefold axes and, therefore, will belong to one of the lower-symmetry systems and not to the cubic system.

The shapes of the unit cells in all the crystal systems are shown in Fig. 2.

A note about the trigonal and hexagonal systems is necessary. In both systems, the same unit cell is chosen, although in the former case only a threefold symmetry is present, whereas the hexagonal system is characterized by the presence of a sixfold axis. For this reason, the trigonal and hexagonal systems are sometimes referred to jointly as the 'hexagonal family'. In addition, trigonal symmetry can be realized in a different way, with a single threefold axis along the body diagonal of a rhombohedral cell, which resembles a 'stretched'

**Figure 2**

The shape of the unit cells in different crystal systems. The unit-cell edges are in general a , b , c , but when there are relations of equality among them, this is indicated by repeating the same symbol. For instance, in the cubic system, the three edges are of equal length (and mutually perpendicular). The rhombohedral cell is a special case of a trigonal cell. It has a threefold axis along its body diagonal (extended direction); therefore, the three unit-cell edges must have the same length and the three unit-cell angles must be equal.

(or 'squeezed') cube with equal cell dimensions ($a = b = c$) and equal cell angles ($\alpha = \beta = \gamma \neq 90^\circ$).

2.2. Symmetry operations and point groups

A symmetry operation is a transformation of an object such that the resulting situation is undistinguishable from the initial one. All symmetry operations (or the corresponding symmetry elements) can be divided into proper rotations around certain axes and improper rotations (rotoinversions) arising as a combination of a rotation with inversion at a point. The crystallographic notation (called international or Hermann–Mauguin notation) represents a proper axis by a number (1, 2, 3, 4 or 6) corresponding to its order, that is to the number of consecutive elementary rotations that will restore the object to its initial orientation. For example, 4 represents the fourfold axis, which consists of four possible rotations: by 90° , 180° , 270° and 360° , where the last rotation, by 360° (effectively equivalent to 0° rotation), is trivial and does not move the object at all. The axis N involves N individual rotations by $n \times 360^\circ/N$ (where $1 \leq n \leq N$). Rotoinversions are represented by a number with a bar above, e.g. $\bar{6}$ (pronounced six bar).

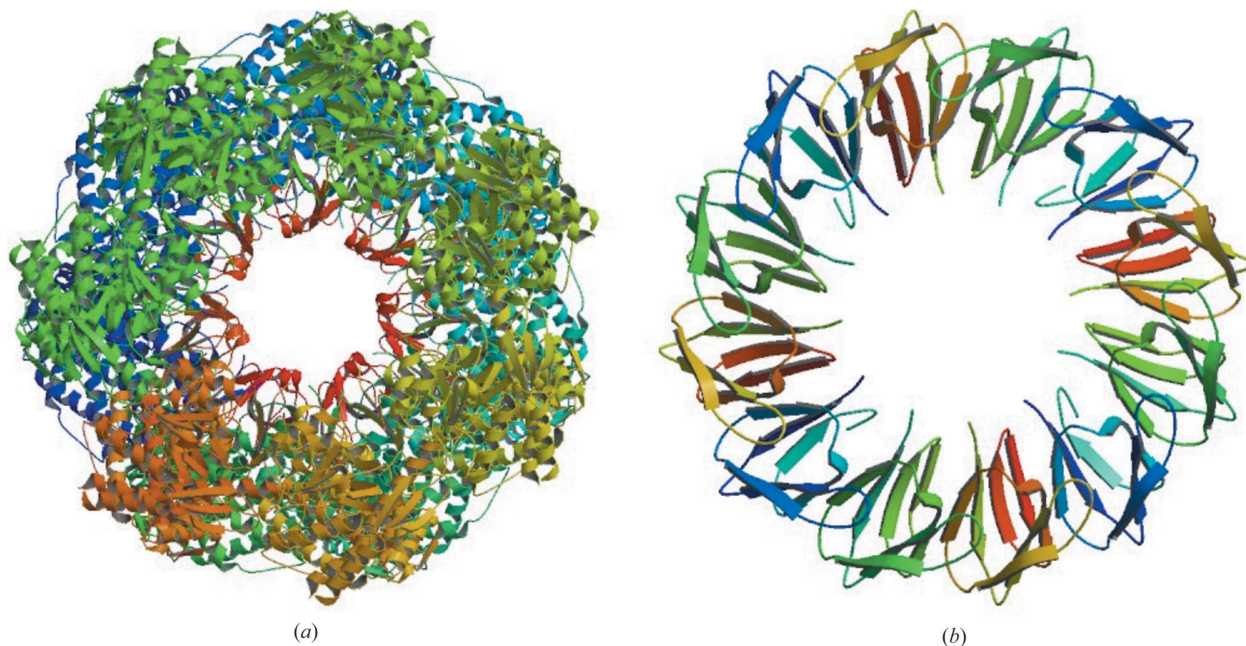
In principle, physical objects (e.g. molecules) may be characterized by a rotation axis of any order. The extreme example is a sphere, possessing an infinite number of all possible rotation and rotoinversion axes. Fig. 3 shows some examples from the Protein Data Bank (PDB; Berman *et al.*, 2000) of oligomeric protein complexes with high rotational symmetry.

However, because crystals have periodic lattices, built from identical unit cells, their rotational symmetry is restricted to the above five types of symmetry axes. Together with the inversion axes, the inventory of individual symmetry elements possible for the external shapes of crystals is thus as follows: 1, 2, 3, 4, 6, $\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$, $\bar{6}$.

A note about the inversion axes is required. The $\bar{1}$ axis effectively represents a center of symmetry, since the rotational component of this axis (360°) is trivial. The operation of $\bar{2}$ is equivalent to reflection in a mirror plane that is perpendicular to the direction of the axis. For this reason, the symbol $\bar{2}$ is not used and the symbol m (mirror) is used instead. Since the improper, or rotoinversion, axes involve inversion, they change the handedness of chiral objects. As a consequence, optically pure compounds (such as natural proteins or nucleic acids) cannot form crystals possessing rotoinversion symmetry elements.

The action of proper rotations is rather easy to visualize, but improper rotations require a certain degree of abstraction to visualize their effect. For a chemist, it may be instructive to analyze the transformations of the molecule of methane, CH_4 , illustrated in Fig. 4.

Real, finite, objects can (and usually do) possess several symmetry elements simultaneously. However, the combined action of two symmetry operations must result in a transformation that corresponds to an existing symmetry element of that object. This, and some other formal requirements, are the principles of the mathematical group theory that is the rigorous framework for the theory of crystallographic

**Figure 3**

(a) Sevenfold symmetry of the chaperone GP3 complex (PDB code 2cgt; Clare *et al.*, 2006); (b) 12-fold symmetry of an oligomeric molecule of the Trap3 mutant (PDB code 2zd0; Watanabe *et al.*, 2008).

symmetry. All the rotation axes (proper and improper) must pass through the center of the object; hence there is always at least one point that remains invariant, *i.e.* does not move under the action of any of the symmetry operations. These two properties are the reason why the set of all symmetry operations of a finite object is called a point group.

The examples in Fig. 5 illustrate the point symmetry of the molecules of chloromethane and dichloromethane. Chloromethane (CH_3Cl) has a threefold axis and three mirror planes intersecting at this axis, and it belongs to the point group $3m$ (C_{3v}). Dichloromethane (CH_2Cl_2) has a twofold axis and two intersecting mirror planes and belongs to the point group $mm2$ (C_{2v}). The symbols used in these examples are in the Hermann–Mauguin notation used in crystallography and (in parentheses) in the Schönflies notation that is more popular in spectroscopy.

There are 32 possible consistent combinations of the proper and rotoinversion axes restricted to order 1, 2, 3, 4 and 6. There are therefore only 32 possible crystallographic point groups, also known as crystal classes, and they are listed in Table 2. Again, the concept of a point group is relevant to finite objects and is appropriate, for example, for the description of the shapes of crystals. This concept was introduced and used to classify crystalline specimens to various crystal classes even before their internal structures became known.

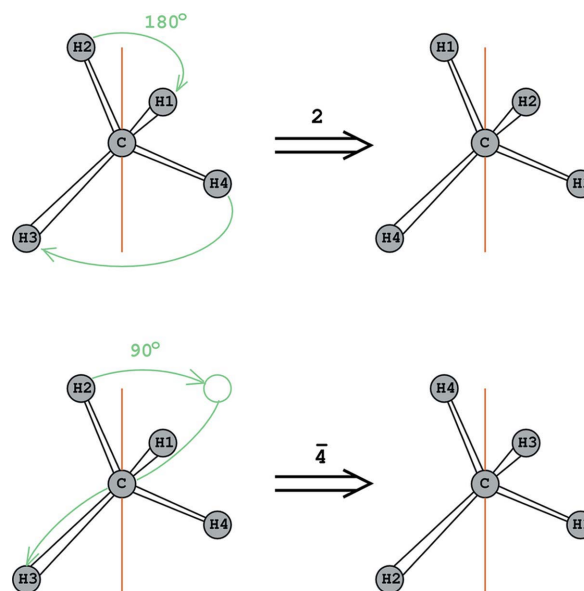
Out of the 32 crystallographic point groups, 11 possess only proper rotations and may characterize crystals of chiral compounds. Nonchiral molecules or racemic mixtures can form crystals in any point group, with or without rotoinversions.

The Hermann–Mauguin symbols of symmetry groups allow a complete reconstruction of the symmetry because they are

based on a set of logical rules. A point-group symbol consists of a maximum of three places describing the symmetry of various directions according to the crystal system.

(a) In the triclinic system, the single place describes the presence ($\bar{1}$) or absence (1) of an inversion center.

(b) In the monoclinic system, the single place describes the character of the y -axis direction.

**Figure 4**

The molecule of methane, CH_4 , with its H atoms labeled to guide the eye, can be transformed by the action of a proper twofold axis (upper panel) and by the action of the $\bar{4}$ rotoinversion axis (lower panel). In addition, the molecule has (not shown) four threefold axes along the C–H bonds, and six mirror planes defined by the six possible H–C–H planes (H1–C–H2, H3–C–H4, H1–C–H3, H2–C–H4 *etc.*).

Table 2

The 32 crystallographic point groups.

The point groups indicated in bold contain only proper rotations, *i.e.* they are applicable to chiral objects, whereas the remaining ones are not.

| System | International notation | Schönflies notation |
|--------------|---|--|
| Triclinic | 1 , $\bar{1}$ | C_1 , C_i |
| Monoclinic | 2 , m , $2/m$ | C_2 , C_s , C_{2h} |
| Orthorhombic | 222 , $mm2$, mmm | D_2 , C_{2v} , D_{2h} |
| Tetragonal | 4 , $\bar{4}$, $4/m$ | C_4 , S_4 , C_{4h} |
| | 422 , $42m$, $4mm$, $4/m\ mm$ | D_4 , D_{2d} , C_{4v} , D_{4h} |
| Trigonal | 3 , $\bar{3}$, 32 , $3m$, $\bar{3}m$ | C_3 , C_{3i} , D_3 , C_{3v} , D_{3d} |
| Hexagonal | 6 , $\bar{6}$, $6/m$ | C_6 , C_{3h} , C_{6h} |
| | 622 , $\bar{6}2m$, $6mm$, $6/m\ mm$ | D_6 , D_{3h} , C_{6v} , D_{6h} |
| Cubic | 23 , $m\bar{3}$, 432 , $43m$, $m\bar{3}m$ | T , T_h , O , T_d , O_h |

(c) The three consecutive places in an orthorhombic symbol describe the symmetry of the x , y and z axes, in that order.

(d) The first place of a tetragonal symbol describes the symmetry of the z axis. If in the equatorial plane (xy) there are also symmetrical directions, they are described in the second (x and y) and third (their diagonals) place.

(e) The convention in the hexagonal and trigonal systems is as in the tetragonal system.

(f) A cubic symbol is distinguished by '3' in the second place, which refers to the four body diagonals of a cube. The first place describes the symmetry of the equivalent x , y and z axes. The third place (if necessary) is reserved for the plane diagonals between the axial directions.

(g) An axis with a perpendicular mirror plane is denoted in the form of a fraction, *e.g.* $2/m$ (pronounced two-upon- m).

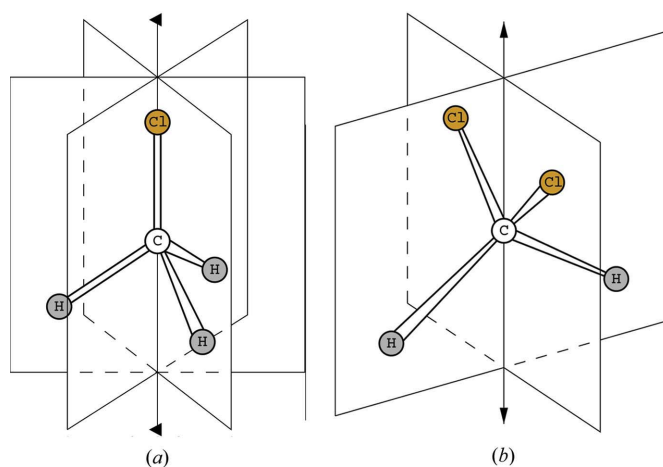
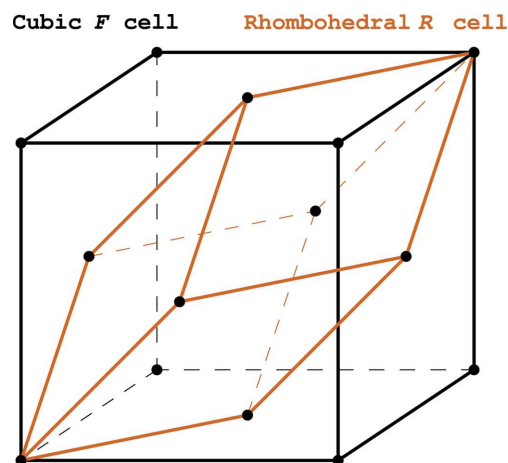
Briefly, in the Schönflies notation, C (cyclic) denotes an axis with its order specified in subscript, S (*Spiegel*) denotes an improper axis (in variance with the crystallographic roto-inversions, Schönflies uses roto-reflections, *i.e.* combinations of rotations with mirror reflection), O refers to symmetry characteristic for an octahedron, T refers to that for a tetrahedron and D (dihedral) denotes a dyad perpendicular to the principal axis. There can be 0, 1 or 2 indices [general form $A_{n\sigma}$, where n denotes the order of the principal axis (1, 2, 3, 4 or 6) and σ denotes a plane of symmetry], which can be horizontal (h), vertical (v) or in a diagonal direction (d). Exceptionally, the index can be i (inversion center) or s (only a mirror plane present).

2.3. Lattices and space groups

The concept of a point group is applicable to finite objects, displaying the symmetry of rotation axes proper or combined with inversion around a point. However, periodic crystals consist of very large numbers of identical unit cells, stacked in a parallel fashion in three dimensions. The principle governing this architecture is periodicity or translation. The individual unit cell can be translated by any integer number of its edges, which are defined by three vectors \mathbf{a} , \mathbf{b} and \mathbf{c} . These shifts can be expressed as $n_1\mathbf{a} + n_2\mathbf{b} + n_3\mathbf{c}$, where n_1 , n_2 and n_3 are arbitrary integers (positive, negative or zero). The set of points generated by all these translations is called a lattice, and it can be considered as an abstract representation of the crystal

interior. In the simplest, or primitive (P), case, the lattice points, called nodes, have only integral coordinates, *i.e.* are located only at unit-cell corners [(0, 0, 0) and all translation equivalents]. In some situations, however, in order to properly reflect the symmetry of the entire crystal interior, a larger unit cell must be selected, with an additional node at its center (I), with a node on a pair of opposite faces (C) or with an extra node on each face (F). The extra nodes in the centered lattices have the following coordinates: I : $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$; C : $\frac{1}{2}, \frac{1}{2}, 0$; and F : $\frac{1}{2}, \frac{1}{2}, 0$; $\frac{1}{2}, 0, \frac{1}{2}$; $0, \frac{1}{2}, \frac{1}{2}$. As a result, the P cells form a single lattice, the C and I cells form double lattices, and the F cells form a quadruple lattice.

To illustrate the need for centered unit cells, let us consider the example of Fig. 6. The rhombohedron (with $\alpha = 60^\circ$) shown in brown forms a primitive cell but has only one threefold axis, whereas the lattice as a whole is cubic and displays four threefold axes, in the directions of the four body diagonals of the cube (plus three fourfold axes, six twofold axes and a number of other symmetry elements). The higher cubic symmetry is apparent if the unit cell is expressed as a

**Figure 5**Point-group symmetry: (a) $3m$ of chloromethane (CH_3Cl) and (b) $mm2$ of dichloromethane (CH_2Cl_2).**Figure 6**Rhombohedral R cell (brown) inscribed in an F -centered cubic cell (black).

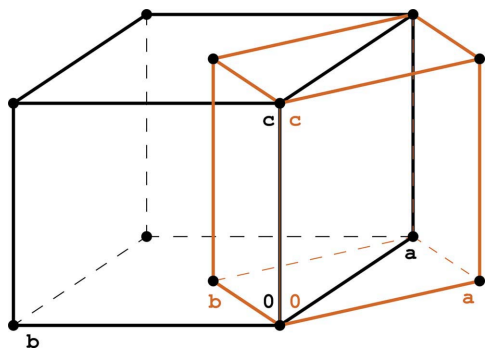


Figure 7
The tetragonal *P* unit cell (brown) has the same symmetry as the *C* cell (black), but is two times smaller.

cube with additional nodes at the centers of all faces, as shown in black.

The rules for selection of the unit cell are as follows: the cell should be the smallest and the simplest, but have the highest possible symmetry, with increasing priority of these three conditions.

Not all centering types exist in some crystal systems. For example, centering of the triclinic cell, with no conditions imposed on its shape and no symmetry higher than an inversion center, makes no sense, since it is always possible to define a smaller and primitive cell of the same, triclinic symmetry. *C*-centering of a tetragonal cell would not lead to any benefit, since such a cell could be reduced to a primitive cell with half the size and the same tetragonal symmetry, after a rotation by 45° around *z*, as illustrated in Fig. 7. *C*-centering of a cubic cell would violate the threefold symmetry, which requires the faces to be equivalent, and so on.

Taking into account all unique possibilities, there are 14 types of unit cells, also known as the Bravais lattices, as presented in Fig. 8.

A special situation occurs in the case of rhombohedral cells, which are primitive from the point of view of centering but have a threefold axis aligned with a body diagonal. The shape of this rhombohedral *R* cell is thus different from the shape of the trigonal and hexagonal *P* cells expressed in hexagonal axes, where the threefold (or sixfold) axis is perpendicular to the *ab* base of the unit cell. It is possible to express the rhombohedral *R* cell in hexagonal axes, as shown in Fig. 9. The hexagonal cell is, however, three times larger than the *R* cell and has additional nodes at $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$ and $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$. It is sometimes denoted *H*, to emphasize the use of hexagonal axes, but this notation is not part of the current crystallographic convention.

The presence of lattice centering and, therefore, of additional nodes means that any object (for example an atom) present at coordinates (x, y, z) will be repeated after parallel translation by the centering vector(s) to the following locations:

$$C\text{-centering: } x + \frac{1}{2}, y + \frac{1}{2}, z$$

$$I\text{-centering: } x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$$

$$F\text{-centering: } x + \frac{1}{2}, y + \frac{1}{2}, z; x + \frac{1}{2}, y, z + \frac{1}{2}; \text{ and } x, y + \frac{1}{2}, z + \frac{1}{2}$$

Translation can be combined with other symmetry operations, namely rotations and mirror reflections, resulting in symmetry elements with translational components, called, respectively, screw axes and glide planes. A screw axis combines a rotation with a translation along the axis. The translation is not arbitrary: when all elementary rotations sum up to a full rotation, the combined translations must bring us to a lattice point equivalent to the starting one in a neighboring unit cell. A screw axis is denoted by N_n , where *N* is the axis order and *n* is a natural number $1 \leq n < N$. In its elementary action, the axis rotates a point by $360^\circ/N$ and at the same time moves it by n/N of its translation vector. If $n/N < \frac{1}{2}$, the axis is right-handed, *i.e.* a clockwise rotation, when viewed along the axis vector, is accompanied by a movement of n/N of this vector. If $n/N > \frac{1}{2}$, the axis is left-handed, which means that a counterclockwise rotation is coupled with an axial transla-

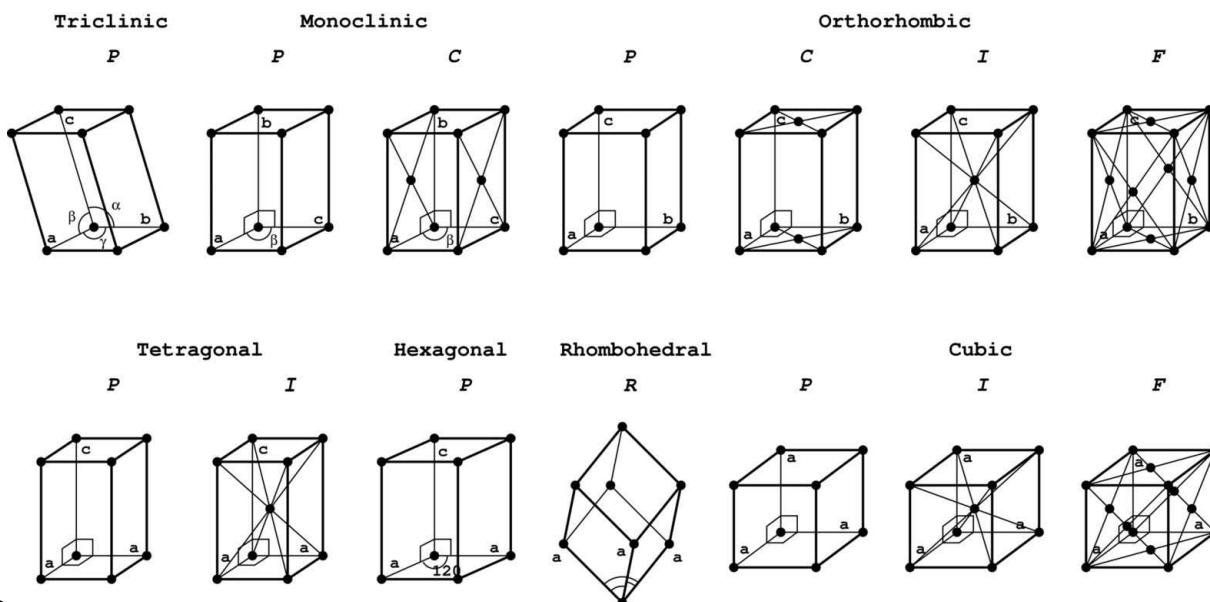
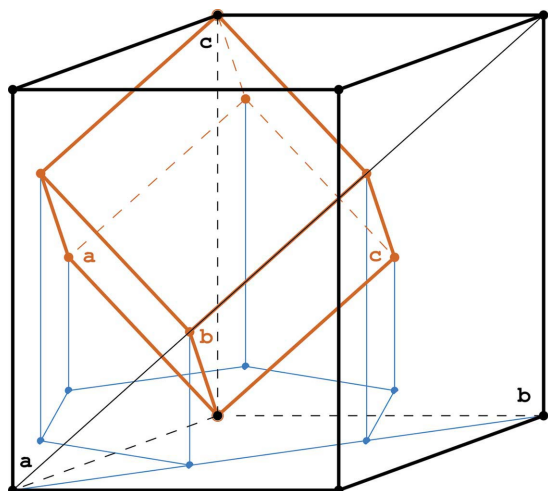


Figure 8
The 14 Bravais lattices.


Figure 9

The relation between the rhombohedral R cell (brown) and the hexagonal H cell (black). The projection of the rhombohedron onto the ab base of the hexagonal cell is also shown (in blue).

tion complementing n/N , i.e. $(1 - n/N)$. A screw axis with $n/N = \frac{1}{2}$ is neutral (Fig. 10). To properly assign handedness to a screw axis, imagine that you are climbing up a spiral staircase. If you grip the outer railing with your right hand, the axis of this staircase is right-handed.

A glide plane combines a mirror reflection with a translation by (usually, albeit not always) $1/2$ of a lattice translation parallel to its plane (Fig. 11). A glide with $\mathbf{a}/2$ translation is called a . It can be normal to \mathbf{y} or to \mathbf{z} . Similarly, glide planes b ($\mathbf{b}/2$ translation) can be normal to \mathbf{x} or \mathbf{z} , but not to \mathbf{y} . Glide planes c ($\mathbf{c}/2$ translation) obey analogous rules. In some centered lattices, a ‘double’ glide plane can be present, with

two translations possible simultaneously along two lattice directions. Such planes are denoted e .

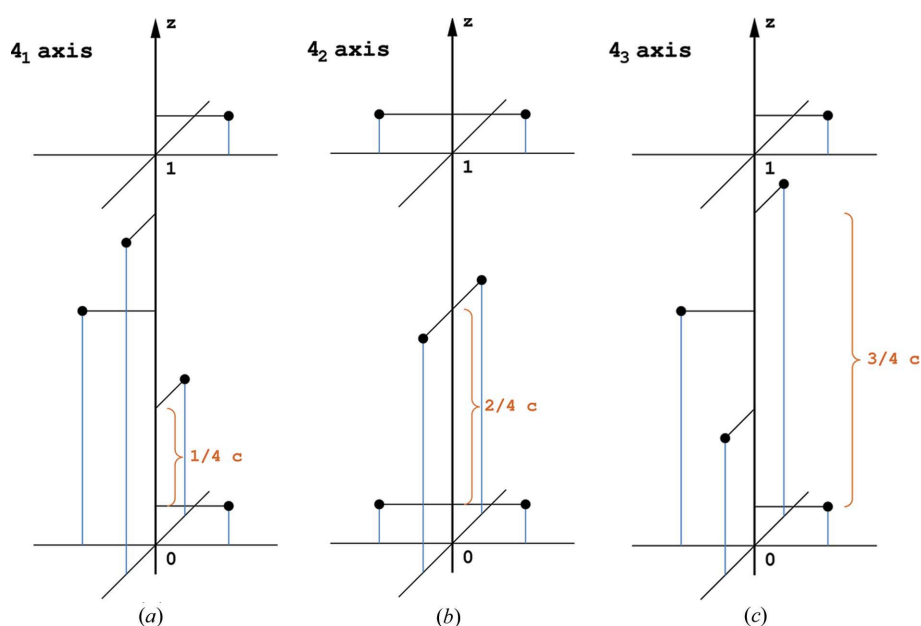
The gliding translation can also have a diagonal direction. If it is equal to $1/2$ of a diagonal translation then the glide plane is termed n and can be perpendicular to \mathbf{x} , \mathbf{y} or \mathbf{z} . Such gliding translations can be $(\mathbf{b} + \mathbf{c})/2$, $(\mathbf{a} + \mathbf{c})/2$ or $(\mathbf{a} + \mathbf{b})/2$. In special cases, only in centered lattices, the gliding vector can be equal to $1/4$ of a diagonal translation. This elegant glide plane is called a ‘diamond’ plane (d) owing to its presence in the crystals of diamond. Because of various diagonal combinations, there are different d planes with the following translations: $(\mathbf{a} \pm \mathbf{b})/4$, $(\mathbf{a} \pm \mathbf{c})/4$, $(\mathbf{b} \pm \mathbf{c})/4$. Again, a repeated operation of a glide plane moves the point to a position equivalent to the original one, but located in the next unit cell.

Special graphical symbols are used to mark various operators in symmetry diagrams (Fig. 12). Blackened lenses, triangles, squares or hexagons depict the two-, three-, four- or sixfold axes perpendicular to the plane of projection. Additional ‘arms’ or ‘blades’ ornamenting these shapes correspond to screw axes of various kinds. The inversion six- and fourfold axes have special symbols, and the center of inversion is represented by a small circle, which is also found in the graphical symbol of the $\bar{3}$ axis. Twofold proper or screw axes in the plane of the diagram are shown as full or half arrows, respectively. Mirror and glide planes in the plane of the diagram are shown as angular corners, if necessary equipped with arrows along the direction of a glide translation. Symmetry planes perpendicular to the diagram are shown with a full line (mirror), dashed line (glide with a translation in the plane of the diagram), dotted line (glide with a translation perpendicular to the plane of the diagram), dash-dot line (glide plane n , with translation 45° out of plane), dash-double-dot line (glide plane e , with translations both in and out of the

plane of the diagram) or dash-dot line with arrows (glide plane d , with 45° translation of $1/4$). A symmetry element parallel to the plane of the diagram, but lying above its zero level, is accompanied by a number (fraction of the perpendicular cell length) corresponding to its height.

Higher-symmetry axes include the simultaneous presence of some lower-symmetry operations, as shown in the list below. For example, if a fourfold axis is present then a twofold rotation around the same axis must also be present.

- 4 includes 2
- 4_1 includes 2_1
- 4_2 includes 2
- 6 includes 3 and 2
- 6_1 includes 3_1 and 2_1
- 6_2 includes 3_2 and 2
- 6_3 includes 3 and 2_1
- 6_4 includes 3_1 and 2
- 6_5 includes 3_2 and 2_1


Figure 10

The operation of the three fourfold screw axes: (a) the right-handed 4_1 axis, (b) the neutral 4_2 axis and (c) the left-handed 4_3 axis.

Table 3
Examples of space-group symbols in all crystal systems.

| Crystal system | Example | Explanation |
|----------------|--------------------|--|
| Triclinic | $P1, P\bar{1}$ | Only center of inversion is possible |
| Monoclinic | $C2, P2_1/m$ | Only twofold symmetry in one direction (y) is possible |
| Orthorhombic | $P222_1, Fdd2$ | Twofold symmetry along x , then y , then z |
| Tetragonal | $P4_3, I4_1/amd$ | Fourfold symmetry along z , then x (y), then xy diagonal |
| Trigonal | $P3_2, P\bar{3}m2$ | Threefold symmetry along z , then x (y), then xy diagonal |
| | $R3, R\bar{3}2$ | Threefold symmetry along space diagonal, then perpendicular to it |
| Hexagonal | $P6_2, P6/mcc$ | Sixfold symmetry along z , then x (y), then xy diagonal |
| Cubic | $P2_13, F432$ | Symmetry along x (y, z), then threefold space diagonals, then face diagonals |

Much in the same way as sets of point-symmetry elements combined into point groups were used to describe the symmetry of finite objects (crystals), combinations of symmetry operations of infinite and periodic crystal lattices correspond to the 230 space groups. Only 65 of the space groups do not include improper symmetry elements. As the name 'space group' suggests, there are no invariant points, since the lattice translations, always present, do not leave any point unmoved.

The Hermann–Mauguin symbol of a space group is constructed by specifying first the Bravais lattice and then, in the same order as in the symbol of the corresponding point group, the symmetry of the characteristic directions (Table 3). It is not possible to construct a Schönflies symbol for a space group in a logical way. Therefore, all space groups belonging to the same point group (with a unique Schönflies symbol) are distinguished by a consecutive number in superscript, e.g. C_{2h}^5 ($P2_1/c$).

In the triclinic system, there are only two space groups possible, $P1$ and $P\bar{1}$. In the monoclinic system, where symmetry is restricted to the y direction, we can have a twofold axis (proper or screw) parallel to y , or/and a plane (mirror or glide) perpendicular to y , but the full symbol, e.g. $C_{12/m1}$, is usually shortened to look like $C2/m$. Orthorhombic

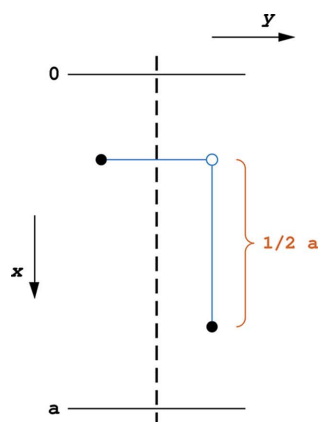


Figure 11

The operation of glide plane a perpendicular to y . The x axis runs down the page and is perpendicular to the y axis (across the page).

space groups require specification of symmetry in three directions, x , y and z , in that order. In tetragonal, trigonal and hexagonal space groups the first place after the Bravais symbol refers to the z direction, the second to the x or y directions (both are equivalent), and the third to the diagonal direction between x and y . If there are no symmetry elements in the last two directions, these positions are omitted and only that related to z is present. In cubic symmetry, the first position refers to x (or y or z , which are all equivalent), the second (3 or $\bar{3}$) to space diagonals (all four of them) of the cube and the third (if it exists, a twofold axis or a mirror) to the directions (six of them) parallel to the diagonals of the cube faces. In the rhombohedral (R) lattice, the first character (3 or $\bar{3}$) denotes the unique space diagonal of the cell and the next defines the directions that are perpendicular to the threefold axis. It is important to remember that an axis in a given direction is parallel to this direction, while a symmetry plane in a given direction is perpendicular to it. Thus, in the monoclinic space group $P2_1/c$, the two symmetry elements listed in the space-group symbol, 2_1 and c , refer to the y direction, but have, of course, mutually perpendicular geometrical disposition.

The main purpose of Volume A of *International Tables for Crystallography* is to present a detailed dissection of each of the space groups with special emphasis on graphical representation. The diagrams are usually drawn in projection along z . All three projections are shown for the low-symmetry systems (triclinic, monoclinic, orthorhombic), whereas a complicated system for illustrating the complex symmetry is used for the highest-symmetry cubic space groups.

The diagrams for two trigonal space groups, $P321$ and $P312$, are shown in Fig. 13. These two space groups should not be confused, although both belong to the same 32 class and have the same assortment of symmetry operations. However, in $P321$ the twofold axes are parallel to the cell edges a and b , whereas in $P312$ the twofold axes, although also lying in the xy plane, are rotated 30° from the former directions and are oriented diagonally between the three equivalent lattice directions in the xy plane.

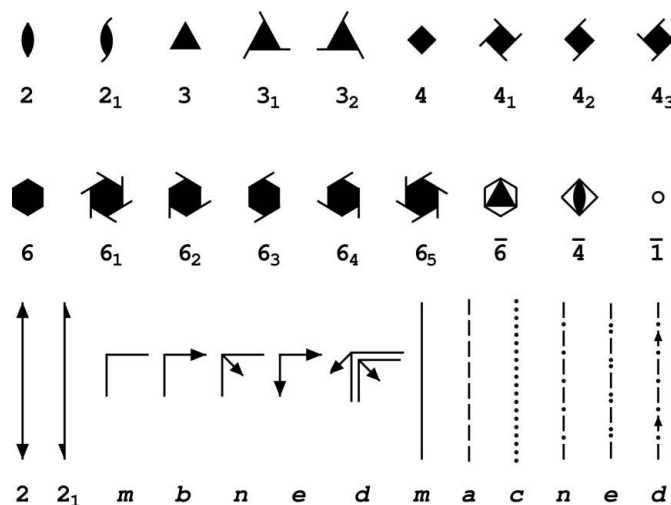


Figure 12

Graphical symbols of crystallographic symmetry elements.

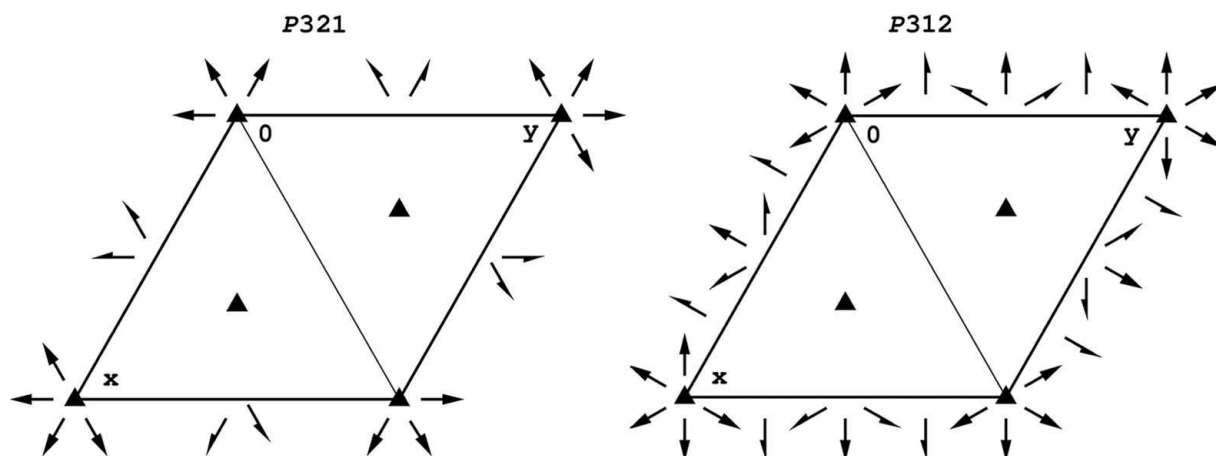


Figure 13
Diagrams of symmetry operations for two trigonal space groups: (left) *P321* and (right) *P312*.

Fig. 14 shows the symmetry diagrams for the orthorhombic space group *Pbcn* in three projections. Different glide planes are marked with appropriate symbols in each projection,

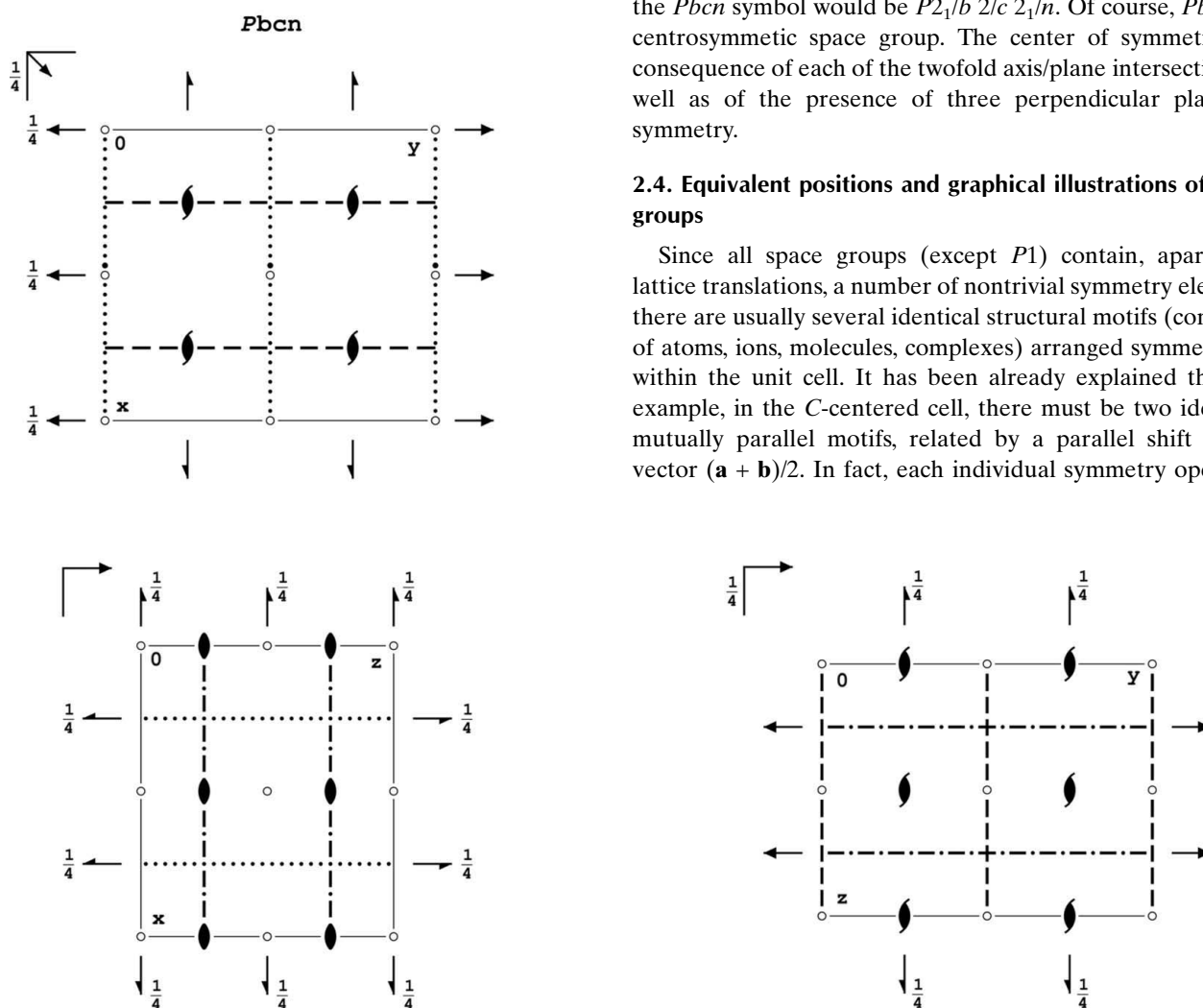


Figure 14
Symmetry diagrams of the orthorhombic space group *Pbcn*, shown in projections along *z* (top), *y* (lower left) and *x* (lower right).

depending on the gliding translation, which can be in the plane of the drawing, perpendicular to it or in a diagonal direction. Two perpendicular planes of symmetry generate a twofold axis parallel to the line of intersection, and thus the full version of the *Pbcn* symbol would be $P2_1/b\ 2/c\ 2_1/n$. Of course, *Pbcn* is a centrosymmetric space group. The center of symmetry is a consequence of each of the twofold axis/plane intersections, as well as of the presence of three perpendicular planes of symmetry.

2.4. Equivalent positions and graphical illustrations of space groups

Since all space groups (except *P1*) contain, apart from lattice translations, a number of nontrivial symmetry elements, there are usually several identical structural motifs (consisting of atoms, ions, molecules, complexes) arranged symmetrically within the unit cell. It has been already explained that, for example, in the *C*-centered cell, there must be two identical, mutually parallel motifs, related by a parallel shift by the vector $(\mathbf{a} + \mathbf{b})/2$. In fact, each individual symmetry operation

always relates a pair of motifs by a specific spatial relation. If two motifs in the crystal are related by a certain symmetry operation, then each part of one motif (a single molecule, group, atom, bond *etc.*) has its counterpart in the other motif, related by the same symmetry operation. It is, therefore, sufficient to represent the symmetry relations within a crystal by specifying the spatial relations between mathematical points placed inside the unit cell. The relation between two points related by a given symmetry element can be illustrated graphically or expressed analytically using their coordinates measured along the three principal directions of the unit cell. Because the unit-cell translations are always present in any space group, it is most convenient to express the coordinates as fractions x , y and z of the unit-cell edges a , b and c , respectively. This simplifies the symmetry considerations, because any unit-cell translation is then simply equivalent to adding an integer number to any or all three fractional coordinates x , y and z . Both methods, graphical and analytical, of describing space-group symmetry relations are found in ITA. For graphical representation, two systems are used: either the unit cell with all symmetry elements is shown in projection, or the unit cell is drawn with all equivalent points generated by the various symmetry operations, also in projection. For low-symmetry groups (triclinic, monoclinic and orthorhombic), three projections with symmetry operators are displayed. For other space groups, only one projection, along the unique threefold or fourfold axis, is present, with the x axis pointing down the page, the y axis to the right and the z axis up towards the viewer.

An example for the space group $P4_32_12$ is shown in Fig. 15.

In Fig. 15(a), the left diagram shows all the symmetry operators present in this space group, represented by their graphical symbols. Visible here are the fourfold screw axes 4_3 and twofold screw axes 2_1 parallel to \mathbf{z} (viewing direction), and also the screw and ordinary twofold axes parallel to the \mathbf{x} , \mathbf{y} and diagonal directions (in the plane of the drawing). Some of the axes with orientation perpendicular to \mathbf{z} are accompanied by fractional numbers, denoting their elevation (expressed as a fraction of the c edge of the unit cell) above the base of the unit cell. Moreover, it is implicitly assumed that these axes (as well as mirror or glide planes, and a center of symmetry, if present) are always accompanied by additional symmetry elements of the same kind located one-half of the unit cell higher. For example, in $P4_32_12$, the 2_1 axes parallel to \mathbf{x} lie at $\frac{1}{8}$ of the c cell parameter above the base, but there also exist 2_1 axes at the level of $(\frac{1}{8} + \frac{1}{2}) = \frac{5}{8}$. Similarly, parallel to \mathbf{y} , there are 2_1 axes at $\frac{3}{8}$ and at $\frac{7}{8}$.

In the right diagram, the symmetry elements are not marked, but a set of small circles is drawn, representing all points that are equivalent by those symmetry operations, within and around the unit cell. Again, a fractional number beside a circle corresponds to the elevation of the point above the base of the cell. The '+' sign designates a point with a positive z coordinate, the '-' sign indicates $-z$. If '+' was assumed to stand for $z = 0.1$, then ' $\frac{1}{2}-$ ' would mean $z = 0.50 - 0.1 = 0.4$ and ' $\frac{1}{4}+$ ' would correspond to $z = 0.25 + 0.1 = 0.35$. The positions of the points presented graphically are also listed

below the diagrams in Fig. 15 in terms of their fractional coordinates.

In Fig. 15(b), the point with coordinates (x, y, z) is marked in brown, together with its equivalents, generated by one lattice translation along the \mathbf{x} and \mathbf{y} directions, which lie in the neighboring unit cells. According to the principle of fractional coordinates, the equivalent points are located at $(x + 1, y, z)$, $(x, y + 1, z)$ and $(x + 1, y + 1, z)$. The four marked points have the same z coordinate but, of course, equivalent points at $z + 1$ (and $z + 2, 3, 4, \dots$) also exist. The lists of general coordinates printed in ITA exclude equivalents generated by pure lattice translation.

In Fig. 15(c), two points are shown related by the 2_1 axis coincident with the cell z axis. If the first point has coordinates (x, y, z) , the second lies at $(\bar{x}, \bar{y}, z + \frac{1}{2})$, and is therefore located in a neighboring unit cell.

The point at $(\bar{x}, \bar{y} + 1, z + \frac{1}{2})$ is also related to (x, y, z) by a 2_1 axis parallel to \mathbf{z} , but shifted to $y = \frac{1}{2}$ (Fig. 15d). This twofold screw axis is implicitly contained in the 4_3 fourfold screw present in the same place, since two individual 90° rotations coupled with two translations by $c/4$ are equivalent to the action of a 2_1 screw along \mathbf{z} .

The two graphical diagrams and the list of equivalent positions are consistent and allow one to deduce which pair of positions (coordinates) is related by which symmetry operation.

2.5. Coordinates and special positions

The number of equivalent points in the unit cell is equal to the number of independent symmetry operations of the space group (disregarding pure lattice translations), *i.e.* to the rank of the group. The coordinates of all symmetry-equivalent positions within the unit cell are listed in ITA in terms of fractional coordinates related to the initial position (x, y, z) .

However, if two positions related, for instance, by a diagonal twofold axis, as in Fig. 16, move toward each other, their coordinates, here (x, y, z) and (y, x, \bar{z}) , become more and more similar. Eventually, these two points coalesce and their common coordinates become $(x, x, 0)$, as illustrated in Fig. 16. Obviously, other pairs of points, related by other twofold axes, will also coalesce to one point; after all, they are symmetry equivalents of the first pair. In conclusion, if a point or a structural motif lies on a nontranslational symmetry element (*i.e.* on a nonscrew axis, mirror or center of inversion), the number of equivalent points or motifs is reduced. Such positions are called 'special', in contrast to the 'general' positions located away from such symmetry elements. Screw axes and glide planes do not constitute special positions, because the translational component always separates the equivalent points. It is important to note that any moiety lying on a special position must itself possess the symmetry of this site. For example, a molecule of water or a sulfate ion in a protein crystal may be located on a twofold axis, but a single polypeptide chain of a protein molecule may not.

In ITA, all special positions (if they exist) are listed immediately under the list of general positions; the multi-

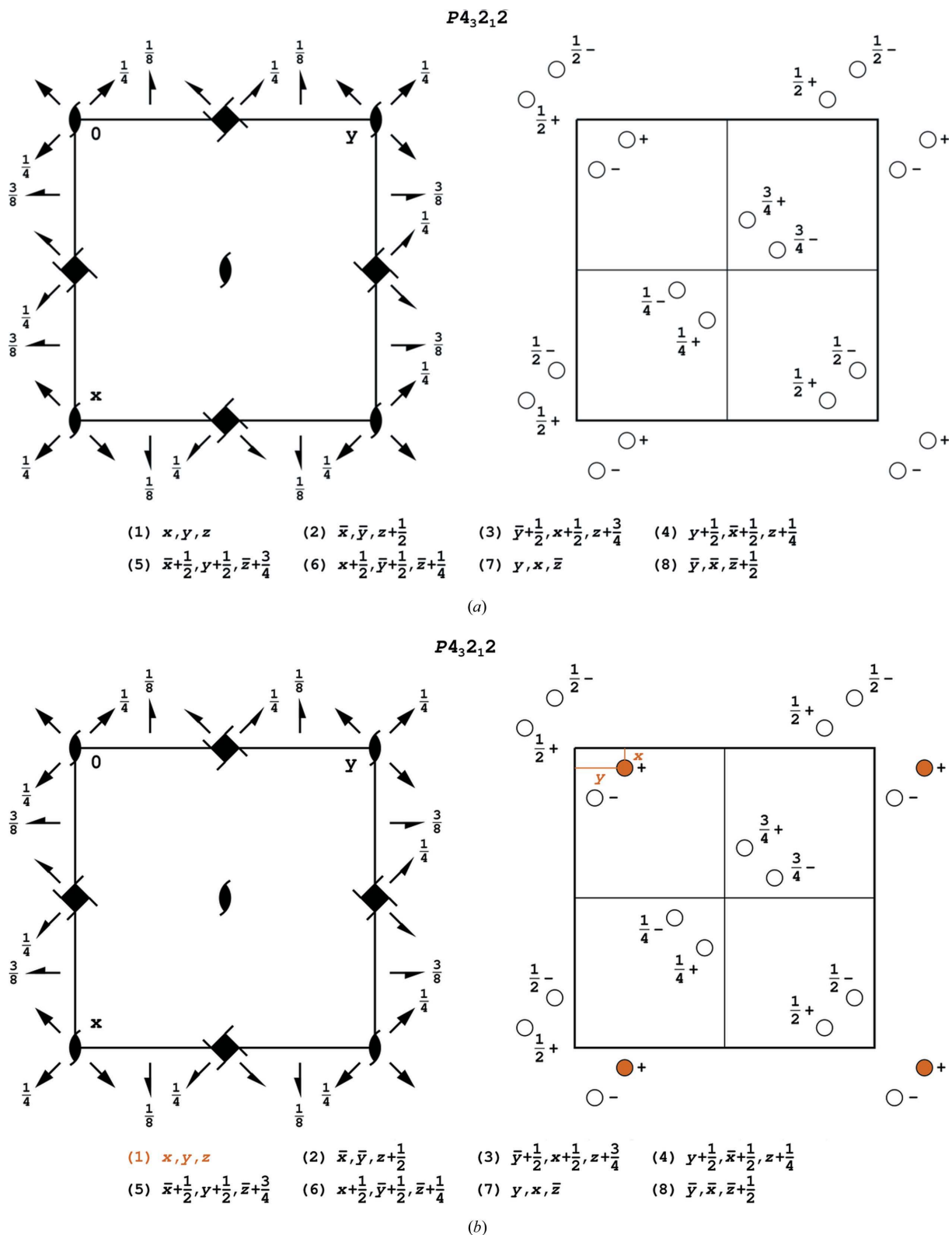
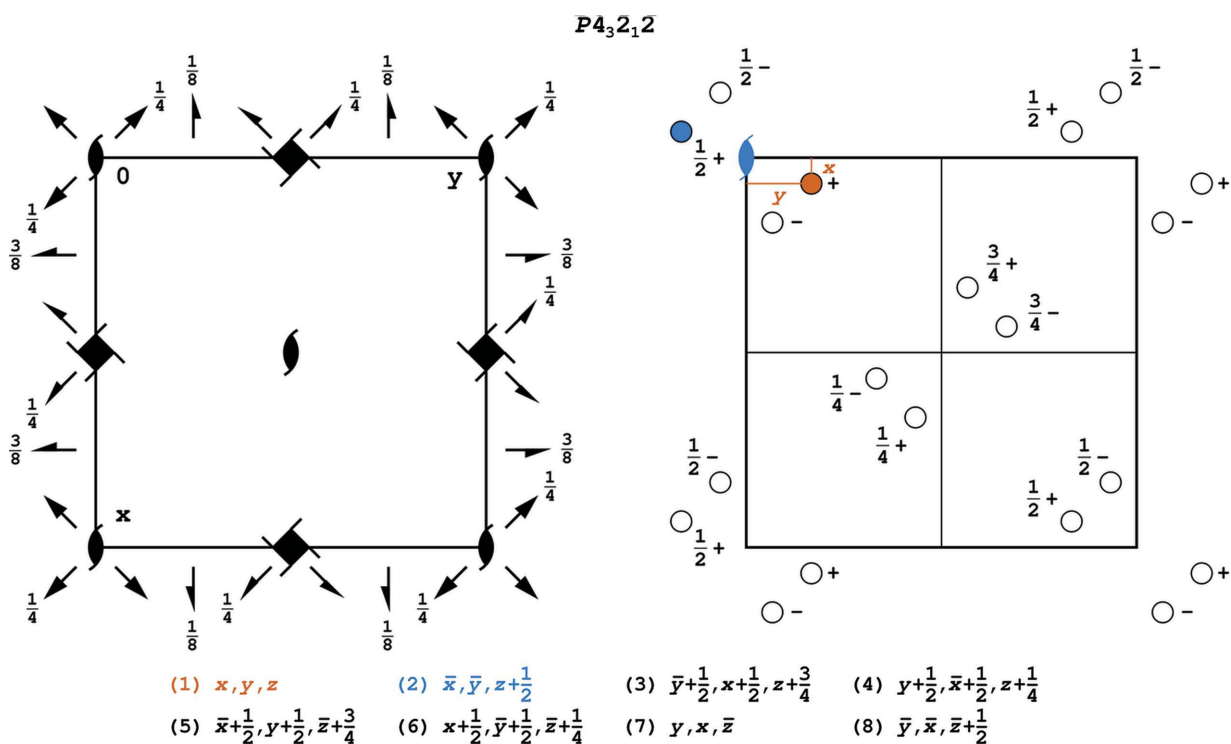
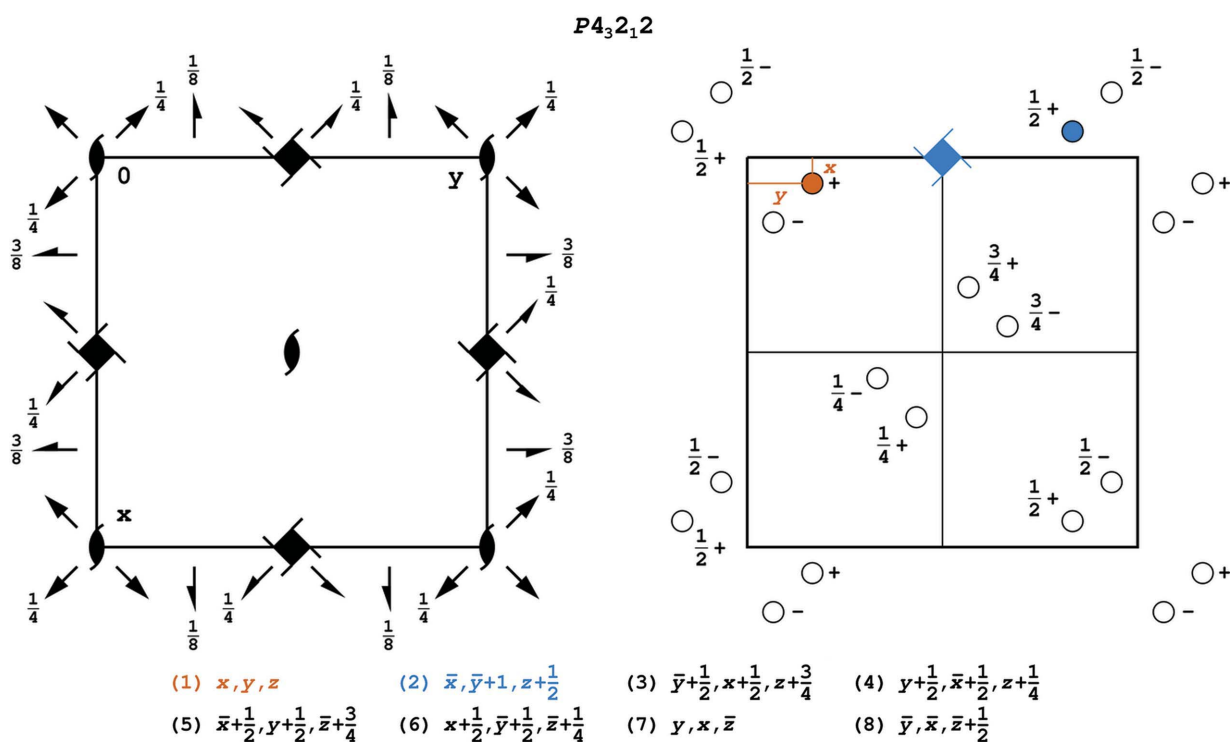


Figure 15 (a) A diagram with symmetry elements (left) and with equivalent points (represented by circles) in general positions (right), together with the fractional coordinates (numbered) of those equivalent positions (bottom list) presented for the space group $P4_32_12$ in the style of ITA. The numbers near the equivalent points refer to their elevation above (or below) the ab base of the unit cell (for example, $\frac{1}{2}-$ stands for $\frac{1}{2} - z$). (b) The same diagrams as in (a) but with the principal point with coordinates (x, y, z) highlighted in brown. Also highlighted are its x - and y -translation equivalents. Coordinates like these (brown), generated by pure lattice translations, are not listed in ITA.



(c)



(d)

Figure 15 (continued)

(c) Two points (colored) in space group $P4_32_12$, related by the 2_1 axis parallel to z located at $(0, 0, z)$. Their coordinates are highlighted by matching colors in the list of equivalent positions below the diagrams. (d) Two points (colored) in space group $P4_32_12$, related by the 2_1 axis parallel to z located at $(0, \frac{1}{2}, z)$, contained within the 4_3 axis at this position. The blue point in this diagram is equivalent to the blue point in (c) by a unit translation along y .

plicity, the Wyckoff letter and the site symmetry are also provided, as in the following examples. The Wyckoff letter corresponds to the traditional nomenclature and has no meaning other than naming all the special positions from the highest to the lowest site symmetry. The site symmetry lists symmetry elements passing through this site in the same order as in the point-group symbol, with the absence of any symmetry in a given direction marked by a dot.

In $P4_32_12$ (Fig. 17), the multiplicity of the general positions is 8 and such a position has no symmetry (onefold axis only).

There is only one type of special position, located on the diagonal dyad, with a multiplicity of 4 and site symmetry 2 (or $\cdot 2$ in full notation).

In $P4_22_12$ (Figs. 18 and 19), there are six sets of special positions, since in this space group there are more proper twofold axes than in $P4_32_12$. Two of these special sets, with a multiplicity of 4, are positioned at the xy diagonal dyads, and another two at the twofold axes parallel to z . The remaining two sets are located at intersections of three twofold axes (two diagonal dyads and one parallel to z), having a multiplicity of 2

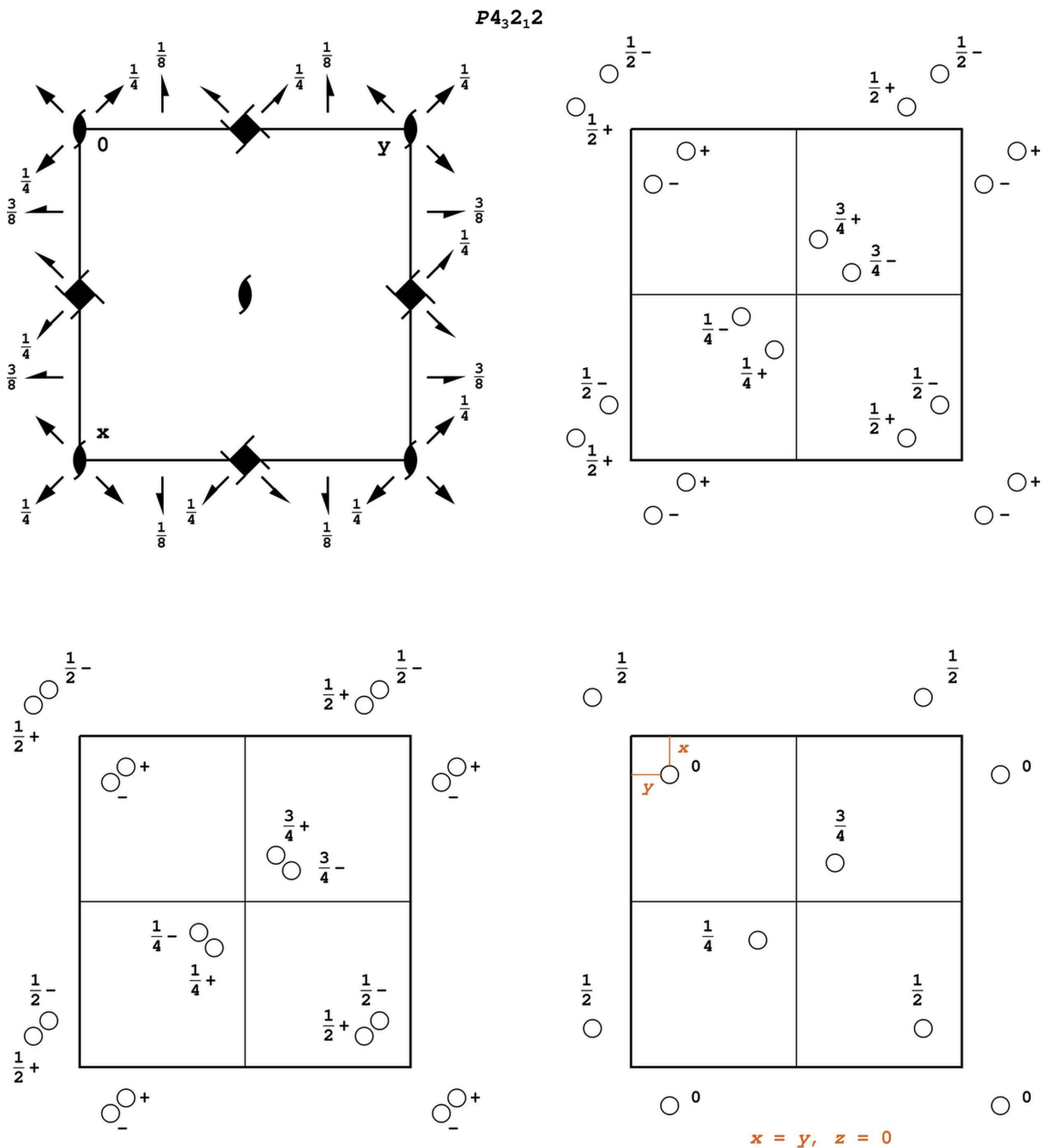


Figure 16

If a point with coordinates (x, y, z) moves toward a point-symmetry element (here a twofold axis in the diagonal direction), the distance to its replica generated by that symmetry operation becomes smaller and smaller. When the point finally lands on this symmetry element (the diagonal twofold axis in this case), the two positions coalesce into one, with coordinates constrained by this particular symmetry element, here $(x, x, 0)$.

and site symmetry 222 . The notation 2.22 indicates that the site symmetry is 222 but that it does not involve any symmetry in the crystallographic x (or y) direction (thus the dot).

For centered lattices, the list of coordinates contains only the set of basic positions, excluding cell centering. However, in a header there is a list of all vectors that have to be added to those coordinates to obtain all positions generated by this space group: see, for instance, the entry for space group $C222_1$ shown in Fig. 20. The multiplicity of the general positions is 8 (Fig. 21), although only four of them are listed. To obtain all positions, it is necessary to add either $(0, 0, 0)$ or $(\frac{1}{2}, \frac{1}{2}, 0)$ to the four positions printed in this list. Analogously, the same centering vectors have to be added to the special positions.

The section 'Symmetry of special projections' defines the unit cells (parallelograms) and their symmetries, obtained when the crystallographic unit cell is projected onto a plane along some characteristic directions. The symmetries of the projections belong to one of the 17 plane groups (analogous to

the 230 three-dimensional space groups), presented in detail in a separate chapter of ITA, but we are not concerned with these aspects here.

2.6. Definition of cell origin

In order to draw the symmetry diagram of a space group and to specify the corresponding equivalent positions, one needs to define the location of the unit cell with respect to all symmetry elements in the lattice. Usually the cell origin is defined at a special point, such as a center of inversion (if it exists) or an intersection of rotation axes. In certain space groups, there are no obvious 'best' places for fixing the unit-cell origin, and it is defined arbitrarily (and always used as specified in ITA). Obviously, in $P1$ the cell origin can be assumed anywhere, since, without any symmetry elements, all positions are equally appropriate. An analogous situation occurs in crystal classes 2, 3, 4 and 6, which possess only a

Space group $P4_32_12$:

| Multiplicity, Wyckoff letter, Site symmetry | Coordinates |
|---|--|
| 8 <i>b</i> 1 | (1) x, y, z (2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{3}{4}$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{4}$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{3}{4}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{4}$ (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z} + \frac{1}{2}$ |
| 4 <i>a</i> ..2 | $x, x, 0$ $\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{4}$ |

Figure 17
Special positions for $P4_32_12$, presented in the style of ITA.

Space group $P4_22_12$:

| Multiplicity, Wyckoff letter, Site symmetry | Coordinates |
|---|--|
| 8 <i>g</i> 1 | (1) x, y, z (2) \bar{x}, \bar{y}, z (3) $\bar{y} + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}$ (4) $y + \frac{1}{2}, \bar{x} + \frac{1}{2}, z + \frac{1}{2}$ (5) $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (6) $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$ (7) y, x, \bar{z} (8) $\bar{y}, \bar{x}, \bar{z}$ |
| 4 <i>f</i> ..2 | $x, x, \frac{1}{2}$ $\bar{x}, \bar{x}, \frac{1}{2}$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, 0$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, 0$ |
| 4 <i>e</i> ..2 | $x, x, 0$ $\bar{x}, \bar{x}, 0$ $\bar{x} + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}$ $x + \frac{1}{2}, \bar{x} + \frac{1}{2}, \frac{1}{2}$ |
| 4 <i>d</i> 2.. | $0, \frac{1}{2}, z$ $0, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z} + \frac{1}{2}$ $\frac{1}{2}, 0, \bar{z}$ |
| 4 <i>c</i> 2.. | $0, 0, z$ $\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, \bar{z} + \frac{1}{2}$ $0, 0, \bar{z}$ |
| 2 <i>b</i> 2.22 | $0, 0, \frac{1}{2}$ $\frac{1}{2}, \frac{1}{2}, 0$ |
| 2 <i>a</i> 2.22 | $0, 0, 0$ $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ |

Figure 18
Special positions for $P4_22_12$, presented in the style of ITA.

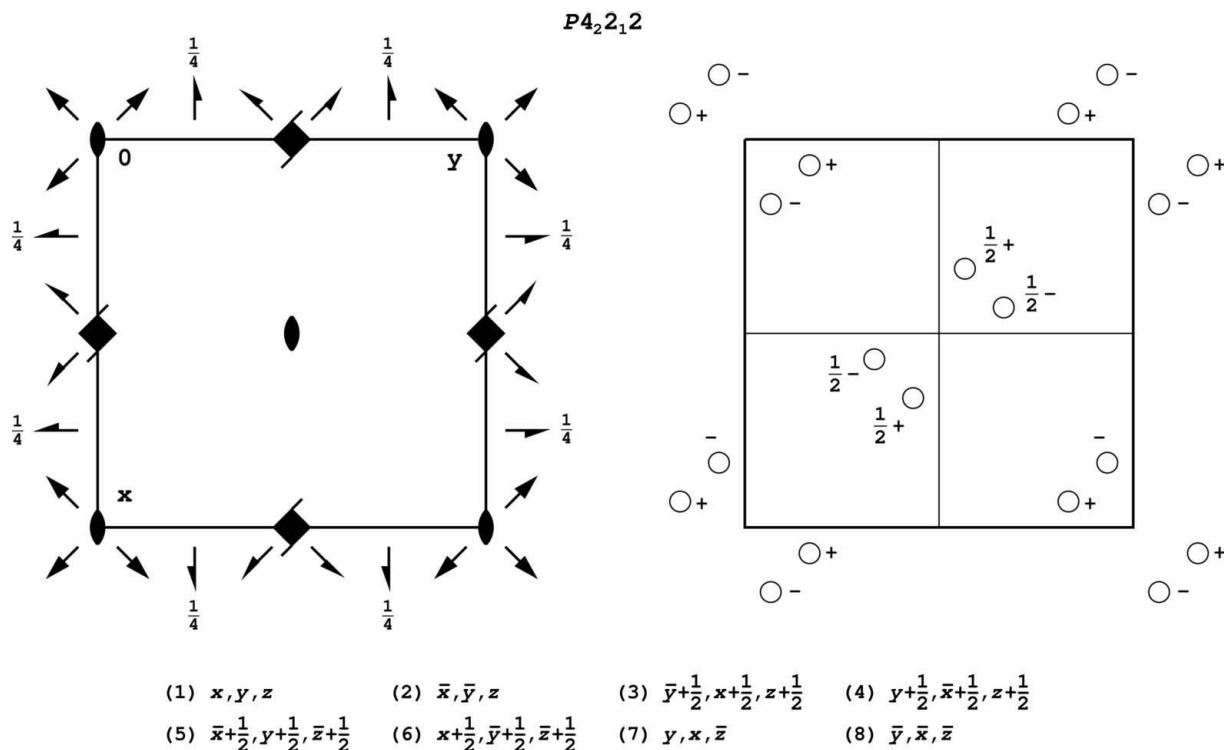


Figure 19 A diagram with symmetry elements (left) and with equivalent points in general positions (right), together with the fractional coordinates (numbered) of those equivalent positions (bottom list) presented for the space group $P4_22_12$ in the style of ITA.

Space group $C222_1$:

| Multiplicity, Wyckoff letter, Site symmetry | Coordinates | | | |
|---|---|---|---|---------------------------|
| | $(0, 0, 0)+ \quad (\frac{1}{2}, \frac{1}{2}, 0)+$ | | | |
| 8 <i>c</i> 1 | (1) x, y, z | (2) $\bar{x}, \bar{y}, z + \frac{1}{2}$ | (3) $\bar{x}, y, \bar{z} + \frac{1}{2}$ | (4) x, \bar{y}, \bar{z} |
| 4 <i>b</i> . 2 . | $0, y, \frac{1}{4}$ | $0, \bar{y}, \frac{3}{4}$ | | |
| 4 <i>a</i> 2 . . | $x, 0, 0$ | $\bar{x}, 0, \frac{1}{2}$ | | |

Figure 20 Basic positions, and vectors needed to obtain all positions generated by space group $C222_1$, presented in the style of ITA.

single polar (*i.e.* directional) axis, and in the monoclinic class *m*, since in these groups there are no other symmetry elements and it does not matter where the origin is defined along the axis (or on the mirror plane). In such space groups, the origin is ‘floating’ in one or more directions.

In $P4_32_12$, the origin could be defined on the 2_1 or 4_3 axes parallel to the *z* direction. However, the *xy* diagonal dyads cross only the 2_1 axis, but not the 4_3 axis, and the former location has been chosen as the unit-cell origin for this space group. This is specified below the symmetry diagram and unambiguously locates the unit-cell origin with respect to all symmetry elements of the space group.

Changing the location of the origin affects the positions of symmetry elements in the unit cell, as illustrated in Fig. 22. It also changes the definition of equivalent positions, as evidenced by the following transformations:

| ITA standard | After origin shift by $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ | Substituting $x' = x + \frac{1}{4},$ $y' = y + \frac{1}{4}, z' = z + \frac{1}{4}$ |
|---|--|--|
| x, y, z | $x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$ | x', y', z' |
| $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ | $\bar{x} + \frac{3}{4}, \bar{y} + \frac{1}{4}, z + \frac{3}{4}$ | $\bar{x}', \bar{y}' + \frac{1}{2}, z' + \frac{1}{2}$ |
| $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ | $\bar{x} + \frac{1}{4}, y + \frac{3}{4}, \bar{z} + \frac{3}{4}$ | $\bar{x}' + \frac{1}{2}, y' + \frac{1}{2}, \bar{z}'$ |
| $x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$ | $x + \frac{3}{4}, \bar{y} + \frac{3}{4}, \bar{z} + \frac{1}{4}$ | $x' + \frac{1}{2}, \bar{y}', \bar{z}' + \frac{1}{2}$ |

2.7. The asymmetric unit

Each unit cell contains as many identical structural motifs at general positions as there are different unique symmetry operations of the corresponding space group. It is, therefore, sufficient to define the contents of only one part of the unit-cell volume, the asymmetric unit (ASU), chosen in such a way that all symmetry-equivalent asymmetric units fill the whole

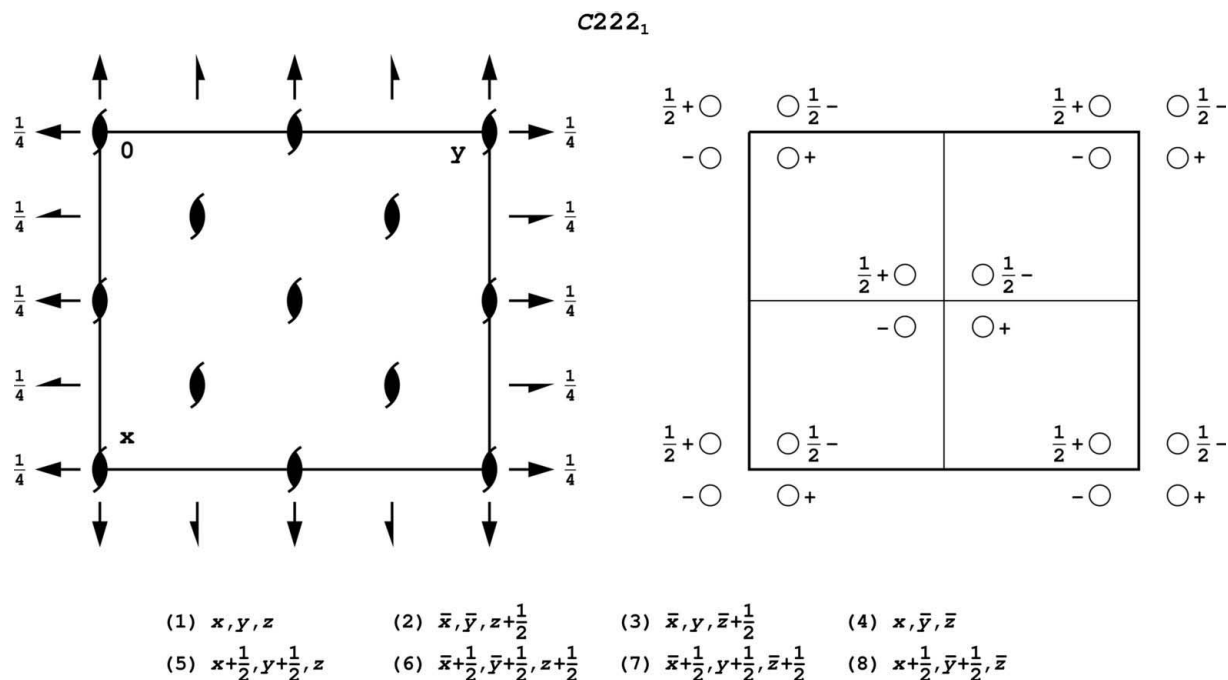


Figure 21 A diagram with symmetry elements (left) and with equivalent points in general positions (right), together with the fractional coordinates (numbered) of those equivalent positions (bottom list) presented for the space group $C222_1$ in the style of ITA.

lattice without any gaps (and without overlap). It is the easiest and usual practice to define the ASU as a convex polyhedron, typically a parallelepiped. (More complicated shapes of the asymmetric unit are necessary only in cubic space groups.) In $P1$, the whole unit cell constitutes the ASU, since there are no symmetry elements at all. Proper rotation axes, mirrors and inversion centers cannot pass through or lie inside the ASU; they can only lie on the boundary, *i.e.* faces, edges or corners, of the ASU. Otherwise, there would be (some) symmetry relation within the ASU volume that would contradict its definition. In many space groups, several satisfactory definitions of the ASU are possible, as illustrated for $P2_1$ in Fig. 23.

There is only one unique twofold screw axis in this space group and, therefore, two equivalent general positions. Accordingly, the volume of the ASU is one-half of the unit-cell volume. Each of the three possibilities shown in Fig. 23 is acceptable, since in all three cases the action of the 2_1 axis transforms the ASU marked in orange to the remaining volume (white) of the unit cell and thus fills the whole lattice. In ITA, the first choice (with $0 \leq z \leq \frac{1}{2}$) is recommended.

2.8. Symmetry operations and generators

For each space group, all symmetry operations are listed, specifying the type of operation, its translational component in parentheses (if one exists) and its location. For $P4_32_12$, the list of its eight symmetry operations is as follows:

- (1) 1
- (2) $2(0, 0, \frac{1}{2}) 0, 0, z$
- (3) $4^+(0, 0, \frac{3}{4}) 0, \frac{1}{2}, z$
- (4) $4^-(0, 0, \frac{1}{4}) \frac{1}{2}, 0, z$
- (5) $2(0, \frac{1}{2}, 0) \frac{1}{4}, y, \frac{3}{8}$
- (6) $2(\frac{1}{2}, 0, 0) x, \frac{1}{4}, \frac{1}{8}$
- (7) $2 x, x, 0$
- (8) $2 x, \bar{x}, \frac{1}{4}$

All listed operations correspond to and are illustrated in the symmetry diagram for this space group. The first operation (1) is the trivial rotation by 0° . The second position describes a

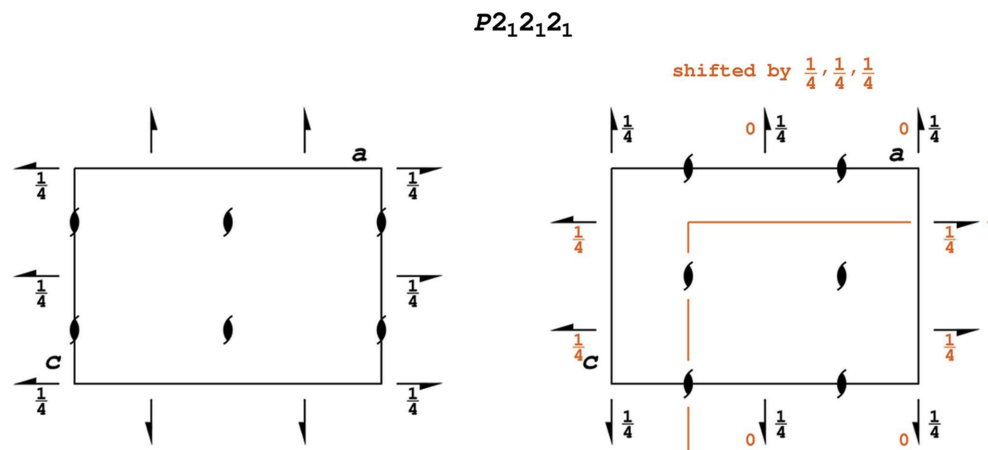


Figure 22 Two possible choices of the unit-cell origin in the space group $P2_12_12_1$, both at the midpoint of three non-intersecting pairs of parallel 2_1 axes. These two choices differ by a shift of the cell origin of $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. In ITA, the variant shown on the left is adopted.

twofold rotation with a translation of $c/2$ and with all points of this axis having coordinates $(0, 0, z)$, which means that it is parallel to the z direction. The third operation is a fourfold rotation with a translation of $3c/4$ along z , around an axis parallel to z but shifted by one-half of the cell parameter in the y direction. The fourth operation is also a fourfold rotation around the z direction, but with $c/4$ translation along z , and shifted by one-half of the unit-cell a edge. Symmetry operations (5) and (6) are the twofold screw axes parallel to the y and x directions, respectively, the first shifted from the cell origin by $a/4$ and $3c/8$, and the second by $b/4$ and $c/8$. The last two operations, (7) and (8), are the ordinary twofold axes (with no translational component), the first one running diagonally between x and y and passing through the origin [points with coordinates $(x, x, 0)$], the second running in the diagonal direction between x and $-y$ with a shift of $c/4$ [points with coordinates $(x, -x, \frac{1}{4})$]. The listed symmetry operations transform a point with general coordinates (x, y, z) into other locations, presented previously in the same order in the list of general positions.

The ‘Generators selected’ listed in ITA after the symmetry operations are a subset of symmetry elements, which by consecutive pairwise combinations will generate all the symmetry elements of the space group.

2.9. Subgroups and supergroups

In principle, in each space (and point) group it is possible to select only a subset of the symmetry elements, corresponding to another group of lower rank. In the trivial extreme, each space group can be expressed as $P1$, but containing multiple copies of the same structural motif in its asymmetric unit (which in $P1$ is the entire unit cell). For example, in the orthorhombic space group $P222$, by combining 1 with each of

the twofold axes, one would generate the three possible realizations of the monoclinic $P2$ space group. $P2$ is, therefore, a subgroup of $P222$ which, in turn, is a supergroup of $P2$. It may be noted that, in all three $P2$ variants, the β angle is equal to 90° . In each crystal system, the space groups of low symmetry are subgroups of some higher-symmetry groups, e.g. $P4_3$ is a subgroup of $P4_322$, $P4_32_12$, $I4_1$, $I4_1/a$, $I4_122$, $I4_1md$, $I4_1cd$, $I4_1/amd$ and $I4_1/acd$, as well as of several cubic space groups. Note that, in the listed I -centered groups, both 4_1 and 4_3 screw axes are present. The rank (*i.e.* number of symmetry elements) of a subgroup is always a divisor of the rank of the supergroup, since addition of a new symmetry element to any group automatically adds all its combinations with the existing elements.

The example in Fig. 24 shows that the $P4_3$ space group is a subgroup of $P4_32_12$. The latter has eight symmetry operations (the trivial 1, three rotations around 4_3 and four twofold axes in the xy plane). In the $P4_3$ space group, there are no axes in the xy plane and the rank is reduced to four. In contrast to $P4_32_12$, the origin in $P4_3$ is defined in ITA on the 4_3 axis.

Another subgroup of $P4_32_12$ is obtained by removing the 4_3 axes (leaving only the 2_1 axes parallel to z) and the 2_1 axes parallel to x and y , as illustrated in Fig. 25. The resulting non-standard group $P2_112$ (in non-standard tetragonal notation) is equivalent to the standard orthorhombic space group $C222_1$, after rotation of the unit cell by 45° and doubling of its volume (Fig. 25).

Yet another possible subgroup of $P4_32_12$ is obtained by removing the 4_3 axes and the twofold axes in the diagonal directions, as in Fig. 26. The resulting space group, $P2_12_11$ (in non-standard tetragonal notation), after an origin shift by $a/4$ and $c/8$, is equivalent to the standard orthorhombic space group $P2_12_12_1$.

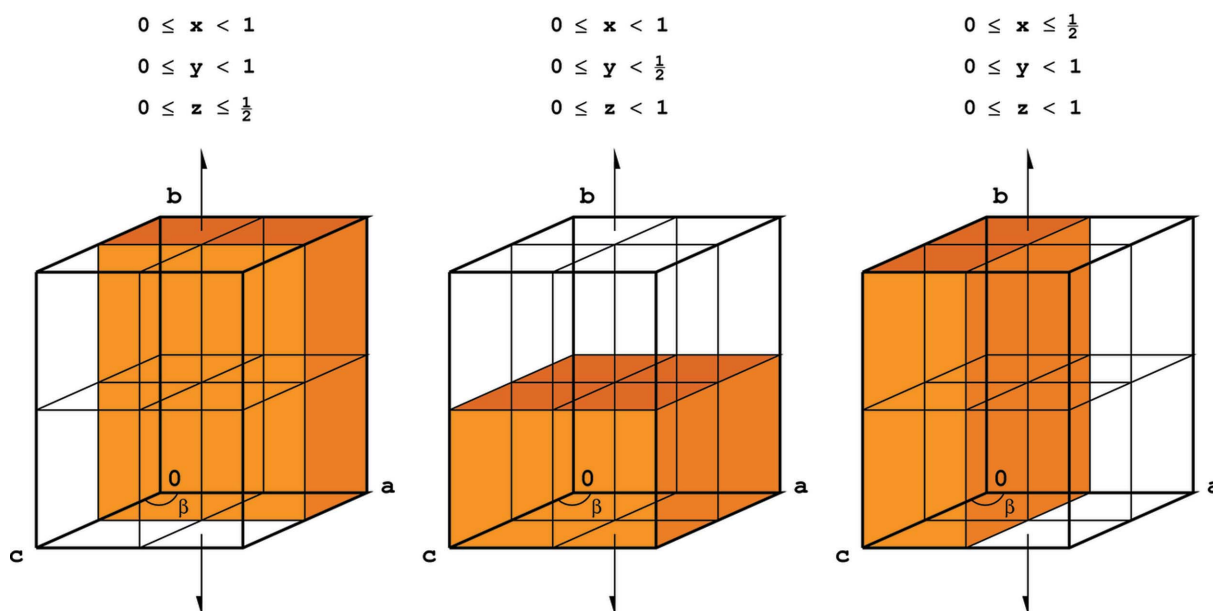


Figure 23

Three possible choices (orange) of the asymmetric unit (ASU) in a unit cell with $P2_1$ space-group symmetry. In all three cases, the 2_1 screw shown in the diagrams generates the second half of the unit cell, *i.e.* fills in the white volume.

There are no more possible subgroups of $P4_32_12$ of rank four. Further subgroups can be obtained by reducing the symmetry of these three subgroups.

ITA lists, for each space group, all subgroups of a rank lowered by one level (maximal subgroups) and supergroups of a rank higher by one level (minimal supergroups).

2.10. Patterson symmetry

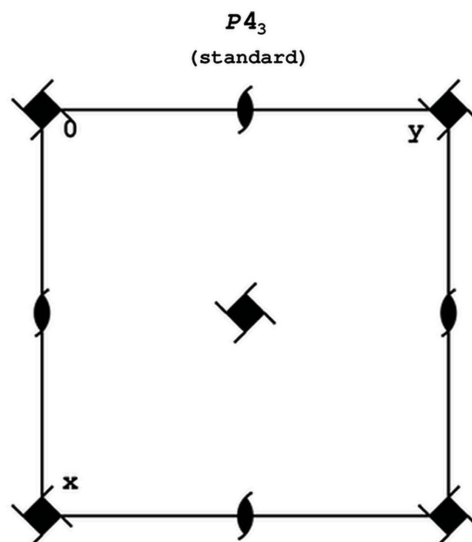
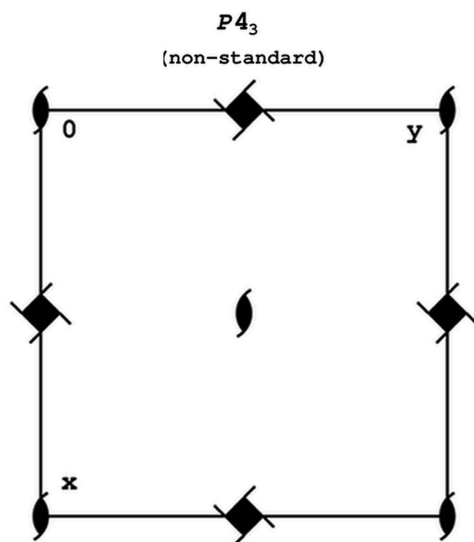
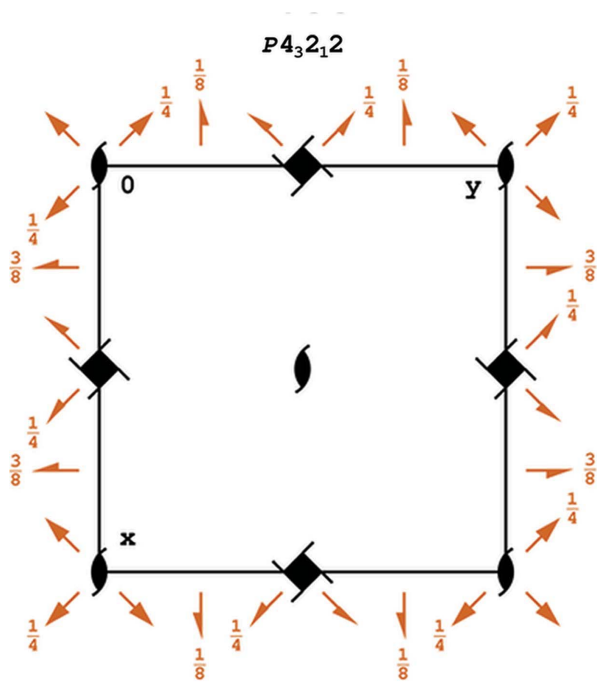
Mathematically, the Patterson function is a self-convolution of the crystal structure (represented, for example, by its electron-density map) with its centrosymmetric image. It can be calculated in a very simple way, by Fourier summation of

the reflection intensities alone. (In contrast, computing of an electron-density map, the ultimate goal of X-ray structure determination, requires the use of reflection amplitudes and phases.) The Patterson function has maxima corresponding to vectors between peaks in the electron-density map, *i.e.* between atoms in the crystal structure, and the height of these maxima is proportional to the product of the atomic numbers of the atoms involved. Therefore, the Patterson function is defined in the so-called vector space. For multi-atomic structures, the Patterson function is highly complicated and very difficult to interpret, but structures consisting of just a few atoms can be deciphered from their Patterson maps. An interesting case is the substructure of the heavy atoms in a protein crystal derivatized by a suitable heavy-atom compound. The symmetry of the Patterson function is usually simpler than that of the original crystal structure because it contains essentially the same symmetry elements but without the translational component, although the lattice centering is preserved. The Patterson function is, however, always centrosymmetric. For example, for the $P4_32_12$ space group the corresponding Patterson symmetry is $P4/mmm$, similarly as for space groups $P422$, $P4_12_12$, $P4_22_12$, $P4mm$, $P4_2cm$, $P4_2bc$, $P\bar{4}2_1c$, $P\bar{4}c2$, $P4/mmm$, $P4/ncc$ or $P4_2/nbc$. For space groups $I422$, $I4_122$, $I4mm$, $I4_1cd$, $I\bar{4}2d$, $I4_1/amd$ or $I4_1/acd$, the Patterson symmetry is $I4/mmm$.

The corresponding Patterson symmetry is specified in ITA for each of the 230 space groups.

2.11. Reflection conditions

The diffraction phenomena produced by crystals on interaction with X-rays (and also with neutrons or electrons) are usually described using the Bragg model, in which the diffracted rays arise as reflections from lattice planes. The reflections are related to the planes from which they have arisen by the use of indices, written as hkl . The Bragg equation



governing these phenomena, $\lambda = 2d_{hkl}\sin\theta_{hkl}$ (where λ is the wavelength of the diffracted radiation), clearly shows that the relation between the interplanar distance of the reflecting

planes d_{hkl} and the angle of reflection θ_{hkl} is reciprocal, *i.e.* that closely spaced planes give rise to large diffraction angles.

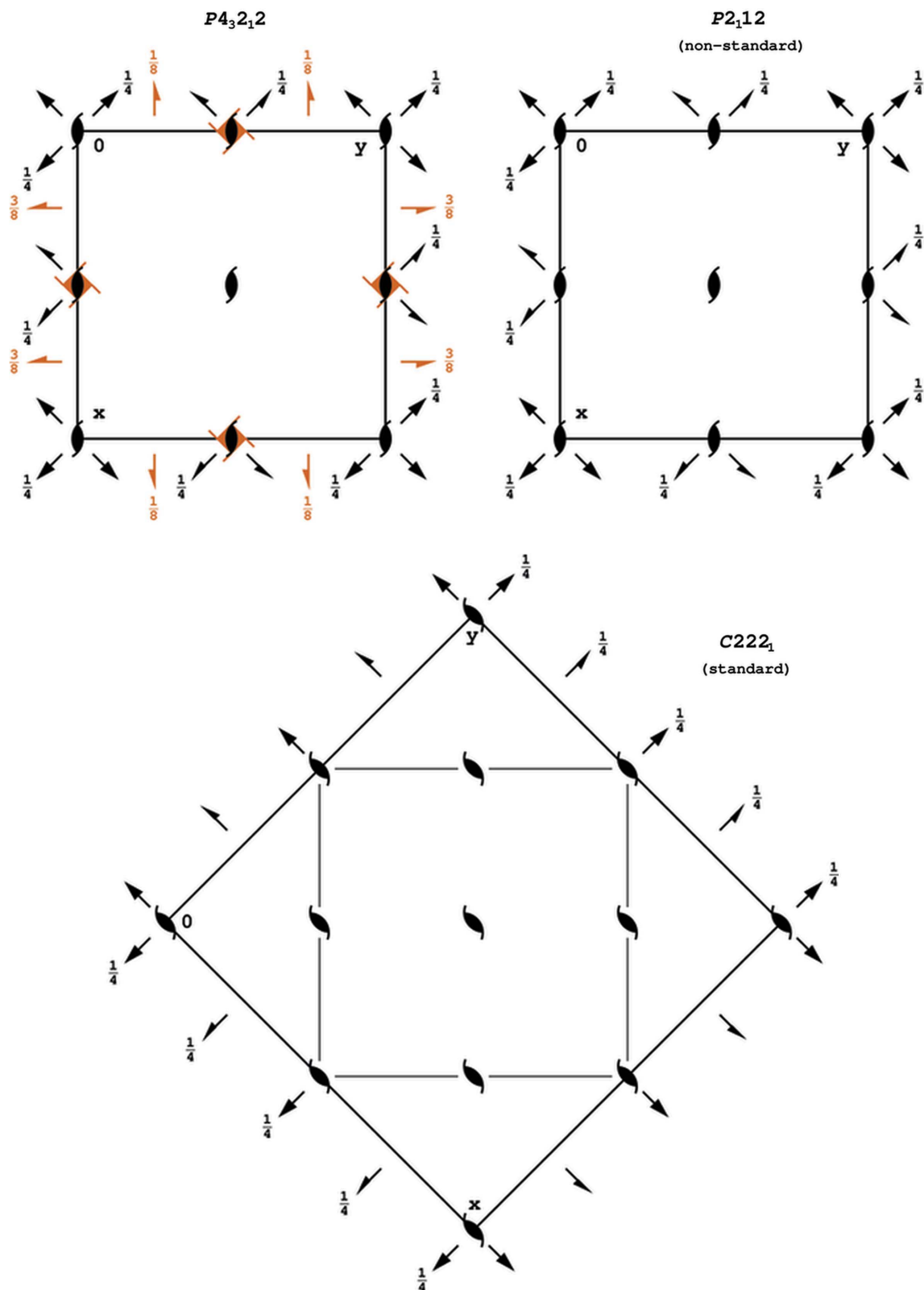


Figure 25

Reduction of $P4_32_12$ to its subgroup $C222_1$, by the removal of the symmetry elements shown in brown. Note the reorientation of the unit cell and doubling of its volume.

Even a very superficial analysis of the diffraction phenomena shows that it is the periodic nature of the crystal that leads to the disappearance of the scattering in most directions and to concentration of the diffracted beams only in very specific, discrete directions in space. It can be easily shown that the introduction of additional translational symmetry (in the form of nonprimitive lattice centering, glide planes or screw axes) must result in the additional disappearance of certain groups of reflections from the diffraction pattern. We shall explain this using some examples.

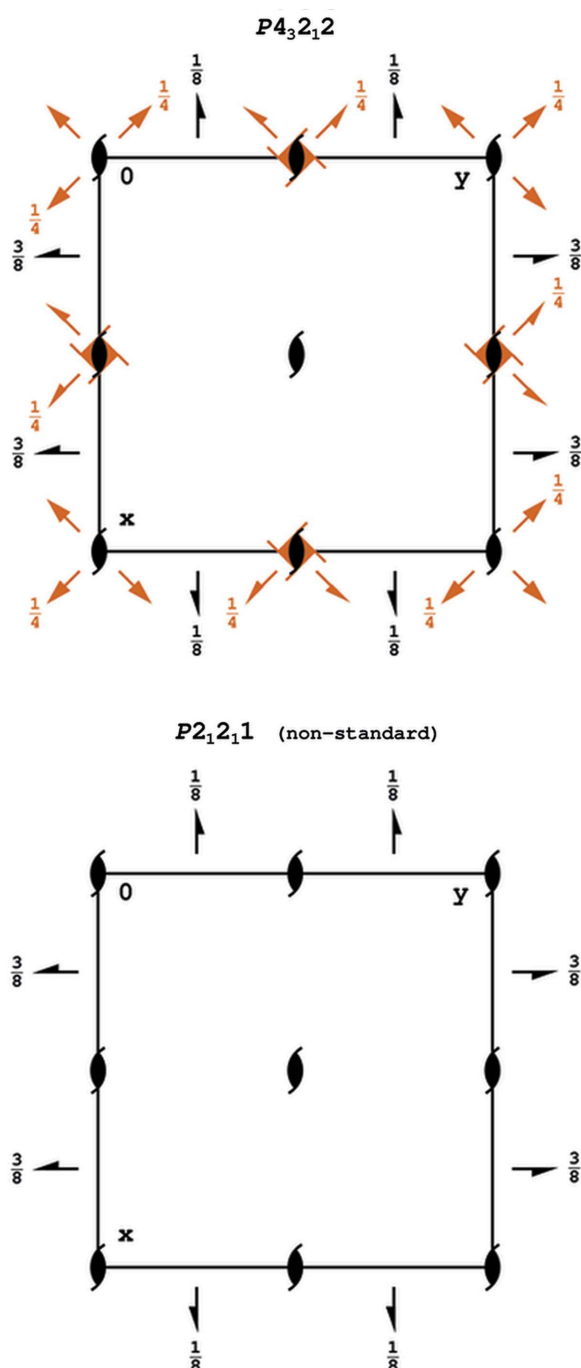


Figure 26
Reduction of $P4_32_12$ to its subgroup $P2_12_12_1$, by the removal of the symmetry elements shown in brown.

Let us consider a primitive lattice, in which the lattice planes (001), represented by the bottom and top 'floors' of a P unit cell, give rise to a strong reflection. The optical path difference between two rays reflected from these two 'floors' is 1λ , *i.e.* after bouncing off the planes, the rays travel 'in phase' (this is why rays reflected from consecutive planes will reinforce each other). Now, let us assume that the cell becomes I -centered, which means that an extra plane, identically populated by nodes, is inserted between each pair of previously existing (001) planes. Thus, the optical path difference between two consecutive planes becomes $\lambda/2$, which means that the rays reflected from these planes will exactly cancel each other (since they will travel 'out of phase', combining a maximum of one wave with a minimum of the other). This is why there will be no 001 reflection from a crystal with an I -centered lattice. Using a more precise mathematical argument, it can be shown that, for an I lattice, all reflections with $h + k + l$ odd will be absent. This condition ('reflection condition' in ITA) is usually written as $h + k + l = 2n$ (where n is any integer), meaning that only reflections for which the sum of indices is even will be present. In a more general argument, cell centering can be viewed as equivalent to halving of the cell dimensions in a projection on any direction in space. Therefore, all general reflections hkl are present only if their appropriate sums fulfill the conditions given in Table 4.

In another example, let us consider the effect of a 2_1 screw axis. Its presence means that an identical structural motif is repeated twice within the unit cell along the direction of the axis, so that the periodicity of the whole structure projected onto this axis is effectively halved, as shown in Fig. 27. In the diffraction pattern, the distance between reflections in this

Table 4
Systematic absences caused by translational symmetry.

| Translational symmetry | Reflections affected | Reflections systematically absent if these conditions are not fulfilled |
|-------------------------------------|----------------------|---|
| Nonprimitive lattice | All | |
| I | hkl | $h + k + l = 2n$ |
| C | hkl | $h + k = 2n$ |
| R | hkl | $-h + k + l = 3n$ |
| F | hkl | $h + k = 2n$ and $h + l = 2n$ and $k + l = 2n$ (h, k, l of the same parity, all even or all odd) |
| Glide planes (examples) | Zone | |
| $a \perp \mathbf{b}$ | $h0l$ | $h = 2n$ |
| $n \perp \mathbf{c}$ | $hk0$ | $h + k = 2n$ |
| $c \perp (xy)$ diagonal | hhl | $l = 2n$ |
| $d \perp \mathbf{a}$ | $0kl$ | $k + l = 4n$ |
| Screw axes | Axial | |
| $2_1 \parallel \mathbf{b}$ | $0k0$ | $k = 2n$ |
| 3_1 or $3_2 \parallel \mathbf{c}$ | $00l$ | $l = 3n$ |
| 4_1 or $4_3 \parallel \mathbf{c}$ | $00l$ | $l = 4n$ |
| $4_2 \parallel \mathbf{c}$ | $00l$ | $l = 2n$ |
| 6_1 or $6_5 \parallel \mathbf{c}$ | $00l$ | $l = 6n$ |
| 6_2 or $6_4 \parallel \mathbf{c}$ | $00l$ | $l = 3n$ |
| $6_3 \parallel \mathbf{c}$ | $00l$ | $l = 2n$ |

(and only this) direction will be doubled, which means that only every other reflection will be present in that particular direction. If the screw axis is parallel to the \mathbf{y} direction (as in the monoclinic $P2_1$ space group), then only every second reflection is present among the reflections along this direction (i.e. $0k0$), so that the k index must be even ($k = 2n$) for reflections $0k0$.

If a threefold screw axis exists along the \mathbf{z} direction, then only those $00l$ reflections are present for which $l = 3n$, i.e. the l index is divisible by 3. It is impossible to know if such systematic absences are caused by the 3_1 or 3_2 axes, since in both cases the effective repeat distance decreases three times. The 6_2 and 6_4 axes generate similar absences (when $l \neq 3n$, for $00l$ reflections), since they also involve a translation by $2/6 = 1/3$ of the c cell dimension. In the case of the 6_1 or 6_5 axes, only $00l$ reflections with $l = 6n$ are present. Similarly, when either 4_1

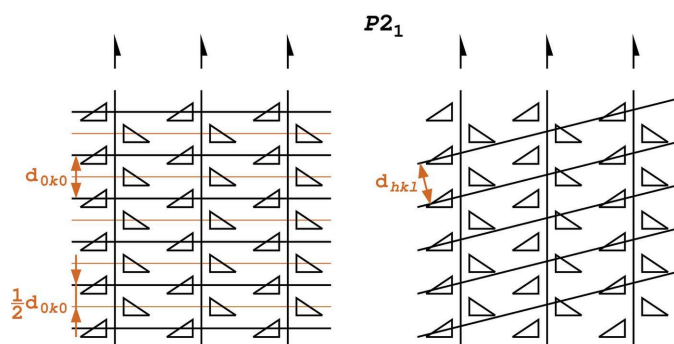


Figure 27

The repeat distance along the 2_1 axis is effectively halved and constellations of identical motifs are repeated in this direction every half of the cell length (left). In consequence, for space group $P2_1$, reflections $0k0$ with k odd are absent. There is no such effect in directions that are not exactly parallel to the screw axis (right).

or 4_3 is present, only $00l$ reflections with $l = 4n$ are seen, whereas in the case of 4_2 , the corresponding condition is $l = 2n$, the same as for the 6_3 axis (both of them implicitly include the 2_1 axis).

The presence of a glide plane causes halving of the effective repeat distance in the direction of the gliding translation if the content of the cell is projected on any direction within this plane. As a consequence, only every second row of reflections is present in the corresponding layer of reflections in the diffraction pattern. For instance, the a -glide plane perpendicular to \mathbf{y} causes systematic absence of all $h0l$ reflections with $h \neq 2n$ (i.e. with $h = 2n + 1$). The c -glide perpendicular to \mathbf{x} causes the absence of $0kl$ reflections with $l = 2n + 1$. An n -glide causes the absence of reflections for which an appropriate sum of indices is odd. For example, in space group $Pbcn$ the following reflections are absent: $0kl$ with $k = 2n + 1$, $h0l$ with $l = 2n + 1$ and $hk0$ with $h + k = 2n + 1$.

In a diffraction pattern, all those systematic extinctions or absences can be traced back to the translational symmetry elements that have caused them, providing a very useful method for space-group determination. The rules for systematic absences are summarized in Table 4. The situation of nonprimitive lattice centering is simple because the extinctions are found in all index groups. The situation with glide planes is more complicated because the effect is only seen in zonal reflections and the extinction rule is dictated by the translational component. A zone of a principal axis (e.g. z) is characterized by a zero index corresponding to that axis ($hk0$), but other zonal directions are more complicated (e.g. hhl for a zone of the xy diagonal). Table 4 includes four examples of glide-plane extinctions. Screw axes affect only the corresponding axial reflections, with the extinction rule again dictated by the translational component.

3. Conclusions

With crystallography quickly disappearing from university curricula, we may be facing a situation when the next generation will lack properly trained scientists able to apply the crystallographic method in structural research, especially in structural biology, to say nothing about advancing the field. Indeed, there are already protein 'crystallographers' who, when asked about the space group of their protein crystal structure, are not sure about the meaning of the question. Some might argue that this is the natural way things evolve and that we should 'move forward', thus leaving the legacy of crystallographic fundamentals to science history and dusty library shelves. In this view, the basics of crystallography are a 'closed science' and formal training is no longer necessary, because we have excellent black-box-style computerized tools that can do almost anything 'automagically', without human intervention. The situation is somewhat similar to questioning the need to teach mathematics, because a lot of things can be done in smart and flashy spreadsheet programs. In our opinion this view is very wrong. Firstly, while indeed some easy and routine cases can be handled by automata, the truly challen-

ging scientific problems almost invariably require input from a human brain. Secondly, if we allow for this generation gap to occur, we may be really facing a serious danger that even progress in tool development will stall in the next decade. Thirdly, practicing science in a conscious, well informed way is really what the whole business of doing science is about. In addition, understanding crystallography brings a lot of fun and intellectual satisfaction. This is why we have decided to write this teaching material – to help those who have no formal training in crystallography but want to be comfortable with its language and understand its methods. We hope that it may also be useful as an additional teaching material in various crystallographic schools and workshops. If our readers enjoy practicing conscious crystallography as much as we do, we will feel gratified that it was well worth the effort.

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