

programs for addressing crystallographic problems related to the study of group–subgroup relations between space groups.

The aim of this contribution is to present the programs and visualizers of the *Symmetry Database* and to provide examples showing how they can be used. Basic definitions and explanations of the notation used in the description of symmetry operations, coordinate transformations, and subgroups and supergroups of space groups can be found in Appendix A.

The programs, visualizers and component databases of the *Symmetry Database* use the *standard* or *default* settings of the space groups. These are specific settings of the space groups that coincide with the conventional space-group descriptions found in *ITA*. For space groups with more than one description in *ITA*, the following settings are chosen as standard: unique axis *b* setting, cell choice 1 for monoclinic groups, hexagonal axes setting for rhombohedral groups, and the origin choice 2 description (*i.e.* with the origin at a centre of inversion) for those centrosymmetric groups that are listed with respect to two origins in *ITA*.

The *Symmetry Database* is arranged into three parts (see Fig. 1). The first part provides access to the crystallographic space-group database, which includes the generators, general and special Wyckoff positions, and affine, Euclidean and

chirality-preserving Euclidean normalizers. This part also includes an interactive visualizer allowing the user to explore the general-position diagrams and symmetry elements of the space groups. The data that are provided in this part are in fact valid for all space groups that belong to the same *space-group type*. (For the definition and a detailed discussion of the term *space-group type*, see Section 1.3.4.1 of *ITA*.) The second part of the *Symmetry Database* provides access to a database of the maximal subgroups and the minimal supergroups of the space groups together with an interactive visualizer allowing the study of the group–subgroup relations between space groups. The third part focuses on the three-dimensional crystallographic point groups, providing access to databases of generators, general positions and Wyckoff positions. This part also includes interactive visualization of point-group symmetry elements. These three parts are described in detail in Sections 2, 3 and 4, respectively.

The *Symmetry Database* provides 14 server-side crystallographic programs and three interactive visualizers. There are 12 main programs and two auxiliary programs. The main programs, which carry out a variety of calculations based on the input submitted by the user, include six programs for space groups and point groups (Generators, General

The screenshot shows the main page of the International Tables Symmetry Database. At the top, there is a green navigation bar with links for home, resources, purchase, contact us, and help. Below this, the page title 'INTERNATIONAL TABLES Symmetry database' is displayed, along with a secondary navigation bar containing links for various crystallographic categories (A, A1, B, C, D, E, F, G, H, I). The main content area is divided into three columns:

- Space-group symmetry data:**
 - Generators:** Set of generators for a given space group
 - General position:** General-position coordinate triplets for a given space group
 - Wyckoff positions:** Wyckoff-positions data for a given space group
 - Normalizers:** Euclidean, chirality-preserving Euclidean and affine normalizers for a given space group
 - Interactive 3D visualization:** Interactively visualize a 3D unit cell containing the symmetry-equivalent points of a general position. Click on points and symmetry operations to see how they are related
- Symmetry relations between space groups:**
 - Maximal subgroups:** Maximal subgroups of indices 2, 3 and 4 (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis)
 - Series of isomorphic subgroups:** Maximal isomorphic subgroups of indices higher than 4 (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis)
 - Minimal supergroups:** Minimal supergroups of indices up to 9 (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis)
 - Group-subgroup relations:** Group-subgroup pair specified by the transformation between the conventional bases of the group and the subgroup (Wyckoff-position splitting schemes, coset decomposition and transformation to the supergroup basis)
 - Graph of maximal subgroups:** Graph of maximal subgroups for a group-subgroup pair (with and without a specific index)
 - Supergroups:** Supergroups of specific index
- 3D Crystallographic point groups:**
 - Generators:** Set of generators for a given point group
 - General position:** General-position coordinate triplets for a given point group
 - Wyckoff positions:** Wyckoff-positions data for a given point group
 - Interactive 3D visualization:** Interactive visualization for a given point group

Figure 1

The main page of the *International Tables Symmetry Database* (<https://symmdb.iucr.org/>) is arranged in three parts. The first part (the left-hand column) provides access to the programs and visualizer associated with space-group symmetry: Generators (see Section 2.1), General position (see Section 2.1), Wyckoff positions (see Section 2.2), Normalizers (see Section 2.3) and Interactive 3D visualization (see Section 2.4). The second part (the middle column) provides access to databases, programs and a visualizer related to symmetry relations between space groups: Maximal subgroups (see Section 3.1), Series of isomorphic subgroups (see Section 3.2), Minimal supergroups (see Section 3.3), Group-subgroup relations (see Section 3.4), Graph of maximal subgroups (see Section 3.5) and Supergroups (see Section 3.6). The third part (the right-hand column) provides access to programs and a visualizer related to the database of three-dimensional crystallographic point groups: Generators, General position and Wyckoff positions (see Section 4.1), and Interactive 3D visualization (see Section 4.2).

position and Wyckoff positions) and six programs for space groups only (Normalizers, Maximal subgroups, Series of isomorphic subgroups, Minimal supergroups, Group-subgroup relations and Supergroups). In addition, two auxiliary programs, coset decomposition and Wyckoff-position splittings, are used to perform some calculations using the data stored in the databases as input. The three interactive visualization programs include a 3D space-group general position and symmetry element visualizer that uses *JSmol* (Interactive 3D general-position visualizer), a JavaScript-based 3D crystallographic point-group symmetry visualizer (Interactive visualization), and a graph-based application for exploring the group-subgroup relationships between space groups (Graph of maximal subgroups).

2. Space-group symmetry

This part of the *Symmetry Database* hosts the data for all 230 space groups in their conventional settings. In addition, crystallographic data for the 530 settings for the monoclinic and orthorhombic space groups listed in Table 1.5.4.4 of *ITA* ('the *ITA* settings') are also available. The data for the generators, general and special Wyckoff positions, and affine, Euclidean and chirality-preserving Euclidean normalizers can be explored here. A 3D interactive visualizer of the points of the general position and the symmetry elements that relate them completes this part. The input for the programs in this part is the space-group numbers according to *ITA*, which can be selected directly from a table that lists them along with their associated Hermann-Mauguin symbols.

2.1. Generators and general position

The generators and general position of a space group are shown by the programs *Generators* and *General position*, respectively. The generators and the general-position entries are given as coordinate triplets, as matrix-column representations of the corresponding symmetry operations and as geometric interpretations (see Appendix A1).

(i) The list of coordinate triplets (x, y, z) reproduces the data from the *General position* blocks of the space-group tables found in *ITA*. The coordinate triplets may also be interpreted as shorthand descriptions of the matrix forms of the corresponding symmetry operations [see (ii) below].

(ii) For the matrix-column representations, the symmetry operations of the space groups are described by (3×4) matrix-column pairs (\mathbf{W}, \mathbf{w}) with reference to a coordinate system consisting of an origin O and a basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$.

(iii) The geometric interpretation of the symmetry operations is given (a) following the conventions in *ITA* [including the symbol of the symmetry operation, its glide or screw component (if relevant), and the location of the related geometric element] and (b) using Seitz notation [see Glazer *et al.* (2014)].

Fig. 2 shows the general position for the space group *Pba2* (No. 32) in the standard setting.

General position		Symmetry operation	
Coordinate triplets	Matrix form	Geometric description	Seitz notation
x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	$(1 0)$
$-x, -y, z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$2, 0, 0, z$	$\{2_{001} 0\}$
$x+1/2, -y+1/2, z$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$a, x, 1/4, z$	$\{m_{110} 1/2, 1/2, 0\}$
$-x+1/2, y+1/2, z$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$b, 1/4, y, z$	$\{m_{1\bar{1}0} 1/2, 1/2, 0\}$

Figure 2

The general position of the space group *Pba2* (No. 32) given by the program *General position* (see Section 2.1).

The programs *Generators* and *General position* list the generators and general-position entries of the space groups in the standard setting as well as in any of the *ITA* settings. Clicking on 'Change settings' gives a list of the *ITA* settings of the space group; the corresponding data can be calculated with respect to one of these settings by choosing it directly from this list. If a particular setting is not in this list (*i.e.* it is not one of the *ITA* settings), it can be obtained by clicking on 'Change basis' and specifying the coordinate transformation that relates the basis of the non-conventional setting $(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\text{non-conv}}$ to that of the standard setting $(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\text{stand}}$ (for details on coordinate transformations, see Appendix A2). The coordinate transformation is described by a matrix-column pair (\mathbf{P}, \mathbf{p}) and consists of two parts: a linear part \mathbf{P} given by a (3×3) matrix, which describes the change of direction and/or length of the basis vectors, $(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\text{non-conv}} = (\mathbf{a}, \mathbf{b}, \mathbf{c})_{\text{stand}}\mathbf{P}$, and an origin shift $\mathbf{p} = (p_1, p_2, p_3)$ given by a (3×1) column, whose coefficients describe the position of the non-conventional origin with respect to the standard one. A matrix-column pair

$$(\mathbf{P}, \mathbf{p}) = \left[\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}, \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} \right]$$

is often written in the following concise form:

$$P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c}, P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c}, P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c}; \\ p_1, p_2, p_3.$$

2.2. Wyckoff positions

The program *Wyckoff positions* lists the Wyckoff positions for a designated space group. The listing follows that of *ITA* (see Fig. 3): the Wyckoff-position block starts with the general position at the top, followed downwards by the various special Wyckoff positions with decreasing multiplicity and increasing site symmetry. The data for each Wyckoff position include (i) the multiplicity, *i.e.* the number of equivalent positions in the conventional unit cell; (ii) the Wyckoff letter, which is an alphabetical label; (iii) the site symmetry described by the point group isomorphic to the site-symmetry group; and (iv) a set of coordinate triplets of the equivalent Wyckoff-

Pmma No. 51

Wyckoff positions Specific orbit Change basis Change setting

Multiplicity, Wyckoff letter, Site symmetry	Coordinates					
8 <i>i</i> 1	x, y, z	$-x+1/2, -y, z$	$-x, -y, z$	$x+1/2, -y, z$	$-x, -y, z$	$x+1/2, -y, z$
4 <i>k</i> m	$1/4, y, z$	$1/4, -y, z$	$3/4, y, z$	$3/4, -y, z$		
4 <i>j</i> m	$x, 1/2, z$	$-x+1/2, 1/2, z$	$-x, 1/2, z$	$x+1/2, 1/2, z$		
4 <i>l</i> m	$x, 0, z$	$-x+1/2, 0, z$	$-x, 0, z$	$x+1/2, 0, z$		
4 <i>h</i> 2	$0, y, 1/2$	$1/2, -y, 1/2$	$0, -y, 1/2$	$1/2, y, 1/2$		
4 <i>g</i> 2	$0, y, 0$	$1/2, -y, 0$	$0, -y, 0$	$1/2, y, 0$		
2 <i>f</i> mm2	$1/4, 1/2, z$	$3/4, 1/2, z$				
2 <i>e</i> mm2	$1/4, 0, z$	$3/4, 0, z$				
2 <i>d</i> 2/m	$0, 1/2, 1/2$	$1/2, 1/2, 1/2$				
2 <i>c</i> 2/m	$0, 0, 1/2$	$1/2, 0, 1/2$				
2 <i>b</i> 2/m	$0, 1/2, 0$	$1/2, 1/2, 0$				
2 <i>a</i> 2/m	$0, 0, 0$	$1/2, 0, 0$				

Figure 3

A screenshot of the output of the program `Wyckoff positions` (see Section 2.2) showing the Wyckoff positions for the space group *Pmma* (No. 51).

Pmma No. 51

Site-symmetry group

The point you have selected 2, 5/4, 1/2 belongs to Wyckoff position 4*h*.

Site-symmetry group: 2.

Coordinate triplet	Matrix form	Geometric description	Seitz notation
x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1	{1 0}
$-x+4, y, -z+1$	$\begin{pmatrix} -1 & 0 & 0 & 4 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \end{pmatrix}$	2 2, $y, 1/2$	$\{2_{011} 401\}$

Figure 4

The site-symmetry group for the point with coordinates 2, 5/4, 1/2 in the space group *Pmma* (No. 51), calculated using the option 'Specific orbit' of the program `Wyckoff positions` (see Section 2.2).

position points in the unit cell, shown under 'Coordinates'. For centred space groups, the centring translations are listed above the coordinate triplets. The point groups isomorphic to the site-symmetry groups (see the third column in Fig. 3) are described using *oriented symbols*: these are modified Hermann–Mauguin point-group symbols that show how the symmetry elements of a site are related to the symmetry elements of the crystal lattice (for more details, see Section 2.1.3.12 of *ITA*). An explicit listing of the symmetry operations of the site-symmetry group of a point is obtained by clicking directly on its coordinate triplet. The symmetry operations of the site-symmetry group of an arbitrary point (specified by its coordinates but not necessarily within the unit cell) can be also be calculated using the option 'Specific orbit'. Fig. 4 shows the list of the symmetry operations of the site-symmetry group for the point 2, 5/4, 1/2 of the space group *Pmma* (No. 51). This point belongs to the Wyckoff position 4*h* and its site-symmetry group is '2'.

The program `Wyckoff positions` provides a list of the Wyckoff positions in different space-group settings, either by specifying the coordinate transformation (\mathbf{P}, \mathbf{p}) to a new basis ('Change basis'), or by selecting one of the *ITA* settings of the corresponding space group directly, using ('Change setting').

2.3. Normalizers

The normalizers of space groups play an important role in a number of applications (see Chapter 3.5 of *ITA*). For example, the number of different but equivalent structure descriptions (even after fixing the space-group setting and origin choice) is

F432 No. 209

Euclidean normalizer Chirality-preserving Euclidean normalizer Affine normalizer

Euclidean normalizer (general metric) $Pm\bar{3}m$ (1/2a, 1/2b, 1/2c)

Index of F432 (209) in $Pm\bar{3}m$ (1/2a, 1/2b, 1/2c): 4
with $i_k = 2$ and $i_s = 2$

Additional generators of $Pm\bar{3}m$ (1/2a, 1/2b, 1/2c) with respect to F432 (209)

Coordinate triplets	Matrix form	Geometric description
$x+1/2, y+1/2, z+1/2$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	$t(1/2, 1/2, 1/2)$
$-x, -y, -z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0, 0, 0

Coset representatives of the decomposition of the normalizer $Pm\bar{3}m$ (1/2a, 1/2b, 1/2c) with respect to F432

Coset 1

Coordinate triplets	Matrix form	Geometric description
x, y, z	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	1

Coset 2

Coordinate triplets	Matrix form	Geometric description
$x+1/2, y+1/2, z+1/2$	$\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1/2 \\ 0 & 0 & 1 & 1/2 \end{pmatrix}$	$t(1/2, 1/2, 1/2)$

Coset 3

Coordinate triplets	Matrix form	Geometric description
$-x, -y, -z$	$\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}$	-1 0, 0, 0

Coset 4

Coordinate triplets	Matrix form	Geometric description
$-x+1/2, -y+1/2, -z+1/2$	$\begin{pmatrix} -1 & 0 & 0 & 1/2 \\ 0 & -1 & 0 & 1/2 \\ 0 & 0 & -1 & 1/2 \end{pmatrix}$	-1 1/4, 1/4, 1/4

Figure 5

Output of the program `Normalizers` (see Section 2.3) for the Euclidean normalizer of the space group *F432* (No. 209). Note that the affine normalizer of the group *F432* coincides with the Euclidean one.

determined by the Euclidean normalizer of the corresponding space group. For more details see Section 5.1. Following *ITA*, the program `Normalizers` shows the Euclidean, chirality-preserving Euclidean and affine normalizers of the space groups (see Appendix A4). The normalizers are described with respect to the standard space-group settings. For triclinic and monoclinic groups (whose affine normalizers are not isomorphic to groups of motions), parametric representations of the matrix–column pairs of the mappings of the affine normalizers are shown together with the appropriate restrictions on the coefficients. Fig. 5 shows the output of the program `Normalizers` for the Euclidean normalizer of the space group *F432* (No. 209). (Note that the type of normalizer can be selected by clicking on the tabs near the top of the page, below the space-group symbol.) The output of the program is organized into three blocks. In the first block of the output, general information about the normalizer is displayed: the Hermann–Mauguin symbol of the normalizer, the basis of the normalizer described in terms of the basis of the space group \mathcal{G} and the index of \mathcal{G} in the normalizer. The second block shows the *additional generators*, i.e. the additional symmetry operations that can generate the normalizer successively from the space group \mathcal{G} (see *ITA*, Tables 3.5.2.3, 3.5.2.4 and 3.5.2.5). These additional symmetry operations are represented by their coordinate triplets, their matrix–column representations and their corresponding geometric interpretations. For example, the Euclidean normalizer $\mathcal{N}_e(\mathcal{G})$ of the space group *F432*(**a, b, c**) is $Pm\bar{3}m$ with basis vectors (1/2**a**, 1/2**b**, 1/2**c**) and

index 4 (see Fig. 5). There are two additional generators that can be used to generate $Pm\bar{3}m(1/2a, 1/2b, 1/2c)$ from $F432$: a translation $t(1/2, 1/2, 1/2)$ and an inversion through the point $0, 0, 0$. The coset representatives of the decomposition of the normalizer with respect to the space group are listed in the last block of the output. Each coset representative is specified by its coordinate triplet, matrix-column representation and geometrical interpretation (see Fig. 5). The affine normalizer $\mathcal{N}_A(\mathcal{G})$ of the space group $F432$ coincides with the Euclidean one, so the output of the program for the space group $F432$ is the same for the Euclidean and affine normalizers.

2.4. Interactive 3D visualization

The visualizer in this section allows the user to explore the symmetry operations that relate the various coordinate triplets of the general position of a space group. It uses *JSmol*, the JavaScript implementation of *Jmol* (Hanson, 2013). The starting point for interaction is a table showing the general position of the space group along with an interactive panel where the three-dimensional general-position diagram is displayed (see Fig. 6; the video in the supporting information also gives a detailed explanation of how to use this visualizer).

The table of the general-position triplets and their interpretation as symmetry operations is interactive: clicking on a specific symmetry operation shows its action on the initial general-position point depicted within the yellow ring on the general-position diagram. If the image point is outside the unit cell, its equivalent point in the unit cell (as reached by a lattice translation) is also indicated. Points in red rings are obtained by symmetry operations of the second kind, *i.e.* those that would change the handedness of a chiral object, such as inversion. The colours of the points distinguish their heights along the *b* axis for triclinic and monoclinic space groups, and along the *c* axis for the other space groups. The action of the symmetry operation can be visualized by clicking on the ‘animate’ button.

The general-position diagram is also interactive: the unit cell can be dragged with the mouse in order to see it from

different perspectives. Clicking on a general-position point shows the operation that transforms the initial general-position point x, y, z to that position. The geometric description of the symmetry operation (type, orientation, screw or glide component, location) is displayed at the top of the diagram. The corresponding symmetry-equivalent position and the related symmetry operation (*modulo* lattice translation) is highlighted in the general-position table. The option ‘animate’ can be used to visualize its action.

Fig. 6 shows a screenshot of the output of *Interactive 3D general-position visualizer* for the space group $P4_2nm$ (No. 102). Clicking on the sixth coordinate triplet $-x + 1/2, y + 1/2, z + 1/2$ in the general-position table shows the user the corresponding *n*-glide reflection with glide vector $0, 1/2, 1/2$, located at $1/4, y, z$ (the blue plane in the diagram). The animation shows the action of the selected symmetry operation on the initial general-position point to a symmetry-equivalent point inside the unit cell.

The potential for *Interactive 3D general-position visualizer* in teaching crystallography is enhanced by the ability to animate the action of the different symmetry operations, in particular those with an intrinsic translation part different from zero, such as screw rotations or glide reflections.

3. Symmetry relations between space groups

This part of the *Symmetry Database* focuses on the study of group-subgroup relations between space groups. The data in Volume A1 of *International Tables for Crystallography* on maximal subgroups of space groups of indices 2, 3 and 4 are extended to include the series of all isomorphic subgroups for indices up to 27 (125 for some cubic groups). In contrast to *ITA1*, where only space-group types of supergroups are indicated, our database contains individual information for each minimal supergroup, including the transformation matrix that relates the conventional bases of the group and the supergroup. Additional programs in this part allow a detailed study of supergroups of space groups of any index (not just minimal supergroups) and the generation of interactive graphs of chains of maximal subgroups.

3.1. Maximal subgroups

All maximal non-isomorphic and maximal isomorphic subgroups \mathcal{H} of a space group \mathcal{G} of indices 2, 3 and 4 can be retrieved from the *Symmetry Database* using the program *Maximal subgroups*. The maximal-subgroup information is presented in blocks of *translationengleiche* and *klassengleiche* subgroups (Hermann, 1929) as defined in Appendix A3.2 (see Section 2.2.4 of *ITA1*, and Fig. 7). The maximal subgroups are distributed into classes of conjugate subgroups and the classes are distinguished by different background colours. Each subgroup $\mathcal{H} < \mathcal{G}$ is specified by (i) the index of \mathcal{H} in \mathcal{G} ; (ii) the Hermann–Mauguin symbol of \mathcal{H} , referred to the coordinate system of \mathcal{G} (this symbol is a link to the class of conjugate subgroups); (iii) the conventional short Hermann–Mauguin symbol and the space-group number of \mathcal{H} (the space-group

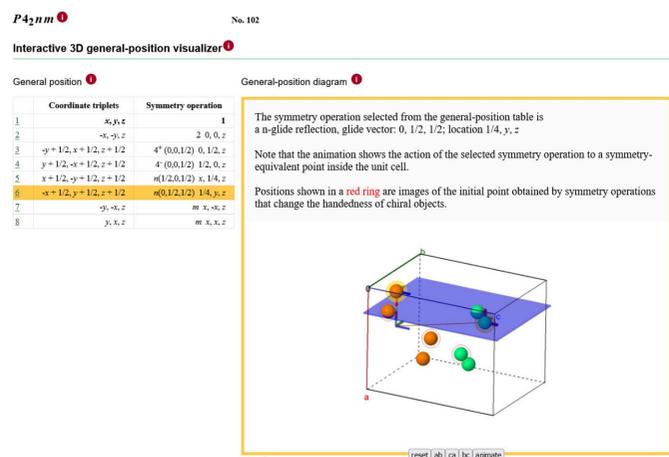


Figure 6
A screenshot of *Interactive 3D general-position visualizer* (see Section 2.4) for the space group $P4_2nm$ (No. 102).

I23 (197) > P23 (195) index 2

Transformation matrix (P, p)

$$a, b, c = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Wyckoff-position splittings

Splitting for specific orbit

I23 (197) P23 (195)

24f: 12j 12j [show relations](#)

12e: 6h 6g [show relations](#)

12d: 6f 6i [show relations](#)

8c: 4e 4e [show relations](#)

6b: 3c 3d [show relations](#)

2a: 1a 1b

Group Wyckoff position 2a representatives		Subgroup	
Group basis	Subgroup basis	Wyckoff position multiplicity and letter	Coordinate triplets
0, 0, 0	0, 0, 0	1a	0, 0, 0
1/2, 1/2, 1/2	1/2, 1/2, 1/2	1b	1/2, 1/2, 1/2

Figure 7
The maximal subgroups of the space group *I23* (No. 197) shown by the program Maximal subgroups (see Section 3.1).

number is a link to a list of maximal subgroups of \mathcal{H}); (iv) the coordinate triplets of the symmetry operations of \mathcal{G} that are used as generators for the subgroup \mathcal{H} ; and (v) the transformation matrix–column pair (P, p) that relates the standard bases of \mathcal{H} and \mathcal{G} (see Appendix A3.2). For certain applications it is necessary to represent the subgroups \mathcal{H} as subsets of elements of \mathcal{G} . This is achieved by clicking on the transformation matrix, which is a link to an auxiliary tool that transforms the general-position representatives of \mathcal{H} to the coordinate system of \mathcal{G} . In addition, for each subgroup the splittings of all Wyckoff positions of \mathcal{G} to that of \mathcal{H} and the coset decomposition of \mathcal{G} with respect to \mathcal{H} can be calculated by the auxiliary programs Wyckoff-position splittings and coset decomposition.

3.1.1. Wyckoff-position splittings. The relations between the Wyckoff positions of a space group and those of its subgroups can involve splittings of the Wyckoff positions, reduction of the site symmetries or both. The auxiliary program Wyckoff-position splittings, used by many of the programs of this part, calculates the splitting of the Wyckoff positions for a given group–subgroup pair $\mathcal{G} > \mathcal{H}$ and the transformation matrix–column pair (P, p) that relates the standard bases of \mathcal{H} and \mathcal{G} . The splitting of the Wyckoff positions of \mathcal{G} into the Wyckoff positions of \mathcal{H} is specified by their multiplicities and Wyckoff letters. This program provides further information on Wyckoff-position splittings that is not listed in *ITA1*, namely the relations between the unit-cell representatives of the orbit of \mathcal{G} and the corresponding representatives of the suborbits of \mathcal{H} . For example, Fig. 8 shows the Wyckoff-position splitting schemes for the group–maximal-subgroup pair *I23* (No. 197) > *P23* (No. 195), $(P, p) = (I, o)$ [here *I* is the three-dimensional unit matrix and *o* is the (3×1) column matrix containing zeros as coefficients]. The Wyckoff position *2a* of *I23* splits into two independent positions of *P23* with no site-symmetry reduction:

$$2a \ 23. (0, 0, 0) \rightarrow 1a \ 23. (0, 0, 0) \cup 1b \ 23. (1/2, 1/2, 1/2).$$

The relations between the coordinate triplets of the Wyckoff positions are displayed under the link ‘show relations’. These relations are presented in a table form showing the Wyckoff-position coordinate triplets with respect to the standard group basis and the corresponding triplets referred to the basis of the

subgroup. Each of these triplets is further interpreted as a coordinate triplet of a subgroup Wyckoff position. As an example, see the yellow table shown at the bottom of Fig. 8.

The link ‘Splitting for a specific orbit’ permits the calculation of the Wyckoff-position splitting schemes for an arbitrary orbit of \mathcal{G} specified by the coordinate triplet of any point of the orbit.

3.1.2. Coset decomposition. The auxiliary program coset decomposition performs the left or right coset decomposition of a group \mathcal{G} with respect to a subgroup $\mathcal{H} < \mathcal{G}$ (see Appendix A3.1):

$$\mathcal{G} = \mathcal{H} + (W_2, w_2)\mathcal{H} + \dots + (W_n, w_n)\mathcal{H}, \quad (1)$$

where *n* is the index of \mathcal{H} in \mathcal{G} and (W_i, w_i) with $i = 1, \dots, n$ are the coset representatives. The coset representative (W_1, w_1) is assumed to be the identity element (I, o) of \mathcal{G} . By default, the program calculates the right coset decomposition of the group with respect to the subgroup, and the coset representatives that are shown are described in the basis of the subgroup. To calculate the left coset decomposition, one has to click on the option ‘Left cosets’. Clicking on ‘show complete cosets’ lists the members of the coset $(W_i, w_i)\mathcal{H}$, where \mathcal{H} is decomposed with respect to its translational subgroup $T_{\mathcal{H}}$.

As an example, Fig. 9 shows the output of coset decomposition for the right coset decomposition of the space group *I23* (No. 197) with respect to one of its maximal subgroups, *R3* (No. 146), $(P, p) = a - b, b + c, -1/2a - 1/2b + 1/2c; 0, 0, 0$.

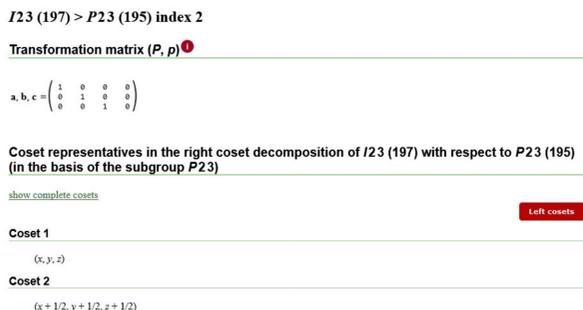


Figure 9
Coset decomposition of the space group *I*23 (No. 197) with respect to the maximal subgroup *R*3 (No. 146) for the transformation matrix **a – b, b + c, –1/2a – 1/2b + 1/2c; 0, 0, 0** calculated by the auxiliary program coset decomposition (see Section 3.1.2).

3.2. Series of isomorphic subgroups

The maximal subgroups of index higher than 4 with indices p , p^2 and p^3 , where p is a prime number, are isomorphic subgroups and infinite in number. In *ITA1* the isomorphic subgroups of indices higher than four, $[i] > 4$, are listed not individually but as members of series under the heading *Series of maximal isomorphic subgroups*. The program *Series of isomorphic subgroups* provides access to the database of maximal isomorphic subgroups. Apart from the parametric descriptions of the series, the program provides an individual listing of all maximal isomorphic subgroups of indices as high as 27 for all space groups, except for the cubic ones, where for some groups the isomorphic subgroups of indices up to 125 are shown. For each series, the Hermann–Mauguin symbol of the subgroup, the selected generators, the restrictions on the parameters describing the series, and the transformation

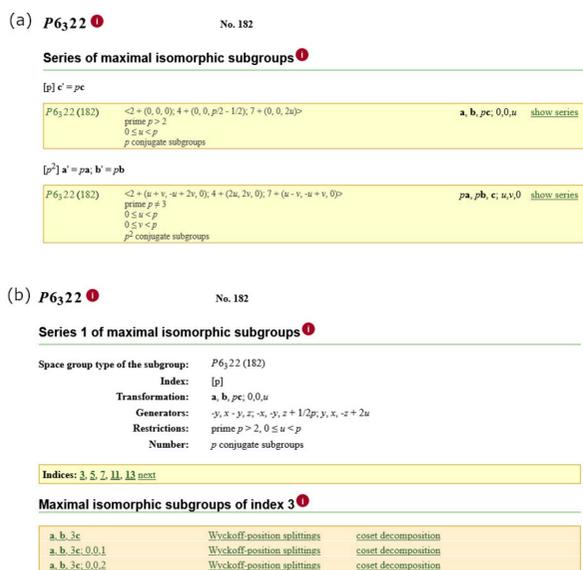


Figure 10
(a) The series of maximal isomorphic subgroups and (b) the maximal isomorphic subgroup of index 3 of the space group *P*6₃22 (No. 182) calculated by the program *Series of isomorphic subgroups* (see Section 3.2).

matrix relating \mathcal{G} and \mathcal{H} are listed [see Fig 10(a)]. The option ‘show series’ generates maximal isomorphic subgroups of any allowed index ‘on the fly’. The format and content of the subgroup data are similar to those of the program *Maximal subgroups* (see Section 3.1). Fig. 10(b) shows the maximal isomorphic subgroups of index 3 of the space group *P*6₃22 (No. 182) generated using this option. For each of the indices, a list of the maximal subgroups is presented together with links to the auxiliary programs *Wyckoff-position splittings* (see Section 3.1.1) and *coset decomposition* (see Section 3.1.2).

3.3. Minimal supergroups

The program *Minimal supergroups* lists the isomorphic and non-isomorphic minimal supergroups of indices 2, 3 and 4 (see Appendix A3.3) for any space group. For triclinic and monoclinic space groups, this list includes minimal isomorphic supergroups of indices up to 7. The minimal-supergroup information is presented in blocks of *translationengleiche* and *non-isomorphic klassengleiche* supergroups, as defined in Appendix A3.3 (see also Section 2.1.6 of *ITA1*). For each minimal supergroup, the index, the Hermann–Mauguin symbol, the space-group number and the transformation matrix (**P, p**) relating the standard bases of the supergroup and the group are specified (see Fig. 11). As in other programs of the *Symmetry Database*, the transformation matrix is a link to an auxiliary tool that calculates the general position of the supergroup with respect to the basis of the group. For each group–supergroup relation, links to the auxiliary programs *Wyckoff-position splittings* (see Section 3.1.1) and *coset decomposition* (see Section 3.1.2) are also provided.

3.4. Group–subgroup relations

A group–subgroup pair $\mathcal{G} > \mathcal{H}$ is specified by the group \mathcal{G} , subgroup \mathcal{H} and transformation matrix–column pair (**P, p**) relating the standard basis of the group to that of the subgroup. For a given group–subgroup pair, the program *Group–subgroup relations* calculates (i) the Wyckoff-position splitting scheme of the group \mathcal{G} with respect to the subgroup \mathcal{H} , (ii) the left and right coset decomposition of \mathcal{G}

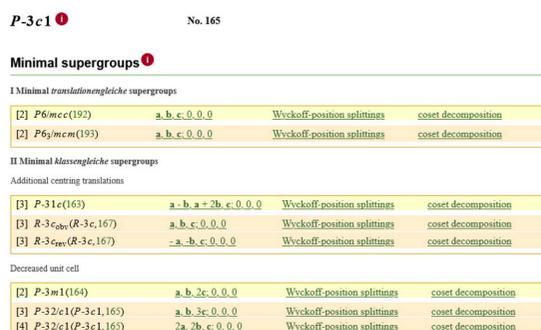


Figure 11
The minimal supergroups of the space group *P*3c1 (No. 165) obtained using the program *Minimal supergroups* (see Section 3.3).

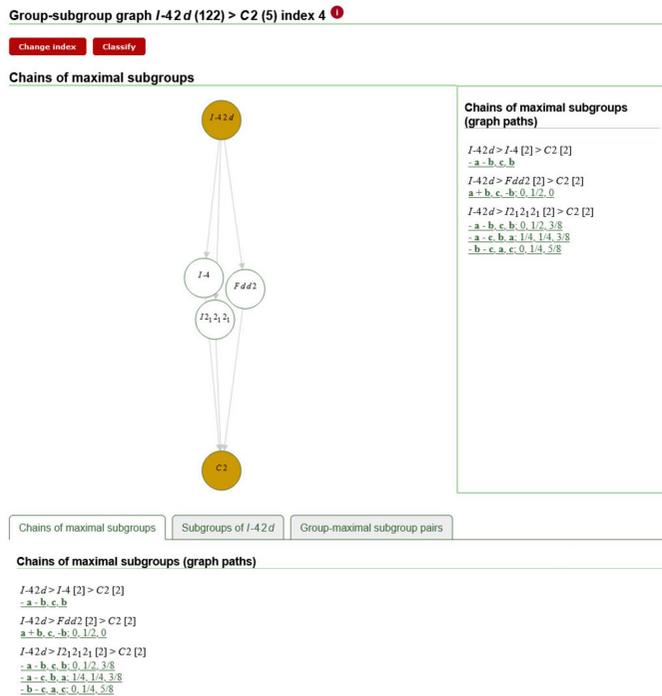


Figure 12

A screenshot of Graph of maximal subgroups (see Section 3.5), where the contracted graph for the pair of space groups $I\bar{4}2d$ (No. 122) > C2 (No. 5) with index 4 is shown.

with respect to \mathcal{H} , and (iii) the transformation of the general position of \mathcal{G} with respect to the basis of \mathcal{H} . As input, the group, the subgroup and the transformation matrix relating the standard basis of the group to that of the subgroup have to be specified. The group and the subgroup can be specified by typing in either the space-group number or the Hermann–Mauguin symbol. Before performing any calculation, the program checks the matrix–column pair (\mathbf{P}, \mathbf{p}) and if it is not valid an error message is displayed. When the transformation matrix for the group–subgroup pair is not known, the auxiliary program Step-by-step calculation of the program Group–subgroup relations can be used to find it.

3.5. Graph of maximal subgroups

Group–subgroup symmetry relations can be visualized as graphs of chains of maximal subgroups using Graph of maximal subgroups. For a given group–subgroup pair $\mathcal{G} > \mathcal{H}$, the program calculates all possible group–subgroup chains of intermediate maximal subgroups \mathcal{Z}_k : $\mathcal{G} > \mathcal{Z}_1 > \dots > \mathcal{Z}_n = \mathcal{H}$ and displays the results in an interactive graph. The auxiliary program Step-by-step calculation can be used to find the transformation matrix–column pairs (\mathbf{P}, \mathbf{p}) defining the group–subgroup relations when the correct transformation matrices are not known. This can also be used to calculate the shortest maximal-subgroup path between the group and the subgroup (Aljazzar & Leue, 2011). The input to Graph of maximal subgroups is the group \mathcal{G} and the subgroup \mathcal{H} ; the index of \mathcal{H} in \mathcal{G} is optional. If the index of the subgroup \mathcal{H} in \mathcal{G} is specified, the group–

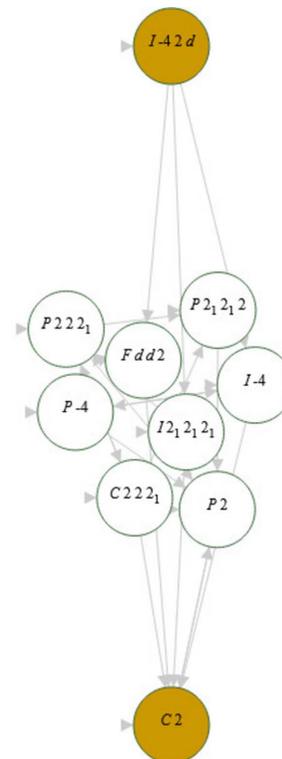


Figure 13

The general contracted graph for $I\bar{4}2d$ (No. 122) > C2 (No. 5), as shown by Graph of maximal subgroups (see Section 3.5).

subgroup relations are shown in a *contracted graph* (see Fig. 12); if not, the group–subgroup relations are represented by a *general contracted graph* (see Fig. 13). The general contracted graph contains all possible groups \mathcal{Z}_k that appear as intermediate maximal subgroups between \mathcal{G} and \mathcal{H} . It is important to note that in both the contracted and general contracted graphs a node specified by a space-group symbol indicates a space-group type, *i.e.* a node might represent different space groups belonging to the same space-group type.

As one can see in Fig. 12, the output of Graph of maximal subgroups is divided into three main sections. The first section hosts the auxiliary programs Change index and Classify. While with Change index one can repeat the calculations with a different index, Classify is used to display the conjugacy classes of maximal subgroups for the given type and index. For each of the conjugacy classes of subgroups, the program indicates the corresponding Hermann group and the factorization of the index $[i] = [i_l] \cdot [i_k]$, where the index $[i_l]$ indicates the reduction of point-group symmetry $[i_l] = |\mathcal{P}_{\mathcal{G}}|/|\mathcal{P}_{\mathcal{H}}|$ while $[i_k]$ reflects the loss of translation symmetry $[i_k] = |\mathcal{T}_{\mathcal{G}}|/|\mathcal{T}_{\mathcal{H}}|$ (see Appendix A3.2; for more details, see Section 1.2.7 of ITA1). For example, in the case of the group–subgroup relation $I\bar{4}2d$ (No. 122) > C2 (No. 5) of index 4, there are three different subgroups C2 distributed between two classes of conjugate subgroups. The three different subgroups correspond to the three sets of twofold rotation axes in $I\bar{4}2d$: those pointing along [100] and [010] of the tetragonal cell give rise to the two conjugate subgroups,

and the twofold axes of the third one (which forms a class of conjugate subgroups by itself) are along the tetragonal axis. The three subgroups C_2 are *translationengleiche* subgroups of $I\bar{4}2d$, i.e. the Hermann group for the pair $I\bar{4}2d > C_2$ of index 4 coincides with the subgroup C_2 with $[i] = [i_l] = 4$ and $[i_k] = 1$.

The transformation matrices for the different chains of maximal subgroups for the selected group–subgroup pair are listed on the right-hand side of the second section of the output, entitled ‘Chains of maximal subgroups’. On the left-hand side, the interactive group–subgroup graph is displayed. When hovering over any graph node, the corresponding space group with its maximal subgroups and minimal supergroups is shown. When clicking on any node, the chains that go through this node are highlighted on the right-hand side. In the last section of the output there are three tabs with more detailed information regarding the graph and the chains of the maximal subgroups. All the chains are listed under the tab ‘Chains of maximal subgroups’. For each chain, the space groups involved are shown and all transformations that correspond to the chain are displayed. The transformation matrices are links and calculate the general position of the subgroup \mathcal{H} in the basis of the group \mathcal{G} . The tab ‘Group–maximal subgroup pairs’ contains all the transformation matrix–column pairs for each group–maximal subgroup pair in the graph. The other tab shows all subgroups of \mathcal{G} involved in the graph.

3.6. Supergroups

The last program available in this part of the *Symmetry Database* is the program *Supergroups*, which calculates all supergroups of a specific space-group type and index (see Appendix A3.3). In contrast to *ITA1*, where only the space-group types of supergroups are indicated, in the *Symmetry Database* each supergroup is listed individually and specified by the transformation matrix that relates the conventional bases of the group and the supergroup. As input, the group, supergroup and index have to be specified. The program lists all the transformation matrices that specify different supergroups, and it is possible to calculate the general position of the group in the basis of each supergroup. The coset decomposition and Wyckoff-position splittings of each group–supergroup relation can also be calculated.

4. 3D crystallographic point groups

For those interested in molecular symmetry and in the physical properties of materials, the generators, general positions and Wyckoff positions of the three-dimensional crystallographic point groups are available in the third part of the *Symmetry Database*. These data can be transformed to different settings, enhancing and extending the data presented in Chapter 3.2 of *ITA*. Moreover, simple, clear and instructive interactive visualization of the symmetry elements and the stereographic projections of the three-dimensional crystallographic point groups is also available. The input for the programs in this part is the point group, which can be selected directly from a table

that lists the Hermann–Mauguin and Schönflies symbols for all 32 three-dimensional crystallographic point groups.

4.1. Data for the crystallographic point groups

In this section of the *Symmetry Database*, there are three programs called *Generators*, *General position* and *Wyckoff positions* (analogous to the programs for the space groups) that list the generators, general positions and Wyckoff positions for the 32 three-dimensional crystallographic point groups, respectively. The crystallographic data retrieved by these programs can be transformed to different settings by clicking on the options ‘Change basis’ or ‘Change setting’. The output of these three programs is similar to the output of the programs *Generators*, *General position* and *Wyckoff positions* for the space groups (see Sections 2.1 and 2.2 for more details).

4.2. Interactive 3D visualization

The program *Interactive visualization* for point groups (Arribas *et al.*, 2014), which was inspired by classical wooden crystallographic models, is an interactive visualizer of the symmetry elements and their stereographic projections for the crystallographic point groups. Interactive three-dimensional polyhedra are used to represent idealized crystals and their corresponding symmetry elements (see Fig. 14). The user can explore different shapes of polyhedra compatible with the selected point group and view them from different angles, and can also selectively enable or disable the visualization of the symmetry elements. It is an excellent program for learning about essential symmetry concepts and the international Hermann–Mauguin notation of point-symmetry groups.

5. Applications

Besides providing access to the crystallographic databases for the point and space groups, the programs and visualizers of the *Symmetry Database* are very useful in the study of symmetry relations between space groups. Information about symmetry

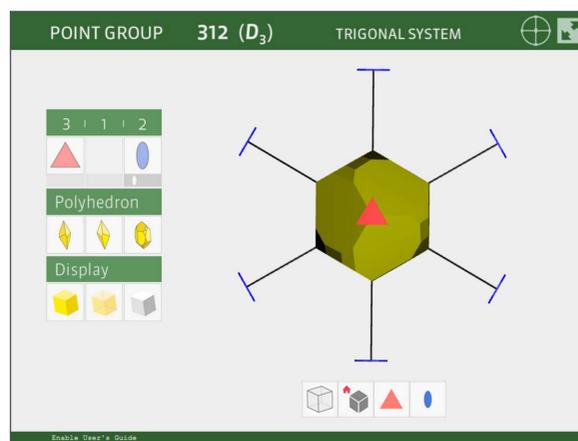


Figure 14
The output of *Interactive visualization* (see Section 4.2) for the point group 312.

relations is essential for the resolution of a number of crystallographic problems, such as the analysis of domain structures, the study of phase transitions and the prediction of new crystal structures. The use of some of these programs and visualizers is demonstrated in this section with several illustrative examples.

5.1. Equivalent crystal-structure descriptions

In general, crystal structures are described through their space-group symmetry, the unit-cell parameters and the atomic positions in the asymmetric unit. The description of a structure is not unique and depends on the coordinate systems, *i.e.* on the chosen setting of the space group. Even after fixing the setting of the space group, in most cases there are several equivalent possible but different descriptions of the same crystal structure (Koch & Fischer, 2006).

Consider, for example, the simple and well known structure of caesium chloride (CsCl), which crystallizes in the cubic space group $Pm\bar{3}m$ (No. 221). The origin can be chosen to be at the centre of a Cs or a Cl atom, which results in two different sets of coordinates (see Fig. 15):

Structure No. 1	Structure No. 2
Cs 1a 0, 0, 0	Cs 1b $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
Cl 1b $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	Cl 1a 0, 0, 0

The equivalence of the two descriptions is easy to recognize [see Fig. 15: they are related by a translation of the type $t(1/2, 1/2, 1/2)$]. But how many equivalent descriptions of the CsCl structure exist? How can we calculate all possible symmetry-equivalent descriptions of a given crystal structure?

The *Euclidean normalizer* $\mathcal{N}_\varepsilon(\mathcal{G})$ plays an important role in the determination of all symmetry-equivalent descriptions of a given structure with space group \mathcal{G} . The number of different equivalent coordinate descriptions of a crystal structure is equal to the index $[i]$ of the group \mathcal{G} in its Euclidean normalizer $\mathcal{N}_\varepsilon(\mathcal{G})$:

$$[i] = \frac{|\mathcal{N}_\varepsilon(\mathcal{G})|}{|\mathcal{G}|}. \quad (2)$$

There are only two space groups, $Im\bar{3}m$ (No. 229) and $Ia\bar{3}d$ (No. 230), that give rise to only one description of a crystal structure. This is due to the fact that the Euclidean normalizer $\mathcal{N}_\varepsilon(\mathcal{G})$ coincides with the space group \mathcal{G} . For all other space groups, there exist at least two equivalent descriptions.

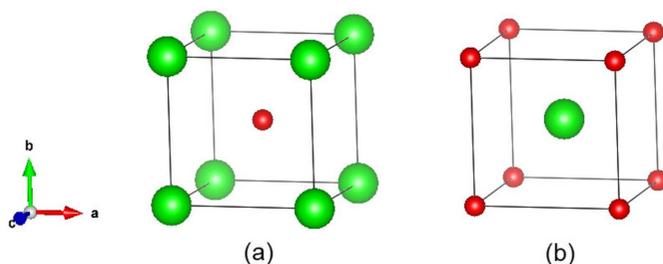


Figure 15
The structure of CsCl described with respect to the cubic space group $Pm\bar{3}m$ (No. 221) with the origin at (a) Cs and (b) Cl.

The transformations generating the set of symmetry-equivalent descriptions of a given crystal structure can be calculated easily by the coset decomposition of $\mathcal{N}_\varepsilon(\mathcal{G})$ with respect to \mathcal{G} :

$$\mathcal{N}_\varepsilon(\mathcal{G}) = \mathcal{G} + (\mathbf{W}_2, \mathbf{w}_2)\mathcal{G} + \dots + (\mathbf{W}_n, \mathbf{w}_n)\mathcal{G}, \quad (3)$$

where n is the index of \mathcal{G} in $\mathcal{N}_\varepsilon(\mathcal{G})$, $(\mathbf{W}_i, \mathbf{w}_i)$ with $i = 1, \dots, n$ represents the coset representatives and $(\mathbf{W}_1, \mathbf{w}_1)$ is assumed to be the identity element (\mathbf{I}, \mathbf{o}) . The transformation of the initial structure by the coset representatives in equation (3) yields all symmetry-equivalent descriptions:

$$X' = (\mathbf{W}_i, \mathbf{w}_i)X, \quad (4)$$

where X represents the coordinates of the atoms in the initial structure, X' corresponds to the coordinates of the atoms of the equivalent descriptions and $(\mathbf{W}_i, \mathbf{w}_i)$ acts as the transformation matrix.

The symmetry-equivalent descriptions of a given structure and their generation can be easily obtained using the program *Normalizers* (see Section 2.3). In the case of CsCl, the Euclidean normalizer of the space group $Pm\bar{3}m(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is $Im\bar{3}m$ with basis vectors $(1/2\mathbf{a}, 1/2\mathbf{b}, 1/2\mathbf{c})$. The index of $Pm\bar{3}m$ in $Im\bar{3}m$ is two; this means that there are only two different symmetry-equivalent descriptions for the structure of CsCl. The coset decomposition of the Euclidean normalizer with respect to the space group,

$$Im\bar{3}m = Pm\bar{3}m + t(1/2, 1/2, 1/2)Pm\bar{3}m, \quad (5)$$

shows that the second equivalent description of CsCl is generated from the initial description by a translation of the type $t(1/2, 1/2, 1/2)$.

Crystal structures with space groups that are polar have infinitely many symmetry-equivalent descriptions, since they are not fixed by symmetry (for more details, see Appendix A4 and Chapter 3.5 of *ITA*). This is the case for the co-crystallization of caffeine and 4-chloro-3-nitrobenzoic acid (Ghosh & Reddy, 2012), which gives a structure with a polar space group $Fdd2$ (No. 43). This structure is available from the Cambridge Crystallographic Data Centre as CCDC reference 88530 (BEDYIU). The Euclidean normalizer of $Fdd2(\mathbf{a}, \mathbf{b}, \mathbf{c})$ is $P^1ban(1/2\mathbf{a}, 1/2\mathbf{b}, \epsilon\mathbf{c})$, a normalizer that contains continuous translations in one direction. This is indicated by $\epsilon\mathbf{c}$ for the third basis vector of the normalizer and by the superscript 1 to the Bravais letter (see Chapter 3.5 of *ITA*). The index of P^1ban in $Fdd2$ is $2 \cdot \infty$; this means that there are two symmetry-equivalent descriptions, and for each one, infinitely many symmetry-equivalent descriptions exist. The translations of the type $t(0, 0, t)$ give rise to infinite equivalent descriptions that differ only in their z coordinates.

5.2. Symmetry relations between space groups

5.2.1. Phase transitions. Consider two phases of the same compound whose symmetries are described by the space group \mathcal{G} (*parent* structure) and \mathcal{H} (*derivative* structure), such that $\mathcal{G} > \mathcal{H}$. The relationship between these two structures can be characterized by a *global distortion* that is decomposed into a *strain*, describing the global distortion of the lattice of the

derivative structure relative to the parent structure, and an *atomic displacement field*, representing the displacements of the atoms of the low-symmetry phase from their positions in the high-symmetry phase. The global distortion can be characterized if the description of the parent structure is transformed by an appropriate transformation (\mathbf{P}, \mathbf{p}) to an equivalent description that is most similar to that of the derivative structure. This new description of the parent structure is usually called the *reference description* of the parent structure relative to the derivative structure. The metric deformation accompanying the phase transition can be determined by the comparison of the bases of the derivative and the reference structures. Similarly, the difference between the atomic positions of the reference and the derivative structure provides information related to the atomic displacements occurring during the phase transition.

As an illustrative example consider the structural phase transition of CaCl_2 . At room temperature CaCl_2 crystallizes in the orthorhombic space group $Pn\bar{m}$ (No. 58). At about 235°C a structural phase transition takes place to a high-symmetry tetragonal phase of the rutile type. The following descriptions of the two phases of CaCl_2 (Howard *et al.*, 2005) are taken from the Inorganic Crystal Structure Database (Fachinformationszentrum Karlsruhe and National Institute of Standards and Technology, <https://www.fiz-karlsruhe.de/icsd.html>, abbreviated as ICSD):

(a) ICSD No. 246417. The symmetry of the high-temperature phase is described by the tetragonal space group $P4_2/m\bar{m}$ (No. 136) with cell parameters $a_t = 6.38310$ (10) Å and $c_t = 4.20409$ (7) Å. The coordinates of the atoms in the asymmetric unit are given as

Ca: $2a$ 0, 0, 0,

Cl: $4f$ 0.3047, 0.3047, 0.

(b) ICSD No. 246416. The low-symmetry structure is described by the orthorhombic space group $Pn\bar{m}$ with cell parameters $a_{\text{orth}} = 6.43763$ (5) Å, $b_{\text{orth}} = 6.28765$ (5) Å and $c_{\text{orth}} = 4.17823$ (1) Å. The coordinates of the atoms in the asymmetric unit are given as

Ca: $2a$ 0, 0, 0,

Cl: $4g$ 0.3249, 0.2822, 0.

The subgroup $Pn\bar{m}$ is a maximal subgroup of index 2 of the group $P4_2/m\bar{m}$. The transformation matrix relating the group with the subgroup, determined by the program *Maximal subgroups* (see Section 3.1), is the identity matrix, *i.e.* $(\mathbf{P}, \mathbf{p}) = (\mathbf{a}, \mathbf{b}, \mathbf{c}; 0, 0, 0)$. This means that the lattice parameters of the reference and parent structures are equal (for details of the unit-cell lattice transformation see Appendix A2). From the comparison of the lattice parameters of the reference and the derivative structures, the lattice deformation accompanying the phase transition can be determined.

The coordinates of the representative Ca atom occupying the position $2a$ 0, 0, 0 in $P4_2/m\bar{m}$ are transformed to $2a$ 0, 0, 0, while those of Cl are transformed from $4f$ 0.3047, 0.3047, 0 in $P4_2/m\bar{m}$ to $4g$ 0.3047, 0.3047, 0 (results provided by the auxiliary program *Wyckoff-position splittings*, see Section 3.1.1). A comparison between the transformed atomic coordinates and the atomic coordinates of the low-symmetry

phase, Ca 0, 0, 0 and Cl 0.3249, 0.2822, 0, reveals the corresponding atomic displacements associated with the phase transition, which, in this case, are related to the displacements of the Cl atoms.

5.2.2. Domain structure analysis. A displacive or order-disorder phase transition often results in the formation of domain structures. A homogeneous single phase with space group \mathcal{G} , known as the *parent* or *prototypic phase*, is transformed to a crystalline phase, known as the *daughter* or *distorted phase*, with space group \mathcal{H} such that $\mathcal{H} < \mathcal{G}$. The distorted phase is usually inhomogeneous, and consists of an infinite number of homogeneous regions called *domains*. Note that domains differ in their location in space, in their size and/or orientation, and potentially in their space groups $\mathcal{H}_i < \mathcal{G}$, which, however, belong to the same space-group type \mathcal{H} .

The domains in the distorted phase can be classified into a finite and small number of *domain states*. Two domains belong to the same domain state if their crystal patterns are identical, *i.e.* if they occupy regions of space that are part of the same crystal pattern. The number and types of domain states that might form during the phase transition can be predicted by the analysis of the group-subgroup relation $\mathcal{G} > \mathcal{H}$ between the prototype and the distorted phases. The domain states can be classified into two types:

(i) *Twin domain states* are formed if the point group $\mathcal{P}_{\mathcal{H}}$ of the distorted phase is a subgroup of the point group $\mathcal{P}_{\mathcal{G}}$ of the parent phase, $\mathcal{P}_{\mathcal{H}} < \mathcal{P}_{\mathcal{G}}$. For example, twin domain states occur if \mathcal{H} is a *translationengleiche* (*equi-translational*) subgroup of the space group \mathcal{G} (see Appendix A3.2) of the prototype phase.

(ii) *Antiphase domain states* are formed if the translation subgroup $\mathcal{T}_{\mathcal{H}}$ of the distorted phase is a subgroup of the translation subgroup $\mathcal{T}_{\mathcal{G}}$ of the parent phase, $\mathcal{T}_{\mathcal{H}} < \mathcal{T}_{\mathcal{G}}$. For example, antiphase domain states occur if the space group \mathcal{H} of the distorted phase is a *klassengleiche* (*equi-class*) subgroup of \mathcal{G} (see Appendix A3.2).

Twin and antiphase domain states can also be simultaneously observed if \mathcal{H} is a *general* subgroup of \mathcal{G} (see Appendix A3.2).

The number of single domain states (\mathbf{S}_i) can be determined by the index $[i]$ of \mathcal{H} in \mathcal{G} . Following Hermann's theorem, the index $[i]$ can also be factorized as

$$[i] = [i_k] \cdot [i_t], \quad (6)$$

where $[i_t]$ is the *t*-index, the *translationengleich* index, and $[i_k]$ is the *k*-index, the *klassengleich* index (see Appendix A3.2); these represent the number of different twin and antiphase domain states that might be formed during the phase transition, respectively.

Let us consider BaTiO_3 , which exhibits a ferroelectric phase transition from a prototype (non-polar) phase with cubic space group $Pm\bar{3}m$ (No. 221) to a distorted polar phase with tetragonal space group of the type $P4mm$ (No. 99). The type and number of domain states that might occur in the low-symmetry phase can be calculated using Group-subgroup relations (see Section 3.4) or Graph of maximal subgroups (see Section 3.5). The Hermann group in this

Table 1

The twinning operation g_i and polarization vector \mathbf{P}_i for each of the domain states \mathbf{S}_i for the phase transition $Pm\bar{3}m$ (No. 221) $\rightarrow P4mm$ (No. 99) of BaTiO₃.

Domain state	Twinning operation (g_i)		Polarization
	Coordinate triplets	Seitz symbols	
\mathbf{S}_1	(x, y, z)	$\{1 0\}$	$\begin{pmatrix} 0 \\ 0 \\ V \end{pmatrix}$
\mathbf{S}_2	$(\bar{x}, \bar{y}, \bar{z})$	$\{\bar{1} 0\}$	$\begin{pmatrix} 0 \\ 0 \\ -V \end{pmatrix}$
\mathbf{S}_3	(z, x, y)	$\{3^+ 0\}$	$\begin{pmatrix} V \\ 0 \\ 0 \end{pmatrix}$
\mathbf{S}_4	$(\bar{z}, \bar{x}, \bar{y})$	$\{\bar{3}^+ 0\}$	$\begin{pmatrix} -V \\ 0 \\ 0 \end{pmatrix}$
\mathbf{S}_5	(y, z, x)	$\{3^- 0\}$	$\begin{pmatrix} 0 \\ V \\ 0 \end{pmatrix}$
\mathbf{S}_6	$(\bar{y}, \bar{z}, \bar{x})$	$\{\bar{3}^- 0\}$	$\begin{pmatrix} 0 \\ -V \\ 0 \end{pmatrix}$

example is $P4mm$ (No. 99) with $i_t = 6$ and $i_k = 1$. Since $P4mm$ is a *translationengleiche* subgroup of $Pm\bar{3}m$ of index 6, six different twin domain states are expected to be formed during the phase transition. For the space group $Pm\bar{3}m$ there are three different (but conjugate in $P4mm$, see Appendix A3.1) subgroups \mathcal{H}_i isomorphic to $P4mm$ of index 6 [with their fourfold axes directed along the \mathbf{a} , \mathbf{b} and \mathbf{c} directions, *i.e.* $\mathcal{H}_1 = P4_a mm$ with $(\mathbf{P}, \mathbf{p}) = (\mathbf{b}, \mathbf{c}, \mathbf{a})$, often written as $\mathcal{H}_1 = P4mm(\mathbf{b}, \mathbf{c}, \mathbf{a})$, $\mathcal{H}_2 = P4_b mm = P4mm(\mathbf{c}, \mathbf{a}, \mathbf{b})$ and $\mathcal{H}_3 = P4_c mm = P4mm(\mathbf{a}, \mathbf{b}, \mathbf{c})$].

Different domain states can exhibit different tensor properties and different diffraction patterns and can differ in other physical properties. The tensor properties of the crystal can be used to distinguish the different domain states if the relation between the domain states is known, *i.e.* if the twinning operation is known. This can be obtained from the coset decomposition of the space group \mathcal{G} of the prototype phase with respect to \mathcal{H}_i , where each of the coset representatives might act as a twinning operation. In this example, the coset decomposition of $\mathcal{G} = Pm\bar{3}m$ with respect to $\mathcal{H}_3 = P4_c mm$ is calculated using the auxiliary program `coset decomposition` (see Section 3.1.2) within `Group-subgroup pair` or `Graph of maximal subgroups` (see Table 1).

Let us analyse the polarization \mathbf{P} , a tensor of rank one, in the low-symmetry phase of BaTiO₃. The polarization in each domain state \mathbf{S}_i can be determined by

$$\mathbf{P}_i = g_i \mathbf{P}, \quad (7)$$

where $i = 1, \dots, 6$ represents the number of domain states \mathbf{S}_i and g_i are the corresponding twinning operations. The polarization vector \mathbf{P} compatible with $\mathcal{H}_3 = P4_c mm$ is of the type

$$\mathbf{P} = \begin{pmatrix} 0 \\ 0 \\ V \end{pmatrix}.$$

Table 1 shows the polarization \mathbf{P}_i in the different domain states calculated by equation (7).

5.2.3. Hierarchical trees. The structural relationships between group-subgroup-related crystal structures can be presented in a concise and comprehensive form using *Bärnighausen trees* (Bärnighausen, 1980). Starting from a high-symmetry structure type (*aristotype*) and reducing the symmetry, by distortions or substitutions of atoms, lower-symmetry structure types (*hettotypes*) are derived. Detailed information on how to construct Bärnighausen trees is available in Chapter 1.6 of *ITA1* and in the book by Müller (2013).¹ The programs `Maximal subgroups` (see Section 3.1), `Graph of maximal subgroups` (see Section 3.5) and `Wyckoff-position splittings` (see Section 3.1.1) are very useful for obtaining the information needed to construct Bärnighausen trees.

Such *hierarchical trees* can also be constructed by searching in the opposite direction (Kitaev *et al.*, 2015), *i.e.* the highest possible structure types (*archetypes*) are reached by starting from a hettotype or *root* structure. In an *ascending group-supergroup tree* the space group \mathcal{G} of the high-symmetry structure is a supergroup of the space group \mathcal{H} of the root structure. Taking into account that any group-supergroup relation $\mathcal{H} < \mathcal{G}$ can be represented by a chain of minimal supergroups, $\mathcal{H} < \mathcal{Z}_1 < \mathcal{Z}_2 < \dots < \mathcal{G}$, the search for possible archetypes can be performed as a stepwise procedure over a chain of minimal supergroups of the space group of the root structure. Starting from the space group \mathcal{H} of the root structure, a list of the minimal supergroups $\mathcal{G}_i > \mathcal{H}$ can be fetched, along with the transformation matrices (\mathbf{P}, \mathbf{p}) relating the supergroup with the group, via the program `Minimal supergroups` (see Section 3.3). The validity of each (\mathbf{P}, \mathbf{p}) has to be evaluated with respect to the splitting of the supergroup's Wyckoff positions into the starting space group \mathcal{H} . For each transformation matrix, the splitting of the Wyckoff positions is directly calculated by the auxiliary program `Wyckoff-position splittings` within the program `Minimal supergroups`, and those supergroups that split their Wyckoff positions into the occupied positions of the root structure are selected. Note that the calculated splitting of the Wyckoff positions has to be checked against the occupied positions in the root structure along with all its

¹ The book by Müller is also available in German (*Symmetriebeziehungen zwischen verwandten Kristallstrukturen*; Vieweg+Teubner, 2012) and in Spanish (*Relaciones de simetría entre estructuras cristalinas*; Síntesis, 2013).

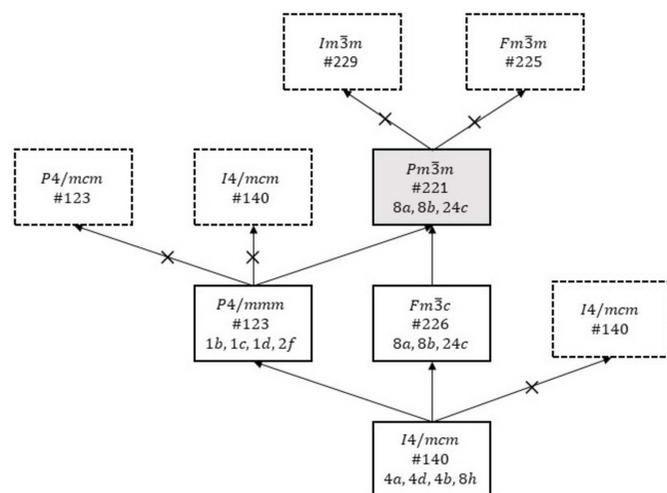


Figure 16
The ascending group-subgroup tree for the $I4/mcm$: $4a, 4d, 4b, 8h$ root structure constructed with the help of Minimal supergroups (see Section 3.3) and Wyckoff-position splittings (see Section 3.1.1). The archetype is shaded in grey, and dashed lines outline the structure types into which transitions are forbidden.

symmetry-equivalent structures as calculated by applying the Euclidean normalizer, using the program *Normalizers* (see Section 2.3). The search then continues upward until the highest possible structure type whose space groups do not have any supergroups fulfilling the conditions for the splitting of the Wyckoff positions is reached. In addition to these symmetry conditions, one has to take into account that a higher-symmetry phase can only be reached if the strain and the atomic displacement relating the two structures are small enough [see Capillas *et al.* (2007)]. More detailed information about the procedure for deriving and constructing group-supergraph trees is provided by Kitaev *et al.* (2015).

Let us construct the group-supergraph tree ascending from a root structure of $KCuF_3$ belonging to the space group $I4/mcm$ (No. 140) with the atoms occupying the $4a, 4d, 4b$ and $8h$ Wyckoff positions. The space group $I4/mcm$ has three minimal supergroups: $Fm\bar{3}c$ (No. 226), $P4/mmm$ (No. 123) and $I4/mcm$ (No. 140). $I4/mcm$ does not satisfy the Wyckoff-position splitting conditions, and thus the upward transition into a structure type with space group $I4/mcm$ is forbidden, as shown in Fig. 16. Upward in this tree, there is only one supergroup for the space group $Fm\bar{3}c$ and three for $P4/mmm$. Among these four supergroups only $Pm\bar{3}m$ (No. 221) meets the splitting conditions of the Wyckoff positions for both $Fm\bar{3}c$ and $P4/mmm$. In the next step, the two supergroups of the group $Pm\bar{3}m$ do not satisfy the splitting conditions of the Wyckoff positions. Therefore the $Pm\bar{3}m$: $1a, 1b, 1c$ structure type should be considered as the archetype for the $I4/mcm$: $4a, 4d, 4b, 8h$ structure type.

Note that there are cases in which the use of non-standard settings is more convenient for describing the symmetry relationships between crystal structures clearly. The results of the programs of the *Symmetry Database* should be used with care, as the programs used the standard setting as a default.

6. Conclusions

The *Symmetry Database* forms part of *International Tables for Crystallography* and hosts (i) crystallographic databases and visualizers for the point and space groups and (ii) programs and an interactive visualizer for studying the symmetry relations between space groups. These programs do not need local installation; the only requirement is to be subscribed to the online version of *International Tables for Crystallography*.

The *Symmetry Database* provides access to the generators, general positions and Wyckoff positions for the point and space groups, and enables transformation of this information to different settings. Databases of the affine, Euclidean and chirality-preserving Euclidean normalizers of the space groups and of the maximal subgroups and minimal supergroups of the space groups are included. There are programs for calculating the supergroups of space groups of any index and for generating interactive graphs of maximal subgroups. Programs for visualizing the symmetry elements and the stereographic projections of the point groups and the general-position diagrams of the space groups are also provided and may be useful for teaching.

APPENDIX A

Some definitions and information on notation

This appendix is based on Chapters 1.3, 1.5 of 1.7 of the *Teaching Edition of International Tables for Crystallography* (2021) and Chapter 3.5 of *ITA* (see also Chapters 8.1, 8.2 and 8.3 of the 5th edition of *International Tables for Crystallography* Volume A, 2006).

A1. Crystallographic symmetry operations

The notation for the space-group symmetry operations in the *Symmetry Database* closely follows the conventions adopted in *ITA*.

In order to describe the symmetry operations analytically, one introduces a coordinate system $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$ consisting of a set of basis vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ and an origin O . A symmetry operation can be regarded as an instruction for how to calculate the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$ of the image point \tilde{X} from the coordinates x, y, z of the original point X .

The equations are

$$\begin{aligned}\tilde{x} &= W_{11}x + W_{12}y + W_{13}z + w_1, \\ \tilde{y} &= W_{21}x + W_{22}y + W_{23}z + w_2, \\ \tilde{z} &= W_{31}x + W_{32}y + W_{33}z + w_3.\end{aligned}\quad (8)$$

These equations can be written using the matrix formalism:

$$\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w} = (\mathbf{W}, \mathbf{w})\mathbf{x}.$$

Here, the symmetry operations (\mathbf{W}, \mathbf{w}) are given in a matrix-column form consisting of a (3×3) matrix (linear) part \mathbf{W} and a (3×1) column (translation) part \mathbf{w} :

$$(\mathbf{W}, \mathbf{w}) = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \end{array} \right). \quad (9)$$

The vertical line in equation (9) is to guide the eye and has no mathematical meaning.

Apart from the matrix–column pair representation of (\mathbf{W}, \mathbf{w}) , a *shorthand notation* for the symmetry operations is often used. It is obtained from the left-hand side of equation (8) by omitting the terms with coefficients 0 and writing the three different rows of equation (8) in one line, separated by commas. For example, consider the last symmetry operation in the general position list obtained by `General position` for the space group $P4_1$ (No. 76):

$$\tilde{\mathbf{x}} = (\mathbf{W}, \mathbf{w})\mathbf{x} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 3/4 \end{pmatrix}$$

would be $\tilde{x} = 0x + 1y + 0z$, $\tilde{y} = -1x + 0y + 0z$, $\tilde{z} = 0x + 0y + 1z + 3/4$. The shorthand notation for (\mathbf{W}, \mathbf{w}) thus reads: $y, \bar{x}, z + 3/4$.

A2. Coordinate transformations: basic results

Let a coordinate system be given with a basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ and an origin O . The general (affine) transformation between two coordinate systems consists of two parts, a *linear part* and a *shift of the origin*.

(1) The linear part is described by a (3×3) matrix

$$\mathbf{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

that relates the primed ('new') basis $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)$ to the unprimed ('old') basis $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$ according to

$$\begin{aligned} (\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3) &= (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)\mathbf{P} \\ &= (\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}. \end{aligned} \quad (10)$$

(2) A shift of the origin is defined by the *shift vector*

$$\mathbf{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}.$$

The basis vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ are fixed at the origin O while the new basis vectors $(\mathbf{a}'_1, \mathbf{a}'_2, \mathbf{a}'_3)$ are fixed at the new origin O' . The new origin has the coordinates (p_1, p_2, p_3) in the old coordinate system.

The general affine transformation of the coordinates of a point X in direct space, given by the column

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix},$$

is given by the following formula:

$$\mathbf{x}' = (\mathbf{P}, \mathbf{p})^{-1}\mathbf{x} = \mathbf{P}^{-1}\mathbf{x} - \mathbf{P}^{-1}\mathbf{p} = \mathbf{P}^{-1}(\mathbf{x} - \mathbf{p}). \quad (11)$$

The metric tensor \mathbf{G} of the unit cell of the crystal lattice is transformed by the matrix \mathbf{P} as follows:

$$\mathbf{G}' = \mathbf{P}^t\mathbf{G}\mathbf{P}, \quad (12)$$

where \mathbf{G}' represents the metric tensor of the new unit cell and \mathbf{P}^t is the transposed matrix of \mathbf{P} .

The volume of the unit cell V changes with the transformation. The volume of the new unit cell V' is obtained by

$$V' = \det(\mathbf{P})V, \quad (13)$$

with $\det(\mathbf{P})$ being the determinant of the matrix \mathbf{P} .

The matrix–column pairs of the symmetry operations are also changed by a change of the coordinate system. If a symmetry operation is described in the 'old' (unprimed) coordinate system by the matrix–column pair (\mathbf{W}, \mathbf{w}) and in the 'new' (primed) coordinate system by the pair $(\mathbf{W}', \mathbf{w}')$, then the relation between the pairs (\mathbf{W}, \mathbf{w}) and $(\mathbf{W}', \mathbf{w}')$ is given by

$$(\mathbf{W}', \mathbf{w}') = (\mathbf{P}, \mathbf{p})^{-1}(\mathbf{W}, \mathbf{w})(\mathbf{P}, \mathbf{p}). \quad (14a)$$

This equation may be written more explicitly as follows:

$$(\mathbf{W}', \mathbf{w}') = (\mathbf{P}^{-1}\mathbf{W}\mathbf{P}, \mathbf{P}^{-1}(\mathbf{w} + (\mathbf{W} - \mathbf{I})\mathbf{p})). \quad (14b)$$

A3. Group–subgroup relations of space groups

A3.1. Basic definitions. A subset \mathcal{H} of elements of a group \mathcal{G} is called a *subgroup* of \mathcal{G} ($\mathcal{G} > \mathcal{H}$) if it fulfils the group postulates with respect to the law of composition of \mathcal{G} . In general, the group \mathcal{G} itself is included among the set of subgroups of \mathcal{G} , i.e. $\mathcal{G} \geq \mathcal{H}$. If $\mathcal{G} > \mathcal{H}$ is fulfilled, then the subgroup \mathcal{H} is called a *proper* subgroup of \mathcal{G} .

Let $\mathcal{H} < \mathcal{G}$ be a subgroup of \mathcal{G} of order $|\mathcal{H}|$. Because \mathcal{H} is a proper subgroup of \mathcal{G} there must be elements $g_i \in \mathcal{G}$ that are not elements of \mathcal{H} . Let $g_2 \in \mathcal{G}$ be one of them. Then the set of elements $g_2\mathcal{H} = \{g_2h_j | h_j \in \mathcal{H}\}^2$ is a subset of the elements of \mathcal{G} with the property that all its elements are different, and that the sets \mathcal{H} and $g_2\mathcal{H}$ have no element in common. Thus, the set $g_2\mathcal{H}$ also contains $|\mathcal{H}|$ elements of \mathcal{G} . If there is another element $g_3 \in \mathcal{G}$ that belongs neither to \mathcal{H} nor to $g_2\mathcal{H}$, one can form another set $g_3\mathcal{H} = \{g_3h_j | h_j \in \mathcal{H}\}$. All elements of $g_3\mathcal{H}$ are different and none occurs already in \mathcal{H} or in $g_2\mathcal{H}$. This procedure can be continued until each element of \mathcal{G} belongs to one of these sets. In this way the group \mathcal{G} can be partitioned into sets (called *cosets*) such that each element $g \in \mathcal{G}$ belongs to exactly one of these cosets.

The partition just described is called a *decomposition* ($\mathcal{G} : \mathcal{H}$) into *left cosets* of the group \mathcal{G} relative to the group \mathcal{H} .

$$\mathcal{G} = \mathcal{H} \cup g_2\mathcal{H} \cup \dots \cup g_i\mathcal{H}. \quad (15)$$

The sets $g_p\mathcal{H}$, $p = 1, \dots, i$ are called left cosets because the elements $h_j \in \mathcal{H}$ are multiplied with the new elements from the left-hand side. The procedure is called a *decomposition*

² The formulation $g_2\mathcal{H} = \{g_2h_j | h_j \in \mathcal{H}\}$ means $g_2\mathcal{H}$ is the set of the products g_2h_j of g_2 with all elements $h_j \in \mathcal{H}$.

into right cosets $\mathcal{H}g_s$ if the elements $h_j \in \mathcal{H}$ are multiplied with the new elements g_s from the right-hand side.

$$\mathcal{G} = \mathcal{H} \cup \mathcal{H}g_2 \cup \dots \cup \mathcal{H}g_i. \quad (16)$$

The elements g_p or g_s are called the *coset representatives*. The number of cosets is called the *index* $[i] = |\mathcal{G} : \mathcal{H}|$ of \mathcal{H} in \mathcal{G} . The coset representative g_1 is always taken as the identity element $g_1 = (\mathbf{I}, \mathbf{o})$.

Two subgroups $\mathcal{H}_j, \mathcal{H}_k < \mathcal{G}$ are called *conjugate* if there is an element $g_q \in \mathcal{G}$ such that $g_q^{-1}\mathcal{H}_jg_q = \mathcal{H}_k$ holds. In this way, the subgroups of \mathcal{G} of the same space-group type and index are distributed into classes of conjugate subgroups that are also called *conjugacy classes of subgroups*. Different conjugacy classes of subgroups may contain different numbers of subgroups, i.e. have different lengths.

A subgroup \mathcal{H} of a group \mathcal{G} is a *normal (invariant) subgroup* $\mathcal{H} \triangleleft \mathcal{G}$ if it is identical to all of its conjugates, $g_q^{-1}\mathcal{H}g_q$, for all $g_q \in \mathcal{G}$, i.e. if its conjugacy class consists of the one subgroup \mathcal{H} only (sometimes called also a *self-conjugated subgroup*).

A3.2. Type of subgroups of space groups. The following types of subgroups of space groups are to be distinguished (Hermann, 1929):

(i) A subgroup \mathcal{H} of a space group \mathcal{G} is called a *translationengleiche (equi-translational) subgroup* or a *t-subgroup* of \mathcal{G} if the set $\mathcal{T}(\mathcal{G})$ of translations is retained, i.e. $\mathcal{T}(\mathcal{H}) = \mathcal{T}(\mathcal{G})$, but the number of cosets of the decomposition $[\mathcal{G} : \mathcal{T}(\mathcal{G})]$, i.e. the order of the point group $\mathcal{P}_{\mathcal{G}}$, is reduced.

(ii) A subgroup $\mathcal{H} < \mathcal{G}$ of a space group \mathcal{G} is called a *klassengleiche (equi-class) subgroup* or a *k-subgroup* if the set $\mathcal{T}(\mathcal{G})$ of all translations of \mathcal{G} is reduced to $\mathcal{T}(\mathcal{H}) < \mathcal{T}(\mathcal{G})$ but all linear parts of \mathcal{G} are retained. Then the number of cosets of the decompositions $(\mathcal{H} : \mathcal{T}(\mathcal{H}))$ and $(\mathcal{G} : \mathcal{T}(\mathcal{G}))$ is the same, i.e. the order of the point group $\mathcal{P}_{\mathcal{H}}$ is the same as that of $\mathcal{P}_{\mathcal{G}}$.

(iii) A *klassengleiche* or *k-subgroup* $\mathcal{H} < \mathcal{G}$ is called *isomorphic* or an *isomorphic subgroup* if it belongs to the same affine space-group type (isomorphism type) as \mathcal{G} .

(iv) A subgroup of a space group $\mathcal{H} < \mathcal{G}$ is called *general* or a *general subgroup* if it is neither a *translationengleiche* nor a *klassengleiche* subgroup. It has lost translations as well as linear parts, i.e. $\mathcal{T}(\mathcal{H}) < \mathcal{T}(\mathcal{G})$ and $\mathcal{P}(\mathcal{H}) < \mathcal{P}(\mathcal{G})$.

Any subgroup \mathcal{H} of a group \mathcal{G} is related to a specific subset of elements of \mathcal{G} and this subset defines the subgroup uniquely: different subgroups of \mathcal{G} , even those isomorphic to \mathcal{H} , correspond to different subsets of the elements of \mathcal{G} .

In the *Symmetry Database* any subgroup \mathcal{H} of a space group \mathcal{G} is specified by its space-group number in *ITA*, the index in the group \mathcal{G} and the transformation matrix–column pair (\mathbf{P}, \mathbf{p}) that relates the standard bases $(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{H}}$ of \mathcal{H} and $(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{G}}$ of \mathcal{G} :

$$(\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{H}} = (\mathbf{a}, \mathbf{b}, \mathbf{c})_{\mathcal{G}}\mathbf{P}. \quad (17)$$

The column $\mathbf{p} = (p_1, p_2, p_3)$ of coordinates of the origin $O_{\mathcal{H}}$ of \mathcal{H} is referred to the coordinate system of \mathcal{G} .

The subgroup data listed in the *Symmetry Database*, i.e. the space-group type of \mathcal{H} and the transformation matrix (\mathbf{P}, \mathbf{p}) , are completely sufficient to define the subgroup uniquely: the transformation of the coordinate triplets of the general posi-

tion of \mathcal{H} (in the standard setting) to the coordinate system of \mathcal{G} by $(\mathbf{P}, \mathbf{p})^{-1}$ yields exactly the subset of elements of \mathcal{G} corresponding to \mathcal{H} .

A very important result on group–subgroup relations between space groups is given by Hermann’s theorem: For any group–subgroup chain $\mathcal{G} > \mathcal{H}$ between space groups there exists a uniquely defined space group \mathcal{M} , called the *Hermann group*, with $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$, where \mathcal{M} is a *translationengleiche* subgroup of \mathcal{G} and \mathcal{H} is a *klassengleiche* subgroup of \mathcal{M} . The decisive point is that any group–subgroup relation between space groups $\mathcal{G} > \mathcal{H}$ of index $[i]$ can be split into a *translationengleiche* subgroup chain between the space groups \mathcal{G} and \mathcal{M} and a *klassengleiche* subgroup chain between the space groups \mathcal{M} and \mathcal{H} . This implies that the index $[i]$ can be expressed as $[i] = [i_k] \cdot [i_l]$, where $[i_k]$ and $[i_l]$ are the indices characterizing the *klassengleiche* and *translationengleiche* subgroup chains, respectively.

It may happen that either $\mathcal{G} = \mathcal{M}$ or $\mathcal{H} = \mathcal{M}$ holds. In particular, one of these equations must hold if $\mathcal{H} < \mathcal{G}$ is a maximal subgroup of \mathcal{G} . In other words, a maximal subgroup of a space group is either a *translationengleiche* subgroup or a *klassengleiche* subgroup, never a general subgroup.

If the maximal subgroups are known for each space group, then in principle each non-maximal subgroup of a space group \mathcal{G} with finite index can be obtained from the data for the maximal subgroups. A non-maximal subgroup $\mathcal{H} < \mathcal{G}$ of finite index $[i]$ is related to the original group \mathcal{G} through a chain of maximal subgroups $\mathcal{Z}_1, \mathcal{Z}_2, \mathcal{Z}_3, \dots, \mathcal{Z}_{k-1}, \mathcal{Z}_k$ such that $\mathcal{H} = \mathcal{Z}_k < \mathcal{Z}_{k-1} < \dots < \mathcal{Z}_1 < \mathcal{Z}_0 = \mathcal{G}$, where \mathcal{Z}_j is a maximal subgroup of \mathcal{Z}_{j-1} of index $[i_j]$ with $j = 1, \dots, k$. The number k is finite and the relation $[i] = \prod_{j=1}^k [i_j]$ holds, i.e. the total index $[i]$ is the product of the indices $[i_j]$. [In general, several chains of maximal subgroups relating the group \mathcal{G} and its subgroup \mathcal{H} could exist. However, the total indices of \mathcal{H} in \mathcal{G} calculated over the different chains should coincide with the index of \mathcal{H} in \mathcal{G} . The transformation matrices (\mathbf{P}, \mathbf{p}) for the symmetry reduction $\mathcal{G} > \mathcal{H}$ calculated over the different chains could differ up to a matrix belonging to the normalizer of \mathcal{H} .]

In a similar way, one can express the transformation matrix (\mathbf{P}, \mathbf{p}) for the symmetry reduction $\mathcal{G} \rightarrow \mathcal{H}$ as a product of the transformation matrices $(\mathbf{P}, \mathbf{p})_j$ characterizing each of the intermediate steps $\mathcal{Z}_{j-1} > \mathcal{Z}_j$: $(\mathbf{P}, \mathbf{p}) = (\mathbf{P}, \mathbf{p})_1(\mathbf{P}, \mathbf{p})_2 \cdots (\mathbf{P}, \mathbf{p})_k$ [here the matrices $(\mathbf{P}, \mathbf{p})_j$ relate the bases of \mathcal{Z}_{j-1} and \mathcal{Z}_j , i.e. $(\mathbf{a}, \mathbf{b}, \mathbf{c})_j = (\mathbf{a}, \mathbf{b}, \mathbf{c})_{j-1}\mathbf{P}_j$].

A3.3. Supergroups of space groups. In the previous section, the relation $\mathcal{H} < \mathcal{G}$ was seen from the viewpoint of the group \mathcal{G} . In this case \mathcal{H} was a subgroup of \mathcal{G} . However, the same relation may be viewed from the group \mathcal{H} . In that case $\mathcal{G} > \mathcal{H}$ is a *supergroup* of \mathcal{H} . As for the subgroups of \mathcal{G} , different kinds of supergroups of \mathcal{H} may be distinguished. The following definitions are obvious:

(i) Let $\mathcal{H} < \mathcal{G}$ be a maximal subgroup of \mathcal{G} . Then $\mathcal{G} > \mathcal{H}$ is called a *minimal supergroup* of \mathcal{H} .

(ii) If \mathcal{H} is a *translationengleiche* subgroup of \mathcal{G} , then \mathcal{G} is a *translationengleiche supergroup (t-supergroup)* of \mathcal{H} .

(iii) If \mathcal{H} is a *klassengleiche* subgroup of \mathcal{G} , then \mathcal{G} is a *klassengleiche supergroup (k-supergroup)* of \mathcal{H} .

(iv) If \mathcal{H} is an isomorphic subgroup of \mathcal{G} , then \mathcal{G} is an *isomorphic supergroup* of \mathcal{H} .

(v) If \mathcal{H} is a general subgroup of \mathcal{G} , then \mathcal{G} is a *general supergroup* of \mathcal{H} .

Following Hermann's theorem, a minimal supergroup of a space group is either a *translationengleiche* (*t*-supergroup) or a *klassengleiche* supergroup (*k*-supergroup).

In general, the search for supergroups of space groups is much more difficult than the search for subgroups. One of the reasons for this is that the search for subgroups $\mathcal{H} < \mathcal{G}$ is restricted to the elements of the space group \mathcal{G} itself, whereas the search for supergroups $\mathcal{G} > \mathcal{H}$ has to take into account the whole (continuous) group of all isometries. For example, there are only a finite number of subgroups \mathcal{H} of any space group \mathcal{G} for any given index $[i]$. On the other hand, there may be not only an infinite number of supergroups \mathcal{G} of a space group \mathcal{H} for a finite index $[i]$ but even an uncountably infinite number of supergroups of \mathcal{H} . As an example, consider the group $\mathcal{H} = P1$. Then there is an infinite number of *t*-supergroups $P\bar{1}$ of index 2 because there is no restriction for the sites of the centres of inversion and thus of the conventional origin of $P\bar{1}$.

A4. Normalizers of space groups

For any group–subgroup pair $\mathcal{G} < \mathcal{S}$ it is possible to define an intermediate group $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$, called the *normalizer of \mathcal{G} with respect to \mathcal{S}* , as the set of all elements $s \in \mathcal{S}$ that map \mathcal{G} onto itself by conjugation:

$$\mathcal{N}_{\mathcal{S}}(\mathcal{G}) = \{s \in \mathcal{S} | s^{-1}\mathcal{G}s = \mathcal{G}\}. \quad (18)$$

The normalizer $\mathcal{N}_{\mathcal{S}}(\mathcal{G})$ is an intermediate group between \mathcal{G} and \mathcal{S} . It is the largest intermediate group that contains \mathcal{G} as a normal subgroup. The normalizer may coincide either with \mathcal{G} or with \mathcal{S} .

For most crystallographic applications it is enough to consider the normalizers with respect to three supergroups of the space groups: the Euclidean group \mathcal{E} is the set of all transformations that preserve the distances and angles, which are also known as isometries; the group \mathcal{E}^+ is the set of all chirality-preserving Euclidean mappings, *i.e.* the isometries of the first kind (all translations and proper rotations, including screw rotations); and the affine group \mathcal{A} is the set of all affine transformations – transformations that preserve angles but not distances.

A4.1. Euclidean normalizer. The Euclidean normalizer of a space group \mathcal{G} is defined as the set of symmetry operations of the Euclidean group \mathcal{E} that leave the space group \mathcal{G} invariant by conjugation:

$$\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \{e \in \mathcal{E} | e^{-1}\mathcal{G}e = \mathcal{G}\}. \quad (19)$$

Each element of the Euclidean normalizer of a space group maps the space group onto itself (as a set) by conjugation.

For most space groups, the Euclidean normalizers $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ are also space groups and can be designated by Hermann–Mauguin symbols. In the case of polar groups their normalizers contain continuous translations due to the fact that their origins cannot be fixed by symmetry. The additional contin-

uous translations can be in one, two or three independent lattice directions and they are used for the designation of the normalizers of polar groups by modified Hermann–Mauguin symbols. These symbols contain a superscript to the lattice symbol (*e.g.* P^1mmm), which indicates the number of independent directions of continuous translations.

A4.2. Chirality-preserving Euclidean normalizer. The group \mathcal{E}^+ is the group of all chirality-preserving Euclidean mappings and a subgroup of the Euclidean group \mathcal{E} , *i.e.* the chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is a subgroup of the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

$$\mathcal{N}_{\mathcal{E}^+}(\mathcal{G}) = \{e' \in \mathcal{E}^+ | e'^{-1}\mathcal{G}e' = \mathcal{G}\}. \quad (20)$$

This normalizer is defined if \mathcal{G} is a *Sohncke space group*, in other words if \mathcal{G} only contains symmetry operations of the first kind (Flack, 2003).

Among the 230 space-group types there are 65 that belong to a Sohncke space-group type. The Sohncke space-group types are composed of 11 pairs of *enantiomorphic* or *chiral* space-group types and the other 43 space-group types are known as *achiral*. A space group is defined as chiral if its Euclidean normalizer does not have any symmetry operation of the second kind. The chirality-preserving Euclidean normalizer $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ coincides with the Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ for the 11 pairs of enantiomorphic space-group types. This means that their normalizers only contain operations of the first kind. For the rest of the space-group types $\mathcal{N}_{\mathcal{E}^+}(\mathcal{G})$ is a non-centrosymmetric subgroup of index 2 of the Euclidean normalizer.

A4.3. Affine normalizer. The affine group \mathcal{A} is the group of all affine mappings, a supergroup of the Euclidean group $\mathcal{E} < \mathcal{A}$ and of all space groups. The affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$ is constructed for each space group \mathcal{G} in the following way:

$$\mathcal{N}_{\mathcal{A}}(\mathcal{G}) = \{a \in \mathcal{A} | a^{-1}\mathcal{G}a = \mathcal{G}\}. \quad (21)$$

Either the affine normalizer of a group is a supergroup of the Euclidean normalizer or they coincide, *i.e.* $\mathcal{N}_{\mathcal{A}}(\mathcal{G}) \supseteq \mathcal{N}_{\mathcal{E}}(\mathcal{G})$.

For cubic, hexagonal, trigonal, tetragonal and some orthorhombic space groups the Euclidean and affine normalizers coincide. For the remaining 38 orthorhombic space groups the affine normalizer is isomorphic to the Euclidean normalizer of highest possible symmetry. The affine normalizers of monoclinic and triclinic space groups are not isomorphic to any space group and cannot be characterized by a modified Hermann–Mauguin symbol. In these cases, the affine normalizers are listed in parametric form (see Table 3.5.2.6 of *ITA*).

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