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Chapter 10

# Unique and Effective Characterization of Space Groups in Computer Applications

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Additional information is available at the end of the chapter

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## 1. Introduction

Any method for the solution of crystal structures or for Rietveld refinement of such structures needs at least the set of symmetry matrices of the given space group (SG). In data bases and concise standard descriptions of crystal structures, the complete list of atoms is reduced to atoms representatives and a space group symbol. Since symmetry operations are tensor objects and their matrix form depend on the origin and the orientation of the coordinate system, the symbol must identify not only the *space group type* but also the *space group description*. For this reason standard space group descriptions called *conventional* were tabulated since the year 1935. Contemporary descriptions are based on the 3rd series of the *International Tables for Crystallography* [1], frequently referred to as ITA83. In a common practice one takes a space-group symbol, usually an international Hermann-Mauguin (H-M) symbol, as the index and obtains the symmetry operators from the printed tables. This approach guarantees the conventional descriptions of space groups, 'standard' ordering of symmetry matrices, its geometric interpretation, etc. but has a disadvantage of being limited to the tabulated representations of space groups. Moreover, huge amount of data and a possibility of human errors in transferring the symmetry information to applications involving crystal symmetry [2,3] leads to the generally accepted conclusion, that the automated derivation of space-group information becomes essential when this information is routinely required, especially in the case of higher symmetry. In the years 1960-1980 well-documented algorithms [4,5] translating H-M symbols into a set of generators, which are then used to build a full set of symmetry matrices, were developed. Differences in the generated space group descriptions, caused by ambiguities in H-M symbols prompted in [6-8], brought to procedures based on explicit-origin generators, that is on symmetry operations with specified complete translation vectors not only on its characteristic components – glide or screw vectors. The explicit-origin generators were organized into lengthy [7,8] or concise space-group symbols and used for the SG generation. The latter

symbol, known as the *Hall symbol*, was applied in [6,9]. It should be also noted, that according to the transformational concept [10], the one from equivalent sets of generators published in ITA83 can serve as the 'starting point' for any space group description in the ITA83-style.

The efficiency of space groups construction from the generators is also considered in the literature. Trivial approaches based on any symmetry operations, treated as the group generators, are redundant and completely ineffective. For example, the number of matrix multiplications and matrix comparisons needed for the generation of space group F$m\bar{3}m$ has been estimated in [9] at 18528 and 1.7 million, respectively. Such huge number of mathematical operations can be drastically reduced at the expense of an algorithm complexity. In the approach described in reference [9], the improved algorithm was approximately 100 times faster than the simplistic method. The natural limit of such improvements corresponds to the non-redundant methods, that is procedures in which each matrix multiplication gives a new symmetry operation and thus matrix comparisons are not needed at all. Such method was based on representation of 32 crystallographic point groups in terms of cyclic groups and their products [7,8]. The 'composition series' method [11], successfully adapted to conventional space group descriptions in ITA83 [12], can also be modified to a non-redundant form [13]. This method is especially interesting, since it repeats the ITA83-type order of symmetry operations, assuming the published sets of generators are used. Basing on the composition series, all space group descriptions, that is conventional or not conventional, may be standardized [13-15].

For specific purposes justified in [8,9], the set of symmetry matrices should be complemented by the 'secondary symmetry information' which originates from the geometric characterizations of the symmetry operations given in ITA83 in the form of the operation symbols and the diagrams of symmetry elements. The symmetry operations are the foundation for the Hermann-Maugin symbols and to derive information important in understanding the Wyckoff positions, to find equivalent descriptions of crystal structures or to find transformations between different algebraic descriptions of the same space group.

The matrix-column pair of a space-group operator contains all the information that is needed for a geometrical characterization of the space-group operator and the corresponding symmetry element. Procedures for doing this are well documented in the literature [8,9,16-18]. Algorithms for the determination of (i) the type of rotation, (ii) the rotation angle $\phi$ given as $n = 360/\phi$, (iii) the sense of rotation, (iv) the orthogonal decomposition of the translation vector of the space group operator into its intrinsic and location-dependent components, (v) the orientation and the location of a geometric element, (vi) the inversion point on a geometric element in case of a rotoinversion symmetry operation, are given in the above references.

Even though the recipes are clear, the geometric meaning of symmetry matrices needs some additional conventions [18] to obtain a unique form, not necessarily presented in algorithms. Difficulties are connected with the positive direction of an axis line or plane traces specifications, or the selection of a point which fixes a geometric element in the space.

Moreover, coding some glide vectors by the letters *a*, *b*, *c*, *g* causes that operation symbols are difficult to generate and are not generally understood, also in the community of crystallographers. Even though there are critical opinions like '*The symbols written under the heading Symmetry operations are actually descriptive symbols which repeat part of the information given by the diagram – actually they correspond to cosets representatives in the decomposition of the space group with respect to its translation subgroup….Solid state physicists would appreciate much more if these symbols are replaced by Seitz operators*' [19], the deriving of geometric descriptions, especially without any relations to the Crystallographic Tables, is crucial. It must be also remembered that symbols were used to give a scientific definition to a term '*symmetry element*' – the collective designation for a number of geometric concepts widely used by crystallographers, mineralogists and spectroscopists [20-22]. They were recommended by the *Ad-hoc committee on the nomenclature of symmetry* [21] for general use.

The analysis of symbol derivations as well as the contents of geometric features in the symbols, given in [15, 18, 23], suggests the possibility of defining new symbols, easier to calculate, universal and richer in geometric meaning.

Taking into account all above remarks, the most important features for the computer generation of space groups and their geometric characterization are: (i) a possibility of unique naming of any SG descriptions, (ii) an easy interpretation of SG symbols, that is a derivation of generators, (iii) effectiveness (non-redundancy) of group generation, (iv) reduced amount of predefined data, (v) full consistency with ITA83, (vi) an effective geometric characterization of obtained set of symmetry matrices. The generators selected by H. Wondratschek and used for the conventional space group descriptions in ITA83 meet some demands from the above list, but the geometric symbols need some modifications.

In this chapter a complete, effective and unique approach to the automated derivation of space-group information for a conventional as well as for a non-conventional space group description is proposed.

## 2. Transformational versus other space-group symbols

There are several systems of space groups naming. They can be divided into three categories in the context of group generations: (i) the *symbolic* one, containing symbols of 'space-group types', like the sequential or the Schőnflies symbols, (ii) the *geometric* one, with the Hermann-Mauguin and the Shubnikov symbols which contain the glide or screw components of symmetry operations given in such a way that the nature of the symmetry elements, their orientation and relative location can be deduced from the symbol, (iii) the *algebraic* category with the Zacharasen, Schmuelli and Hall symbols of complete generators, most convenient for the derivation of 'specific groups'. The Hermann-Mauguin symbols are mainly used in connection with the International Tables for Crystallography for the designation of the conventional space group descriptions. The computer programs transforming these most informative symbols into specific space groups have limited possibilities, are rather complicated, sensitive to changes in space-group symbols and must contain additional conventions, since H-M symbols do not depend on the origin selection. On

the other side, the algebraic SG symbols lose a clear geometric interpretation and should be selected from the 'economic' point of view – minimal stored data, a simple and non-redundant algorithm generation. The presented transformational approach to naming and deriving specific space groups, based on earlier works [10,15], meets the mentioned demands.

| SG No | +1 | +2 | +3 | +4 | +5 | +6 | +7 | +8 | +9 | +10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | P1 | $P\bar{1}$ | P2 | $P2_1$ | C2 | Pm | Pc | Cm | Cc | P2/m |
| 10 | $P2_1/m$ | C2/m | P2/c | $P2_1/c$ | C2/c | P222 | $P222_1$ | $P2_12_12$ | $P2_12_12_1$ | $C222_1$ |
| 20 | C222 | F222 | I222 | $I2_12_12_1$ | Pmm2 | $Pmc2_1$ | Pcc2 | Pma2 | $Pca2_1$ | Pnc2 |
| 30 | $Pmn2_1$ | Pba2 | $Pna2_1$ | Pnn2 | Cmm2 | $Cmc2_1$ | Ccc2 | Amm2 | Aem2 | Ama2 |
| 40 | Aea2 | Fmm2 | Fdd2 | Imm2 | Iba2 | Ima2 | Pmmm | Pnnn | Pccm | Pban |
| 50 | Pmma | Pnna | Pmna | Pcca | Pbam | Pccn | Pbcm | Pnnm | Pmmn | Pbcn |
| 60 | Pbca | Pnma | Cmcm | Cmca | Cmmm | Cccm | Cmma | Ccca | Fmmm | Fddd |
| 70 | Immm | Ibam | Ibca | Imma | P4 | $P4_1$ | $P4_2$ | $P4_3$ | I4 | $I4_1$ |
| 80 | $P\bar{4}$ | $I\bar{4}$ | P4/m | $P4_2/m$ | P4/n | $P4_2/n$ | I4/m | $I4_1/a$ | P422 | $P42_12$ |
| 90 | $P4_122$ | $P4_12_12$ | $P4_222$ | $P4_22_12$ | $P4_322$ | $P4_32_12$ | I422 | $I4_122$ | P4mm | P4bm |
| 100 | $P4_2cm$ | $P4_2nm$ | P4cc | P4nc | $P4_2mc$ | $P4_2bc$ | I4mm | I4cm | $I4_1md$ | $I4_1cd$ |
| 110 | $P\bar{4}2m$ | $P\bar{4}2c$ | $P\bar{4}2_1m$ | $P\bar{4}2_1c$ | $P\bar{4}m2$ | $P\bar{4}c2$ | $P\bar{4}b2$ | $P\bar{4}n2$ | $I\bar{4}m2$ | $I\bar{4}c2$ |
| 120 | $I\bar{4}2m$ | $I\bar{4}2d$ | P4/mmm | P4/mcc | P4/nbm | P4/nnc | P4/mbm | P4/mnc | P4/nmm | P4/ncc |
| 130 | $P4_2/mmc$ | $P4_2/mcm$ | $P4_2/nbc$ | $P4_2/nnm$ | $P4_2/mbc$ | $P4_2/mnm$ | $P4_2/nmc$ | $P4_2/ncm$ | I4/mmm | I4/mcm |
| 140 | $I4_1/amd$ | $I4_1/acd$ | P3 | $P3_1$ | $P3_2$ | R3 | $P\bar{3}$ | $R\bar{3}$ | P312 | P321 |
| 150 | $P3_112$ | $P3_121$ | $P3_212$ | $P3_221$ | R32 | P3m1 | P31m | P3c1 | P31c | R3m |
| 160 | R3c | $P\bar{3}1m$ | $P\bar{3}1c$ | $P\bar{3}m1$ | $P\bar{3}c1$ | $R\bar{3}m$ | $R\bar{3}c$ | P6 | $P6_1$ | $P6_5$ |
| 170 | $P6_2$ | $P6_4$ | $P6_3$ | $P\bar{6}$ | P6/m | $P6_3mc$ | P622 | $P6_122$ | $P6_522$ | $P6_222$ |
| 180 | $P6_422$ | $P6_322$ | P6mm | P6cc | $P6_3cm$ | $P6_3cm$ | $P\bar{6}m2$ | $P\bar{6}c2$ | $P\bar{6}2m$ | $P\bar{6}2c$ |
| 190 | P6/mmm | P6/mcc | $P6_3/mcm$ | $P6_3/mmc$ | P23 | F23 | I23 | $P2_13$ | $I2_13$ | $Pm\bar{3}$ |
| 200 | $Pn\bar{3}$ | $Fm\bar{3}$ | $Fd\bar{3}$ | $Im\bar{3}$ | $Pa\bar{3}$ | $Ia\bar{3}$ | P432 | $P4_232$ | F432 | $F4_132$ |
| 210 | I432 | $P4_332$ | $P4_132$ | $I4_132$ | $P\bar{4}3m$ | $F\bar{4}3m$ | $I\bar{4}3m$ | $P\bar{4}3n$ | $F\bar{4}3c$ | $I\bar{4}3d$ |
| 220 | $Pm\bar{3}m$ | $Pm\bar{3}m$ | $Pn\bar{3}n$ | $Pm\bar{3}n$ | $Fm\bar{3}m$ | $Fm\bar{3}c$ | $Fd\bar{3}m$ | $Fd\bar{3}c$ | $Im\bar{3}m$ | $Ia\bar{3}d$ |

**Table 1.** The Hermann-Mauguin symbols which can appear in the transformational space-group descriptions

The transformational approach was inspired by the fact, that in ITA83 all different descriptions of the same space group (settings, origin choices, cell choices) were generated from the same operations transformed to the new coordinate system. Thus, all multiple descriptions as well as any non-conventional description of a given space-group type may be constructed from one set of generators. In contrary to the generally accepted convention that all multiple descriptions are equivalent, one and only one description (and corresponding information: the conventional cell, origin, H-M symbol, etc.) serves as the reference for other SG descriptions. As a result, the number of H-M symbols is reduced to 230 and each such symbol likewise the sequential number or the Schőnflies symbol denotes the space-group type and points at the 'starting' set of generators.

The selection of the reference descriptions is based on the following conventions. In monoclinic system the settings with *unique axis b*, *cell choice* 1 are chosen. Five groups with *R*

– centred cells are described in the *hexagonal axes*. For the space groups with two origin choices, the description with a centre as the origin is chosen.

Having settled the relation between a space-group type and its well established description, other descriptions of the same space-group type are easily identified by a *transformational space-group symbol* (TSG) obtained from the type symbol and explicitly given coordinate system transformation

$$\text{TSG} = \text{type symbol}\ \left(P_{11},P_{21},P_{31},\ P_{12},P_{22},P_{32},\ P_{13},P_{23},P_{33}\right)\ \left(p_1,p_2,p_3\right), \tag{1}$$

where parameters in the first parenthesis describe the unit cell transformation

$$(\mathbf{a}',\mathbf{b}',\mathbf{c}') = (\mathbf{a},\mathbf{b},\mathbf{c})\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix} = (\mathbf{a},\mathbf{b},\mathbf{c})\ \mathbf{P}, \tag{2}$$

and the remaining parameters define the origin shift

$$t = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}. \tag{3}$$

In most cases some of the parameters are zero and an abbreviated 'short-hand' notation

$$\text{TSG} = \text{type symbol}\ \left(a',b',c'\right)\ \left(t\right) \tag{4}$$

is preferred. The shortening concept is similar to that used in storing the symmetry matrices as the coordinate triplets in ITA83. Moreover, the identity transformation (**a**, **b**, **c**) and the zero origin shift (**0**) are omitted in the symbol.

To be familiar with, some examples of the TSG symbols are given underneath:

Fdd2 (b/2+c/2, a/2+c/2, a/2+b/2) – a primitive description of the space group,
$Pn\bar{3}$ (-1/4,-1/4,-1/4) – *origin choice* 1,
5 (c,a,b) – *unique axis* c, *cell choice* 1, for the group with sequence number 5 or H-M symbol *C*2.

It must be remembered that the Bravais centring letter in an H-M symbol is valid only for the conventional space-group type and generally does not describe the centring vectors resulting from the axis transformation given in the transformational symbols. On the other hand, the use of a sequence number or a Schőnflies symbol to point the space-group type is not very informative. The relation between H-M symbols in the ITA83 and the generators based on the composition series method is lost, but it can be restored by the following trick. Each space group type has one and only one set of generators identified by unique H-M symbol, Schőnflies symbol or even by a sequential number. Thus, the group symbol identifies not only the group type, but also its selected matrix representation (including the axis labelling, the origin). Other group descriptions, conventional or not, need explicit information on the axis transformation and/or the origin shift enabled. In any case an original or transformed generators gives a complete set of symmetry matrices in an unambiguous and effective way.

## 3. Description of symmetry operations

Crystallographic groups are groups in the mathematical sense of the word *group*, i.e. they are the sets of elements which fulfil the group conditions. The elements of a space group are the symmetry operations of a crystal, which can be described in several ways. In ITA83 they are presented in four different forms:

i. by a list of symmetry matrices of *general position* in the form of coordinate triplets,
ii. by a general-position diagram,
iii. by the diagram(s) of symmetry elements,
iv. by a list of geometric interpretations of symmetry matrices from (i).

The great importance of geometrical intuition and the geometric point of view on space groups, their symmetry elements, H-M symbols, Wyckoff positions, origin specifications is clear from the above list. The diagrams are rather complicated constructions and cannot be derived *on line* for any space group description, contrary to the geometric symbols for each symmetry matrix. In the computer applications an operation symbol may be considered as the 'gravity centre' of geometric characterization of a symmetry matrix.

For easer understanding of the further material, in the first part of this section the common facts about 'standard' algebraic and geometric descriptions of symmetry operations will be recalled. Next the new geometric symbolism will be proposed. A *dual symbol* of space-group operation is based on a dual symbol of point operation [23] and a point on *geometric elements* closest to the origin [18]. These modifications improve the informative properties and also reduce some conventions necessary for the standard symbols to be unique.

In the three-dimensional space the general linear mappings, called also the *affine mappings*, transform a point coordinates $x$, $y$, $z$ into the coordinates $\tilde{x}, \tilde{y}, \tilde{z}$ of the image point by the system of equations

$$\begin{aligned} \tilde{x} &= \mathrm{W}_{11}x + \mathrm{W}_{12}y + \mathrm{W}_{13}z + \mathrm{w}_1 \\ \tilde{y} &= \mathrm{W}_{21}x + \mathrm{W}_{22}y + \mathrm{W}_{23}z + \mathrm{w}_2 \\ \tilde{z} &= \mathrm{W}_{31}x + \mathrm{W}_{32}y + \mathrm{W}_{33}z + \mathrm{w}_3 \end{aligned} \tag{5}$$

represented in the matrix form as

$$\tilde{\mathbf{x}} = \mathbf{W}\mathbf{x} + \mathbf{w} \xrightarrow{\text{definition}} (\mathbf{W}, \mathbf{w})\mathbf{x}. \tag{6}$$

For computer applications a more convenient description uses so called augmented matrix $\boldsymbol{\mathcal{W}}$ which combines the (3x3) matrix **W** with a (3x1) column matrix **w** and a row matrix (0 0 0 1). The augmenting of the coordinate column $x$, $y$, $z$ by a fourth dummy coordinate, fixed at 1, leads to a more homogenous form

$$\tilde{\mathbf{x}} = \boldsymbol{\mathcal{W}}\mathbf{x}. \tag{7}$$

Contrary to the affine mappings, which preserve the straight lines, planes and parallelism of such objects, a special case called *isometries* preserves also distances and in consequence the volumes and orthogonalities. In this situation the determinant det(**W**) = ±1. Moreover, for

crystallographic symmetry operations related to the crystallographic coordinate system all elements of the matrix are integers reduced to the values {-1,0,1}, if such coordinate system is based on the shortest lattice vectors or on the Bravais cells. In the latter case, especially simple forms of **W** consisting of three or four non-zero elements are obtained. Therefore, in printed descriptions of space groups, like in ITA83, the space - consuming forms (**W**,**w**) or $\boldsymbol{\mathcal{W}}$ are equivalently given as shorthand notation of the equation systems (5) and called the *coordinate triplets* $\tilde{x},\tilde{y},\tilde{z}$ or the Jones faithful notation.

There are also some advantages in notation (R|**t**) introduced by Seitz in [25] and adopted by solid-states physicists [26]. In this notation 'R' means a point operation **W** given symbolically and '**t**' is an explicitly given translation, equivalent to **w**. Thus, the diversity of R-symbols, corresponding to a set of different symmetry matrices occurring in the conventional space group descriptions, is reduced to 64 items (48 orthogonal matrices with three non-zero elements occuring in the cubic system and 16 additional matrices with four non-zero elements coming from the oriented hexagonal system). The Seitz symbols are very concise and with the help of multiplication tables they identify the product of symmetry operations

$$\left(\mathrm{R}_{\mathbf{1}}\,|\,\mathbf{t}_{\mathbf{1}}\right)\left(\mathrm{R}_{\mathbf{2}}\,|\,\mathbf{t}_{\mathbf{2}}\right) \;=\; \left(\mathrm{R}_1\mathrm{R}_2\,|\,\mathrm{R}_{\mathbf{1}}\mathbf{t}_{\mathbf{2}}+\mathbf{t}_{\mathbf{1}}\right) \;=\; \left(\mathrm{R}\,|\,\mathbf{t}\right), \tag{8}$$

but for explicit values of components **t**, the **W** matrices symbolized by R must be known. Two special actions R on **t** should be distinguished. Assuming the $k$ order of R, that is the equality $\mathbf{W}^k = \mathbf{I}$ is held, these actions can be distinguished by equations

$$\left(\mathrm{R}\,|\,\mathbf{t}_{\mathrm{para}}\right)^k \;=\; \left(\mathrm{I}\,|\,k\mathbf{t}_{\mathrm{para}}\right)\mathrm{and}\left(\mathrm{R}\,|\,\mathbf{t}_{\mathrm{ortho}}\right)^k \;=\; \left(\mathrm{I}\,|\,0\right), \tag{9}$$

where vectors $\mathbf{t}_{\mathrm{para}}$ and $\mathbf{t}_{\mathrm{ortho}}$ are mutually perpendicular.

Recently, the set of geometric symbols for R used in ITA83 was compared with other sets of symbols of point-group operations [24]. Some symbols are purely symbolic, other contain geometric information and are more or less self-defined.

Relations between different spaces, their geometric invariants and group properties of such invariants were 'discovered' before the development of the crystallographic groups. Starting from the Erlangen program announced by Felix Klein in 1872, it is understood that different symmetries represented by the abstract structure-groups are consequences of different geometries and their invariants. Thus, there are two points of view on symmetry: one is algebraic and the second one is geometric. In the case of groups described in ITA83, the three items from the four-element list of equivalent symmetry descriptions possess the geometric nature. The geometric information has played important roles in many aspects of crystallography. The algorithms for the characterization of symmetry operations are the foundation for the Hermann-Maugin symbols. The 'secondary symmetry information' is important in understanding the Wyckoff positions, distinguishing partners in an enantiomorfic pair, finding equivalent descriptions of crystal structures or finding transformations between different algebraic descriptions of the same space group.

The description of a general procedure for deriving symbols for the symmetry operations was included in Chapter 11 of ITA83 [17]. A similar approach was used in [16], different modifications can be found in [7,8]. In all this approaches the basic concepts consist in extracting from **w** (**t** in Seitz notation) its characteristic part $\mathbf{w}_g$ interpreted as screw/glide vectors, finding a set of fixed points of pure rotations or reflections and thus orient and locate so called *geometric element* and find the sense of rotation angle symbolized by a number $n$ = 2,3,4 or 6 (rotation angle = $360^o/n$). The scheme of calculation and some critical remarks is given below.

## 3.1. Type of symmetry operation

The type of symmetry operation is obtained by a modification of point operation symbols according to the characteristic part of translation vector **w**. It is obvious that the type of point operations is completely determined by a matrix part **W** of (**W**,**w**). Table 2 contains the classification of matrices **W** based on the analysis of their traces and determinants.

| | det(**W**)=1 | | | | | det(**W**)=-1 | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| tr(**W**) | 3 | 2 | 1 | 0 | -1 | -3 | -2 | -1 | 0 | 1 |
| type | 1 | 6 | 4 | 3 | 2 | $\bar{1}$ | $\bar{6}$ | $\bar{4}$ | $\bar{3}$ | m |
| order $k$ | 1 | 6 | 4 | 3 | 2 | 2 | 6 | 4 | 6 | 2 |

**Table 2.** Classification of the point symmetry matrices

A vector **w,** if different from **0**, should be decomposed into orthogonal components: a *glide/screw part* $\mathbf{w}_g$ and a *location part* $\mathbf{w}_l$. While the first component changes operation types, namely: rotations into screw rotations and reflections into glide reflections, the second one is responsible for shifting the corresponding symmetry element from the origin. The part $\mathbf{w}_g$ may be derived by projecting **w** onto the space invariant under **W**, but this needs the metrical information about the coordinate system. The metric-free derivation uses the property (9)

$$\left(\mathbf{W},\mathbf{w}\right)^k = \left(\mathbf{W},\mathbf{w_g}+\mathbf{w_l}\right)^k = \left(\mathbf{I},k\mathbf{w_g}\right) \tag{10}$$

and the location part is the difference $\mathbf{w}_l = \mathbf{w} - \mathbf{w}_g$.

## 3.2. Sense of direction and sense of rotation

To complete the characterization of **W**, excluding the cases where W represents a two-fold rotation or a reflection, the sense of rotation must be determined. For this purpose and also for obtaining the compatibility between analytical descriptions of axes, a convention which fixes the positive direction must be adopted. Such convention was not explicitly described in [17] and in consequence other conventions are sometimes applied. For example, from the two equivalent descriptions of the same crystallographic direction $[1\bar{1}\bar{1}]$ and $[\bar{1}11]$ the latter is positively directed according to the rule applied in [13] and the opposite selection is

compatible with geometric descriptions in ITA83. A systematic analysis of 'standard' symbols allowed to specify in [18] six conventions C1 – C6, which together with the algebraic procedures lead to unique symbols. Convention C2, in the detailed form is given in Table 3.

| Stand up element | Two zeroes values | One zero | All non-zero values |
|---|---|---|---|
| $u$ | [+ 0 0] | [0 + +] or [0 + -] | [+ - -] |
| $v$ | [0 + 0] | [+ 0 +] or [- 0 +] | [- + -] |
| $w$ | [0 0 +] | [+ + 0] or [+ - 0] | [- - +] |
| - | | | [+ + +] |

**Table 3.** Selection of the positive direction from a pair [$uvw$] and [$\bar{u}\bar{v}\bar{w}$]. The symbols '-', '0', '+' are used for the positive, zero, negative values, respectively.

According to the convention in Table 3, positive directions characterize the positive product of the non-zero components. Such situation cannot occur if there are only two non-zero elements, which differ in the sign. In this case the rule can be stated as 'a negative component may precede a zero component, but never may follow it'.

Assuming a positive direction of the axis corresponding to a rotation or rotoinversion operation has been determined, one of two commonly used procedures [17, 27] should be applied to obtain the sense of rotation. The Boisen & Gibbs procedure given in [27] is more practical. Having the positive axis direction [$uvw$] derived from **W,** the positive sense of rotation is obtained if one of the following conditions is fulfilled:

$$\text{if } v = w = 0 \text{ and } u\mathrm{W}_{32} > 0 \text{ or } w\mathrm{W}_{21} - v\mathrm{W}_{31} > 0. \tag{11}$$

### 3.3. Orientation – location part

In the classical approaches to the considered topic, the orientation of a geometric element is determined together with its location in one step. Solving of three simultaneous equations of reduced operation (**W**,**w**$_l$), given in a matrix form

$$\left(\mathbf{W} - \mathbf{I}\right)\mathbf{x}_\mathbf{F} + \mathbf{w}_\mathbf{l} = 0, \tag{12}$$

leads to the linear or planar sets of solutions (fixed points) for rotations or reflections, respectively. For a rotoinversion other than a pure inversion, the axis results from the equation

$$\left(\mathbf{W}^2 - \mathbf{I}\right)\mathbf{x}_\mathbf{F} + \mathbf{W}\mathbf{w} + \mathbf{w} = 0. \tag{13}$$

In both cases the set of equations is indeterminate, since det(**W** - **I**) in (12) or det(**W**$^2$ - **I**) in (13) are equal zero. This leads to parametric solutions, which forms depend on the mode of calculation.

Although the procedure may also be applied to cases where space groups are given in non-conventional descriptions, there are situations where it is difficult to obtain a unique result even for coordinate triplets taken from ITA83 [18].

For example the matrix equation

$$\begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 1/6 \\ 1/3 \\ -1/6 \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

gives three solutions presented here as the orientation-location parts:

1. $x$, $-x + 1/3$, $-x + 1/6$ if $x$ is treated as the parameter,
2. $-y + 1/3$, $y$, $y - 1/6$ if $y$ is selected as the parameter,
3. $-z + 1/6$, $z + 1/6$, $z$ if $z$ represents the variable parameter.

Of course, these solutions describe the same symmetry axis, but differ in a selected parameter, in a positive direction and in a location point. Unique solutions require special conventions in programmable algorithms, based for example on the *row echelon forms* [9, 27], or in post-calculation standardization.

### 3.4. Pseudo-inverse and the point closest to origin

Another possibility originates from the linear algebra and from the concept of *pseudo-inverse* matrices. This mathematical formulation allows obtaining single points $\mathbf{x}_F$ from equations (12) and (13). Such unique points have simple interpretation; they represent points from the linear or planar sets closest to origin. The derivation of the pseudo-inverse matrix $(\mathbf{W}\text{-}\mathbf{I})^+$ is rather cumbersome, but this idea inspires the new point of view on the location derivation and specification in the geometric descriptions.

## 4. Dual symbols for space-group operations

As mentioned in the previous section, the geometric interpretation of symmetry operations is vital for many crystallographic topics. But there are some disadvantages in the derivation and application of the pioneers symmetry operation symbols (Fischer, Koch in ITA83). In the published procedure, intended mainly for manual calculations and for a link between symmetry matrices and the diagrams of symmetry elements, there is a lack of conventions needed to cast this approach into a programmable algorithm and to obtain unique relations: given symmetry operation → the operation symbol. In the literature concerning this topic individual conventions are frequently added into specified algorithms [8,9], which causes that the derived symbols are unique, but not necessary agree with ITA83 symbols. Special difficulties arise in deriving the orientation-location part of a symmetry operation. A

systematic analysis of ITA83 symbols resulted in extracting 6 conventions necessary for automatic generation of the orientation-location parts in an unambiguous way [14]. The novel approach presented in that publication contains the derivation of a *point closest to origin* $\mathbf{x}_c$ as an alternative to solving an indeterminate set of equations by the pseudo-inversion matrices. But a methodological advance connected with the unambiguity of $\mathbf{x}_c$ was next lost in the standardization step, in which the obtained result was transformed into a conventional point on a geometric element. The inconveniences of classical symbols can be summarized as follows:

i. the procedure outlined in ITA83 for the classical names of the symmetry operations is not unique and must be supplemented by explicitly given conventions like in [18],
ii. the symbols lost some information in comparing with the source symmetry matrices, for example the point operation symbol 2 0,y,0 and space operations based on it may be obtained from two different matrices,
iii. symbols, especially involving the reflections, are limited to the conventional space groups descriptions,
iv. symbols are laborious for computer derivation and manipulation, *e.g.* they contain the symbols *a*, *b*, *c*, *g* for glide planes, the symbols *x*, *y*, *z* for free parameters.

Some of the listed problems are immanently involved with the specific form of the orientation-location part and they should be overcome or at least simplified by developing a new symbol of symmetry operation. The problems (ii) and partially (iii) and (iv) disappear, if the orientation of a geometric element is presented in the form of the orthogonal lattice splitting (*uvw*)[*hkl*]. Advantages of using splitting indices for the characterization of point operations were described in [23]. The benefits for space operations should be even greater. The conventions for a unique description of a geometric element location in (i) have no meaning for $\mathbf{x}_c$. Moreover, by removing the *a*, *b*, *c*, *g* designations of glide planes, a new symbol will be more consistent.

The splitting indices describe the orientation of the symmetry axes or the symmetry planes in the same way as [*uvw*](*hkl*). They, together with a locating point on the geometric element, fully correspond to the orientation-location parts. More precisely, the informative content of this construction exceeds the analogous information stored classically. Lattice rows [*uvw*] and lattice planes (*hkl*) are orthogonal to each other and exchangeable in the reciprocal space. Specifications of the same lattice direction in direct and reciprocal spaces better characterize the axis system and simplify the crystallographic calculations, that is calculations in non-Cartesian systems. While two point operations given by coordinate triplets $\bar{x}, y, \bar{z}$ and $\bar{x}, \bar{x}+y, \bar{z}$ lead to a common geometric symbol 2 0,*y*,0, the splitting indices are [010](010) in the former case and [010]($\bar{1}$20) in the latter.

The lattice perpendicularities revealed by splitting indices are also important in the orthogonal splitting of the translational part **w** of a space-group operation. The **w** components are parallel/orthogonal to [*uvw*] and also to (*hkl*), what was symbolically drawn in Figure 1.

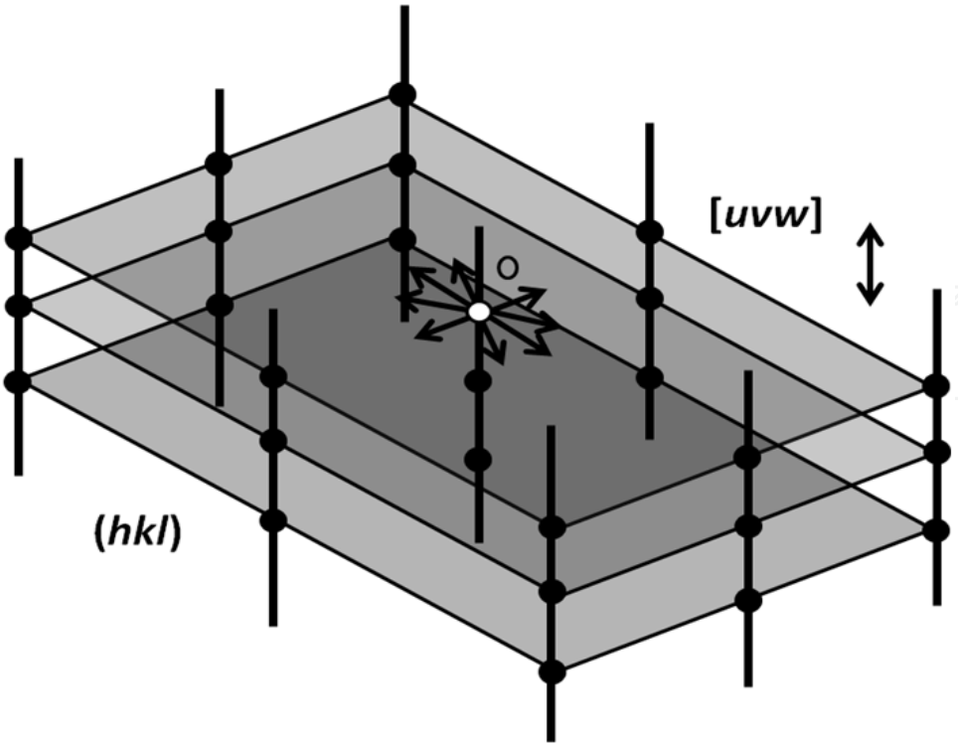


**Figure 1.** Origin - central lattice point of a dual symbol. Each crystallographic point operation (excluding identity and inversion) orthogonally splits the lattice into the lattice rows [*uvw*] and the lattice planes (*hkl*). The decomposition of a translation **w** in the space-group operations is also based on the lattice perpendicular property.

Let $\mathbf{x}_c$ denotes a special point, the point from set $\mathbf{x}_F$ closest to the coordinate system origin. Such points may be found on any geometric element (Fig.2). Thus, every 4x4 symmetry matrix $\mathcal{W}$, excluding only identity operation and pure translations, can be characterized by $\mathbf{x}_c$. Vector $\mathbf{x}_c$ is always perpendicular to the geometric element and to the intrinsic part $\mathbf{w}_g$, if not zero. Two vectors separated by the asterisk, that is $\mathbf{w}_g$* $\mathbf{x}_c$ give complete geometric information about a space-group operation, assuming that the point –group operation was characterized by the dual symbol. For this reason, the new geometric symbol of a space-symmetry operation is also called the *dual symbol*, like in the case of point operations [18]. This should not lead to confusion, since the information concerning the point operation is separated from the characteristics involved with the space-symmetry operation. Such approach reflects the analogy to the algebraic difference between the point operation **W** and the space operation (**W**,**w**). Moreover, the perpendicularity between the lattice row and the lattice planes expressed by splitting indices is reflected also in the pair $\mathbf{w}_g$, $\mathbf{x}_c$. In consequence, the six components of two vectors $\mathbf{w}_g$* $\mathbf{x}_c$ may be presented only by four simple ratios, since in every case $\mathbf{w}_g$ or $\mathbf{x}_c$ is parallel to the integer vector [*uvw*]. Thus, the dual symbol takes the form

$$\begin{aligned} &\pm n^{\pm}\left[uvw\right]\left(hkl\right)r_1 * r_2, r_3, r_4 \text{ for rotations and rotoinversions} \\ &\text{and } m\left[uvw\right]\left(hkl\right)r_1, r_2, r_3 * r_4 \text{ for reflections,} \end{aligned} \tag{14}$$

where: the minus sign before $n$ or a bar over $n$ is the 'inversion sign' = det(**W**)
$n$ – axis symbol, order of $\mathbf{W}_P$,
$m$ – mirror plane ($n$ =2, det(**W**) = -1),
[$uvw$] – symmetry axis direction or a normal to the reflection plane,
[$hkl$] – reflection plane or plane perpendicular to the direction of symmetry axis,
$r_1$ * $r_2$, $r_3$, $r_4$ – specification of vectors $\mathbf{w}_g = (r_1u, r_1v, r_1w)$ and $\mathbf{x}_c = (r_2, r_3, r_4)$,
$r_1$, $r_2$, $r_3$ * $r_4$ – specification of vectors $\mathbf{w}_g = (r_1, r_2, r_3)$ and $\mathbf{x}_c = (r_4u, r_4v, r_4w)$.

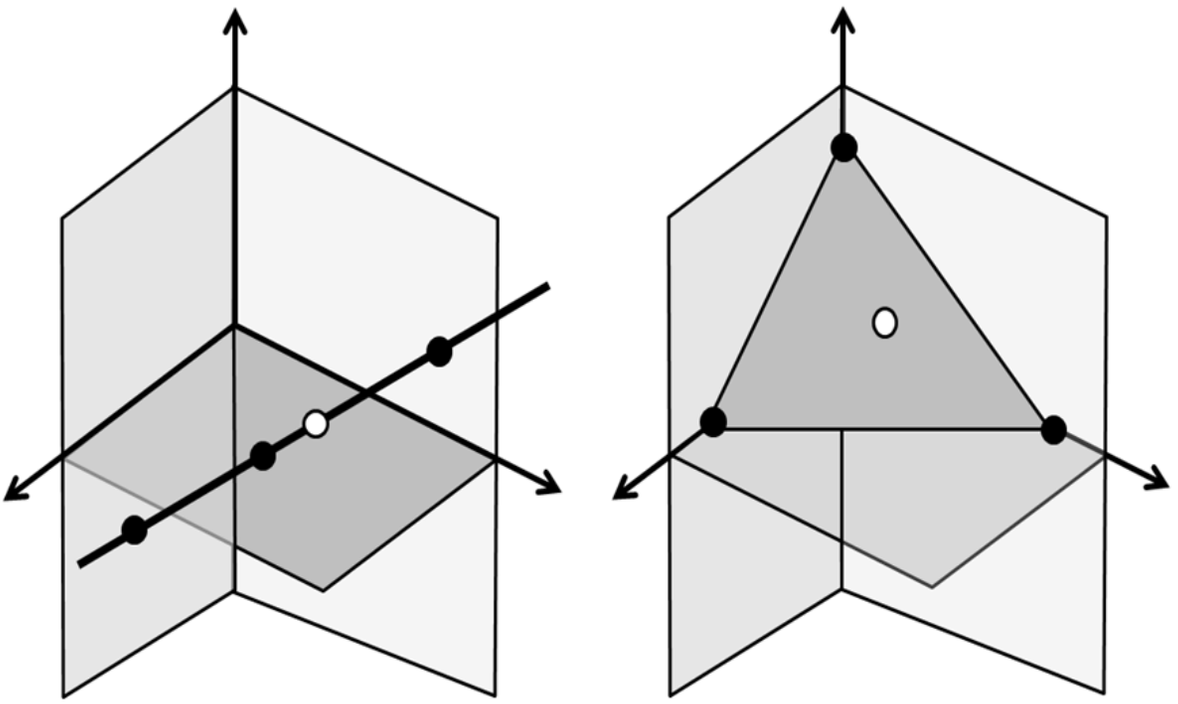

**Figure 2.** Characteristic points of geometric elements in general orientation. For a symmetry axis they defined the intersection of an axis with the basal planes. A symmetry plane is located by its intersection with the coordinate axes. Alternative fixing of geometric element may be based on the unique point $\mathbf{x}_c$ closest to the origin, schematically presented by open circles.

In most cases such complete form can be further reduced. Zero vectors are omitted. If the lattice row indices are equal to the lattice plane indices, a typical situation for a conventional description of space groups, the latter does not need to be specified. Generally, the indices ($hkl$) in dual symbols are related with the indices [$uvw$] by the lattice metric. Since non-orthogonal symmetry matrices occur only in the oriented hexagonal system, the $h$ symbol may designate a unique transformation matrix from [$uwv$] to ($hkl$) according to the scheme:

$$[uvw]h \rightarrow \begin{pmatrix} 2 & \bar{1} & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} h \\ k \\ l \end{pmatrix}, \tag{15}$$

where the matrix elements are scaled to integers and the 3,3 element is arbitrarily set. The common divisor must be removed from the symbol ($hkl$), if present.

It may be surprising that the dual symbols do not contain the specification of an inversion point in the case of rotoinversion. This can be explained by extending the interpretation of

$\mathbf{w}_g$ also on such operations. Vector $\mathbf{w}_g$ 'measures' the intrinsic transformation of the point $\mathbf{x}_c$ into another point, both on a geometric element

$$\mathbf{w_g} = \left(\mathbf{W}, \mathbf{w}\right)\mathbf{x_c} - \mathbf{x_c}. \tag{16}$$

Thus, $\mathbf{w}_g$ describes a classical screw/glide vector and a pure inversion of the point $\mathbf{x}_c$. This means that

$$\mathbf{x_{inv}} = \mathbf{x_c} + \mathbf{w_g} / \mathbf{2} \tag{17}$$

so the calculation and specification of $\mathbf{w}_g$ is reasonable for all operation types. The relations and remarks may be better explained by a few examples.

**Example 1**

The symmetry matrix $\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0 \\ 0.5 \end{bmatrix}$ is described as $\bar{4}^+$ [001] ½ * ¼,-¼,0.

The obtained dual symbols contain the following data. The matrix describes a fourfold rotoinversion operation. Its geometric element is oriented along direction [001], which is orthogonal to the (001) plane. The point on the axis closest to origin $\mathbf{x}_c$ has coordinates: ¼,-¼,0. Mapping $\mathbf{x}_c$ is reduced to a pure inversion and generates the shift ½[0,0,1]. Thus, the inversion point is at ¼,-¼,¼, the middle between $\mathbf{x}_c$ and its image.

**Example 2**

The matrix $\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0.5 \\ 0 \end{bmatrix}$ is described as m[1-10] ½,½,0*.

In this case the matrix describes a glide symmetry operation. The symmetry plane has Miller indices (1-10) and goes through the origin. The glide vector is (½,½,0).

**Example 3**

The matrix $\begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 0.5 \end{bmatrix}$ is described as m[100](2-10) 0,0½* or shorter as m[100]h 0,0,½*.

In this case the matrix also describes a glide symmetry operation, but in a hexagonal system. The symmetry plane has Miller indices $(2\bar{1}0)$ and goes through the origin. The glide vector is (0,0,½).

**Example 4**

The matrix $\begin{bmatrix} \bar{1} & \bar{1} & \bar{1} \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0{,}5 \\ 0 \\ 0 \end{bmatrix}$ occurring in a primitive description of group No 227 is described as $3^+$ $[\bar{1}\bar{1}3](001)$ *1/6,1/6,0.

The matrix generates a three-fold rotation. The axis is oriented along $[\bar{1}\bar{1}3]$direction, which is perpendicular to (001) planes and is located by the point 1/6,1/6,0.

It may be noted from the above examples that – introducing the dual symbols – the inconveniences mentioned at the beginning of this section are avoided. The new notation displays the geometric features of a rotation, a rotoinversion, a screw rotation, a reflection, a glide reflection and even an inversion, in a homogeneous way. All such operations correspond to a geometric element (in the form of a single point, line or plane), for which a point closer to the origin always exists, a unique point $\mathbf{x}_c$. The difference $(\mathbf{W},\mathbf{w})\mathbf{x}_c - \mathbf{x}_c$, defines an 'intrinsic transformation'. These two vectors extend the geometric description of a point operation to the description of a space group operation. The symbols are applicable to space groups presented conventionally as well as non-conventionally. The symbols are rather concise, especially in the context of geometric information, which they contain. The use of the splitting indices [*uvw*](*hkl*) seems to be more applicable for space group then for point groups. Crystallographers interpret [*uvw*] as a family of lattice rows and (*hkl*) as a family of planes. For practical purposes there is only one question: is the determination of $\mathbf{x}_c$ computationally simple?

## 5. Derivation of $\mathbf{x}_c$ points for space-group operations

Point $\mathbf{x}_c$ was geometrically defined as the point on the geometric element closest to the origin or equivalently, as the shortest position vector which tail is fixed at the origin and the head ends on the geometric element. Such definition is rather descriptive and not much useful for practical purposes. Generally, the derivation must be carried out in a non-Cartesian system for which the metric is not known. The splitting indices of the matrix part **W** make a geometric concept based on which the quantitative components of $\mathbf{x}_c$ may be calculated from the translation part **w** of a space-group operation. For any **W** (excluding identity or inversion operations) the indices of the orthogonal lattice splitting orient the reflection plane by (*hkl*) indices and also orient line [*uvw*] in space perpendicular to this plane or orient the symmetry axis [*uvw*] and specify some plane orthogonal to it. If $\mathbf{w} = \mathbf{0}$, the direction [*uvw*] and the plane (*hkl*) intersect in the coordinate system origin O, like in Fig. 1. In this situation the head and the tail of $\mathbf{x}_c$ coincide with O, as for point operations. But if $\mathbf{w} \neq \mathbf{0}$, the head of $\mathbf{x}_c$ may move along line [*uvw*] for reflections or may move on (*hkl*) plane for any type of rotations. Thus, the construction based on the lattice orthogonality given by the splitting indices enables finding $\mathbf{x}_c$ without complete metric information. The meaning of $\mathbf{x}_c$ for the inversion operation is obvious, since a geometric element in this situation is reduced to one point and for a pure translation $\mathbf{x}_c = 0$.

The key to finding $\mathbf{x}_c$ on the (*hkl*) plane or on the [*uvw*] line is the orbit, a set of points interrelated by the analysed operation. Contrary to general operation (**W**,**w**), its reduced version $(\mathbf{W},\mathbf{w}_l)$ leads to the cyclic groups and to a limited number of equivalent points in space. If an arbitrary point is located on direction [*uvw*] for a symmetry plane, or on the (*hkl*) plane for a symmetry axis, then the centre of gravity of the orbit generated by this point and $(\mathbf{W},\mathbf{w}_l)$ defines $\mathbf{x}_c$. Thus, $\mathbf{x}_c$ describes the shift of the orbit generated by $(\mathbf{W},\mathbf{w}_l)$ and points closest to the origin for all $(\mathbf{W},\mathbf{w}_l)^n$ operations. Certainly, for $\mathbf{w}_l = \mathbf{0}$ the gravity centre coincides with the origin. Systematic derivation of $\mathbf{x}_c$ for all types of space-group operations is clearer with the help of sketches presented in Figure 3. The intrinsic translation parts $\mathbf{w}_l$

and the projection planes (*hkl*) are treated as already known. The considered orbits are one- or two-dimensional, assuming the origin is located in the fixed point of an rotoinversion operation. Not all points on the orbit are necessary to derive $\mathbf{x}_c$. For an orbit in the form of square its centre is determined by points in two opposite vertices. The centre of the hexagon may be reached by rotating one side by 60°. In final formulae the rotation sense is guaranteed by the presence of **W,** but in geometric constructions the rotation sense must be taken into account. A systematic derivation of the formulae for $\mathbf{x}_c$ is followed below.

**Figure 3a**

Identity operation (**I**,**0**) can be interpreted as the reduced operation of a pure translation (**I**,**w**). Its geometric element contains all points. Point (0,0,0) is the closest to the origin. Thus, $\mathbf{x}_c$ is defined as the zero vector, not dependent on **w**. Another, somewhat artificial but more consistent with the rest of figures approach, is based on the selection of specific point **-w**/2 for the representation of translation

1. Vector to the special point, $\overrightarrow{01}$ = **x= - w**/2
2. Vector to its image, $\overrightarrow{02}$ = **Wx+w** = - **w**/2

Point $\mathbf{x}_c = (\overrightarrow{01} + \overrightarrow{02})/2 = \mathbf{0}$

**Figure 3b**

The origin is located at the inversion point. The combination of the inversion with the translation is equivalent to shifting the inversion point by a half of the translation vector, hence

1. Vector to any point, $\overrightarrow{01}$ = **x**
2. Vector to its image, $\overrightarrow{02}$ = **Wx+w** = -**x**+**w**

The new position of inversion point $\mathbf{x}_c = (\overrightarrow{01} + \overrightarrow{02})/2 = \mathbf{w}/2$

**Figures 3c and 3d**

The orbit generated by a reduced two-fold operation or reduced reflection contains two points.

1. Vector to any point, $\overrightarrow{01}$ = **x**
2. Vector to its image, $\overrightarrow{02}$ = **Wx+w**$_l$ = -**x**+**w**$_l$

The shortest vector $\mathbf{x}_c = (\overrightarrow{01} + \overrightarrow{02})/2 = \mathbf{w}_l/2$ lies on (*hkl*) for a two-fold rotation or on [*uvw*] for a reflection

**Figures 3e and 3f**

In the case of four–fold rotation or four-fold rotoinversion the calculations are as follows:

1. Vector to any point, $\overrightarrow{01}$ = **x**
2. Vector to its image, $\overrightarrow{02}$ = **Wx+w**$_l$
3. Vector to the image of image, $\overrightarrow{03}$ = **W**(**Wx+w**$_l$ **)+ w**$_l$ = -**x** +**Ww**$_l$+**w**$_l$, since in this case $\mathbf{W}^2\mathbf{x} = -\mathbf{x}$

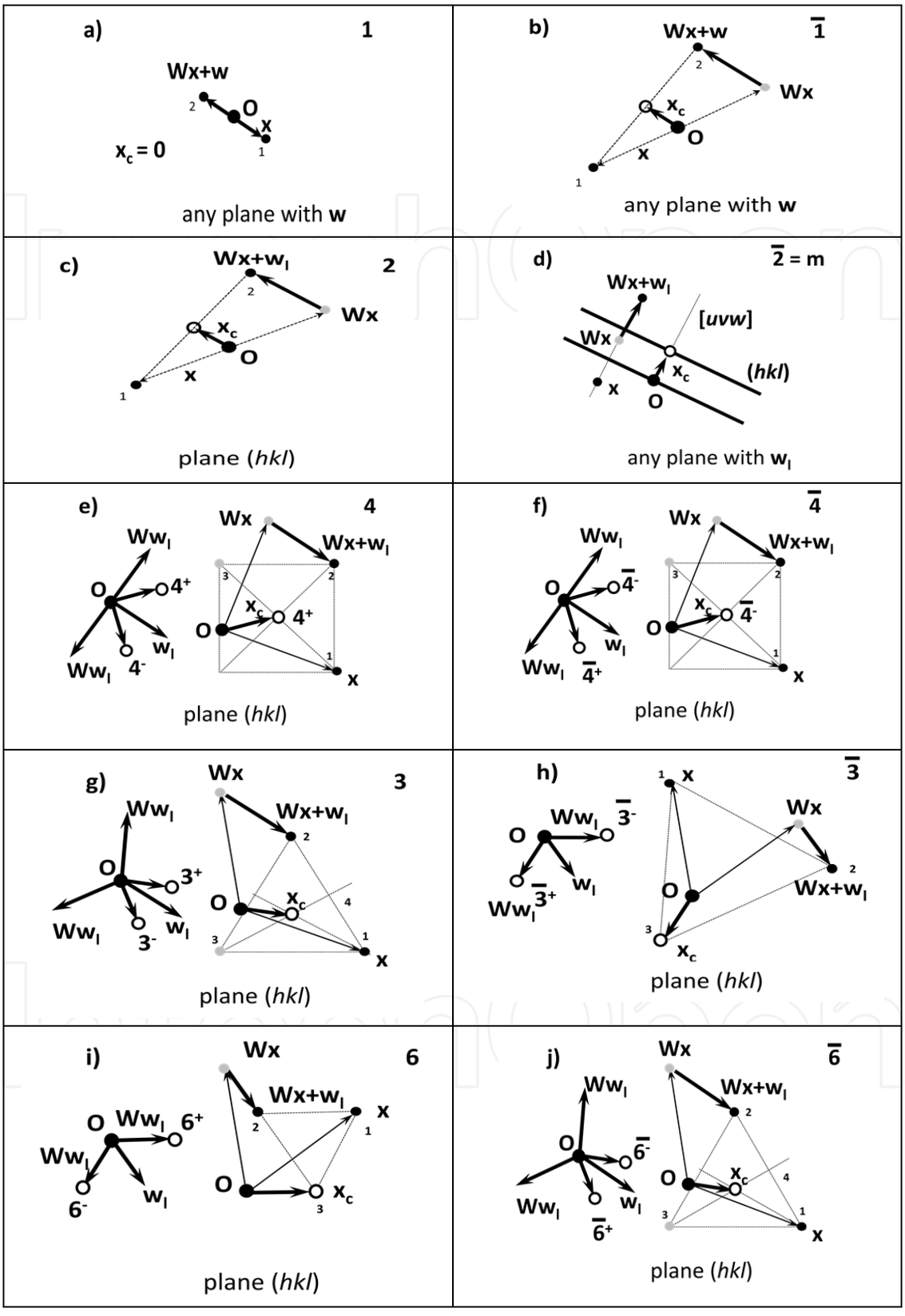


**Figure 3.** Sketches for derivation points $\mathbf{x}_c$ based on any point **x** and its image(s). On all drawings the projection plane is specified, the origin and $\mathbf{x}_c$ are marked as large filled and empty circles, respectively. Other explanations are given in the text.

The centre of gravity for all symmetry equivalent points is the same as for two points of opposite vertices. Thus, the new position of the rotation point is $\mathbf{x}_c = (\overrightarrow{01} + \overrightarrow{03})/2 = (\mathbf{W}\mathbf{w}_l+\mathbf{w}_l)/2$

**Figures 3g and 3j**

In the case of three–fold rotation or six-fold rotoinversion, the location vectors from the origin to the vertices of equilateral triangle are given by any point **x** and its two images:

1. Vector to any point, $\overrightarrow{01} = \mathbf{x}$
2. Vector to its image, $\overrightarrow{02} = \mathbf{W}\mathbf{x}+\mathbf{w}_l$
3. Vector to the image of image, $\overrightarrow{03} = \mathbf{W}(\mathbf{W}\mathbf{x}+\mathbf{w}_l)+ \mathbf{w}_l = \mathbf{W}^2\mathbf{x} +\mathbf{W}\mathbf{w}_l+\mathbf{w}_l$

The centre of gravity determines the new position of the rotation point

$$\mathbf{x}_c = (\overrightarrow{01} + \overrightarrow{02}+ \overrightarrow{03})/3 = (\mathbf{W}\mathbf{w}_l+2\mathbf{w}_l)/3, \text{ since } \mathbf{W}^2\mathbf{x} + \mathbf{W}\mathbf{x} + \mathbf{x} = \mathbf{0}.$$

**Figures 3h and 3i**

In the case of six–fold rotation or three-fold rotoinversion, the location vectors from the origin to the vertices of regular hexagon are given by any point **x** and its consecutive images. But a simpler way may be based on a rotation of a hexagon side by 60°

1. Vector to any point, $\overrightarrow{01} = \mathbf{x}$
2. Displacement vector between **x** and its image, $\overrightarrow{12} = \mathbf{W}\mathbf{x}+\mathbf{w}_l - \mathbf{x}$, a hexagon side
3. Rotation of $\overrightarrow{12}$ by 60° = $\mathbf{W}(\mathbf{W}\mathbf{x}+\mathbf{w}_l -\mathbf{x}) = \mathbf{W}^2\mathbf{x} +\mathbf{W}\mathbf{w}_l - \mathbf{W}\mathbf{x}$

The centre of gravity determines the new position of the rotation point

$$\mathbf{x}_c = (\overrightarrow{01} +\mathbf{W}\overrightarrow{12}) = \mathbf{W}\mathbf{w}_l, \text{ since } \mathbf{W}^2\mathbf{x} - \mathbf{W}\mathbf{x} + \mathbf{x} = \mathbf{0}, \text{ if } \mathbf{W} \text{ describe rotation by } 60°.$$

The obtained results are summarized in Table 4.

| Axis symbol | $\mathbf{x}_c$ | Axis symbol | $\mathbf{x}_c$ |
|---|---|---|---|
| 1 | **0** | $\bar{1}$ | $\mathbf{w}/2$ |
| $2, \bar{2}(m)$ | $\mathbf{w}_l/2$ | $4, \bar{4}$ | $(\mathbf{W}\mathbf{w}_l+\mathbf{w}_l)/2$ |
| $3, \bar{6}$ | $(\mathbf{W}\mathbf{w}_l+2\mathbf{w}_l)/3$ | $\bar{3}$, 6* | $\mathbf{W}\mathbf{w}_l$ |

* erroneously stated in [18].

**Table 4.** Formulae for calculation points $\mathbf{x}_c$.

It may be seen from Table 4 that having classified the matrix part **W** and having decomposed translation part **w**, the derivation of $\mathbf{x}_c$ for any space-group operation is unique and extremely simple. Calculations are based on the standard matrix arithmetic: multiplication of a matrix by a vector, adding two vectors or multiplying a vector by a constant. The geometric interpretation of specified rules as well as their explanation is also simple. A comparison of derived formulae with those described in article [18] reveals an incorrect equation for the axis symbol 6 in the published data. The error was overlooked, since in all conventional descriptions of the space groups, the origin is located on the hexagonal axis.

## 6. Predefined data for space groups generation

For practical and technical convenience the amount of predefined data needed for all 230 space group generation in computer applications should be minimal and the generation process should be most effective. In the case of space group generation in ITA83 style the latter demand is obtained by the composition series method, which on the other hand leads to some redundancy in the sets of non-translational 'generators selected'. This extension may be avoided by reselecting the generators in such a way, that their number is minimal but they can easily restore the original composition series. The concept leads to extending slightly the set of predefined point symmetry operations and to significant reduction of the generators specification for each group, remembering that SG belonging to the same crystal class are based on the same point generators. Since the arithmetic class may be extracted from a space-group symbol or a space-group number, the space generators may be composed of the point generators and individually given translations. Next, the obtained list should be slightly modified to produce a full list of generators needed in a very effective composition method.

This paragraph specifies complete data needed for effective and unique generation of all space groups:

a. 18 matrices (point operations)
b. 37 ranges of space group numbers which correspond to conventional point group descriptions specified by its generators – numbers of matrices from list (a)
c. 230 specification of Bravais letter and one or two translation parts which together with point operations from (b) define space group generators

Matrices needed for restoring the composition series are compiled in Table 5. According to [18] and possible future extensions of the algorithms, they are coded by single numbers. Only proper rotations should be explicitly defined.

| No | Code | Symbol | No | Code | Symbol | No | Code | Symbol | No | Code | Symbol |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 16484 | 1 | 5 | 7410 | 2 [1-10] | 10 | 16482 | m x,y,0 | 15 | 5223 | -6+ 0,0,z; 0,0,0 |
| 1 | 3200 | 2 [001] | 6 | 14459 | 6+ 0,0,z | 11 | 16322 | m x,0,z | 16 | 11865 | -3+ 0,0,z;0,0,0 |
| 2 | 3360 | 2 [010] | 7 | 7817 | 3+ 0,0,z | 12 | 11784 | -4+ 0,0,z; 0,0,0 | 17 | 8866 | -3+ x,x,x;0,0,0 |
| 3 | 7898 | 4+ [001] | 8 | 10816 | 3+ x,x,x | 13 | 7412 | m x,-x,z | | | |
| 4 | 12270 | 2 [110] | 9 | 3198 | -1 | 14 | 12272 | m x,x,z | | | |

**Table 5.** Symmetry matrices used as point groups generators

Matrices of improper rotation haves numbers increased by 9 and codes complemented to 19682: No = No(proper)+9, code=19682-code (proper). The obvious relation **PntGen** = -1***PntGen** (proper) may be also applied. A code is converted into the 3x3 matrix **PntGen** by the following procedure:

```
For k = 3 To 1 Step -1
For j = 3 To 1 Step -1
PntGen(k, j) = (code Mod 3) - 1
code = code \ 3 'integral division
Next j
Next k
```

The relations between the space groups from Table 1 and corresponding point groups are compiled in Table 6. The sequence of point-group generators taken from Table 5 is associated with a space group by its number, according to the order of space-group types unchanged since the first edition of Tables in 1935. A range of space-group numbers compatible with a given list (point group) is defined by its maximal value (SG column). Some subranges or individual SG numbers are needed for the alternative description of point groups, what is seen in the last 5 rows.

| SG max | PG symbol | Genera-tors | SG max | PG symbol | Genera-tors | SG max | PG symbol | Genera-tors | SG max | PG symbol | Genera-tors |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | - | 82 | $\bar{4}$ | 12 | 161 | 3m1 | 7,10 | 199 | 23 | 1,8 |
| 2 | $\bar{1}$ | 9 | 88 | 4/m | 3,9 | 167 | $\bar{3}$m1 | 16,4 | 206 | m$\bar{3}$ | 1,17 |
| 5 | 2 | 2 | 98 | 422 | 3,2 | 173 | 6 | 6 | 214 | 432 | 1,8,4 |
| 9 | m | 11 | 110 | 4mm | 3,11 | 174 | $\bar{6}$ | 15 | 220 | $\bar{4}$3m | 1,8,13 |
| 15 | 2/m | 2,9 | 122 | $\bar{4}$2m | 12,2 | 176 | 6/m | 6,9 | 230 | m$\bar{3}$m | 1,17,4 |
| 24 | 222 | 1,2 | 142 | 4/mmm | 3,2,9 | 182 | 622 | 6,4 | 115-120 | $\bar{4}$m2 | 12,11 |
| 46 | mm2 | 1,11 | 146 | 3 | 7 | 186 | 6mm | 6,10 | 149,151, 153 | 312 | 7,5 |
| 74 | mmm | 1,2,9 | 148 | $\bar{3}$ | 16 | 190 | $\bar{6}$m2 | 15,10 | 157,159 | 31m | 7,13 |
| 80 | 4 | 3 | 155 | 321 | 7,4 | 194 | 6/mmm | 6,4,9 | 162-163 | $\bar{3}$1m | 16,5 |
| | | | | | | | | | 189-190 | $\bar{6}$2m | 15,4 |

**Table 6.** 32 point groups (+ 5 additional orientations), its generators and the maximal numbers of space groups to which the group corresponds

There are 73 *symmorphic* space groups, which in the conventional description need only additional information on the centring type. In other groups the space generators must contain partial translations. A proper selection of the origin makes that only one or two non-zero vectors must be specified. Based on the 'conventional origins' from ITA83, the information necessary to convert point generators into the space generators was compiled in Table 7.

The lack of Bravais letter in the items of Table 7 means the primitive lattice or the symbol P. Only translation parts different from the zero vector are specified; their ordering positions are fixed by the asterisks. In order to overcome ratios, translation vectors are multiplied by 4, or by 6 in the trigonal and hexagonal crystal systems. Moreover, in the latter systems only the *z*-component differs from zero and thus is specified. The items can be treated as a

concise information on the system of primitive as well as non-primitive translations including: lattice centring, origin specification, relative position of symmetry elements differing space groups in the arithmetic class.

Based on the unique identifier of a space-group type, which can be related to the space-group sequence number, the list of space-group generators organized in the composition series can be obtained from condensed data included in Tables 5-7.

| SG No | +1 | +2 | +3 | +4 | +5 | +6 | +7 | +8 | +9 | +10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | | | | 020 | C | | 002 | C | C002 | |
| 10 | 020 | C | 002 | 022 | C002 | | 002002 | *220 | 202022 | C002002 |
| 20 | C | F | I | I202022 | | 002002 | *002 | *200 | 002200 | *022 |
| 30 | 202202 | *220 | 002220 | *222 | C | C002002 | C*002 | A | A*020 | A*200 |
| 40 | A*220 | F | F*111 | I | I*220 | I*200 | | 220202 | *002 | 220200 |
| 50 | 200 | 200222 | 202202 | 200002 | *220 | 220022 | 002022 | *222 | 220020 | 222002 |
| 60 | 202022 | 202020 | C002002 | C022022 | C | C*002 | C020020 | C200002 | F | F330303 |
| 70 | I | I*220 | I202022 | I020020 | | 001 | 002 | 003 | I | I021 |
| 80 | | I | | 002 | 200 | 022 | I | I311 | | 220220 |
| 90 | 001 | 221221 | 002 | 222222 | 003 | 223223 | I | I021203 | | *220 |
| 100 | 002002 | 222222 | *002 | *222 | 002 | 002220 | I | I*002 | I021 | I021002 |
| 110 | | *002 | *220 | *222 | | *002 | *220 | *222 | I | I*002 |
| 120 | I | I*203 | | *002 | 200200 | 200202 | *220 | *222 | 200020 | 200022 |
| 130 | 002 | 002002 | 202200 | 202202 | 002220 | 222222 | 202020 | 202022 | I | I*002 |
| 140 | I131202 | I131200 | | 2 | 4 | R | | R | | |
| 150 | 24 | 2 | 42 | 4 | R | | | *3 | *3 | R |
| 160 | R*3 | | *3 | | *3 | R | R*3 | | 1 | 5 |
| 170 | 2 | 4 | 3 | | | 3 | | 12 | 54 | 24 |
| 180 | 42 | 3 | | *3 | 33 | 3 | | 33 | | 3 |
| 190 | | *3 | 33 | 3 | | F | I | 202 | I202 | |
| 200 | 220 | F | F330 | I | 202 | I202 | | **222 | F | F022*313 |
| 210 | I | 202*133 | 202*311 | I202*311 | | F | I | **222 | F*222 | I202*111 |
| 220 | | 220*002 | **222 | 220*220 | F | F**222 | F312*312 | F132*310 | I | I202*311 |

**Table 7.** Bravais symbols and the translation parts of generators

## 7. Composition series and space groups generation

It is well known and seen in Table 6 that maximally three generators are necessary for obtaining all symmetry operations in the point groups, even in group $m\bar{3}m$. But for effective generation of groups based on a series of normal subgroups, the listed set of generators should be extended to the complete composition series. The following action leads to the non-translational sets of generators used in ITA83:

i. generators 4 and $\bar{4}$ (matrices 3 and 12) are preceded by their squares.
ii. generator $\bar{3}$ is replaced by the 3 and the generator $\bar{1}$ is added as the last generator.

iii. generators 6 and $\bar{6}$ (matrices 6 and 15) are replaced by their third and second powers.
iv. in the case of a cubic system the two-fold rotation in $z$ direction (matrix 1) is followed by the two-fold rotation in $y$ direction (matrix 2). The situation is a little more cumbersome for the space groups: the translation part of generator 2[010] occurring in the composition series is not explicitly specified and must be obtained by a cyclic permutation of the translation components ($t_x$, $t_y$, $t_z$) →($t_z$, $t_x$, $t_y$) given for 2[001] generator.

The construction of composition series of generators is shown on the example of the tetragonal group *P*42/*nnm* in its initial description. According to Table 1 the input, from which the non-modified generators shown in Table 8 have been obtained, is reduced to number '134'. Comparing this space-group number with the data contained in Table 3, 132<= 134 < 136, gives the point group 4/*mmm* and point generators 3,2,9, which matrix forms are derived from the integers 7898, 3360 and 3198. The 'space' information is presented in Table 7. The given group number corresponds to string '202202', and defines translation parts for the first and the second generator. According to rule (i) in the above list, the first generator of composition series is obtained by squaring the generator with their matrix part no 3. As a result, four generators described in Table 8 are obtained.

| | | | |
|---|---|---|---|
| $\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&1\end{pmatrix},\begin{pmatrix}1/2\\1/2\\0\end{pmatrix}$ | $\begin{pmatrix}0&\bar{1}&0\\1&0&0\\0&0&1\end{pmatrix},\begin{pmatrix}1/2\\0\\1/2\end{pmatrix}$ | $\begin{pmatrix}\bar{1}&0&0\\0&1&0\\0&0&\bar{1}\end{pmatrix},\begin{pmatrix}1/2\\0\\1/2\end{pmatrix}$ | $\begin{pmatrix}\bar{1}&0&0\\0&\bar{1}&0\\0&0&\bar{1}\end{pmatrix},\begin{pmatrix}0\\0\\0\end{pmatrix}$ |

**Table 8.** Composition series of generators for the space group type No 134, consistent with ITA83.

Having completed a composition series set of generators, the derivation of all symmetry matrices or more precisely obtaining the *coset representatives* is a trivial task. Each non-translational generator doubles, or triples in the case of $3^+$ operation, the current set of symmetry operations and thus the process is non-redundant and needs only one matrix multiplication per one new symmetry operation item.

The generating process needs only one list of 4x4 matrices for storing as well the original or transformed generators as new generated operations. It is assumed that the GensNo generators are located in the upper part of the **SymMtx** list starting from position 49, the current number of symmetry operators **SymsNo** is set to 1 and the unit matrix is introduced as the first element of **SymMtx**. Let the procedure **NewSymMtx** with three input indices **gen**, **oldsym**, **newsym** multiplies the matrix 48+**gen** by the matrix **oldsym**, reduces translation components modulo 1 and locates the new symmetry operation in the **newsym** position**.** The complete space group generation procedure can be as follows:

```
For i = 1 To GensNo          'main loop

If SymMtx(48+i,1,1) + SymMtx(48+i,2,2) + SymMtx(48+i,3,3) = 0 Then     'test for 3+
triple = True
Else
triple = False
```

```
Endif
For j = 1 To SymsNo 'generation of the successive normal subgroups
Call NewSymMtx(i, j, SymsNo + j)
If triple = True Then Call NewSymMtx(i, SymsNo + j, 2 * SymsNo + j)
Next j
If triple = True Then SymsNo = SymsNo * 3 Else SymsNo = SymsNo * 2 'current number of
symmetry operation
Next i 'end of main loop
```

The advantages of the composition series method are clear from the above scheme – every new symmetry matrix is obtained by a single multiplication without checking for redundancy. Since the complete list of generators corresponds to the explicitly given ones in ITA83, the obtained result repeats the corresponding conventional space group description in ITA83, including also the order of the symmetry matrices. This is also the base for the other unique space group descriptions, irrespective of whether they are conventional or not, since before the process starts, the generators can be recalculated according to any given coordinate transformation **T** by standard equation $\mathbf{G}' = \mathbf{T}^{-1}\mathbf{G}\mathbf{T}$. Such approach is especially simple in connection with the *translational space group symbols,* where transformations are described explicitly.

## 8. Deriving dual symbols for symmetry operations

The derivation of a dual symbol from a symmetry operation (**W**,**w**) involves the following:

a. Characterizing the point operation **W** by: (i) rotation type, that is 1, 2, 3, 4, 6, $\bar{1}$, m, $\bar{3}$, $\bar{4}$, $\bar{6}$, (ii) sense of rotation, (iii) orthogonal lattice splitting indices [*uvw*](*hkl*)
b. Characterizing the space operation (**W**,**w**) by: (i) orthogonal splitting of the translation part $\mathbf{w} = \mathbf{w}_g + \mathbf{w}_l$, (ii) point $\mathbf{x}_c$ on geometric element closest to the origin.

The type of point operation is easily recognized from the determinant and trace of **W** using a look-up Table 2. Splitting indices are the same for both matrices **W** and **–W**. Let $\mathbf{W}_p$ denotes the proper rotation matrix det(**W**)**W.** A lattice vector [*uvw*] parallel to the rotation axis as well its reciprocal (*hkl*) are defined by any non-zero column and any non-zero row of the matrices constructed in dependence on the order *k* of $\mathbf{W}_p$:

$$k = \mathbf{2} : \mathbf{I} + \mathbf{W_p}, k = \mathbf{3} : \mathbf{I} + \mathbf{W_p} + \mathbf{W_p}^{\mathbf{2}},\ k = \mathbf{4} : \mathbf{I} + \mathbf{W_p}^{\mathbf{2}} \text{ and } k = \mathbf{6} : \mathbf{I} + \mathbf{W_p}^{\mathbf{3}}$$

where **I** denotes a unit matrix.

Next, a positive scalar product is required, if necessary by multiplying (*hkl*) by -1. If vectors [*uvw*] and (*hkl*) have common divisors, indices should be divided. At last all indices can change the signs in order to obtain the positive axis direction according to Table 3. Having determined the direction [*uvw*] of an axis, the sense of rotation is simply determined from the inequalities (11). These are all steps needed for a complete geometric description of a point symmetry operation. Practically, the conventions are reduced to the one rule about the positive direction of [*uvw*].

The orthogonal splitting of a translation part **w** depends on the axis direction [*uvw*]. The same results are obtained for (**W**,**w**) and (-**W**,**w**), thus calculations can be reduced to the pair ($\mathbf{W}_p$,**w**). Since ($\mathbf{W}_p$,**w**)$^k$ = (**I**,$k\mathbf{w}_g$), the *k*-th part of the resulting translation defines the intrinsic component of the translation, and in consequence also the location component $\mathbf{w}_l = \mathbf{w}-\mathbf{w}_g$. In the presented procedure such decomposition is also valuable for a rotoinversion operation. As usual, for a reflection the numerical values of $\mathbf{w}_g$ and $\mathbf{w}_l$ must be interchanged. The central problem of deriving the point $\mathbf{x}_c$ (an invariant relative to a reduced operation and closest to the origin) is to find such point on the [*uvw*] lattice vector or on the (*hkl*) plane for a rotation and rotoinversion in the first case and for a reflection in the latter. Geometrical considerations showed that $\mathbf{x}_c$ are rather simply calculated from $\mathbf{w}_l$ according to relations given in Table 4.

The derivation of $\mathbf{x}_c$ ends the calculation needed to describe the space symmetry operation. But vectors $\mathbf{x}_c$ in the case of reflections and $\mathbf{w}_g$ in the case of rotations or rotoinversions are parallel to [*uvw*] and may be represented by a single ratio r. Thus, an intrinsic component $\mathbf{w}_g$ and a shift vector (orthogonal to the geometric element) are presented by four simple ratios. An asterisk mark serves as a separation mark between vectors and thus a dual symbol of space-group operation takes the form of ±n ± [*uvw*](*hkl*) $\mathbf{w}_g$*$\mathbf{x}_c$.

## 9. Origin problem

In the non-symmorphic space groups the symmetry elements are not constrained to pass through the origin. The selection of a reasonable origin for a coordinate system relative to non-intersecting symmetry elements is not unique. The symbol of space-group type, like Hermann-Mauguin symbol, fixes in space only relative positions of symmetry elements. Absolute positions need complete translational parts in the space-group generators. The presented technique of space group derivation based on predefined generators favours one and the only one origin for each space group, even if this group is tabulated in ITA83 relative to two origins.

Finding a transformation between two descriptions of the same space group differing only by the origin shift is arithmetically at least cumbersome. In this case, similarly like in other space-group considerations, the geometric information is very practical. A typical way of resolving the mentioned problem consists of a geometrical interpretation of the symmetry matrices in both descriptions and of deduction of the transformation from the diagram of symmetry elements in ITA83. Such analysis is impossible for a non-conventional space group description, but in every case may be carried out on dual symbols.

Since the dual symbols described in the preceding section are easy to obtain, they should be routinely derived together with the space group generation. Their role in the origin control is rather evident, but we illustrate this feature by means of an example. Let column 2 of Table 9 lists the dual symbols of the *P*42/*nnm* operations obtained from the generators presented in Table 8. The items 1, 7, 9, 15 have reduced $\mathbf{x}_c$ parts. It is visible that the origin is located at the inversion point, the intersection of 2[110] and m[110]. A full symmetry of the origin is 2/m (this is the second origin choice tabulated in ITA83).

A higher symmetry of the origin can be obtain by placing it on $\bar{4}$. The origin shifted from that in the first column by (1/4,-1/4,0) leads to a group description symbolized by TSG = *P*42/*nnm* (1/4,-1/4,0) (this is the first origin choice in ITA83). The result is listed in column 3 of Table 9. It can be seen that rotoinversion operations 11,12 contain the intrinsic part ½ and the inversion point according to (17) in (0,0,1/4).

Another possibility to select the origin in a high symmetry point is to put it on $\bar{4}$ , but exactly at the inversion point. In this situation the origin is shifted by (1/4,-1/4,1/4) in comparison with column 2. The symmetry matrices of the group description TSG = *P*42/*nnm* (1/4,-1/4,1/4) presented by dual symbols are given in the last column of Table 9.

| No | TSG | | |
|---|---|---|---|
| | *P*42/*nnm* | *P*42/*nnm* (¼,-¼,0) | *P*42/*nnm* (¼,-¼,¼) |
| 1 | 1 | 1 | 1 |
| 2 | 2 [001] * 1/4,1/4,0 | 2 [001] | 2 [001] |
| 3 | 4+[001] 1/2 * 1/4,1/4,0 | 4+[001] 1/2 * 0,1/2,0 | 4+[001] 1/2 * 0,1/2,0 |
| 4 | 4-[001] 1/2 * 1/4,1/4,0 | 4-[001] 1/2 * 1/2,0,0 | 4-[001] 1/2 * 1/2,0,0 |
| 5 | 2 [010] * 1/4,0,1/4 | 2 [010] * 0,0,1/4 | 2 [010] |
| 6 | 2 [100] * 0,1/4,1/4 | 2 [100] * 0,0,1/4 | 2 [100] |
| 7 | 2 [110] | 2 [110] 1/2 * | 2 [110] 1/2 * 0,0,1/4 |
| 8 | 2 [1-10] * 1/4,1/4,0 | 2 [1-10] * 1/4,1/4,0 | 2 [1-10] * 1/4,1/4,1/4 |
| 9 | -1 | -1 * 1/4,1/4,0 | -1 * 1/4,1/4,1/4 |
| 10 | m [001] 1/2,1/2,0 * | m [001] 1/2,1/2,0 * | m [001] 1/2,1/2,0 * 1/4 |
| 11 | -4+[001] 1/2 * 1/4,-1/4,0 | -4+[001] 1/2 * | -4+[001] |
| 12 | -4-[001] 1/2 * -1/4,1/4,0 | -4-[001] 1/2 * | -4-[001] |
| 13 | m [010] 1/2,0,1/2 * | m [010] 1/2,0,1/2 * 1/4 | m [010] 1/2,0,1/2 * 1/4 |
| 14 | m [100] 0,1/2,1/2 * | m [100] 0,1/2,1/2 * 1/4 | m [100] 0,1/2,1/2 * 1/4 |
| 15 | m [110] | m [110] | m [110] |
| 16 | m [1-10] 1/2,1/2,0 * | m [1-10] | m [1-10] |

**Table 9.** Different descriptions of the space group type *P*42/*nnm*

In order to show different group-subgroup relations, other descriptions of space groups may be desirable. Contrary to rather difficult manipulation based on coordinate triplets [28], the determination of shift vectors with the help of geometric information is simple. For this purpose the classical symbols of symmetry operations as well dual symbols are similarly useful, but the latter may be also applicable in a non-conventional space-group description. Since the multiplication of symmetry matrices is based on modulo 1 arithmetic, the origin control should involve only the generators of space groups.

## 10. Axes problem

A rigorous classification of space groups, that is their specific descriptions, into space-group type can be given in an algebraic or a geometric way. Typically, the matrix algebra and the

group-theoretical approach is preferred. For this classification, each space group description is referred to a primitive base and an origin. Two space groups **G** and **G′** belong to the same space-group type if a transformation pair **P**, **p** exists, for which the 3x3 matrix has integral elements with det(**P**) = 1 and the **p** vector consists of three real numbers, such that **G** is transformed into **G**′ (see, Wondratschek in ITA83). This definition is very simple, but finding the transformation between two sets of matrices may be a real challenge.

Let's modify the above equivalence definition for the practical purposes. Now **G′** means a conventionally described *space-group type*, represented by a unique set of generators or symmetry matrices. **G** is still referred to a primitive base. **G** belongs to the space-group type **G′** if a transformation pair **P**, **p** exists, for which the 3x3 matrix has integral elements with det(**P**) = 1,2,3 or 4 and the **p** vector consists of three real numbers, such that **G** is transformed into **G**′. The first step in determining the type of group **G** is to refer it to a centred Bravais base by a proper selection of coordinate axes. It is simple with the help of dual symbols what will be illustrated by the group description TSG = $I4_122$ (1,0,0; 0,1,0; ½,1/2,1/2) (1/4,1/4,0) given in Table 10.

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 0 | 0 | 0 | 2 | -1 | 0 | -1 | 0,5 | 3 | 0 | -1 | -1 | 0,25 | 4 | 0 | 1 | 0 | 0,75 |
| | 0 | 1 | 0 | 0 | | 0 | -1 | -1 | 0,5 | | 1 | 0 | 0 | 0,25 | | -1 | 0 | -1 | 0,75 |
| | 0 | 0 | 1 | 0 | | 0 | 0 | 1 | 0 | | 0 | 0 | 1 | 0,5 | | 0 | 0 | 1 | 0,5 |
| | 1 | | | | | 2 [-1-12]( 0 0 1) * 1/4,1/4,0 | | | | | 4+[-1-12]( 0 0 1) 1/4 * 0,1/2,0 | | | | | 4-[-1-12]( 0 0 1) 1/4 * 1,0,0 | | | |
| 5 | -1 | 0 | 0 | 0,25 | 6 | 1 | 0 | 1 | 0,75 | 7 | 0 | 1 | 1 | 0 | 8 | 0 | -1 | 0 | 0,5 |
| | 0 | 1 | 1 | 0,25 | | 0 | -1 | 0 | 0,75 | | 1 | 0 | 1 | 0 | | -1 | 0 | 0 | 0,5 |
| | 0 | 0 | -1 | 0,5 | | 0 | 0 | -1 | 0,5 | | 0 | 0 | -1 | 0 | | 0 | 0 | -1 | 0 |
| | 2 [010]( 0 2 1) 1/2 * 1/8,-1/8,1/4 | | | | | 2 [100]( 2 0 1) 1 * -1/8,3/8,1/4 | | | | | 2 [110]( 1 1 1) | | | | | 2 [1-10] * 1/4,1/4,0 | | | |

**Table 10.** Symmetry matrices and dual symbols of the group description TSG = $I4_122$ (1,0,0; 0,1,0; ½,1/2,1/2) (1/4,1/4,0)

Items 1,2,3 and 4 define symmetry axis $4_1$ parallel to $[\bar{1}\bar{1}2]$. Matrices (5,6) and (7,8) describe two pairs of orthogonally oriented twofold axes, according to property $u_1h_2 + v_1k_2 + w_1l_2 = u_2h_1 + v_2k_1 + w_2l_1 = 0$ between the corresponding splitting indices. A similar test shows the orthogonality between $4_1$ and all twofold axes. Thus, two orthogonal bases and two transformation matrices may be constructed from [*uvw*] indices. The first transformation matrix **P** with columns [100], [010], $[\bar{1}\bar{1}2]$ has det(**P**) = 2 and leads to *I*-centred basis. The equivalent F-centred Bravais tetragonal cell is involved with P in the form $[1\bar{1}0]$, [110] and $[\bar{1}\bar{1}2]$. The application of the first transformation matrix is equivalent to the selection of the conventional axes for the tetragonal space group.

Moreover, the arithmetic type 422*I* of the analysed group is determined. From the predefined data one can find that only two space-group types, namely the groups with sequence numbers 97 and 98, belong to this arithmetic type. Group 97 is symmorphic. Thus,

$4_1$ axis points directly onto type 98 space group. The origin shift **p** may be determined by comparing points $\mathbf{x}_c$ in dual symbols of the space-group type generators and symmetry operations of the analysed group with identical matrix parts. The generators of group type $I4_122$ are characterized by dual symbols as: 4+[001] 1/4 * -1/4,1/4,0 and 2 [010] * 1/4,0,3/8. Items 3 and 5 from Table 10 transformed according to **P** matrix give 4+[001] 1/4 * 0,1/2,0 and 2 [010] 1/2 * 1/4,0,1/8. The origin shift **p** = -1/4,-1/4,0 predicted from the $4_1^+$ operation equals both descriptions.

The analysed example does not attempt to be a kind of algorithmic approach, but was included to show the advantages of representing symmetry operations in both forms, as a symmetry matrix and as a dual symbol.

## 11. Conclusions

It was assumed that, the choice of the known or modified algorithms should be motivated by obtaining functional relations $f_1$ (*SG symbol*, *ordering number*) = *symmetry matri*x and $f_2$ (*symmetry matrix*) = *geometric description* on the assumption that the needed conventions are reduced to a minimum. This unique arithmetic and geometric description of space groups cannot be obtained at the cost of excessive amount of the predefined data, ineffective or sophisticated algorithms. Moreover, in the case of conventional axes and origins the results cannot differ from that contained in ITA83. It appears that such practical purposes have been achieved.

The commonly accepted Hermann-Mauguin symbol is very informative and useful for controlling group orientation, but is not dependent on the origin choice and is not applicable for a non-conventional space group description. The absolute position of symmetry elements needs an explicit origin specification, by giving a complete information about the translation part of generators. The coding of such generators leads to the elaborated symbols (Zachariassen/Shmueli) or to the concise symbols (Hall), but involved with many conventions and rather sophisticated interpretation of symbols. Moreover, in universal approaches based on arbitrary generators most of the computing time is spent on tests for closure or for redundancy of generated operations.

The '*transformational concept*' presented in this chapter introduces an 'absolute' description of each space group type contrary to the multiple standards for some space group types in ITA83. Thus, all groups belonging to a given SG type may be derived from the same set of optimally selected generators, assuming that the transformation from the SG type to a needed description is known. The TSG symbol was aimed at pointing in a computer program at the set of generators, prepared as 'composition series', and at giving an explicit definition of necessary transformation of these generators. There is no need to interpret the TSG symbol or tests the generators. If generators published in ITA83 serve as predefined type generators, nearly 100% of computing time is spent on non-redundant SG derivation. Programs based on a transformational concept reproduce all conventional descriptions given in ITA83; in the non-conventional cases they lead to descriptions in the ITA83 style.

From this point of view, such algorithms standardize any SG descriptions and their geometric interpretations and may be treated as an electronic extension of the printed ITA83 tables. In this context the classification of space groups into conventionally versus non-conventionally described, and the evolutionary changes between different editions of Tables are unsubstantial.

The generation schema based on composition series leads also to a considerable reduction of predefined data, what is an important feature in the implementing and testing of SG derivation programs. Since all the space groups which are based on a given point group are generated in the same way, only the translational parts of generators should be stored. Using small improvements discussed in the text, the non-redundant number of composition series generators is 3, and thus the non-redundant number of translations for each space-group type is 0,1 or maximum 2.

The introduced dual symbol of symmetry operation sheds some light on the lattice properties and thus changes a rather informative character of the geometric symbols into a valuable tool for finding the transformation between different descriptions of the same groups. Since the symbol is universal, convention free, easy to derive and to manipulate on a computer, it is advised to generate space group descriptions simultaneously in two forms, as coordinate triplets and as dual symbols. Any new information can be obtained from the additional Seitz symbol.

The simplicity of the considered approach is evident and seems to be valuable also for teaching purposes. Algorithms were implemented in the Visual Basic, in the Excel environment. All procedures need less than 600 programming lines including 200-line subroutine for transforming a symmetry matrix into a dual symbol. This procedure may be also used as stand-alone item to characterize any symmetry matrix. The source code included in the Excel worksheet may be obtained from the author on request.

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