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Space of symmetry matrices with elements 0, ±1 and complete geometric description; its properties and application

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A *fixed set*, that is the set of all lattice metrics corresponding to the arithmetic holohedry of a primitive lattice, is a natural tool for keeping track of the symmetry changes that may occur in a deformable lattice [Ericksen (1979). *Arch. Rat. Mech. Anal.* **72**, 1–13; Michel (1995). *Symmetry and Structural Properties of Condensed Matter*, edited by T. Lulek, W. Florek & S. Walcerz. Singapore: Academic Press; Pitteri & Zanzotto (1996). *Acta Cryst.* A**52**, 830–838; and references quoted therein]. For practical applications it is desirable to limit the infinite number of arithmetic holohedries, and simplify their classification and construction of the fixed sets. A space of 480 matrices with cyclic consecutive powers, determinant 1, elements from {0, ±1} and geometric description were analyzed and offered as the framework for dealing with the symmetry of reduced lattices. This matrix space covers all arithmetic holohedries of primitive lattice descriptions related to the three shortest lattice translations in direct or reciprocal spaces, and corresponds to the unique list of 39 fixed points with integer coordinates in six-dimensional space of lattice metrics. Matrices are presented by the introduced *dual symbol*, which sheds some light on the lattice and its symmetry-related properties, without further digging into matrices. By the orthogonal lattice distortion the lattice group–subgroup relations are easily predicted. It was proven and exemplified that new symbols enable classification of lattice groups on an absolute basis, without metric considerations. In contrast to long established but sophisticated methods for assessing the metric symmetry of a lattice, simple filtering of the symmetry operations from the predefined set is proposed. It is concluded that the space of symmetry matrices with elements from {0, ±1} is the natural environment of lattice symmetries related to the reduced cells and that complete geometric characterization of matrices in the arithmetic holohedry provides a useful tool for solving practical lattice-related problems, especially in the context of lattice deformation.

1. Introduction

The 14 Bravais types of three-dimensional lattices based both on the *geometric holohedry* (seven crystal systems) and the centring mode can be distinguished by the topological, metrical or symmetry properties of the lattices. The approach presented here originates from the fact that small variations in input lattice dimensions may lead, under special circumstances, to a discontinous change in referring the lattice descriptions to the privileged primitive bases. In the symmetry approach, a lattice type is defined as the class of all primitive lattices whose lattice groups (*arithmetic holohedries*) are conjugated within the 'global symmetry group' $GL(3, \mathbb{Z})$, the infinite group of invertible 3×3 matrices with integral entries. Collecting the symmetry matrices with elements from {0, ±1} into one set and changing the abstract form of the symmetry operation into a complete geometric description is a profitable task since it provides a conceptual and practical framework for easier study of the 'arithmetic symmetry' of deformable crystals, *i.e.* the derivation of a lattice group, its classification, analysis of the group–subgroup context, selecting centred conventional cell *etc*.

Determination of matrices relating any primitive cell of the lattice to itself is not an algorithmic process and consists of searching potential solutions to see whether they represent the isometric transformation for a given lattice metric.[1] The

[1] Finding the arithmetic holohedry is similar to the solution of *diophanthine* systems (Le Page, 2002). For instance, the Pitagoras (integer) numbers which satisfy the equation $a^2 + b^2 = c^2$ cannot be obtained algorithmically.

Table 1
Hierarchical subsets of matrices with cyclic consecutive powers (symmetry matrices): $GL(3, \mathbb{Z}) \supset \boldsymbol{U} \supset \boldsymbol{V} \supset \boldsymbol{W}$.

	Matrices	Maximal groups	Matrix elements	Mapped basis vectors	Cell kind	Holohedry
$\boldsymbol{U}$	∞	∞	Integer	Lattice vectors	Any primitive cell	Arithmetric
$\boldsymbol{V}$	960†	39	0, ±1 (3–7)‡	Cell vectors	(Reduced) Buerger cell	Arithmetric
$\boldsymbol{W}$	64	2	0, ±1 (3, 4)‡	Basis vectors§	(Centred) Bravais cell	Geometric

† In applications only 480 matrices with det = 1 are needed. ‡ Number of non-zero elements. § In the hexagonal system $-(\boldsymbol{a} + \boldsymbol{b})$ is treated as the fourth basis vector.

practical procedures of lattice group derivation [by *B* matrices in Santoro & Mighell (1970), Mighell*et al.* (1981) and Himes & Mighell (1987) or by space distribution of twofold operations in the geometric approach (Le Page, 1982)] are in fact tests of some matrices from $GL(3, \mathbb{Z})$. The number of possible lattice bases and thus the arithmetic holohedries is infinite, but privileged bases in crystallography significantly reduce the variety of symmetry matrices and generally limit their elements to values of 0, ±1. The *Buerger cell* is defined as that based upon the three shortest non-coplanar translations of the lattice (Buerger, 1957). In a number of cases further restrictive rules have to be applied for a unique choice – the *Niggli cell* (Niggli, 1928). The three shortest vectors in the Delaunay reduction $|\boldsymbol{a}|^2 + |\boldsymbol{b}|^2 + |\boldsymbol{c}|^2 + |\boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c}|^2 = min$ lead to the *Delaunay cell*. Recently, Lebedev *et al.* (2006) introduced the idea of combinatorial generation of all 3 × 3 matrices with elements in {−1, 0, 1}, finite order with respect to the matrix multiplication and with the determinant equal to 1. They claimed that the resulting set of 504 matrices covers all possible isometries of the Buerger or Niggli reduced cells. A similar, but reduced in number, set of 480 elements was constructed by Zwart *et al.* (2006) to find all the possible orientations of dyads in Buerger-restricted cells. Despite rather intuitive arguments, both applications gave useful ranges for algebraic or geometric descriptions of arithmetic holohedries in the reduced cells. The finiteness of the symmetry operation set also implies limits on the number of maximal groups and their *fixed sets*, where the latter term means all lattices described in the six-dimensional space $C^+(Q_3)$[2] of lattice metrics and which are compatible with a given lattice group [see Pitteri & Zanzotto (1996) for an introduction to these ideas].

Generally, the conjugacy between lattice groups cannot be found in the set of symmetry operations (it does not contain shear operations) and a geometric criterion is needed for arithmetic holohedry classification. The following remark is essential regarding this point. While the classical operation symbol (Fischer & Koch, 1983) was designed for the symmetry matrices related to Bravais-centred cells and it contains information limited to one direction ($\boldsymbol{u}$ for rotations and rotoinversions or $\boldsymbol{h}$ for reflections; Stróż, 2007), in the primitive cells the scalar product $\boldsymbol{u} \cdot \boldsymbol{h}$ explicitly gives information on lattice centring in the $\boldsymbol{u}$ direction (Le Page, 1982) and thus both directions are needed for determination of a lattice group type.

In this paper the *space* $\boldsymbol{V}$ of 480 symmetry matrices with elements 0, ±1 is proposed as an 'analogue to some extent' of $GL(3, \mathbb{Z})$ in considerations involving the symmetry of reduced lattices. A simple lattice metric filter over $\boldsymbol{V}$ may be used as a practical method for totally branching free determinations of arithmetic holohedries. The central focus of the method described herein is on the application of geometric information extracted from the matrices rather than on using the matrices themselves. The geometric data contained in a new symbol are based on the concept of lattice orthogonal splitting caused by a symmetry operation (see, for example, Fuksa & Engel, 1994), which takes into account both invariant directions $\boldsymbol{u}$ and $\boldsymbol{h}$, and corresponds to complete specification of the symmetry matrix eigenvectors. Based on dual symbols one can predict which symmetry matrices in $\boldsymbol{V}$ are not compatible with the Buerger-reduced bases, classify lattice groups without conjugacy tests in the infinite $GL(3, \mathbb{Z})$ or construct the transformation from the primitive to the Bravais cell and in consequence assign the cell type to any lattice group in $\boldsymbol{V}$. The pairs of mutually reciprocal lattice bases in which holohedries are maximal groups and exhaust symmetry matrices in $\boldsymbol{V}$ were determined. At least one cell in each pair is based on the shortest lattice vectors. This defines the criterion for a given metric tensor to represent a lattice whose holohedry comprises $\boldsymbol{V}$. The lattice group–subgroup relations can be analyzed by orthogonal lattice distortion. Examples included in the text show that the space $\boldsymbol{V}$ with well defined internal structure can be effectively used to solve practical lattice-related problems.

2. The reduced lattice holohedries and space *V* of matrices with elements 0, ±1

It is well known that conventional space-group descriptions in *International Tables for Crystallography*, Vol. A (*ITA*), are based on Bravais cells and *geometric holohedries*. Thus, the $\boldsymbol{W}$ set of all point operations is limited to 64 matrices, compiled and characterized by geometric symbols in the 1983 edition of *ITA* (Tables 11.2 and 11.3). The 48 orthogonal matrices covered by $m\bar{3}m$ transform basis vectors into basis vectors and the same is done by 16 additional matrices covered by 6/*mmm*, if $-(\boldsymbol{a} + \boldsymbol{b})$ is also considered as a basis vector.

In the case of any primitive lattice descriptions and *arithmetic holohedries*, symmetry operations transform the basis vector into any lattice vector so the $\boldsymbol{U}$ set of all the potential symmetry matrices is infinite. This implies many problems with practical considerations based on the lattice symmetry referred to a primitive description.

The concept of emphasizing *reduced-lattice holohedries*, *i.e.* symmetry lattice descriptions by symmetry matrices with elements 0, ±1, as a special case of the arithmetic holohedries

[2] Following the notation of Michel (1995), the space of all symmetric 3 × 3 positive-definite matrices is denoted by $C^+(Q_3)$. The lattice metric tensors $\boldsymbol{M}$ belong to this space. This guarantees that for any vector $\boldsymbol{x} \neq \boldsymbol{0}$, $\boldsymbol{x}^T\boldsymbol{M}\boldsymbol{x} > 0$.

Table 2
Reduced-form tensors of the highest-symmetry primitive cells whose holohedries are maximal groups in $\boldsymbol{V}$.

Tensors are scaled to the minimal integer values. Settings of the same lattice are distinguished by the sequence number added to the lattice symbol. Tensors of non-Buerger cells are given in bold.

Direct space		Reciprocal space		Direct space		Reciprocal space	
Lattice	Reduced form	Lattice	Reduced form	Lattice	Reduced form	Lattice	Reduced form
*cP*1	1, 1, 1, 0, 0, 0			*cF*7	2, 2, 2, 0, −1, −1	***cI*7**	**4, 3, 3, 1, 2, 2**
*hP*1	2, 2, 1, 0, 0, −1	*hP*4	2, 2, 1, 0, 0, 1	*cF*8	2, 2, 2, 1, 1, 0	***cI*8**	**3, 3, 4, −2, −2, 1**
*hP*2	2, 1, 2, 0, −1, 0	*hP*5	2, 1, 2, 0, 1, 0	*cF*9	2, 2, 2, 1, 0, 1	***cI*9**	**3, 4, 3, −2, 1, −2**
*hP*3	1, 2, 2, −1, 0, 0	*hP*6	1, 2, 2, 1, 0, 0	*cF*10	2, 2, 2, 0, 1, 1	***cI*10**	**4, 3, 3, 1, −2, −2**
*cF*1	2, 2, 2, 1, 1, 1	*cI*1	3, 3, 3, −1, −1, −1	*cF*11	2, 2, 2, 1, −1, 0	***cI*11**	**3, 3, 4, −2, 2, −1**
*cF*2	2, 2, 2, −1, −1, 1	*cI*2	3, 3, 3, 1, 1, −1	*cF*12	2, 2, 2, 1, 0, −1	***cI*12**	**3, 4, 3, −2, −1, 2**
*cF*3	2, 2, 2, −1, 1, −1	*cI*3	3, 3, 3, 1, −1, 1	*cF*13	2, 2, 2, 0, 1, −1	***cI*13**	**4, 3, 3, −1, −2, 2**
*cF*4	2, 2, 2, 1, −1, −1	*cI*4	3, 3, 3, −1, 1, 1	*cF*14	2, 2, 2, −1, 1, 0	***cI*14**	**3, 3, 4, 2, −2, −1**
*cF*5	2, 2, 2, −1, −1, 0	***cI*5**	**3, 3, 4, 2, 2, 1**	*cF*15	2, 2, 2, −1, 0, 1	***cI*15**	**3, 4, 3, 2, −1, −2**
*cF*6	2, 2, 2, −1, 0, −1	***cI*6**	**3, 4, 3, 2, 1, 2**	*cF*16	2, 2, 2, 0, −1, 1	***cI*16**	**4, 3, 3, −1, 2, −2**

(Table 1), originates from the practical advances of such an approach (the finite number of symmetry matrices) and natural interpretation of the 'reduced' matrices. Matrices with elements 0, ±1 transform basis vectors into cell vectors, *i.e.* the cell edges, face or body diagonals, and are intuitively assigned to lattice descriptions based on the shortest lattice translations (Buerger-reduced cells). $\boldsymbol{V}$ proves useful in the analysis based on arithmetic holohedries, especially if all the maximal groups and their 'fixed sets' will be determined.

Space $\boldsymbol{V}$ can be dynamically obtained by:

(i) filtering of all combinations of −1, 0, 1 in a 3 × 3 array $\boldsymbol{v}$ [restrictions: 3 ≤ number of non-zero elements ≤ 7, $\det(\boldsymbol{v}) = 1$, elements of $\boldsymbol{v}^n \in \{-1, 0, 1\}$ for $n < 6$],

(ii) selecting a few generators and duplicating them by raising to the power n ($n < 6$), transposing and transforming by the orthogonal transformations.

Both approaches are not very effective, but once generated matrices are easily replaceable by single natural numbers (*Appendix A*), stored, retrieved and decoded on demand.

3. Maximal groups

It is clear that maximal groups are holohedries of the highest-symmetry lattices, but in contrast to the subset $\boldsymbol{W}$ already mentioned, the holohedries in $\boldsymbol{V}$ should form complete (orthogonal) conjugacy classes and be paired by transposition if different. The groups distinguished by transposition relate to pseudo-inverse lattices (Grimmer, 2003): (*cF*, *cI*) or (*hP* with 120°, *hP* with 60°), while the holohedry of *cP* is single. In the *cF* lattice there are two Buerger cells (Gruber, 1973). Orthogonal transformation leads to one lattice setting of *cP*, three of *hP* (if 120° is demanded), four and 12 variants of the corresponding two Buerger cells in *cF*. Together with pseudo-reciprocal lattice settings this gives 39 maximal groups in $\boldsymbol{V}$, denoted by the corresponding metric tensor and symbolized by the indexed lattice symbols (Table 2). Each matrix $\boldsymbol{v} \in \boldsymbol{V}$ occurs at least in one of these maximal groups, so $\boldsymbol{V}$ is covered by the enumerated holohedries. The list obtained is also minimal, since each group contains some matrices occurring exclusively in it.

Lemma 1. The combinatorial space $\boldsymbol{V}$ of matrices with cyclic consecutive powers and elements from {0, ±1} is covered by its 39 maximal groups (six orthogonal conjugacy classes), also represented as unique points with the smallest integer coordinates in the six-dimensional space $C^+(Q_3)$ of lattice metrics.

Some comments on the compiled data seem to be interesting:

(i) The contents of Table 2 are unique up to the numbering of the settings.

(ii) The symmetry of *cP*1 and *hP*1 lattices covers all point operations in the conventional space-group descriptions (*e.g.* in *ITA*).

(iii) The elements in $\boldsymbol{V}$ can be grouped into complete orthogonal conjugacy classes.

(iv) The maximal groups in $\boldsymbol{V}$ also form full conjugacy classes: *cP*1, *hP*1–*hP*6, *cF*1–*cF*4, *cF*5–*cF*16, *cI*1–*cI*4, *cI*5–*cI*16.

(v) Since the *cI* lattice is characterized by a single Buerger cell (Gruber, 1973), some *cI* settings (*cI*5–*cI*16, in bold) represent the non-Buerger cell.

Matrices in $\boldsymbol{V}$, which only occur in the holohedries of these settings, are not consistent with the symmetry of any Buerger-reduced cell. These matrices correspond to threefold operations along axes orthogonal to {123} or {112} planes. It is easy to prove by a geometric construction (*Appendix B*) that they need non-Buerger lattice descriptions.

The above consideration and maximality of compiled holohedries leads to the following lemma:

Lemma 2 (criterion for the description of a lattice symmetry in $\boldsymbol{V}$*)*. A lattice referred to its three shortest non-coplanar translations or a lattice which in reciprocal space is defined by the three shortest non-coplanar vectors has symmetry matrices that belong to $\boldsymbol{V}$. The subset $\boldsymbol{V}'$, without matrices representing threefold operations along axes orthogonal to {123} or {112}, covers the symmetry operations of any lattice related to the Buerger-reduced cell in a given space.

4. Geometric interpretation of matrices

It is well known (see, for example, Fuksa & Engel, 1994) that any proper rotation (excluding the identity operation) or its cyclic group orthogonally splits the lattice[3] into one-dimensional and two-dimensional sublattices given by the lattice row [*uvw*] and the lattice plane (*hkl*).

The sum $\sum_{i=1}^{n} v^i$ of the cyclic group elements generated by $\boldsymbol{v} \in \boldsymbol{V}$, $\det(\boldsymbol{v}) = 1$, $\boldsymbol{v}^n = \boldsymbol{I}$ (identity operation) can be presented by the matrix form

[3] As was kindly commented by the referee, this property was discovered by Euler in 1775.

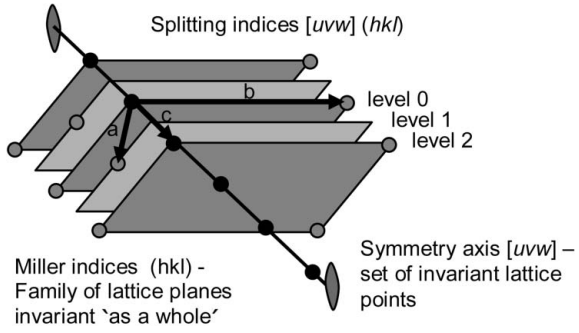

Figure 1
Geometric information contained in a splitting index [*uvw*](*hkl*). The symbol [001](102) means that the symmetry axis is parallel to ***c*** and orthogonal to the planes (102). The basis vectors ***a***, ***b***, ***c*** end on lattice points on the 0, 1, 2 level of the (102) family planes. In this case the lattice is *b*-centred.

$$\frac{n}{uh+vk+wl}\begin{pmatrix} u \\ v \\ w \end{pmatrix}\cdot(hkl), \tag{1}$$

or equivalently given by the expression

$$n[uvw](hkl), \tag{2}$$

since information contained in the denominator in equation (1) is redundant.

Equation (2) has an interesting geometric interpretation (Fig. 1). The first triplet in square brackets [*uvw*] characterizes the row of invariant lattice points (direction ***u*** in direct space) and the second triplet in round brackets (*hkl*) defines the normal (direction ***h*** in the reciprocal space) to the 'invariant as a whole' lattice planes under *n*-fold rotation. The coprime indices written side by side as [*uvw*](*hkl*) are considered here as (*lattice orthogonal*) *splitting indices* of the symmetry operation ***v*** and its cyclic group. The directions in splitting indices are unique up to a sign.

The convention for sign selection cannot be based on one direction only, since the triplets [*uvw*] and (*hkl*) replace each other if the symmetry of reciprocal lattice is considered. This problem can be overcome by the following procedure:

(i) from the [*uvw*], (*hkl*) pair select the one with indices 0, ±1 and the greater number of zeros,

(ii) if the chosen triplet does not describe the positive direction (Stróż, 2007, convention C2), change the signs in the two sets of indices.

If the sign of rotation is of interest it can be derived by standard methods (*e.g.* Fischer & Koch, 1983) and included in expression (2) between the axis symbol and the splitting indices, forming the *dual operation symbol*, the complete geometric description of a point operation ***v***.

The dual symbols integrate information contained separately in two classical symbols of a symmetry matrix and its transposition and thus bring to light more lattice properties:

(i) Centring of a lattice in the axis direction ***u***. If ***uh*** = 2 or 3 then the axis encounters the lattice points on every second or third plane of the family planes ***h***.

(ii) Matrices ***v*** and $(\boldsymbol{v}^T)^{-1}$ describe the same symmetry operation as those considered in pseudo-inversion lattices. This is reflected in dual symbols, *e.g.* $4^+[\bar{1}11](011)$ and $4^-[011](\bar{1}11)$, deeply hidden in coordinate triplet notation $\bar{y}, x+y+z, \bar{x}$ and $y-z, \bar{x}+y, y$, and lost in standard symbols $4^-\, x, \bar{x}, \bar{x}$ and $4^-\, 0, y, y$.

(iii) In the case of twofold rotation, the symmetry matrix can be reconstructed from the symbol

$$\boldsymbol{v} = 2/(\boldsymbol{u}\cdot\boldsymbol{h})\cdot\begin{pmatrix} uh & uk & ul \\ vh & vk & vl \\ wh & wk & wl \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3}$$

(iv) If $\boldsymbol{g}^{-1}\boldsymbol{v}_1\boldsymbol{g} = \boldsymbol{v}_2$, *i.e.* the symmetry matrix $\boldsymbol{v}_1$ is conjugated to $\boldsymbol{v}_2$ by an element $g \in GL(3, \mathbb{Z})$, then the corresponding splitting indices are similarly related,

$$\boldsymbol{g}^{-1}\,[u_1v_1w_1]\,(h_1k_1l_1)\,\boldsymbol{g} = [u_2v_2w_2]\,(h_2k_2l_2), \tag{4}$$

where direct row indices $[u_1v_1w_1]$ are treated as the column matrix.

(v) Two symmetry axes of the lattice are orthogonal if

$$[u_1v_1w_1]\,(h_2k_2l_2) = [u_2v_2w_2]\,(h_1k_1l_1) = 0. \tag{5}$$

(vi) Orthogonal distortion of a lattice along a given symmetry axis. The symmetry matrix ***v*** represented by the geometric symbol [*uvw*](*hkl*) is retained in the lattice group if the reduced lattice tensor ***M*** = (***aa***, ***bb***, ***cc***, ***bc***, ***ca***, ***ab***) is modified according to the equation

$$\boldsymbol{M}' = \boldsymbol{M} + \varepsilon(hh, kk, ll, kl, hl, hk), \tag{6}$$

where ε is a distortion parameter.

Each symbol points to one matrix from ***V*** and thus can represent it. The two non-orthogonal symmetry matrices only share the dual symbol in the [*uvw*] = (*hkl*) case. It should be clear from the properties (i) to (vi) that dual symbols can be applied for easier classification of arithmetic holohedries, simpler derivation of the transformation matrix to the Bravais description or to predict symmetry changes caused by the orthogonal lattice distortion.

5. Lattice classification and Bravais cell derivation

The crystal system is known from the group order by determining the holohedry. Thus, the only remaining problem is to determine the lattice centring type (*P*, *I*, *F*, *A*, *B*, *C*) corresponding to transformation ***T*** from the current primitive base (***a***, ***b***, ***c***) to the centred base (***a***, ***b***, ***c***)***T*** = (***a***′, ***b***′, ***c***′), where

$$\boldsymbol{T} = \begin{pmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \\ w_1 & w_2 & w_3 \end{pmatrix} \tag{7}$$

is defined by indices of three mutually orthogonal symmetry axes. The lattice centring type depends on the 'centring properties': the number of centred directions in equation (7) and the multiplicity $m = \det(\boldsymbol{T})$ of the resulting cell.

Table 3
Classification of lattice groups in $\boldsymbol{V}$.

The crystal system is recognized by the holohedry order. The centring properties (the number of centred directions *cd* and the multiplicity *m* of the cell based on three mutually orthogonal symmetry axes) determine the Bravais cell (lattice type).

Holohedry order $\lvert H\rvert$	Centring properties (*cd*, *m*) and cell type
48	(0, 1) *cP*, (3, 2) *cI*, (3, 4) *cF*
16	(0, 1) *tP*, (3, 2) *tI*
8	(0, 1) *oP*, (2, 2) *oC*, (3, 2) *oI*, (3, 4) *oF*
4	(0†) *mP*, (1†) *mC* or *mI*
24	*hP*
12	*hR*
2	*aP*

† Centring property along unique twofold axis.

Four systems with centred lattice types must be analyzed:

(*a*) *Cubic system*: Matrix $\boldsymbol{T}$ is composed of three fourfold axis directions, $m = 4$ corresponds to the *cF* type and $m = 2$ points to the *cI* type.

(*b*) *Tetragonal system*: Columns of $\boldsymbol{T}$ are defined by the directions of one fourfold axis and two mutually perpendicular twofold axes. From two these systems, that with $m = 2$ is preferred.

(*c*) *Orthorhombic system*: Matrix $\boldsymbol{T}$ is composed of three twofold axis directions, $m = 4$ indicates the *oF* type. If $m = 2$ there are two possible centring types recognized by centring properties (i) of the axes considered. The lack of centring in one direction corresponds to *C*-centring, in the opposite case there is *I*-centring.

(*d*) *Monoclinic system*: The scalar products $\boldsymbol{uh}$ of the unique twofold axis allow the distinction between primitive and centred lattice types.

The above considerations, summarized in Table 3, allow one to propose a convenient criterion for practical classification of Bravais lattices.

Lemma 3 (lattice classification). A (Bravais) lattice type is defined as the class of all lattices referred to its three shortest non-coplanar lattice translations whose arithmetic holohedries are of the same order and have the same centring properties.

Example 1. Let a Buerger-reduced cell be given by the parameters: $a = b = 1.3$, $c = 1.358$ Å, $\alpha = \beta = 118.59$, $\gamma = 90^\circ$. Filtering of $\boldsymbol{V}'$ gives 16 matrices consistent with the metric tensor

$$\boldsymbol{M} = \begin{pmatrix} a^2 & ab\cos\gamma & ca\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ca\cos\beta & bc\cos\alpha & c^2 \end{pmatrix} = \begin{pmatrix} 1.69 & 0 & -0.845 \\ 0 & 1.69 & -0.845 \\ -0.845 & -0.845 & 1.845 \end{pmatrix}. \quad (8)$$

The dual symbols of the symmetry matrices with positive determinants are given in Table 4.

Table 4
Lattice symmetry related to the primitive cell $a = b = 1.3$, $c = 1.358$ Å, $\alpha = \beta = 118.59$, $\gamma = 90^\circ$ given by dual symbols.

Matrices are printed only for clarity.

$\boldsymbol{v}_1 = \begin{pmatrix} \bar1 & 0 & 0 \\ 0 & 1 & \bar1 \\ 0 & 0 & \bar1 \end{pmatrix}$	$\boldsymbol{v}_2 = \begin{pmatrix} \bar1 & 0 & 1 \\ 0 & \bar1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$	$\boldsymbol{v}_3 = \begin{pmatrix} 0 & \bar1 & 0 \\ \bar1 & 0 & 0 \\ 0 & 0 & \bar1 \end{pmatrix}$	$\boldsymbol{v}_4 = \begin{pmatrix} 0 & \bar1 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$2\,[010](02\bar1)$	$2[112](001)$	$2[1\bar10](1\bar10)$	$4^+[112](001)$
$\boldsymbol{v}_5 = \begin{pmatrix} 0 & 1 & \bar1 \\ 1 & 0 & \bar1 \\ 0 & 0 & \bar1 \end{pmatrix}$	$\boldsymbol{v}_6 = \begin{pmatrix} 0 & 1 & 0 \\ \bar1 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$	$\boldsymbol{v}_7 = \begin{pmatrix} 1 & 0 & \bar1 \\ 0 & \bar1 & 0 \\ 0 & 0 & \bar1 \end{pmatrix}$	$\boldsymbol{v}_8 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
$2[110](11\bar1)$	$4^-[112](001)$	$2[100](20\bar1)$	$1[]()$

Matrices $\boldsymbol{v}_2$, $\boldsymbol{v}_4$, $\boldsymbol{v}_6$ and $\boldsymbol{v}_8$ define the fourfold axis. According to property (v) twofold axes given by $\boldsymbol{v}_1$ and $\boldsymbol{v}_7$ are orthogonal. The same is true for the axes given by $\boldsymbol{v}_3$ and $\boldsymbol{v}_5$. Thus, there are two transformation matrices

$$\boldsymbol{T}_1 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix} \quad \text{or} \quad \boldsymbol{T}_2 = \begin{pmatrix} 1 & 1 & 1 \\ \bar1 & 1 & 1 \\ 0 & 0 & 2 \end{pmatrix}, \quad (9)$$

with $\det(\boldsymbol{T}_1) = 2$ and $\det(\boldsymbol{T}_2) = 4$. In the tetragonal system *F*-centring is equivalent to *I*-centring, but conventionally the smaller one is selected. Thus, the Bravais cell is given by the tensor

$$\boldsymbol{T}_1^T \boldsymbol{M} \boldsymbol{T}_1 = \begin{pmatrix} 1.69 & 0 & 0 \\ 0 & 1.69 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \quad (10)$$

or by parameters $a = b = 1.13$, $c = 2$ Å, $\alpha = \beta = \gamma = 90^\circ$. The centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ results from the multiplication of $(\boldsymbol{T}_1)^{-1}$ and integer vectors, *e.g.* (1, 1, 1).

In sharp contrast to the conjugacy tests of lattice holohedries in the group theory (special comparison of two or more holohedries), the type of lattice can be deduced from a single holohedry (absolute manner) and the Bravais cell can be selected from any lattice description. The procedure based on the developed lemmas and illustrated by the above example can be outlined as follows:

(*a*) Buerger reduction to the cell described by the metric tensor $\boldsymbol{M}$.

(*b*) Filtering $\boldsymbol{V}'$: $\boldsymbol{H} = (\boldsymbol{v}_i \mid \boldsymbol{v}_i{}^T \boldsymbol{M}\, \boldsymbol{v}_i = \boldsymbol{M})$, $\boldsymbol{v}_i \in \boldsymbol{V}'$ and presenting holohedry by dual symbols.

(*c*) Composing the transformation matrix $\boldsymbol{T}$ and calculation $\boldsymbol{T}^T\boldsymbol{M}\boldsymbol{T}$.

The selection of Bravais cells for orthogonal systems is automatic; the case of the monoclinic system needs further clarification.

6. Analysis of lattice group–subgroup relations by breaking symmetry

The number of maximal groups in $\boldsymbol{V}$ is limited. This is a good reason to analyze group–subgroup relations by 'distortion paths' originated in the lattice tensors given in Table 2. From equation (10) the distortion orthogonal or parallel to a given symmetry axis is easily constructed. The symmetry operation $n[uvw](hkl)$ is retained in the holohedry of the lattice with the metric tensor modified by $\Delta\boldsymbol{M} = \alpha(hh, kk, ll, kl, hl, hk)$. Distortion is equivalent to changing the interplanar distance $d_{(hkl)}$. Deformations corresponding to $\Delta d_{(h'k'l')}$ retain the orthogonality property [but can break symmetry on planes (hkl) and change the type of symmetry axis] assuming that the scalar product $[uvw](h'k'l') = 0$.

Example 2. We are interested in distortion paths leading to the symmetry operation 2[001](012) or to *mC* lattice holohedry containing this operation. Only *hP*6, *cF*9 and *cF*12 metrics from Table 2 comply with the requirements $(012) \parallel \boldsymbol{M} \cdot [001]$. The given operation is retained in corresponding groups after successive modification of the interplanar distances $d_{(012)}$ and $d_{(110)}$. This destroys other orthogonalities, but not [001](012). Thus, in all three cases the distortion $\alpha d_{(012)} + \beta d_{(110)} = \alpha(0, 1, 4, 2, 0, 0) + \beta(1, 1, 0, 0, 0, 1)$ leads to the centred monoclinic lattices *hP*6: $\rightarrow$ (1.07, 2.12, 2.2, 1.1, 0, 0.07), *cF*9: $\rightarrow$ (2.07, 2.12, 2.2, 1.1, 0, 1.07), *cF*12: $\rightarrow$ (2.07, 2.12, 2.2, 1.1, 0, −0.93) assuming $\alpha = 0.05$ and $\beta = 0.07$. The holohedries of the resulting lattices contain the 2[001](012) operation.

Breaking symmetry in all the highest-symmetry lattices given by 39 metric tensors leads to the diagram shown in Fig. 2. Three branches on the distortion paths distinguished by small circles corresponding to the *Bravais connection* (Pitteri & Zanzotto, 1996) relate two inequivalent lattices by infinitesimal deformation without symmetry lowering. One bifurcation point corresponds to a tetragonal primitive lattice (Table 5).

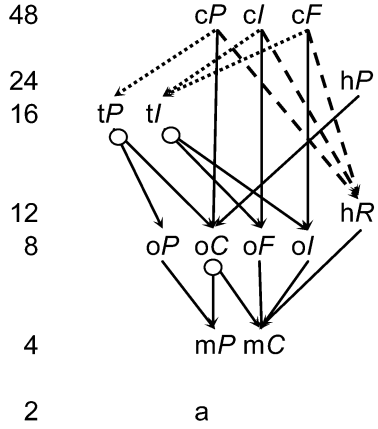

Figure 2
Breaking symmetry of lattices deformed orthogonally along directions parallel to fourfold (dotted lines), threefold (broken lines) and twofold (solid lines) axes. Every lattice deformed along the direction inclined to all the symmetry axes represents a triclinic system (not shown on the diagram).

Table 5
Exemplary holohedry of *tP* lattice (*cP*1 lattice distorted by $\alpha d_{(010)}$) with two systems of mutually orthogonal symmetry axes.

Dual symbol	Centring	Axis system	Dual symbol	Centring	Axis system
2[001](001)	No	1	4^+[010](010)	No	1, 2
2[100](100)	No	1	2[010](010)	No	1, 2
2[$\bar{1}$01]($\bar{1}$01)	Yes	2	4^-[010](010)	No	1, 2
2[101](101)	Yes	2	1 []()	–	–

Owing to property (v) of the dual symbol it is easy to recognize two systems of mutually orthogonal symmetry axes in the lattice group *tP*. These systems differ by centring properties. Distortion along the twofold axis from the first system ($\beta d_{(001)}$ or $\beta d_{(100)}$) destroys the twofold axes in centred directions, reduces the fourfold axis and leads to the *oP* lattice while analogous distortion ($\gamma d_{(\bar{1}01)}$ or $\gamma d_{(101)}$) along the axis in the non-centred direction gives the *oB* lattice. By varying the parameters β and γ from zero to some finite values four Bravais connections between *oP* and *oB* may be defined. A similar analysis can be performed for the two remaining bifurcation points. The above result is well known from the work of Pitteri & Zanzotto, but in contrast to a more sophisticated analysis of fixed sets in six-dimensional space $C^+(Q_3)$, the present approach based on dual symbols of symmetry operations is simple and more intuitive. The Bravais connections between inequivalent lattices are consequences of subgroups in the lattice holohedry, which correspond to the same crystal system but differ in centring properties.

7. Symmetry matrices of Delaunay reduced cells

Since the Niggli cells are also Buerger cells with additional conditions, it is clear that only some subset of $\boldsymbol{V}'$ is necessary to cover all their holohedries. However, in the Delaunay reduction this does not need to be a rule. The following procedure was used to find such matrices based on the special forms of the Selling tetrahedron (Table 9.1.8.1 in the 2005 edition of *ITA*; Burzlaff & Zimmermann, 2005). First, the parameters of the primitive cells are generated such that $a, b, c \leq |\boldsymbol{a} + \boldsymbol{b} + \boldsymbol{c}|$ and all the requirements of a given special form are fullfiled. Next, the symmetry matrices and their dual symbols of the holohedries are determined by filtering the $\boldsymbol{V}$ file. In most cases, as in all Delaunay cells with centred monoclinic symmetry, the relation $M \cdot [uvw] = (hkl)$ points to the maximal group *cF*5. According to the consideration in §6 it was easy to define the deformation path from the Delaunay cell with maximal symmetry (*cP*1, *cI*1, *cF*5, *hP*1) to a given Delaunay cell. However, in four cases (Table 6) not all symmetry matrices can be found in $\boldsymbol{V}$. This problem can be overcome if 16 additional matrices are appended to the file. These matrices describe fourfold symmetry axes in the cubic primitive lattice referred to the bases given by the reduced metric tensors (1, 2, 1, −1, 0, 0) and (1, 1, 2, 0, 0, −1), and designed as *cP*2 and *cP*3 accordingly. They are not compatible with Buerger reduced cells, even if in eight cases the matrices have elements restricted to values of (−1, 0, 1). Moreover, the

Table 6
Four Delaunay cells designed by Bravais symbols and components of Selling tetrahedron whose holohedries are subgroups of *cP*2 and *cP*3.

Delaunay cell	Highest-symmetry cell	Deformation
cP (0, 0, 14, 14, 14, 0)	*cP*2	–
tP (0, 0, 14, 14, 24, 0)	*cP*2	$\alpha d_{(010)}$
tP (0, 0, 14, 23, 0, 23)	*cP*3	$\alpha d_{(100)}$
oP (0, 0, 14, 23, 24, 0)	*cP*2	$\alpha d_{(100)} + \beta d_{(010)}$

relation between matrices and their dual symbols cease being unique.

Thus, holohedries of Delaunay cells are covered by the set of 104 symmetry matrices occurring in lattice descriptions *cP*1, *cP*2, *cP*3, *cI*1, *cF*5, *hP*1.

8. Discussion

While the set of symmetry matrices that cover geometric holohedries of lattices referred to conventional bases is well characterized, no systematic attempts were made to define such sets for privileged primitive bases. The collection of matrices related to Buerger-reduced or Niggli-reduced bases was roughly limited by a combinatorial set of matrices with elements 0, ±1, determinant 1 and finite consecutive powers (Lebedev *et al.*, 2006; Zwart *et al.*, 2006). The presented work proves that the mentioned set, named '$\boldsymbol{V}$ space', plays a fundamental role in analysis based on the arithmetic holohedries of reduced lattices. In the analysed context, the term 'reduced' is understood as 'related to a base, in which all symmetry matrices satisfy the condition: $\boldsymbol{v} \in \boldsymbol{V}'$. In this sense all Buerger and Niggli cells, most Delaunay cells (with the exception of four cases) and also some non-Buerger cells are arithmetically reduced. Some properties of $\boldsymbol{V}$ seem to be interesting and useful: the set is covered by 39 maximal groups which are holohedries of *cP*, *cF*, *cI* and *hP* lattices uniquely represented by metric tensors with smaller integers, and is closed relative to powering, negating, transposing and orthogonal transformation of all the elements. Matrices in $\boldsymbol{V}$ can be easily and reversibly coded by single numbers and thus effectively stored, compared and sorted. For symmetry operations contained in $\boldsymbol{V}$ there is one-to-one correspondence between the matrix form and its dual symbol. Only in the case of $[uvw] = (hkl)$ is the dual symbol shared between two non-orthogonal symmetry matrices, $\boldsymbol{v}$ and $(\boldsymbol{v}^T)^{-1}$.

It is open to doubt whether searching 384 matrices (space $\boldsymbol{V}'$) to determine lattice holohedry is effective. In the matrix approach to this problem (Santoro & Mighell, 1970; Mighell *et al.*, 1981; Himes & Mighell, 1987) and a highly skewed unit cell, a computer program seeks the matrix elements in a wide range of integers and consequently a huge number of potential symmetry matrices must be tested. A similar situation also takes place in the geometric approach based on searching for the orthogonalities between a lattice row $\boldsymbol{u}$ and a lattice plane $\boldsymbol{h}$ (Le Page, 1982). With original limitations on $\boldsymbol{u}$ and $\boldsymbol{h}$ there are still thousands of pairs $(\boldsymbol{u}, \boldsymbol{h})$ which require the evaluation. However, in $\boldsymbol{V}$ there are 81 twofolds and only this number of corresponding pairs should be tested (Zwart *et al.*, 2006). However, remembering that in the Le Page method lattice symmetry is obtained by additional calculations based on the space distribution of twofolds, even in this situation simple filtering of the matrices from $\boldsymbol{V}'$ should be acknowledged as being effective.

The notion of dual symbols, or more precisely the description of lattice orthogonality by the pair lattice plane (uvw)/lattice row $[uvw]$ has a long tradition in the crystallographic literature and practical applications. Deviation from the exact orthogonality as *twin obliquity* has been introduced by Friedel (1926) to characterize pseudosymmetries of lattices and their relation to twinning. Identification of twofolds by generating indices $\boldsymbol{h}$ and $\boldsymbol{u}$ ($\boldsymbol{u} \cdot \boldsymbol{h} = 1$ or 2, obliquity less than some arbitrary limit for pseudo-symmetry) is the first step in the Le Page algorithm for derivation of the conventional unit cell from the Buerger-reduced cell. Some advances in naming symmetry operations by the dual symbols (especially in the case of twofolds and reflection planes) were also considered by Zimmermann (1976).

It has been proven in this article that dual symbols of a lattice holohedry contain similar information to its fixed set and give an alternative framework for the analysis of deformable lattices symmetry. They are sufficient to classify arithmetic holohedries in $\boldsymbol{V}$ (and corresponding lattices) into Bravais types without conjugacy tests in $GL(3, \mathbb{Z})$. It can be concluded that for many practical lattice-related problems, the geometric information contained in symmetry matrices is more useful than the matrices themselves. Thus, dual symbols have not only 'descriptive' but also 'methodic' sense. Their form is also convenient for computer manipulation.

APPENDIX *A*
Concise list of symmetry matrices related to reduced lattices

According to the analogy between the solution of diophantine systems and determination of a lattice symmetry, it is essential to consider the limited sets of potential symmetry matrices with elements 0, ±1 related to different lattice metrical restrictions. Hierarchical sets of matrices presented by single natural numbers $ord(\boldsymbol{v})$ in the ternary counting system[4] are compiled in Table 7.

APPENDIX *B*
A symmetry matrix whose dual symbol contains Miller indices of type {123} or {112} cannot describe the symmetry of a Buerger-reduced cell

Matrices in lines 27–32 of Table 7 represent threefold rotations with dual symbols containing Miller indices of the type {123} or {112} and occur in holohedries of *cI*5–*cI*16 lattices. They

[4] A matrix $\boldsymbol{v}$ with elements 0, $\pm$ 1 is coded into the natural number $ord(\boldsymbol{v})$ by the expression $\sum_{i,j=1}^{3} 3^{[2-3i-j]}(v_{ij} + 1)$. The *ord* can be decoded into matrix $\boldsymbol{v}$ by integer division *div* and the following procedure: *i*, *j*: = 3: 1: dum: = ord *div* 3: $v(i, j)$: = ord − 3dum − 1: ord: = dum: *j*: = *j* − 1: *if j* = 0 *then* (*j*: = 3, *i*: = *i* − 1): *if i* > 0 *then goto* 1.

Table 7
Hierarchical sets of symmetry matrices (det = 1) and corresponding lattice restrictions.

Matrices together with their negatives cover the holohedries of: the primitive cubic cell (lines 1–3), conventional centred cells (lines 1–4, set ***W***), Buerger cells (lines 1–26, set ***V′***), Buerger cells in direct or in reciprocal spaces (lines 1–32, set ***V***).

(1)	3200,	3250,	3310,	3360,	7410,	7636,	7672,	7898								
(2)	8872,	9022,	9202,	9352,	10324,	10498,	10642,	10816								
(3)	11786,	11992,	12064,	12270,	16320,	16378,	16426,	16484								
(4)	3117,	5225,	5547,	7817,	11867,	14133,	14459,	16563								
(5)	394,	454,	457,	608,	635,	698,	1170,	1173,	1176,	1310,	1328,	1337,	1346,	1364,	1399,	1435
(6)	1792,	1891,	1894,	2039,	2066,	2138,	2321,	2398,	2444,	2471,	2498,	2638,	2641,	2644,	2801,	2884
(7)	3016,	3058,	3090,	3144,	3173,	3188,	3191,	3194,	3197,	3203,	3206,	3209,	3212,	3227,	3333,	3357
(8)	3363,	3387,	3484,	3562,	3576,	3603,	3630,	3755,	3838,	3902,	3929,	3956,	4078,	4081,	4084,	4247
(9)	4324,	4469,	4496,	4586,	4708,	4825,	4828,	5198,	5216,	5234,	5252,	5269,	5341,	5544,	5550,	5954
(10)	5981,	6026,	6226,	6268,	6271,	6658,	6664,	6668,	6708,	6838,	6908,	6940,	7011,	7014,	7015,	7061
(11)	7088,	7156,	7169,	7246,	7264,	7404,	7416,	7559,	7589,	7640,	7670,	7720,	7750,	7790,	7814,	7820
(12)	7844,	7871,	7876,	7889,	7895,	7901,	7907,	7918,	7925,	7960,	7979,	7996,	8112,	8156,	8158,	8164
(13)	8308,	8368,	8402,	8454,	8455,	8457,	8546,	8573,	8627,	8638,	8692,	8710,	8806,	8846,	8882,	8908
(14)	8925,	8926,	8959,	9174,	9175,	9198,	9199,	9201,	9203,	9204,	9205,	9228,	9229,	9238,	9334,	9362
(15)	9380,	9445,	9459,	9460,	10228,	10288,	10316,	10352,	10399,	10431,	10432,	10614,	10615,	10638,	10639,	10641
(16)	10643,	10644,	10645,	10668,	10669,	10768,	10790,	10808,	10834,	10869,	10870,	10885,	10976,	11003,	11050,	11057
(17)	11104,	11140,	11206,	11266,	11336,	11388,	11389,	11391,	11514,	11566,	11576,	11578,	11678,	11702,	11705,	11708
(18)	11732,	11746,	11759,	11777,	11783,	11789,	11795,	11813,	11824,	11830,	11902,	11915,	11981,	11996,	12062,	12076
(19)	12142,	12258,	12282,	12407,	12434,	12515,	12520,	12592,	12628,	12688,	12722,	12790,	12825,	12828,	12829,	12964
(20)	12968,	12976,	13026,	13404,	13467,	13468,	13645,	13708,	13726,	14110,	14158,	14191,	14239,	14354,	14402,	14440
(21)	14476,	14862,	14961,	14962,	15109,	15190,	15208,	15442,	15591,	15648,	15649,	15696,	15697,	15738,	15763,	15786
(22)	15922,	16054,	16063,	16068,	16077,	16086,	16093,	16102,	16125,	16134,	16135,	16182,	16183,	16191,	16288,	16297
(23)	16306,	16311,	16329,	16336,	16345,	16354,	16368,	16369,	16377,	16379,	16386,	16387,	16416,	16417,	16425,	16427
(24)	16434,	16435,	16459,	16507,	16531,	16540,	16554,	16572,	16588,	16597,	16620,	16621,	16629,	16659,	16668,	16669
(25)	16876,	17049,	17106,	17107,	17154,	17155,	17178,	17203,	17226,	17368,	17539,	17620,	17656,	17778,	17895,	17896
(26)	18242,	18290,	18310,	18347,	18382,	18484,	18507,	18532,	18565,	18613,	18991,	19036,	19072,	19236,	19281,	19282
(27)	347,	685,	1325,	1334,	1340,	1349,	1841,	2149,	2371,	2614,	2668,	2911,	3865,	4054,	4108,	4297
(28)	4579,	4775,	5219,	5222,	5228,	5231,	6031,	6161,	6694,	6904,	7138,	7186,	7396,	7426,	7719,	7749
(29)	7808,	7811,	7823,	7826,	8128,	8404,	8608,	8656,	8765,	8836,	8958,	8985,	9299,	9370,	9417,	9444
(30)	10271,	10360,	10371,	10398,	10709,	10798,	10884,	10911,	11020,	11086,	11338,	11548,	11693,	11696,	11714,	11717
(31)	12075,	12141,	12238,	12304,	12484,	12550,	12718,	12994,	13381,	13509,	14190,	14238,	14359,	14395,	14887,	14919
(32)	15441,	15568,	15616,	15921,	16875,	17026,	17074,	17367,	17803,	17835,	18229,	18301,	18564,	18612,	19213,	19341

need something other than Buerger-reduced lattice descriptions. This can be proved geometrically. For example, the matrix '1340' represents operation 3^+ [001](123) depicted in Fig. 3.

Proof. A threefold axis intersects levels 1 and 2 of the family of lattice planes in threefold symmetry points (Fig. 3*a*). The shortest distance from the axis to any lattice point on level 1 or level 2 is the same. This implies that a cell translation which ends at level 2 is longer than three (owing to threefold symmetry) non-coplanar vectors ending in level 1 (Fig. 3*b*). This is contrary to the assumption that the cell is constructed on the three shortest translations.

Similar arguments can be applied to the symmetry matrices with Miller indices of type {112} in their dual symbols.

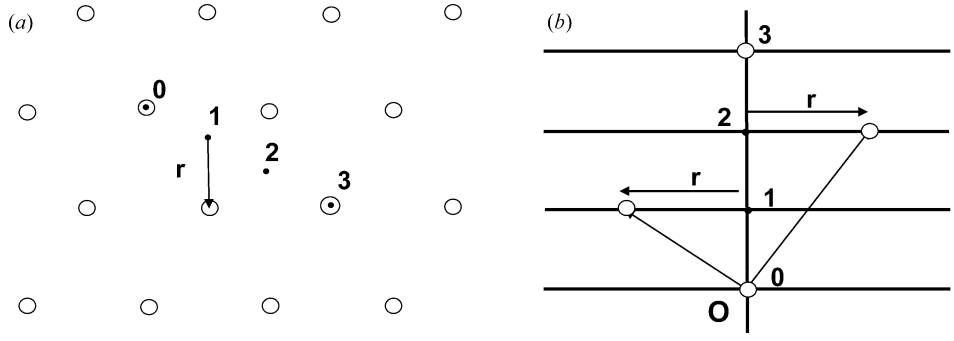

Figure 3
The intersections of the levels of the lattice plane family with a threefold axis. The intersection points to (*a*) the hexagonal plane and (*b*) the stacking of such planes. The shortest lattice translation from origin O to level 2 is longer than the shortest lattice vector to level 1.

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