Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 18 May 2007
Accepted 13 September 2007

A systematic approach to the derivation of standard orientation-location parts of symmetry-operation symbols

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Automatically generated orientation-location parts, or coordinate triplets describing the geometric elements, differ frequently from the corresponding parts of the symmetry-operation symbols listed in *International Tables for Crystallography* [(1983), Vol. A, *Space-Group Symmetry*, edited by Th. Hahn. Dordrecht: Reidel]. An effective algorithm enabling the derivation of standard orientation-location parts from any symmetry matrix is described and illustrated. The algorithm is based on a new concept alternative to the 'invariant points of reduced operation'. First, the geometric element that corresponds to a given symmetry operation is oriented and located in a nearly convention free manner. The application of the direction indices [*uvw*] or Miller indices (*hkl*) gives a unique orientation provided the convention about the positive direction is defined. The location is fixed by the specification of a unique point on the geometric element, *i.e.* the point closest to the origin. Next, both results are converted into the standard orientation-location form. The standardization step can be incorporated into other existing methods of derivation of the symmetry-operation symbols. A number of standardization examples are given.

1. Introduction

Volume A of *International Tables for Crystallography* edited by Th. Hahn (referred to hereafter as ITA83) contains new features describing space groups. Among them, a symmetry-operation block is found. The block forms a link between the algebraic way (coordinate triplets of general position) and the geometric way (symmetry-elements diagram) of space-group characterization. An entry in the block consists of a symmetry-operation-type symbol, specification of glide/screw vector if present, followed by 'a coordinate triplet indicating the *location* and *orientation* of the symmetry element which corresponds to the symmetry operation' (Hahn & Looijenga-Vos in ITA83, 5th edition, p. 27), called here the orientation-location part.[1]

The set of points defined by an orientation-location part is considered as a geometric element. The idea of a geometric element (GE) was introduced for precise definition of a symmetry element and for assigning the symmetry operations to the symmetry element (de Wolf *et al.*, 1989). The symmetry-operation symbols were recommended for general use in the Report of the IUCr *Ad hoc* Committee on the Nomenclature of Symmetry (de Wolf *et al.*, 1992). Hence the symbols contained in ITA83 became standard geometrical descriptions of symmetry operations.

The procedure of deriving the symbol from the matrix form of a symmetry operation described by Fischer & Koch in the explanatory part of ITA83 is based on an earlier approach developed by Wondratschek & Neubüser (1967). The type of symmetry operation, the intrinsic translation and the inversion point for a rotoinversion can be uniquely derived from the symmetry matrix. In this classical approach, the orientation-location part is obtained in one step by solving three simultaneous equations. In other methods, the solution is preceded by determining the orientation of the given rotation axis (Grosse-Kunstleve, 1999). In some cases, this information can be used to describe a system of equations in a more convenient coordinate system where one of the basis vectors is parallel to the rotation axis (Shmueli, 1984).

As pointed out in literature on this subject (Fischer & Koch, 1983; Shmueli, 1984; Boisen & Gibbs, 1990; Hahn & Wondratschek, 1994; Grosse-Kunstleve, 1999), the invariant subspace of reduced operation is obtained by solving the system of three simultaneous equations. Such a system is undetermined and may be solved in many ways. However, unique particular solutions can be obtained after applying some algebraic conventions. The general rules relevant to all systems have not been described so far. Consequently, standard symbols are frequently replaced by other geometric

[1] The term 'orientation-location part' is preferred in comparison to the commonly used term 'location' because it reflects two functions of the coordinates which describe the geometric element of the operation.

information based on the authors' own conventions (Shmueli, 1984; Grosse-Kunstleve, 1999).

The aim of this work is to describe the derivation of the orientation-location parts from any symmetry matrix in an algorithmic way. The emphasis on derivation of the standard descriptions is greater than that found in literature elsewhere. First, the orientation-location parts of symbols given in ITA83 are analysed and conventions which correspond to the applied algebraic rules are defined. Then the final form of the orientation-location parts are constructed in three steps: (i) derivation and classification of the GE orientations, (ii) determination of the unique point on the GE, *i.e.* the point closest to the origin, (iii) transformation of the unique point into the standard point for each type of GE orientation.

2. Analysis of the orientation-location parts of geometric descriptions listed in ITA83

2.1. Conventions

The orientation-location part is interpreted as a parametric equation of a line or a plane. With reference to the coordinate system, the GE of rotation, screw rotation or rotoinversion is described by the system of equations $x = at + x_0$, $y = bt + y_0$, $z = ct + z_0$ written in the abbreviated form as $at + x_0, bt + y_0, ct + z_0$. The geometrical significance of these equations is invariant under dummy variable (parameter) t transformations: (i) scaling of variable, $t = kt$ ($k > 0$); (ii) inversion of variable, $t = -t$; (iii) symbol change, $t = x$ (or y or z); or (iv) origin shift, $t = t + t_0$. The plane of reflection or glide reflection is characterized in a similar way but with two dummy variables. The algebraic conventions applied in derivation of the standard orientation-location part correspond to the rules which fix each of the above transformations.

For standardization purposes, the coefficients $[a, b, c]$ are relatively prime integers and the point x_0, y_0, z_0 is characteristic for the GE. The problem is that there are several characteristic points (Fig. 1), namely, the set of one, two or three

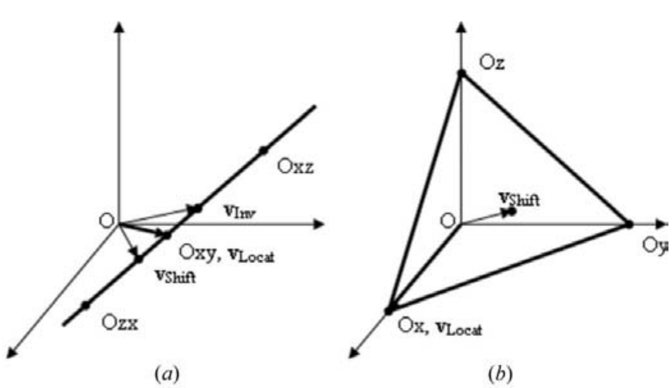

Figure 1
Characteristic points of geometric elements in general orientation. Point $\mathbf{v}_{\rm Inv}$ occurs only for rotoinversion. $\mathbf{v}_{\rm Shift}$ corresponds to the point closest to the origin O. $\mathbf{v}_{\rm Locat}$ terminates on the point conventionally chosen from the set of special points. (*a*) The set contains the points of intersection of a line with the basal planes. (*b*) The set contains the points of intersection of the coordinate axes with a plane.

special points (intersection of GE and basal planes or coordinate axes), the point closest to the origin represented by the position vector $\mathbf{v}_{\rm Shift}$, and the inversion point applicable only to rotoinversion.

From the standard symbols printed in ITA83, a number of conventions are derived. These rules are listed below in the form of concise notation, where the symbol '↺' is used for cyclic permutation and '$-$', '$+$', '0', 'n', '*' for negative, positive, zero, non-zero and any value, respectively.

C1 (scaling): coefficients $[a, b, c]$ should be scaled into relatively prime integers.

C2 (positive sense): from the scaled pair $[a, b, c]$ and $[-a, -b, -c]$, the selected one must fit the pattern [100]↺, $[+n0]$↺, $[+--]$↺ or $[+++]$.

C3 (variable symbol): $t = x$ for $[n**]$, $t = y$ for $[0n*]$, $t = z$ for $[00n]$.

C4 (variable origin for axis): the zero value of the dummy variable corresponds to the point of intersection selected in the order of descending priority: (*, *, 0), (0, *, *), (*, 0, *).

C5 (variable origin for plane): the zero value of the dummy variables correspond to the point of intersection selected in the order of descending priority: (*, 0, 0), (0, *, 0), (0, 0, *).

C6 (traces of the plane): the symbol for a reflection or glide reflection defines two traces which span the plane. For a plane in general orientation,[2] the traces $[mn0]$ and $[p0r]$ are selected for construction of the orientation-location part and the letter z is used as the dummy-variable symbol for the second trace.

The conventions were tested by checking the consistency of the descriptions in ITA83 (printed in 1995). They showed only a few inconsistencies for the glide reflections (Stróż, 1997*a*,*b*), corrected in the 5th edition of ITA83 (printed in 2002, pp. xix, xx). Other, non-standard, geometric symbols differ in convention C2 (Grosse-Kunstleve, 1999) or in conventions C4 and C5 (Shmueli, 1984).

It is evident that the above rules are dependent on the orientation of geometric elements. In order to implement them into an automatic procedure, it is reasonable to classify the symmetry operations by their GE's orientation in space.

2.2. The vector form of the orientation-rotation part

For further considerations, it is crucial to present a standard orientation-location part in one of the following vector forms:

$$\begin{aligned} t\mathbf{v}_{\rm Axis} + \mathbf{v}_{\rm Locat} &\overset{\rm NORM}{\longrightarrow} t[uvw] + X_0, \\ t_1\mathbf{v}_{\rm Trace1} + t_2\mathbf{v}_{\rm Trace2} + \mathbf{v}_{\rm Locat} &\overset{\rm NORM}{\longrightarrow} t_1[mno] + t_2[pqr] + X_0. \end{aligned} \quad (1)$$

The first expression in (1) defines a line and the second one describes a plane spanned by two vectors, $\mathbf{v}_{\rm Trace1}$ and $\mathbf{v}_{\rm Trace2}$, parallel to the intersections of the plane with the basal planes. Let NORM symbolize the procedure which scales a vector represented by the integer or rational numbers to the shortest vector with the integer components. If necessary, the vector sense is changed according to C2. This guarantees that the GE

[2] Conventions relevant to symmetry planes in general orientation cannot be derived from the standard symbols (given in ITA83). This proposed extension is applicable to non-conventional space-group settings.

Table 1
Normalized traces for different types of plane orientation.

Miller indices type	Trace **Oxy** NORM $(k, -h, 0)$	Trace **Oyz** NORM $(0, l, -k)$	Trace **Ozx** NORM $(-l, 0, h)$
(100)	$\mathbf{v}_{\rm Trace1}$ = [010]	[000]	$\mathbf{v}_{\rm Trace2}$ = [001]
(010)	$\mathbf{v}_{\rm Trace2}$ = [100]	$\mathbf{v}_{\rm Trace1}$ = [001]	[000]
(001)	[000]	$\mathbf{v}_{\rm Trace2}$ = [010]	$\mathbf{v}_{\rm Trace1}$ = [100]
(0*kl*)	$\mathbf{v}_{\rm Trace1}$ = [100]	$\mathbf{v}_{\rm Trace2}$ = [0*qr*]	$\mathbf{v}_{\rm Trace1}$ = [100]
(*h*0*l*)	$\mathbf{v}_{\rm Trace1}$ = [010]	$\mathbf{v}_{\rm Trace1}$ = [010]	$\mathbf{v}_{\rm Trace2}$ = [*p*0*r*]
(*hk*0)	$\mathbf{v}_{\rm Trace2}$ = [*pq*0]	$\mathbf{v}_{\rm Trace1}$ = [001]	$\mathbf{v}_{\rm Trace1}$ = [001]
(*hkl*)	$\mathbf{v}_{\rm Trace1}$ = [*mn*0]	$\mathbf{v}_{\rm Trace3}$ = [0*tu*]	$\mathbf{v}_{\rm Trace2}$ = [*p*0*r*]

Table 2
Normalized direction vectors for different types of axis/plane orientation.

Direction indices	[100]	[010]	[001]	[0*vw*]	[*u*0*w*]	[*uv*0]	[*uvw*]
Orientation type	1	2	3	4	5	6	7
Miller indices	(100)	(010)	(001)	(0*kl*)	(*h*0*l*)	(*hk*0)	(*hkl*)
Orientation type	8	9	10	11	12	13	14

orientation is described uniquely by the direction indices [*uvw*] for an axis or by the pair of trace indices [*mno*] and [*pqr*] for a plane. In the latter case, there are one or two zeroed components in each trace description. Moreover, it is assumed that standard point X_0 represented by $\mathbf{v}_{\rm Locat}$ is selected in accordance with C4 or C5. In non-standard descriptions, any point on GE, *e.g.* the point closest to the origin, fixes the GE location.

It may be of interest to compare the traditional interpretation of the orientation-location parts with the one given in (1). Classically, a coordinate triplet is treated in a more algebraic way as a solution of an 'invariant-points equation'. As was pointed out earlier, even for symmetry operations occurring in conventional space-group descriptions (ITA83), the standardization of all solutions is difficult. In the present approach, the orientation-location part is understood as a geometric object composed of a point and one or two direction indices. The explicit separation of orientation and location, together with the following algorithmic considerations, ensures that unique forms (1) and standard descriptions of the coordinate triplets are obtained.

3. Orientation of a geometric element

3.1. A short review of existing approaches

The matrix-vector $(\mathbf{W}, \mathbf{w})$ form of symmetry operation contains all the information required for a complete geometrical characterization of the considered space-group operation. Let $\mathbf{R} = \det(\mathbf{W})\mathbf{W}$ be a proper rotation matrix with order n defined by equation $\mathbf{R}^n = \mathbf{I}$, where $\mathbf{I}$ is the identity matrix. Each operation with $n > 1$ has a characteristic direction $\mathbf{v}_{\rm Axis}$, *i.e.* the eigenvector of the matrix $\mathbf{R}$ (*e.g.* Wondratschek & Neubüser, 1967). A systematic solution of the eigenvalue equation $\mathbf{R}\mathbf{v}_{\rm Axis} = \mathbf{v}_{\rm Axis}$ may be obtained by row echelon forms (Grosse-Kunstleve, 1999). Another approach is based on the matrix $[\mathbf{P}]_1 = \mathbf{I} + \sum_{i=1}^{n-1}\mathbf{W}^i$ for $\det(\mathbf{W}) = 1$ or $[\mathbf{P}]_2 = \mathbf{I} + \sum_{i=1}^{n-1}(-1)^i\mathbf{W}^i$ for $\det(\mathbf{W}) = -1$, and the relation $\mathbf{v}_{\rm Axis} = [\mathbf{P}]_1\mathbf{v}$ for $\det(\mathbf{W}) = 1$ or $\mathbf{v}_{\rm Axis} = [\mathbf{P}]_2\mathbf{v}$ for $\det(\mathbf{W}) = -1$, where $\mathbf{v} = (1, 3, 5)$ (Shmueli, 1984). As the author has commented, the matrix $[\mathbf{P}]_1$ was frequently used by Zachariasen (1967) and is required for the decomposition of the translation part $\mathbf{w}$ into its components along and normal to the axis (*e.g.* Fischer & Koch, 1983).

3.2. Axis direction

Shmueli's method of axis-direction calculation can be somewhat simplified. The sum of the vectors symmetrically distributed around the rotation axis, equivalent to $[\mathbf{P}]_1\mathbf{v}$, can be limited to only two or three such vectors. Moreover, one can notice that the result of calculation is equal to a column of the matrix if $\mathbf{v}$ is equal to a basis vector. Thus, any column of $[\mathbf{P}]_1$ defines the zero vector or the vector parallel to the rotation direction.

Let us construct the following matrix:

$$\begin{aligned} \mathbf{S} &= (\mathbf{I} + \mathbf{R}^{n/2}), \qquad n = 2, 4, 6, \\ \mathbf{S} &= (\mathbf{I} + \mathbf{R} + \mathbf{R}^2), \quad n = 3, \end{aligned} \tag{2}$$

similar to $[\mathbf{P}]_1$. If column $\mathbf{S}_{*j} \neq \mathbf{0}$, then the axis direction (or direction perpendicular to the plane) is directly determined,

$$\mathbf{v}_{\rm Axis} = \mathbf{S}_{*j}, \tag{3}$$

and uniquely described,

$$[uvw] = {\rm NORM}(\mathbf{v}_{\rm Axis}). \tag{4}$$

Direction indices [*uvw*] are used in orientation-location parts of rotations, screw rotations and rotoinversions.

3.3. Plane orientation

In the case of reflection $[n = 2, \det(\mathbf{W}) = -1]$, the vector $\mathbf{v}_{\rm Axis}$ or [*uvw*] should be transformed to the pair of traces. The calculations are simple if the plane normal $\mathbf{v}_{\rm Axis}$ is referred to the reciprocal-coordinate system

$$\mathbf{v}_{\rm Plane} = \mathbf{M}\mathbf{v}_{\rm Axis}, \tag{5}$$

where $\mathbf{M}$ is the metric tensor. The normalized $\mathbf{v}_{\rm Plane}$,

$$(hkl) = {\rm NORM}(\mathbf{v}_{\rm Plane}), \tag{6}$$

gives the plane orientation in the form of the Miller indices. Three traces, *i.e.* the intersections of the (*hkl*) plane with the basal planes, are represented by the vectors denoted by basal-plane symbols:

$$\begin{aligned} \mathbf{Oxy} &= (k, -h, 0), \\ \mathbf{Oyz} &= (0, l, -k), \\ \mathbf{Ozx} &= (-l, 0, h). \end{aligned} \tag{7}$$

One normalized trace, selected according to Table 1, with components m, n, o is denoted as $\mathbf{v}_{\rm Trace1}$ and the second one with components p, q, r as $\mathbf{v}_{\rm Trace2}$.

All planes in Table 1, neglecting the (*hkl*) plane, define two different traces. Each plane that corresponds to the reflection or glide reflection is oriented by the unique Miller indices or by a unique pair of traces ($\mathbf{v}_{\rm Trace1}$, $\mathbf{v}_{\rm Trace2}$). The last row in

Table 3
Projection subspaces corresponding to geometric elements.

GE subspace	Dim. of GE	Projection subspace	Dim. of subspace
Point	0	Whole space	3
Line	1	Points on plane perpendicular to the GE through origin	2
Plane	2	Points on line perpendicular to the GE through origin	1

Table 1 describes the case occurring only in non-conventional settings of space groups and the pair of traces is selected according to C6.

3.4. Classification of symmetry operations

To obtain standard orientation-rotation descriptions, it is reasonable to divide rotations, screw rotations or rotoinversions into seven orientation types according to the indices type of the corresponding axis. Similarly, reflections or glide reflections can be divided into seven types on the basis of the Miller indices type of the corresponding plane (Table 2).

Hence symmetry operations are divided into 15 types according to the orientation of their geometric elements, where orientation type 0 is assigned to an inversion point and means 'no orientation'. Such a classification simplifies the incorporation of conventions (especially C4 and C5) into the derivation procedure and justifies the corresponding orientation-rotation parts classification.

4. Fixing a geometric element by the unique location point

4.1. Splitting the translation part

Decomposition of the translation vector $\mathbf{w}$ into intrinsic and location-dependent components ($\mathbf{w} = \mathbf{w}_g + \mathbf{w}_L$) is given separately in all cited references. The alternative calculation can be based on the matrix $\mathbf{S}$ defined in (2):

$$\mathbf{w}_g = \mathbf{S}\mathbf{w}/2 \text{ for } n = 2, 4, 6, \quad \mathbf{w}_g = \mathbf{S}\mathbf{w}/3 \text{ for } n = 3 \text{ and } \mathbf{w}_L = \mathbf{w} - \mathbf{w}_g. \tag{8}$$

The component $\mathbf{w}_g$ in (8) is parallel to the rotation axis of the operation $\det(\mathbf{W})\mathbf{W}$. This direction in the case of reflections [$n = 2$, $\det(\mathbf{W}) = -1$] is normal to the reflection plane of the original symmetry operation $\mathbf{W}$ and hence the standard meaning of symbols $\mathbf{w}_L$ and $\mathbf{w}_g$ is retained after their interchange.

Unlike the 'classical' approaches, splitting the translation part (8) is also relevant to rotoinversions. The location-dependent component allows for the location of all geometrical elements in a similar way. $\mathbf{w}_g$ relates the point on the rotation axis closest to the origin to the inversion point [see equation (11)]. Thus it is not necessary to solve the determinate equation $(\mathbf{W}, \mathbf{w})\mathbf{v}_{\rm Inv} = \mathbf{v}_{\rm Inv}$, where $\mathbf{v}_{\rm Inv}$ denotes the inversion point.

Table 4
The formulae for calculation of vector $\mathbf{v}_{\rm Shift}$ from component $\mathbf{w}_L$.

For simplicity, $\mathbf{w}_k$ stands for $\mathbf{w}_L + \mathbf{W}\mathbf{w}_L$.

Det(**W**)n	$\mathbf{v}_{\rm Shift}$
-1	$\mathbf{w}/2$
$2, -2$ (m)	$\mathbf{w}_L/2$
$3, -6$	$(\mathbf{w}_L + \mathbf{w}_k)/3$
-3	$\mathbf{W}\mathbf{w}_L$
$4, -4$	$\mathbf{w}_k/2$
6	$\mathbf{w}_k$

4.2. Existing approaches to GE fixing

As mentioned in all references, when dealing with symbols of symmetry operations, any particular solution of the indeterminate equation

$$\mathbf{W}\mathbf{x} + \mathbf{w}_L = \mathbf{x} \tag{9}$$

defines a point on the geometric element and thus fixes its location in space. A typical solution can be found by zeroing the free variable(s) and by solving the system (*e.g.* Fischer & Koch, 1983). Without additional conventions like C4, C5 (or C6 in the case of the non-standard setting of a space group), one can obtain two or three valid solutions. The selected solution used in standard operation symbols is called here *the standard location point* and denoted by $\mathbf{v}_{\rm Locat}(x_0, y_0, z_0)$.

Another method is the transformation of (9) to such a coordinate system that one of its basis vectors is parallel to the $\mathbf{v}_{\rm Axis}$. Then the new system is solved and the result is transformed back to the original system (Shmueli, 1984). This method is algorithmically complicated, especially in non-standard settings of space groups.

A general approach, avoiding the special treatment mentioned above, was proposed by Grosse-Kunstleve (1999). Equation (9) rearranged to the form $(\mathbf{I} - \mathbf{W})\mathbf{x} = \mathbf{w}_L$ gives the solution $\mathbf{v}_{\rm Shift} = \mathbf{x} = (\mathbf{I} - \mathbf{W})^{+}\mathbf{w}_L$, where $(\mathbf{I} - \mathbf{W})^{+}$ is the pseudoinverse of $(\mathbf{I} - \mathbf{W})$. In practice, calculation of $(\mathbf{I} - \mathbf{W})^{+}$ is not easy. The application of the matrix pseudoinverse gives a unique result which corresponds to the solution of determinate equation(s) in the subspace obtained by orthogonal projection of the original space (Stoer & Bulirsch, 1983).

4.3. New approach to the fixing problem

The projection concept together with the specific features of matrices $\mathbf{W}$ are used for construction of relations similar to equation $\mathbf{v}_{\rm Shift} = (\mathbf{I} - \mathbf{W})^{+}\mathbf{w}_L$.

First, the projection subspaces, *i.e.* the orthogonal complements of the GE subspaces are defined (Table 3).

Next, the general relation $\Pr(\mathbf{W}\mathbf{v}_{\rm Shift} + \mathbf{w}) = \mathbf{v}_{\rm Shift}$ is rewritten into the form of (9):

$$\Pr(\mathbf{W}\mathbf{v}_{\rm Shift}) + \mathbf{w}_L = \mathbf{v}_{\rm Shift}, \tag{10}$$

where Pr denotes the orthogonal projection according to Table 3. For considered projections, a necessary condition for $\mathbf{W}$ to be retained as symmetry operation in projection subspace (Hahn & Wondratschek, 1994) is fulfilled. Details

Table 5
Composition of the standard orientation-location part from the direction indices $\mathbf{v}_{\rm Axis}$ or ($\mathbf{v}_{\rm Trace1}$, $\mathbf{v}_{\rm Trace2}$) and the coordinates of the standard location point $\mathbf{v}_{\rm Locat}(x_0, y_0, z_0)$.

Orientation type	GE orientation and dummy variable(s) symbol(s)	x_0	y_0	z_0	Template of standard orientation-location part
0	–	s_1	s_2	s_3	x_0, y_0, z_0
1	$x\mathbf{v}_{\rm Axis}$	0	s_2	s_3	x, y_0, z_0
2	$y\mathbf{v}_{\rm Axis}$	s_1	0	s_3	x_0, y, z_0
3	$z\mathbf{v}_{\rm Axis}$	s_1	s_2	0	x_0, y_0, z
4	$y\mathbf{v}_{\rm Axis}$	s_1	$s_2 - s_3v/w$	0	$x_0, vy + y_0, wy$
5	$x\mathbf{v}_{\rm Axis}$	$s_1 - s_3u/w$	s_2	0	$ux + x_0, y_0, wx$
6	$x\mathbf{v}_{\rm Axis}$	0	$s_2 - s_1v/u$	s_3	$ux, vx + y_0, z_0$
7	$x\mathbf{v}_{\rm Axis}$	$s_1 - s_3u/w$	$s_2 - s_3v/w$	0	$ux + x_0, vx+ y_0, wx$
8	$y\mathbf{v}_{\rm Trace1} + z\mathbf{v}_{\rm Trace2}$	s_1	0	0	x_0, y, z
9	$z\mathbf{v}_{\rm Trace1} + x\mathbf{v}_{\rm Trace2}$	0	s_2	0	x, y_0, z
10	$x\mathbf{v}_{\rm Trace1} + y\mathbf{v}_{\rm Trace2}$	0	0	s_3	x, y, z_0
11	$x\mathbf{v}_{\rm Trace1} + y\mathbf{v}_{\rm Trace2}$	0	$s_2 - s_3q/r$	0	$x, qy + y_0, ry$
12	$y\mathbf{v}_{\rm Trace1} + x\mathbf{v}_{\rm Trace2}$	$s_1 - s_3p/r$	0	0	$px + x_r, y, rx$
13	$z\mathbf{v}_{\rm Trace1} + x\mathbf{v}_{\rm Trace2}$	$s_1 - s_2p/q$	0	0	$px + x_0, qx, z$
14	$x\mathbf{v}_{\rm Trace1} + z\mathbf{v}_{\rm Trace2}$	$s_1 - s_2m/n - s_3p/r$	0	0	$mx + pz + x_0, nx, rz$

concerning the geometry of projections were described by Buerger (1965).

In each subspace, there is only one point s_1, s_2, s_3 represented by the location vector $\mathbf{v}_{\rm Shift}$. It characterizes the shortest vector which starts at the coordinate-system origin and terminates at the GE. $\mathbf{v}_{\rm Shift}$ is unique with a precise geometric meaning and is characteristic for all geometric elements. Such a non-standard point is called *the unique location point*. Calculation of $\mathbf{v}_{\rm Shift}$ for a GE in the form of a plane or a point is trivial. For a GE in the form of a line, equation (10) also has an algebraic solution (Table 4). Projection of a rotation, rotoinversion or screw rotation corresponds to the rotation by the angle from the set $\pm 2\pi/k$ (k = 2, 3, 4, 6) around the rotation point on the projection plane. Translation $\mathbf{w}_L$ in conjunction with rotation shifts the rotation point from the origin to the invariant point $\mathbf{v}_{\rm Shift}$. For acceptable rotation angles of the symmetry operations, simple relations between $\mathbf{w}_L$ and $\mathbf{v}_{\rm Shift}$ exist and their corresponding formulae can be obtained in a geometric way (see Appendix *A*).

Thus every geometric element is fixed by its unique location point, the point closest to the origin. Such a point also occurs in some geometrical descriptions obtained by Shmueli. It frequently differs from the standard location point applied in standard descriptions.

In the case of rotoinversions [$n > 2$, det($\mathbf{W}$) = -1], the orientation-location part is followed by the specification of the inversion point $\mathbf{v}_{\rm Inv}$, which is directly related to $\mathbf{v}_{\rm Shift}$:

$$\mathbf{v}_{\rm Inv} = \mathbf{v}_{\rm Shift} + \mathbf{w}_g/2. \quad (11)$$

5. Standard orientation-location forms

5.1. Composing the standard symbol

In order to obtain standard description of an orientation-location part, the unique location vector must be transformed into the standard location vector. This is achieved by shifting the origin of the dummy variable(s) in (1). For example, in the case of a rotation axis, if the jth component of $\mathbf{v}_{\rm Locat}$ is zeroed then

$$\mathbf{v}_{\rm Locat}(i) = \mathbf{v}_{\rm Shift}(i) - \mathbf{v}_{\rm Shift}(j)/\mathbf{v}_{\rm Axis}(j)\mathbf{v}_{\rm Axis}(i), \quad \text{for } i = 1, 2, 3. \quad (12)$$

Derivation of $\mathbf{v}_{\rm Locat}$ for the planes is performed similarly. Transformation formulae for different orientation types of GE, corresponding to conventions C4, C5 and C6, have been derived.

In Table 5, standard forms of orientation-location parts, including the proposed symbol for a plane in general orientation, are compiled. The standard forms are composed of the orientation specification based on conventions C1, C2, C3 and of the coordinates of the standard location point. The transformation formulae $\mathbf{v}_{\rm Shift} \Rightarrow \mathbf{v}_{\rm Locat}$ are given in columns 3, 4 and 5 and depend on the orientation type of the geometric element.

The last column of Table 5 lists all the templates of standard orientation-rotation parts including the proposed one. The outlined algorithmic approach transforms any symmetry matrix automatically into the orientation-rotation part in accordance with one of the 15 templates. Formulae in columns 3, 4, 5 transform not only the unique location point s_1, s_2, s_3 but generally any point on the GE into the standard location point x_0, y_0, z_0.

5.2. Testing the orientation-location parts

The orientation-location part obtained by any derivation routine can be converted into the standard form, provided this part corresponds to (1). In the testing procedure, both orientation and location are checked independently. One or two direction indices are easily extracted from the orientation-location parts. Denoting the expressions in (1) by GE(t) and GE(t_1, t_2), [uvw] = GE(1) − GE(0) and [mno] = GE(1, 0) − GE(0, 0), [pqr] = GE(0, 1) − GE(0, 0). The evaluated indices should be consistent with C2 found in the NORM procedure.

In order to check or transform the location point s_1, s_2, s_3 into the standard location point x_0, y_0, z_0, the orientation type of a geometric element must be known. For a symmetry plane, the Miller-indices type is first derived from the pair of trace indices by look-up in Table 1. Next, the orientation type may be assigned to a given orientation-location part according to Table 2. In the standard symmetry-operation symbol, the location point s_1, s_2, s_3 should be mapped onto itself by the formulae selected from the columns 3, 4 and 5 of Table 5.

The following examples will illustrate the testing procedure.

Examples concerning the orientation:

(i) $x + 1/4, y, \bar{x}$ (S.G. 225, ITA83, 1995) $\rightarrow \mathbf{v}_{\rm Trace1} = (0, 1, 0)$, $\mathbf{v}_{\rm Trace2} = (1, 0, -1) \rightarrow {\rm NORM}(\mathbf{v}_{\rm Trace1}) = [010], {\rm NORM}(\mathbf{v}_{\rm Trace2}) = [\bar{1}01] \rightarrow \bar{x} + 1/4, y, x$ (ITA83, 2002).

(ii) $\bar{x} + 1/2, y, x$ (S.G. 225, ITA83, 1995) $\rightarrow \mathbf{v}_{\rm Trace1} = (0, 1, 0)$, $\mathbf{v}_{\rm Trace2} = (-1, 0, 1) \rightarrow {\rm NORM}(\mathbf{v}_{\rm Trace1}) = [010], {\rm NORM}(\mathbf{v}_{\rm Trace2}) = [\bar{1}01] \rightarrow \bar{x} + 1/2, y, x$ (ITA83, 2002).

(iii) $-x, x - 1/6, x$ (S.G. not given, Grosse-Kunstleve, 1999) $\rightarrow \mathbf{v}_{\rm Axis} = (\bar{1}, 1, 1) \rightarrow {\rm Norm}(\mathbf{v}_{\rm Axis}) = [uvw] = [1\bar{1}\bar{1}] \rightarrow x, \bar{x} - 1/6, \bar{x}$ (in ITA83 style).

Examples concerning the location:

(iv) $x, 2x - 1/2, z$ (S.G. 160, ITA83, 1995) $\rightarrow [mno] = [001]$, $[pqr] = [120] \rightarrow$ Orient. type = 13; $s_1, s_2, s_3 = 0, -1/2, 0 \rightarrow x_0, y_0, z_0 = 1/4, 0, 0$ and $x + 1/4, 2x, z$ (ITA83, 2002).

(v) $-1/6 - x, 1/3 - x, 1/6 + x$ (S.G. 205, Shmueli, 1984) $\rightarrow [uvw] = [\bar{1}\bar{1}1] \rightarrow$ Orient. type = 7; $s_1, s_2, s_3 = -1/6, 1/3, 1/6 \rightarrow x_0, y_0, z_0 = 0, 1/2, 0$ and $\bar{x}, \bar{x} + 1/2, x$ (ITA83, 2002).

As far as the first three examples are concerned, only the second item adheres to the C2 convention. It is worth recalling that change in the sense of the rotation axis vector [see example (iii)] involves the change in the sense of rotation and finally changes the signs '+' or '−' found in the operation-type specification.

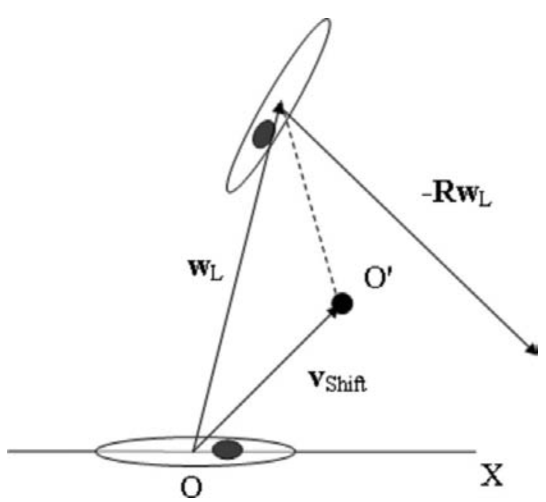

Figure 2
Two-dimensional model of space transformation on the projection plane, orthogonal to the GE of symmetry operation ($\bar{6}$, $\mathbf{w}_{g+}\mathbf{w}_L$). The location part $\mathbf{w}_L$ shifts the rotation point from the origin O to the invariant point O'. Rotations are defined with reference to line OX.

6. Metric tensor

The metric properties of crystal space do not influence the derivation of the operation symbols. However, a given symbol can be obtained from different matrices (*e.g.* $\bar{x}, y, \bar{z}$ in the cubic system or $\bar{x}, \bar{x} + y, \bar{z}$ in the hexagonal system $\rightarrow$ 2 $0, y, 0$), and thus the reverse transformation[3] would require coordinate system data to be specified. By including the metric tensor into the calculation system, the symmetry matrices and operation symbols can be mutually transformed and finally it is possible to compose symmetry operations given in the geometric descriptions.

In all cited references, the metric properties were not used for calculations. They are also not necessary in the presented approach but allow for an elegant calculation of both Miller indices and the indices of plane traces. We may use another method based on the fact that the columns of the matrix $\mathbf{I} + \mathbf{W}$ define two linearly independent vectors parallel to the plane. By their linear combination, the pair of trace indices can be obtained. This way is algorithmically more cumbersome in comparison with the described one.

The Miller indices (hkl) obtained from $\mathbf{v}_{\rm Axis}$, by equations (5) and (6) depend only on the structure of the metric tensor and not on the particular numerical values of its elements. Hence, for practical calculations, the default metric tensors can be used (one predefined metric tensor per crystallographic axis system). Evidently, in the non-standard space-group description, the default metric tensor must be transformed in accordance with the coordinate-axis system change.

7. Conclusions

Orientation of a geometric element is uniquely determined by direction indices (for a rotation axis) or a pair of trace indices (for a symmetry plane), provided the convention on the positive direction in space is defined. Only for a plane in general orientation where three different traces exist is the pair selected according to the new convention.

The unique point on any geometric element closest to the origin fixes this element in space. However, a standard operation symbol represents the standard location point, *viz* the intersection point of the corresponding geometric element with the basal plane or with the system axis. Generally, there are one, two or three such points; the ambiguity is avoided by special conventions.

Classification of geometric element orientations allows us to define the explicit equations for transformation of any point on a geometric element into the standard one (used in ITA83). Thus, the description of the fixing point does not depend on the derivation algorithm.

The proposed approach for derivation of orientation and location of geometric elements uses only simple vector/matrix manipulations and no special procedures (like row echelon form, Gauss reduction procedure, matrix inversion or axis system rotation) are required. The method is algorithmically

[3] The general method of matrix form derivation from the symbols for symmetry operations is not considered here.

simple, relatively compact and applicable to symmetry operations described both in standard and in non-standard settings of space groups.

APPENDIX *A*
Derivation of vector $\mathbf{v}_{\rm Shift}$ for sixfold rotoinversion

Suppose that the matrix pair $(\mathbf{W},\mathbf{w})$ corresponds to the sixfold rotoinversion $\bar{6}^{+}$ with the proper rotation matrix $\mathbf{R} = -\mathbf{W}$ and location part $\mathbf{w}_L$. The original points on the projection plane in the vicinity of O are plotted in the form of a disc with the solid object in it (Fig. 2).

Projection of the transformed points maps this disc onto the copy, rotated by an angle of 240° (360°/6 + 180°) and translated by $\mathbf{w}_L$. Three points, the origin O and ends of the vectors $\mathbf{w}_L$, $\mathbf{w}_L - \mathbf{R}\mathbf{w}_L$, form an equilateral triangle with O' as its centre. Rotation by an angle of −120° about this point gives the same two-dimensional mappings. Trigonometric manipulation yields $\mathbf{v}_{\rm shift} = 1/3(2\mathbf{w}_L - \mathbf{R}\mathbf{w}_L)$ or $1/3(2\mathbf{w}_L + \mathbf{W}\mathbf{w}_L)$. Similar simple relations exist for other types of crystallographic symmetry operations.

APPENDIX *B*
Glide reflection by a plane in a general orientation – a comparative study

Consider the operation $(0, 1/2, 1/2) + (46)$ of the group $Fd\bar{3}c$ (origin choice 1) described as the coordinate triplet $\bar{z} + 1/2, y + 1/2, \bar{x} + 1/2$ or symbolized by $b\ \bar{x} + 1/2, y, x$. When referred to the primitive basis, the coordinate triplet takes the following form:

$$x + 1/2, \bar{x} - y - z + 1/2, z + 1/2$$
$$\Rightarrow \mathbf{W} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{w} = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}.$$

First the type of the transformed operation is identified by calculating the trace and the determinant of $\mathbf{W}$. In this case, $\mathrm{tr}(\mathbf{W}) = 1$, $\det(\mathbf{W}) = -1$ and the operation corresponds to a reflection or a glide reflection. Next the order of the matrix $\mathbf{R}$ is determined ($n = 2$) and the translation vector $\mathbf{w}$ is decomposed into $\mathbf{w}_g = (1/2, -1/2, 1/2)$ and $\mathbf{w}_L = (0, 1, 0)$. Finally, the orientation-location part is derived by two different methods.

B1. The classical approach

The orientation-location part follows from the equation system

$$(\mathbf{W}, \mathbf{w}_L)\mathbf{x} = \mathbf{x} \Rightarrow \begin{pmatrix} 1 & 0 & 0 \\ -1 & -1 & -1 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

The possible solution, $x = -2y - z + 1$ with undetermined y and z, can be rewritten as the coordinate triplet $-2y - z + 1, y, z$. By changing the dummy variable from y to $\bar{x}$, the full symbol of the glide reflection takes the form $g(1/2, -1/2, 1/2)\ 2x - z + 1, \bar{x}, z$ as intended by C6. Generally, the above equations are easy to define but it is rather difficult, like in this case, to formalize their standard solutions.

B2. The algorithmic approach

If one chooses the identity matrix $\mathbf{I}$ as the default metric tensor $\mathbf{M}$ for the cubic system then the lattice transformation $F \rightarrow P$ gives $M_{ij} = 0.25$ for $i \neq j$ and $M_{ij} = 0.5$ for $i = j$. Any scaled column of the matrix $\mathbf{S} = \mathbf{I} - \mathbf{W}$ leads to $\mathbf{v}_{\rm Axis} = [010]$. This vector transformed to the reciprocal space

$$\begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/4 & 1/2 & 1/4 \\ 1/4 & 1/4 & 1/2 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1/4 \\ 1/2 \\ 1/4 \end{pmatrix}$$

and then normalized gives the Miller indices $\mathbf{v}_{\rm Plane} = (121)$. Hence the corresponding traces are $\mathbf{v}_{\rm Trace1} = [2\bar{1}0]$ and $\mathbf{v}_{\rm Trace2} = [\bar{1}01]$ (orientation type = 14, see Table 1). According to Table 4, the relation $\mathbf{v}_{\rm Shift} = \mathbf{w}_L/2$ determines the point $(0, \frac{1}{2}, 0)$ on the plane. The transformations $x_0 = s_1 - s_2 m/n - s_3 p/r$, $y_0 = 0$ and $z_0 = 0$ (the last row in Table 5) give the following solutions: $x_0 = 0 - 0.5 \times 2/(-1) - 0(-1)/1 = 1$, $y_0 = 0$ and $z_0 = 0$. Thus, the unique location point $(0, \frac{1}{2}, 0)$ is converted into the standard location point $(1, 0, 0)$, *i.e.* the intersection of the symmetry plane with the axis Ox.

Therefore the orientation-location part takes the form $x[2\bar{1}0] + z[\bar{1}01] + 1, 0, 0 = 2x - z + 1, \bar{x}, z$ proposed for description of planes in general orientation. Finally, the operation symbol is $g(1/2, -1/2, 1/2)\ 2x - z + 1, \bar{x}, z$.

APPENDIX *C*
Examples for the derivation of the orientation-location part

C1. Example 1. Glide reflection by a plane parallel to two crystal axes

The operation $(0, 1/2, 1/2) + (4)$ of the group $C2/c$ (unique axis c, cell choice 1) is described as the coordinate triplet $x + 1/2, y + 1/2, \bar{z} + 1/2$. The type of the operation is $\mathrm{tr}(\mathbf{W}) = 1$, $\det(\mathbf{W}) = -1 \Rightarrow$ reflection or glide reflection, $n = 2$. For the order $n = 2$, equation (2) gives the matrix $\mathbf{S} = (\mathbf{I} + \mathbf{R})$. Recalling that $\mathbf{R} = \det(\mathbf{W})\mathbf{W}$, one can obtain

$$\mathbf{S} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

with two zero columns. Hence, $\mathbf{v}_{\rm Axis} = \mathrm{NORM}(\mathbf{S}_{*3}) = [001]$.

The metric tensor and its possible numerical representation for the selected setting of the monoclinic group are the following:

$$\mathbf{M} = \begin{pmatrix} a^2 & ab\cos\gamma & 0 \\ ab\cos\gamma & b^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix} = \begin{pmatrix} 0.7 & -0.2 & 0 \\ -0.2 & 1 & 0 \\ 0 & 0 & 0.9 \end{pmatrix}.$$

According to equation (3), the normalized results of the multiplication $\mathbf{M}\mathbf{v}_{\rm Axis}$ determine the Miller indices of the symmetry plane $(hkl) = (001)$. The orientation type 10 corresponds to the pair of traces $\mathbf{v}_{\rm Trace1} = [100]$ and $\mathbf{v}_{\rm Trace2} = [010]$.

As was earlier explained, in the case of planes the splitting formulae given in (8) should be interchanged. Hence the location dependent part $\mathbf{w}_L = \mathbf{S}\mathbf{w}/2 = (0, 0, 1/2)$, and $\mathbf{w}_g = \mathbf{w} - \mathbf{w}_L = (1/2, 1/2, 0)$. According to Table 4, the plane is fixed by the point closest to the origin, $\mathbf{v}_{\rm Shift} = \mathbf{w}_L/2 = (0, 0, 1/4)$. This is also the standard location point, $\mathbf{v}_{\rm Locat} = \mathbf{v}_{\rm Shift}$. Therefore, the orientation-location part takes the form $x[100] + y[010] + (0, 0, 1/4) = x, y, \frac{1}{4}$, consistent with the appropriate template in the last column of Table 5. The derived result corresponds to the operation symbol $n(1/2, 1/2, 0) = x, y, \frac{1}{4}$ printed in ITA83.

C2. Example 2. Rotoinversion operation

The operation $(0, 0, 0) + (18)$ of the group $Fd\bar{3}$ (origin choice 1) has the following coordinate triplet representation: $\bar{z} + 1/4,\ x + 1/4,\ y + 1/4$. Its type is identified as threefold rotoinversion, according to $\mathrm{tr}(\mathbf{W}) = 0$ and $\det(\mathbf{W}) = -1$. In this case, the proper rotation matrix $\mathbf{R} = -\mathbf{W}$ and its order $n = 3$. From equation (2), the matrix $\mathbf{S}$ is given as the expression $\mathbf{I} + \mathbf{R} + \mathbf{R}^2$:

$$\mathbf{S} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix}.$$

Any column of $\mathbf{S}$ after normalization uniquely characterizes the axis direction $\mathbf{v}_{\rm Axis} = [uvw] = [\bar{1}1\bar{1}]$ and the orientation type 7. $\mathbf{w}_g = \mathbf{S}\mathbf{w}/3 = (1/12, -1/12, 1/12)$ and $\mathbf{w}_L = (1/6, 1/3, 1/6)$. According to Table 4, the unique location point $\mathbf{v}_{\rm Shift}(s_1, s_2, s_3)$ is determined by formula $\mathbf{W}\mathbf{w}_L = (-1/6, 1/6, 1/3)$. This point can be converted into the standard location point by equations found in Table 5, appropriate for the orientation type:

$$x_0 = s_1 - s_3 u/w = -1/6 - (1/3)(-1)/(-1) = -1/2$$
$$y_0 = s_2 - s_3 v/w = 1/6 - (1/3)(1)/(-1) = 1/2$$
$$z_0 = 0.$$

The orientation-location part is defined by the expression $x[-1, 1, -1] + (-\frac{1}{2}, \frac{1}{2}, 0)$ and takes the form $\bar{x} - \frac{1}{2},\ x + \frac{1}{2},\ \bar{x}$. The inversion point is calculated from equation (11): $\mathbf{v}_{\rm Inv} = \mathbf{v}_{\rm Shift} + \mathbf{w}_g/2 = (-1/6, 1/6, 1/3) + (1/24, -1/24, 1/24) = (-1/8, 1/8, 3/8)$. Both results are consistent with the standard operation symbol $\bar{3}^{+}\ \bar{x} - \frac{1}{2}, x + \frac{1}{2}, \bar{x}; -1/8, 1/8, 3/8$.

To make this example complete, the sense of the rotoinversion is determined. There are two commonly used procedures given by Fischer & Koch (1983) and Boisen & Gibbs (1990). The latter method is more practical. It uses the quantities $\mathbf{v}_{\rm Axis} = [uvw]$ and $\mathbf{R}$. The sense of rotation is positive if one of the following conditions is true: (i) $v = w = 0$ and $uR_{32} > 0$ or (ii) $R_{21}w - R_{31}v > 0$. In our example, condition (ii) is fulfilled: $(-1)(-1) - (0)(1) = 1 > 0$. The positive sense of rotation is indicated by the superscript '+' in the full operation symbol.

The author wishes to thank the referees for reading and revising the first and second versions of the submitted manuscript. Their remarks, critical comments and suggestions have stimulated the author to reconstruct the whole article and to clarify the presented ideas.

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