J. Appl. Cryst. (1982). **15**, 255–259

The Derivation of the Axes of the Conventional Unit Cell from the Dimensions of the Buerger-Reduced Cell†

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(*Received* 24 *June* 1981; *accepted* 16 *October* 1981)

Abstract

The identification of twofold axes is straightforward if the cell is based on three of the shortest lattice translations. The distribution of twofold axes in space fixes the lattice symmetry and most conventional cell edges. A program based on this approach has been written. It works for the seven cases with minimum branching of the algorithm.

Introduction

The traditional way of assessing the metric symmetry of a lattice is based on numerical relationships in the matrix of scalar products of the Niggli-reduced cell. It is summarized in § 5.1 of *International Tables for X-ray Crystallography* Vol. 1 (1969), pp. 530–535. The editions prior to 1969 do not contain this section. Forty-four cases are distinguished and a corresponding computer program would therefore require a considerable amount of branching and would be likely to suffer from the drawbacks commonly associated with such a structure.

The present approach is based on the identification of twofold axes according to the following three criteria which are developed in Appendices I, II and III.

(1) A row with period **t** is a twofold axis of a lattice if and only if there is a reciprocal-lattice row with period τ such that $\mathbf{t}\times\tau=0$ and $\mathbf{t}.\tau=1$ or 2.

(2) If the lattice is referred to three of its shortest non-coplanar translations, the moduli of the Miller indices of such direct and reciprocal rows cannot exceed 2.

(3) A lattice symmetry is uniquely determined by the space distribution of its twofold axes.

Application of the above remarks to the problem

The first two remarks provide a simple way of finding all the twofold axes in the lattice to be studied. Comparison of their distribution in space with the well-known distributions of even-order symmetry axes (=twofold axes) in six of the seven possible lattice symmetries allows the lattice symmetry to be identified according to the third criterion. This process places the lattice in a conventional orientation and the choice of rows to be selected as edges of the conventional cell is guided by the coincidence of lattice rows with pre-determined symmetry axes. This process is described in more detail under *The algorithm*.

A difficulty associated with the problem itself is that the metric symmetry of a given lattice is to be found using measured cell parameters. Uncertainties are associated with such measurements, therefore the collinearity of the direct and reciprocal-lattice rows can only be determined within the limits of experimental error. The angle δ between these rows is calculated with $\tan\delta=|(\mathbf{t}\times\tau)|/|(\mathbf{t}.\tau)|$. If this angle is small but still larger than the limits of experimental error on angles, the row is a pseudo-axis of metric symmetry. If δ is less than the limit, the row can be a true or a pseudo-symmetry axis. In other words this approach, in common with all others, might attribute to the lattice a metric symmetry higher than its true symmetry.

The calculation of the δ angle is achieved by referring the direct and reciprocal lattices to the same Cartesian system as shown by Rollett (1965) by means of the matrix

$$\mathbf{L}=\begin{vmatrix} a\sin\beta\sin\gamma^* & 0 & 0 \\ -a\sin\beta\cos\gamma^* & b\sin\alpha & 0 \\ a\cos\beta & b\cos\alpha & c \end{vmatrix}.$$

The orthogonal components **t** of a direct lattice vector **U** are given by $\mathbf{t}=\mathbf{L}\,\mathbf{U}$ while the orthogonal components τ of a reciprocal-lattice vector **h** are $\tau=(\mathbf{L}^T)^{-1}\mathbf{h}$ and it is then a simple matter to evaluate δ knowing **t** and τ.

The algorithm

The algorithm for deriving the conventional cell is shown in Table 1. The sequence of operations is as follows.

The input cell is first reduced to a primitive set of translations retaining its handedness. The three shortest non-coplanar translations are found by Buerger reduction (Buerger, 1960). In the ambiguous cases, *e.g.*

† NRC No. 19969.

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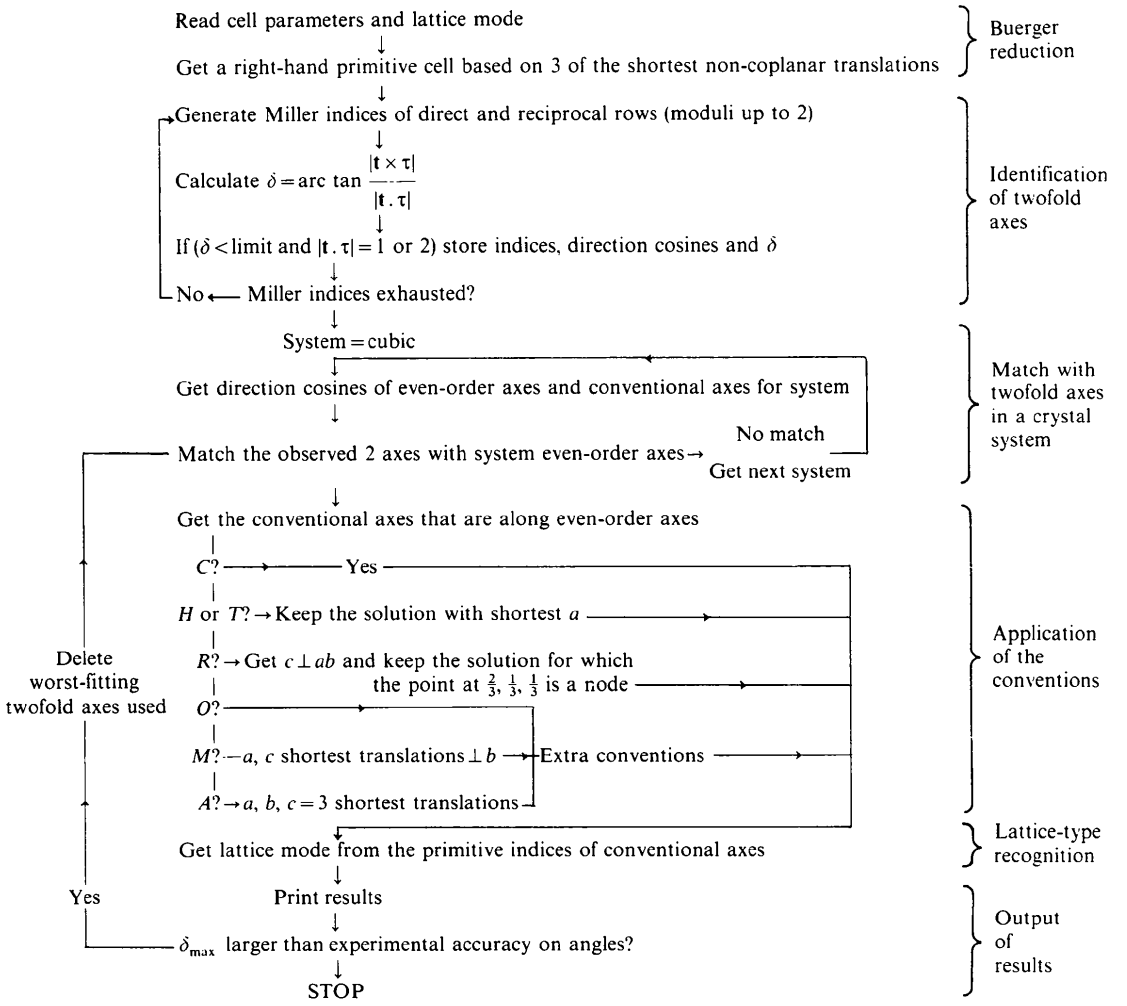
Table 1. *The algorithm*



when the third- and fourth-shortest translations are of equal lengths, it does not matter which triplet is actually selected. Gruber (1973) has shown that when the Buerger-reduced cell is not unique, the triplets on which the different cells are based have the same lengths as the triplet on which the Niggli cell is based. The discussion in Appendix II shows the existence of strictly shorter translations in the cases where indices of three or more would be required to index the twofold axis or the plane perpendicular to it. The labeling of the cell edges does not matter as long as the handedness of the cell is preserved. The matrix **B** of correspondence between the direct indices $\mathbf{U}_B$ in the Buerger-reduced cell and the indices $\mathbf{U}_I$ in the input cell is given by $\mathbf{U}_I = \mathbf{B}\mathbf{U}_B$. The rows of the **B** matrix are the indices of the edges of the Buerger-reduced cell.

The twofold axes are then found in the Buerger cell by generating indices of real and reciprocal rows **U** and **h** with moduli up to 2. If $\mathbf{U} . \mathbf{h} = 1$ or 2, the δ angle is calculated. If this angle is less than some arbitrary limit for pseudo symmetry, *e.g.* 3°, the indices **U** of the direct row, the direction cosines of its period and the δ angle are kept.

If nine or more twofold axes have been found, a match is sought between the well-known space distribution of even-order axes in the cubic lattice symmetry and the observed distribution. The match is based on the similarity of angles between symmetry directions calculated using their direction cosines. If all cubic directions have a counterpart in the lattice studied, a solution has been found. The rows to be selected as edges of the conventional cell are the ones which match the three fourfold axes forming a right-handed system. The correspondence matrix **C** between the conventional indices $\mathbf{U}_C$ and the indices $\mathbf{U}_B$ with the Buerger cell is given by $\mathbf{U}_B = \mathbf{C}\mathbf{U}_C$. Its rows are the indices of the conventional axes in the Buerger-cell axial system. The correspondence matrix **D** of the

input indices and the conventional indices is therefore given by $\mathbf{U}_I = \mathbf{D}\mathbf{U}_C$ with $\mathbf{D} = \mathbf{B}\mathbf{C}$. It follows that the correspondence between the input and conventional reciprocal indices $\mathbf{h}_I$ and $\mathbf{h}_C$ is $\mathbf{h}_I = (\mathbf{D}^T)^{-1}\mathbf{h}_C$.

The Bravais type of the conventional cell is found from the **C** matrix. If the determinant of **C** is 1, 3 or 4 the cell is respectively *P*, *R* or *F* centered in general (obviously, no *R*-centered cubic lattice will be found). If the determinant is 2, the indices of the conventional direct nodes 011, 101, 110 and 111 with the primitive Buerger-reduced cell are calculated using $\mathbf{U}_B = \mathbf{C}\mathbf{U}_C$. If they are not coprime, the conventional cell is respectively *A*, *B*, *C* or *I* centered.

The input indices of the direct rows selected to be the conventional axes are printed together with the periods along these rows and the angles they make with one another: they are the parameters of the conventional cell. The indices $\mathbf{h}_I$ of the axes of the reciprocal of the conventional cell are also output.

The largest δ angle used in the solution, δ_{max}, is printed. If this angle is no larger than the experimental error limit, the solution is called 'metrically cubic' and the search is stopped. If the angle is larger, the solution is called 'pseudo cubic' and the search is resumed after deleting from the list of observed twofold axes all rows with δ angles larger than or equal to δ_{max}. This ensures that further solutions can only be better fits.

Hexagonal, rhombohedral, tetragonal, orthorhombic, monoclinic and anorthic symmetries (*h*, *r*, *t*, *o*, *m* and *a*) are then examined in turn until a metric agreement is found. Contrary to the cubic case, several possibilities exist in these six cases for the correspondence between symmetry elements and conventional cell edges. In the *h*, *r* and *t* cases two possibilities are due to the symmetry itself: the symmetry is invariant under a 30, 60 or 45° rotation about the *z* axis (assuming an *hR* cell for the rhombohedral lattice; see Donnay, 1977), although such rotations are not symmetry elements of the lattice. Consequently, two possibilities have to be examined in this case and the one giving the smallest value of **a** is retained for *h* and *t* symmetries. The solution for which the point $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$ in the hexagonal cell corresponds to a lattice node is kept for *r* symmetry, which ensures the obverse setting of the hexagonal cell in the rhombohedral lattice. For orthorhombic symmetry, **a**, **b** and **c** are taken along the three mutually perpendicular twofold axes. For monoclinic symmetry, the two shortest translations in the plane perpendicular to the twofold axis are selected to be **a** and **c**. For triclinic symmetry, the edges of the Buerger-reduced cell are accepted. In the last three cases, the labeling of the axes requires extra conventions which are applied separately.

Discussion

This approach is essentially geometrical and is based on a simple criterion to identify twofold axes. Starting from any cell based on three of the shortest lattice translations, it finds the metric symmetry and most conventional cell edges by superposition with the even-order axes present in six of the seven well-known possible cases. It then applies the metric conventions in the *o*, *m* and *a* cases. Finally, the Bravais type of the conventional cell is derived.

This approach separates the logical steps involved in the problem permitting more flexibility in the solution than the approach in *International Tables for X-ray Crystallography* (1969), in which the metric conventions of the Niggli-reduced cell are intermingled with an arbitrary selection of possible lattice modes in order to limit the number of cases to 44. The resulting cell has in some cases to be transformed in order to conform with a consistent set of metric rules [see footnote in *International Tables for X-ray Crystallography* Vol. I (1969), p. 535]. In the present approach, the metric conventions are a separate step in the process prior to obtaining the lattice mode. This step can be altered independently from the system and lattice-mode recognition.

The handling of pseudo symmetry is straightforward in the present approach. When searching the crystal systems ranked in the order *c*, *h*, *r*, *t*, *o*, *m*, *a*, each time a solution is found, all the twofold axes with a δ angle not smaller than the largest one used in the match are deleted from the list of twofold axes, ensuring that only better solutions can be found. For example, if a crystal is pseudo-tetragonal but metrically monoclinic (Table 2) only the better of the two orthorhombic pseudo-cells will be mentioned with the two best of the five implied monoclinic cells. The process converges towards the metric symmetry while mentioning increasingly better solutions of decreasing symmetry until a metric agreement is found.

It should be noted that, in the case of pseudo-symmetry, the δ angle is the obliquity of a possible twin law with index 1 because the rotation by 180° about the row **U** or about the normal to the plane **h** would approximately restore all the lattice nodes. The list of 'possible twofold axes' in Table 2 is truly an exhaustive list of the twofold axes augmented by all the possible twin laws of index 1 up to the arbitrary maximum obliquity of 3°. The largest obliquity in a solution can be used as a quantitative criterion for pseudo-cells in the same way as it is used for twin laws.

Finally, the present approach is well suited for computer-controlled diffractometers. The NRC Fortran diffractometer program contains the present approach as an overlay and checks that the trial cell used obeys some set of conventions before diffracted intensity measurement. If the cell used is unconventional, the crystal can be reset or not in the conventional orientation at the wish of the user. This resetting can be performed automatically because the program derives the correspondence matrices between

Table 2. *The computer output*

The column labeled 'dot product' is $|\mathbf{t}.\tau|$ and that labeled 'vector product' is in fact $\arctan(|\mathbf{t}\times\tau|\ |\mathbf{t}.\tau|)$ in degrees.

```
INPUT CELL:    4.000      4.472      4.583     79.030     64.130     64.150 LATTICE MODE P
A BUERGER CELL
               4.000      4.472      4.583     79.030     64.130     64.150
THE INPUT-TO-BUERGER CELL MATRIX
                          1.0    0.0    0.0
                          0.0    1.0    0.0
                          0.0    0.0    1.0

              POSSIBLE 2-FOLD AXES:
             ROWS                          PRODUCTS
      DIRECT        RECIPROCAL          DOT     VECTOR
    1   0   -2      0   0   1            2       0.005
    0   1   -1      0   1  -1            2       1.480
    1  -2    0      0   1   0            2       0.714
    1  -1   -1      0   1   1            2       1.482
    1   0    0      2   1   1            2       0.714

              PSEUDO   TETRAGONAL I     MAX DELTA      1.482
A =   0.0  1.0 -1.0    5.7622  ALPHA=    90.501  A* =   0.000   0.500  -0.500
B =   1.0 -1.0 -1.0    5.7625  BETA =    89.505  B* =   0.000  -0.500  -0.500
C =  -1.0  0.0  0.0    4.0000  GAMMA=    88.610  C* =  -1.000  -0.500  -0.500
              PSEUDO ORTHORHOMBIC F     MAX DELTA      0.714
A =  -1.0  0.0  0.0    4.0000  ALPHA=    90.003  A* =  -1.000  -0.500  -0.500
B =   1.0 -2.0  0.0    8.0497  BETA =    89.996  B* =   0.000  -0.500   0.000
C =  -1.0  0.0  2.0    8.2474  GAMMA=    90.714  C* =   0.000   0.000   0.500
              PSEUDO   MONOCLINIC C     MAX DELTA      0.714
A =  -1.0  0.0  0.0    4.0000  ALPHA=    89.692  A* =  -1.000  -0.500   0.000
B =   1.0 -2.0  0.0    8.0497  BETA =   115.870  B* =   0.000  -0.500   0.000
C =   0.0  0.0  1.0    4.5830  GAMMA=    90.714  C* =   0.000   0.000   1.000
          METRICALLY   MONOCLINIC C     MAX DELTA      0.005
A =  -1.0  0.0  0.0    4.0000  ALPHA=    89.999  A* =  -1.000   0.000  -0.500
B =  -1.0  0.0  2.0    8.2474  BETA =   115.850  B* =   0.000   0.000   0.500
C =   0.0  1.0  0.0    4.4720  GAMMA=    89.996  C* =   0.000   1.000   0.000
```

both the direct and reciprocal input and conventional cells as explained above. At the same time, eventual metric pseudo-symmetry of the lattice is disclosed for later investigation. Such an approach ensures, for example, that triclinic lattices will be referred to their three shortest direct translations, in agreement with all accepted sets of conventions. A surprisingly high proportion of recently published triclinic structures do not follow this unanimously accepted rule.

Conclusion

A geometrical derivation of the conventional cells has been obtained which can accommodate any set of metric conventions for the orthorhombic, monoclinic and triclinic lattice symmetries. It does not require the use of the Niggli reduced cell and avoids the extensive branching of algorithms based on the approach in *International Tables for X-ray Crystallography* (1969). The program runs on PDP8-E, PDP11, UNIVAC 1100 and CDC 7400 computers.

I thank Dr A. D. Mighell from NBS, Washington, USA, for the programs and especially the test deck used at NBS. I also thank Drs L. D. Calvert and E. J. Gabe for fruitful discussions.

APPENDIX I

Condition for a row to be a twofold axis

A twofold axis is at the same time a direct-lattice row and a reciprocal-lattice row because the sum of two lattice vectors **v** and **v**′ related by a 180° rotation about the symmetry axis is a lattice vector **V** parallel to the axis (Fig. 1*a*). This holds for direct lattice vectors as well as reciprocal ones. This collinearity can be expressed by the relation $\mathbf{t}\times\tau=0$, where t and τ are

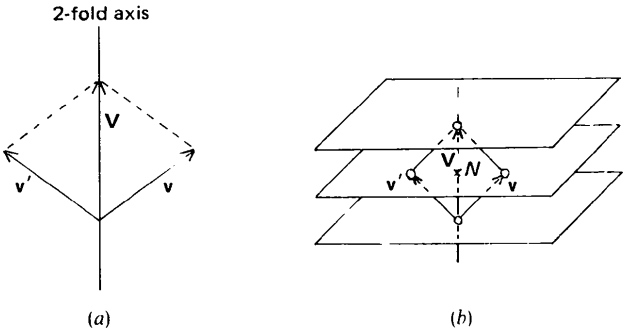


Fig. 1. (*a*) A twofold axis is parallel to a lattice translation. (*b*) The scalar product of the direct and reciprocal periods along an even-order axis can only be 1 or 2.

respectively the direct and the reciprocal periods along the axis. The existence of a reciprocal row along the symmetry axis implies the existence of direct-lattice planes perpendicular to it. If we consider a lattice vector **v** joining two neighboring planes, the dot product $\mathbf{v}.\tau$ is equal to 1 because the reciprocal period is the inverse of the interplanar distance in the direct lattice. The same relation is true for **v**′ obtained by rotating **v** by 180° about the axis. The vector $\mathbf{V}=\mathbf{v}+\mathbf{v}'$ is either the period along the axis or twice that period because **V** is a lattice vector crossing only one lattice plane at a point N which can be, but which is not necessarily, a lattice node. As $\mathbf{V}.\tau$ is equal to 2, this implies $\mathbf{t}.\tau=1$ or 2 (Fig. 1*b*).

Conversely, the conditions $\mathbf{t}\times\tau=0$ and $\mathbf{t}.\tau=1$ or 2 imply that the lattice planes perpendicular to the collinear direct and reciprocal rows are mirror planes because the levels $+n$ and $-n$ of this family of direct planes are separated by $2n$ interplanar distances, *i.e.* an integer number of periods of the direct row which is perpendicular to them. Owing to the center of symmetry in all lattice nodes, it follows that the row is a twofold axis.

Conclusion

A lattice row with period **t** is an even-order symmetry axis of a lattice if and only if there is a reciprocal-lattice row with period τ such that $\mathbf{t}\times\tau=0$ with $\mathbf{t}.\tau=1$ or 2.

APPENDIX II
The indices of the direct and reciprocal rows along a twofold axis cannot be larger than 2

The direct lattice is assumed to be referred to a Buerger-reduced cell, *i.e.* to its three shortest lattice translations. It is shown below that this implies that the moduli of the Miller indices of its even-order symmetry axes cannot be larger than 2.

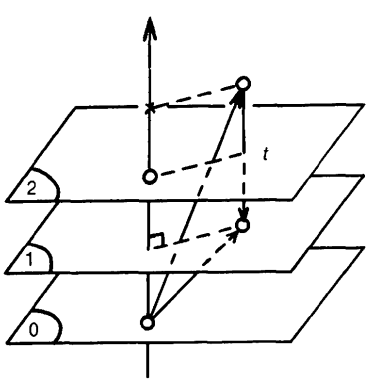


Fig. 2. The three shortest non-coplanar translations can only end in the levels 0, 1 or 2 of the family of lattice planes perpendicular to a twofold axis.

A. The reciprocal row

The indices of the reciprocal row are equal to the indices of the family of direct lattice planes perpendicular to it. From the definitions, the ith Miller index of the plane is the sequence number of the level of that family of planes in which ends the ith cell translation. If a cell translation ends in level j with $j>2$, a strictly shorter but non-zero translation exists in level 1 if j is odd and in level 2 if j is even, owing to the period along the twofold axis perpendicular to the planes (Fig. 2). As this would be contrary to the hypothesis that the cell is based on the three shortest translations, no Miller index of the reciprocal row can be larger than 2.

B. The direct row

No simple proof of this simple property could be devised for the direct row and a proof by mutually exclusive cases can be obtained from the author. The duality of the direct and reciprocal lattices cannot be used because the fact that the direct cell is based on the three shortest translations does not imply the same property for the reciprocal cell.

Conclusion

If the cell is Buerger-reduced, *i.e.* is based on three of the shortest non-coplanar lattice translations, the moduli of the Miller indices of the direct and reciprocal rows along its even-order axes cannot be larger than 2.

APPENDIX III
The complete lattice symmetry is implied by the pattern of its even-order symmetry axes

The following two statements are well-known theorems whose proofs can be found in textbooks:

1. The normal to a plane containing p intersecting twofold axes is a p axis.
2. In a lattice, perpendicular to an even-order axis there is a mirror plane.

Remark 1 implies the existence of the threefold axes in the rhombohedral and cubic cases when the twofold axes have been identified. It allows one to label the even-order symmetry axes as twofold, fourfold or sixfold axes depending on the number of twofold axes perpendicular to them.

Remark 2 then gives the complete lattice symmetry in the seven possible cases.

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