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## RESEARCH AND DEVELOPMENT REPORT

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IS-1141

Chemistry (UC-4)
TID-4500, July 1, 1965

UNITED STATES ATOMIC ENERGY COMMISSION

Research and Development Report

# THE REDUCED CELL AND ITS CRYSTALLOGRAPHIC APPLICATIONS

by

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April, 1965

Ames Laboratory

at

Iowa State University of Science and Technology
F. H. Spedding, Director,
Contract W-7405 eng-82

IS-1141

This report is distributed according to the category Chemistry (UC-4) as listed in TID-4500, July, 1965.



Printed in USA. Price $ 6.00 . Available from the Clearinghouse for Federal Scientific and Technical Information, National Bureau of Standards, U. S. Department of Commerce, Springfield, Virginia

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# THE REDUCED CELL AND ITS CRYSTALLOGRAPHIC APPLICATIONS

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## ABSTRACT

This report describes the reduced cell and its applications to structural crystallography. Typical applications which are discussed are its use as the standard choice of the unit cell in a triclinic lattice and the use of its scalars in identifying in a lattice the cell of highest symmetry. The report also describes two FORTRAN computer programs which may be used to locate the reduced cell in a lattice, to calculate its parameters and to derive the matrix for the transformation of the original cell to the reduced cell.

## I. INTRODUCTION

Preliminary investigations of a crystalline substance usually begin with an identification of its crystal symmetry, such as its crystal system, lattice type, space group and cell parameters. Such information may be obtained either by powder or single crystal X-ray diffraction techniques. Once the symmetry has been established, however, it is sometimes desirable to locate and identify its reduced cell as well.

The "true" reduced cell is defined as that cell whose axes are the three shortest non-coplanar translations in the lattice; consequently there is only one such cell in any one lattice. It is, by convention, the standard choice for the triclinic cell. But more important, this cell, and the method of finding it, provides a simple direct method for identifying and locating in the lattice the cell of highest symmetry,

starting from any cell in any arbitrary orientation. This fact alone immediately suggests two useful applications: its use in powder work in assigning the cell of highest symmetry to a pattern indexed in the triclinic system by a method such as that due to Ito, and for the alignment of single crystals on a single crystal orienter in which the crystals are mounted in a completely random orientation. It also serves as a "fingerprint" and can thus be used not only for comparing two crystalline forms of a compound for similarities in their lattice but can also be used to verify whether or not two crystalline forms actually correspond to the same compound. Furthermore, by the same reasoning, any two or more cells in a lattice may be linked together via the reduced cell since the same reduced cell can always be found regardless of the starting point. The reduced cell is thus an important one; consequently the method of finding it, as well as a discussion of its applications, is the purpose of this report and is fully discussed with the aid of detailed examples.

The concluding portion of this report describes two computer programs written in full Fortran for the IBM 7074 computer. The first of the two programs, RCELL, is strictly a cell reduction program which obtains the reduced cell by the method discussed in this report. The second, TRACER, is an expanded version of RCELL and may be used not only for obtaining the reduced cell, but also for general cell transformations as well as matrix multiplication and matrix inversion of 3 x 3 transformation matrices.

The Delaunay cell and the method of finding it is not discussed in this report. It is a cell whose shortest three non-coplanar translations are chosen so as to enable all three interaxial angles to be non-acute; they are not necessarily the shortest translations in the lattice.

## II. THE REDUCED CELL

### A. THEORY

Of the seven systems into which crystals may be classified, the triclinic system is the only one which possesses no symmetry at all. Through lack of symmetry the three axes may be unequal in length, unequally inclined and at angles other than right angles. This means that any three non-coplanar vectors suffice in outlining a triclinic cell in a lattice, that there is no restriction as to which three are chosen and that they are not restricted to those shortest in magnitude.

Of the infinite number of possible triclinic cells, most of them are quite impractical. One cell which has now been accepted as standard is defined as the smallest cell whose axes are the three shortest non-coplanar translations in the lattice. This particular cell is referred to as the reduced cell and the method of finding it is known as cell reduction. For a triclinic cell to be a reduced cell the following conditions must be satisfied:

(i). The cell must be primitive.

(ii). Each cell edge must be shorter than the diagonals of the faces bordering it[1], so that (vectorially)

$$|\vec{a}| < |\vec{a} + \vec{b}|, \qquad |\vec{b}| < |\vec{a} + \vec{b}|, \qquad |\vec{c}| < |\vec{a} + \vec{c}|,$$
$$|\vec{a}| < |\vec{a} - \vec{b}|, \qquad |\vec{b}| < |\vec{a} - \vec{b}|, \qquad |\vec{c}| < |\vec{a} - \vec{c}|,$$
$$|\vec{a}| < |\vec{a} + \vec{c}|, \qquad |\vec{b}| < |\vec{b} + \vec{c}|, \qquad |\vec{c}| < |\vec{b} + \vec{c}|,$$
$$|\vec{a}| < |\vec{a} - \vec{c}|, \qquad |\vec{b}| < |\vec{b} - \vec{c}|, \qquad |\vec{c}| < |\vec{b} - \vec{c}|,$$

Condition (ii) may be rewritten into a more suitable form as a test by squaring each side of each inequality and expressing the vectors as scalar products. For instance, by squaring both sides of

$$|\vec{b}| < |\vec{a} - \vec{b}|,$$

we obtain

$$|\vec{b}|^2 < |\vec{a} - \vec{b}|^2,$$
$$|\vec{b} \cdot \vec{b}| < |\vec{a} \cdot \vec{a}| + |\vec{b} \cdot \vec{b}| - 2|\vec{a} \cdot \vec{b}|,$$
$$2|\vec{a} \cdot \vec{b}| < |\vec{a} \cdot \vec{a}|,$$
$$|\vec{a} \cdot \vec{b}| < \tfrac{1}{2}a^2.$$

By a similar treatment with the others, the twelve inequalities reduce to the following six:

(iii).
$$|\vec{a} \cdot \vec{b}| \leq \tfrac{1}{2}a^2$$
$$|\vec{a} \cdot \vec{b}| \leq \tfrac{1}{2}b^2$$
$$|\vec{b} \cdot \vec{c}| \leq \tfrac{1}{2}b^2$$
$$|\vec{b} \cdot \vec{c}| \leq \tfrac{1}{2}c^2$$
$$|\vec{c} \cdot \vec{a}| \leq \tfrac{1}{2}c^2$$
$$|\vec{c} \cdot \vec{a}| \leq \tfrac{1}{2}a^2$$

where $|\vec{a} \cdot \vec{b}| = ab\cos\gamma$, etc.

If a cell defining a particular lattice is primitive but fails to satisfy all six conditions under (iii), it is possible to search for shorter translations in a systematic way utilizing directly the three vectors

defining the edges of the original cell. One method of doing this is due to Azároff and Buerger[2] and is the method discussed here. The use of this method requires that (1) the cell to be reduced is primitive and (2) the three vectors describe the cell in direct space, as the reciprocal of the reduced primitive cell of the reciprocal lattice is not necessarily the reduced primitive cell of the direct lattice[1, 2]. The method of searching for shorter vectors in a lattice may be achieved in at least one of two ways, either graphically or analytically.

The graphical method of finding the reduced cell simply involves constructing the lattice on paper and searching for the shortest translations directly. This may be achieved by drawing a two-dimensional lattice of points, or net, according to a fixed scale containing two of the three axes and searching for the shortest translations, one axis at a time.

The analytical procedure is a much more exact approach for it not only allows the more demanding accuracy but it also lends itself well for use on a computer (Chapter III). Briefly, the analytic reduction proceeds as follows: First, of the three scalar products $\vec{a} \cdot \vec{b}$, $\vec{b} \cdot \vec{c}$, $\vec{c} \cdot \vec{a}$, the one largest in absolute value is selected as the first candidate for the reduction of a vector. The particular vector which is reduced first is the larger of the two vectors comprising the scalar product just selected; thereafter, the second longest remaining translation of $\vec{a}$, $\vec{b}$ and $\vec{c}$ is reduced next and finally the remaining translation reduced last. After all three translations (vectors) have been reduced, the six

conditions (iii) are again tested. If one or more of the axes can be reduced still further, the new parameters are recycled for further reduction.

The procedure of reducing the length of a vector is achieved by vector addition or subtraction. Figure 1 illustrates this procedure for the reduction of vector $\vec{b}_1$ in the $\vec{a}\,\vec{b}_1$ -plane. Shorter vectors of $\vec{b}$ are found by adding (vectorially) integral values of $\vec{a}$ to $\vec{b}_1$ if the angle between $\vec{a}$ and $\vec{b}_1$ is greater than 90° or by subtracting (vectorially) integral values of $\vec{a}$ from $\vec{b}_1$ if the angle between them is less than 90°. In this case the angle between them is less than 90° so that by successive subtraction of vector $\vec{a}$ from $\vec{b}_1$ the shortest vector $\vec{b}_3$ is ultimately obtained in this net, where $|\vec{b}_1| > |\vec{b}_2| > |\vec{b}_3| < |\vec{b}_4| < \cdots < |\vec{b}_\infty|$

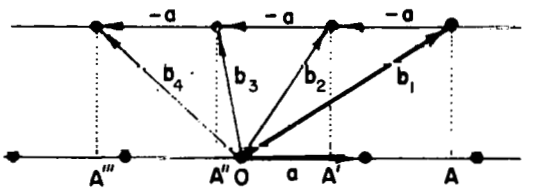



Fig. 1. The vectorial reduction of a vector.

That $|\vec{b}_3|$ is the smallest may be verified mathematically in the following manner. Let the projection of vector $\vec{b}_1$ on the lattice row containing vector $\vec{a}$ be defined as the distance OA. Similarly, let the projection of $\vec{b}_2$ on the same row be OA' and that of $\vec{b}_3$ be OA'', etc. In going from $\vec{b}_1$ to $\vec{b}_2$ to $\vec{b}_3$ the magnitude of $\vec{b}_n$ is seen to decrease as does its

projection, and from $\vec{b}_4$ to $\vec{b}_\infty$ they start to increase again. For $\vec{b}_1$ the projection OA is longer than $|a|$ but both OA' and OA'' are shorter than $|a|$. Now if $\vec{b}_2 = \vec{b}_3$ then OA' = OA'' = $\frac{1}{2}|a|$. If, however, the vectors $\vec{b}_2$ and $\vec{b}_3$ are of unequal length, then their projections are also of unequal length, one projection (in this case OA') being greater than $\frac{1}{2}|a|$ and the other (in this case OA'') being less than $\frac{1}{2}|a|$. Thus, the shortest translation $\vec{b}_n$, in general, is obtained when

$$\cos\gamma \leq \frac{\frac{1}{2}|a|}{|b|}$$

or

$$|b \cos\gamma| \leq \tfrac{1}{2}|a|.$$

If both sides are multiplied by $\vec{a}$, the following expression is obtained:

$$|ab \cos\gamma| \leq \tfrac{1}{2} a^2.$$

But $$|ab \cos\gamma| = |\vec{a} \cdot \vec{b}|,$$

whence $$|\vec{a} \cdot \vec{b}| \leq \tfrac{1}{2}a^2,$$

which is just one of the six expressions of (iii) on page 4. Note that this is merely equivalent to saying that $\vec{b}$ is the shortest translation in the ab-plane when

$$|\vec{b}| < |\vec{a} \pm \vec{b}|.$$

As the length of a vector is reduced, that is, as shorter vectors are located in a net, the angle between the two vectors involved in the reduction approaches 90° with a corresponding approach of the scalar product to zero. For instance, as $\vec{b}$ is reduced in the ab-plane, $\gamma \rightarrow 90°$ and $|\vec{a} \cdot \vec{b}| \rightarrow 0$. This immediately suggests an analytical approach to locating shorter vectors in a lattice. Suppose we can locate shorter

vectors of $\vec{b}$ as follows:

$$\vec{b}_n = \vec{b}_1 - n\vec{a}$$

where $|\vec{b}_n| < |\vec{b}_1|$. If we multiply (vertically) both sides by $\vec{a}$, we obtain

$$\vec{a} \cdot \vec{b}_n = \vec{a} \cdot \vec{b}_1 - na^2 ,$$

an expression now in a usable mathematical form for locating shorter vectors of $\vec{b}$, a form which is in terms of variables which are known, since it is equivalent (in expanded form) to

$$ab_n \cos\gamma_n = ab_1 \cos\gamma_1 - na^2 .$$

If

$$\vec{b}_n = \vec{b}_1 + n\vec{a}$$

then

$$\vec{a} \cdot \vec{b}_n = \vec{a} \cdot \vec{b}_1 + na^2 .$$

In otherwords, if $\vec{a} \cdot \vec{b}_1$ is positive, we subtract $na^2$; if $\vec{a} \cdot \vec{b}_1$ is negative, we add $na^2$. In this way $\vec{a} \cdot \vec{b}_1$ is made smaller; the net affect is reduction of $\vec{b}$ ($\vec{a}$ held constant) in the $ab_1$-plane which in turn yields a vector more orthorgonal to $\vec{a}$, that is $|\vec{b}_n| < |\vec{b}_1|$ and $|\cos\gamma_n| < |\cos\gamma_1|$. If it is desired to reduce $\vec{a}$ instead of $\vec{b}$ in the ab-plane, then $nb^2$ is appropriately added or subtracted from $\vec{a} \cdot \vec{b}$. Once the smallest $|\vec{a} \cdot \vec{b}|$ is calculated, the new cell parameters may be determined according to the usual methods (Appendix IV).

According to the foregoing discussion integral values of $a^2$, $b^2$ or $c^2$ are either added or subtracted from an unsymmetrical scalar product for reduction of a vector. These integers, n, may be used to obtain the final matrix for transforming the original triclinic cell to the reduced

cell. We first note that before any axis is reduced the initial matrix is always the identity matrix. After reduction of a vector has taken place in a particular net, the integer, n, which is obtained becomes the element $n_{ij}$ introduced into the identity matrix to form the particular matrix corresponding to the transformation of the cell before reduction to the cell obtained after reduction of the vector. Each time this process is carried out one simply starts again with the identity matrix and reduces the vector to determine its magnitude and the integer $n_{ij}$. Finally after the entire cell has been reduced, the matrix for the transformation of the original triclinic cell to the reduced cell becomes

$$N_{1\rightarrow n} = (N_{n-1\rightarrow n}) \cdots (N_{4\rightarrow 5})(N_{3\rightarrow 4})(N_{2\rightarrow 3})(N_{1\rightarrow 2})$$

where $N_{p\rightarrow q}$, whose modulus is always unity, is the matrix for the transformation of cell (p) to cell (q), cell (1) being the original cell and cell (n) the reduced cell.

To illustrate this procedure of deducing the matrix suppose we reduce a particular cell by first reducing vector $\vec{c}$ in the ac-plane, holding $\vec{a}$ fixed in magnitude. This means vector $\vec{a}$ will be added or subtracted n-times from vector $\vec{c}$ until the shortest magnitude of $\vec{c}$ is obtained; mathematically this corresponds to the addition or subtraction of $na^2$ from $\vec{a} \cdot \vec{c}$ until $|\vec{a} \cdot \vec{c}| \leq \frac{1}{2}a^2$. The integer n is therefore $n_{31}$, so that the matrix of the resulting transformation is

$$N_{1\rightarrow 2} = \begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ n_{31} & 0 & 1 \end{Vmatrix} .$$

The modulus of this matrix is unity. Now suppose we further reduce vector $\vec{c}$ this time in the new bc-plane, holding vector $\vec{b}$ fixed in magnitude. The matrix then for the transformation of the cell before reduction to that obtained after reduction of vector $\vec{c}$ in the new bc-plane is

$$N_{2\rightarrow 3} = \begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & n_{32} & 1 \end{Vmatrix} .$$

The matrix for the transformation of the original triclinic cell to the cell obtained at this stage of the reduction is

$$N_{1\rightarrow 3} = (N_{2\rightarrow 3})(N_{1\rightarrow 2}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & n_{32} & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ n_{31} & 0 & 1 \end{pmatrix} .$$

In like manner if vector $\vec{b}$ is next reduced, say in the new bc-plane holding $\vec{c}$ fixed in magnitude, the matrix for the original cell to the cell obtained at this new stage of the reduction becomes

$$N_{1\rightarrow 4} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & n_{23} \\ 0 & 0 & 1 \end{pmatrix} (N_{1\rightarrow 3})$$

etc.

The reduced cell is, as previously stated, always a primitive cell. This is required in order for it to have the smallest volume and the three shortest non-coplanar translations in the lattice. Therefore, since the cell reduction technique just described involves no change in volume,

the original cell from which the reduced cell is obtained must also be primitive. There is no restriction, of course, in subjecting centered cells to cell reduction. Since no change in volume occurs the cell obtained after reduction can never, then, be primitive with one lattice point but may still be centered in the usual sense and will have the same volume and total number of lattice points as before. Thus, if a C-centered triclinic cell undergoes reduction in its parameters, the final cell will still have the same volume, even though shorter axes, and will still contain two lattice points, being either A-, B- or C-centered, body-centered, or even a primitive cell which is centered along an edge, depending upon the particular transformation involved. Our discussion will pertain only to reduction of true primitive cells containing only one lattice point.

Of the seven crystal systems, only two may be reduced. According to the procedure heretofore described, cells may be reduced only if their unsymmetrical scalars (i.e., $\vec{a} \cdot \vec{b}$, $\vec{b} \cdot \vec{c}$, $\vec{c} \cdot \vec{a}$) are not equal to zero and are not at their minimum possible absolute value. Thus, in addition to the triclinic system in which all three axes may be reduced, the monoclinic cells may also be reduced but only in the plane containing the non-90° angle. In the monoclinic system, c-unique, only $\vec{a}$ and/or $\vec{b}$ may be reduced, the reduction being in the ab-plane; for b-unique, only $\vec{a}$ and/or $\vec{c}$ may be reduced, the reduction being in the ac-plane. All other systems have their unsymmetrical scalars either all zero or at their minimum absolute value. This simply means, then, that the primitive cells in the other five crystal systems are actually the reduced

cells. (This is not so for the centered cells, which may be reduced to their reduced cells only by first transforming them to a primitive triclinic or monoclinic cell. This is discussed in more detail in Section E-3 of this chapter.)

## B. THE REDUCED CELL IN ITS CONVENTIONAL ORIENTATION

A convention has been established for the reduced cell defining a triclinic lattice and may be stated as follows:

> The reduced cell defining a triclinic lattice is that cell which is primitive in nature (contains no centering), whose edges are the three shortest non-coplanar translations in the lattice, labelled so as to have $c < a < b$ and oriented so that the angles $\alpha$ and $\beta$ are non-acute.

(A full discussion of the convention for all seven crystal systems may be found in Crystal Data Determinative Tables, ACA Monograph No. 5, 2nd ed., (1963), p. 2.)

It may turn out that after the triclinic reduced cell has been found -- that is, after the shortest translations have been located and they satisfy conditions (i) and (ii) on page 4 -- it may not correspond to the convention stated above. A rearrangement of the axes and redefinition of the angles is thus required. To do this one simply rearranges the translations into the proper order, carrying along the corresponding angles, and then converts the angles $\alpha$ and $\beta$ to obtuse if found to be acute, obeying the rules which are discussed in the next section, rules to which one must strictly adhere for proper conversion.

## C. RULES ASSOCIATED WITH CHANGES IN CELL ORIENTATION

A cell defined by three axes and three angles is not restricted soley to one orientation. One is free to interchange the axes, to reverse the direction of the axes, to reverse the so-called character of the angles or to revert from a right-handed coordinate system to a left-handed system and vice versa. All these changes must be executed following a certain set of basic rules. Failure to do so may result in reversal of the axial sense and, even more seriously, a possible inadvertent destruction of the lattice accompanied by a change in volume.

The rules of interest are summarized below. The term "character" of an interaxial angle refers to its acute or obtuse nature, indicated by the sign of its cosine, (+) for acute and (-) for obtuse.

(i). The "reversal" in the direction of any axis directly involves two angles, the new angles always being the supplement of the old (viz., $\theta \rightarrow \pi - \theta$), since two of the three scalar products involve the reversed axis.

(a). If <u>one</u> axis is reversed (e.g., abc$\rightarrow\bar{a}$bc), the character of the angles opposite the other two axes is reversed (e.g., $\beta_{new} = \pi - \beta_{old}$ and $\gamma_{new} = \pi - \gamma_{old}$). Accompanying this change is a reverse in the sense of a, b, c, that is, there results a conversion of a right-handed coordinate system to a left-handed system, and vice versa (viz., $V = (-\vec{a}) \cdot \vec{b} \times \vec{c} = -V$).

(b). If two axes are reversed (e. g., abc→$\overline{ab}$c), the character of the two angles opposite the reversed axes is changed (e. g., $\alpha$ and $\beta$, indicated by the fact that $\bar{b}\cdot c = -(b\cdot c)$ and $\bar{a}\cdot c = -(a\cdot c)$ ); the new angles are the supplement of the old. The axial sense is not changed, since $V = (-\vec{a})\cdot(-\vec{b}) \times \vec{c} = +V$.

(c). If all three axes are reversed (e. g., abc →$\overline{abc}$), the character of no angle is changed. The axial sense is changed, however, since $V = (-\vec{a})\cdot(-\vec{b}) \times (-\vec{c}) = -V$.

(ii). If the character of any angle is changed, a second must also be changed. Thus, if the character of $\gamma$ is changed, then $(\vec{a}\cdot\vec{b})\rightarrow -(\vec{a}\cdot\vec{b})$, implying either $\vec{a}$ or $\vec{b}$ has reversed direction, thus involving a change in sign of a second unsymmetrical scalar product.

(iii). If two axes are "interchanged", the sense of the axes is also changed (e. g., if abc→acb then $+V\rightarrow -V$). To prevent this change in the axial sense, the direction of either one (namely, the unchanged axis) or all three axes must be reversed. Accompanying this change, (a) if the one axis is reversed (viz., $\bar{a}\rightarrow -\vec{a}$) the character of the angles opposite the interchanged axes (viz., opposite $\bar{b}$ and $\vec{c}$) is reversed, and (b) if all three axes are reversed, the character of no angles is changed (rule (i) above). Thus,

if $abc \rightarrow ba\bar{c}$, then ($\alpha' = \pi - \beta$ and $\beta' = \pi - \alpha$)

or if $abc \rightarrow bac$, then ($\alpha' = \beta$, $\beta' = \alpha$),

the system remains right-handed, or left-handed as the case may be.

(iv). If three axes are "interchanged" they merely permute, with no change in the axial sense (e.g., if $abc \rightarrow cab \rightarrow bca$, then +V remains +V).

Transformation matrices are affected by reversing the direction of one or more axes. Suppose a cell is transformed to a new cell and it is then desired to reverse the direction of one or more of the axes of the new cell to give a third cell with the same axial lengths. The transformation matrix from cell (1) to cell (3) can be obtained by left multiplying the transformation matrix of cell (1) to cell (2) with the matrix used for reversing the direction of the axes. Consider, for example, the reversal in the direction of axes $\vec{a}$ and $\vec{c}$ in cell (2). The matrix for transforming cell (1) to cell (3) is then

cell (2) to cell (3) (a and c reversed) | cell (1) to cell (2) | cell (1) to cell (3)

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix} \cdot \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} = \begin{pmatrix} -n_{11} & -n_{12} & -n_{13} \\ n_{21} & n_{22} & n_{23} \\ -n_{31} & -n_{32} & -n_{33} \end{pmatrix}$$

Notice this simply involves reversing the sign of the matrix elements in the rows corresponding to the axes being reversed in cell (2). This type of change holds in general for one, two, or three axes being reversed.

This leads to the following rule:

(v). Let the transformation of cell (1) to cell (2) be given by

$$\begin{pmatrix} \vec{A} \\ \vec{B} \\ \vec{C} \end{pmatrix}_{\text{Cell (2)}} = \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}_{\text{Cell (1)}}$$

The reversal in the direction of $\vec{A}$, $\vec{B}$, and/or $\vec{C}$ reverses the signs of the corresponding "row" elements of the transformation matrix. That is, if $\vec{A} \rightarrow -\vec{A}$, then $n_{11} \rightarrow -n_{11}$, $n_{12} \rightarrow -n_{12}$, $n_{13} \rightarrow -n_{13}$, and similarly for $\vec{B}$ and/or $\vec{C}$ if they are reversed.

In a three-dimensional lattice there are only four ways of obtaining a right-handed system of labelled axes differing only in the character of the angles $\alpha$, $\beta$, $\gamma$ between them; likewise there are only four ways of obtaining a left-handed system. These may be seen to comprise the eight corners of a unit cell:

| right-handed | left-handed |
|---|---|
| a b c | $\overline{\text{a b c}}$ |
| a $\overline{\text{b}}$ $\overline{\text{c}}$ | $\overline{\text{a}}$ b c |
| $\overline{\text{a}}$ b $\overline{\text{c}}$ | a $\overline{\text{b}}$ c |
| $\overline{\text{a b}}$ c | a b $\overline{\text{c}}$ |

Figure 2 shows those for the right-handed axial cross situated at the corners [000], [011], [101] and [110]. The angles $\alpha$, $\beta$, $\gamma$ which the three vectors make at one of the corners, say [000], will be $\alpha$, $\beta'$, $\gamma'$

at [011], $\alpha'$, $\beta$ , $\gamma'$ at [101] and $\alpha', \beta', \gamma$ at [110], where the primed letters designate supplementary angles ($\alpha' = 180° - \alpha$, ···, etc.)

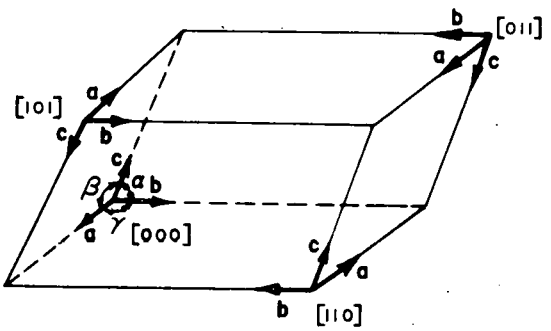



Fig. 2. The four right-handed axial representations of labelled axes in a three-dimensional lattice.

The angles $\alpha$, $\beta$, $\gamma$ at any one corner may, in general, be acute or obtuse. Consequently, there are a total of eight possible combinations, shown in tabulated form in Table 1 for each of the four right-handed axial representations[3], where the character of the angle is indicated by the sign of its cosine, (+) for acute and (-) for obtuse.

Inspection of Table 1 reveals one significant property of a lattice. In only four of the eight cases (Nos. 1, 2, 3, 4) is it possible to find all three angles obtuse. In every case, on the other hand, there exists a right-handed system with at least two angles obtuse. This fact has thus been a basis for the convention established for the triclinic reduced cell (page 12) which sets two angles obtuse and allows the third to be

Table 1. The four right-handed axial representations of labelled axes and the characters of the interaxial angles.

| Possi-bilities | Corner [[000]] | | | Corner [[011]] | | | Corner [[101]] | | | Corner [[110]] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $\alpha$ | $\beta$ | $\gamma$ | $\alpha$ | $\beta'$ | $\gamma'$ | $\alpha'$ | $\beta$ | $\gamma'$ | $\alpha'$ | $\beta'$ | $\gamma$ |
| 1 | - | - | - | - | + | + | + | - | + | + | + | - |
| 2 | - | + | + | - | - | - | + | + | - | + | - | + |
| 3 | - | - | - | - | - | - | - | - | - | - | - | - |
| 4 | + | + | - | + | - | + | - | + | + | - | - | - |
| 5 | - | - | + | - | + | - | + | - | - | + | + | + |
| 6 | - | + | - | - | - | + | + | + | + | + | - | - |
| 7 | + | - | - | + | + | + | - | - | + | - | + | - |
| 8 | + | + | + | + | - | - | - | + | + | - | - | + |

either obtuse or acute. In this way the triclinic cell whose axes are the three shortest non-coplanar translations in the lattice may be satisfied at all times; to restrict all three angles obtuse leads to a solution in only 50% of the cases.

## D. SAMPLE CELL REDUCTIONS OF SOME TRICLINIC CELLS

The following examples are intended to illustrate in principle the methods associated with the reduced cell technique. Example 1 illustrates the complete step-by-step process of obtaining the reduced cell of triclinic 16-DL methyloctadecanoic acid. Example 2 illustrates the method of converting a reduced cell to its conventional orientation for iodine trichloride in which only the angles have to be redefined. A third example may be found in Example 3, particularly step 2 and 3 on page 69, which illustrates extremely well each one of the basic rules of the previous

section for conversion of a reduced cell to its conventional orientation in a lattice. If other examples are desired for practice, the reader is referred to the excellent comprehensive reference Crystal Data Determinative Tables referred to in Section B of this chapter. All the triclinic cells defined in that volume are the "true" reduced cells; for each triclinic compound the editors have indicated the original lattice parameters reported in the literature, the parameters of the reduced cell in its conventional orientation and the matrix for transformation of the original cell to the reduced cell.

Example 1.

Crystals of 16-DL methyloctadecanoic acid, $C_{19}H_{38}O_2$, are triclinic, space group $P\bar{1}$, with lattice parameters[6]

| | |
|---|---|
| a = 5.40 Å | $\alpha$ = 145° 38' |
| b = 7.54 | $\beta$ = 105° 42' |
| c = 51.8 | $\gamma$ = 60° 18' |

Determine its reduced cell.

Solution. First a test is made to determine if this cell is already the reduced cell. To do this we will need to know the six scalar products.

$$\vec{a} \cdot \vec{b} = ab \cos\gamma = (5.40)(7.54) \cos 60° 18' = +20.17$$

$$\vec{b} \cdot \vec{c} = bc \cos\alpha = (7.54)(51.8) \cos 145° 38' = -322.39$$

$$\vec{c} \cdot \vec{a} = ca \cos\beta = (51.8)(5.40) \cos 105° 42' = -75.69$$

$$\vec{a} \cdot \vec{a} = a^2 = (5.40)^2 = 29.16$$

$$\vec{b} \cdot \vec{b} = b^2 = (7.54)^2 = 56.85$$

$$\vec{c} \cdot \vec{c} = c^2 = (51.8)^2 = 2683.24$$

(i). Test

Is $|+20.17| \leq \frac{1}{2}(29.16)$ ? No.

Is $|+20.17| \leq \frac{1}{2}(56.85)$ ? Yes.

Is $|-322.39| \leq \frac{1}{2}(56.85)$ ? No.

Is $|-322.39| \leq \frac{1}{2}(2683.24)$ ? Yes.

Is $|-75.69| \leq \frac{1}{2}(2683.24)$ ? Yes.

Is $|-75.69| \leq \frac{1}{2}(29.16)$ ? No.

Since three of the six tests fail, it may be concluded that the cell is not a reduced cell. We therefore proceed to part (ii).

(ii). The Cell Reduction

Reduction of c.

Inspection of the three scalar products $\vec{a} \cdot \vec{b}$, $\vec{b} \cdot \vec{c}$, and $\vec{c} \cdot \vec{a}$ reveals that $\vec{b} \cdot \vec{c}$ is the largest in absolute value. Furthermore, of vectors $\vec{b}$ and $\vec{c}$, $\vec{c}$ is the larger. Therefore, $\vec{c}$ is reduced first and $\vec{b}$ is held constant in magnitude. The product $\vec{b} \cdot \vec{c}$ is negative in value, so integral values of $b^2$ $(= \vec{b} \cdot \vec{b})$ must be added to the scalar product to reduce its value.

$$\vec{b}_2 \cdot \vec{c}_2 = \vec{b}_1 \cdot \vec{c}_1 + nb_1^2 = (-322.39) + n\,(56.85)$$

$= -322.39$ when $n=0$

$= -265.54$ $n=1$

$= -208.69$ $n=2$

$= -151.84$ $n=3$

$= -94.99$ $n=4$

$= -38.14$ $n=5$

$= +18.71$ $n=6$ ←

$= +75.56$ $n=7$

When n = 6 the scalar product $\vec{b}_2 \cdot \vec{c}_2$ is seen to attain its minimum absolute value. Figure 3 illustrates the reduction in $\vec{c}$ that has just occurred.

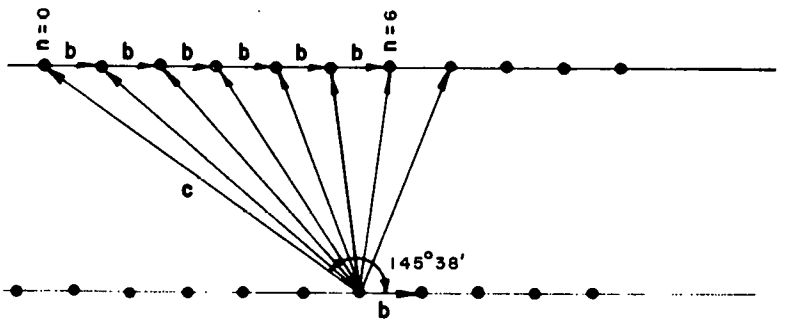



Fig. 3. The vectorial reduction of vector $\vec{c}$ by vector $\vec{b}$ in the $\vec{b}\,\vec{c}$ -plane.

The relationships of the vectors in the old and new cell are thus the following:

| Original Cell | New Cell |
|---|---|
| $\vec{a}_1$ | $\vec{a}_2 = \vec{a}_1$ |
| $\vec{b}_1$ | $\vec{b}_2 = \vec{b}_1$ |
| $\vec{c}_1$ | $\vec{c}_2 = \vec{c}_1 + 6\vec{b}_1$ |
| $\vec{a}_1 \cdot \vec{b}_1$ | $\vec{a}_2 \cdot \vec{b}_2 = \vec{a}_1 \cdot \vec{b}_1$ |
| $\vec{b}_1 \cdot \vec{c}_1$ | $\vec{b}_2 \cdot \vec{c}_2 = \vec{b}_1 \cdot (\vec{c}_1 + 6\vec{b}_1) = \vec{b}_1 \cdot \vec{c}_1 + 6b_1^2$ |
| $\vec{c}_1 \cdot \vec{a}_1$ | $\vec{c}_2 \cdot \vec{a}_2 = (\vec{c}_1 + 6\vec{b}_1) \cdot \vec{a}_1 = \vec{c}_1 \cdot \vec{a}_1 + 6\vec{b}_1 \cdot \vec{a}_1$ |

Their calculated values in the new cell are

$$a_2 = a_1 = 5.40$$

$$b_2 = b_1 = 7.54$$

$$c_2 = \sqrt{(\vec{c}_1 + 6\vec{b}_1)\cdot(\vec{c}_1 + 6\vec{b}_1)} = 29.35$$

i.e., $$c_2^2 = \vec{c}_2 \cdot \vec{c}_2 = (\vec{c}_1 + 6\vec{b}_1)\cdot(\vec{c}_1 + 6\vec{b}_1)$$

$$= c_1^2 + 12\,\vec{b}_1 \cdot \vec{c}_1 + 36 b_1^2$$

$$= (51.8)^2 + 12\,(-322.39) + 36\,(7.54)^2$$

$$= 861.22$$

$$c_2 = \sqrt{861.22} = 29.35$$

$$\vec{a}_2 \cdot \vec{b}_2 = \vec{a}_1 \cdot \vec{b}_1 = +20.17$$

$$\vec{b}_2 \cdot \vec{c}_2 = \vec{b}_1 \cdot \vec{c}_1 + 6b_1^2 = +18.71$$

$$\vec{c}_2 \cdot \vec{a}_2 = \vec{c}_1 \cdot \vec{a}_1 + 6\vec{b}_1 \cdot \vec{a}_1 = -75.69 + 6\,(+20.17) = +45.33$$

The transformation matrix from the original cell to the new cell is

$$\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 6 & 1 \end{Vmatrix} .$$

Further Reduction of c.

A test may now be made to determine if the vector $\vec{c}$ can be reduced even further, this time in the ac plane.

Is $$|\vec{c}_2 \cdot \vec{a}_2| \leq \tfrac{1}{2} a_2^2 \quad ?$$

$$|+45.33| \leq \tfrac{1}{2}\,(29.16) \quad ? \qquad \text{No.}$$

Therefore, $\vec{c}$ can be reduced still further. The reduction will occur in the new ac plane and values of $a^2$ must be subtracted from $\vec{c}_2 \cdot \vec{a}_2$, a positive quantity.

$$\vec{c}_3 \cdot \vec{a}_3 = \vec{c}_2 \cdot \vec{a}_2 - n a_2^2 = (+45.33) - n\,(29.16)$$

$= +45.33$ when $n=0$

$= +16.17$ $n=1$

$= -12.99$ $n=2$ ←

$= -42.15$ $n=3$

The relationships of the vectors in the old and new cell are now the following:

| Original Cell | New Cell |
|---|---|
| $\vec{a}_2$ | $\vec{a}_3 = \vec{a}_2$ |
| $\vec{b}_2$ | $\vec{b}_3 = \vec{b}_2$ |
| $\vec{c}_2$ | $\vec{c}_3 = \vec{c}_2 - 2\vec{a}_2$ |
| $\vec{a}_2 \cdot \vec{b}_2$ | $\vec{a}_3 \cdot \vec{b}_3 = \vec{a}_2 \cdot \vec{b}_2$ |
| $\vec{b}_2 \cdot \vec{c}_2$ | $\vec{b}_3 \cdot \vec{c}_3 = \vec{b}_2 \cdot (\vec{c}_2 - 2\vec{a}_2) = \vec{b}_2 \cdot \vec{c}_2 - 2\vec{b}_2 \cdot \vec{a}_2$ |
| $\vec{c}_2 \cdot \vec{a}_2$ | $\vec{c}_3 \cdot \vec{a}_3 = (\vec{c}_2 - 2\vec{a}_2) \cdot \vec{a}_2 = \vec{c}_2 \cdot \vec{a}_2 - 2\vec{a}_2^2$ |

Their calculated values in the new cell are

$$a_3 = a_2 = 5.40$$

$$b_3 = b_2 = 7.54$$

$$c_3 = \sqrt{(\vec{c}_2 - 2\vec{a}_2) \cdot (\vec{c}_2 - 2\vec{a}_2)} = 28.22$$

$$\vec{a}_3 \cdot \vec{b}_3 = \vec{a}_2 \cdot \vec{b}_2 = +20.17$$

$$\vec{b}_3 \cdot \vec{c}_3 = \vec{b}_2 \cdot \vec{c}_2 - 2\vec{b}_2 \cdot \vec{a}_2 = -21.63$$

$$\vec{c}_3 \cdot \vec{a}_3 = \vec{c}_2 \cdot \vec{a}_2 - 2a_2^2 = -12.99$$

The new transformation matrix (from the original cell) is now

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \overline{2} & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 6 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \overline{2} & 6 & 1 \end{pmatrix}$$

Reduction of b.

Of the original parameters $\vec{a}_1$, $\vec{b}_1$ and $\vec{c}_1$, $\vec{b}_1$ was seen to have the second largest value. It may thus be reduced next. A test may be made to determine in which plane the reduction will have to be made.

Is $|\vec{b}_3 \cdot \vec{c}_3| \leq \frac{1}{2} c_3^2$ ?

$|-21.63| \leq \frac{1}{2}(796.54)$. Yes.

Is $|\vec{a}_3 \cdot \vec{b}_3| \leq \frac{1}{2} a_3^2$ ?

$|+20.17| \leq \frac{1}{2}(29.16)$. No.

Therefore, the vector $\vec{b}\,(=\vec{b}_3)$ can be reduced in the ab plane, using $\vec{a}_3 \cdot \vec{b}_3$.

$$\vec{a}_4 \cdot \vec{b}_4 = \vec{a}_3 \cdot \vec{b}_3 - n\, a_3^2 = (+20.17) - n\,(29.16)$$

$= +20.17$ when $n=0$

$= -8.99$ $n=1$ ←

$= -38.15$ $n=2$

The relationships of the vectors in the old and new cell are now the following:

| Original Cell | New Cell |
|---|---|
| $\vec{a}_3$ | $\vec{a}_4 = \vec{a}_3$ |
| $\vec{b}_3$ | $\vec{b}_4 = \vec{b}_3 - \vec{a}_3$ |
| $\vec{c}_3$ | $\vec{c}_4 = \vec{c}_3$ |
| $\vec{a}_3 \cdot \vec{b}_3$ | $\vec{a}_4 \cdot \vec{b}_4 = \vec{a}_3 \cdot (\vec{b}_3 - \vec{a}_3) = \vec{a}_3 \cdot \vec{b}_3 - a_3^2$ |
| $\vec{b}_3 \cdot \vec{c}_3$ | $\vec{b}_4 \cdot \vec{c}_4 = (\vec{b}_3 - \vec{a}_3) \cdot \vec{c}_3 = \vec{b}_3 \cdot \vec{c}_3 - \vec{a}_3 \cdot \vec{c}_3$ |
| $\vec{c}_3 \cdot \vec{a}_3$ | $\vec{c}_4 \cdot \vec{a}_4 = \vec{c}_3 \cdot \vec{a}_3$ |

Their calculated values in the new cell are

$$a_4 = a_3 = 5.40$$

$$b_4 = \sqrt{(\vec{b}_3 - \vec{a}_3)\cdot(\vec{b}_3 - \vec{a}_3)} = 6.76$$

$$c_4 = c_3 = 28.22$$

$$\vec{a}_4 \cdot \vec{b}_4 = -8.99$$

$$\vec{b}_4 \cdot \vec{c}_4 = \vec{b}_3 \cdot \vec{c}_3 - \vec{a}_3 \cdot \vec{c}_3 = -8.64$$

$$\vec{c}_4 \cdot \vec{a}_4 = \vec{c}_3 \cdot \vec{a}_3 = -12.99$$

The new transformation matrix (from the original cell) is now

$$\begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \bar{2} & 6 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & 1 & 0 \\ \bar{2} & 6 & 1 \end{pmatrix} .$$

Testing the new scalar product $\vec{b}_4 \cdot \vec{c}_4$ against $\frac{1}{2}c_4^2$ indicates reduction of vector $\vec{b}$ is essentially complete.

Reduction of a.

The remaining translation, $\vec{a}$, is now reduced next. A test is made to determine in which plane the reduction will be necessary or if reduction can occur at all.

Is $|\vec{c}_4 \cdot \vec{a}_4| \leq \frac{1}{2} c_4^2$ ?

$|-12.99| \leq \frac{1}{2}(796.54)$ ? Yes.

Is $|\vec{a}_4 \cdot \vec{b}_4| \leq \frac{1}{2} b_4^2$ ?

$|-8.99| \leq \frac{1}{2}(45.67)$, ? Yes.

Reduction of the original triclinic cell is thus complete. Testing the original six conditions using the values obtained for $a_1$, $b_1$, $c_1$,

$\vec{a}_4 \cdot \vec{b}_4$, $\vec{b}_4 \cdot \vec{c}_4$ and $\vec{c}_4 \cdot \vec{a}_4$ verifies this and additional cycles are unnecessary. The cell parameters of the reduced triclinic cell are thus

$$a_4 = 5.40 \text{ Å}$$

$$b_4 = 6.76$$

$$c_4 = 28.22$$

$$\cos \alpha = \frac{\vec{b}_4 \cdot \vec{c}_4}{b_4 c_4} = \frac{-8.64}{(6.76)(28.22)} = -0.04529$$

$$\alpha = \cos^{-1} (-0.04529) = 92° 36'$$

$$\cos \beta = \frac{\vec{c}_4 \cdot \vec{a}_4}{c_4 a_4} = \frac{-12.99}{(28.22)(5.40)} = -0.08524$$

$$\beta = \cos^{-1} (-0.08524) = 94° 53'$$

$$\cos \gamma = \frac{\vec{a}_4 \cdot \vec{b}_4}{a_4 b_4} = \frac{-8.99}{(5.40)(6.76)} = -0.24627$$

$$\gamma = \cos^{-1} (-0.24627) = 104° 15'$$

The transformation matrix from the original triclinic cell to the reduced cell is thus

$$\begin{Vmatrix} 1 & 0 & 0 \\ \bar{1} & 1 & 0 \\ \bar{2} & 6 & 1 \end{Vmatrix} .$$

Now, the conventional orientation of the reduced cell in a triclinic lattice is

$$c < a < b$$

$\alpha$, $\beta$ obtuse.

Therefore, the lattice parameters of the reduced cell become (upon rearrangement)

| | |
|---|---|
| a = 6.76 Å | $\alpha$ = 94° 53' |
| b = 28.22 | $\beta$ = 104° 15' |
| c = 5.40 | $\gamma$ = 92° 36' |

The corresponding transformation matrix is

$$\begin{Vmatrix} \bar{1} & 1 & 0 \\ \bar{2} & 6 & 1 \\ 1 & 0 & 0 \end{Vmatrix} .$$

Example 2.

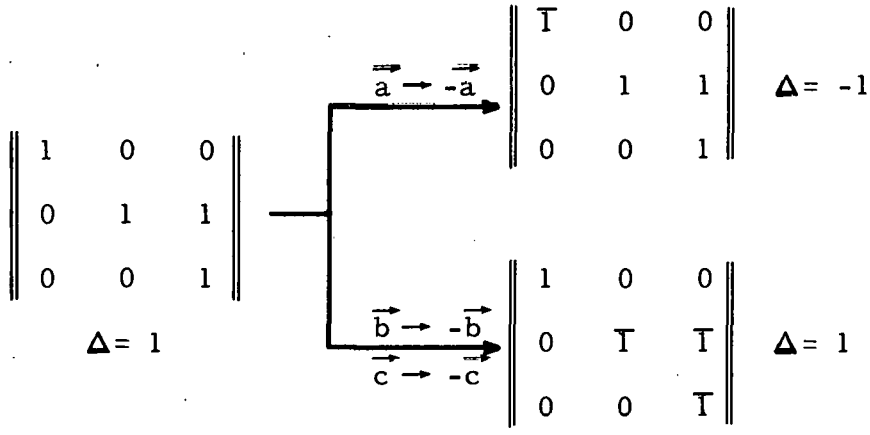
Crystals of iodine trichloride, $I_2Cl_6$, are triclinic, space group $P\bar{1}$, with lattice parameters a = 5.71, b = 10.88, c = 5.48 Å and $\alpha$ = 130° 50', $\beta$ = 80° 50', $\gamma$ = 108° 30'. Upon transformation to its reduced cell the parameters become a = 5.71, b = 8.39, c = 5.48 Å and $\alpha$ = 101° 13', $\beta$ = 80° 50' and $\gamma$ = 107° 54'. The corresponding transformation matrix is 100/011/001. Determine the parameters of the reduced cell in its conventional orientation.

Solution. The convention is $c < a < b$ with $\alpha$, $\beta$ obtuse. The axial lengths of the reduced cell in the orientation indicated are seen to be in the proper order. The angle $\beta$ however does not conform to the convention and must be corrected. The change which is required is the following:

$$\beta' = \pi - \beta = \pi - 80° 50' = 99° 10'$$

$$\gamma' = \pi - \gamma = \pi - 107° 54' = 72° 6' .$$

Such a change results from two possible changes in the axes: a reversal in the direction of the a-axis only or the reversal in the directions of both the b- and c-axes. We may take our choice. The transformation matrix corresponding to the two possible changes are illustrated below.




Notice that one is related to the other by a change in sign of all nine elements. The former ($\Delta = -1$) involves a conversion from say, a right-handed system to a left-handed system; the latter ($\Delta = 1$) a retention of sense.

## E. APPLICATIONS

Once a unit cell has been identified from single crystal or powder diffraction data, one question often asked is whether or not a unit cell of symmetry higher than the observed one actually exists and if so what is it, how is it oriented relative to the observed one, and what are its dimensions? The reduced cell and the method of finding it provides the answer.

## 1. THE 43 REDUCED CELLS

In 1928 P. Niggli showed that there are only 43 unique reduced cell types[4]. He showed that by considering all the possible combinations of axial lengths and interaxial angles in the fourteen Bravais lattices, there result just these 43 cells whose axes correspond to the three shortest non-coplanar translations in the lattice. Its six scalars -- $\vec{a}\cdot\vec{a}$, $\vec{b}\cdot\vec{b}$, $\vec{c}\cdot\vec{c}$, $\vec{b}\cdot\vec{c}$, $\vec{c}\cdot\vec{a}$, $\vec{a}\cdot\vec{b}$ -- consequently contain complete information about the Bravais lattice of highest symmetry which it represents. In representing the reduced cell by its scalar products the following matrix representation was proposed by him:

$$\begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{c}\cdot\vec{c} \\ \vec{b}\cdot\vec{c} & \vec{c}\cdot\vec{a} & \vec{a}\cdot\vec{b} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{22} & r_{33} \\ r_{23} & r_{31} & r_{12} \end{pmatrix}$$

where $a < b < c$ with $\alpha$, $\beta$, $\gamma$ all obtuse or all acute.

As examples of three of the 43 reduced cell types, let us consider the three cubic lattices shown in Figure 4. In each lattice the reduced cell is outlined in bold lines with axes labelled **e** (after Niggli[4]).

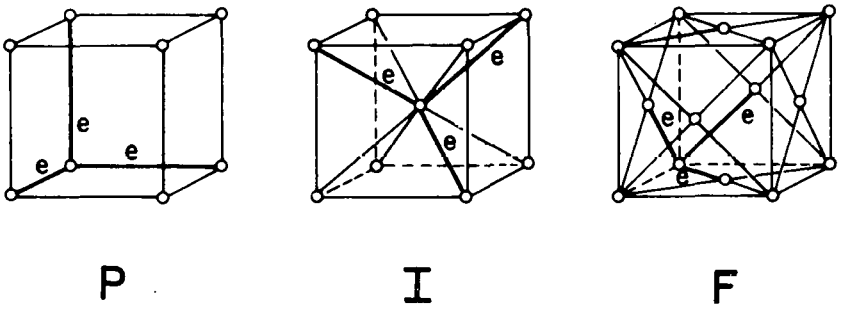



Fig. 4. The three cubic lattices and their reduced cell.

In the primitive case the three shortest vectors correspond to the edges of the cell itself. Its scalar products are thus

$$r_{11} = r_{22} = r_{33} = \vec{e} \cdot \vec{e} = a^2$$

$$r_{23} = r_{31} = r_{12} = \vec{e} \cdot \vec{e} = e^2 \cos 90° = 0,$$

its reduced form therefore being

$$\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ 0 & 0 & 0 \end{pmatrix}.$$

The three shortest vectors in the body-centered cubic lattice correspond to the lines joining three non-adjacent corners of the cube with the center of the cube, thus lying along the body-diagonals. These three vectors are thus seen to actually form a rhombohedral cell with $\alpha = 109° 28' 16.4''$, $\cos \alpha = -1/3$. For this reduced cell we have

$$r_{11} = r_{22} = r_{33} = e^2 = \left(\frac{\sqrt{3}a}{2}\right)^2 = \frac{3a^2}{4}$$

$$r_{23} = r_{31} = r_{12} = \vec{e} \cdot \vec{e} = e^2 \cos \alpha = e^2\left(-\frac{1}{3}\right) = -\frac{r_{11}}{3}.$$

Its reduced form is thus

$$\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \frac{-}{r}_{11} & \frac{-}{r}_{11} & \frac{-}{r}_{11} \\ \overline{3} & \overline{3} & \overline{3} \end{pmatrix}.$$

The three shortest vectors in a face-centered cubic lattice correspond to the reduced cell whose axes join a corner of the cube with the three nearest face-centers, thus lying along the face-diagonals to form a rhombohedral cell with $\alpha = 60°$, $\cos \alpha = \frac{1}{2}$. This reduced cell is a reciprocal of the reduced cell in a body-centered cubic lattice. For this cell we have

$$r_{11} = r_{22} = r_{33} = e^2 = \left(\frac{\sqrt{2}a}{2}\right)^2 = \frac{a^2}{2}$$

$$r_{23} = r_{31} = r_{12} = \vec{e} \cdot \vec{e} = e^2 \cos 60° = e^2\left(\tfrac{1}{2}\right) = \frac{r_{11}}{2} .$$

Its reduced form is thus

$$\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \frac{r_{11}}{2} & \frac{r_{11}}{2} & \frac{r_{11}}{2} \end{pmatrix} .$$

The reduced cell is thus seen to be a special one. Its six scalars are seen to characterize a particular Bravais lattice, its axial lengths and interaxial angles. Herein lies the "link" between any cell in a lattice and cells of higher symmetry. By the method outlined in the preceding sections of this chapter, the cell is transformed to its reduced cell. Its reduced form will be one of the 43 possible reduced forms. By comparing its six scalars with those in Tables 2 and 3, the crystal system and lattice type of highest symmetry in the lattice may be readily identified, keeping in mind, of course, the possibility of pseudo-cells since the reduced form says nothing about symmetry, just axial lengths and interaxial angles.

## 2. ORGANIZATION AND USE OF TABLES 2 AND 3

The 43 reduced cell types and their reduced forms are listed in Tables 2 and 3. Their corresponding orientation in the Bravais lattice appear in Figure 5 where $\vec{a}$, $\vec{b}$, $\vec{c}$ are the axes of the reduced cell in its conventional orientation and $\vec{A}$, $\vec{B}$, $\vec{C}$ are the axes of the unit cell. The reduced forms appearing in these two tables appear in revised form from

those found in Niggli's original work[4] and from the reduced forms tabulated in Azároff and Buerger[2], which are based directly on Niggli's work. Niggli defined the orientation of his reduced cell as $a < b < c$ with $\alpha$, $\beta$, $\gamma$ either all obtuse or all acute, giving rise to what he called "positive" reduced forms and "negative" reduced forms respectively. The reduced cell has since been standardized to be $c < a < b$ with $\alpha$, $\beta$ obtuse (p. 12). Tables 2 and 3 are based on this convention. In most cases only one reduced form is possible; that is, only one orientation of the reduced cell in the lattice is possible which conforms to this convention. In other cases there are two possibilities, one with $\gamma$ acute and the other with $\gamma$ obtuse, just as in the case of the convention used by Niggli where a positive reduced form and a negative reduced form could co-exist in the same lattice. When two such orientations are possible, both are given to facilitate quick and rapid reference. (Note that a, b, c, $\alpha$ and $\beta$ remain unchanged in the two orientations. Note also that the reduced cell is defined soley by its three axial vectors; the character of its interaxial angles defines its orientation.) Consequently, if a reduced cell is converted to its conventional orientation, these tables may be used directly.

In practice the procedure of identifying the unit cell and lattice type from a knowledge of the reduced cell is as follows: First, the symmetrical scalars (i.e., $\vec{a} \cdot \vec{a}$, $\vec{b} \cdot \vec{b}$, $\vec{c} \cdot \vec{c}$ - in that order) of the conventional reduced cell are placed into one of the following four categories, as defined on page 29in terms of $r_{11}$, $r_{22}$ and $r_{33}$:

$r_{11} = r_{22} = r_{33}$

$r_{11} = r_{22} \neq r_{33}$

$r_{11} \neq r_{22} \neq r_{33}$ (where $r_{11} = r_{33} \neq r_{22}$)

$r_{11} \neq r_{22} \neq r_{33}$

Using Table 2 and the catagory established for the symmetrical scalars, to within reasonable experimental error, the unsymmetrical scalars (i.e., $\vec{b} \cdot \vec{c}$, $\vec{c} \cdot \vec{a}$, $\vec{a} \cdot \vec{b}$ - in that order) are examined next to determine to which subcatagory they belong. In doing this they are searched for specializations, such as one or more being zero, one or more being related to each other or related to the symmetrical scalars. From this it is possible to deduce immediately the crystal system of highest symmetry, if one exists. Finally, using Table 3 and the cell number in parentheses obtained from Table 2, the transformation from the reduced cell to the unit cell, and its lattice type, may be obtained.

Using Table 3 the cell parameters of the unit cell may be found by two different methods, using either the direct transformation matrix appearing in column 4 or the formulas appearing in column 5. If the matrix in column 4 is used, the method proceeds according to that given in Appendix IV. If the formulas in column 5 are used, the actual scalars are simply inserted directly into the expressions listed.

The expressions in column 5 of Table 3 are based directly on the matrix appearing in column 4 and the reduced form appearing in column 3. The following illustration shows their derivation for Orthorhombic (26a). According to Table 3 the reduced form (whose general form is defined on page 29) and the transformation matrix for this cell are, respectively

$$\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \frac{1}{2}\overline{r}_{33} & \frac{1}{2}\overline{r}_{33} & r_{12} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 1 & 1 \\ \overline{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} .$$

The formula for $A^2$ in terms of the reduced cell scalars is

$$\begin{aligned} A^2 &= (\vec{a} + \vec{b} + \vec{c}) \cdot (\vec{a} + \vec{b} + \vec{c}) \\ &= \vec{a} \cdot \vec{a} + \vec{b} \cdot \vec{b} + \vec{c} \cdot \vec{c} + 2\vec{b} \cdot \vec{c} + 2\vec{c} \cdot \vec{a} + 2\vec{a} \cdot \vec{b} \\ &= r_{11} + r_{11} + r_{33} + \frac{2\overline{r}_{33}}{2} + \frac{2\overline{r}_{33}}{2} + 2r_{12} \\ &= 2(r_{11} + r_{12}) - r_{33} . \end{aligned}$$

The expressions for $B^2$ and $C^2$ may be similarly obtained using

$$B^2 = (-\vec{a} + \vec{b}) \cdot (-\vec{a} + \vec{b})$$

and

$$C^2 = (\vec{c}) \cdot (\vec{c}) .$$

Figure 5, as previously indicated, consists of the schematic diagrams of the various reduced cells(with axes $\vec{a}$, $\vec{b}$, $\vec{c}$) outlined in their respective Bravais space-lattice (with axes $\vec{A}$, $\vec{B}$, $\vec{C}$). They are based directly on Niggli's original figures (Figures 44 - 58)[4] with a few modifications.*

*Permission to use Figures 44 - 58 due to Niggli[4] was kindly granted by Akademische Verlagsgesellschaft, Frankfurt Am Main, Germany.

Table 2 (pages 36-39)

Table 3 (pages 40-60)

Table 2. The "Unsymmetrical" Scalars of the 43 reduced cell types in their conventional orientation ($c < a < b$; $\alpha$, $\beta$ obtuse).

A. Symmetrical Scalars: $r_{11} = r_{22} = r_{33}$

| Unsym. Scalars: | | | | |
|---|---|---|---|---|
| 0 | 0 | 0 | | Cubic (41) |
| $\frac{1}{2}\bar{r}_{11}$ | $\frac{1}{2}\bar{r}_{11}$ | $\frac{1}{2}r_{11}$ | | Cubic (43) |
| $\bar{r}_{23}$ | $\bar{r}_{23}$ | $r_{23}$ | | Rhombohedral (36) |
| $\bar{r}_{23}$ | $\bar{r}_{23}$ | $\bar{r}_{23}$ | | Rhombohedral (37) |
| $\frac{1}{3}\bar{r}_{11}$ | $\frac{1}{3}\bar{r}_{11}$ | $\frac{1}{3}r_{11}$ | | Cubic (42) |
| two equal | | (sum = $-r_{11}$) | | Tetragonal (34a,b,c) |
| three unequal | | (sum = $-r_{11}$) | | Orthorhombic (25a,b,c) |

B. Symmetrical Scalars: $r_{11} = r_{22} \neq r_{33}$

| Unsym. Scalars: | | | | |
|---|---|---|---|---|
| 0 | 0 | 0 | | Tetragonal (31) |
| 0 | 0 | $\frac{1}{2}r_{11}$ | | Hexagonal (40a) |
| 0 | 0 | $\frac{1}{2}\bar{r}_{11}$ | | Hexagonal (40b) |
| 0 | 0 | $r_{12}$ | | Orthorhombic (24a) |
| 0 | 0 | $\bar{r}_{12}$ | | Orthorhombic (24b) |

Table 2. (continued).

B. con't.

| | | | |
|---|---|---|---|
| $\frac{1}{2}\bar{r}_{33}$ | $\frac{1}{2}\bar{r}_{33}$ | $\frac{1}{4}r_{33}$ | Tetragonal (33) |
| $\frac{1}{2}\bar{r}_{33}$ | $\frac{1}{2}\bar{r}_{33}$ | $r_{12}$ | Orthorhombic (26a) |
| $\frac{1}{2}\bar{r}_{33}$ | $\frac{1}{2}\bar{r}_{33}$ | $\bar{r}_{12}$ | Orthorhombic (26b) |
| $\frac{1}{3}\bar{r}_{33}$ | $\frac{1}{3}\bar{r}_{33}$ | $\frac{1}{2}(\bar{r}_{11} - \frac{1}{3}\bar{r}_{33})$ | Rhombohedral (38) |
| $\bar{r}_{23}$ | $\bar{r}_{23}$ | $r_{12}$ | Monoclinic (14) |
| $\bar{r}_{23}$ | $\bar{r}_{23}$ | $\bar{r}_{12}$ | Monoclinic (15) |

C. Symmetrical Scalars: $r_{11} \neq r_{22} \neq r_{33}$ (where $r_{11} = r_{33} \neq r_{22}$)

| | | | | |
|---|---|---|---|---|
| Unsym. Scalars: | 0 | 0 | 0 | Tetragonal (30) |
| | 0 | $\frac{1}{2}\bar{r}_{11}$ | 0 | Hexagonal (39) |
| | 0 | $\bar{r}_{31}$ | 0 | Orthorhombic (23) |
| | $\frac{1}{2}\bar{r}_{11}$ | 0 | $\frac{1}{2}r_{11}$ | Tetragonal (32a) |
| | $\frac{1}{2}\bar{r}_{11}$ | 0 | $\frac{1}{2}\bar{r}_{11}$ (sum $= -r_{11}$) | Tetragonal (32b) |
| | $\bar{r}_{23}$ | $\bar{r}_{31}$ | $r_{23}$ | Monoclinic (12) |
| | $\bar{r}_{23}$ | $\bar{r}_{31}$ | $\bar{r}_{23}$ | Monoclinic (13) |
| | $\frac{1}{2}\bar{r}_{11}$ | $\frac{1}{2}\bar{r}_{11}$ | $\frac{1}{2}r_{11}$ | Rhombohedral (35) |
| $\bar{r}_{23}$ | $(\bar{r}_{11} - 2\bar{r}_{23})$ | $\bar{r}_{23}$ | (sum $= -r_{11}$) | Orthorhombic (28) |
| $\bar{r}_{23}$ | $(\bar{r}_{11} - \bar{r}_{23} - \bar{r}_{12})$ | $\bar{r}_{12}$ | (sum $= -r_{11}$) | Monoclinic (7) |

Table 2. (continued).

D. Symmetrical Scalars: $r_{11} \neq r_{22} \neq r_{33}$

| | | | | |
|---|---|---|---|---|
| Unsym. Scalars: | 0 | 0 | 0 | Orthorhombic (19) |
| | 0 | 0 | $\frac{1}{2}r_{11}$ | Orthorhombic (22a) |
| | 0 | 0 | $\frac{1}{2}\bar{r}_{11}$ | Orthorhombic (22b) |
| | 0 | 0 | $r_{12}$ | Monoclinic (4a) |
| | 0 | 0 | $\bar{r}_{12}$ | Monoclinic (4b) |
| | 0 | $\frac{1}{2}\bar{r}_{33}$ | 0 | Orthorhombic (20) |
| | 0 | $\bar{r}_{31}$ | 0 | Monoclinic (5) |
| | 0 | $\frac{1}{2}\bar{r}_{33}$ | $r_{12}$ | Monoclinic (9a) |
| | 0 | $\frac{1}{2}\bar{r}_{33}$ | $\bar{r}_{12}$ | Monoclinic (9b) |
| | $\frac{1}{2}\bar{r}_{33}$ | 0 | 0 | Orthorhombic (21) |
| | $\bar{r}_{23}$ | 0 | 0 | Monoclinic (3) |
| | $\frac{1}{2}\bar{r}_{33}$ | 0 | $\frac{1}{2}r_{11}$ | Orthorhombic (27a) |
| | $\frac{1}{2}\bar{r}_{33}$ | 0 | $\frac{1}{2}\bar{r}_{11}$ | Orthorhombic (27b) |
| | $\frac{1}{2}\bar{r}_{33}$ | 0 | $r_{12}$ | Monoclinic (11a) |
| | $\frac{1}{2}\bar{r}_{33}$ | 0 | $\bar{r}_{12}$ | Monoclinic (11b) |
| | $\bar{r}_{23}$ | 0 | $\frac{1}{2}r_{11}$ | Monoclinic (10a) |
| | $\bar{r}_{23}$ | 0 | $\frac{1}{2}\bar{r}_{11}$ | Monoclinic (10b) |

Table 2. (continued).

D. con't.

| | |
|---|---|
| $\frac{1}{2}\bar{r}_{33}$ $\frac{1}{2}\bar{r}_{33}$ $\frac{1}{4}r_{33}$ | Orthorhombic (29) |
| $\frac{1}{2}\bar{r}_{33}$ $\frac{1}{2}\bar{r}_{33}$ $r_{12}$ | Monoclinic (8) |
| $\frac{1}{2}\bar{r}_{33}$ $\bar{r}_{31}$ $\frac{1}{2}r_{31}$ | Monoclinic (16) |
| $\frac{1}{2}\bar{r}_{31}$ $\bar{r}_{31}$ $\frac{1}{2}r_{11}$ | Monoclinic (17) |
| $\bar{r}_{23}$ $\frac{1}{2}\bar{r}_{33}$ $\frac{1}{2}r_{23}$ | Monoclinic (18) |
| $\frac{1}{2}(\bar{r}_{33}-\bar{r}_{31})$ $\bar{r}_{31}$ $\frac{1}{2}(\bar{r}_{11}-\bar{r}_{31})$ [sum $= \frac{1}{2}(r_{11} + r_{33})$] | Monoclinic (6) |
| $\bar{r}_{23}$ $\bar{r}_{31}$ $r_{12}$ | Triclinic (1) |
| $\bar{r}_{23}$ $\bar{r}_{31}$ $\bar{r}_{12}$ | Triclinic (2) |

Table 3. The reduced forms and transformation matrices for the 43 reduced cells.

## TRICLINIC

| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 1 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & \bar{r}_{31} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | |
| 2 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & \bar{r}_{31} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | |

## MONOCLINIC (c-unique)

| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 3 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = r_{22}$<br>$C^2 = r_{11}$<br>$\cos\gamma = \bar{r}_{23}/AB$ |
| 4a | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & 0 & r_{12} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = r_{22}$<br>$C^2 = r_{33}$<br>$\cos\gamma = -r_{12}/AB$ |
| 4b | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & 0 & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = r_{22}$<br>$C^2 = r_{33}$<br>$\cos\gamma = \bar{r}_{12}/AB$ |
| 5 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & \bar{r}_{31} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$ | $A = r_{33}$<br>$B = r_{11}$<br>$C = r_{22}$<br>$\cos\gamma = \bar{r}_{31}/AB$ |

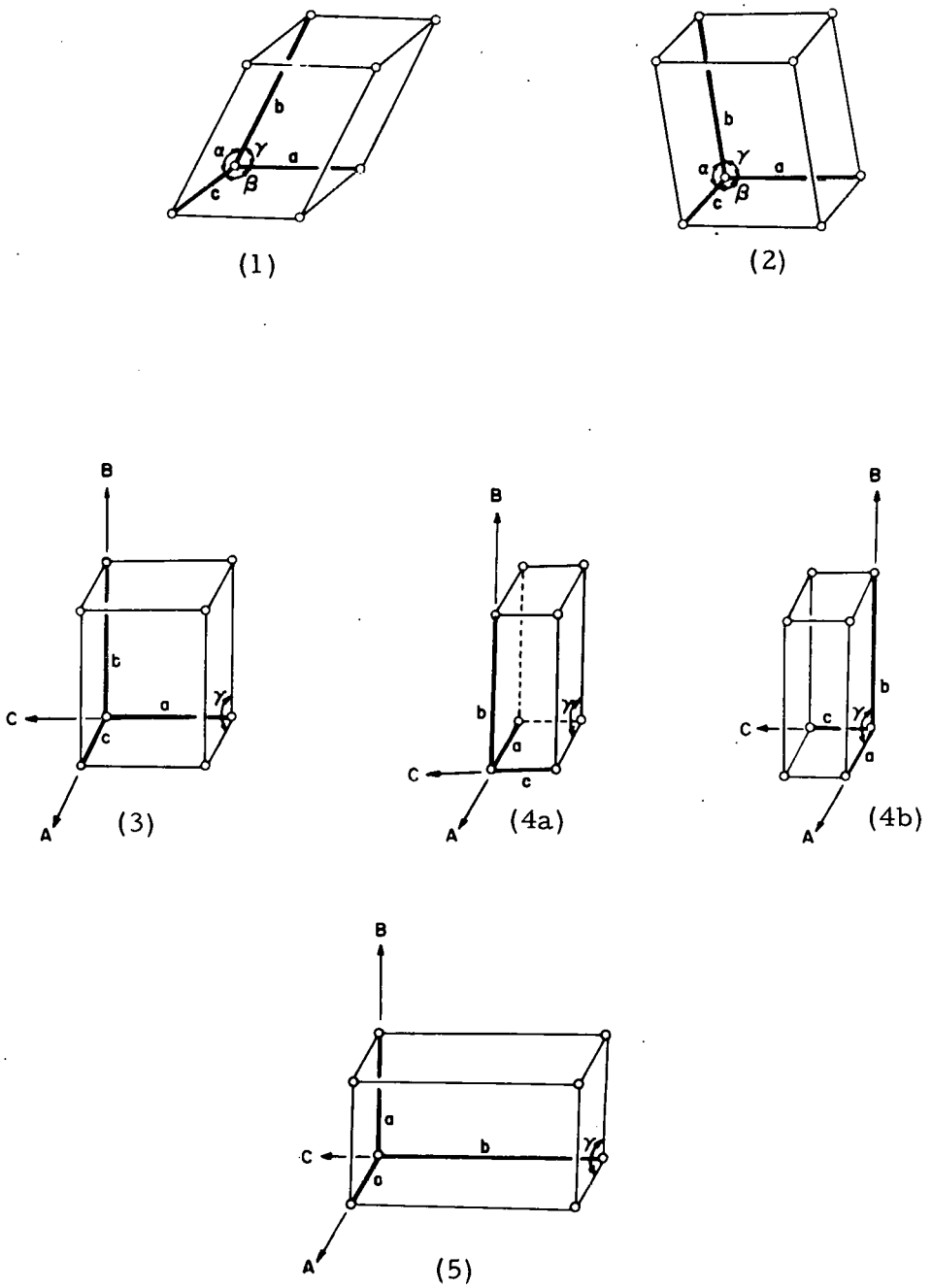
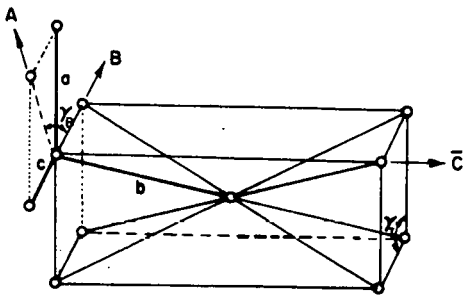



Fig. 5. The fourteen Bravais lattices and their reduced cells.

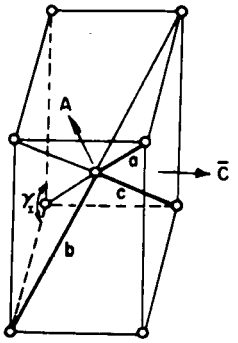
Table 3. (continued).

## MONOCLINIC (c-unique)

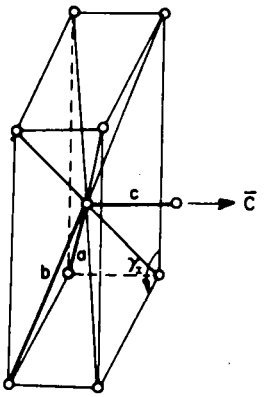
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 6 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33} - \bar{r}_{31}}{2} & \bar{r}_{31} & \frac{\bar{r}_{11} - \bar{r}_{31}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & \bar{1} \\ \bar{1} & \bar{2} & \bar{1} \end{pmatrix}$ | $A^2 = r_{11} + r_{33} + 2\bar{r}_{31}$<br>$B^2 = r_{33}$<br>$C^2 = 4r_{22} - r_{11} - r_{33} - 2\bar{r}_{31}$<br>$\cos\gamma = (-r_{33} - \bar{r}_{31})/AB$ |
| 7 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \bar{r}_{23} & (\bar{r}_{11} - \bar{r}_{23} - \bar{r}_{12}) & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & \bar{1} \\ \bar{1} & \bar{1} & 0 \\ \bar{1} & 0 & \bar{1} \end{pmatrix}$ | $A^2 = 4r_{11} + 2\bar{r}_{23} + 2\bar{r}_{12}$<br>$B^2 = r_{11} + r_{22} + 2\bar{r}_{12}$<br>$C^2 = -2(\bar{r}_{23} + \bar{r}_{12})$<br>$\cos\gamma = -2(r_{11} + \bar{r}_{12})/AB$ |
| 8 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & \frac{\bar{r}_{33}}{2} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} \bar{2} & 0 & \bar{1} \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | $A^2 = 4r_{11} - r_{33}$<br>$B^2 = r_{11} + r_{22} - 2r_{12}$<br>$C^2 = r_{33}$<br>$\cos\gamma = 2(r_{12} - r_{11})/AB$ |
| 9a | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & \frac{\bar{r}_{33}}{2} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 2 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | $A^2 = 4r_{11} - r_{33}$<br>$B^2 = r_{22}$<br>$C^2 = r_{33}$<br>$\cos\gamma = (-2r_{12})/AB$ |
| 9b | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & \frac{\bar{r}_{33}}{2} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 2 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | $A^2 = 4r_{11} - r_{33}$<br>$B^2 = r_{22}$<br>$C^2 = r_{33}$<br>$\cos\gamma = 2\bar{r}_{12}/AB$ |
| 10a | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ r_{23} & 0 & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 2 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ | $A^2 = 4r_{22} - r_{11}$<br>$B^2 = r_{33}$<br>$C^2 = r_{11}$<br>$\cos\gamma = 2\bar{r}_{23}/AB$ |
| 10b | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & 0 & \frac{\bar{r}_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 2 & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | $A^2 = 4r_{22} - r_{11}$<br>$B^2 = r_{33}$<br>$C^2 = r_{11}$<br>$\cos\gamma = 2\bar{r}_{23}/AB$ |



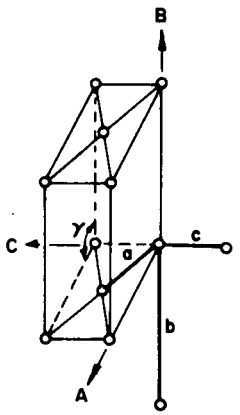

(6)



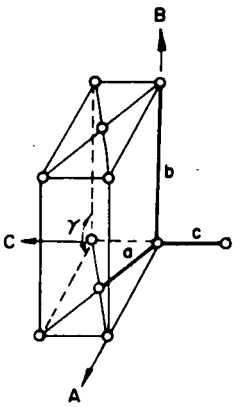

(7)



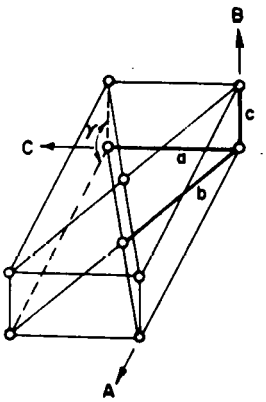

(8)



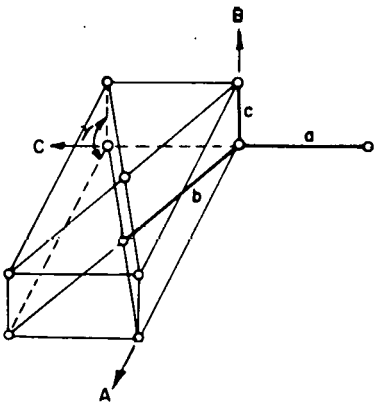

(9a)




(9b)




(10a)



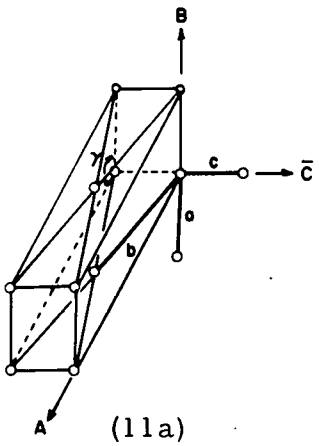

(10b)

Fig. 5. (continued).

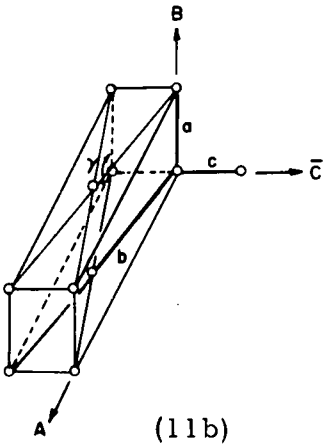
Table 3. (continued).

# MONOCLINIC (c-unique)

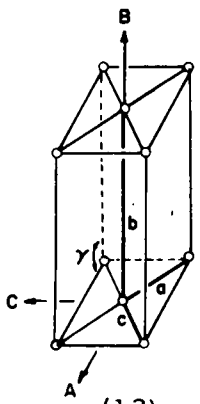
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 11a | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & 0 & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 0 & 2 & 1 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | $A^2 = 4r_{22} - r_{33}$<br>$B^2 = r_{11}$<br>$C^2 = r_{33}$<br>$\cos\gamma = (-2r_{12})/AB$ |
| 11b | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & 0 & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 0 & 2 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 4r_{22} - r_{33}$<br>$B^2 = r_{11}$<br>$C^2 = r_{33}$<br>$\cos\gamma = 2\bar{r}_{12}/AB$ |
| 12 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \bar{r}_{23} & \bar{r}_{31} & r_{23} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & \bar{1} \end{pmatrix}$ | $A^2 = 2(r_{11} - \bar{r}_{31})$<br>$B^2 = r_{22}$<br>$C^2 = 2(r_{11} + \bar{r}_{31})$<br>$\cos\gamma = 2\bar{r}/AB$ |
| 13 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \bar{r}_{23} & \bar{r}_{31} & \bar{r}_{23} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{31})$<br>$B^2 = r_{22}$<br>$C^2 = 2(r_{11} - \bar{r}_{31})$<br>$\cos\gamma = 2\bar{r}_{23}/AB$ |
| 14 | B | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \bar{r}_{23} & \bar{r}_{23} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & \bar{1} & 0 \end{pmatrix}$ | $A^2 = 2(r_{11} + r_{12})$<br>$B^2 = r_{33}$<br>$C^2 = 2(r_{11} - r_{12})$<br>$\cos\gamma = 2\bar{r}_{23}/AB$ |
| 15 | B | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \bar{r}_{23} & \bar{r}_{23} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & \bar{1} & 0 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{12})$<br>$B^2 = r_{33}$<br>$C^2 = 2(r_{11} - \bar{r}_{12})$<br>$\cos\gamma = 2\bar{r}_{23}/AB$ |
| 16 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & \bar{r}_{31} & \frac{r_{31}}{2} \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & \bar{2} & \bar{1} \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = r_{11}$<br>$C^2 = 4r_{22} - r_{33}$<br>$\cos\gamma = \bar{r}_{31}/AB$ |



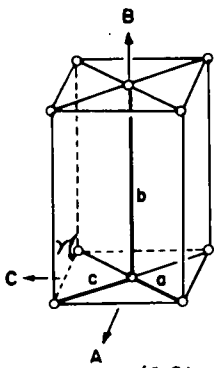

(11a)



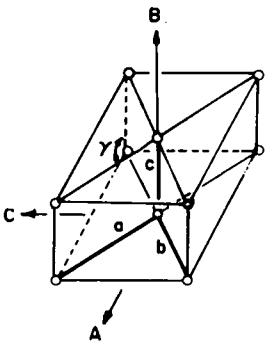

(11b)



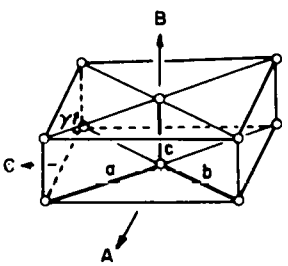

(12)



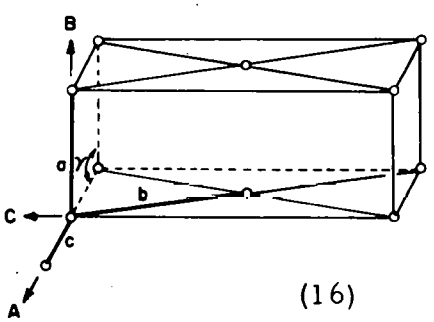

(13)




(14)




(15)




(16)

Fig. 5. (continued).

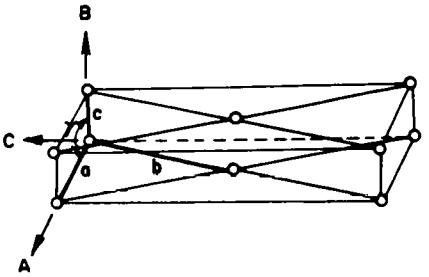
Table 3. (continued).

## MONOCLINIC (c-unique)

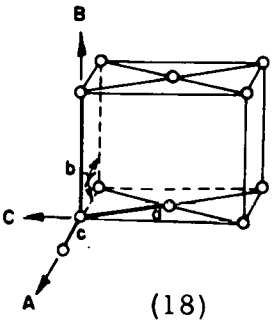
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 17 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{31}}{2} & \bar{r}_{31} & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & \bar{2} & 0 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = r_{33}$<br>$C^2 = 4r_{22} - r_{11}$<br>$\cos\gamma = \bar{r}_{31}/AB$ |
| 18 | B | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & \frac{\bar{r}_{33}}{2} & \frac{r_{23}}{2} \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{2} & 0 & \bar{1} \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = r_{22}$<br>$C^2 = 4r_{11} - r_{33}$<br>$\cos\gamma = \bar{r}_{23}/AB$ |

## MONOCLINIC (b-unique)

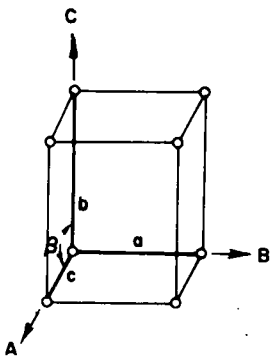
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 3 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = r_{11}$<br>$C^2 = r_{22}$<br>$\cos\beta = \bar{r}_{23}/AC$ |
| 4a | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & 0 & r_{12} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = r_{33}$<br>$C^2 = r_{22}$<br>$\cos\beta = -r_{12}/AC$ |
| 4b | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & 0 & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = r_{33}$<br>$C^2 = r_{22}$<br>$\cos\beta = \bar{r}_{12}/AC$ |
| 5 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & \bar{r}_{31} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = r_{22}$<br>$C^2 = r_{11}$<br>$\cos\beta = \bar{r}_{31}/AC$ |



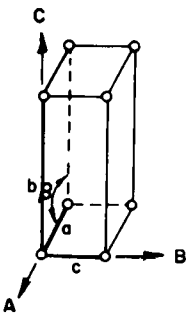

(17)



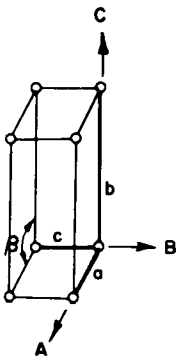

(18)



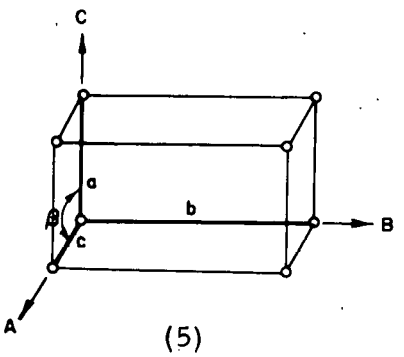

(3)




(4a)




(4b)



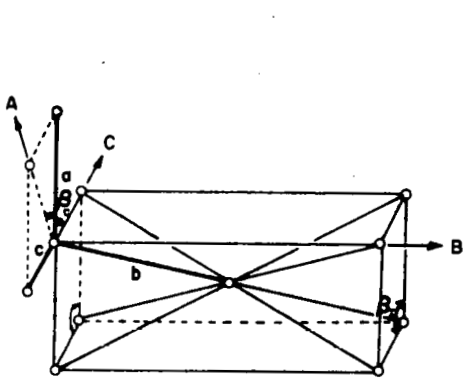

(5)

Fig. 5. (continued).

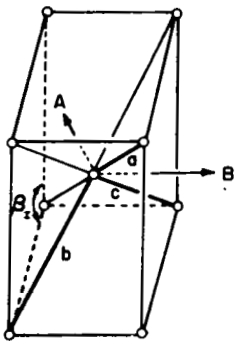
Table 3. (continued).

# MONOCLINIC (b-unique)

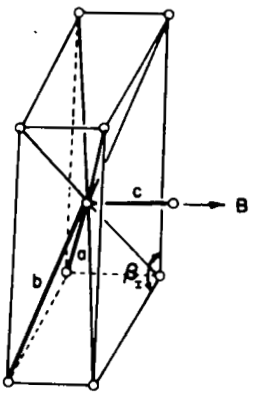
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 6 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33} - \bar{r}_{31}}{2} & \bar{r}_{31} & \frac{\bar{r}_{11} - \bar{r}_{31}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 1 \\ 1 & 2 & 1 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | $A^2 = r_{11} + r_{33} + 2r_{31}$<br>$B^2 = 4r_{22} - r_{11} - r_{33} - 2r_{31}$<br>$C^2 = r_{33}$<br>$\cos\beta = (-r_{33} - r_{31})/AC$ |
| 7 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \bar{r}_{23} & (\bar{r}_{11} - \bar{r}_{23} - \bar{r}_{12}) & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & \bar{1} \\ 1 & 0 & 1 \\ \bar{1} & \bar{1} & 0 \end{pmatrix}$ | $A^2 = 4r_{11} + 2\bar{r}_{23} + 2\bar{r}_{12}$<br>$B^2 = -2(\bar{r}_{23} + \bar{r}_{12})$<br>$C^2 = r_{11} + r_{22} + 2\bar{r}_{12}$<br>$\cos\beta = -2(r_{11} + \bar{r}_{12})/AC$ |
| 8 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & \frac{\bar{r}_{33}}{2} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} \bar{2} & 0 & \bar{1} \\ 0 & 0 & 1 \\ 1 & \bar{1} & 0 \end{pmatrix}$ | $A^2 = 4r_{11} - r_{33}$<br>$B^2 = r_{33}$<br>$C^2 = r_{11} + r_{22} - 2r_{12}$<br>$\cos\beta = 2(r_{12} - r_{11})/AC$ |
| 9a | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & \frac{\bar{r}_{33}}{2} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 2 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$ | $A^2 = 4r_{11} - r_{33}$<br>$B^2 = r_{33}$<br>$C^2 = r_{22}$<br>$\cos\beta = (-2r_{12})/AC$ |
| 9b | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & \frac{\bar{r}_{33}}{2} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 2 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = 4r_{11} - r_{33}$<br>$B^2 = r_{33}$<br>$C^2 = r_{22}$<br>$\cos\beta = 2\bar{r}_{12}/AC$ |
| 10a | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & 0 & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 2 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 4r_{22} - r_{11}$<br>$B^2 = r_{11}$<br>$C^2 = r_{33}$<br>$\cos\beta = 2\bar{r}_{23}/AC$ |
| 10b | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & 0 & \frac{\bar{r}_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 2 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 4r_{22} - r_{11}$<br>$B^2 = r_{11}$<br>$C^2 = r_{33}$<br>$\cos\beta = 2\bar{r}_{23}/AC$ |
| 11a | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & 0 & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 0 & 2 & 1 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | $A^2 = 4r_{22} - r_{33}$<br>$B^2 = r_{33}$<br>$C^2 = r_{11}$<br>$\cos\beta = (-2r_{12})/AC$ |
| 11b | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & 0 & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 0 & 2 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ | $A^2 = 4r_{22} - r_{33}$<br>$B^2 = r_{33}$<br>$C^2 = r_{11}$<br>$\cos\beta = 2\bar{r}_{12}/AC$ |



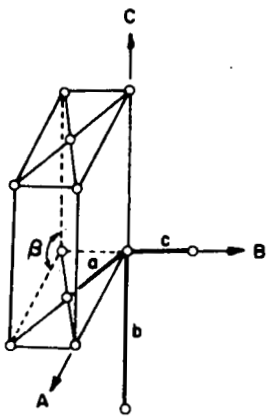

(6)



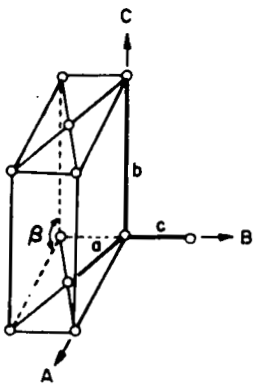

(7)



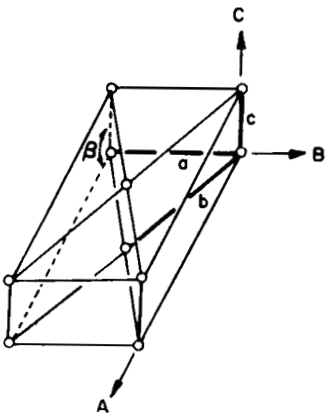

(8)



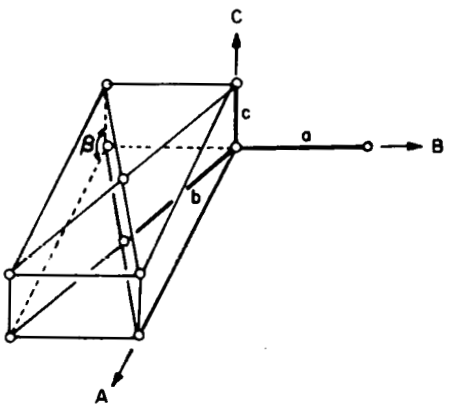

(9a)



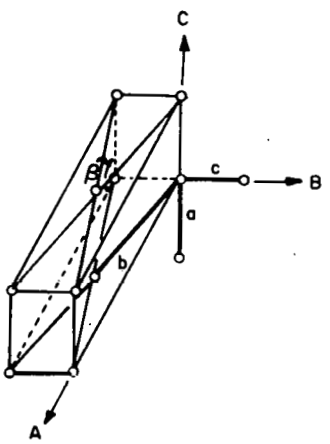

(9b)



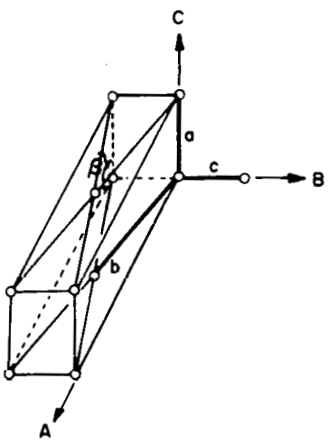

(10a)




(10b)




(11a)




(11b)

Fig. 5. (continued).

Table 3. (continued).

# MONOCLINIC (b-unique)

| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 12 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \bar{r}_{23} & \bar{r}_{31} & r_{23} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = 2(r_{11} - \bar{r}_{31})$<br>$B^2 = 2(r_{11} + \bar{r}_{31})$<br>$C^2 = r_{22}$<br>$\cos\beta = 2\bar{r}_{23}/AC$ |
| 13 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \bar{r}_{23} & \bar{r}_{31} & \bar{r}_{23} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{31})$<br>$B^2 = 2(r_{11} - \bar{r}_{31})$<br>$C^2 = r_{22}$<br>$\cos\beta = 2\bar{r}_{23}/AC$ |
| 14 | C | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \bar{r}_{23} & \bar{r}_{23} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} + r_{12})$<br>$B^2 = 2(r_{11} - r_{12})$<br>$C^2 = r_{33}$<br>$\cos\beta = 2\bar{r}_{23}/AC$ |
| 15 | C | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \bar{r}_{23} & \bar{r}_{23} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{12})$<br>$B^2 = 2(r_{11} - \bar{r}_{12})$<br>$C^2 = r_{33}$<br>$\cos\beta = 2\bar{r}_{23}/AC$ |
| 16 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \dfrac{\bar{r}_{33}}{2} & \bar{r}_{31} & \dfrac{r_{31}}{2} \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = 4r_{22} - r_{33}$<br>$C^2 = r_{11}$<br>$\cos\beta = \bar{r}_{31}/AC$ |
| 17 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \dfrac{\bar{r}_{31}}{2} & \bar{r}_{31} & \dfrac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = 4r_{22} - r_{11}$<br>$C^2 = r_{33}$<br>$\cos\beta = \bar{r}_{31}/AC$ |
| 18 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \bar{r}_{23} & \dfrac{\bar{r}_{33}}{2} & \dfrac{r_{23}}{2} \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 2 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = 4r_{11} - r_{33}$<br>$C^2 = r_{22}$<br>$\cos\beta = \bar{r}_{23}/AC$ |

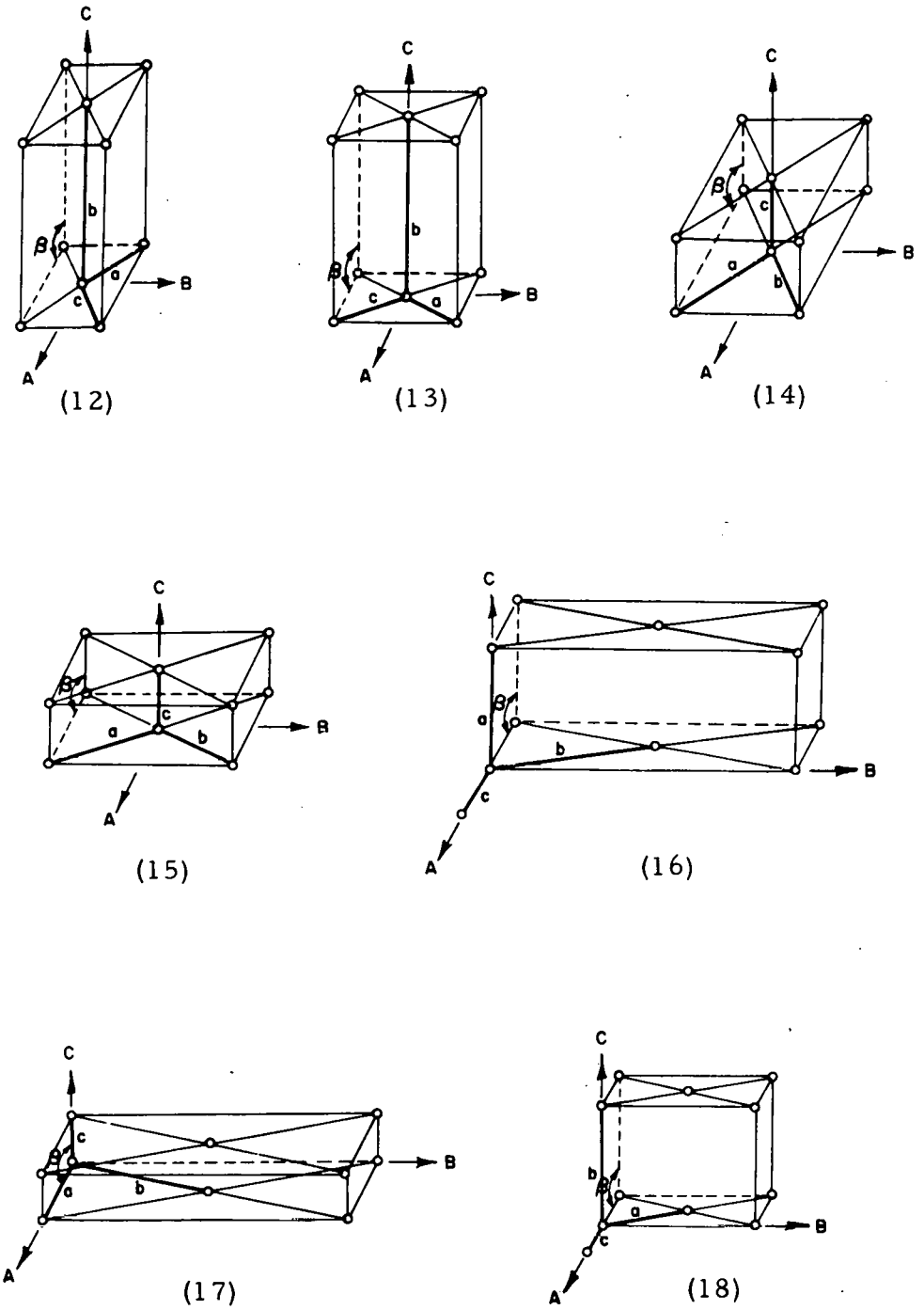
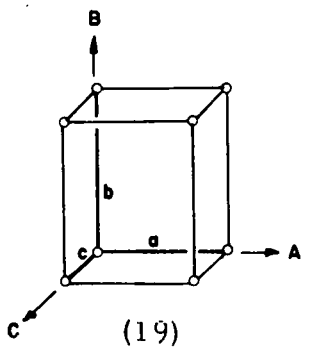



Fig. 5. (continued).

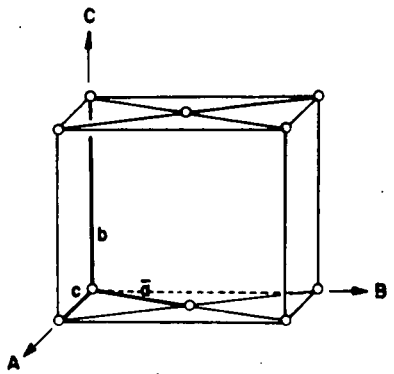
Table 3. (continued).

# ORTHORHOMBIC

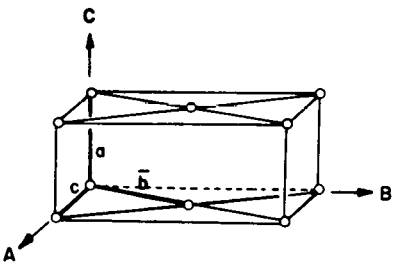
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 19 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = r_{22}$<br>$C^2 = r_{33}$ |
| 20 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & \frac{\bar{r}_{33}}{2} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ \bar{2} & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = 4r_{11} - r_{33}$<br>$C^2 = r_{22}$ |
| 21 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{2} & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$ | $A^2 = r_{33}$<br>$B^2 = 4r_{22} - r_{33}$<br>$C^2 = r_{11}$ |
| 22a | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & 0 & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = 4r_{22} - r_{11}$<br>$C^2 = r_{33}$ |
| 22b | C | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ 0 & 0 & \frac{\bar{r}_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & \bar{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = 4r_{22} - r_{11}$<br>$C^2 = r_{33}$ |
| 23 | C | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ 0 & \bar{r}_{31} & 0 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{31})$<br>$B^2 = 2(r_{11} - \bar{r}_{31})$<br>$C^2 = r_{33}$ |
| 24a | C | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ 0 & 0 & r_{12} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} - r_{12})$<br>$B^2 = 2(r_{11} + r_{12})$<br>$C^2 = r_{33}$ |
| 24b | C | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ 0 & 0 & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{12})$<br>$B^2 = 2(r_{11} - \bar{r}_{12})$<br>$C^2 = r_{33}$ |



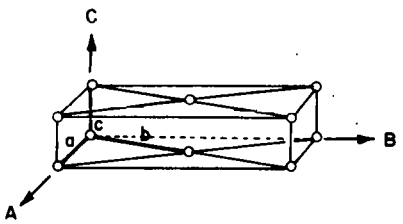

(19)



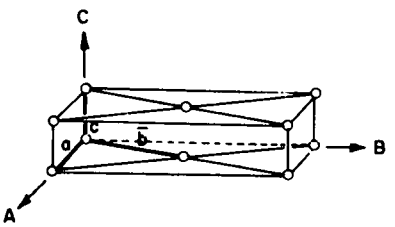

(20)



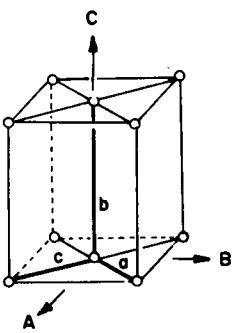

(21)



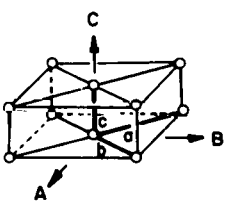

(22a)



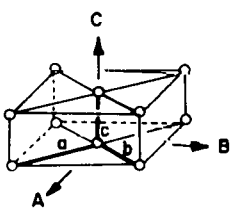

(22b)




(23)




(24a)



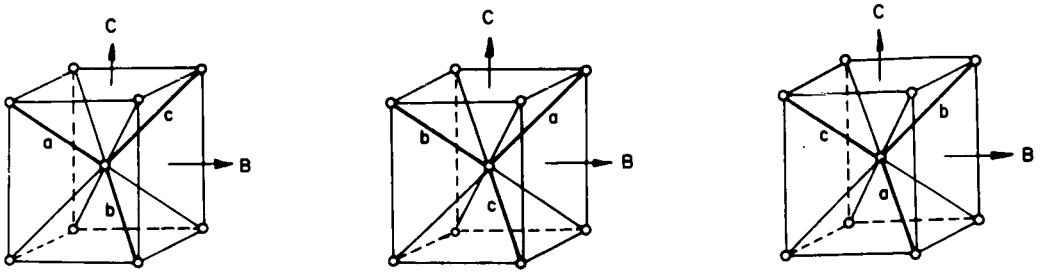

(24b)

Fig. 5. (continued).

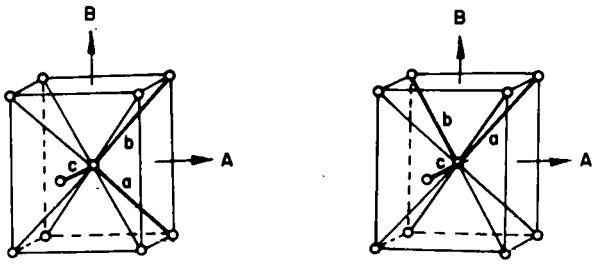
Table 3. (continued).

# ORTHORHOMBIC

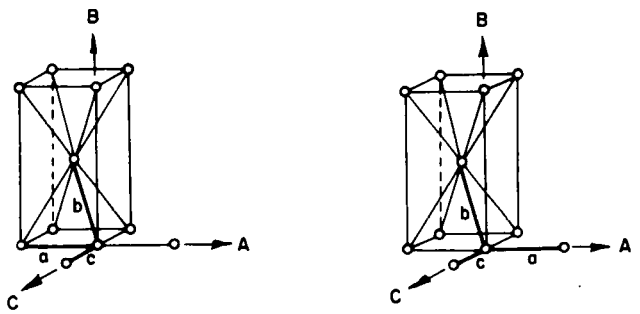
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 25a | I | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ (\bar{r}_{11} - \bar{r}_{31} - \bar{r}_{12}) & \bar{r}_{31} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{12})$<br>$B^2 = -2(\bar{r}_{31} + \bar{r}_{12})$<br>$C^2 = 2(r_{11} + \bar{r}_{31})$ |
| 25b | I | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \bar{r}_{23} & (\bar{r}_{11} - \bar{r}_{23} - \bar{r}_{12}) & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{23})$<br>$B^2 = -2(\bar{r}_{23} + \bar{r}_{12})$<br>$C^2 = 2(r_{11} + \bar{r}_{12})$ |
| 25c | I | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \bar{r}_{23} & \bar{r}_{31} & (\bar{r}_{11} - \bar{r}_{23} - \bar{r}_{31}) \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} + \bar{r}_{31})$<br>$B^2 = -2(\bar{r}_{23} + \bar{r}_{31})$<br>$C^2 = 2(r_{11} + \bar{r}_{23})$ |
| 26a | I | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \frac{\bar{r}_{33}}{2} & \frac{\bar{r}_{33}}{2} & r_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 1 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} + r_{12}) - r_{33}$<br>$B^2 = 2(r_{11} - r_{12})$<br>$C^2 = r_{33}$ |
| 26b | I | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \frac{\bar{r}_{33}}{2} & \frac{\bar{r}_{33}}{2} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} - \bar{r}_{12})$<br>$B^2 = 2(r_{11} + \bar{r}_{12}) - r_{33}$<br>$C^2 = r_{33}$ |
| 27a | I | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & 0 & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 0 & 0 \\ \bar{1} & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = 4r_{22} - r_{11} - r_{33}$<br>$C^2 = r_{33}$ |
| 27b | I | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & 0 & \frac{\bar{r}_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 1 & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$B^2 = 4r_{22} - r_{11} - r_{33}$<br>$C^2 = r_{33}$ |
| 28 | F | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \bar{r}_{23} & (\bar{r}_{11} - 2\bar{r}_{23}) & \bar{r}_{23} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 2 & 1 \\ \bar{1} & 0 & \bar{1} \end{pmatrix}$ | $A^2 = 4(r_{11} + \bar{r}_{23})$<br>$B^2 = 4(r_{22} + \bar{r}_{23}) + r_{11}$<br>$C^2 = -4\bar{r}_{23}$ |
| 29 | F | $\begin{pmatrix} r_{11} & r_{22} & r_{33} \\ \frac{\bar{r}_{33}}{2} & \frac{\bar{r}_{33}}{2} & \frac{r_{33}}{4} \end{pmatrix}$ | $\begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 4r_{11} - r_{33}$<br>$B^2 = 4r_{22} - r_{33}$<br>$C^2 = r_{33}$ |



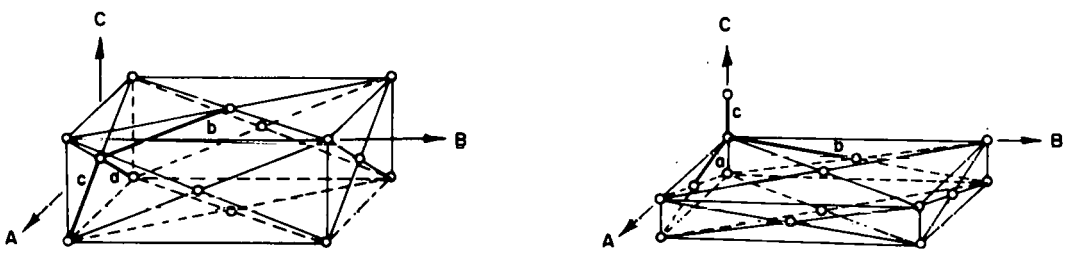

(25a) (25b) (25c)




(26a) (26b)




(27a) (27b)



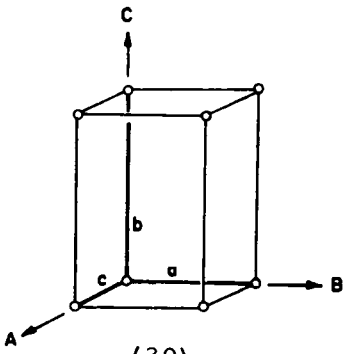

(28) (29)

Fig. 5. (continued).

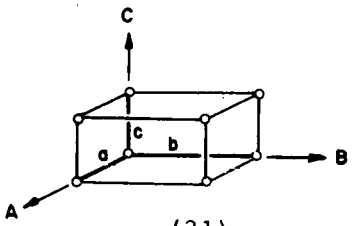
Table 3. (continued).

# TETRAGONAL

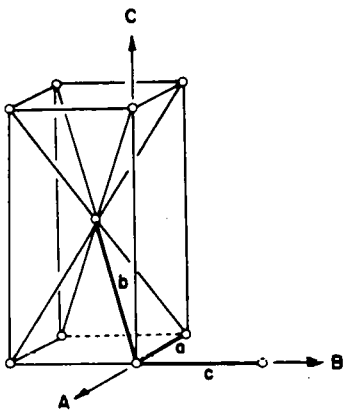
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 30 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = r_{22}$ |
| 31 | P | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = r_{33}$ |
| 32a | I | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \frac{\bar{r}_{11}}{2} & 0 & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ \bar{1} & 2 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = 4r_{22} - 2r_{11}$ |
| 32b | I | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \frac{\bar{r}_{11}}{2} & 0 & \frac{\bar{r}_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 2 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = 4r_{22} - 2r_{11}$ |
| 33 | I | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \frac{\bar{r}_{33}}{2} & \frac{\bar{r}_{33}}{2} & \frac{r_{33}}{4} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 2r_{11} + \frac{1}{2}\bar{r}_{33}$<br>$C^2 = r_{33}$ |
| 34a | I | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \bar{r}_{23} & \frac{\bar{r}_{11} - \bar{r}_{23}}{2} & \frac{\bar{r}_{11} - \bar{r}_{23}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$ | $A^2 = r_{11} - \bar{r}_{23}$<br>$C^2 = 2(r_{11} + \bar{r}_{23})$ |
| 34b | I | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \frac{\bar{r}_{11} - \bar{r}_{31}}{2} & \bar{r}_{31} & \frac{\bar{r}_{11} - \bar{r}_{31}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11} - \bar{r}_{31}$<br>$C^2 = 2(r_{11} + \bar{r}_{31})$ |
| 34c | I | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \frac{\bar{r}_{11} - \bar{r}_{12}}{2} & \frac{\bar{r}_{11} - \bar{r}_{12}}{2} & \bar{r}_{12} \end{pmatrix}$ | $\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{11} - \bar{r}_{12}$<br>$C^2 = 2(r_{11} + \bar{r}_{12})$ |



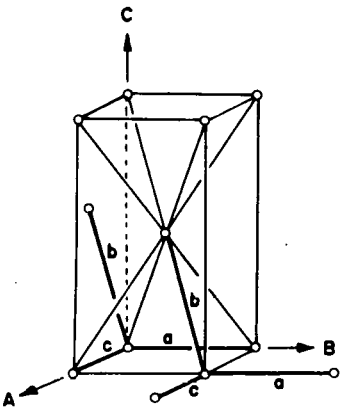

(30)



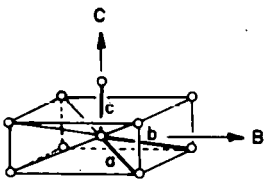

(31)



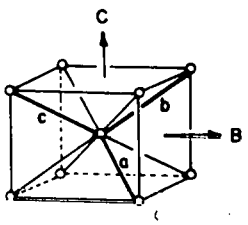

(32a)



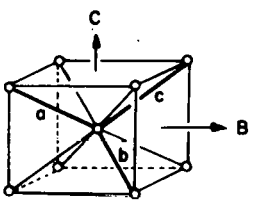

(32b)



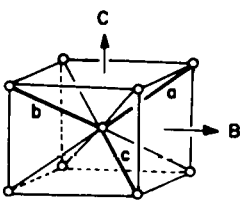

(33)




(34a)




(34b)



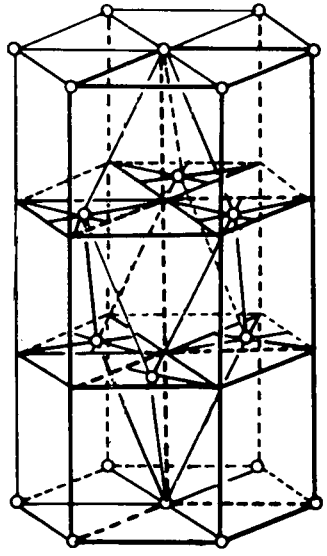

(34c)

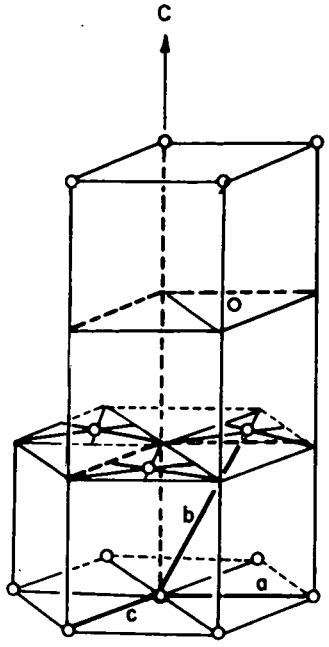
Fig. 5. (continued).

Table 3. (continued).

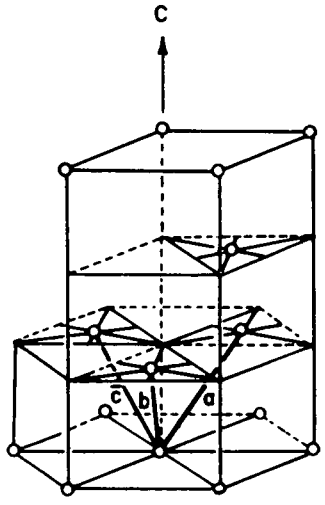
# RHOMBOHEDRAL

| No. | Reduced form | RHOMBOHEDRAL (Primitive) | | HEXAGONAL (Triply-primitive) | |
|---|---|---|---|---|---|
| | | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
| 35 | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ \frac{\bar{r}_{11}}{2} & \frac{\bar{r}_{11}}{2} & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 1 & 0 \end{pmatrix}$ | $A^2 = r_{22}$<br>$r_{11} = 2r_{22}(1 - \cos\alpha)$<br>$(\alpha < 60^\circ)$ | $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ \bar{1} & 3 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = 3(3r_{22} - r_{11})$<br>$\gamma = 120^\circ$ |
| 36 | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \bar{r}_{23} & \bar{r}_{23} & r_{23} \end{pmatrix}$ | $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | $A^2 = r_{11}$<br>$r_{23} = r_{11}\cos\alpha$<br>$(60^\circ < \alpha < 90^\circ)$ | $\begin{pmatrix} \bar{1} & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & \bar{1} \end{pmatrix}$ | $A^2 = 2(r_{11} - r_{23}) = 2(r_{11} + \bar{r}_{23})$<br>$C^2 = 3(r_{11} + 2r_{23}) = 3(r_{11} - 2\bar{r}_{23})$<br>$\gamma = 120^\circ$ |
| 37 | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \bar{r}_{23} & \bar{r}_{23} & \bar{r}_{23} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$\bar{r}_{23} = r_{11}\cos\alpha$<br>$(90^\circ < \alpha < 109^\circ 28' 16.4'')$ | $\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & 1 & \bar{1} \\ 1 & 1 & 1 \end{pmatrix}$ | $A^2 = 2(r_{11} - \bar{r}_{23})$<br>$C^2 = 3(r_{11} + 2\bar{r}_{23})$<br>$\gamma = 120^\circ$ |
| 38 | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \frac{\bar{r}_{33}}{3} & \frac{\bar{r}_{33}}{3} & \frac{\bar{r}_{11} - \frac{\bar{r}_{33}}{3}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{11}$<br>$r_{33} = 3r_{11}(1 + 2\cos\alpha)$<br>$(\alpha > 109^\circ 28' 16.4'')$ | $\begin{pmatrix} 2 & 1 & 1 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = 3r_{11} - \frac{r_{33}}{3} = 3r_{11} + \frac{\bar{r}_{33}}{3}$<br>$C^2 = r_{33}$<br>$\gamma = 120^\circ$ |

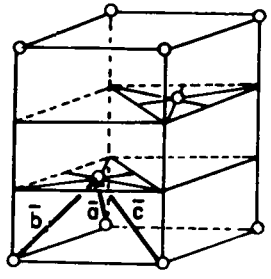




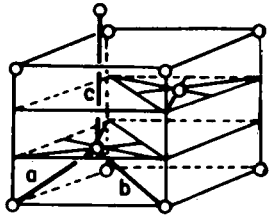

(35)




(36)




(37)




(38)

Fig. 5. (continued).

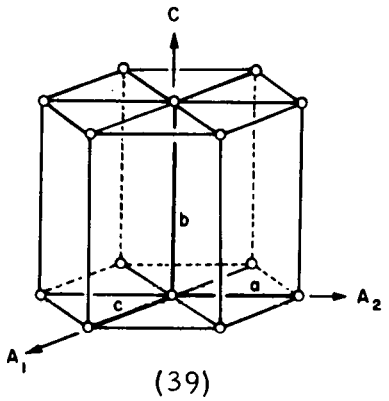
Table 3. (continued).

## HEXAGONAL

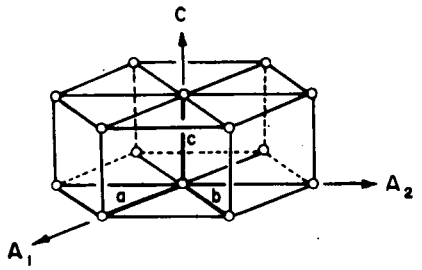
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 39 | P | $\begin{pmatrix} r_{11} & r_{22} & r_{11} \\ 0 & \frac{\bar{r}_{11}}{2} & 0 \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = r_{22}$<br>$\gamma = 120^\circ$ |
| 40a | P | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ 0 & 0 & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = r_{33}$<br>$\gamma = 120^\circ$ |
| 40b | P | $\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ 0 & 0 & \frac{\bar{r}_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$<br>$C^2 = r_{33}$<br>$\gamma = 120^\circ$ |

## CUBIC

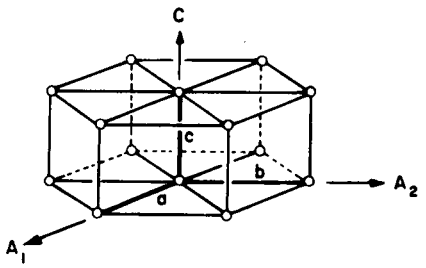
| No. | Unit cell lattice type | Reduced form | Transformation matrix for reduced cell to unit cell | Cell parameters of unit cell in terms of reduced cell scalars |
|---|---|---|---|---|
| 41 | P | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ 0 & 0 & 0 \end{pmatrix}$ | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | $A^2 = r_{11}$ |
| 42 | I | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \frac{\bar{r}_{11}}{3} & \frac{\bar{r}_{11}}{3} & \frac{\bar{r}_{11}}{3} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$ | $A^2 = \frac{4}{3} r_{11}$ |
| 43 | F | $\begin{pmatrix} r_{11} & r_{11} & r_{11} \\ \frac{\bar{r}_{11}}{2} & \frac{\bar{r}_{11}}{2} & \frac{r_{11}}{2} \end{pmatrix}$ | $\begin{pmatrix} 1 & 1 & 1 \\ 1 & \bar{1} & \bar{1} \\ \bar{1} & 1 & \bar{1} \end{pmatrix}$ | $A^2 = 2r_{11}$ |



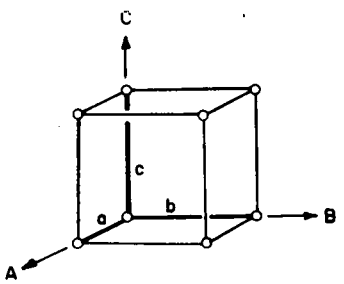

(39)



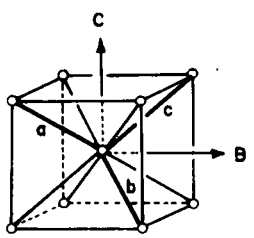

(40a)



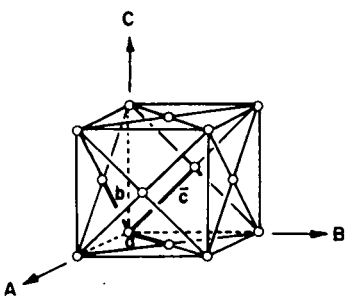

(40b)




(41)




(42)




(43)

Fig. 5. (continued).

## 3. USES OF THE REDUCED CELL

Because of the uniqueness of the reduced cell, because it can always be readily found without difficulty and because its scalars identify the cell of highest symmetry in the lattice, it thus provides many far-reaching uses as a tool in lattice studies and transformations. The following are a few typical examples.

The reduced cell as the standard choice for the triclinic cell in a triclinic lattice has already been discussed.

By making use of the fact that the Bravais lattice imposes restrictions on the cell parameters of the reduced cell and thus its scalars, the reduced cell may therefore be used to identify cells of highest symmetry in a lattice. This use is not restricted soley to using the reduced cell as a test on primitive triclinic cells but may be used equally well on any cell in any crystal system, primitive or centered, in any orientation. The object in each case is always to convert the cell to its reduced cell so its scalars can be analyzed with use of Tables 2 and 3. If the original cell is triclinic or monoclinic, it must be reduced before testing. If the original cell is primitive but of symmetry higher than monoclinic, it always corresponds to the reduced cell without previous reduction. If the original cell (any system) is centered it necessarily does not correspond to the reduced cell and must first be converted to a primitive cell before reduction to its reduced cell. In routine work the triclinic transformations appearing on pages 174 and 175 may be used

successfully on any crystal system for achieving conversion to a primitive lattice. Thus, if it is desired to test a C-centered monoclinic lattice for a higher symmetry cell, it may first be transformed to a primitive cell by the transformation $\frac{1}{2}\frac{1}{2}0/\frac{\bar{1}}{2}\frac{1}{2}0/001$ (obtained from page 32) and the primitive cell then reduced by the method of Section A of this chapter. If the reduced form reveals a higher symmetry cell, the matrix in column 4 of Table 3 provides the necessary link to that unit cell.

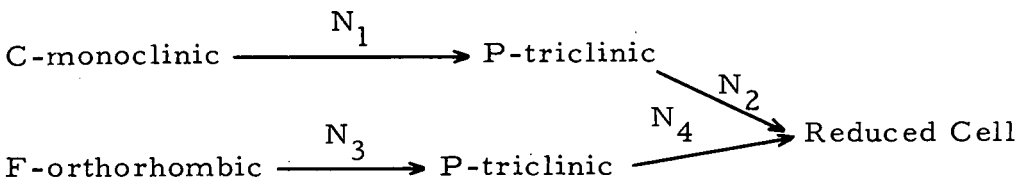
Another frequent use is the application of cell reduction to primitive monoclinic cells in order to find the $\beta$-angle, or $\gamma$-angle as the case may be, nearest 90°. At the same time the cell so obtained is the reduced cell and its scalars can be quickly analyzed to verify whether or not the original monoclinic cell is actually the cell of highest symmetry in the lattice. Since monoclinic cells are so frequently encountered in structural work, this is recommended as routine practice and a good habit to get into "before" the actual structure determination begins. By making this a common practice it is possible to transform the Miller indices to the better cell in the initial stages of the determination and thus save needless extra work later.

A fourth example is its use in aligning a single crystal on a single crystal orienter. Suppose a crystal fragment or sphere is to be used for the collection of intensity data. Such crystal shapes often give little or no direct indication of cell orientation. Using the cell reduction technique, however, the problem of cell orientation is solved rapidly

and easily. A cell -- any arbitrary cell -- is first located and then transformed to its reduced cell; the original cell may, for example, be triclinic, primitive or centered. An analysis of the reduced cell scalars will immediately identify the unit cell and its relative orientation, using Tables 2 and 3 (see Example 3).

A fifth example is its use in proving whether or not two crystals are of the same compound; they may, for instance, be different in crystal habit. There is always only one reduced cell in any one lattice. Thus, if the lattices are identical, the reduced cells will also be identical.

The reduced cell can also be used to provide the "link" between two cells in a lattice. Suppose, for instance, a crystal structure is reported in the literature as being Cc monoclinic. Suppose a reinvestigation is carried out by a different investigator and it is discovered that the crystals are really face-centered orthorhombic. He may first check to make sure the face-centered orthorhombic cell describes the same lattice as the C-centered monoclinic cell reported in the literature by transforming both cells to their respective reduced cell. If the crystals are of the same compound their reduced cells will be identical, as pointed out above. If it is shown that the two lattices are indeed identical, it may then be desired to transform the cell parameters, the fractional atomic coordinates and the Miller indices of the monoclinic cell to those in the orthorhombic orientation; the matrices for achieving these transformations may be obtained from the matrix for the transformation of lattice axes in direct space, a matrix obtained by multiplication of the four matrices involved in the following sequence of operations:




so that the matrix, N, for the transformation of the C-centered monoclinic cell to the face-centered orthorhombic cell is

$$N = (N_3^{-1})(N_4^{-1})(N_2)(N_1) .$$

In this way the reduced cell is seen to provide the link between the monoclinic cell and the face-centered cell in the same lattice. In practice, of course, in order for the reduced cell to be the link it must be brought into the same "orientation" from both cells (page 32). For convenience, the orientation may be that established by convention, namely $c < a < b$ with $\alpha$, $\beta$ obtuse. If it should turn out that the reduced cell obtained from the one unit cell has $\gamma$ acute and the other reduced cell has $\gamma$ obtuse, the other five parameters identical, one of the two conventional reduced cells must be reoriented to make the one $\gamma$-angle agree in numerical value with the $\gamma$-angle in the other cell before calculating the matrix for linking the two cells - via the reduced cell (see page 32). (For comments on rules governing the reorientation, see pages 13 to 18 . See also Example 3, part B, pages 80 - 86 for further comments on the existence of two possible orientations for the same reduced cell in a lattice.) In using the computer programs described in Chapter III of this report, the reduced cell defined on the last page of output will be that in its conventional orientation, with no restriction on the character of the angle $\gamma$.

In view of the foregoing discussion one may wish to extend the convention for the orientation of the reduced cell to "$c < a < b$ with $\alpha$, $\beta$ obtuse and $\gamma$ obtuse, if possible". In reporting a true reduced cell in the literature, however, it will usually - if not always - be used soley for reporting a triclinic cell in a triclinic lattice, a cell for which there can be no alternative choices in the character of the angle $\gamma$ once $\alpha$ and $\beta$ are restricted to obtuse in nature. It is to be recalled that the convention was originally established only for the orientation of the reduced cell in a triclinic lattice.

Before concluding, one important point must be emphasized. It is very important that the appropriate matrices be selected for conversion of a centered Bravais lattice to a primitive lattice. It is not sufficient merely to reduce the volume of the cell by a factor of two, for instance, in transforming an A-, B-, C- or I-centered lattice to a primitive lattice. It can be shown quite easily that any cell subjected to a transformation specified for A→P, B→P, C→P and I→P results in a different reduced cell in each case. On the other hand, of the numerous possible transformations for, say, A→P applied specifically to an A-centered cell, results in only one reduced cell in the end.

Finally, it may be concluded that the reduced cell is also useful in identifying all cells of possible lower symmetry in a particular lattice. Consider, for instance, hexagonal (40b) whose reduced form is

$$\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ 0 & 0 & \frac{1}{2}\overline{r}_{11} \end{pmatrix} .$$

By disregarding $r_{12}$ as being the observed specialization $\frac{1}{2}\bar{r}_{11}$ and by considering "0" to be $\bar{r}_{23}$ we find, upon inspection of Table 2 under ($r_{11} = r_{22} \neq r_{33}$), the following reduced forms as well

$$\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ 0 & 0 & \bar{r}_{12} \end{pmatrix} \qquad \text{orthorhombic (24b)}$$

and

$$\begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \bar{r}_{23} & \bar{r}_{23} & \bar{r}_{12} \end{pmatrix} \qquad \text{monoclinic (15),}$$

Orthorhombic (24b) and monoclinic (15) are both C-centered cells, both of which do exist in a hexagonal lattice. This clearly shows that inspection of the reduced cell scalars for the greatest number of specializations will reveal the cell of highest symmetry.

Example 3

PART A

In an investigation of nickel dimethylglyoxime a single crystal fragment of the compound was mounted on a fiber in a completely random orientation and aligned on a single crystal orienter. A face-centered triclinic cell was located and observed to have the following lattice parameters: a = 10.360, b = 18.037, c = 25.760 A., $\alpha$ = 127.03°, $\beta$ = 129.81°, $\gamma$ = 90.51°. The problem is the following: we wish to locate in the lattice the unit cell of highest symmetry, identify its crystal system, lattice type and cell parameters, and to derive the transformation

matrix for transforming the face-centered triclinic cell to the newly chosen unit cell.

Solution. Before proceeding with the calculations, let us outline the procedure we shall follow.

Step 1. Transform the face-centered cell to a primitive cell.

Step 2. Reduce the primitive cell to its reduced cell.

Step 3. Convert the reduced cell to its conventional orientation, defined as $c < a < b$ with $\alpha$, $\beta$ obtuse. This will allow us to use Tables 2 and 3.

Step 4. Identify the reduced cell scalars (of the conventional reduced cell) with one of the reduced forms in Table 2, thereby identifying immediately the crystal system of highest symmetry in the lattice.

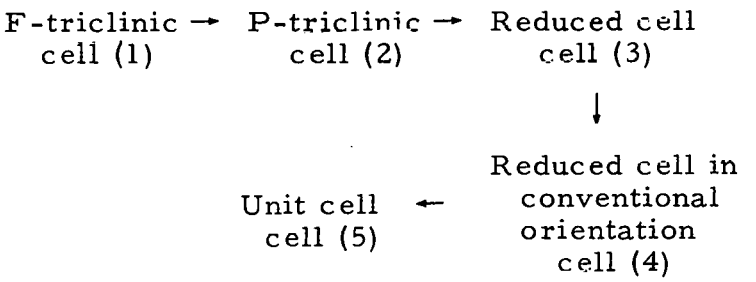
Step 5. Using Table 3 and the information obtained in Table 2

a) deduce the lattice type,

b) calculate the cell parameters of the new unit cell.

Step 6. Using matrix multiplication, deduce the transformation matrix for transformation of the original face-centered triclinic cell to the unit cell.

The series of transformations to be executed will thus be



Step 1. Transformation of face-centered triclinic to primitive triclinic; Cell (1) to cell (2).

Our ultimate goal is to reach the reduced cell, the unique cell which contains information about the unit cell of highest symmetry in the lattice, its relative orientation and parameters. But it is a primitive cell and since it can only be obtained directly from a primitive triclinic cell, we must first transform the face-centered cell to a primitive one, with a subsequent reduction in volume. Theoretically the primitive triclinic cell may be any one of the infinite such cells in the lattice; consequently we are free to select any transformation matrix we desire, so long as it carries out the desired reduction. In routine work we may select the (F → P) transformation on page 175, which is

$$\begin{Vmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{Vmatrix} .$$

If the face-centered cell is subjected to this transformation, the new parameters belonging to cell (2) become

| | |
|---|---|
| a = 10.3602 Å | $\alpha$ = 120.2543° |
| b = 10.4402 | $\beta$ = 143.4895° |
| c = 10.3583 | $\gamma$ = 59.7430° |

Step 2. Reduction of primitive cell to reduced cell; Cell (2) to cell (3).

The primitive triclinic cell obtained in Step 1 may now be reduced by the method outlined in Section A of this chapter. If this is done it is

observed that the primitive triclinic cell transforms to the reduced cell by the following transformation matrix:

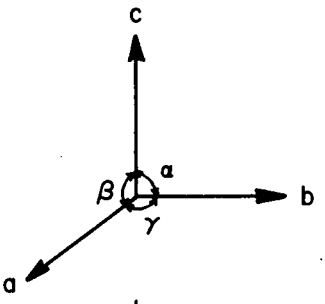
$$\begin{Vmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{Vmatrix} \qquad \text{[cell (2) to cell (3)]}$$

to yield lattice parameters

| | |
|---|---|
| a = 6.4901 Å | $\alpha$ = 60.5197° |
| b = 10.3595 | $\beta$ = 71.7607° |
| c = 10.3583 | $\gamma$ = 71.7498° . |

Step 3. Conversion of reduced cell to conventional orientation; cell (2) to cell (4).

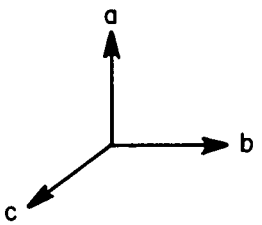
We wish to use Tables 2 and 3 where the crystal system of highest symmetry may be identified. To use them, however, the reduced cell must be in its conventional orientation, namely $c < a < b$ with $\alpha$, $\beta$ obtuse. The reorientation of axes and angles may be done in several ways, three of which are shown in detail below. The affects of the changes on the transformation matrix for cell (2) to cell (3) is also shown. When the entire processed is finished, the resulting matrix will be that for cell (2) to cell (4), where cell (4) is now the reduced cell in its conventional orientation. The rules set forth in Chapter II, Section C, are used throughout.




Interchange a and c,

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix},$$

System goes left-handed.




Return to right-handed system by reversing direction of b. This sets

$\alpha = \pi - \alpha$
$\gamma = \pi - \gamma$

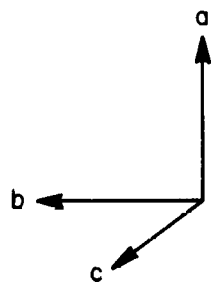
$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & \bar{1} \\ 1 & 0 & 1 \end{pmatrix}$$

Set $\alpha = \pi - \alpha$
$\beta = \pi - \beta$

Reverse direction of a and b;

$$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & \bar{1} & \bar{1} \\ 1 & 0 & 1 \end{pmatrix}$$

System remains left-handed.

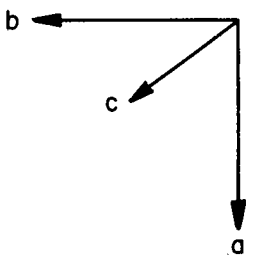



Set $\alpha = \pi - \alpha$
$\beta = \pi - \beta$

Reverse direction of c;

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & \bar{1} \end{pmatrix}$$

System returns to right-handed.




Set $\beta = \pi - \beta$
$\gamma = \pi - \gamma$

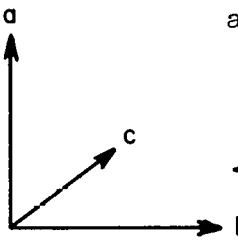
Reverse direction of b and c

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & \bar{1} \end{pmatrix}$$

System remains right-handed.

Return to right-handed system by reversing the direction of all three axes;

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & \bar{1} \end{pmatrix}$$



Upon completion of the necessary changes to obtain the reduced cell in its conventional orientation, the following lattice parameters for cell (4) and transformation matrix of cell (2) to cell (4) are obtained:

$$\begin{array}{lll} a = 10.3583\ \text{Å} & \alpha = 108.2502^\circ & \left\| \begin{array}{ccc} 0 & 0 & 1 \\ 0 & 1 & 1 \\ \bar{1} & 0 & \bar{1} \end{array} \right\| \\ b = 10.3595 & \beta = 108.2393^\circ & \\ c = 6.4901 & \gamma = 60.5197^\circ, & \end{array} .$$

Step 4. Identification of unit cell of highest symmetry in lattice.

We now look at the reduced form of the conventional reduced cell, cell (4), and analyze its scalars.

$$\begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{c}\cdot\vec{c} \\ \vec{b}\cdot\vec{c} & \vec{c}\cdot\vec{a} & \vec{a}\cdot\vec{b} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{22} & r_{33} \\ r_{23} & r_{31} & r_{12} \end{pmatrix} = \begin{pmatrix} 107.29 & 107.32 & 42.12 \\ -21.06 & -21.04 & 52.81 \end{pmatrix}$$

Its inspection reveals the following relationships (to within experimental error):

$$r_{11} = r_{22}$$
$$r_{23} = r_{31} = -\tfrac{1}{2}r_{33} .$$

We now go to Table 2, which is divided into four divisions according to the four classes of "symmetrical" scalars. In our case we observe $(\vec{a}\cdot\vec{a} = \vec{b}\cdot\vec{b} \neq \vec{c}\cdot\vec{c})$, that is $(r_{11} = r_{22} \neq r_{33})$, which appears on page 36-37. Within this division a search is made for the set of three "unsymmetrical" scalars coinciding with our observed set, namely $(\vec{b}\cdot\vec{c}\ \ \vec{c}\cdot\vec{a}\ \ \vec{a}\cdot\vec{b}) = (\tfrac{1}{2}\bar{r}_{33}\ \ \tfrac{1}{2}\bar{r}_{33}\ \ r_{12})$. It turns out to be the seventh entry, indicating an orthorhombic cell. The number in parentheses, (26a), refers to the cell number in Table 3, appearing on page 54, and to the corresponding diagram in Figure 5 on page 55.

Step 5. Identification of lattice type and calculation of cell parameters.

Referring now to Table 3 and cell number (26a), we find all the remaining information we need to know. According to this table nickel dimethylglyoxime is body-centered orthorhombic and the matrix for transforming the conventional reduced cell to the orthorhombic cell is $111/\bar{1}10/001$.

The orthorhombic cell parameters may be calculated from the conventional reduced cell parameters in one of two ways, using either the direct transformation matrix appearing in column 4 or the formulas appearing in column 5. Both methods are illustrated below.

Method A. (discussed in Appendix IV).

I-orthorhombic cell — Conventional reduced cell

$$\begin{pmatrix} \vec{A} \\ \vec{B} \\ \vec{C} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}$$

$\vec{A} = \vec{a} + \vec{b} + \vec{c}$

$\vec{B} = -\vec{a} + \vec{b}$

$\vec{C} = \vec{c}$

$$A^2 = (\vec{a} + \vec{b} + \vec{c}) \cdot (\vec{a} + \vec{b} + \vec{c})$$

$$= \vec{a} \cdot \vec{a} + \vec{b} \cdot \vec{b} + \vec{c} \cdot \vec{c} + 2\vec{b} \cdot \vec{c} + 2\vec{c} \cdot \vec{a} + 2\vec{a} \cdot \vec{b}$$

$$= a^2 + b^2 + c^2 + 2bc \cos \alpha + 2ca \cos \beta + 2ab \cos \gamma$$

$$= (10.3583)^2 + (10.3595)^2 + (6.4901)^2$$

$$+ 2(-21.0557) + 2(-21.0412) + 2(52.8078)$$

$$= 278.15785 \qquad A = 16.68 \text{ Å}.$$

Similarly,

$$B^2 = (-\vec{a} + \vec{b}) \cdot (-\vec{a} + \vec{b}) = 108.99802, \qquad B = 10.44 \text{ Å}$$

$$C^2 = (\vec{c}) \cdot (\vec{c}), \qquad C = 6.49 \text{ Å}.$$

Method B.

$$A^2 = 2(r_{11} + r_{12}) - r_{33}$$
$$= 2(107.30681 + 52.8078) - 42.1214$$
$$= 278.10783 \qquad A = 16.68 \text{ Å}.$$

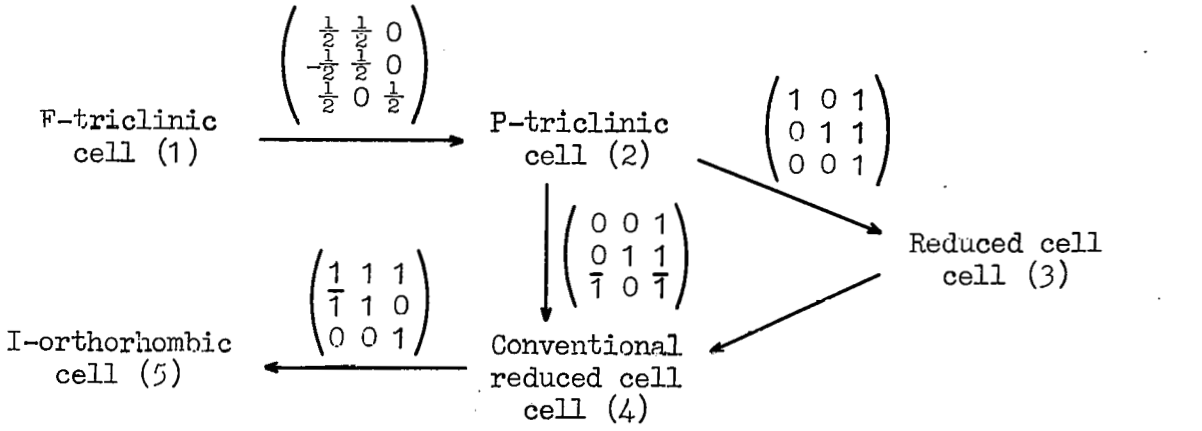
$$B^2 = 2(r_{11} - r_{12})$$
$$= 2(107.30681 - 52.8078)$$
$$= 108.99802 \qquad B = 10.44 \text{ Å}.$$

$$C^2 = r_{33} = 42.1214 \qquad C = 6.49 \text{ Å}.$$

where $r_{11}$ in this case was taken as the average of $a^2 + b^2$. These values agree quite well, within experimental error, with the observed values[7] of a = 16.68, b = 10.44 and c = 6.49 Å.

Step 6. Generation of matrix for transformation of the face-centered triclinic cell to body-centered orthorhombic cell.

The series of transformations which were executed in the preceding series of steps, together with the transformation matrices used and generated, were the following:



The matrix, N, for the transformation of the original face-centered triclinic cell to the orthorhombic cell is given by

$$N = KJI = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & -1 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} .$$

This is solved by matrix multiplication (Appendix VI). First J and I are multiplied together, as written, and the resultant left multiplied by K. The result becomes

$$N = \begin{Vmatrix} -\frac{1}{2} & 0 & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ -1 & -\frac{1}{2} & -\frac{1}{2} \end{Vmatrix} , \qquad [\text{cell (1) to cell (5)}].$$

We may check this matrix to verify its correctness by first calculating its modulus. The value is observed to be $+\frac{1}{2}$, verifying that the system has remained right-handed (indicated by the + sign) and that a reduction in volume of one-half has occurred in going from a face-centered lattice to a body-centered lattice, which is just what we should expect. If we then calculate the orthorhombic cell parameters using matrix N, we find that precisely the same values are obtained for A, B, C as before.

With appropriate application of matrix N to the face-centered triclinic cell, the body-centered orthorhombic cell may be located on the single crystal orienter and a check made on the intensities to verify the presence of three intersecting mirror planes, thereby confirming the true existence of the orthorhombic cell rather than a pseudo-orthorhombic cell.

Having obtained the matrix for the transformation of the original triclinic cell to the final orthorhombic cell, we may quite easily construct a schematic diagram of the lattice containing both cells to visualize just how they are oriented relative to each other. To do this we could first draw the triclinic lattice and then, using the transformation matrix N, construct the orthorhombic vectors within this lattice, or we could draw the orthorhombic lattice first, constructing the triclinic vectors in the lattice second. Obviously, the latter approach would be the easier since the axes describe an orthogonal system which is easier to draw. But to do this we need to know the inverse of matrix N since we will want to go "from" the orthorhombic cell constructed first "to" the triclinic cell. The inverse matrix and the appropriate vectorial transformation of axes in direct space is

$$N^{-1} = \begin{Vmatrix} -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{3}{2} & -\frac{1}{2} \\ \frac{3}{2} & -\frac{1}{2} & -\frac{1}{2} \end{Vmatrix}$$

| F-triclinic cell | | I-orthorhombic cell |
|---|---|---|
| $\vec{A}$ | = | $-\frac{1}{2}\vec{a} - \frac{1}{2}\vec{b} - \frac{1}{2}\vec{c}$ |
| $\vec{B}$ | = | $-\frac{1}{2}\vec{a} + \frac{3}{2}\vec{b} - \frac{1}{2}\vec{c}$ |
| $\vec{C}$ | = | $\frac{3}{2}\vec{a} - \frac{1}{2}\vec{b} - \frac{1}{2}\vec{c}$ . |

The net result is shown in Fig. 6 in which the vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ correspond to the axes of the orthorhombic cell and the vectors $\vec{A}$, $\vec{B}$, $\vec{C}$ to the axes of the original face-centered triclinic cell.

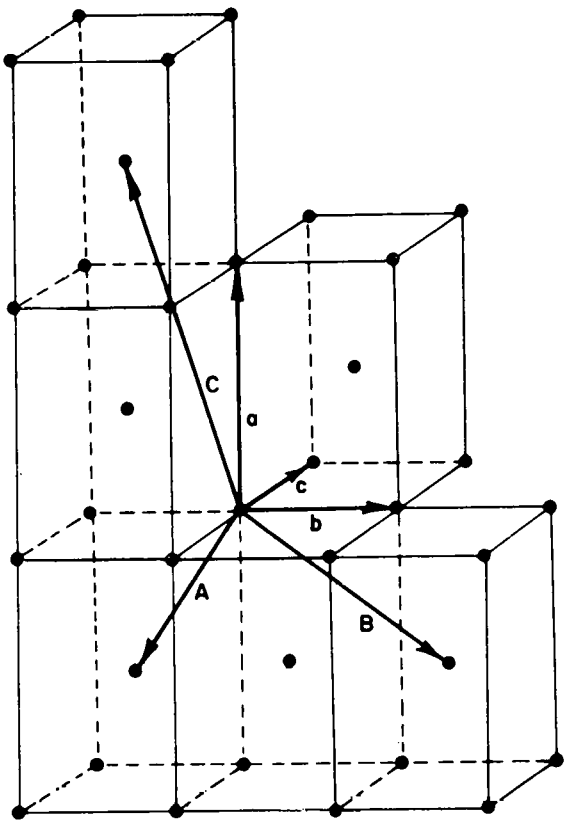



Fig. 6. The face-centered triclinic cell outlined in the body-centered orthorhombic lattice of nickel dimethylglyoxime.

Once we know the matrix for transforming the original cell to the final cell in direct space, we automatically know three other matrices, namely the original cell to the final cell in reciprocal space and the final cell back to the original cell in both direct and reciprocal space. Knowing these, of course, we then automatically know the matrices for transforming Miller indices as well as atomic coordinates of atoms because the former transforms by the same matrix as the transformation of axes in direct space (Appendix III) and the atomic coordinates transform by the same matrix as the transformation of axes in reciprocal space (Appendix III).

The matrices of interest may be summarized as follows: Let cell (1) be the original face-centered triclinic cell and cell (5) the final body-centered orthorhombic cell. In addition, let N be the matrix for transforming cell (1) to cell (5) and its inverse, $N^{-1}$, be that for cell (5) to cell (1), both in direct space; that is

CELL (1) TO CELL (5) CELL (5) TO CELL (1)

$$N = \begin{Vmatrix} -\frac{1}{2} & 0 & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ -1 & -\frac{1}{2} & -\frac{1}{2} \end{Vmatrix} \qquad N^{-1} = \begin{Vmatrix} -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{3}{2} & -\frac{1}{2} \\ \frac{3}{2} & -\frac{1}{2} & -\frac{1}{2} \end{Vmatrix}$$

From these two matrices we may establish the following for the transformation of axes:

CELL (1) TO CELL (5)

in direct space:
$$\begin{Vmatrix} -\frac{1}{2} & 0 & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ -1 & -\frac{1}{2} & -\frac{1}{2} \end{Vmatrix} = N$$

in reciprocal space:
$$\begin{Vmatrix} -\frac{1}{2} & -\frac{1}{2} & \frac{3}{2} \\ -\frac{1}{2} & \frac{3}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{Vmatrix} = \text{transpose of } N^{-1}$$

CELL (5) TO CELL (1)

in direct space:
$$\begin{Vmatrix} -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{3}{2} & -\frac{1}{2} \\ \frac{3}{2} & -\frac{1}{2} & -\frac{1}{2} \end{Vmatrix} = N^{-1}$$

in reciprocal space:
$$\begin{Vmatrix} -\frac{1}{2} & -\frac{1}{2} & -1 \\ 0 & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & 0 & -\frac{1}{2} \end{Vmatrix} = \text{transpose of } N$$

Problem 3, Part A, just completed by hand calculation may be solved for the most part through the use of the computer program TRACER, discussed in the next chapter. The input and output to this problem are shown on pages 120 through 125.

## PART B

To illustrate a phenomenon which may occur, not often but occassionally, let us modify one of the lattice parameters, say c, by an amount +0.004 Å to that which was observed for the face-centered triclinic cell stated in Part A of this problem, thus paralleling a situation which may occur in experimental measurements of lattice parameters. Suppose we change the parameter c = 25.760 to c = 25.764 Å., leaving the others unchanged. Now repeat the series of transformations executed in Part A.

Solution. First, the face-centered triclinic cell is transformed to the primitive cell, yielding the parameters a = 10.3602, b = 10.4402, c = 10.3602 Å, $\alpha$ = 120.2510°, $\beta$ = 143.4914°, $\gamma$ = 59.7430°.

Next, the reduced cell is found. Using the method of Section A of this chapter (or programs RCELL or TRACER), it is observed that the primitive triclinic cell transforms to a reduced cell this time, not by the transformation matrix observed in Part A of this problem, but by the following matrix:

$$\begin{Vmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & 0 & 1 \end{Vmatrix} \quad \text{[cell (2) to cell (3)]},$$

to yield lattice parameters a = 6.4904, b = 10.3600, c = 10.3602 Å., $\alpha$ = 72.7766°, $\beta$ = 71.7461°, $\gamma$ = 108.2460°.

Next the reduced cell in its conventional orientation is obtained, giving

$$a = 10.3600\ \text{Å}. \qquad \alpha = 108.2539°$$

$$b = 10.3602 \qquad \beta = 108.2460°$$

$$c = 6.4904 \qquad \gamma = 107.2234°$$

and the matrix for cell (2) to cell (4) being

$$\begin{Vmatrix} 1 & \bar{1} & \bar{1} \\ 0 & 0 & 1 \\ \bar{1} & 0 & \bar{1} \end{Vmatrix} .$$

If we compare the conventional reduced cell just obtained with the one obtained in Part A, Step 3, we notice a conspicuous difference. All six cell parameters are essentially the same (within experimental error) except the angle $\gamma$. The questions which might be asked at this point are: What happened? Are the conventional reduced cells obtained in both cases really the same or are they actually different? Is it still possible to arrive at the same orthorhombic cell as that obtained in Part A of this problem?

Before explaining what happened, let us first answer the last of the three questions by analyzing the scalars of the conventional reduced cell just obtained. These are

$$\begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{c}\cdot\vec{c} \\ \vec{b}\cdot\vec{c} & \vec{c}\cdot\vec{a} & \vec{a}\cdot\vec{b} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{22} & r_{33} \\ r_{23} & r_{31} & r_{12} \end{pmatrix} = \begin{pmatrix} 107.33 & 107.33 & 42.12 \\ -21.06 & -21.05 & -31.78 \end{pmatrix} .$$

This reduced form is seen to be identical to that obtained in Part A except that $r_{12}$ is now negative with a value of -31.78 instead of +52.81. Inspection of Table 2 for the observed form of

$$\begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{c}\cdot\vec{c} \\ \vec{b}\cdot\vec{c} & \vec{c}\cdot\vec{a} & \vec{a}\cdot\vec{b} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \frac{1}{2}\bar{r}_{33} & \frac{1}{2}\bar{r}_{33} & \bar{r}_{12} \end{pmatrix}$$

shows that the lattice is again orthorhombic, the number in parentheses being (26b).

Turning to Table 3 and looking up cell number (26b) it is discovered that the reduced cell actually describes the same body-centered orthorhombic lattice as does (26a) and can be verified visually upon inspection of the corresponding figure.

Let us now analyze what happened to cause this change in the reduced cell and to show mathematically that the two reduced cells do indeed describe the same orthorhombic cell. First, notice the similarities, and differences, in the matrices for the transformation of the primitive triclinic cell, cell (2), to the reduced cell, cell (3), obtained in Parts A and B. They were

Part A

$$\begin{Vmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{Vmatrix}$$

Part B

$$\begin{Vmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & 0 & 1 \end{Vmatrix} .$$

The only difference in the two is the difference in element $n_{21}$; in the former matrix it is a "0", in the latter a "-1". This means the change toward the apparently different reduced cells took place during the cell reduction when the following test was made:

$$|\vec{a}_n \cdot \vec{b}_n| \overset{?}{\leq} \tfrac{1}{2} a^2 ,$$

the point at which a test was made for the possible reduction of vector $\vec{b}$ in the ab-plane, holding vector $\vec{a}$ fixed in both magnitude and direction. In the reduction routine it is observed that this occurs when subscript n = 3. In part A the actual test and results are


(a) Part A (b) Part B

Fig. 7. Vectors in $a_3b_3$-plane in Example 3, parts A and B respectively.

$$|+21.0547| < \tfrac{1}{2}\,(42.1214) = 21.0607$$

and in part B

$$|+21.0752| > \tfrac{1}{2}\,(42.1253) = 21.0626\ .$$

The scalar product $\vec{a}_3 \cdot \vec{b}_3$ is seen to be so close in absolute value to $\frac{1}{2}a_3^2$ that the slightest change in either of the two quantities influenced whether or not reduction was to occur (see Fig. 7). In part A the scalar product was less than $\frac{1}{2}a_3^2$ so that no reduction took place and the angle $\gamma$ remained acute; in part B the scalar product was greater than $\frac{1}{2}a_3^2$ so that reduction took place and the angle $\gamma$ became obtuse.

It is to be recalled from the discussion in section A of this chapter that if the projection of say, vector $\vec{b}$, onto say, vector $\vec{a}$, is exactly

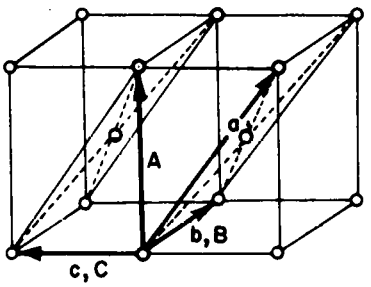
equal to $|\frac{1}{2}\vec{a}|$, then the magnitude of vector $\vec{b}$ remains unchanged if the character of the angle between $\vec{a}$ and $\vec{b}$ is reversed. Thus, in experimental work where lattice parameters have a certain amount of error associated with them, it is of no serious consequence if a vector is or is not capable of being reduced in this situation. In one case the angle is acute, in the other obtuse, and the vector being shifted undergoes only a very small to negligible change in magnitude, depending on how close the situation above is described.

Let us now assume for the moment that entry number (26b) is not in Tables 2 or 3. Since the reduced form obtained in part B contains a negative $r_{12}$, it would appear that we could not use reduced form (26a). The reduced form to which one must resort would then be the choice

$$\begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{b}\cdot\vec{b} & \vec{c}\cdot\vec{c} \\ \vec{b}\cdot\vec{c} & \vec{c}\cdot\vec{a} & \vec{a}\cdot\vec{b} \end{pmatrix} = \begin{pmatrix} r_{11} & r_{11} & r_{33} \\ \bar{r}_{23} & \bar{r}_{23} & \bar{r}_{12} \end{pmatrix}, \text{ (Monoclinic 15)}$$

which technically matches the observed ($r_{12}$ negative).

Now, monoclinic (15) is an end-centered cell, being C-centered b-unique or B-centered c-unique. Since the observed reduced form matches so closely reduced form (26a), except for $r_{12}$ being negative, we should be highly suspicious of the existence of the body-centered orthorhombic lattice. To confirm our suspicions it may be recalled that an end-centered monoclinic cell may be transformed to a body-centered monoclinic cell by the following transformation (shown for C-centered b-unique)




$$\vec{A} = \vec{a} + \vec{c}$$
$$\vec{B} = \vec{b}$$
$$\vec{C} = \vec{c}$$

Fig. 8. Transformation of a C-centered monoclinic lattice to a Body-centered lattice.

If the body-centered monoclinic cell has $\beta = 90°$ and three intersecting mirror planes are found, the cell is then body-centered orthorhombic. Thus, let us transform the conventional reduced cell to the body-centered monoclinic cell, using the following series of transformations:

$$\text{conventional reduced cell} \xrightarrow[\text{(from table 9)}]{\begin{Vmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix}} \text{C-centered monoclinic 13b (b-unique)} \xrightarrow{\begin{Vmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix}} \text{I-centered cell}$$

The matrix for the transformation of the conventional reduced cell to the body-centered cell becomes

$$N = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which, when solved by matrix multiplication, is seen to give a transformation matrix which gives the same body-centered lattice parameters

as those obtained in part A. This means that although the reduced cell obtained in part B appears to differ from that obtained in part A in the angle $\gamma$, the same body-centered orthorhombic lattice is described by the reduced cell in either case, regardless of whether $r_{12}$ is negative or positive. Using this transformation matrix just obtained the cell parameters are calculated to be A = 10.44, B = 16.68, C = 6.49 Å.; the values for A and B have simply been interchanged in value.

In this particular example the conventional reduced cells gave reduced forms in which $|r_{12}|_a \neq |-r_{12}|_b$. In some cases this is, indeed, found to occur. In others $|r_{12}|_a = |-r_{12}|_b$, an example being monoclinic (4a and 4b). These cases arise soley from the convention set upon the reduced cell, which explicitly states that while $\alpha$ and $\beta$ are restricted to obtuse, no such restriction exists on $\gamma$. So it is that in some cases two reduced cells satisfying the convention may result for a particular lattice, differing only in the angle $\gamma$, the result being different orientations of the "same" reduced cell in the lattice.

## III. COMPUTER PROGRAMS FOR LATTICE TRANSFORMATIONS AND CELL REDUCTIONS

Two Fortran computer programs are described in this chapter for general lattice transformations and cell reductions in direct space. The first described is RCELL, a computer program used soley for obtaining reduced cells directly from primitive triclinic or monoclinic cells. The second described is TRACER, a much more general program which

may be used for general cell transformations in direct space, for cell reductions only or for general cell transformations followed by cell reduction. TRACER is designed to perform the same operations as RCELL with the added feature that if cell reduction is desired,the input cell may be primitive or centered, and if centered,may be transformed by the program to a primitive cell and then reduced without reloading the program. Program RCELL is restricted to the reduction of primitive cells only in obtaining reduced cells.

## A. RCELL,

## A Fortran Cell Reduction Program

### 1. GENERAL INFORMATION

Program RCELL, written in IBM 7074 Fortran language, is a computer program for the reduction of primitive cells by the procedure discussed in Chapter II. The orientation of the reduced cell defined in this program is that established for a triclinic lattice, that cell whose edges are the three shortest non-coplanar translations in the lattice, labelled so as to have $c < a < b$ and oriented so that the angles $\alpha$ and $\beta$ are non-acute.

The essential input consists of four cards: a title card, a card specifying the form of the six cell parameters of the cell to be reduced, a card containing the six lattice parameters, and a stopper card coded so as to allow more than one cell to be reduced without reloading the program.

The output consists of the input data, the old parameters (real and reciprocal), the new parameters (real and reciprocal) of the reduced cell together with the transformation matrix and its inverse for the original cell to the reduced cell, the new parameters (real and reciprocal) of the reduced cell in its conventional orientation together with the transformation matrix and its inverse for the original cell to the reduced cell in its conventional orientation, the trigonometric values (sine and cosine) of the real and reciprocal angles of the conventional reduced cell and the scalars corresponding to the conventional reduced cell for use with Tables 2 and 3 for the determination of unit cells of higher symmetry.

The program has been written in full Fortran with a minimum of indexing. All arrays are one-dimensional. There are no subroutines. The sequential instructions in the program follow exactly the reduction procedure outlined in Chapter II, Example 1, and the rules outlined on pages 13-17. Example 1 in Chapter 1 has been included in this report for a twofold purpose. It illustrates the step-by-step detailed mechanics of solving for the reduced cell and it provides a worked out example to aid in following and interpreting the Fortran statements in the Symbolic Program Listing.

The program itself is divided into five parts according to its function. Part 1 is used for reading in the input data and setting it up for use in Part 2. It is used in calculating the cell parameters in direct or reciprocal space, depending upon the form of the input, and for calculating the trigonometric values of the cell angles. The formulas which are used are the following (from Buerger[1], Tables 20 and 21):

$$a^* = \frac{1}{a \sin\beta^* \sin\gamma} \qquad \cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$$

$$b^* = \frac{1}{b \sin\alpha^* \sin\gamma} \qquad \cos\beta^* = \frac{\cos\alpha\cos\gamma - \cos\beta}{\sin\alpha\sin\gamma}$$

$$c^* = \frac{1}{c \sin\alpha^* \sin\beta} \qquad \cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$$

$$a = \frac{1}{a^* \sin\beta \sin\gamma^*} \qquad \cos\alpha = \frac{\cos\beta^*\cos\gamma^* - \cos\alpha^*}{\sin\beta^*\sin\gamma^*}$$

$$b = \frac{1}{b^* \sin\alpha \sin\gamma^*} \qquad \cos\beta = \frac{\cos\alpha^*\cos\gamma^* - \cos\beta^*}{\sin\alpha^*\sin\gamma^*}$$

$$c = \frac{1}{c^* \sin\alpha \sin\beta^*} \qquad \cos\gamma = \frac{\cos\alpha^*\cos\beta^* - \cos\gamma^*}{\sin\alpha^*\sin\beta^*}$$

$$V = abc \sin\alpha \sin\beta \sin\gamma^*$$

$$V^* = 1/V \quad .$$

Part 2 transforms the original cell to its reduced cell, which may or may not conform to convention. The final matrix elements which are generated for the transformation of the original cell to its reduced cell are represented in the program as a one-dimensional array, N(I), where I is a subscript, and is defined as follows:

$$\begin{matrix} \text{original} \\ \text{cell} \end{matrix} \begin{pmatrix} \vec{A} \\ \vec{B} \\ \vec{C} \end{pmatrix} = \begin{pmatrix} N_1 & N_2 & N_3 \\ N_4 & N_5 & N_6 \\ N_7 & N_8 & N_9 \end{pmatrix} \begin{matrix} \text{reduced} \\ \text{cell} \end{matrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix} .$$

The matrices printed out in the output correspond to the direct transformation matrix defined as

$$\begin{matrix}\text{original}\\ \text{cell}\end{matrix} \qquad\qquad \begin{matrix}\text{reduced}\\ \text{cell}\end{matrix}$$

$$\begin{pmatrix}\vec{A}\\ \vec{B}\\ \vec{C}\end{pmatrix} = \begin{pmatrix}n_{11} & n_{12} & n_{13}\\ n_{21} & n_{22} & n_{23}\\ n_{31} & n_{32} & n_{33}\end{pmatrix} \begin{pmatrix}\vec{a}\\ \vec{b}\\ \vec{c}\end{pmatrix}$$

where $n_{11} = N_1$, $n_{12} = N_2$, etc.

Part 3 transforms the reduced cell obtained in Part 2 to the conventional orientation established for the triclinic system. Part 4 calculates the trigonometric sines and cosines of the angles of the conventional reduced cell. Part 5 calculates the six Niggli scalars, which are defined on page 29.

As indicated in Chapter II a primitive monoclinic cell may be reduced to obtain a new cell with more orthogonal axes. For a discussion regarding this use of RCELL, see page 110.

## 2. INPUT DATA

1. Title card -- 1 card -- FORMAT (16A5)

   Any alphanumeric information. This will be printed back out as a heading on each page of output.

2. Control card -- 1 card -- FORMAT (I1)

   = 1 if the cell parameters on the Parameter card are in direct space.

   = 2 if the cell parameters on the Parameter card are in reciprocal space.

3. Parameter card -- 1 card

| Column | |
|---|---|
| 1 - 10 | FORMAT (F10.6), lattice parameter a (or a*). |
| 11 - 20 | FORMAT (F10.6), lattice parameter b (or b*). |
| 21 - 30 | FORMAT (F10.6), lattice parameter c (or c*). |
| 31 - 40 | FORMAT (F10.6), lattice parameter $\alpha$ (or $\alpha^*$). |
| 41 - 50 | FORMAT (F10.6), lattice parameter $\beta$ (or $\beta^*$). |
| 51 - 60 | FORMAT (F10.6), lattice parameter $\gamma$ (or $\gamma^*$). |

Note: The cell edges are in (Å) in direct space and ($Å^{-1}$) in reciprocal space; the angles are in degrees and decimal fraction.

4. Stopper card -- 1 card -- FORMAT (I1)

= 0 (or blank) if no more cells are to be reduced.

= 1 if another cell is to be reduced.

Note: This card allows reduction of more than one cell without reloading the program. Thus, any number of sets of data may be processed. Each set consists of items 1 through 4.

## 3. RUNNING DECK ARRANGEMENT

Program RCELL is on the Iowa State IBM 7074 library tape under the name RCELL44SLL. In using the tape a typical run will consist of the following cards:

| | 14 16 | 76 |
|---|---|---|
| 1 card: | (Start Account Card) | POGO |
| 1 card: | ALTSW ALL OFF | POGO |
| 1 card: | Z LLOAD @RCELL44SLL@ | POGO |

76

4 cards per cell: (Data Cards)

1 card: WTM

1 card: (End Account Card) POGO

All variables are stored in COMMON, locations 19800 - 19975, and may be called with a POGOZ dump. The time estimate is approximately 1 minute for reduction of 10 cells.

## 4. SAMPLE INPUT AND OUTPUT

Example 1 on page 19 showed by hand calculation the reduction of primitive 16-DL methyloctadecanoic acid whose lattice parameters are reported in the literature[6] as being

| | |
|---|---|
| a = 5.40 Å | $\alpha$ = 145° 38' |
| b = 7.54 | $\beta$ = 105° 42' |
| c = 51.8 | $\gamma$ = 60° 18' . |

The same cell may be reduced by this program, using the following input data:

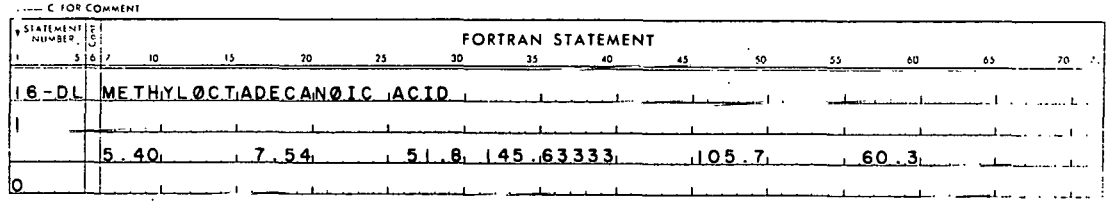



Fig. 9. Input data for sample problem.

The output is shown on the next two pages.

16-DL METHYLOCTADECANOIC ACID

INPUT DATA IN DIRECT SPACE

OLD PARAMETERS (ORIGINAL CELL)

| | | | |
|---|---|---|---|
| A | = 5.4000 | ALPHA | = 145.6333 |
| B | = 7.5400 | BETA | = 105.7000 |
| C | = 51.8000 | GAMMA | = 60.3000 |
| A* | = 0.222224 | ALPHA* | = 34.2310 |
| B* | = 0.271423 | BETA * | = 106.3917 |
| C* | = 0.035648 | GAMMA* | = 120.0464 |
| V | = 992.119 | | |
| V* | = 0.001008 | | |

NEW PARAMETERS (REDUCED CELL)

| | | | |
|---|---|---|---|
| A | = 5.4000 | ALPHA | = 92.6019 |
| B | = 6.7576 | BETA | = 94.8837 |
| C | = 28.2209 | GAMMA | = 104.2573 |
| A* | = 0.192023 | ALPHA* | = 86.0595 |
| B* | = 0.153046 | BETA * | = 84.2910 |
| C* | = 0.035648 | GAMMA* | = 75.4449 |
| V | = 992.119 | | |
| V* | = 0.001008 | | |

TRANSFORMATION MATRICES

| DIRECT | INVERSE |
|---|---|
| 1 0 0 | 1 0 0 |
| -1 1 0 | 1 1 0 |
| -2 6 1 | -4 -6 1 |
| MOD = 1.00 | MOD = 1.00 |

16-DL METHYLOCTADECANOIC ACID

NEW PARAMETERS (CONVENTICNAL REDUCED CELL)

| | | | |
|---|---|---|---|
| A = | 6.7576 | ALPHA = | 94.8837 |
| B = | 28.2209 | BETA = | 104.2573 |
| C = | 5.4000 | GAMMA = | 92.6019 |
| A* = | 0.153046 | ALPHA* = | 84.2910 |
| B* = | 0.035648 | BETA * = | 75.4449 |
| C* = | 0.192023 | GAMMA* = | 86.0595 |
| V = | 992.119 | | |
| V* = | 0.001008 | | |

TRANSFORMATION MATRICES

| DIRECT | | | INVERSE | | |
|---|---|---|---|---|---|
| -1 | 1 | 0 | 0 | 0 | 1 |
| -2 | 6 | 1 | 1 | 0 | 1 |
| 1 | 0 | 0 | -6 | 1 | -4 |

TRIGONOMETRIC VALUES OF THE ANGLES OF THE CONVENTICNAL REDUCED CELL

| | ANGLE | SIN | COS |
|---|---|---|---|
| ALPHA | 94.8837 | 0.99637 | -0.08513 |
| BETA | 104.2573 | 0.96920 | -0.24628 |
| GAMMA | 92.6019 | 0.99897 | -0.04540 |
| ALPHA* | 84.2910 | 0.99504 | 0.09948 |
| BETA * | 75.4449 | 0.96791 | -0.25131 |
| GAMMA* | 86.0595 | 0.99764 | 0.06872 |

SCALARS CORRESPONDING TO CONVENTIONAL REDUCED CELL

R(1,1) = 45.67 R(2,2) = 796.42 R(3,3) = 29.16

R(2,3) = -12.97 R(3,1) = -8.99 R(1,2) = -8.66

R(2,3) + R(3,1) + R(1,2) = -30.62

# 5. SYMBOLIC PROGRAM LISTING

```
C                              PROGRAM RCELL
C
C
C
C     DESCRIPTION.    CELL REDUCTION PROGRAM
C     LANGUAGE.       FULL FORTRAN FOR IBM 7074
C     DATE.           FEBRUARY 1965 (FINAL VERSION)
C     PROGRAMMER.     STEPHEN L. LAWTON
C
C
C     GLOSSARY OF SYMBOLS
C
C     A           DIRECT CELL PARAMETER, A
C     AA          A*A
C     AB          A*B*COSGA = SCALAR PRODUCT OF A WITH B
C     ABSAB       ABSF(AB)
C     ABSBC       ABSF(BC)
C     ABSCA       ABSF(CA)
C     AL          DIRECT CELL PARAMETER, ALPHA, IN RADIANS
C     ALPHA       DIRECT CELL PARAMETER, ALPHA, IN DEGREES
C     ALS         RECIPROCAL CELL PARAMETER, ALPHA-STAR, IN RADIANS
C     ALSTAR      RECIPROCAL CELL PARAMETER, ALPHA-STAR, IN DEGREES
C     ANGLE(3)    DIRECT CELL PARAMETERS ALPHA, BETA, GAMMA IN NEW CELL
C     AS          RECIPROCAL CELL PARAMETER, A-STAR
C     B           DIRECT CELL PARAMETER, B
C     BB          B*B
C     BC          B*C*COSAL = SCALAR PRODUCT OF B WITH C
C     BE          DIRECT CELL PARAMETER, BETA, IN RADIANS
C     BES         RECIPROCAL CELL PARAMETER, BETA-STAR, IN RADIANS
C     BESTAR      RECIPROCAL CELL PARAMETER, BETA-STAR, IN DEGREES
C     BET         MODULUS OF INVERSE MATRIX, IN FLOATING POINT
C     BETA        DIRECT CELL PARAMETER, BETA, IN DEGREES
C     BS          RECIPROCAL CELL PARAMETER, B-STAR
C     C           DIRECT CELL PARAMETER, C
C     CA          C*A*COSBE = SCALAR PRODUCT OF C WITH A
C     CC          C*C
C     COSAL       COSF(AL)
C     COSALS      COSF(ALS)
C     COSBE       COSF(BE)
C     COSBES      COSF(BES)
C     COSGA       COSF(GA)
C     COSGAS      COSF(GAS)
C     CS          RECIPROCAL CELL PARAMETER, C-STAR
C     D(3)        DIRECT CELL PARAMETERS A, B, C IN NEW ORIENTED CELL
C     DET         MODULUS OF DIRECT MATRIX, IN FLOATING POINT
C     GA          DIRECT CELL PARAMETER, GAMMA, IN RADIANS
C     GAMMA       DIRECT CELL PARAMETER, GAMMA, IN DEGREES
C     GAS         RECIPROCAL CELL PARAMETER, GAMMA-STAR, IN RADIANS
C     GASTAR      RECIPROCAL CELL PARAMETER, GAMMA-STAR, IN DEGREES
C     I           INDEX
C     IAXIS       AXIS (VECTOR) HELD CONSTANT. 1=A, 2=B, 3=C
C     ICONT       CODE FOR NEXT JOB
C     ICYCLE      NUMBER OF CYCLES IN REDUCED CELL ROUTINE
C     INPUT       SPECIFICATION CODE FOR CELL PARAMETERS READ AT INPUT
C     IOUTPT      PROGRAM SECTION NUMBER
C     ISIGN       NUMBER OF ACUTE ANGLES IN REDUCED CELL
C     J           INDEX
```

```
C      JA          CODE FOR SHIFT IN A-AXIS.  JA=0 NO SHIFT, JA=1 SHIFT
C      JB          CODE FOR SHIFT IN B-AXIS.  JB=0 NO SHIFT, JB=1 SHIFT
C      JC          CODE FOR SHIFT IN C-AXIS.  JC=0 NO SHIFT, JC=1 SHIFT
C      JF          JA + JB + JC
C      JJ          INDEX.
C      JL          INDEX.
C      K2          CODE FOR REDUCTION OF REMAINING TWO AXES
C      KK          CODE FOR PARAMETERS IN CONVENTIONAL CELL. 1=A, 2=B, 3=C
C      L           INDEX
C      LM          INDEX
C      M           INDEX
C      MAX         LARGEST CELL PARAMETER READ AT INPUT. 1=A, 4=B, 7=C
C      N(9)        ELEMENTS OF DIRECT TRANSFORMATION MATRIX
C      NA(9)       MATRIX ELEMENTS OF CELL (N) TO CELL (N+1)
C      NB(9)       MATRIX ELEMENTS OF CELL (1) TO CELL (N+1)
C      NCHECK      INDEX CONTROLLING REDUCTION OF CELL PARAMETER
C      NET         MODULUS OF DIRECT TRANSFORMATION MATRIX, IN FIXED POINT
C      NI(9)       ELEMENTS OF INVERSE TRANSFORMATION MATRIX
C      NSTOP       INDEX CONTROL. WHEN NSTOP = 3, REDUCTION CYCLE COMPLETE
C      NTEMP(9)    TEMPORARY STORAGE LOCATION FOR MATRIX ELEMENTS
C      NTURN       INDEX CONTROL
C      PN          INTEGER (FLOATING PT.)
C      QMAX        THE LARGER OF TWO CELL PARAMETERS
C      QQMAX       THE LARGEST OF (ABSAB, ABSBC, ABSCA)
C      SINAL       SINF(AL)
C      SINALS      SINF(ALS)
C      SINBE       SINF(BE)
C      SINBES      SINF(BES)
C      SINGA       SINF(GA)
C      SINGAS      SINF(GAS)
C      STORE       TEMPORARY STORAGE LOCATION FOR NEW SCALAR PRODUCT
C      SUM         BC + CA + AB
C      TITLE(16)   ALPHANUMERIC TITLE READ AT START OF PROGRAM
C      V           CELL VOLUME IN DIRECT SPACE
C      VS          CELL VOLUME IN RECIPROCAL SPACE
C      X           TEMPORARY LOCATION FOR CELL PARAMETER A, B OR C
C      XX          X*X
C      XY          TEMPORARY LOCATION FOR SCALAR PRODUCT AB, BC OR CA
C      XY2         TEMPORARY LOCATION OF NEW SCALAR PRODUCT
C      Y           TEMPORARY LOCATION FOR CELL PARAMETER A, B OR C
C      YY          Y*Y
C      YZ          TEMPORARY LOCATION FOR SCALAR PRODUCT AB, BC OR CA
C      Z           TEMPORARY LOCATION FOR CELL PARAMETER A, B OR C
C      ZX          TEMPORARY LOCATION FOR SCALAR PRODUCT AB, BC OR CA
C      ZX2         TEMPORARY LOCATION OF NEW SCALAR PRODUCT
C      ZZ          Z*Z
C
C
      DIMENSION TITLE(16), N(9), NA(9), NB(9), NI(9), D(3), ANGLE(3),
     1          NTEMP(9)
      COMMON  TITLE,INPUT,A,B,C,ALPHA,BETA,GAMMA,AS,BS,CS,ALSTAR,BESTAR,
     1        GASTAR,SINAL,SINBE,SINGA,COSAL,COSBE,COSGA,SINALS,SINBES,
     2        SINGAS,COSALS,COSBES,COSGAS,AL,BE,GA,ALS,BES,GAS,V,VS,AB,
     3        BC,CA,X,Y,Z,XY,YZ,ZX,XX,YY,ZZ,XY2,ZX2,QMAX,MAX,N,D,ANGLE,
     4        IOUTPT,NSTOP,K2,KK,NCHECK,PN,STORE,I,JJ,JL,M,L,LM,NTURN,
     5        NTEMP,ISIGN,ICONT,ABSAB,ABSBC,ABSCA,QQMAX,IAXIS,ICYCLE,
     6        JA,JB,JC,JF,SUM,NA,NB,NI,NET,DET,BET,J
C
C
C          PART 1.   INPUT
C
C
 9999 READ 1000, (TITLE(I), I = 1,16)
```

```
      READ 1001, INPUT
 1000 FORMAT (16A5)
 1001 FORMAT (I1)
      IOUTPT = 1
      IF (INPUT - 1) 61, 61, 62
   61 READ 1002, A, B, C, ALPHA, BETA, GAMMA
      GO TO 71
   62 READ 1002, AS, BS, CS, ALSTAR, BESTAR, GASTAR
 1002 FORMAT (6F10.6)
      GO TO 72
C
   71 SINAL = SINF(ALPHA * 0.01745329)
      SINBE = SINF(BETA  * 0.01745329)
      SINGA = SINF(GAMMA * 0.01745329)
      COSAL = COSF(ALPHA * 0.01745329)
      COSBE = COSF(BETA  * 0.01745329)
      COSGA = COSF(GAMMA * 0.01745329)
   81 ALS = ACOSF((COSBE * COSGA - COSAL) / (SINBE * SINGA))
      BES = ACOSF((COSAL * COSGA - COSBE) / (SINAL * SINGA))
      GAS = ACOSF((COSAL * COSBE - COSGA) / (SINAL * SINBE))
      SINALS = SINF(ALS)
      SINBES = SINF(BES)
      SINGAS = SINF(GAS)
      AS = 1. / (A * SINBES * SINGA)
      BS = 1. / (B * SINALS * SINGA)
      CS = 1. / (C * SINALS * SINBE)
      ALSTAR = ALS * 57.295780
      BESTAR = BES * 57.295780
      GASTAR = GAS * 57.295780
      GO TO 99
C
   72 SINALS = SINF(ALSTAR * 0.01745329)
      SINBES = SINF(BESTAR * 0.01745329)
      SINGAS = SINF(GASTAR * 0.01745329)
      COSALS = COSF(ALSTAR * 0.01745329)
      COSBES = COSF(BESTAR * 0.01745329)
      COSGAS = COSF(GASTAR * 0.01745329)
      AL = ACOSF((COSBES * COSGAS - COSALS) / (SINBES * SINGAS))
      BE = ACOSF((COSALS * COSGAS - COSBES) / (SINALS * SINGAS))
      GA = ACOSF((COSALS * COSBES - COSGAS) / (SINALS * SINBES))
      SINAL = SINF(AL)
      SINBE = SINF(BE)
      SINGA = SINF(GA)
      COSAL = COSF(AL)
      COSBE = COSF(BE)
      COSGA = COSF(GA)
      A = 1. / (AS * SINBE * SINGAS)
      B = 1. / (BS * SINAL * SINGAS)
      C = 1. / (CS * SINAL * SINBES)
      ALPHA = AL * 57.295780
      BETA  = BE * 57.295780
      GAMMA = GA * 57.295780
C
   99 V  = A*B*C*SINAL*SINBE*SINGAS
      VS = 1./V
      GO TO (65, 501, 67), IOUTPT
C
C
C          OUTPUT OF PART 1.   OUTPUT OF INPUT AND THE OTHER
C     CALCULATED CELL DATA.   (ORIGINAL CELL)
C
C
   65 PRINT 1004
```

```
      PRINT 1005, (TITLE(I), I = 1,16)
 1004 FORMAT (1H1)
 1005 FORMAT (1HK, 4X, 16A5 // )
      IF (INPUT - 1) 13, 13, 14
   13 PRINT 1006
 1006 FORMAT (1HJ, 3X, 27H INPUT DATA IN DIRECT SPACE // )
      GO TO 16
   14 PRINT 1007
 1007 FORMAT (1HJ, 3X, 31H INPUT DATA IN RECIPROCAL SPACE // )
   16 PRINT 1008
 1008 FORMAT (1HL, 9X, 33H OLD PARAMETERS   (ORIGINAL CELL)   )
   75 PRINT 1011, A, ALPHA
      PRINT 1012, B, BETA
      PRINT 1013, C, GAMMA
      PRINT 1014, AS, ALSTAR
      PRINT 1015, BS, BESTAR
      PRINT 1016, CS, GASTAR
      PRINT 1017, V
      PRINT 1018, VS
 1011 FORMAT (1HK, 15X, 6H A  = F9.4, 14X, 10H ALPHA  = F10.4)
 1012 FORMAT (1H , 15X, 6H B  = F9.4, 14X, 10H BETA   = F10.4)
 1013 FORMAT (1H , 15X, 6H C  = F9.4, 14X, 10H GAMMA  = F10.4)
 1014 FORMAT (1HJ, 15X, 6H A* = F9.6, 14X, 10H ALPHA* = F10.4)
 1015 FORMAT (1H , 15X, 6H B* = F9.6, 14X, 10H BETA * = F10.4)
 1016 FORMAT (1H , 15X, 6H C* = F9.6, 14X, 10H GAMMA* = F10.4)
 1017 FORMAT (1HJ, 15X, 6H V  = F9.3)
 1018 FORMAT (1H , 15X, 6H V* = F9.6, // )
      GO TO (174, 701, 889), IOUTPT
C
C
C           PART 2.   TRANSFORMATION OF ORIGINAL CELL TO REDUCED CELL
C
C
  174 IOUTPT = 2
      ICYCLE = 1
      AB = A * B * COSGA
      BC = B * C * COSAL
      CA = C * A * COSBE
      DO 175 J = 1,9
      N(J) = 0
  175 NA(J) = 0
      N(1) = 1
      N(5) = 1
      N(9) = 1
      NA(1) = 1
      NA(5) = 1
      NA(9) = 1
  382 NSTOP = 1
      K2 = 0
      ABSAB = ABSF(AB)
      ABSBC = ABSF(BC)
      ABSCA = ABSF(CA)
      QQMAX = MAX1F(ABSAB, ABSBC, ABSCA)
      IF (QQMAX - ABSAB) 176, 401, 176
  176 IF (QQMAX - ABSBC) 890, 404, 407
  401 QMAX = MAX1F(A,B)
      IF (QMAX - A) 84, 91, 92
  404 QMAX = MAX1F(B,C)
      IF (QMAX - B) 84, 93, 94
  407 QMAX = MAX1F(C,A)
      IF (QMAX - C) 84, 95, 96
   91 IAXIS = 2
      GO TO 1
```

```
   92 IAXIS = 1
      GO TO 4
   93 IAXIS = 3
      GO TO 4
   94 IAXIS = 2
      GO TO 7
   95 IAXIS = 1
      GO TO 7
   96 IAXIS = 3
      GO TO 1
C
    1 MAX = 1
      GO TO 10
    2 IAXIS = 1
      QMAX = MAX1F(B,C)
      IF (QMAX - B) 87, 101, 102
  101 K2 = 1
      GO TO 30
  102 K2 = 2
      GO TO 50
    3 IF (K2 - 1) 88, 121, 122
  121 IAXIS = 2
      GO TO 50
  122 IAXIS = 3
      GO TO 30
C
    4 MAX = 4
      GO TO 30
    5 IAXIS = 2
      QMAX = MAX1F(A,C)
      IF (QMAX - A) 87, 201, 202
  201 K2 = 1
      GO TO 10
  202 K2 = 2
      GO TO 50
    6 IF (K2 - 1) 88, 123, 124
  123 IAXIS = 1
      GO TO 50
  124 IAXIS = 3
      GO TO 10
C
    7 MAX = 7
      GO TO 50
    8 IAXIS = 3
      QMAX = MAX1F(A,B)
      IF (QMAX - A) 87, 301, 302
  301 K2 = 1
      GO TO 10
  302 K2 = 2
      GO TO 30
    9 IF (K2 - 1) 88, 125, 126
  125 IAXIS = 1
      GO TO 30
  126 IAXIS = 2
      GO TO 10
   84 PRINT 2010
 2010 FORMAT (1HL, 83H $ERROR$ - STATEMENT NO. 401 PLUS 001 CARD, 404 PL
     1US 001 CARD OR 407 PLUS 001 CARD.)
      GO TO 890
   87 PRINT 2011
 2011 FORMAT (1HL, 77H $ERROR$ - STATEMENT NO. 2 PLUS 001 CARD, 5 PLUS 0
     101 CARD OR 8 PLUS 001 CARD.)
      GO TO 890
```

```
   88 PRINT 2012
 2012 FORMAT (1HL, 35H $ERROR$ - STATEMENT NO. 3, 6 OR 9.)
      GO TO 890
C
C           REDUCTION OF A.    (QMAX = A)
C
   10 X  = A
      Y  = B
      Z  = C
      XY = AB
      YZ = BC
      ZX = CA
C
      NCHECK = 1
      GO TO (85, 11, 12), IAXIS
   11 I = 2
      GO TO 100
   12 I = 3
      GO TO 300
C
   15 A  = X
      B  = Y
      C  = Z
      AB = XY
      BC = YZ
      CA = ZX
C
      NCHECK = NCHECK - 1
      IF (NCHECK) 46, 17, 17
   17 IF (I - 2) 86, 12, 11
   46 MAX = MAX + 1
      NSTOP = NSTOP + 1
      IF (NSTOP - 3) 18, 18, 601
   18 GO TO (1, 2, 3, 4, 5, 6, 7, 8, 9), MAX
C
C           REDUCTION OF B.    (QMAX = B)
C
   30 X  = B
      Y  = C
      Z  = A
      XY = BC
      YZ = CA
      ZX = AB
C
      NCHECK = 1
      GO TO (32, 85, 31), IAXIS
   31 I = 6
      GO TO 100
   32 I = 4
      GO TO 300
C
   35 A  = Z
      B  = X
      C  = Y
      AB = ZX
      BC = XY
      CA = YZ
C
      NCHECK = NCHECK - 1
      IF (NCHECK) 46, 37, 37
   37 IF (I - 4) 86, 31, 32
C
C           REDUCTION OF C.    (QMAX = C)
```

```
C
   50 X  = C
      Y  = A
      Z  = B
      XY = CA
      YZ = AB
      ZX = BC
C
      NCHECK = 1
      GO TO (51, 52, 85), IAXIS
   51 I = 7
      GO TO 100
   52 I = 8
      GO TO 300
C
   55 A  = Y
      B  = Z
      C  = X
      AB = YZ
      BC = ZX
      CA = XY
C
      NCHECK = NCHECK - 1
      IF (NCHECK) 46, 57, 57
   57 IF (I - 7) 86, 52, 51
C
   85 PRINT 2015
 2015 FORMAT (1HL, 47H $ERROR$ - ERROR IN AXIS DESIGNATION IN PART 2.)
      GO TO 890
   86 PRINT 2014
 2014 FORMAT (1HL, 38H $ERROR$ - STATEMENT NO. 17, 37 OR 57.)
      GO TO 890
C
C           REDUCTION OF X.  ABSF(X.Y) GREATER THAN (Y**2)/2
C
  100 XX = X*X
      YY = Y*Y
      PN = 0.
      IF (ABSF(XY) - 0.5 * YY) 444, 444, 110
  110 IF (XY) 120, 444, 200
  120 XY2 = XY + PN*YY
      IF (XY2) 130, 150, 150
  130 STORE = XY2
      PN = PN + 1.
      GO TO 110
  150 IF (ABSF(XY2) - ABSF(STORE)) 143, 142, 142
  142 PN = PN - 1.
  143 NA(I) = PN
      X =  SQRTF(XX + 2.*PN*XY + PN*PN*YY)
      ZX = ZX + PN*YZ
  144 IF (ABSF(XY2) - ABSF(STORE)) 160, 170, 170
  160 XY = XY2
      GO TO 520
  170 XY = STORE
      GO TO 520
C
  200 XY2 = XY - PN*YY
      IF (XY2) 250, 250, 230
  230 STORE = XY2
      PN = PN + 1.
      GO TO 200
  250 IF (ABSF(XY2) - ABSF(STORE)) 243, 243, 242
  242 PN = PN - 1.
```

```
  243 NA(I) = -PN
      X = SQRTF(XX - 2.*PN*XY + PN*PN*YY)
      ZX = ZX - PN*YZ
      GO TO 144
C
C           REDUCTION OF X.  ABSF(Z.X) GREATER THAN (Z**2)/2
C
  300 XX = X*X
      ZZ = Z*Z
      PN = 0.
      IF (ABSF(ZX) - 0.5 * ZZ) 444, 444, 310
  310 IF (ZX) 320, 444, 400
  320 ZX2 = ZX + PN*ZZ
      IF (ZX2) 330, 350, 350
  330 STORE = ZX2
      PN = PN + 1.
      GO TO 310
  350 IF (ABSF(ZX2) - ABSF(STORE)) 343, 342, 342
  342 PN = PN - 1.
  343 NA(I) = PN
      X = SQRTF(XX + 2.*PN*ZX + PN*PN*ZZ)
      XY = XY + PN*YZ
  344 IF (ABSF(ZX2) - ABSF(STORE)) 360, 370, 370
  360 ZX = ZX2
      GO TO 520
  370 ZX = STORE
      GO TO 520
C
  400 ZX2 = ZX - PN*ZZ
      IF (ZX2) 450, 450, 430
  430 STORE = ZX2
      PN = PN + 1.
      GO TO 400
  450 IF (ABSF(ZX2) - ABSF(STORE)) 463, 463, 462
  462 PN = PN - 1.
  463 NA(I) = -PN
      X = SQRTF(XX - 2.*PN*ZX + PN*PN*ZZ)
      XY = XY - PN*YZ
      GO TO 344
C
  520 NB(1) = NA(1)*N(1) + NA(2)*N(4) + NA(3)*N(7)
      NB(2) = NA(1)*N(2) + NA(2)*N(5) + NA(3)*N(8)
      NB(3) = NA(1)*N(3) + NA(2)*N(6) + NA(3)*N(9)
      NB(4) = NA(4)*N(1) + NA(5)*N(4) + NA(6)*N(7)
      NB(5) = NA(4)*N(2) + NA(5)*N(5) + NA(6)*N(8)
      NB(6) = NA(4)*N(3) + NA(5)*N(6) + NA(6)*N(9)
      NB(7) = NA(7)*N(1) + NA(8)*N(4) + NA(9)*N(7)
      NB(8) = NA(7)*N(2) + NA(8)*N(5) + NA(9)*N(8)
      NB(9) = NA(7)*N(3) + NA(8)*N(6) + NA(9)*N(9)
      DO 521 J = 1,9
      N(J) = NB(J)
      IF (N(J)) 521, 540, 521
  540 N(J) = 0
  521 NA(J) = 0
      NA(1) = 1
      NA(5) = 1
      NA(9) = 1
  444 GO TO (601, 15, 15, 35, 601, 35, 55, 55, 601), I
C
C
C           OUTPUT OF PART 2.    (REDUCED CELL)
C
C
```

```
  601 COSAL = BC / (B*C)
      COSBE = CA / (C*A)
      COSGA = AB / (A*B)
      AL = ACOSF(COSAL)
      BE = ACOSF(COSBE)
      GA = ACOSF(COSGA)
      SINAL = SINF(AL)
      SINBE = SINF(BE)
      SINGA = SINF(GA)
      ALPHA = 57.295780 * AL
      BETA  = 57.295780 * BE
      GAMMA = 57.295780 * GA
      GO TO 81
C
C          A TEST IS NOW MADE TO DETERMINE IF THE CELL JUST OBTAINED
C     IS THE REDUCED CELL.  IF ONE OR MORE OF THE AXES CAN BE FURTHER
C     REDUCED, THE PROGRAM RETURNS TO STMNT 382 FOR ANOTHER CYCLE.
C
  501 IF (ABSF(AB) - 0.5 * A*A) 502, 502, 381
  502 IF (ABSF(AB) - 0.5 * B*B) 503, 503, 381
  503 IF (ABSF(BC) - 0.5 * B*B) 504, 504, 381
  504 IF (ABSF(BC) - 0.5 * C*C) 505, 505, 381
  505 IF (ABSF(CA) - 0.5 * C*C) 506, 506, 381
  506 IF (ABSF(CA) - 0.5 * A*A) 66, 66, 381
  381 ICYCLE = ICYCLE + 1
      GO TO 382
C
   66 NET = N(1)*(N(5)*N(9) - N(8)*N(6)) - N(2)*(N(4)*N(9) - N(7)*N(6))
     1     + N(3)*(N(4)*N(8) - N(7)*N(5))
      DET = NET
      NI(1) =  (N(5)*N(9) - N(8)*N(6)) / NET
      NI(2) = -(N(2)*N(9) - N(8)*N(3)) / NET
      NI(3) =  (N(2)*N(6) - N(5)*N(3)) / NET
      NI(4) = -(N(4)*N(9) - N(7)*N(6)) / NET
      NI(5) =  (N(1)*N(9) - N(7)*N(3)) / NET
      NI(6) = -(N(1)*N(6) - N(4)*N(3)) / NET
      NI(7) =  (N(4)*N(8) - N(7)*N(5)) / NET
      NI(8) = -(N(1)*N(8) - N(7)*N(2)) / NET
      NI(9) =  (N(1)*N(5) - N(4)*N(2)) / NET
      BET = NI(1)*(NI(5)*NI(9) - NI(8)*NI(6))
     1     - NI(2)*(NI(4)*NI(9) - NI(7)*NI(6))
     2     + NI(3)*(NI(4)*NI(8) - NI(7)*NI(5))
      DO 64 I = 1,9
      IF (NI(I)) 64, 63, 64
   63 NI(I) = 0
   64 CONTINUE
      IF (IOUTPT - 2) 582, 582, 583
C
  582 PRINT 1027
 1027 FORMAT (1HL,      9X, 32H NEW PARAMETERS   (REDUCED CELL)    )
      GO TO 75
  701 PRINT 1028
      PRINT 1029
      PRINT 1030, N(1), N(2), N(3), NI(1), NI(2), NI(3)
      PRINT 1030, N(4), N(5), N(6), NI(4), NI(5), NI(6)
      PRINT 1030, N(7), N(8), N(9), NI(7), NI(8), NI(9)
      PRINT 1031, DET, BET
 1028 FORMAT (1HJ, 25X, 25H TRANSFORMATION MATRICES )
 1029 FORMAT (1HJ, 23X, 7H DIRECT, 13X, 8H INVERSE )
 1030 FORMAT (1HJ, 20X, 3I4, 8X, 3I4 )
 1031 FORMAT (1HJ, 21X, 6H MOD = F5.2, 9X, 6H MOD = F5.2 )
C
C
```

```
C          PART 3.   TRANSFORMATION OF REDUCED CELL TO CONVENTIONAL
C      REDUCED CELL.  THE CONVENTION IS C LESS THAN A LESS THAN B,
C      WITH ALPHA, BETA OBTUSE.
C
C
      IOUTPT = 3
      JA = 0
      JB = 0
      JC = 0
      NTURN = 1
      KK = 3
      IF (MIN1F(A,B,C) - A) 702, 611, 999
  611 JJ = 7
      M = -6
      GO TO 721
  702 IF (MIN1F(A,B,C) - B) 612, 613, 999
  612 JC = 1
      JJ = 7
      M = 0
      GO TO 723
  613 JJ = 7
      M = -3
      GO TO 722
  703 NTURN = 2
      KK = 2
      IF (MAX1F(A,B,C) - A) 999, 614, 704
  614 JJ = 4
      M = -3
      GO TO 721
  704 IF (MAX1F(A,B,C) - B) 999, 615, 616
  615 JB = 1
      JJ = 4
      M = 0
      GO TO 722
  616 JJ = 4
      M = 3
      GO TO 723
  706 NTURN = 3
      KK = 1
      IF (D(2) - A) 710, 707, 710
  710 IF (D(2) - B) 999, 708, 709
  707 IF (MIN1F(B,C) - B) 622, 621, 999
  621 JJ = 1
      M = 6
      GO TO 723
  622 JJ = 1
      M = 3
      GO TO 722
  708 IF (MIN1F(A,C) - A) 623, 621, 999
  623 JA = 1
      JJ = 1
      M = 0
      GO TO 721
  709 IF (MIN1F(A,B) - A) 623, 622, 999
C
  721 D(KK) = A
      ANGLE (KK) = ALPHA
  664 JL = JJ + 2
      DO 665 L = JJ,JL
      LM = L + M
  665 NTEMP(L) = N(LM)
      GO TO (703, 706, 739), NTURN
  722 D(KK) = B
```

```
      ANGLE (KK) = BETA
      GO TO 664
  723 D(KK) = C
      ANGLE (KK) = GAMMA
      GO TO 664
C
  739 DO 730 I = 1,9
  730 N(I) = NTEMP(I)
      A = D(1)
      B = D(2)
      C = D(3)
      ALPHA = ANGLE(1)
      BETA  = ANGLE(2)
      GAMMA = ANGLE(3)
C
C          THE FOLLOWING SECTION CHECKS TO MAKE SURE ALPHA AND BETA ARE
C     EACH EQUAL TO OR GREATER THAN 90 DEGREES.  IF ONE OR BOTH ARE
C     LESS THAN 90 DEGREES, THE PROPER ADJUSTMENTS ARE MADE.
C
      ISIGN = 0
      IF (ALPHA - 90.0) 21, 801, 801
   21 ISIGN = ISIGN + 1
  801 IF (BETA - 90.0) 22, 802, 802
   22 ISIGN = ISIGN + 1
  802 IF (ISIGN - 1) 831, 69, 79
C
C     ISIGN = 1
C          EITHER ALPHA OR BETA IS LESS THAN 90 DEGREES.  REDEFINE THAT
C          ANGLE AS ITS SUPPLEMENT AND SET GAMMA = 180.0 - GAMMA.
C          (TWO ANGLES MUST ALWAYS BE TRANSFORMED SIMULTANEOUSLY.)
C
   69 GAMMA = 180.0 - GAMMA
      DO 6661 I = 7,9
      N(I) = -N(I)
      IF (N(I)) 6661, 4441, 6661
 4441 N(I) = 0
 6661 CONTINUE
      IF (ALPHA - 90.0) 43, 44, 44
   43 ALPHA = 180.0 - ALPHA
      DO 6662 I = 1,3
      N(I) = -N(I)
      IF (N(I)) 6662, 4442, 6662
 4442 N(I) = 0
 6662 CONTINUE
      GO TO 831
   44 BETA = 180.0 - BETA
      DO 6663 I = 4,6
      N(I) = -N(I)
      IF (N(I)) 6663, 4443, 6663
 4443 N(I) = 0
 6663 CONTINUE
      GO TO 831
C
C     ISIGN = 2
C          REDEFINE ALPHA AND BETA AS ITS OWN SUPPLEMENT AND REVERSE THE
C          DIRECTIONS OF A AND B.
C
   79 ALPHA = 180.0 - ALPHA
      BETA = 180.0 - BETA
      DO 6664 I = 1,6
      N(I) = -N(I)
      IF (N(I)) 6664, 4444, 6664
 4444 N(I) = 0
```

```
 6664 CONTINUE
C
C          A CHECK IS MADE TO DETERMINE IF THE SYSTEM HAS GONE FROM
C     RIGHT-HANDED TO LEFT-HANDED OR VICE VERSA.  IF JF = 1 THE SYSTEM
C     HAS REVERSED.  IF JF = 0 OR 3, IT HAS NOT REVERSED.
C
  831 JF = JA + JB + JC
      IF (JF - 1) 71, 832, 71
  832 DO 835 I = 1,9
      N(I) = -N(I)
      IF (N(I)) 835, 833, 835
  833 N(I) = 0
  835 CONTINUE
      GO TO 71
C
C
C          OUTPUT OF PART 3
C
C
   67 GO TO 66
  583 PRINT 1026, (TITLE(I), I = 1,16)
 1026 FORMAT (1H4, 4X, 16A5 // )
   68 PRINT 1038
 1038 FORMAT (1HJ, 9X, 45H NEW PARAMETERS   (CONVENTIONAL REDUCED CELL))
      GO TO 75
  889 PRINT 1028
      PRINT 1029
      PRINT 1030, N(1), N(2), N(3), NI(1), NI(2), NI(3)
      PRINT 1030, N(4), N(5), N(6), NI(4), NI(5), NI(6)
      PRINT 1030, N(7), N(8), N(9), NI(7), NI(8), NI(9)
      GO TO 633
  999 PRINT 1054
 1054 FORMAT (1HL, 17H $ERROR$ - PART 3)
C
C
C          OUTPUT OF PART 4.   TRIGONOMETRIC VALUES OF THE ANGLES OF THE
C     CONVENTIONAL REDUCED CELL.
C
C
  633 PRINT 634
  634 FORMAT (1HL, 9X, 73H TRIGONOMETRIC VALUES OF THE ANGLES OF THE CON
     1VENTIONAL REDUCED CELL      )
      SINAL  = SINF(ALPHA  * 0.01745329)
      SINBE  = SINF(BETA   * 0.01745329)
      SINGA  = SINF(GAMMA  * 0.01745329)
      COSAL  = COSF(ALPHA  * 0.01745329)
      COSBE  = COSF(BETA   * 0.01745329)
      COSGA  = COSF(GAMMA  * 0.01745329)
      SINALS = SINF(ALSTAR * 0.01745329)
      SINBES = SINF(BESTAR * 0.01745329)
      SINGAS = SINF(GASTAR * 0.01745329)
      COSALS = COSF(ALSTAR * 0.01745329)
      COSBES = COSF(BESTAR * 0.01745329)
      COSGAS = COSF(GASTAR * 0.01745329)
      PRINT 635
  635 FORMAT (1HK, 28X, 7H ANGLE , 6X, 5H SIN , 7X, 5H COS )
      PRINT 641, ALPHA, SINAL, COSAL
      PRINT 642, BETA,  SINBE, COSBE
      PRINT 643, GAMMA, SINGA, COSGA
      PRINT 644, ALSTAR, SINALS, COSALS
      PRINT 645, BESTAR, SINBES, COSBES
      PRINT 646, GASTAR, SINGAS, COSGAS
  641 FORMAT (1HJ, 15X, 7H ALPHA , F13.4, 2F12.5)
```

```
  642 FORMAT (1H , 15X, 7H BETA  , F13.4, 2F12.5)
  643 FORMAT (1H , 15X, 7H GAMMA , F13.4, 2F12.5)
  644 FORMAT (1HJ, 15X, 7H ALPHA*, F13.4, 2F12.5)
  645 FORMAT (1H , 15X, 7H BETA *, F13.4, 2F12.5)
  646 FORMAT (1H , 15X, 7H GAMMA*, F13.4, 2F12.5)
C
C
C          OUTPUT OF PART 5.   SCALARS CORRESPONDING TO THE CONVENTIONAL
C     REDUCED CELL.
C
C
  871 PRINT 880
  880 FORMAT (1HL, 9X, 56H SCALARS CORRESPONDING TO CONVENTIONAL REDUCED
     1 CELL     )
      AA = A*A
      BB = B*B
      CC = C*C
      AB = A*B*COSGA
      BC = B*C*COSAL
      CA = C*A*COSBE
      SUM = BC + CA + AB
      PRINT 881, AA, BB, CC
      PRINT 882, BC, CA, AB
      PRINT 883, SUM
  881 FORMAT (1HK, 15X, 9H R(1,1) = F7.2, 5X, 9H R(2,2) = F7.2, 5X,
     1         9H R(3,3) = F7.2)
  882 FORMAT (1HJ, 15X, 9H R(2,3) = F7.2, 5X, 9H R(3,1) = F7.2, 5X,
     1         9H R(1,2) = F7.2)
  883 FORMAT (1HK, 15X, 28H R(2,3) + R(3,1) + R(1,2)  =  F7.2)
C
  890 READ 1070, ICONT
 1070 FORMAT (I1)
      IF (ICONT) 89, 89, 9999
   89 STOP 89
      END
```

## B. TRACER

### A General Fortran Lattice Transformation - Cell Reduction Program

### 1. GENERAL INFORMATION

Program TRACER, written in IBM 7074 Fortran language, is an expanded version of RCELL. It is a computer program for general cell transformations in direct space (using matrices supplied by the user), for cell reductions only or for general cell transformations followed by cell reduction. Typical examples of its uses are

1. Transformation of lattice axes in direct space and reciprocal space ($Å^{-1}$) from an old cell to a new cell, e.g., Monoclinic $P2_1/n$ to $P2_1/c$, using a transformation matrix supplied by the user.

2. Transformation of a primitive triclinic or monoclinic cell to its reduced cell.

3. Reduction of primitive monoclinic cells, using the cell reduction technique incorporated in the program, to locate a better monoclinic cell with shorter and more orthogonal axes.

4. Two or more transformations in sequence, using matrices supplied by the user, to transform each cell consecutively to the next cell and to calculate the cell parameters of each intermediate cell and the final cell, e.g., F-triclinic to P-triclinic to I-orthorhombic.

5. Two or more transformations in sequence, transforming the first N cells to new cells using matrices supplied by the user and then letting the program transform the Nth cell to its reduced cell, e.g., F-triclinic to P-triclinic to reduced cell.

6. Matrix multiplication of two or more transformation matrices.

The tabulated transformations of lattices for the triclinic and monoclinic systems appearing in Appendix VII cover transformations frequently encountered in crystallography and may be used in routine work with the program. Suppose, for instance, one has a face-centered triclinic cell and it is desired to obtain the reduced cell. Before the reduced cell can be found the face-centered cell must first be converted to a primitive cell. Being unique, the program is always able to locate it starting with any arbitrary primitive triclinic cell in the lattice. The same reduced cell is always obtained, as will the matrix for the transformation of the original centered cell to the reduced cell, regardless of the intermediate primitive cell. The transformations on pages 174 - 175 will be found particularly useful in this regard for obtaining such intermediate primitive cells at this step. (Note that they may be used on any centered cell belonging to any one of the seven crystal systems.)

The essential input consists of the six lattice parameters (real or reciprocal), the matrices to be used for the consecutive transformations of cells which will not be reduced by the program as well as any alphanumeric information identifying each cell. The reduced cell, if desired, does not have to be obtained directly from the original cell but may be obtained from a cell previously obtained by other transformations (see No. 5 above); it must; however, be the last cell in any sequence of transformations, that is, after the reduced cell is obtained "by the program" one may not transform the cell to a new cell without reloading the

program. A maximum of eight consecutive transformations may be applied to any one original cell (controlled by the DIMENSION statement for output only). Provision has been made for allowing more than one compound to be run without reloading the program.

The output consists of the matrices used and generated for the lattice axes in direct space, the lattice parameters (real and reciprocal) of the original cell, all intermediate cells and the final cell, and the sine and cosine values of all angles in each cell. In the case of the reduced cell the program prints out two cells, as in the case of program RCELL, the second being just as rearrangement of the first and corresponds to the convention established for the triclinic reduced cell, namely, that cell whose edges are the three shortest non-coplanar translations in the lattice, labelled so as to have $c < a < b$ and oriented so that the angles $\alpha$ and $\beta$ are non-acute. Included also are the scalars of the reduced cell for use with Tables 2 and 3 for the determination of unit cells of higher symmetry. (For a discussion of the use of the "direct" and "inverse" matrices in the output, see Appendix III.)

As indicated above, this program (and RCELL, as well) may be used to reduce a primitive monoclinic cell to find a monoclinic cell with shorter and more orthogonal axes. This is one of the reasons why the two orientations of the reduced cell are printed in the output. The first of the two reduced cells is that obtained directly from the original cell "before" reorientation of axes. In using the program for this purpose the new angle will, in 50% of the cases, become acute after reduction.

This results from the natural sequence in the reduction process. According to Section C in Chapter II, the appropriate "obtuse" angle of the new cell is the supplement of the acute angle with the corresponding changes in axial directions and transformation matrices (rules i - v, Section C). Consider, for example, the reduction of a primitive monoclinic cell to a new monoclinic cell with the following new lattice parameters and transformation matrix:

$$\begin{array}{lll} a = 10.65\ \text{Å}. & \alpha = 90^\circ & \\ b = 16.81 & \beta = 87.62^\circ & , \quad \text{matrix:} \begin{Vmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix} . \\ c = 8.44 & \gamma = 90^\circ & \end{array}$$

If it is desired that $\beta$ be non-acute, the changes to be made are as follows (two choices):

(a). Set $\beta = 180^\circ - 87.62^\circ = 92.38^\circ$,

set abc $\rightarrow \overline{a}bc$

and set $\begin{Vmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix} \rightarrow \begin{Vmatrix} \overline{1} & 0 & \overline{1} \\ 0 & \overline{1} & 0 \\ 0 & 0 & 1 \end{Vmatrix}$ ,

or (b). Set $\beta = 180^\circ - 87.62^\circ = 92.38^\circ$ (as in (a) above),

set abc $\rightarrow a\overline{bc}$

and set $\begin{Vmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix} \rightarrow \begin{Vmatrix} 1 & 0 & 1 \\ 0 & \overline{1} & 0 \\ 0 & 0 & \overline{1} \end{Vmatrix}$ .

The program has been written in full Fortran using one-, two- and three-dimensional arrays. The generation of the matrices in the output

is defined in the usual sense on page 90. The matrix elements of all primitive cells to their reduced cells are in fixed point; all other matrices are in floating point. TRACER is essentially an expanded version of RCELL so that the cell reduction routine is virtually the same. The routine which calculates a new cell from an old using the matrix supplied at input uses the method and formulas in Appendix IV. After all axial transformations have been completed, a test is made to determine the total number of consecutive transformations executed for any one compound; if more than two have been made, all N matrices are multiplied together according to the rules of matrix multiplication outlined in Appendix VI.

## 2. INPUT DATA

1. Title card -- 1 card -- FORMAT (16A5)

   Any alphanumeric information. This will be printed back out as a heading on each page of output.

2. Control card -- 1 card

   Column

   1 - 3 FORMAT (I3), = 1 if the cell parameters on the Parameter card are in direct space.

   = 2 if the cell parameters on the Parameter card are in reciprocal space.

   4 - 6 FORMAT (I3), number of Cell Specification cards to be read; (ITOTAL).

   7 - 9 FORMAT (I3), number of Transformation cards to be read; (MATRIX).

3. Parameter card -- 1 card

   Column

   1 - 10 FORMAT (F10.6), lattice parameter a (or a*).

   11 - 20 FORMAT (F10.6), lattice parameter b (or b*).

   21 - 30 FORMAT (F10.6), lattice parameter c (or c*).

   31 - 40 FORMAT (F10.6), lattice parameter $\alpha$ (or $\alpha^*$).

   41 - 50 FORMAT (F10.6), lattice parameter $\beta$ (or $\beta^*$).

   51 - 60 FORMAT (F10.6), lattice parameter $\gamma$ (or $\gamma^*$).

   Note: The cell edges are in (Å) in direct space and ($Å^{-1}$) in reciprocal space; the angles are in degrees and decimal fraction.

4. Cell Specification cards -- ITOTAL cards

| Column | | |
|---|---|---|
| 1 | FORMAT (I1), | cell number. (The original cell is cell number 1.) |
| 2 | | (blank) |
| 3 | FORMAT (I1), | = 1 if the cell is to be transformed to a new cell using the matrix supplied on the Transformation card.<br>= 2 if the cell is to be reduced to its reduced cell by the program.<br>= 3 final cell. No transformation to be applied. |
| 4 - 5 | | (blank) |
| 6 - 80 | FORMAT (15A5), | Any alphanumeric information describing the cell, e.g., lattice type and crystal system. Left justify. This will be printed back out as a heading. |

Note (1). These ITOTAL cards include the original cell, all intermediate cells and the final cell. They must be arranged in increasing order of cell number.

Note (2). The reduced cell is to be considered as one cell, not two, even though the program will output the reduced cell in two orientations: one whose lattice parameters were obtained by direct transformation from the previous cell and the same

reduced cell but with its lattice parameters rearranged so as to conform to the convention established for the triclinic system.

5. Transformation cards -- MATRIX cards -- FORMAT (9F8.5)

   One card per matrix, arranged in order of use. Each matrix is used for transforming one cell to a new cell, e.g.,

   Cell (1) to Cell (2) -- 1 card

   Cell (2) to Cell (3) -- 1 card, etc.

   These cards are included only when needed; if MATRIX = 0, these cards are omitted (see sample problems). The order of punching is P(1, 1), P(1, 2), P(1, 3) P(2, 1), P(2, 2), P(2, 3), P(3, 1), P(3, 2), P(3, 3).

6. Stopper card -- 1 card -- FORMAT (I1)

   = 0 (or blank) if no more compounds are to be processed,

   = 1 if another compound is to be processed.

   Note: This card allows more than one compound to be processed without reloading the program. Thus, any number of sets of data may be processed. Each set consists of items 1 through 6.

## 3. RUNNING DECK ARRANGEMENT

Program TRACER is on the Iowa State IBM 7074 library tape under the name TRACER3SLL. In using the tape a typical run will consist of the following cards:

| | 14 16 | 76 |
|---|---|---|
| 1 card: | (Start Account Card) | POGO |
| 1 card: | ALTSW ALL OFF | POGO |
| 1 card: | Z LLOAD @TRACER3SLL@ | POGO |
| | (Data Cards) | |
| 1 card: | | WTM |
| 1 card: | (End Account Card) | POGO |

All variables are stored in COMMON, locations 19000 - 19975, and may be called with a POGOZ dump. The time estimate is approximately 1 minute for transformation or reduction of 10 cells.

# 4. SAMPLE INPUT AND OUTPUT

## SAMPLE PROBLEM 1

It is desired to find the reduced cell of triclinic 16-DL methyloctadecanoic acid, space group $P\bar{1}$, with lattice parameters a = 5.40, b = 7.54, c = 51.8 A., $\alpha$ = 145° 38', $\beta$ = 105° 42', $\gamma$ = 60° 18'. The desired transformation is

P-triclinic cell (1) ⟶ Reduced cell (2)

C FOR COMMENT

| STATEMENT NUMBER | CONTINUE | FORTRAN STATEMENT |
|---|---|---|
| 16-DL | | METHYLØCTADECANØIC ACID |
| 1 | 2 | 0 |
| | | 5.40, 7.54, 51.8, 145.63333, 105.7, 60.3 |
| 1 2 | | TRICLINIC - PRIMITIVE |
| 2 3 | | REDUCED CELL |
| 0 | | |

Fig. 10. Input data for sample problem 1.

The computer output for sample problem 1 has not been included in this report.

## SAMPLE PROBLEM 2

It is desired to carry out two separate transformations, using matrices found in Table 9. The transformations of interest are

a) Compound A

$$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

Monoclinic $P2_1/n$ → Monoclinic $P2_1/c$

cell (1) cell (2)

b) Compound B

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$$

Monoclinic Ia → Monoclinic Cc

cell (1) cell (2)

The lattice parameters of cell (1), compound A, are a = 7.62, b = 4.10, c = 13.2 A., $\beta$ = 110° 20' (b-unique) and those of cell (1), compound B, are a = 10.2, b = 12.4, c = 16.8 A., $\beta$ = 99° 00' (b-unique).

C FOR COMMENT

| STATEMENT NUMBER | C O N T | FORTRAN STATEMENT |
|---|---|---|
| | | 1 5 6 7 10 15 20 25 30 35 40 45 50 55 60 65 70 7 |
| COMPOUND A | | |
| 1 | 2 | 1 |
| | | 7.62, 4.10, 13.2, 90.0, 110.33333, 90.0, |
| 1 1 | | MONOCLINIC - P2,1/N |
| 2 3 | | MONOCLINIC - P2,1/C |
| | -1 | 1.0 0.0 0.0 0.0 -1.0 0.0 1.0 0.0 1.0 |
| 1 | | |
| COMPOUND B | | |
| 1 | 2 | 1 |
| | | 10.2, 12.4, 16.8, 90.0, 99.0, 90.0, |
| 1 1 | | MONOCLINIC - IA |
| 2 3 | | MONOCLINIC - CC |
| | 1 | 1.0 0.0 1.0 0.0 1.0 0.0 -1.0 0.0 0.0 |
| 0 | | |

Fig. 11. Input data for sample problem 2.

The output for sample problem 2 has not been included in this report.

SAMPLE PROBLEM 3

It is desired to find the reduced cell of face-centered triclinic nickel dimethylglyoxime whose lattice parameters were observed on a single crystal orienter to be a = 10.360, b = 18.037, c = 25.760 A., $\alpha$ = 127.03°, $\beta$ = 129.81°, $\gamma$ = 90.51°. The matrix for the transformation of the face-centered triclinic cell to a primitive triclinic cell is $\frac{1}{2}\frac{1}{2}0/\bar{\frac{1}{2}}\frac{1}{2}0/\frac{1}{2}0\frac{1}{2}$ (obtained from page 175). The consecutive transformations of interest are

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$$

F-triclinic cell (1) ⟶ P-triclinic cell (2) ⟶ Reduced cell (3).

C FOR COMMENT

| STATEMENT NUMBER | CONT. | FORTRAN STATEMENT |
|---|---|---|
| NICKEL | | DIMETHYLGLYØXIME |
| 1 | 3 | 1 |
| | 10 | .360, 18.037, 25.760, 127.03, 129.81, 90.51 |
| 1 1 | | TRICLINIC - F-CENTERED |
| 2 2 | | TRICLINIC - PRIMITIVE |
| 3 3 | | REDUCED CELL |
| | 0 | .5, 0.,5, 0.0, -0,.5, 0.5, 0.0, 0.,5, 0.0, 0,.5 |
| 0 | | |

Fig. 12. Input data for sample problem 3.

The output to this problem is shown on the next six pages. For a discussion and an analysis of the output, see Example 3, page 67, particularly steps 4-6.

NICKEL DIMETHYLGLYOXIME

INPUT DATA OF ORIGINAL CELL IN DIRECT SPACE

LATTICES USED IN PROGRAM

CELL (1) TRICLINIC - F-CENTERED
CELL (2) TRICLINIC - PRIMITIVE
CELL (3) REDUCED CELL
CELL (4) REDUCED CELL CONFORMING TO TRICLINIC CONVENTION

TRANSFORMATION MATRICES

CELL (1) TO CELL (2)

| | | |
|---|---|---|
| 0.50 | 0.50 | 0.00 |
| -0.50 | 0.50 | 0.00 |
| 0.50 | 0.00 | 0.50 |

MOD = 0.2500

CELL (2) TO CELL (1)

| | | |
|---|---|---|
| 1.00 | -1.00 | 0.00 |
| 1.00 | 1.00 | 0.00 |
| -1.00 | 1.00 | 2.00 |

MOD = 4.0000

CELL (2) TO CELL (3)

| | | |
|---|---|---|
| 1 | 0 | 1 |
| 0 | 1 | 1 |
| 0 | 0 | 1 |

MOD = 1.0000

CELL (3) TO CELL (2)

| | | |
|---|---|---|
| 1 | 0 | -1 |
| 0 | 1 | -1 |
| 0 | 0 | 1 |

MOD = 1.0000

CELL (2) TO CELL (4)

| | | |
|---|---|---|
| 0 | 0 | 1 |
| 0 | 1 | 1 |
| -1 | 0 | -1 |

MOD = 1.0000

CELL (4) TO CELL (2)

| | | |
|---|---|---|
| -1 | 0 | -1 |
| -1 | 1 | 0 |
| 1 | 0 | 0 |

MOD = 1.0000

NICKEL DIMETHYLGLYOXIME

CELL (1) TO CELL (3)

| | | |
|---|---|---|
| 1.00 | 0.50 | 0.50 |
| 0.00 | 0.50 | 0.50 |
| 0.50 | 0.00 | 0.50 |

MOD = 0.2500

CELL (3) TO CELL (1)

| | | |
|---|---|---|
| 1.00 | -1.00 | 0.00 |
| 1.00 | 1.00 | -2.00 |
| -1.00 | 1.00 | 2.00 |

MOD = 4.0000

CELL (1) TO CELL (4)

| | | |
|---|---|---|
| 0.50 | 0.00 | 0.50 |
| 0.00 | 0.50 | 0.50 |
| -1.00 | -0.50 | -0.50 |

MOD = 0.2500

CELL (4) TO CELL (1)

| | | |
|---|---|---|
| 0.00 | -1.00 | -1.00 |
| -2.00 | 1.00 | -1.00 |
| 2.00 | 1.00 | 1.00 |

MOD = 4.0000

NICKEL DIMETHYLGLYOXIME

LATTICE PARAMETERS OF CELL (1) -- TRICLINIC - F-CENTERED

| | | | |
|---|---|---|---|
| A | = 10.3600 | ALPHA | = 127.0300 |
| B | = 18.0370 | BETA | = 129.8100 |
| C | = 25.7600 | GAMMA | = 90.5100 |
| A* | = 0.164116 | ALPHA* | = 37.6805 |
| B* | = 0.090704 | BETA * | = 36.0275 |
| C* | = 0.082674 | GAMMA* | = 49.9648 |
| V | = 2260.142 | | |
| V* | = 0.000442 | | |

NATURAL TRIGONOMETRIC VALUES OF THE ANGLES

| | ANGLE | SIN | COS |
|---|---|---|---|
| ALPHA | 127.0300 | 0.79832 | -0.60223 |
| BETA | 129.8100 | 0.76817 | -0.64024 |
| GAMMA | 90.5100 | 0.99996 | -0.00890 |
| ALPHA* | 37.6805 | 0.61126 | 0.79143 |
| BETA * | 36.0275 | 0.58817 | 0.80873 |
| GAMMA* | 49.9648 | 0.76565 | 0.64326 |

NICKEL DIMETHYLGLYOXIME

LATTICE PARAMETERS OF CELL (2) -- TRICLINIC - PRIMITIVE

| | | | |
|---|---|---|---|
| A | = 10.3602 | ALPHA | = 120.2543 |
| B | = 10.4402 | BETA | = 143.4895 |
| C | = 10.3583 | GAMMA | = 59.7430 |
| A* | = 0.165323 | ALPHA* | = 78.9107 |
| B* | = 0.113000 | BETA * | = 42.5259 |
| C* | = 0.165349 | GAMMA* | = 101.0974 |
| V | = 565.035 | | |
| V* | = 0.001770 | | |

NATURAL TRIGONOMETRIC VALUES OF THE ANGLES

| | ANGLE | SIN | COS |
|---|---|---|---|
| ALPHA | 120.2543 | 0.86380 | -0.50384 |
| BETA | 143.4895 | 0.59497 | -0.80375 |
| GAMMA | 59.7430 | 0.86377 | 0.50388 |
| ALPHA* | 78.9107 | 0.98133 | 0.19234 |
| BETA * | 42.5259 | 0.67592 | 0.73697 |
| GAMMA* | 101.0974 | 0.98130 | -0.19248 |

NICKEL DIMETHYLGLYOXIME

LATTICE PARAMETERS OF CELL (3) -- REDUCED CELL

| | | | |
|---|---|---|---|
| A | = 6.4901 | ALPHA | = 60.5197 |
| B | = 10.3595 | BETA | = 71.7607 |
| C | = 10.3583 | GAMMA | = 71.7498 |
| A* | = 0.165323 | ALPHA* | = 115.9084 |
| B* | = 0.113000 | BETA * | = 101.0792 |
| C* | = 0.113006 | GAMMA* | = 101.0974 |
| V | = 565.035 | | |
| V* | = 0.001770 | | |

NATURAL TRIGONOMETRIC VALUES OF THE ANGLES

| | ANGLE | SIN | COS |
|---|---|---|---|
| ALPHA | 60.5197 | 0.87053 | 0.49212 |
| BETA | 71.7607 | 0.94976 | 0.31299 |
| GAMMA | 71.7498 | 0.94970 | 0.31317 |
| ALPHA* | 115.9084 | 0.89549 | -0.43693 |
| BETA * | 101.0792 | 0.98136 | -0.19217 |
| GAMMA* | 101.0974 | 0.98130 | -0.19248 |

SCALARS CORRESPONDING TO THIS REDUCED CELL

| | | |
|---|---|---|
| R(1,1) = 42.12 | R(2,2) = 107.32 | R(3,3) = 107.29 |
| R(2,3) = 52.81 | R(3,1) = 21.04 | R(1,2) = 21.06 |

R(2,3) + R(3,1) + R(1,2) = 94.90

NICKEL DIMETHYLGLYOXIME

LATTICE PARAMETERS OF CELL (4) -- CONVENTIONAL REDUCED CELL

| | | | |
|---|---|---|---|
| A | = 10.3583 | ALPHA | = 108.2502 |
| B | = 10.3595 | BETA | = 108.2393 |
| C | = 6.4901 | GAMMA | = 60.5197 |
| A* | = 0.113006 | ALPHA* | = 78.9026 |
| B* | = 0.113000 | BETA * | = 78.9208 |
| C* | = 0.165323 | GAMMA* | = 115.9084 |
| V | = 565.035 | | |
| V* | = 0.001770 | | |

NATURAL TRIGONOMETRIC VALUES OF THE ANGLES

| | ANGLE | SIN | COS |
|---|---|---|---|
| ALPHA | 108.2502 | 0.94970 | -0.31317 |
| BETA | 108.2393 | 0.94976 | -0.31299 |
| GAMMA | 60.5197 | 0.87053 | 0.49212 |
| ALPHA* | 78.9026 | 0.98130 | 0.19248 |
| BETA * | 78.9208 | 0.98136 | 0.19217 |
| GAMMA* | 115.9084 | 0.89949 | -0.43693 |

SCALARS CORRESPONDING TO THIS REDUCED CELL

| | | |
|---|---|---|
| R(1,1) = 107.29 | R(2,2) = 107.32 | R(3,3) = 42.12 |
| R(2,3) = -21.06 | R(3,1) = -21.04 | R(1,2) = 52.81 |

R(2,3) + R(3,1) + R(1,2) = 10.71

# 5. SYMBOLIC PROGRAM LISTING

```
C                              PROGRAM TRACER
C
C
C
C     DESCRIPTION.    LATTICE TRANSFORMATION - CELL REDUCTION PROGRAM
C     LANGUAGE.       FULL FORTRAN FOR IBM 7074
C     DATE.           FEBRUARY 1965 (FINAL VERSION)
C     PROGRAMMER.     STEPHEN L. LAWTON
C
C
C     GLOSSARY OF SYMBOLS
C
C     A           DIRECT CELL PARAMETER, A
C     AA          A*A
C     AB          A*B*COSGA = SCALAR PRODUCT OF A WITH B
C     ABSAB       ABSF(AB)
C     ABSBC       ABSF(BC)
C     ABSCA       ABSF(CA)
C     AL          DIRECT CELL PARAMETER, ALPHA, IN RADIANS
C     ALPHA       DIRECT CELL PARAMETER, ALPHA, IN DEGREES
C     ALS         RECIPROCAL CELL PARAMETER, ALPHA-STAR, IN RADIANS
C     ALSTAR      RECIPROCAL CELL PARAMETER, ALPHA-STAR, IN DEGREES
C     ANGLE(3)    DIRECT CELL PARAMETERS ALPHA, BETA, GAMMA IN NEW CELL
C     AS          RECIPROCAL CELL PARAMETER, A-STAR
C     AXIS(3)     DIRECT CELL PARAMETERS A, B, C OF NEW CELL
C     B           DIRECT CELL PARAMETER, B
C     BB          B*B
C     BC          B*C*COSAL = SCALAR PRODUCT OF B WITH C
C     BE          DIRECT CELL PARAMETER, BETA, IN RADIANS
C     BES         RECIPROCAL CELL PARAMETER, BETA-STAR, IN RADIANS
C     BESTAR      RECIPROCAL CELL PARAMETER, BETA-STAR, IN DEGREES
C     BET         MODULUS OF TRANSF. MATRIX FOR CELL(N+1) TO CELL(N)
C     BETA        DIRECT CELL PARAMETER, BETA, IN DEGREES
C     BS          RECIPROCAL CELL PARAMETER, B-STAR
C     C           DIRECT CELL PARAMETER, C
C     CA          C*A*COSBE = SCALAR PRODUCT OF C WITH A
C     CC          C*C
C     CELL(15,12)    ANY ALPHANUMERIC INFORMATION DESCRIBING THE CELL
C     COS(3)      COSF OF NEW ALPHA, BETA, GAMMA
C     COSAL       COSF(AL)
C     COSALS      COSF(ALS)
C     COSBE       COSF(BE)
C     COSBES      COSF(BES)
C     COSGA       COSF(GA)
C     COSGAS      COSF(GAS)
C     CS          RECIPROCAL CELL PARAMETER, C-STAR
C     D(3)        DIRECT CELL PARAMETERS A, B, C IN NEW ORIENTED CELL
C     DET         MODULUS OF TRANSF. MATRIX FOR CELL(N) TO CELL(N+1)
C     DIM(6,12)   STORAGE LOCATIONS FOR A, B, C, ALPHA, BETA, GAMMA
C     GA          DIRECT CELL PARAMETER, GAMMA, IN RADIANS
C     GAMMA       DIRECT CELL PARAMETER, GAMMA, IN DEGREES
C     GAS         RECIPROCAL CELL PARAMETER, GAMMA-STAR, IN RADIANS
C     GASTAR      RECIPROCAL CELL PARAMETER, GAMMA-STAR, IN DEGREES
C     I           INDEX
C     IAXIS       AXIS (VECTOR) HELD CONSTANT. 1=A, 2=B, 3=C
```

```
C      ICONT       CODE FOR NEXT JOB
C      ICYCLE      NUMBER OF CYCLES IN REDUCED CELL ROUTINE
C      ICYCLT      NUMBER OF CYCLES IN ROUTINE
C      IDENT       (NOT USED IN PROGRAM)
C      IHKL(12)    CODE FOR PROGRAM SECTION
C      INPUT       SPECIFICATION CODE FOR CELL PARAMETERS READ AT INPUT
C      IOUTPT      PROGRAM SECTION NUMBER
C      ISIGN       NUMBER OF ACUTE ANGLES IN REDUCED CELL
C      ISUM        TOTAL NUMBER OF CELLS INVOLVED IN PROGRAM
C      ITOTAL      TOTAL NUMBER OF CELL IDENTIFICATION CARDS READ IN
C      J           INDEX
C      JA          CODE FOR SHIFT IN A-AXIS.  JA=0 NO SHIFT, JA=1 SHIFT
C      JB          CODE FOR SHIFT IN B-AXIS.  JB=0 NO SHIFT, JB=1 SHIFT
C      JB2         INDEX
C      JC          CODE FOR SHIFT IN C-AXIS.  JC=0 NO SHIFT, JC=1 SHIFT
C      JF          JA + JB + JC
C      JJ          INDEX
C      JL          INDEX
C      K           INDEX
C      K2          CODE FOR REDUCTION OF REMAINING TWO AXES
C      K4          CODE FOR TRANSFER TO + FROM MATRIX INVERSION ROUTINE
C      K8          STORAGE FOR K
C      KK          CODE FOR PARAMETERS IN CONVENTIONAL CELL. 1=A, 2=B, 3=C
C      KX          INDEX
C      L           INDEX
C      L2          INDEX
C      LINE        PAGE CONTROL FOR OUTPUT
C      LL          INDEX
C      LM          INDEX
C      M           INDEX
C      MATRIX      NUMBER OF TRANSFORMATION CARDS READ IN
C      MAX         LARGEST CELL PARAMETER READ AT INPUT. 1=A, 4=B, 7=C
C      MM(3,3,3)   MATRIX ELEMENTS (IN FIXED PT.) FOR CELL(N+1) TO CELL(N)
C      N(9)        ELEMENTS OF DIRECT TRANSFORMATION MATRIX TO RED. CELL
C      NA(9)       MATRIX ELEMENTS OF CELL (N) TO CELL (N+1) IN RED. SECT.
C      NB(9)       MATRIX ELEMENTS OF CELL (1) TO CELL (N+1) IN RED. SECT.
C      NCHECK      INDEX CONTROLLING REDUCTION OF CELL PARAMETER
C      NN(3,3,3)   MATRIX ELEMENTS (IN FIXED PT.) FOR CELL(N) TO CELL(N+1)
C      NQ(12)      IDENTIFICATION VARIABLE
C      NSTOP       INDEX CONTROL. WHEN NSTOP = 3, REDUCTION CYCLE COMPLETE
C      NTEMP(9)    TEMPORARY STORAGE LOCATION FOR MATRIX ELEMENTS
C      NTURN       INDEX CONTROL
C      P(3,3,3)    MATRIX ELEMENTS (IN FLOATING POINT)
C      PN          INTEGER (FLOATING PT.)
C      Q(3,3,3)    MATRIX ELEMENTS (IN FLOATING POINT)
C      QMAX        THE LARGER OF TWO CELL PARAMETERS
C      QQMAX       THE LARGEST OF (ABSAB, ABSBC, ABSCA)
C      S(3,3,14)   MATRIX ELEMENTS (IN FLOAT PT.) FOR CELL(N+1) TO CELL(N)
C      SINAL       SINF(AL)
C      SINALS      SINF(ALS)
C      SINBE       SINF(BE)
C      SINBES      SINF(BES)
C      SINGA       SINF(GA)
C      SINGAS      SINF(GAS)
C      STORE       TEMPORARY STORAGE LOCATION FOR NEW SCALAR PRODUCT
C      SUM         BC + CA + AB
C      TITLE(16)   ALPHANUMERIC TITLE READ AT START OF PROGRAM
C      V           CELL VOLUME IN DIRECT SPACE
C      VS          CELL VOLUME IN RECIPROCAL SPACE
C      W(3,3,3)    MATRIX ELEMENTS OF ORIGNAL CELL TO FINAL CELL
C      X           TEMPORARY LOCATION FOR CELL PARAMETER A, B OR C
C      XX          X*X
C      XY          TEMPORARY LOCATION FOR SCALAR PRODUCT AB, BC OR CA
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C      XY2         TEMPORARY LOCATION OF NEW SCALAR PRODUCT
C      Y           TEMPORARY LOCATION FOR CELL PARAMETER A, B OR C
C      YY          Y*Y
C      YZ          TEMPORARY LOCATION FOR SCALAR PRODUCT AB, BC OR CA
C      Z           TEMPORARY LOCATION FOR CELL PARAMETER A, B OR C
C      ZX          TEMPORARY LOCATION FOR SCALAR PRODUCT AB, BC OR CA
C      ZX2         TEMPORARY LOCATION OF NEW SCALAR PRODUCT
C      ZZ          Z*Z
C
C
C
C                          ****************************
C
C                               FORMAT STATEMENTS
C
C                          ****************************
C
C
 1000 FORMAT (16A5)
 1001 FORMAT (3I3)
 1002 FORMAT (6F10.6)
 1003 FORMAT (1X, I2, 2X, 15A5)
 1004 FORMAT (9F8.5)
 1005 FORMAT (1H1)
 1006 FORMAT (1HK, 4X, 16A5)
 1007 FORMAT (1HL, 3X, 44H INPUT DATA OF ORIGINAL CELL IN DIRECT SPACE )
 1008 FORMAT (1HL, 3X, 48H INPUT DATA OF ORIGINAL CELL IN RECIPROCAL SPA
     1CE )
 1009 FORMAT (1HL, 3X, 40H LATTICES USED IN PROGRAM                  / )
 1010 FORMAT (1H , 9X, 7H CELL (,I1,4H)   , 15A5)
 1011 FORMAT (1H , 9X, 7H CELL (,I1,51H)   REDUCED CELL CONFORMING TO TR
     1ICLINIC CONVENTION )
 1012 FORMAT (1HL, 83H $ERROR$ - STATEMENT NO. 401 PLUS 001 CARD, 404 PL
     1US 001 CARD OR 407 PLUS 001 CARD.  )
 1013 FORMAT (1HL, 77H $ERROR$ - STATEMENT NO. 2 PLUS 001 CARD, 5 PLUS 0
     101 CARD OR 8 PLUS 001 CARD.  )
 1014 FORMAT (1HL, 35H $ERROR$ - STATEMENT NO. 3, 6 OR 9.  )
 1015 FORMAT (1HL, 47H $ERROR$ - ERROR IN AXIS DESIGNATION IN PART 1. )
 1016 FORMAT (1HL, 38H $ERROR$ - STATEMENT NO. 17, 37 OR 57.     )
 1017 FORMAT (1HL, 18H $ERROR$ - PART 2. )
 1018 FORMAT (1HL, 3X, 39H TRANSFORMATION MATRICES                   / )
 1019 FORMAT (1HK, 12X, 7H CELL (,I1,11H) TO CELL (,I1,1H),
     1             12X, 7H CELL (,I1,11H) TO CELL (,I1,1H) // )
 1020 FORMAT (1H , 11X, 3F7.2, 12X, 3F7.2 / )
 1021 FORMAT (1HK, 12X, 19H CELL (1) TO CELL (,I1,1H),
     1             12X,  7H CELL (,I1,13H) TO CELL (1) // )
 1022 FORMAT (1H4, 4X, 16A5 / )
 1023 FORMAT (1HK, 9X, 29H LATTICE PARAMETERS OF CELL (,I1,5H) -- ,15A5)
 1024 FORMAT (1HK, 15X, 6H A  = F9.4, 14X, 10H ALPHA  = F10.4)
 1025 FORMAT (1H , 15X, 6H B  = F9.4, 14X, 10H BETA   = F10.4)
 1026 FORMAT (1H , 15X, 6H C  = F9.4, 14X, 10H GAMMA  = F10.4)
 1027 FORMAT (1HJ, 15X, 6H A* = F9.6, 14X, 10H ALPHA* = F10.4)
 1028 FORMAT (1H , 15X, 6H B* = F9.6, 14X, 10H BETA * = F10.4)
 1029 FORMAT (1H , 15X, 6H C* = F9.6, 14X, 10H GAMMA* = F10.4)
 1030 FORMAT (1HJ, 15X, 6H V  = F9.3)
 1031 FORMAT (1H , 15X, 6H V* = F9.6, // )
 1032 FORMAT (1HK, 9X, 44H NATURAL TRIGONOMETRIC VALUES OF THE ANGLES )
 1033 FORMAT (1HK, 28X, 7H ANGLE , 6X, 5H SIN , 7X, 5H COS )
 1034 FORMAT (1HJ, 15X, 7H ALPHA , F13.4, 2F12.5)
 1035 FORMAT (1H , 15X, 7H BETA  , F13.4, 2F12.5)
 1036 FORMAT (1H , 15X, 7H GAMMA , F13.4, 2F12.5)
 1037 FORMAT (1HJ, 15X, 7H ALPHA*, F13.4, 2F12.5)
 1038 FORMAT (1H , 15X, 7H BETA *, F13.4, 2F12.5)
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 1039 FORMAT (1H , 15X, 7H GAMMA=, F13.4, 2F12.5)
 1040 FORMAT (1HL, 9X, 44H SCALARS CORRESPONDING TO THIS REDUCED CELL  )
 1041 FORMAT (1HK, 15X, 9H R(1,1) = F7.2, 5X, 9H R(2,2) = F7.2, 5X,
     1                  9H R(3,3) = F7.2)
 1042 FORMAT (1HJ, 15X, 9H R(2,3) = F7.2, 5X, 9H R(3,1) = F7.2, 5X,
     1                  9H R(1,2) = F7.2)
 1043 FORMAT (1HK, 15X, 28H R(2,3) + R(3,1) + R(1,2)  =  F7.2)
 1044 FORMAT (1H , 16X, 3I4, 21X, 3I4 / )
 1045 FORMAT (1HK, 9X, 29H LATTICE PARAMETERS OF CELL (,I1,31H) -- CONVE
     1NTIONAL REDUCED CELL          )
 1046 FORMAT (1H , 16X, 6H MOD = F8.4, 19X, 6H MOD = F8.4 / )
 1070 FORMAT (I1)
C
C
C                                    ***************
C
C                                        INPUT
C                                    ***************
C
C
      DIMENSION TITLE(16), NQ(12), CELL(15,12), P(3,3,12), Q(3,3,12),
     1          W(3,3,12), IHKL(12), DIM(6,12), AXIS(3), COS(3),
     2          ANGLE(3), KG(9), N(9), D(3), NTEMP(9), NN(3,3,3),
     3          MM(3,3,4), S(3,3,15), DET(15), BET(15), NA(9), NB(9)
      COMMON  INPUT,ITOTAL,MATRIX,A,B,C,ALPHA,BETA,GAMMA,AS,BS,CS,
     1        ALSTAR,BESTAR,GASTAR,ICYCLT,ICYCLE,IOUTPT,ISUM,SINAL,
     2        SINBE,SINGA,COSAL,COSBE,COSGA,ALS,BES,GAS,SINALS,SINBES,
     3        SINGAS,COSALS,COSBES,COSGAS,AL,BE,GA,V,VS,NSTOP,K2,AB,BC,
     4        CA,ABSAB,ABSBC,ABSCA,MAX,QMAX,QQMAX,IAXIS,X,Y,Z,XY,YZ,ZX,
     5        NCHECK,XX,YY,ZZ,PN,XY2,ZX2,STORE,NTURN,AA,BB,CC,I,J,K,L,M,
     6        KK,JJ,JL,LM,ISIGN,SUM,KX,LL,K4,L2,TITLE,NQ,IHKL,AXIS,COS,
     7        ANGLE,LINE,N,D,NTEMP,CELL,DIM,NN,MM,P,Q,W,DET,BET,K8,
     8        JA,JB,JC,JF,JB2,NA,NB
C
 9999 READ 1000, (TITLE(I), I = 1,16)
      READ 1001, INPUT, ITOTAL, MATRIX
      GO TO (61, 62), INPUT
   61 READ 1002, A, B, C, ALPHA, BETA, GAMMA
      GO TO 70
   62 READ 1002, AS, BS, CS, ALSTAR, BESTAR, GASTAR
   70 DO 82 J = 1,ITOTAL
   82 READ 1003, NQ(J), (CELL(I,J), I = 1,15)
      IF (MATRIX) 600, 600, 78
   78 DO 83 K = 1,MATRIX
   83 READ 1004, ((P(I,J,K), J = 1,3), I = 1,3)
      K4 = 1
C
C
C                              *************************
C
C                                  MATRIX INVERSION
C
C                              *************************
C
C
 5550 GO TO (5551, 5552, 5553, 5553), K4
 5551 L = 1
      GO TO 5554
 5552 L = K
      GO TO 5554
 5553 L = L2
 5554 DET(L) = P(1,1,L)*(P(2,2,L)*P(3,3,L) - P(3,2,L)*P(2,3,L))
```

```
     1       - P(1,2,L)*(P(2,1,L)*P(3,3,L) - P(3,1,L)*P(2,3,L))
     2       + P(1,3,L)*(P(2,1,L)*P(3,2,L) - P(3,1,L)*P(2,2,L))
      S(1,1,L) =  (P(2,2,L)*P(3,3,L) - P(3,2,L)*P(2,3,L)) / DET(L)
      S(1,2,L) = -(P(1,2,L)*P(3,3,L) - P(3,2,L)*P(1,3,L)) / DET(L)
      S(1,3,L) =  (P(1,2,L)*P(2,3,L) - P(2,2,L)*P(1,3,L)) / DET(L)
      S(2,1,L) = -(P(2,1,L)*P(3,3,L) - P(3,1,L)*P(2,3,L)) / DET(L)
      S(2,2,L) =  (P(1,1,L)*P(3,3,L) - P(3,1,L)*P(1,3,L)) / DET(L)
      S(2,3,L) = -(P(1,1,L)*P(2,3,L) - P(2,1,L)*P(1,3,L)) / DET(L)
      S(3,1,L) =  (P(2,1,L)*P(3,2,L) - P(3,1,L)*P(2,2,L)) / DET(L)
      S(3,2,L) = -(P(1,1,L)*P(3,2,L) - P(3,1,L)*P(1,2,L)) / DET(L)
      S(3,3,L) =  (P(1,1,L)*P(2,2,L) - P(2,1,L)*P(1,2,L)) / DET(L)
      DO 5555 I = 1,3
      DO 5555 J = 1,3
      IF (S(I,J,L)) 5555, 5559, 5555
 5559 S(I,J,L) = 0.0
 5555 CONTINUE
      BET(L) = 1./DET(L)
      IF (K4 - 1) 5558, 5556, 5558
 5556 IF (L - MATRIX) 5557, 5558, 5558
 5557 L = L + 1
      GO TO 5554
 5558 GO TO (600, 603, 68, 7772), K4
C
C
C                    ************************************
C
C                         MISCELLANEOUS PROCESSING
C
C                    ************************************
C
C
  600 ICYCLT = 0
      ICYCLE = 0
      IOUTPT = 1
      K = 1
      IHKL(1) = 1
      I = NQ(ITOTAL - 1)
      GO TO (112, 116), I
  112 ISUM = ITOTAL
      GO TO 80
  116 ISUM = ITOTAL + 1
   80 GO TO (71, 72), INPUT
C
   71 SINAL = SINF(ALPHA * 0.01745329)
      SINBE = SINF(BETA  * 0.01745329)
      SINGA = SINF(GAMMA * 0.01745329)
      COSAL = COSF(ALPHA * 0.01745329)
      COSBE = COSF(BETA  * 0.01745329)
      COSGA = COSF(GAMMA * 0.01745329)
   81 ALS = ACOSF((COSBE * COSGA - COSAL) / (SINBE * SINGA))
      BES = ACOSF((COSAL * COSGA - COSBE) / (SINAL * SINGA))
      GAS = ACOSF((COSAL * COSBE - COSGA) / (SINAL * SINBE))
      SINALS = SINF(ALS)
      SINBES = SINF(BES)
      SINGAS = SINF(GAS)
      COSALS = COSF(ALS)
      COSBES = COSF(BES)
      COSGAS = COSF(GAS)
      AS = 1. / (A * SINBES * SINGA)
      BS = 1. / (B * SINALS * SINGA)
      CS = 1. / (C * SINALS * SINBE)
      ALSTAR = ALS * 57.295780
      BESTAR = BES * 57.295780
```

```
      GASTAR = GAS * 57.295780
      GO TO 99
C
   72 SINALS = SINF(ALSTAR * 0.01745329)
      SINBES = SINF(BESTAR * 0.01745329)
      SINGAS = SINF(GASTAR * 0.01745329)
      COSALS = COSF(ALSTAR * 0.01745329)
      COSBES = COSF(BESTAR * 0.01745329)
      COSGAS = COSF(GASTAR * 0.01745329)
      AL = ACOSF((COSBES * COSGAS - COSALS) / (SINBES * SINGAS))
      BE = ACOSF((COSALS * COSGAS - COSBES) / (SINALS * SINGAS))
      GA = ACOSF((COSALS * COSBES - COSGAS) / (SINALS * SINBES))
      SINAL = SINF(AL)
      SINBE = SINF(BE)
      SINGA = SINF(GA)
      COSAL = COSF(AL)
      COSBE = COSF(BE)
      COSGA = COSF(GA)
      A = 1. / (AS * SINBE * SINGAS)
      B = 1. / (BS * SINAL * SINGAS)
      C = 1. / (CS * SINAL * SINBES)
      ALPHA = AL * 57.295780
      BETA  = BE * 57.295780
      GAMMA = GA * 57.295780
C
   99 V  = A*B*C*SINAL*SINBE*SINGAS
      VS = 1./V
      GO TO (65, 65, 777), IOUTPT
C
   65 DIM(1,K) = A
      DIM(2,K) = B
      DIM(3,K) = C
      DIM(4,K) = ALPHA
      DIM(5,K) = BETA
      DIM(6,K) = GAMMA
      I = IHKL(K)
      GO TO (67, 501, 41), I
   67 IF (K - 1) 64, 64, 63
   63 IF (ISUM - K) 41, 41, 113
C
   64 PRINT 1005
      PRINT 1006, (TITLE(I), I = 1,16)
      GO TO (107, 108), INPUT
  107 PRINT 1007
      GO TO 73
  108 PRINT 1008
   73 PRINT 1009
      DO 13 J = 1,ITOTAL
   13 PRINT 1010, J, (CELL(I,J), I = 1,15)
      I = NQ(ITOTAL - 1)
      GO TO (113, 111), I
  111 J = J + 1
      PRINT 1011, J
  113 I = NQ(K)
      GO TO (5000, 5001), I
C
C
C     ***************************************************************
C
C           TRANSFORMATION USING MATRIX SUPPLIED THRU INPUT
C
C     ***************************************************************
C
```

```
C
C           CALCULATION OF THE NEW A, B, C
C
 5000 ICYCLT = ICYCLT + 1
      DO 117 I = 1,3
  117 AXIS(I)= SQRTF((P(I,1,K)*A)**2 + (P(I,2,K)*B)**2 + (P(I,3,K)*C)**2
     1          + 2.*(P(I,1,K)*P(I,2,K)*A*B*COSGA
     2          +     P(I,1,K)*P(I,3,K)*A*C*COSBE
     3          +     P(I,2,K)*P(I,3,K)*B*C*COSAL))
C
C           CALCULATION OF THE NEW ALPHA, BETA, GAMMA
C
      J = 2
      L = 3
      DO 19 I = 1,3
      COS(I) = (P(J,1,K)*P(L,1,K)*A*A + P(J,2,K)*P(L,2,K)*B*B
     1          + P(J,3,K)*P(L,3,K)*C*C
     2          + (P(J,1,K)*P(L,2,K) + P(J,2,K)*P(L,1,K))*A*B*COSGA
     3          + (P(J,1,K)*P(L,3,K) + P(J,3,K)*P(L,1,K))*A*C*COSBE
     4          + (P(J,2,K)*P(L,3,K) + P(J,3,K)*P(L,2,K))*B*C*COSAL)
     5          / (AXIS(J)*AXIS(L))
      ANGLE(I) = ACOSF(COS(I)) * 57.295780
      GO TO (115, 16, 19), I
  115 J = 1
      GO TO 19
   16 L = 2
   19 CONTINUE
      A = AXIS(1)
      B = AXIS(2)
      C = AXIS(3)
      ALPHA = ANGLE(1)
      BETA  = ANGLE(2)
      GAMMA = ANGLE(3)
      K = K + 1
      IHKL(K) = 1
      GO TO 71
C
C
C           ************************************************************
C
C                          TRANSFORMATION TO REDUCED CELL
C
C           ************************************************************
C
C
C           PART 1.  TRANSFORMATION.
C
C
 5001 K = K + 1
      IHKL(K) = 2
      ICYCLE = 1
      AB = A * B * COSGA
      BC = B * C * COSAL
      CA = C * A * COSBE
      DO 175 J = 1,9
      N(J) = 0
  175 NA(J) = 0
      N(1) = 1
      N(5) = 1
      N(9) = 1
      NA(1) = 1
      NA(5) = 1
      NA(9) = 1
```

```
  382 NSTOP = 1
      K2 = 0
      ABSAB = ABSF(AB)
      ABSBC = ABSF(BC)
      ABSCA = ABSF(CA)
      QQMAX = MAX1F(ABSAB, ABSBC, ABSCA)
      IF (QQMAX - ABSAB) 176, 401, 176
  176 IF (QQMAX - ABSBC) 890, 404, 407
  401 QMAX = MAX1F(A,B)
      IF (QMAX - A) 84, 91, 92
  404 QMAX = MAX1F(B,C)
      IF (QMAX - B) 84, 93, 94
  407 QMAX = MAX1F(C,A)
      IF (QMAX - C) 84, 95, 96
   91 IAXIS = 2
      GO TO 1
   92 IAXIS = 1
      GO TO 4
   93 IAXIS = 3
      GO TO 4
   94 IAXIS = 2
      GO TO 7
   95 IAXIS = 1
      GO TO 7
   96 IAXIS = 3
      GO TO 1
C
    1 MAX = 1
      GO TO 10
    2 IAXIS = 1
      QMAX = MAX1F(B,C)
      IF (QMAX - B) 87, 101, 102
  101 K2 = 1
      GO TO 30
  102 K2 = 2
      GO TO 50
    3 IF (K2 - 1) 88, 121, 122
  121 IAXIS = 2
      GO TO 50
  122 IAXIS = 3
    4 MAX = 4
      GO TO 30
    5 IAXIS = 2
      QMAX = MAX1F(A,C)
      IF (QMAX - A) 87, 201, 202
  201 K2 = 1
      GO TO 10
  202 K2 = 2
      GO TO 50
    6 IF (K2 - 1) 88, 123, 124
  123 IAXIS = 1
      GO TO 50
  124 IAXIS = 3
      GO TO 10
C
    7 MAX = 7
      GO TO 50
    8 IAXIS = 3
      QMAX = MAX1F(A,B)
      IF (QMAX - A) 87, 301, 302
  301 K2 = 1
      GO TO 10
  302 K2 = 2
```

```
      GO TO 30
    9 IF (K2 - 1) 88, 125, 126
  125 IAXIS = 1
      GO TO 30
  126 IAXIS = 2
      GO TO 10
   84 PRINT 1012
      GO TO 890
   87 PRINT 1013
      GO TO 890
   88 PRINT 1014
      GO TO 890
C
C           REDUCTION OF A.    (QMAX = A)
C
   10 X  = A
      Y  = B
      Z  = C
      XY = AB
      YZ = BC
      ZX = CA
C
      NCHECK = 1
      GO TO (85, 11, 12), IAXIS
   11 I = 2
      GO TO 100
   12 I = 3
      GO TO 300
C
   15 A  = X
      B  = Y
      C  = Z
      AB = XY
      BC = YZ
      CA = ZX
C
      NCHECK = NCHECK - 1
      IF (NCHECK) 46, 17, 17
   17 IF (I - 2) 86, 12, 11
   46 MAX = MAX + 1
      NSTOP = NSTOP + 1
      IF (NSTOP - 3) 18, 18, 601
   18 GO TO (1, 2, 3, 4, 5, 6, 7, 8, 9), MAX
C
C           REDUCTION OF B.    (QMAX = B)
C
   30 X  = B
      Y  = C
      Z  = A
      XY = BC
      YZ = CA
      ZX = AB
C
      NCHECK = 1
      GO TO (32, 85, 31), IAXIS
   31 I = 6
      GO TO 100
   32 I = 4
      GO TO 300
C
   35 A  = Z
      B  = X
      C  = Y
```

```
      AB = ZX
      BC = XY
      CA = YZ
C
      NCHECK = NCHECK - 1
      IF (NCHECK) 46, 37, 37
   37 IF (I - 4) 86, 31, 32
C
C           REDUCTION OF C.    (QMAX = C)
C
   50 X  = C
      Y  = A
      Z  = B
      XY = CA
      YZ = AB
      ZX = BC
C
      NCHECK = 1
      GO TO (51, 52, 85), IAXIS
   51 I = 7
      GO TO 100
   52 I = 8
      GO TO 300
C
   55 A  = Y
      B  = Z
      C  = X
      AB = YZ
      BC = ZX
      CA = XY
C
      NCHECK = NCHECK - 1
      IF (NCHECK) 46, 57, 57
   57 IF (I - 7) 86, 52, 51
C
   85 PRINT 1015
      GO TO 890
   86 PRINT 1016
      GO TO 890
C
C           REDUCTION OF X.  ABSF(X,Y) GREATER THAN (Y**2)/2
C
  100 XX = X*X
      YY = Y*Y
      PN = 0.
      IF (ABSF(XY) - 0.5 * YY) 444, 444, 110
  110 IF (XY) 120, 444, 200
  120 XY2 = XY + PN*YY
      IF (XY2) 130, 150, 150
  130 STORE = XY2
      PN = PN + 1.
      GO TO 110
  150 IF (ABSF(XY2) - ABSF(STORE)) 143, 142, 142
  142 PN = PN - 1.
  143 NA(I) = PN
      X =  SQRTF(XX + 2.*PN*XY + PN*PN*YY)
      ZX = ZX + PN*YZ
  144 IF (ABSF(XY2) - ABSF(STORE)) 160, 170, 170
  160 XY = XY2
      GO TO 520
  170 XY = STORE
      GO TO 520
C
```

```
  200 XY2 = XY - PN*YY
      IF (XY2) 250, 250, 230
  230 STORE = XY2
      PN = PN + 1.
      GO TO 200
  250 IF (ABSF(XY2) - ABSF(STORE)) 243, 243, 242
  242 PN = PN - 1.
  243 NA(I) = -PN
      X = SQRTF(XX - 2.*PN*XY + PN*PN*YY)
      ZX = ZX - PN*YZ
      GO TO 144
C
C           REDUCTION OF X.  ABSF(Z.X) GREATER THAN (Z**2)/2
C
  300 XX = X*X
      ZZ = Z*Z
      PN = 0.
      IF (ABSF(ZX) - 0.5 * ZZ) 444, 444, 310
  310 IF (ZX) 320, 444, 400
  320 ZX2 = ZX + PN*ZZ
      IF (ZX2) 330, 350, 350
  330 STORE = ZX2
      PN = PN + 1.
      GO TO 310
  350 IF (ABSF(ZX2) - ABSF(STORE)) 343, 342, 342
  342 PN = PN - 1.
  343 NA(I) = PN
      X = SQRTF(XX + 2.*PN*ZX + PN*PN*ZZ)
      XY = XY + PN*YZ
  344 IF (ABSF(ZX2) - ABSF(STORE)) 360, 370, 370
  360 ZX = ZX2
      GO TO 520
  370 ZX = STORE
      GO TO 520
C
  400 ZX2 = ZX - PN*ZZ
      IF (ZX2) 450, 450, 430
  430 STORE = ZX2
      PN = PN + 1.
      GO TO 400
  450 IF (ABSF(ZX2) - ABSF(STORE)) 463, 463, 462
  462 PN = PN - 1.
  463 NA(I) = -PN
      X = SQRTF(XX - 2.*PN*ZX + PN*PN*ZZ)
      XY = XY - PN*YZ
      GO TO 344
C
  520 NB(1) = NA(1)*N(1) + NA(2)*N(4) + NA(3)*N(7)
      NB(2) = NA(1)*N(2) + NA(2)*N(5) + NA(3)*N(8)
      NB(3) = NA(1)*N(3) + NA(2)*N(6) + NA(3)*N(9)
      NB(4) = NA(4)*N(1) + NA(5)*N(4) + NA(6)*N(7)
      NB(5) = NA(4)*N(2) + NA(5)*N(5) + NA(6)*N(8)
      NB(6) = NA(4)*N(3) + NA(5)*N(6) + NA(6)*N(9)
      NB(7) = NA(7)*N(1) + NA(8)*N(4) + NA(9)*N(7)
      NB(8) = NA(7)*N(2) + NA(8)*N(5) + NA(9)*N(8)
      NB(9) = NA(7)*N(3) + NA(8)*N(6) + NA(9)*N(9)
      DO 521 J = 1,9
      N(J) = NB(J)
      IF (N(J)) 521, 540, 521
  540 N(J) = 0
  521 NA(J) = 0
      NA(1) = 1
      NA(5) = 1
```

```
      NA(9) = 1
  444 GO TO (601, 15, 15, 35, 601, 35, 55, 55, 601), I
C
C
C          OUTPUT OF PART 1.    (REDUCED CELL)
C
C
  601 COSAL = BC / (B*C)
      COSBE = CA / (C*A)
      COSGA = AB / (A*B)
      AL = ACOSF(COSAL)
      BE = ACOSF(COSBE)
      GA = ACOSF(COSGA)
      SINAL = SINF(AL)
      SINBE = SINF(BE)
      SINGA = SINF(GA)
      ALPHA = 57.295780 * AL
      BETA  = 57.295780 * BE
      GAMMA = 57.295780 * GA
      LL = 1
      GO TO 602
C
C          A TEST IS NOW MADE TO DETERMINE IF THE CELL JUST OBTAINED
C     IS THE REDUCED CELL.  IF ONE OR MORE OF THE AXES CAN BE FURTHER
C     REDUCED, THE PROGRAM RETURNS TO STMNT 382 FOR ANOTHER CYCLE.
C
  501 IF (ABSF(AB) - 0.5 * A*A) 502, 502, 381
  502 IF (ABSF(AB) - 0.5 * B*B) 503, 503, 381
  503 IF (ABSF(BC) - 0.5 * B*B) 504, 504, 381
  504 IF (ABSF(BC) - 0.5 * C*C) 505, 505, 381
  505 IF (ABSF(CA) - 0.5 * C*C) 506, 506, 381
  506 IF (ABSF(CA) - 0.5 * A*A) 66, 66, 381
  381 ICYCLE = ICYCLE + 1
      GO TO 382
C
C
C          PART 2.   TRANSFORMATION OF REDUCED CELL TO CONVENTIONAL
C     REDUCED CELL.  THE CONVENTION IS C LESS THAN A LESS THAN B,
C     WITH ALPHA, BETA OBTUSE.
C
C
   66 JA = 0
      JB = 0
      JC = 0
      K = K + 1
      IHKL(K) = 3
      NTURN = 1
      KK = 3
      IF (MIN1F(A,B,C) - A) 702, 611, 999
  611 JJ = 7
      M = -6
      GO TO 721
  702 IF (MIN1F(A,B,C) - B) 612, 613, 999
  612 JC = 1
      JJ = 7
      M = 0
      GO TO 723
  613 JJ = 7
      M = -3
      GO TO 722
  703 NTURN = 2
      KK = 2
      IF (MAX1F(A,B,C) - A) 999, 614, 704
```

```
  614 JJ = 4
      M = -3
      GO TO 721
  704 IF (MAX1F(A,B,C) - B) 999, 615, 616
  615 JB = 1
      JJ = 4
      M = 0
      GO TO 722
  616 JJ = 4
      M = 3
      GO TO 723
  706 NTURN = 3
      KK = 1
      IF (D(2) - A) 710, 707, 710
  710 IF (D(2) - B) 999, 708, 709
  707 IF (MIN1F(B,C) - B) 622, 621, 999
  621 JJ = 1
      M = 6
      GO TO 723
  622 JJ = 1
      M = 3
      GO TO 722
  708 IF (MIN1F(A,C) - A) 623, 621, 999
  623 JA = 1
      JJ = 1
      M = 0
      GO TO 721
  709 IF (MIN1F(A,B) - A) 623, 622, 999
C
  721 D(KK) = A
      ANGLE (KK) = ALPHA
  664 JL = JJ + 2
      DO 665 L = JJ,JL
      LM = L + M
  665 NTEMP(L) = N(LM)
      GO TO (703, 706, 739), NTURN
  722 D(KK) = B
      ANGLE (KK) = BETA
      GO TO 664
  723 D(KK) = C
      ANGLE (KK) = GAMMA
      GO TO 664
C
  739 DO 730 I = 1,9
  730 N(I) = NTEMP(I)
      A = D(1)
      B = D(2)
      C = D(3)
      ALPHA = ANGLE(1)
      BETA  = ANGLE(2)
      GAMMA = ANGLE(3)
C
C          THE FOLLOWING SECTION CHECKS TO MAKE SURE ALPHA AND BETA ARE
C     EACH EQUAL TO OR GREATER THAN 90 DEGREES.  IF ONE OR BOTH ARE
C     LESS THAN 90 DEGREES, THE PROPER ADJUSTMENTS ARE MADE.
C
  223 LL = 2
      ISIGN = 0
      IF (ALPHA - 90.0) 21, 801, 801
   21 ISIGN = ISIGN + 1
  801 IF (BETA - 90.0) 22, 802, 802
   22 ISIGN = ISIGN + 1
  802 IF (ISIGN - 1) 602, 69, 79
```

```
C
C      ISIGN = 1
C           EITHER ALPHA OR BETA IS LESS THAN 90 DEGREES.  REDEFINE THAT
C           ANGLE AS ITS SUPPLEMENT AND SET GAMMA = 180.0 - GAMMA.
C           (TWO ANGLES MUST ALWAYS BE TRANSFORMED SIMULTANEOUSLY.)
C
   69 GAMMA = 180.0 - GAMMA
      DO 6661 I = 7,9
      N(I) = -N(I)
      IF (N(I)) 6661, 4441, 6661
 4441 N(I) = 0
 6661 CONTINUE
      IF (ALPHA - 90.0) 43, 44, 44
   43 ALPHA = 180.0 - ALPHA
      DO 6662 I = 1,3
      N(I) = -N(I)
      IF (N(I)) 6662, 4442, 6662
 4442 N(I) = 0
 6662 CONTINUE
      GO TO 602
   44 BETA = 180.0 - BETA
      DO 6663 I = 4,6
      N(I) = -N(I)
      IF (N(I)) 6663, 4443, 6663
 4443 N(I) = 0
 6663 CONTINUE
      GO TO 602
C
C      ISIGN = 2
C           REDEFINE ALPHA AND BETA AS ITS OWN SUPPLEMENT AND REVERSE THE
C           DIRECTIONS OF A AND B.
C
   79 ALPHA = 180.0 - ALPHA
      BETA = 180.0 - BETA
      DO 6664 I = 1,6
      N(I) = -N(I)
      IF (N(I)) 6664, 4444, 6664
 4444 N(I) = 0
 6664 CONTINUE
C
  602 GO TO (821, 831), LL
C
C           A CHECK IS MADE TO DETERMINE IF THE SYSTEM HAS GONE FROM
C      RIGHT-HANDED TO LEFT-HANDED OR VICE VERSA.  IF JF = 1 THE SYSTEM
C      HAS REVERSED.  IF JF = 0 OR 3, IT HAS NOT REVERSED.
C
  831 JF = JA + JB + JC
      IF (JF - 1) 821, 832, 821
  832 DO 835 I = 1,9
      N(I) = -N(I)
      IF (N(I)) 835, 833, 835
  833 N(I) = 0
  835 CONTINUE
C
  821 K = K - 1
      NN(1,1,LL) = N(1)
      NN(1,2,LL) = N(2)
      NN(1,3,LL) = N(3)
      NN(2,1,LL) = N(4)
      NN(2,2,LL) = N(5)
      NN(2,3,LL) = N(6)
      NN(3,1,LL) = N(7)
      NN(3,2,LL) = N(8)
```

```
      NN(3,3,LL) = N(9)
      P(1,1,K) = N(1)
      P(1,2,K) = N(2)
      P(1,3,K) = N(3)
      P(2,1,K) = N(4)
      P(2,2,K) = N(5)
      P(2,3,K) = N(6)
      P(3,1,K) = N(7)
      P(3,2,K) = N(8)
      P(3,3,K) = N(9)
      K4 = 2
      GO TO 5550
  603 MM(1,1,LL) = S(1,1,K)
      MM(1,2,LL) = S(1,2,K)
      MM(1,3,LL) = S(1,3,K)
      MM(2,1,LL) = S(2,1,K)
      MM(2,2,LL) = S(2,2,K)
      MM(2,3,LL) = S(2,3,K)
      MM(3,1,LL) = S(3,1,K)
      MM(3,2,LL) = S(3,2,K)
      MM(3,3,LL) = S(3,3,K)
      K = K + 1
      IF (IHKL(K) - 2) 81, 81, 71
C
  999 PRINT 1017
      GO TO 890
C
C
C           ************************************************************
C
C               GENERATION OF MATRIX FOR TRANSFORMATION OF ORIGINAL
C                                CELL TO FINAL CELL
C
C           ************************************************************
C
C
   41 IF (ITOTAL - 3) 68, 45, 45
   45 K4 = 3
      K = K + 1
      IHKL(K) = 4
 8881 DO 8882 L = 1,ISUM
      DO 8882 J = 1,3
      DO 8882 I = 1,3
 8882 Q(I,J,L) = P(I,J,L)
      IF (K4 - 4) 56, 58, 58
   56 K8 = K
      GO TO 59
   58 K = K8
   59 IF (ICYCLE) 53, 53, 54
   53 K = K + 1
   54 L = K - 3
      M = K - 4
      LL = L
  104 DO 105 I = 1,3
      DO 105 J = 1,3
  105 W(I,J,L) = Q(I,1,L)*Q(1,J,M)+Q(I,2,L)*Q(2,J,M)+Q(I,3,L)*Q(3,J,M)
      IF (M - 1) 8890, 8890, 106
  106 DO 8883 I = 1,3
      DO 8883 J = 1,3
 8883 Q(I,J,L) = W(I,J,L)
      M = M - 1
      GO TO 104
 8890 IF (K4 - 3) 890, 8892, 8891
```

```
 8891 L2 = L2 + 1
      GO TO 8893
 8892 L2 = ISUM
 8893 DO 8887 I = 1,3
      DO 8887 J = 1,3
 8887 P(I,J,L2) = W(I,J,L)
      GO TO 5550
C
C
C                                   ***************
C
C                                        OUTPUT
C
C                                   ***************
C
C
   68 IOUTPT = 3
      PRINT 1018
      K = 1
      IF (ISUM - 5) 798, 799, 799
  798 LINE = 2
      GO TO 800
  799 LINE = 3
  800 I = NQ(K)
      GO TO (750, 751), I
  750 KX = K + 1
      PRINT 1019, K, KX, KX, K
      PRINT 1020, P(1,1,K),P(1,2,K),P(1,3,K), S(1,1,K),S(1,2,K),S(1,3,K)
      PRINT 1020, P(2,1,K),P(2,2,K),P(2,3,K), S(2,1,K),S(2,2,K),S(2,3,K)
      PRINT 1020, P(3,1,K),P(3,2,K),P(3,3,K), S(3,1,K),S(3,2,K),S(3,3,K)
      PRINT 1046, DET(K), BET(K)
      GO TO 755
  751 L = 1
      KX = K + 1
      PRINT 1019, K, KX, KX, K
      PRINT 1044, NN(1,1,L),NN(1,2,L),NN(1,3,L), MM(1,1,L),MM(1,2,L),
     1            MM(1,3,L)
      PRINT 1044, NN(2,1,L),NN(2,2,L),NN(2,3,L), MM(2,1,L),MM(2,2,L),
     1            MM(2,3,L)
      PRINT 1044, NN(3,1,L),NN(3,2,L),NN(3,3,L), MM(3,1,L),MM(3,2,L),
     1            MM(3,3,L)
      PRINT 1046, DET(K), BET(K)
      LINE = LINE + 1
      IF (LINE - 5) 752, 743, 743
  743 LINE = 1
      PRINT 1022, (TITLE(I), I = 1,15)
  752 L = 2
      KX = K + 2
      PRINT 1019, K, KX, KX, K
      PRINT 1044, NN(1,1,L),NN(1,2,L),NN(1,3,L), MM(1,1,L),MM(1,2,L),
     1            MM(1,3,L)
      PRINT 1044, NN(2,1,L),NN(2,2,L),NN(2,3,L), MM(2,1,L),MM(2,2,L),
     1            MM(2,3,L)
      PRINT 1044, NN(3,1,L),NN(3,2,L),NN(3,3,L), MM(3,1,L),MM(3,2,L),
     1            MM(3,3,L)
      PRINT 1046, DET(K+1), BET(K+1)
  755 LINE = LINE + 1
      IF (LINE - 5) 741, 740, 740
  740 LINE = 1
      PRINT 1022, (TITLE(I), I = 1,15)
  741 K = K + 1
      IF (ITOTAL - K) 753, 753, 800
  753 IF (ITOTAL - 3) 742, 757, 757
```

```
C
  757 PRINT 1021, ITOTAL,ITOTAL
      PRINT 1020, P(1,1,L2),P(1,2,L2),P(1,3,L2), S(1,1,L2),S(1,2,L2),
     1            S(1,3,L2)
      PRINT 1020, P(2,1,L2),P(2,2,L2),P(2,3,L2), S(2,1,L2),S(2,2,L2),
     1            S(2,3,L2)
      PRINT 1020, P(3,1,L2),P(3,2,L2),P(3,3,L2), S(3,1,L2),S(3,2,L2),
     1            S(3,3,L2)
      PRINT 1046, DET(L2), BET(L2)
      IF (ICYCLE) 742, 742, 758
  758 K4 = 4
      JB2 = ITOTAL - 1
      DO 7771 I = 1,3
      DO 7771 J = 1,3
 7771 P(I,J,JB2) = NN(I,J,2)
      GO TO 8881
 7772 LINE = LINE + 1
      IF (LINE - 5) 761, 760, 760
  760 LINE = 1
      PRINT 1022, (TITLE(I), I = 1,15)
  761 PRINT 1021, ISUM, ISUM
      PRINT 1020, P(1,1,L2),P(1,2,L2),P(1,3,L2), S(1,1,L2),S(1,2,L2),
     1            S(1,3,L2)
      PRINT 1020, P(2,1,L2),P(2,2,L2),P(2,3,L2), S(2,1,L2),S(2,2,L2),
     1            S(2,3,L2)
      PRINT 1020, P(3,1,L2),P(3,2,L2),P(3,3,L2), S(3,1,L2),S(3,2,L2),
     1            S(3,3,L2)
      PRINT 1046, DET(L2), BET(L2)
C
  742 J = 0
  756 J = J + 1
      PRINT 1022, (TITLE(I), I = 1,16)
      IF (IHKL(J) - 3) 771, 772, 771
  771 PRINT 1023, J, (CELL(I,J), I = 1,15)
      GO TO 773
  772 PRINT 1045, J
C
  773 A = DIM(1,J)
      B = DIM(2,J)
      C = DIM(3,J)
      ALPHA = DIM(4,J)
      BETA  = DIM(5,J)
      GAMMA = DIM(6,J)
      GO TO 71
  777 PRINT 1024, A, ALPHA
      PRINT 1025, B, BETA
      PRINT 1026, C, GAMMA
      PRINT 1027, AS, ALSTAR
      PRINT 1028, BS, BESTAR
      PRINT 1029, CS, GASTAR
      PRINT 1030, V
      PRINT 1031, VS
C
      SINAL  = SINF(ALPHA * 0.01745329)
      SINBE  = SINF(BETA  * 0.01745329)
      SINGA  = SINF(GAMMA * 0.01745329)
      COSAL  = COSF(ALPHA * 0.01745329)
      COSBE  = COSF(BETA  * 0.01745329)
      COSGA  = COSF(GAMMA * 0.01745329)
      SINALS = SINF(ALSTAR * 0.01745329)
      SINBES = SINF(BESTAR * 0.01745329)
      SINGAS = SINF(GASTAR * 0.01745329)
      COSALS = COSF(ALSTAR * 0.01745329)
```

```
      COSBES = COSF(BESTAR * 0.01745329)
      COSGAS = COSF(GASTAR * 0.01745329)
C
      PRINT 1032
      PRINT 1033
      PRINT 1034, ALPHA, SINAL, COSAL
      PRINT 1035, BETA,  SINBE, COSBE
      PRINT 1036, GAMMA, SINGA, COSGA
      PRINT 1037, ALSTAR, SINALS, COSALS
      PRINT 1038, BESTAR, SINBES, COSBES
      PRINT 1039, GASTAR, SINGAS, COSGAS
C
      I = IHKL(J)
      GO TO (208, 871, 871), I
C
  871 PRINT 1040
      AA = A*A
      BB = B*B
      CC = C*C
      AB = A*B*COSGA
      BC = B*C*COSAL
      CA = C*A*COSBE
      SUM = AB + BC + CA
      PRINT 1041, AA, BB, CC
      PRINT 1042, BC, CA, AB
      PRINT 1043, SUM
C
  208 IF (ISUM - J) 890, 890, 756
C
C
  890 READ 1070, ICONT
      IF (ICONT) 89, 89, 9998
 9998 PRINT 1005
      GO TO 9999
   89 STOP 89
      END
```

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# APPENDIX I. THE SPACE LATTICE

The periodic arrangement of atomic or molecular units in a crystal may be conveniently expressed by representing the repeating units as points. The result is a three-dimensional network of points in space called a lattice or point lattice and the points making up this network are the lattice points. This framework has the property that it can be moved about in space like a rigid body either by translation or rotation about a given axis so as to bring the lattice points into self-coincidence.

As can be seen from Figure 13 a point lattice may be regarded as dissecting space into a set of parallelepiped cells with a lattice point at each corner. Each cell, or unit cell, is identical in size, shape and

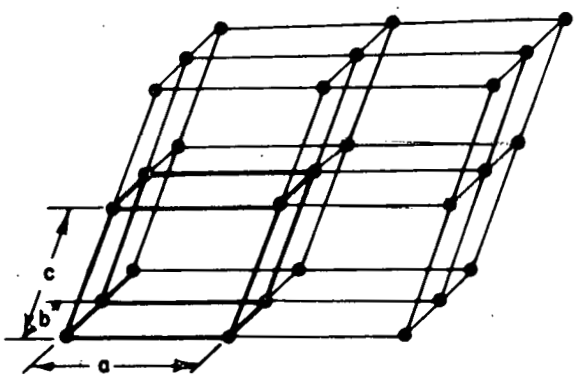



Fig. 13. The Space Lattice

orientation. The number of cells differing in size, shape and orientation in a lattice is infinite since there are an infinite number of possible lattice rows. However, only three non-coplanar rows are required to outline a cell in three-dimensional space. The shape of this cell, and hence the shape of the entire lattice, may be completely described by specifying the repeat distance between points along each of the three chosen directions in the lattice and by specifying the angles between these three intersecting rows (Figure 13). The total number of parameters is thus six: three crystallographic axes a, b, c and three interaxial angles $\alpha$, $\beta$, $\gamma$, where

$\alpha$ is the angle between sides b and c,

$\beta$ is the angle between sides a and c,

$\gamma$ is the angle between sides a and b.

A variety of names are given to the six quantities which specify a three-dimensional lattice. The three most commonly used are lattice parameters, lattice constants and cell dimensions.

Crystals contain symmetry as a consequence of periodicity and only certain types and combinations are allowed, giving rise to 32 point groups and 230 space groups, each corresponding to possible combinations of symmetry in a lattice. The net effect of symmetry is to restrict the axial lengths and angles to special values, resulting in cells of various shapes. By dividing the point groups into classes according to the principle axes of rotation, that is, with n = 1, 2, 3, 4 and 6 and, if necessary, by further subdivision according to a common set of unique

symmetry elements, the seven crystal systems result. These are summarized in Table 4. The minimum essential symmetry elements which define each system are shown in column 3. It is these elements alone which are responsible for fixing one or more of the six lattice parameters summarized in columns 5 and 6.

As is shown in column 4 of Table 4 the threefold axes which define the rhombohedral and cubic systems lie along the body-diagonals rather than coinciding with one or more of the three crystallographic axes. In these two systems it is this element which controls the six parameters. First, a threefold along a body-diagonal restricts a = b = c. The cubic system then differs from the rhombohedral system only in the total number of threefold body-diagonals; the former has only one whereas the latter has four at 109° 28' to each other. Such an arrangement of threefolds restricts the angles $\alpha = \beta = \gamma = 90°$ for the cubic system whereas no such restriction exists in the rhombohedral system.

The cells corresponding to the seven crystal systems and the unique symmetry elements controlling their shape are shown in Figure 14.

It may turn out experimentally that two or more cell parameters which are not required to be equal in magnitude may actually turn out to be accidentally equal, within experimental error. Such a cell is a pseudo-cell and is always of lower symmetry than the parameters indicate. For instance, if the $\beta$-angle of a monoclinic cell is 90°, all three sides still unequal, it is only pseudo-orthorhombic and is still monoclinic

TABLE 4

The Seven Crystal Systems

| Order of Principle Axis | Crystal System | Minimum Symmetry Requirements; unique elements | Location of Unique Elements | Axial Lengths | Interaxial Angles |
|---|---|---|---|---|---|
| 1 | Triclinic (Anorthic) | none | | $a \neq b \neq c$ | $\alpha \neq \beta \neq \gamma$ |
| 2 | Monoclinic | 1 (twofold, mirror) | b-axis | $a \neq b \neq c$ | $\alpha = \gamma = 90°; \beta > 90°$ |
| | Orthorhombic (Rhombic) | 3 (twofolds, mirrors) | a, b, c-axes | $a \neq b \neq c$ | $\alpha = \beta = \gamma = 90°$ |
| 3 | Rhombohedral (Trigonal) | 1 (threefold) | body-diagonal | $a = b = c$ | $\alpha = \beta = \gamma \neq 90°$ |
| 2 or 4 | Cubic (Isometric) | 4 (threefolds) | body-diagonals; 109° 28' to each other | $a = b = c$ | $\alpha = \beta = \gamma = 90°$ |
| 4 | Tetragonal | 1 (fourfold) | c-axis | $a = b \neq c$ | $\alpha = \beta = \gamma = 90°$ |
| 6 | Hexagonal | 1 (sixfold) | c-axis | $a = b \neq c$ | $\alpha = \beta = 90°; \gamma = 120°$ |

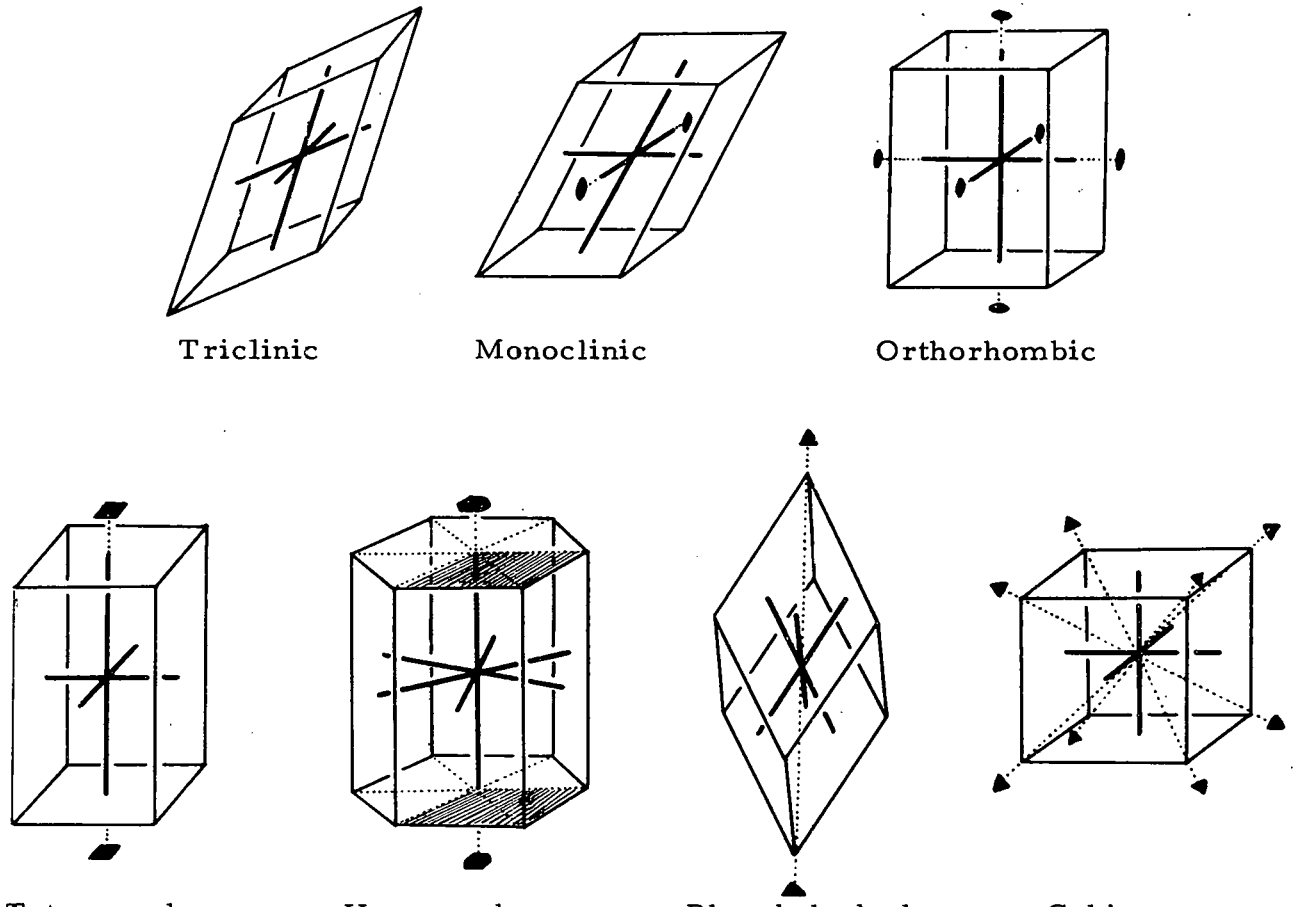



Fig. 14. The seven crystal systems.

by symmetry due to the absence of intersecting mirror planes or two-fold axes. Likewise, an orthorhombic cell whose three sides are equal in length is pseudo-cubic but still remains orthorhombic by symmetry due to the absence of crystal units related by threefolds axes.

Depending upon the three intersecting lattice rows which are chosen, cells of a wide variety of shapes and sizes are possible in a given lattice. As can be seen from Figure 15 such cells are not restricted to so-called primitive cells with a lattice point located at just the corners; non-primitive or centered cells are also possible.

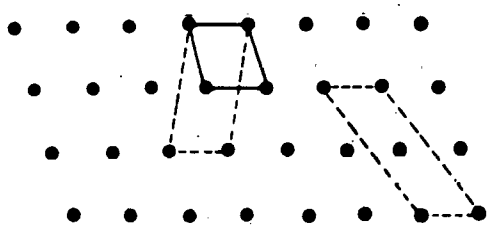


Fig. 15. Examples of different cells outlined in a lattice

There are, in all, only three unique types of centering, namely end-centering, face-centering and body-centering. These, together with primitive, constitute the four lattice types. The primitive, or simple cells, denoted by the symbol P, contain only one

lattice point per cell, each point located at a corner and shared by eight cells. The centered cells contain points in addition to those in the corners. Thus, the body-centered cell, denoted by the symbol I, contains one additional point at the body center. The end-centered cell, denoted by the symbol A, B or C, also contains two points per cell but with centering on two faces, namely those which are parallel and opposite each other. The symbol denotes the face on which the centering occurs and is defined with the A face containing the b- and c-axes, the B face containing the a- and c-axes and the C face containing the a- and b-axes. In orthogonal systems this is equivalent to saying that the A face is normal to the a-axis, the B face normal to the b-axis and the C face normal to the c-axis. The face-centered cell, denoted by the symbol F, exhibits centering on all six faces, thereby increasing to four the number of points per cell; those in the eight corners constitute one and those in the six faces, each shared by two cells, constitute the other three.

The relative volumes of the primitive and centered cells of course vary in exactly the same ratio as the number of lattice points each contains. That is, the volume of the cells of lattice type P:(A, B, C):I:F is in the ratio 1:2:2:4. A cell containing two lattice points is said to be doubly primitive, three points triply primitive and four points quadruply primitive.

In practice it would seem logical to outline the cell in a lattice having the smallest volume, namely a primitive cell. Why then does one concern himself with centered cells at all? The unit cell, it must be

understood, does not literally "exist" as such in a lattice; they are only a mental construction chosen at ones convenience. There are thus an infinite number of cells which can be outlined in a lattice. On the other hand there is always only one unique cell of least volume whose axes correspond to the primary rotation axes of the lattice as a whole. This is the cell in which one is really interested for it is the only cell which displays the full symmetry of the lattice. As a result, this cell may turn out to be centered with a repeating unit of structure in its faces or body center. For this reason it is necessary that we retain centered cells in crystal classification.

All seven crystal systems are capable of possessing centering. Depending upon the system some of these centered cells can be transformed to centered cells of smaller volume or transformed directly to a primitive cell without losing its full symmetry. This merely amounts to redefining in the lattice a new cell without destroying the 90° angles. For instance, a face-centered monoclinic cell may be redefined as an end-centered monoclinic cell with half the volume and no loss in symmetry. It is not possible, however, for each of the seven systems to have each of the three types of centering; some types of centering are not consistent with the symmetry conditions. For instance, a cubic cell cannot have centering on only one pair of opposite faces as the symmetry would then no longer be cubic; rotation about anyone of the four threefold body-diagonal axes would automatically generate centering in the other pair of faces.

As a convenient rule of thumb, the following order of reductions are seen to hold for the "possible" transformations of lattice types within a crystal system:

| | | | | |
|---|---|---|---|---|
| F | → I | → A, B, C | → P | lattice type |
| 4 | 2 | 2 | 1 | pts. per cell; rel. vol. |

The direction of the arrow indicates the direction in which one lattice type may be reduced to another, if possible. Thus, in the tetragonal system two reductions are possible: a C centered lattice may be reduced to a primitive lattice and a face-centered lattice to a body-centered lattice, each with a reduction in both volume and total number of lattice points. Note the order "I before (A, B, C)"; it is written in this way because a monoclinic I lattice may be converted to an A or C monoclinic lattice (b-unique) or A or B lattice (c-unique), the arrow indicating this direction of transformation.

The primitive cells, plus those where the centering is unique, are listed in Table 5 and shown in Figure 16. These are called the fourteen Bravais Lattices.

TABLE 5.

THE FOURTEEN BRAVAIS LATTICES

| System | Unique Lattice Types | Alternative Symbols for Other Orientations | Direct Relationship |
|---|---|---|---|
| Triclinic | P | A, B, C, I, F | P(=A=B=C=I=F) |
| Monoclinic | P, C | A, B, I, F | P(=B), C(=A=I=F) |
| Orthorhombic | P, C, I, F | A, B | C(=A=B) |
| Tetragonal | P, I | C, F | P(=C), I(=F) |
| Hexagonal | P | H | P(H) |
| Rhombohedral | R | | |
| Cubic | P, I, F | | |

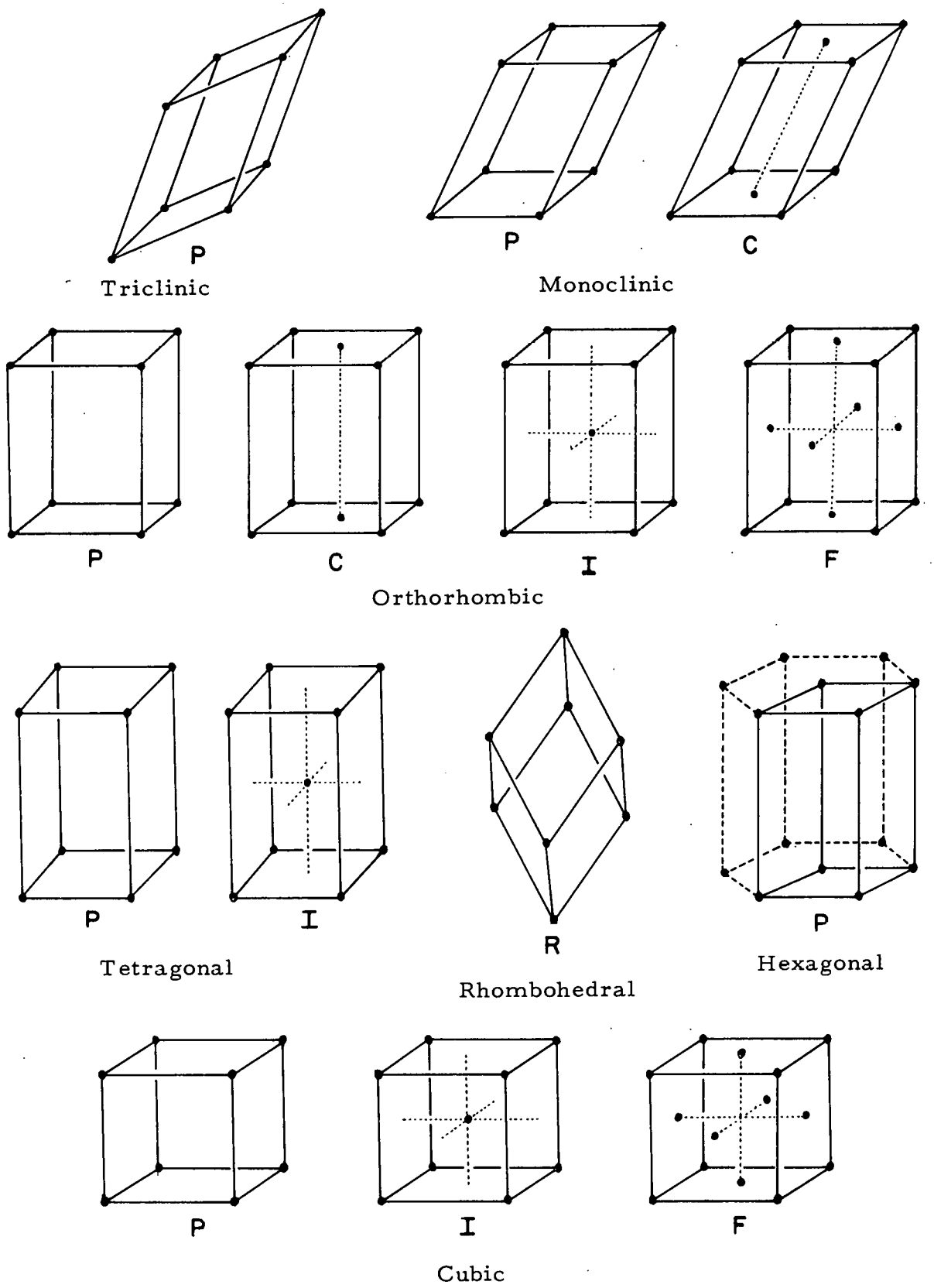



Fig. 16. The fourteen Bravais lattices.

# APPENDIX II. VECTORIAL REPRESENTATION OF AXES IN A DIRECT LATTICE

Since each point in the three-dimensional lattice is related by translation to an adjacent point (or any other point), such an array of points may be defined by three non-coplanar vectors. These three vectors each have magnitude and direction, corresponding to the distance and direction the rigid lattice must be translated to arrive at self-coincidence. Alternately, the three vectors may be considered as representing the three arbitrary distances and directions one point must be moved to generate all the other points to completely fill space.

For convenience, the vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ describing the point lattice may be placed so that all three eminate from a single point, conveniently taken as the corner of a cell (Figure 17). Each vector will then terminate at the next point along the lattice row. The length of the three sides a, b and c of the unit cell correspond to the magnitudes of the vectors and the angles $\alpha$, $\beta$, $\gamma$ to the angles between each pair of vectors.

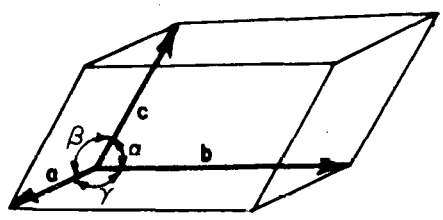



Fig. 17. A three dimensional parallelepiped, or unit cell.

# APPENDIX III

## TRANSFORMATION OF LATTICE AXES, MILLER INDICES AND ATOMIC COORDINATES

Given a cell defined by a set of coordinate axes, or vectors, in a lattice it is sometimes desirable to redefine in the lattice a new cell possessing a new set of coordinate axes. Accompanying this change there is a change in the intercepts which the new axes make with the various planes, that is, a change in the Miller indices, as well as a change in the lattice axes in reciprocal space and the atomic coordinates of the atoms. As is shown in Table 6 when transforming from cell (1), the original cell, to cell (2), a new cell in the same lattice, the Miller indices transform by the same matrix as the vectorial transformation of lattice axes in direct space [1, 5] (no change of origin) whereas the reciprocal axes and atomic coordinates both transform by a matrix which is the transpose of the inverse of the matrix for the vectorial transformation of lattice axes in direct space[5].

Example

Consider the transformation of a C-centered monoclinic cell to a body-centered orthorhombic cell, where A = a, B = b and C = a + c. Let cell (1) be the original monoclinic cell and cell (2) the new orthorhombic cell. Further, let N be the matrix for transforming the lattice axes of cell (1) to cell (2) and its inverse, $N^{-1}$, be that for cell (2) to cell (1), that is

CELL (1) TO CELL (2) CELL (2) TO CELL (1)

$$N = \begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{Vmatrix} \qquad N^{-1} = \begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 1 \end{Vmatrix}$$

Knowing these two, the other transformations of interest are thus known immediately, as summarized below:

CELL (1) TO CELL (2)

Axes in direct space
Miller indices :

$$\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{Vmatrix} = N$$

Axes in reciprocal space
Atomic coordinates :

$$\begin{Vmatrix} 1 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix} = \text{transpose of } N^{-1}$$

CELL (2) TO CELL (1)

Axes in direct space
Miller indices :

$$\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 1 \end{Vmatrix} = N^{-1}$$

Axes in reciprocal space
Atomic coordinates :

$$\begin{Vmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{Vmatrix} = \text{transpose of } N$$

Table 6. The transformation of lattice axes, Miller indices and atomic coordinates.

| Description | Transformation | Matrix | Definitions |
|---|---|---|---|
| (a). Vectorial transformation of lattice axes in direct space, cell (1) to cell (2). | $A = n_{11}a + n_{12}b + n_{13}c$<br>$B = n_{21}a + n_{22}b + n_{23}c$<br>$C = n_{31}a + n_{32}b + n_{33}c$ | N | $a,b,c$ = real axes of cell (1)<br>$A,B,C$ = real axes of cell (2)<br>$n_{ij}$ = elements of matrix N |
| (b). Transformation of Miller indices, cell (1) to cell (2). | $H = n_{11}h + n_{12}k + n_{13}l$<br>$K = n_{21}h + n_{22}k + n_{23}l$<br>$L = n_{31}h + n_{32}k + n_{33}l$ | N | $h,k,l$ = Miller indices of cell (1)<br>$H,K,L$ = Miller indices of cell (2)<br>$n_{ij}$ = elements of matrix N |
| (c). Inverse vectorial transformation of lattice axes in direct space, cell (2) to cell (1). | $a = s_{11}A + s_{12}B + s_{13}C$<br>$b = s_{21}A + s_{22}B + s_{23}C$<br>$c = s_{31}A + s_{32}B + s_{33}C$ | $N^{-1}$ | $a,b,c$ = real axes of cell (1)<br>$A,B,C$ = real axes of cell (2)<br>$s_{ij}$ = matrix elements of N inverse, $N^{-1}$ |
| (d). Vectorial transformation of lattice axes in reciprocal space, cell (1) to cell (2). | $A^* = t_{11}a^* + t_{12}b^* + t_{13}c^*$<br>$B^* = t_{21}a^* + t_{22}b^* + t_{23}c^*$<br>$C^* = t_{31}a^* + t_{32}b^* + t_{33}c^*$ | transpose of $N^{-1}$ | $a^*,b^*,c^*$ = reciprocal axes of cell (1)<br>$A^*,B^*,C^*$ = reciprocal axes of cell (2)<br>$t_{ij}$ = matrix elements of $N^{-1}$ transposed |
| (e). Transformation of atomic coordinates, cell (1) to cell (2). | $x_2 = t_{11}x_1 + t_{12}y_1 + t_{13}z_1$<br>$y_2 = t_{21}x_1 + t_{22}y_1 + t_{23}z_1$<br>$z_2 = t_{31}x_1 + t_{32}y_1 + t_{33}z_1$ | transpose of $N^{-1}$ | $x_1,y_1,z_1$ = fractional atomic coordinates in cell (1)<br>$x_2,y_2,z_2$ = fractional atomic coordinates in cell (2)<br>$t_{ij}$ = matrix elements of $N^{-1}$ transposed |

# APPENDIX IV. THE USE OF VECTOR MULTIPLICATION IN THE TRANSFORMATION OF LATTICE AXES

A cell is transformed to a new cell by expressing the new coordinate axes $\vec{A}$, $\vec{B}$, $\vec{C}$, as vectors, in terms of the old with axes $\vec{a}$, $\vec{b}$, $\vec{c}$. The magnitudes of the six cell parameters in the new cell are then obtained from the scalar products of the new vectors expressed in terms of the original vectors whose magnitudes are known. The method results from the following two properties of the scalar (dot) product:

(i). The dot product of a vector with itself gives the square of its magnitude.

(ii). The dot product of two non-zero vectors, divided by their magnitudes, gives the cosine of the angle between them.

The general form of the vectorial transformation of axes is given by

$$\begin{pmatrix} \vec{A} \\ \vec{B} \\ \vec{C} \end{pmatrix}_{\text{new}} = \begin{pmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}_{\text{old}},$$

or as (a) in Table 6, page 159. To calculate the magnitude of A, B, C, $\alpha$, $\beta$, $\gamma$ in the new cell, the following expressions are used:

$$|A| = \sqrt{\vec{A} \cdot \vec{A}} \qquad \cos \alpha' = \frac{\vec{B} \cdot \vec{C}}{|B||C|}$$

$$|B| = \sqrt{\vec{B} \cdot \vec{B}} \qquad \cos \beta' = \frac{\vec{A} \cdot \vec{C}}{|A||C|}$$

$$|C| = \sqrt{\vec{C} \cdot \vec{C}} \qquad \cos \gamma' = \frac{\vec{A} \cdot \vec{B}}{|A||B|}$$

where

$$\vec{A}\cdot\vec{A} = (n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c})\cdot(n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c})$$
$$\vec{B}\cdot\vec{B} = (n_{21}\vec{a} + n_{22}\vec{b} + n_{23}\vec{c})\cdot(n_{21}\vec{a} + n_{22}\vec{b} + n_{23}\vec{c})$$
$$\vec{C}\cdot\vec{C} = (n_{31}\vec{a} + n_{32}\vec{b} + n_{33}\vec{c})\cdot(n_{31}\vec{a} + n_{32}\vec{b} + n_{33}\vec{c})$$

$$\vec{A}\cdot\vec{B} = (n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c})\cdot(n_{21}\vec{a} + n_{22}\vec{b} + n_{23}\vec{c})$$
$$\vec{B}\cdot\vec{C} = (n_{21}\vec{a} + n_{22}\vec{b} + n_{23}\vec{c})\cdot(n_{31}\vec{a} + n_{32}\vec{b} + n_{33}\vec{c})$$
$$\vec{C}\cdot\vec{A} = (n_{31}\vec{a} + n_{32}\vec{b} + n_{33}\vec{c})\cdot(n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c}) .$$

In expanded form A· B becomes

$$\begin{aligned}\vec{A}\cdot\vec{B} &= (n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c})\cdot(n_{21}\vec{a} + n_{22}\vec{b} + n_{23}\vec{c}) \\ &= (n_{11}\vec{a}\cdot n_{21}\vec{a} + n_{11}\vec{a}\cdot n_{22}\vec{b} + n_{11}\vec{a}\cdot n_{23}\vec{c} \\ &\quad + n_{12}\vec{b}\cdot n_{21}\vec{a} + n_{12}\vec{b}\cdot n_{22}\vec{b} + n_{12}\vec{b}\cdot n_{23}\vec{c} \\ &\quad + n_{13}\vec{c}\cdot n_{21}\vec{a} + n_{13}\vec{c}\cdot n_{22}\vec{b} + n_{13}\vec{c}\cdot n_{23}\vec{c} \\ &= (n_{11}n_{21})a^2 + (n_{12}n_{22})b^2 + (n_{13}n_{23})c^2 \\ &\quad + (n_{12}n_{23} + n_{13}n_{22})\, b\, c\cos\alpha \\ &\quad + (n_{11}n_{23} + n_{13}n_{21})\, a\, c\cos\beta \\ &\quad + (n_{11}n_{22} + n_{12}n_{21})\, a\, b\cos\gamma\end{aligned}$$

When $\vec{A} = \vec{B}$ this reduces to

$$\vec{A}\cdot\vec{A} = (n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c})\cdot(n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c})$$

$$= (n_{11}a)^2 + (n_{12}b)^2 + (n_{13}c)^2$$

$$+ 2n_{12}n_{13}b\,c\cos\alpha$$

$$+ 2n_{11}n_{13}a\,c\cos\beta$$

$$+ 2n_{11}n_{12}a\,b\cos\gamma$$

The other dot products may be similarly obtained.

The following example illustrates the use of these expressions.

Example

Consider the following axial transformation in a direct lattice:

$$\begin{pmatrix} \vec{A} \\ \vec{B} \\ \vec{C} \end{pmatrix}_{\text{new}} = \begin{pmatrix} \bar{1} & 1 & 0 \\ \bar{2} & 6 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}_{\text{old}}$$

The lattice parameters in the original cell are a = 5.40, b = 7.54, c = 51.8 Å., $\alpha = 145°38'$, $\beta = 105°42'$, $\gamma = 60°18'$. Calculate the parameters A, B, C, $\alpha'$, $\beta'$, $\gamma'$ in the new cell.

$$|A| = \sqrt{\vec{A}\cdot\vec{A}} = \sqrt{(-\vec{a}+\vec{b})\cdot(-\vec{a}+\vec{b})}$$

$$|B| = \sqrt{\vec{B}\cdot\vec{B}} = \sqrt{(-2\vec{a}+6\vec{b}+\vec{c})\cdot(-2\vec{a}+6\vec{b}+\vec{c})}$$

$$|C| = \sqrt{\vec{C}\cdot\vec{C}} = \sqrt{\vec{a}\cdot\vec{a}}$$

$$\cos\alpha' = \frac{\vec{B}\cdot\vec{C}}{|B||C|} = \frac{(-2\vec{a}+6\vec{b}+\vec{c})\cdot\vec{a}}{|B||C|}$$

$$\cos\beta' = \frac{\vec{C}\cdot\vec{A}}{|C||A|} = \frac{\vec{a}\cdot(-\vec{a}+\vec{b})}{|C||A|}$$

$$\cos\gamma' = \frac{\vec{A}\cdot\vec{B}}{|A||B|} = \frac{(-\vec{a}+\vec{b})\cdot(-2\vec{a}+6\vec{b}+\vec{c})}{|A||B|}$$

The length of the A-axis is

$$A^2 = \vec{A}\cdot\vec{A} = (-\vec{a}+\vec{b})\cdot(-\vec{a}+\vec{b})$$

$$= (-\vec{a})\cdot(-\vec{a}) + 2\,\vec{a}\cdot\vec{b} + \vec{b}\cdot\vec{b}$$

$$= a^2 + 2ab\cos\gamma + b^2$$

$$= (5.40)^2 - 2(5.40)(7.54)\cos 60°18' + (7.54)^2$$

$$= 45.67,$$

$$A = \sqrt{45.67} = 6.76\ \text{Å},$$

and similarly $B = 28.2$ Å,

$C = 5.40$ Å.

The magnitude of the angle $\alpha$ is

$$\cos\alpha = \frac{\vec{B}\cdot\vec{C}}{|B||C|} = \frac{(-2\vec{a}+6\vec{b}+\vec{c})\cdot\vec{a}}{|B||C|} = \frac{-2\vec{a}\cdot\vec{a}+6\vec{b}\cdot\vec{a}+\vec{c}\cdot\vec{a}}{|B||C|}$$

$$= \frac{-2a^2 + 6ab\cos\gamma + ac\cos\beta}{|B||C|}$$

$$= \frac{-2(5.40)^2 + 6(5.40)(7.54)\cos 60°18' + (5.40)(51.8)\cos 105°42'}{(28.2)(5.40)}$$

$$= -0.08529,$$

$$\alpha = \cos^{-1}(-0.08529) = 94°\ 54',$$

and similarly $\beta = 104°\ 16'$,

$\gamma = 92°\ 36'$.

## APPENDIX V. THE INVERSE TRANSFORMATION

Suppose a cell with axes a, b, c is transformed to a new cell with axes A, B, C. The vectorial transformation of these axes in direct space is given in the usual way by the following set of equations:

$$\vec{A} = n_{11}\vec{a} + n_{12}\vec{b} + n_{13}\vec{c}$$

$$\vec{B} = n_{21}\vec{a} + n_{22}\vec{b} + n_{23}\vec{c}$$

$$\vec{C} = n_{31}\vec{a} + n_{32}\vec{b} + n_{33}\vec{c} \quad .$$

The matrix for this transformation is

$$N = \begin{Vmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{Vmatrix} \quad .$$

The inverse transformation $N^{-1}$, corresponding to the transformation of the new cell back to the original cell, is then

$$N^{-1} = \begin{Vmatrix} \dfrac{\begin{vmatrix} n_{22} & n_{23} \\ n_{32} & n_{33} \end{vmatrix}}{\Delta} & -\dfrac{\begin{vmatrix} n_{12} & n_{13} \\ n_{32} & n_{33} \end{vmatrix}}{\Delta} & \dfrac{\begin{vmatrix} n_{12} & n_{13} \\ n_{22} & n_{23} \end{vmatrix}}{\Delta} \\ -\dfrac{\begin{vmatrix} n_{21} & n_{23} \\ n_{31} & n_{33} \end{vmatrix}}{\Delta} & \dfrac{\begin{vmatrix} n_{11} & n_{13} \\ n_{31} & n_{33} \end{vmatrix}}{\Delta} & -\dfrac{\begin{vmatrix} n_{11} & n_{13} \\ n_{21} & n_{23} \end{vmatrix}}{\Delta} \\ \dfrac{\begin{vmatrix} n_{21} & n_{22} \\ n_{31} & n_{32} \end{vmatrix}}{\Delta} & -\dfrac{\begin{vmatrix} n_{11} & n_{12} \\ n_{31} & n_{32} \end{vmatrix}}{\Delta} & \dfrac{\begin{vmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{vmatrix}}{\Delta} \end{Vmatrix} \quad .$$

where $\Delta$ is the determinant of the original transformation matrix:

$$\Delta = \begin{vmatrix} n_{11} & n_{12} & n_{13} \\ n_{21} & n_{22} & n_{23} \\ n_{31} & n_{32} & n_{33} \end{vmatrix} .$$

The derivation of the inverse, $N^{-1}$, in actual practice may be carried out in a four step procedure. Starting with the original matrix, N, each element $n_{ij}$ is first replaced by its minor. The minor of $n_{ij}$ is the array of order one less than the original array and corresponds to the array of elements left after striking out row i and column j. Thus, the minor of $n_{11}$ is

$$\begin{vmatrix} n_{22} & n_{23} \\ n_{32} & n_{33} \end{vmatrix}$$

etc. Second, a sign is attached to each minor to convert it to a cofactor, $q_{ij}$, the sign being $(-1)^{i+j}$. Third, the transpose is formed, which simply involves the exchange of each cofactor $q_{ij}$ for $q_{ji}$. The result at this stage is a matrix known as the adjoint of N. Finally, each transposed cofactor--that is, each element in the adjoint--is now divided by the determinant of the original matrix. The final result is the inverse matrix $N^{-1}$.

Example.

Consider the following axial transformation in direct space and its corresponding matrix, N:

$$\begin{aligned} \vec{A} &= -\vec{a} + \vec{b} \\ \vec{B} &= -2\vec{a} + \vec{b} + \vec{c}\,, \\ \vec{C} &= \vec{a} \qquad\quad + \vec{c} \end{aligned} \qquad \text{matrix: } N = \begin{Vmatrix} \bar{1} & 1 & 0 \\ \bar{2} & 1 & 1 \\ 1 & 0 & 1 \end{Vmatrix}$$

It is desired to solve for the inverse transformation, $N^{-1}$, to express the vectors $\vec{a}$, $\vec{b}$, $\vec{c}$ in terms of $\vec{A}$, $\vec{B}$, $\vec{C}$.

Solution. The determinant of this matrix is

$$\Delta = \begin{vmatrix} \bar{1} & 1 & 0 \\ \bar{2} & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix} = \bar{1}\begin{vmatrix} 1 & 1 \\ 0 & 1 \end{vmatrix} - 1\begin{vmatrix} \bar{2} & 1 \\ 1 & 1 \end{vmatrix} + 0\begin{vmatrix} \bar{2} & 1 \\ 1 & 0 \end{vmatrix}$$

$$= -1\,(1 - 0) - 1\,(-2 - 1) + 0(0 - 1)$$

$$= -1 + 3 = 2 \quad .$$

Proceeding by the stepwise process, writing down first the cofactors (minors plus their sign), we have

$$\begin{Vmatrix} \begin{vmatrix} 1 & 1 \\ 0 & 1 \end{vmatrix} & -\begin{vmatrix} \bar{2} & 1 \\ 1 & 1 \end{vmatrix} & \begin{vmatrix} \bar{2} & 1 \\ 1 & 0 \end{vmatrix} \\ -\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} & \begin{vmatrix} \bar{1} & 0 \\ 1 & 1 \end{vmatrix} & -\begin{vmatrix} \bar{1} & 1 \\ 1 & 0 \end{vmatrix} \\ \begin{vmatrix} 1 & 0 \\ 1 & 1 \end{vmatrix} & -\begin{vmatrix} \bar{1} & 0 \\ \bar{2} & 1 \end{vmatrix} & \begin{vmatrix} \bar{1} & 1 \\ \bar{2} & 1 \end{vmatrix} \end{Vmatrix} = \begin{Vmatrix} 1 & 3 & \bar{1} \\ \bar{1} & \bar{1} & 1 \\ 1 & 1 & 1 \end{Vmatrix}$$

$$\Big\downarrow \text{ transpose}$$

$$N^{-1} = \begin{Vmatrix} \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{3}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{Vmatrix} \xleftarrow[\text{by } \Delta]{\text{divide each element}} \begin{Vmatrix} 1 & \bar{1} & 1 \\ 3 & \bar{1} & 1 \\ \bar{1} & 1 & 1 \end{Vmatrix}$$

Hence, the transformation in real space of the cell with axes A, B, C back to the original cell with axes a, b, c is

$$\vec{a} = \tfrac{1}{2}\vec{A} - \tfrac{1}{2}\vec{B} + \tfrac{1}{2}\vec{C}$$

$$\vec{b} = \tfrac{3}{2}\vec{A} - \tfrac{1}{2}\vec{B} + \tfrac{1}{2}\vec{C}$$

$$\vec{c} = -\tfrac{1}{2}\vec{A} + \tfrac{1}{2}\vec{B} + \tfrac{1}{2}\vec{C} \quad .$$

# APPENDIX VI. TWO OR MORE TRANSFORMATIONS IN SEQUENCE-(MATRIX MULTIPLICATION)

If the vectorial transformation from cell 1 to cell 2 is known and that from cell 2 to cell 3 is known, it is sometimes desirable to know the transformation from cell 1 to cell 3. In general, if the transformation matrix from one cell to the next for n cells in succession is known, the matrix for the transformation of the original cell to the nth cell may be found by the method known as matrix multiplication.

The method of matrix multiplication proceeds as follows: Let D represent the matrix for the transformation from cell 1 to cell 2, E the matrix for cell 2 to cell 3, F the matrix for cell 3 to cell 4, etc., and N the matrix for the transformation of cell (n-1) to cell n. The matrix, Q, for the transformation of cell 1 to cell n is then given by

$$Q = N \ldots H G F E D .$$

Each matrix is left multiplied by the next matrix in succession; they are non-commutative. This relationship states that first matrix D is left multiplied by E to yield a new matrix, U, which corresponds to the transformation of cell 1 to cell 3; that is, $U = E D$. Then U is left multiplied by F to yield the matrix V corresponding to the transformation from cell 1 to cell 4; that is, $V = F U = F (E D)$. Proceeding in an analogous manner until all the matrices have been accounted for, the matrix Q becomes the matrix for the transformation of cell 1 to cell n. This is summarized as follows:

cell 1 to cell 3 $\quad U = ED$

cell 1 to cell 4 $\quad V = FU = F(ED)$

cell 1 to cell 5 $\quad W = GV = G(FED)$

cell 1 to cell 6 $\quad X = HW = H(GFED)$

.

.

cell 1 to cell n $\quad Q = N(N\text{-}1 \ldots HGFED)$ .

The actual multiplication of two matrices occurs in a row by column manner; that is, each element of the row in the lefthand matrix is multiplied into the corresponding element of the column in the right-hand matrix and then the products are summed. For the product of the two matrices ED in that order where the elements in matrix $D = [d_{ij}]$ and in matrix $E = [e_{ij}]$, the elements in matrix F become $F = [f_{ij}]$, where

$$f_{ij} = e_{i1}d_{1j} + e_{i2}d_{2j} + \ldots + e_{ip}d_{pj} = \sum_{k=1}^{p} e_{ik}d_{kj}$$

($i = 1, 2, \ldots, m$; $j = 1, 2, \ldots, n$ in an $m$ x $n$ matrix).

In three-dimensional lattice transformations 3 x 3 matrices are used and are thus said to be conformable, that is, the number of columns in D is equal to the number of rows in E, a strict requirement for matrix multiplication.

The following example illustrates the method of multiplying two 3 x 3 matrices together.

Example

cell 1 → cell 2

$$\begin{pmatrix} \vec{A} \\ \vec{B} \\ \vec{C} \end{pmatrix} = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}$$

cell 2 → cell 3

$$\begin{pmatrix} \vec{A}' \\ \vec{B}' \\ \vec{C}' \end{pmatrix} = \begin{pmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{pmatrix} \begin{pmatrix} \vec{A} \\ \vec{B} \\ \vec{C} \end{pmatrix}$$

cell 1 → cell 3

$$\begin{pmatrix} \vec{A}' \\ \vec{B}' \\ \vec{C}' \end{pmatrix} = \begin{pmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{pmatrix} \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ u_{21} & u_{22} & u_{23} \\ u_{31} & u_{32} & u_{33} \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}$$

By matrix multiplication this reduces to

$$\begin{pmatrix} \vec{A}' \\ \vec{B}' \\ \vec{C}' \end{pmatrix} = \begin{pmatrix} w_{11}u_{11} + w_{12}u_{21} + w_{13}u_{31}, & w_{11}u_{12} + w_{12}u_{22} + w_{13}u_{32}, & w_{11}u_{13} + w_{12}u_{23} + w_{13}u_{33} \\ w_{21}u_{11} + w_{22}u_{21} + w_{23}u_{31}, & w_{21}u_{12} + w_{22}u_{22} + w_{23}u_{32}, & w_{21}u_{13} + w_{22}u_{23} + w_{23}u_{33} \\ w_{31}u_{11} + w_{32}u_{21} + w_{33}u_{31}, & w_{31}u_{12} + w_{32}u_{22} + w_{33}u_{32}, & w_{31}u_{13} + w_{32}u_{23} + w_{23}u_{33} \end{pmatrix} \begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{c} \end{pmatrix}$$

# APPENDIX VII.

## THE TABULATED TRANSFORMATION OF LATTICES WITH CHANGE OF AXES, LATTICE TYPE AND SPACE GROUP

As pointed out in Appendix I there are only fourteen Bravais Lattices. Associated with these fourteen there are 230 space groups. But as is shown in Table 5, page 154, other types of centering are also possible, though not unique from the basic fourteen, simply by a change in the orientation of the cell brought about by a change in one or more of the axes defining the system. Consequently, these non-unique lattice types then give rise to the numerous non-standard space groups, which may be found in Appendix VIII.

It is often standard practice to convert cells with non-standard space group symbols to their conventional orientations for at least one of two major reasons: conversion or reduction of lattice types to the standard Bravais lattices (e. g., body-centered monoclinic to C-centered monoclinic, b-unique) or conversion of symmetry elements to alternate orientations (e. g., n-glide to c-glide in the monoclinic system). In order that each or both changes may be made, it is necessary that a change be made in the axes defining the cell. Just exactly what changes are made, of course, depends upon the crystal system involved. To facilitate routine work in such conversions the space group transformations for the triclinic and monoclinic systems have been worked out and appear on the following pages. Also included is the frequently used rhombohedral - hexagonal transformation.

In the triclinic system the five lattice transformations are given for reduction to the "primitive" Bravais lattice. In the case of the three end-centered cells, two have been given for each: that appearing on the left corresponds to a change in magnitude of one axis only, that on the right to a change in two axes. The latter has been included for each of these cases for routine work in cell reductions discussed in Chapter III.

In the monoclinic system both the first setting (c-unique) and second setting (b-unique) are given. Related series of space group transformations are divided according as $b < a$, $a < b$ (c-unique) and $c < a$, $a < c$ (b-unique). In some cases the transformations are the same, in others they are different, a fact which can be verified upon inspection of the corresponding figures. As is shown in Table 7, which is to be used only in conjunction with the transformations appearing on pages 177 through 190, the new $\gamma$ or $\beta$ will increase or decrease depending upon the ratio of the two original axes and the angle between them. In no case should it ever change character, that is, its cosine change sign, a situation occurring only if the scalar product of the two original non-unique axes is greater in absolute value than the square of the shorter original non-unique axis (see Table 7). When this happens the monoclinic cell is capable of being reduced until the new angle is less than the original angle and both are obtuse.

Finally, it may be pointed out that in the monoclinic system the unique end-centered cells for c-unique are A and B and for b-unique A and C. By convention the C-centered cell is taken as unique for the

second setting. The corresponding cell for the first setting, c-unique, would be an A-centered cell if the axes were simply permuted thusly: $b \rightarrow c$, $c \rightarrow a$, $a \rightarrow b$. However, an A-centered cell is common to both settings. So as to distinguish between the two settings when reporting the lattice type, the B-centered cell has been accepted as standard for the first setting and may be obtained directly from the second setting by setting $a = a$, $b \rightarrow c$, and $c \rightarrow -b$; that is

b-unique to c-unique

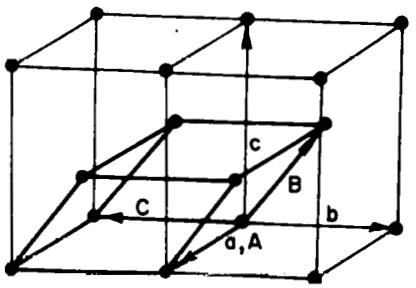
$$\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{Vmatrix}$$

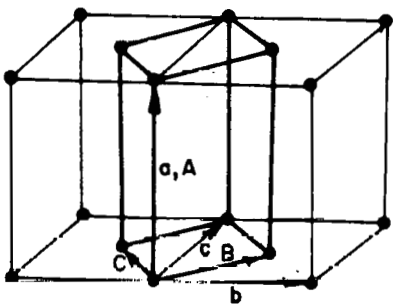
and

c-unique to b-unique

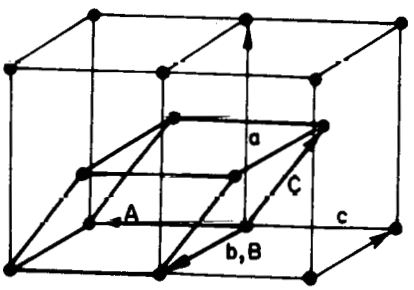
$$\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{Vmatrix} .$$

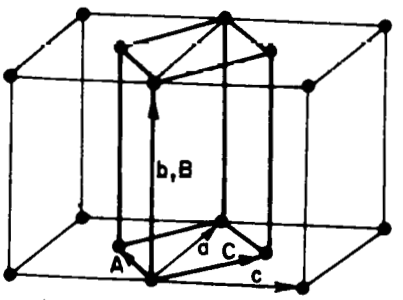
# TRICLINIC



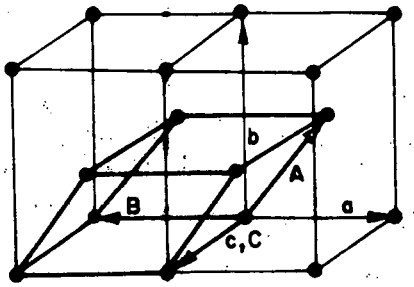

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & \bar{1} & 0 \end{pmatrix} \quad A \longrightarrow P \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$



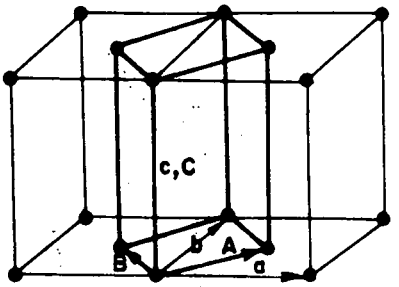

$$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \quad B \longrightarrow P \quad \begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$$

Fig. 18. The five triclinic lattice transformations.

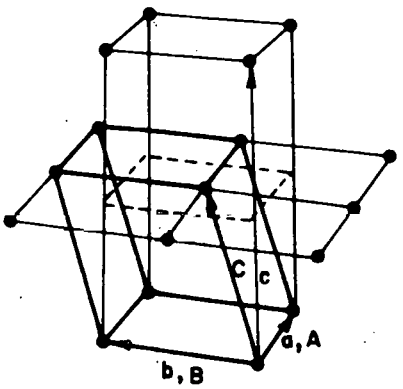



$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$C \longrightarrow P$

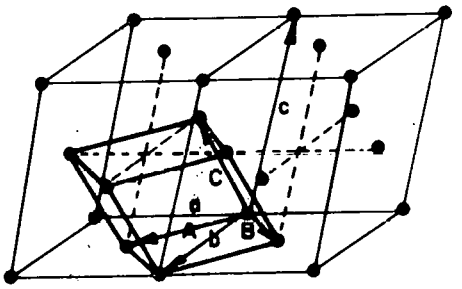



$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$




$I \longrightarrow P$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$




$F \longrightarrow P$

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$$

Fig. 18 (continued).

TABLE 7. The Change in the Monoclinic Angle With Change in Cell Orientation*

MONOCLINIC

1st Setting - Unique Axis c

| | | |
|---|---|---|
| a < b | $0 \leq \lvert a \cdot b \rvert < \frac{1}{2}a^2$ | $\gamma_{new} > \gamma_{old}$ |
| | $\lvert a \cdot b \rvert = \frac{1}{2}a^2$ | $\gamma_{new} = \gamma_{old}$ |
| | $\frac{1}{2}a^2 < \lvert a \cdot b \rvert < a^2$ | $\gamma_{new} < \gamma_{old}$ |
| | $\lvert a \cdot b \rvert = a^2$ | $\gamma_{new} = 90°$ |
| | $a^2 < \lvert a \cdot b \rvert$ | $\gamma$ changes character |
| b < a | $0 \leq \lvert a \cdot b \rvert < \frac{1}{2}b^2$ | $\gamma_{new} > \gamma_{old}$ |
| | $\lvert a \cdot b \rvert = \frac{1}{2}b^2$ | $\gamma_{new} = \gamma_{old}$ |
| | $\frac{1}{2}b^2 < \lvert a \cdot b \rvert < b^2$ | $\gamma_{new} < \gamma_{old}$ |
| | $\lvert a \cdot b \rvert = b^2$ | $\gamma_{new} = 90°$ |
| | $b^2 < \lvert a \cdot b \rvert$ | $\gamma$ changes character |

2nd Setting - Unique Axis b

| | | |
|---|---|---|
| a < c | $0 \leq \lvert a \cdot c \rvert < \frac{1}{2}a^2$ | $\beta_{new} > \beta_{old}$ |
| | $\lvert a \cdot c \rvert = \frac{1}{2}a^2$ | $\beta_{new} = \beta_{old}$ |
| | $\frac{1}{2}a^2 < \lvert a \cdot c \rvert < a^2$ | $\beta_{new} < \beta_{old}$ |
| | $\lvert a \cdot c \rvert = a^2$ | $\beta_{new} = 90°$ |
| | $a^2 < \lvert a \cdot c \rvert$ | $\beta$ changes character |
| c < a | $0 \leq \lvert a \cdot c \rvert < \frac{1}{2}c^2$ | $\beta_{new} > \beta_{old}$ |
| | $\lvert a \cdot c \rvert = \frac{1}{2}c^2$ | $\beta_{new} = \beta_{old}$ |
| | $\frac{1}{2}c^2 < \lvert a \cdot c \rvert < c^2$ | $\beta_{new} < \beta_{old}$ |
| | $\lvert a \cdot c \rvert = c^2$ | $\beta_{new} = 90°$ |
| | $a^2 < \lvert a \cdot c \rvert$ | $\beta$ changes character |

*The cell edges a, b, c correspond to the edges in the "original" cell.

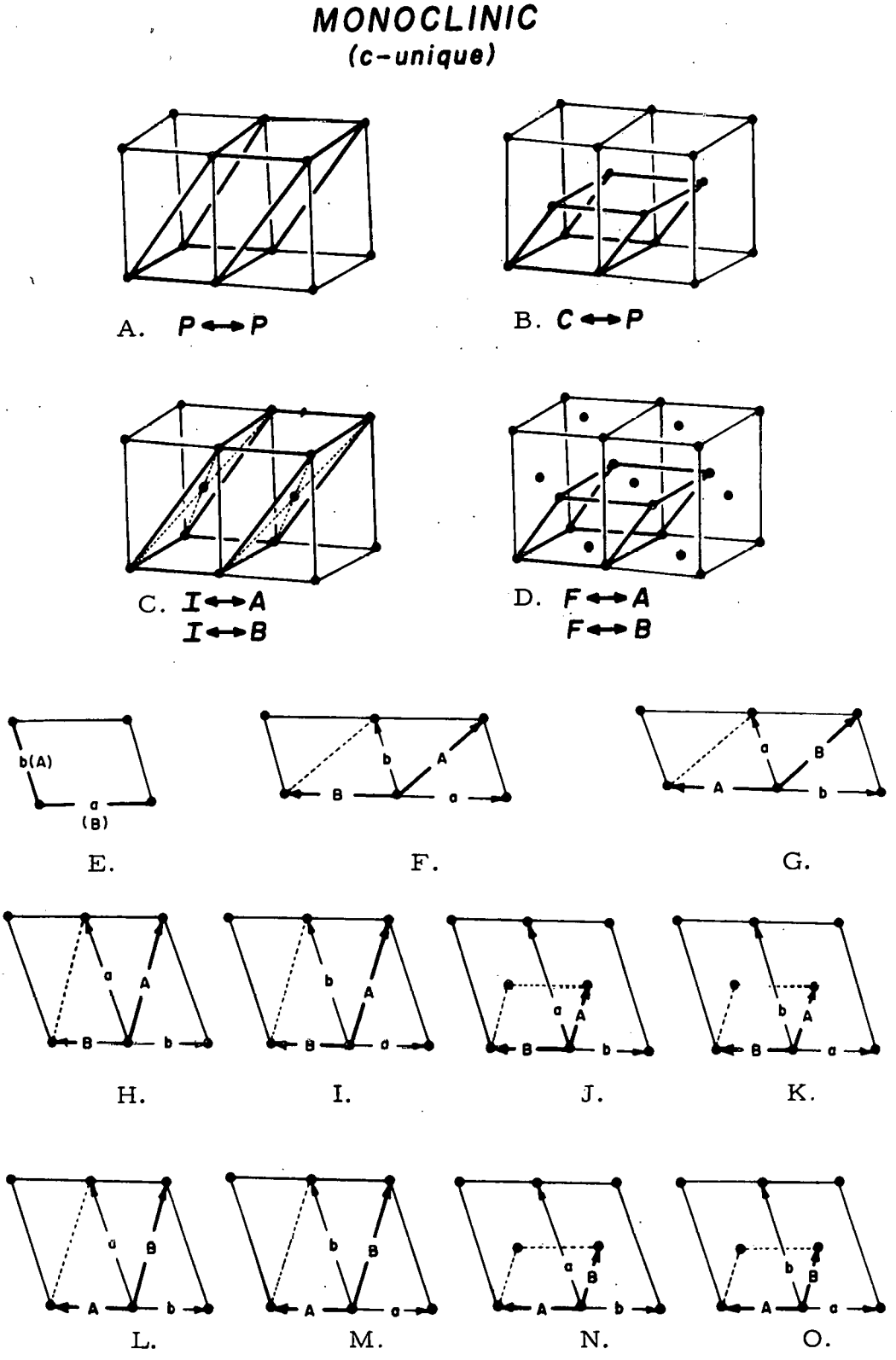



Fig. 19. The vectorial transformation of axes accompanying Monoclinic space group transformations (1st setting).

Table 8. The Monoclinic space group transformations (1st setting).

$P \longrightarrow P$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| $Pa \longrightarrow Pb$<br>$P2/a \longrightarrow P2/b$<br>$P2_1/a \longrightarrow P2_1/b$ | b < a<br>a < b | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$ | E |
| $Pb \longrightarrow Pa$<br>$P2/b \longrightarrow P2/a$<br>$P2_1/b \longrightarrow P2_1/a$ | b < a<br>a < b | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & \bar{1} & 0 \end{pmatrix}$ | E |
| $Pn \longrightarrow Pb$<br>$P2/n \longrightarrow P2/b$<br>$P2_1/n \longrightarrow P2_1/b$ | b < a | $\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | L |
| | a < b | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | M |
| $Pn \longrightarrow Pa$<br>$P2/n \longrightarrow P2/a$<br>$P2_1/n \longrightarrow P2_1/a$ | b < a | $\begin{pmatrix} 1 & 1 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | H |
| | a < b | $\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | I |

Table 8. (cont.). $C \longrightarrow P$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| $C2 \longrightarrow P2$<br>$C2_1 \longrightarrow P2_1$<br>$Cm \longrightarrow Pm$<br>$C2/m \longrightarrow P2/m$<br>$C2_1/m \longrightarrow P2_1/m$ | b < a | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | J |
| | | $\begin{pmatrix} 0 & \bar{1} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | N |
| | a < b | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | K |
| | | $\begin{pmatrix} \bar{1} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |
| $C2/b \longrightarrow P2/b$<br>$C2_1/b \longrightarrow P2_1/b$ | b < a<br>a < b | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | J |
| $C2/a \longrightarrow P2/a$<br>$C2_1/a \longrightarrow P2_1/a$ | b < a<br>a < b | $\begin{pmatrix} \bar{1} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |
| $Ca \longrightarrow Pb$<br>$C2/a \longrightarrow P2/b$<br>$C2_1/a \longrightarrow P2_1/b$ | b < a<br>a < b | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | K |
| $Cc \longrightarrow Pa$<br>$C2/c \longrightarrow P2/a$<br>$C2_1/c \longrightarrow P2_1/a$ | b < a<br>a < b | $\begin{pmatrix} 0 & \bar{1} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | N |

Table 8. (cont.). $C \longrightarrow P$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| $Cd \longrightarrow Pb$<br>$C2/d \longrightarrow P2/b$<br>$C2_1/d \longrightarrow P2_1/b$ | b < a | $\begin{pmatrix} 0 & \bar{1} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | N |
| | a < b | $\begin{pmatrix} \bar{1} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |
| $Cd \longrightarrow Pa$<br>$C2/d \longrightarrow P2/a$<br>$C2_1/d \longrightarrow P2_1/a$ | b < a | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | J |
| | a < b | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | K |

$A \longrightarrow B$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| $A2 \longrightarrow B2$<br>$Am \longrightarrow Bm$<br>$A2/m \longrightarrow B2/m$ | b < a<br>a < b | $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | E |
| $Aa \longrightarrow Bb$<br>$A2/a \longrightarrow B2/b$ | b < a<br>a < b | $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | E |

Table 8. (cont.). $B \longrightarrow A$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| $B2 \longrightarrow A2$<br>$Bm \longrightarrow Am$<br>$B2/m \longrightarrow A2/m$ | b < a<br>a < b | $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | E |
| $Bb \longrightarrow Aa$<br>$B2/b \longrightarrow A2/a$ | b < a<br>a < b | $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | E |

$I \longrightarrow B$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| $I2 \longrightarrow B2$<br>$Im \longrightarrow Bm$<br>$I2/m \longrightarrow B2/m$ | b < a | $\begin{pmatrix} 1 & \bar{1} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | H |
| | a < b | $\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | I |
| $Ia \longrightarrow Bb$<br>$I2/a \longrightarrow B2/b$ | b < a | $\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | F |
| | a < b | $\begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | I |

Table 8. (cont.). $I \longrightarrow A$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| *I2* ⟶ *A2*<br>*Im* ⟶ *Am*<br>*I2/m* ⟶ *A2/m* | b < a | $\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | L |
| | a < b | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | M |
| *Ib* ⟶ *Aa*<br>*I2/b* ⟶ *A2/a* | b < a | $\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | L |
| | a < b | $\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | G |

$F \longrightarrow B$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| *F2* ⟶ *B2*<br>*Fm* ⟶ *Bm*<br>*F2/m* ⟶ *B2/m*<br>*Fd* ⟶ *Bb*<br>*F2/d* ⟶ *B2/b* | b < a | $\begin{pmatrix} 0 & \bar{1} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | N |
| | a < b | $\begin{pmatrix} \bar{1} & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |

Table 8. (cont.). $F \longrightarrow A$

| Space group transformation | Original axes | Transformation matrix | Fig. 19 |
|---|---|---|---|
| $F2 \longrightarrow A2$<br>$Fm \longrightarrow Am$<br>$F2/m \longrightarrow A2/m$<br>$Fd \longrightarrow Aa$<br>$F2/d \longrightarrow A2/a$ | b < a | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | J |
| | a < b | $\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ | K |

# MONOCLINIC
## (b-unique)

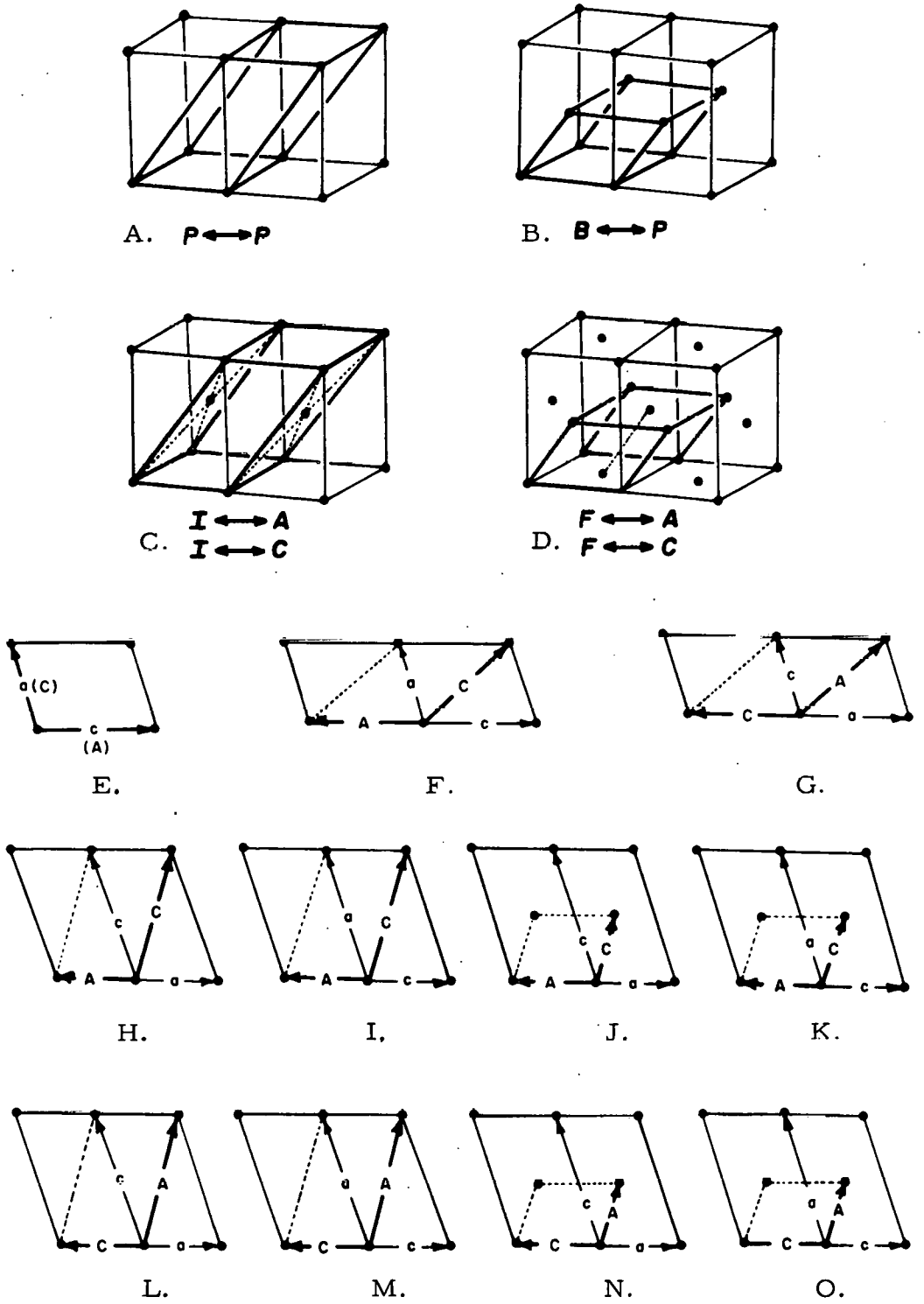



Fig. 20. The vectorial transformation of axes accompanying Monoclinic space group transformations (2nd setting).

Table 9. The Monoclinic space group transformations (2nd setting).

$P \longrightarrow P$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $Pc \longrightarrow Pa$<br>$P2/c \longrightarrow P2/a$<br>$P2_1/c \longrightarrow P2_1/a$ | a < c<br>c < a | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$ | E |
| $Pa \longrightarrow Pc$<br>$P2/a \longrightarrow P2/c$<br>$P2_1/a \longrightarrow P2_1/c$ | a < c<br>c < a | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$ | E |
| $Pn \longrightarrow Pa$<br>$P2/n \longrightarrow P2/a$<br>$P2_1/n \longrightarrow P2_1/a$ | a < c | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | L |
| | c < a | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | M |
| $Pn \longrightarrow Pc$<br>$P2/n \longrightarrow P2/c$<br>$P2_1/n \longrightarrow P2_1/c$ | a < c | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 1 \end{pmatrix}$ | H |
| | c < a | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$ | I |

Table 9. (cont.). $B \longrightarrow P$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $B2 \longrightarrow P2$<br>$B2_1 \longrightarrow P2_1$<br>$Bm \longrightarrow Pm$<br>$B2/m \longrightarrow P2/m$<br>$B2_1/m \longrightarrow P2_1/m$ | a < c | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | J |
| | | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | N |
| | c < a | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | K |
| | | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |
| $B2/a \longrightarrow P2/a$<br>$B2_1/a \longrightarrow P2_1/a$ | a < c<br>c < a | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | J |
| $B2/c \longrightarrow P2/c$<br>$B2_1/c \longrightarrow P2_1/c$ | a < c<br>c < a | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |
| $Bc \longrightarrow Pa$<br>$B2/c \longrightarrow P2/a$<br>$B2_1/c \longrightarrow P2_1/a$ | a < c<br>c < a | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | K |
| $Ba \longrightarrow Pc$<br>$B2/a \longrightarrow P2/c$<br>$B2_1/a \longrightarrow P2_1/c$ | a < c<br>c < a | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | N |

Table 9. (cont.). $B \longrightarrow P$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $Bd \longrightarrow Pa$<br>$B2/d \longrightarrow P2/a$<br>$B2_1/d \longrightarrow P2_1/a$ | a < c | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | N |
| | c < a | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |
| $Bd \longrightarrow Pc$<br>$B2/d \longrightarrow P2/c$<br>$B2_1/d \longrightarrow P2_1/c$ | a < c | $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | J |
| | c < a | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | K |

$C \longrightarrow A$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $C2 \longrightarrow A2$<br>$Cm \longrightarrow Am$<br>$C2/m \longrightarrow A2/m$ | a < c<br>c < a | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$ | E |
| $Cc \longrightarrow Aa$<br>$C2/c \longrightarrow A2/a$ | a < c<br>c < a | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$ | E |

Table 9. (cont.). $A \longrightarrow C$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $A2 \longrightarrow C2$<br>$Am \longrightarrow Cm$<br>$A2/m \longrightarrow C2/m$ | a < c<br>c < a | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$ | E |
| $Aa \longrightarrow Cc$<br>$A2/a \longrightarrow C2/c$ | a < c<br>c < a | $\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$ | E |

$I \longrightarrow A$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $I2 \longrightarrow A2$<br>$Im \longrightarrow Am$<br>$I2/m \longrightarrow A2/m$ | a < c | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 1 \end{pmatrix}$ | H |
| | c < a | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$ | I |
| $Ic \longrightarrow Aa$<br>$I2/c \longrightarrow A2/a$ | a < c | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$ | F |
| | c < a | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$ | I |

Table 9. (cont.). $I \longrightarrow C$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $I2 \longrightarrow C2$<br>$Im \longrightarrow Cm$<br>$I2/m \longrightarrow C2/m$ | a < c | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | L |
| | c < a | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | M |
| $Ia \longrightarrow Cc$<br>$I2/a \longrightarrow C2/c$ | a < c | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | L |
| | c < a | $\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | G |

$F \longrightarrow A$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $F2 \longrightarrow A2$<br>$Fm \longrightarrow Am$<br>$F2/m \longrightarrow A2/m$<br>$Fd \longrightarrow Aa$<br>$F2/d \longrightarrow A2/a$ | a < c | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$ | N |
| | c < a | $\begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$ | O |

Table 9. (cont.). $F \longrightarrow C$

| Space group transformation | Original axes | Transformation matrix | Fig. 20 |
|---|---|---|---|
| $F2 \longrightarrow C2$<br>$Fm \longrightarrow Cm$<br>$F2/m \longrightarrow C2/m$<br>$Fd \longrightarrow Cc$<br>$F2/d \longrightarrow C2/c$ | a < c | $\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | J |
| | c < a | $\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$ | K |

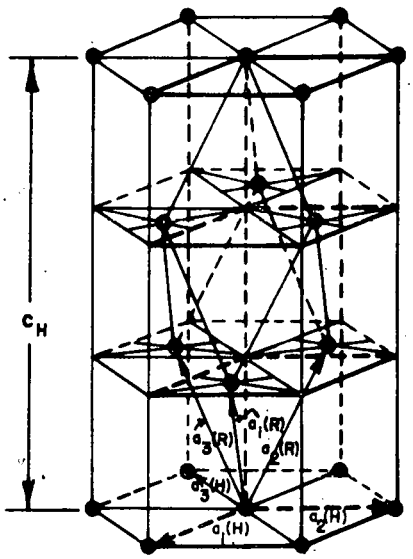



Fig. 21. A primitive rhombohedral cell referred to a hexagonal lattice[4]. The hexagonal cell is triply primitive, has a volume three times the volume of the rhombohedral cell and contains three lattice points per unit cell (at 000, $\frac{2}{3}\frac{1}{3}\frac{1}{3}$ and $\frac{1}{3}\frac{2}{3}\frac{2}{3}$).

## 1. PRIMITIVE RHOMBOHEDRAL TO TRIPLY-PRIMITIVE HEXAGONAL

Vectorial Transformation of Axes

| Hexagonal cell | | Rhombohedral cell |
|---|---|---|
| $a_1(H)$ | = | $a_1(R) - a_2(R)$ |
| $a_2(H)$ | = | $a_2(R) - a_3(R)$ |
| $c(H)$ | = | $a_1(R) + a_2(R) + a_3(R)$ |

Cell Parameters of Hexagonal Cell

$$a_H = 2a_R \sin\frac{\alpha}{2}$$

$$c_H = 3a_R\sqrt{1 - \frac{4}{3}(\sin^2\frac{\alpha}{2})}$$

$$\frac{c_H}{a_H} = \sqrt{\frac{9}{4\sin^2\frac{\alpha}{2}} - 3}$$

$$V_H = 3\,V_R = a_H^{\,2}\,c_H \sin 60^\circ$$

## 2. TRIPLY - PRIMITIVE HEXAGONAL TO PRIMITIVE RHOMBOHEDRAL

### Vectorial Transformation of Axes

Rhombohedral cell — Hexagonal cell

$$a_{1_R} = \frac{1}{3}(2a_{1_H} + a_{2_H} + c_H)$$

$$a_{2_R} = \frac{1}{3}(-a_{1_H} + a_{2_H} + c_H)$$

$$a_{3_R} = \frac{1}{3}(-a_{1_H} - 2a_{2_H} + c_H)$$

### Cell Parameters of Rhombohedral Cell

$$a_R = \frac{1}{3}\sqrt{3a_H^2 + c_H^2}$$

$$\sin\frac{\alpha}{2} = \frac{3a_H}{2\sqrt{3a_H^2 + c_H^2}} = \frac{3}{2\sqrt{3 + (\frac{c_H}{a_H})}}$$

$$V_R = \frac{1}{3} V_H = a^3 (1 + 2\cos^3\alpha - 3\cos^2\alpha)^{\frac{1}{2}}$$

$$= 2a^3 (\sin\frac{\alpha}{2} \cdot \sin\frac{3\alpha}{2})^{\frac{1}{2}} \cdot \sin\frac{\alpha}{2}$$

# Appendix VII

## THE 230 SPACE GROUPS AND THEIR ALTERNATE ORIENTATIONS

| No. | Schoenflies symbol | Standard symbol | Other orientations | | | | |
|---|---|---|---|---|---|---|---|
| Triclinic | | | | | | | |
| 1 | $C_1^1$ | P1 | A1 | B1 | C1 | I1 | F1 |
| 2 | $C_i^1$, $S_2^1$ | $P\bar{1}$ | $A\bar{1}$ | $B\bar{1}$ | $C\bar{1}$ | $I\bar{1}$ | $F\bar{1}$ |
| Monoclinic (1st setting; c-axis unique) | | | | | | | |
| 3 | $C_2^1$ | P2 | C2 | | | | |
| 4 | $C_2^2$ | $P2_1$ | $C2_1$ | | | | |
| 5 | $C_2^3$ | B2 | A2 | I2 | F2 | | |
| 6 | $C_s^1$, $C_{1h}^1$ | Pm | Cm | | | | |
| 7 | $C_s^2$, $C_{1h}^2$ | Pb | Pa | Pn | Ca | Cd | |
| 8 | $C_s^3$, $C_{1h}^3$ | Bm | Am | Im | Fm | | |
| 9 | $C_s^4$, $C_{1h}^4$ | Bb | Aa | Ia | Fd | | |
| 10 | $C_{2h}^1$ | P2/m | C2/m | | | | |
| 11 | $C_{2h}^2$ | $P2_1/m$ | $C2_1/m$ | | | | |
| 12 | $C_{2h}^3$ | B2/m | A2/m | I2/m | F2/m | | |
| 13 | $C_{2h}^4$ | P2/b | P2/a | P2/n | C2/a | C2/b | C2/d |
| 14 | $C_{2h}^5$ | $P2_1/b$ | $P2_1/a$ | $P2_1/n$ | $C2_1/a$ | $C2_1/b$ | $C2_1/d$ |
| 15 | $C_{2h}^6$ | B2/b | A2/a | I2/a | F2/d | | |

| No. | Schoenflies symbol | Standard symbol | Other orientations[a] | | | | |
|---|---|---|---|---|---|---|---|
| Monoclinic (2nd setting; b-axis unique) | | | | | | | |
| 3 | $C_2^1$ | P2 | B2 | | | | |
| 4 | $C_2^2$ | $P2_1$ | $B2_1$ | | | | |
| 5 | $C_2^3$ | C2 | A2 | I2 | F2 | | |
| 6 | $C_s^1$, $C_{1h}^1$ | Pm | Bm | | | | |
| 7 | $C_s^2$, $C_{1h}^2$ | Pc | Pa | Pn | Ba | Bd | |
| 8 | $C_s^3$, $C_{1h}^3$ | Cm | Am | Im | Fm | | |
| 9 | $C_s^4$, $C_{1h}^4$ | Cc | Aa | Ia | Fd | | |
| 10 | $C_{2h}^1$ | P2/m | B2/m | | | | |
| 11 | $C_{2h}^2$ | $P2_1/m$ | $B2_1/m$ | | | | |
| 12 | $C_{2h}^3$ | C2/m | A2/m | I2/m | F2/m | | |
| 13 | $C_{2h}^4$ | P2/c | P2/a | P2/n | B2/a | B2/c | B2/d |
| 14 | $C_{2h}^5$ | $P2_1/c$ | $P2_1/a$ | $P2_1/n$ | $B2_1/a$ | $B2_1/c$ | $B2_1/d$ |
| 15 | $C_{2h}^6$ | C2/c | A2/a | I2/a | F2/d | | |
| Orthorhombic | | | | | | | |
| 16 | $D_2^1$, $V^1$ | P222 | P222 | P222 | P222 | P222 | P222 |
| 17 | $D_2^2$, $V^2$ | $P222_1$ | $P2_122$ | $P22_12$ | $P22_12$ | $P222_1$ | $P2_122$ |
| 18 | $D_2^3$, $V^3$ | $P2_12_12$ | $P22_12_1$ | $P2_122_1$ | $P2_122_1$ | $P2_12_12$ | $P22_12_1$ |
| 19 | $D_2^4$, $V^4$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ |
| 20 | $D_2^5$, $V^5$ | $C222_1$ | $A2_122$ | $B22_12$ | $B22_12$ | $C222_1$ | $A2_122$ |
| 21 | $D_2^6$, $V^6$ | C222 | A222 | B222 | B222 | C222 | A222 |

[a]Orthorhombic: cab, bca, $a\bar{c}b$, $ba\bar{c}$, $\bar{c}ba$

| No. | Schoenflies symbol | Standard symbol | Other orientations[a] | | | | |
|---|---|---|---|---|---|---|---|
| 22 | $D_2^7$, $V^7$ | F222 | F222 | F222 | F222 | F222 | F222 |
| 23 | $D_2^8$, $V^8$ | I222 | I222 | I222 | I222 | I222 | I222 |
| 24 | $D_2^9$, $V^9$ | $I2_12_12_1$ | $I2_12_12_1$ | $I2_12_12_1$ | $I2_12_12_1$ | $I2_12_12_1$ | $I2_12_12_1$ |
| 25 | $C_{2v}^1$ | Pmm2 | P2mm | Pm2m | Pm2m | Pmm2 | P2mm |
| 26 | $C_{2v}^2$ | $Pmc2_1$ | $P2_1ma$ | $Pb2_1m$ | $Pm2_1b$ | $Pcm2_1$ | $P2_1am$ |
| 27 | $C_{2v}^3$ | Pcc2 | P2aa | Pb2b | Pb2b | Pcc2 | P2aa |
| 28 | $C_{2v}^4$ | Pma2 | P2mb | Pc2m | Pm2a | Pbm2 | P2cm |
| 29 | $C_{2v}^5$ | $Pca2_1$ | $P2_1ab$ | $Pc2_1b$ | $Pb2_1a$ | $Pbc2_1$ | $P2_1ca$ |
| 30 | $C_{2v}^6$ | Pnc2 | P2na | Pb2n | Pn2b | Pcn2 | P2an |
| 31 | $C_{2v}^7$ | $Pmn2_1$ | $P2_1mn$ | $Pn2_1m$ | $Pm2_1n$ | $Pnm2_1$ | $P2_1nm$ |
| 32 | $C_{2v}^8$ | Pba2 | P2cb | Pc2a | Pc2a | Pba2 | P2cb |
| 33 | $C_{2v}^9$ | $Pna2_1$ | $P2_1nb$ | $Pc2_1n$ | $Pn2_1a$ | $Pbn2_1$ | $P2_1cn$ |
| 34 | $C_{2v}^{10}$ | Pnn2 | P2nn | Pn2n | Pn2n | Pnn2 | P2nn |
| 35 | $C_{2v}^{11}$ | Cmm2 | A2mm | Bm2m | Bm2m | Cmm2 | A2mm |
| 36 | $C_{2v}^{12}$ | $Cmc2_1$ | $A2_1ma$ | $Bb2_1m$ | $Bm2_1b$ | $Ccm2_1$ | $A2_1am$ |
| 37 | $C_{2v}^{13}$ | Ccc2 | A2aa | Bb2b | Bb2b | Ccc2 | A2aa |
| 38 | $C_{2v}^{14}$ | Amm2 | B2mm | Cm2m | Am2m | Bmm2 | C2mm |
| 39 | $C_{2v}^{15}$ | Abm2 | B2cm | Cm2a | Ac2m | Bma2 | C2mb |
| 40 | $C_{2v}^{16}$ | Ama2 | B2mb | Cc2m | Am2a | Bbm2 | C2cm |
| 41 | $C_{2v}^{17}$ | Aba2 | B2cb | Cc2a | Ac2a | Bba2 | C2cb |
| 42 | $C_{2v}^{18}$ | Fmm2 | F2mm | Fm2m | Fm2m | Fmm2 | F2mm |
| 43 | $C_{2v}^{19}$ | Fdd2 | F2dd | Fd2d | Fd2d | Fdd2 | F2dd |
| 44 | $C_{2v}^{20}$ | Imm2 | I2mm | Im2m | Im2m | Imm2 | I2mm |

[a]Orthorhombic: cab, bca, $a\bar{c}b$, $ba\bar{c}$, $\bar{c}ba$

| No. | Schoenflies symbol | Standard symbol | Other orientations[a] | | | | |
|---|---|---|---|---|---|---|---|
| 45 | $C_{2v}^{21}$ | Iba2 | I2cb | Ic2a | Ic2a | Iba2 | I2cb |
| 46 | $C_{2v}^{22}$ | Ima2 | I2mb | Ic2m | Im2a | Ibm2 | I2cm |
| 47 | $D_{2h}^{1}$, $V_h^1$ | Pmmm | Pmmm | Pmmm | Pmmm | Pmmm | Pmmm |
| 48 | $D_{2h}^{2}$, $V_h^2$ | Pnnn | Pnnn | Pnnn | Pnnn | Pnnn | Pnnn |
| 49 | $D_{2h}^{3}$, $V_h^3$ | Pccm | Pmaa | Pbmb | Pbmb | Pccm | Pmaa |
| 50 | $D_{2h}^{4}$, $V_h^4$ | Pban | Pncb | Pcna | Pcna | Pban | Pncb |
| 51 | $D_{2h}^{5}$, $V_h^5$ | Pmma | Pbmm | Pmcm | Pmcm | Pmmb | Pcmm |
| 52 | $D_{2h}^{6}$, $V_h^6$ | Pnna | Pbnn | Pncn | Pnan | Pnnb | Pcnn |
| 53 | $D_{2h}^{7}$, $V_h^7$ | Pmna | Pbmn | Pncm | Pman | Pnmb | Pcnm |
| 54 | $D_{2h}^{8}$, $V_h^8$ | Pcca | Pbaa | Pbcb | Pbab | Pccb | Pcaa |
| 55 | $D_{2h}^{9}$, $V_h^9$ | Pbam | Pmcb | Pcma | Pcma | Pbam | Pmcb |
| 56 | $D_{2h}^{10}$, $V_h^{10}$ | Pccn | Pnaa | Pbnb | Pbnb | Pccn | Pnaa |
| 57 | $D_{2h}^{11}$, $V_h^{11}$ | Pbcm | Pmca | Pbma | Pcmb | Pcam | Pmab |
| 58 | $D_{2h}^{12}$, $V_h^{12}$ | Pnnm | Pmnn | Pnmn | Pnmn | Pnnm | Pmnn |
| 59 | $D_{2h}^{13}$, $V_h^{13}$ | Pmmn | Pnmm | Pmnm | Pmnm | Pmmn | Pnmm |
| 60 | $D_{2h}^{14}$, $V_h^{14}$ | Pbcn | Pnca | Pbna | Pcnb | Pcan | Pnab |
| 61 | $D_{2h}^{15}$, $V_h^{15}$ | Pbca | Pbca | Pbca | Pcab | Pcab | Pcab |
| 62 | $D_{2h}^{16}$, $V_h^{16}$ | Pnma | Pbnm | Pmcn | Pnam | Pmnb | Pcmn |
| 63 | $D_{2h}^{17}$, $V_h^{17}$ | Cmcm | Amma | Bbmm | Bmmb | Ccmm | Amam |
| 64 | $D_{2h}^{18}$, $V_h^{18}$ | Cmca | Abma | Bbcm | Bmab | Ccmb | Acam |
| 65 | $D_{2h}^{19}$, $V_h^{19}$ | Cmmm | Ammm | Bmmm | Bmmm | Cmmm | Ammm |
| 66 | $D_{2h}^{20}$, $V_h^{20}$ | Cccm | Amaa | Bbmb | Bbmb | Cccm | Amaa |
| 67 | $D_{2h}^{21}$, $V_h^{21}$ | Cmma | Abmm | Bmcm | Bmam | Cmmb | Acmm |

[a]Orthorhombic: cab, bca, $a\bar{c}b$, $ba\bar{c}$, $\bar{c}ba$.

| No. | Schoenflies symbol | Standard symbol | Other orientations[a,b] | | | | |
|---|---|---|---|---|---|---|---|
| 68 | $D_{2h}^{22}$, $V_h^{22}$ | Ccca | Abaa | Bbcb | Bbab | Cccb | Acaa |
| 69 | $D_{2h}^{23}$, $V_h^{23}$ | Fmmm | Fmmm | Fmmm | Fmmm | Fmmm | Fmmm |
| 70 | $D_{2h}^{24}$, $V_h^{24}$ | Fddd | Fddd | Fddd | Fddd | Fddd | Fddd |
| 71 | $D_{2h}^{25}$, $V_h^{25}$ | Immm | Immm | Immm | Immm | Immm | Immm |
| 72 | $D_{2h}^{26}$, $V_h^{26}$ | Ibam | Imcb | Icma | Icma | Ibam | Imcb |
| 73 | $D_{2h}^{27}$, $V_h^{27}$ | Ibca | Ibca | Ibca | Icab | Icab | Icab |
| 74 | $D_{2h}^{28}$, $V_h^{28}$ | Imma | Ibmm | Imcm | Imam | Immb | Icmm |
| Tetragonal | | | | | | | |
| 75 | $C_4^1$ | P4 | C4 | | | | |
| 76 | $C_4^2$ | $P4_1$ | $C4_1$ | | | | |
| 77 | $C_4^3$ | $P4_2$ | $C4_2$ | | | | |
| 78 | $C_4^4$ | $P4_3$ | $C4_3$ | | | | |
| 79 | $C_4^5$ | I4 | F4 | | | | |
| 80 | $C_4^6$ | $I4_1$ | $F4_1$ | | | | |
| 81 | $S_4^1$ | $P\bar{4}$ | $C\bar{4}$ | | | | |
| 82 | $S_4^2$ | $I\bar{4}$ | $F\bar{4}$ | | | | |
| 83 | $C_{4h}^1$ | P4/m | C4/m | | | | |
| 84 | $C_{4h}^2$ | $P4_2/m$ | $C4_2/m$ | | | | |
| 85 | $C_{4h}^3$ | P4/n | C4/a | | | | |
| 86 | $C_{4h}^4$ | $P4_2/n$ | $C4_2/a$ | | | | |

[a]Orthorhombic: cab, bca, $a\bar{c}b$, $ba\bar{c}$, $\bar{c}ba$.
[b]Tetragonal: a- and b-axes in same plane but 45° to those in the standard orientation.

| No. | Schoenflies symbol | Standard symbol | Other orientations[a] |
|---|---|---|---|
| 87 | $C_{4h}^5$ | I4/m | F4/m |
| 88 | $C_{4h}^6$ | $I4_1/a$ | $F4_1/d$ |
| 89 | $D_4^1$ | P422 | C422 |
| 90 | $D_4^2$ | $P42_12$ | $C422_1$ |
| 91 | $D_4^3$ | $P4_122$ | $C4_122$ |
| 92 | $D_4^4$ | $P4_12_12$ | $C4_122_1$ |
| 93 | $D_4^5$ | $P4_222$ | $C4_222$ |
| 94 | $D_4^6$ | $P4_22_12$ | $C4_22_1$ |
| 95 | $D_4^7$ | $P4_322$ | $C4_322$ |
| 96 | $D_4^8$ | $P4_32_12$ | $C4_32_1$ |
| 97 | $D_4^9$ | I422 | F422 |
| 98 | $D_4^{10}$ | $I4_122$ | $F4_122$ |
| 99 | $C_{4v}^1$ | P4mm | C4mm |
| 100[b] | $C_{4v}^2$ | P4bm | C4mb |
| 101 | $C_{4v}^3$ | $P4_2cm$ | $C4_2mc$ |
| 102[b] | $C_{4v}^4$ | $P4_2nm$ | $C4_2mn$ |
| 103 | $C_{4v}^5$ | P4cc | C4cc |
| 104[b] | $C_{4v}^6$ | P4nc | C4cn |
| 105 | $C_{4v}^7$ | $P4_2mc$ | $C4_2cm$ |
| 106[b] | $C_{4v}^8$ | $P4_2bc$ | $C4_2cb$ |
| 107 | $C_{4v}^9$ | I4mm | F4mm |
| 108 | $C_{4v}^{10}$ | I4cm | F4mc |

[a]Tetragonal: a- and b-axes in same plane but 45° to those in the standard orientation.

[b]See footnote, p. 204.

| No. | Schoenflies symbol | Standard symbol | Other orientations[a] |
|---|---|---|---|
| 109 | $C_{4v}^{11}$ | $I4_1md$ | $F4_1dm$ |
| 110 | $C_{4v}^{12}$ | $I4_1cd$ | $F4_1dc$ |
| 111 | $D_{2d}^{1}$, $V_d^1$ | $P\bar{4}2m$ | $C\bar{4}m2$ |
| 112 | $D_{2d}^{2}$, $V_d^2$ | $P\bar{4}2c$ | $C\bar{4}c2$ |
| 113 | $D_{2d}^{3}$, $V_d^3$ | $P\bar{4}2_1m$ | $C\bar{4}m2_1$ |
| 114 | $D_{2d}^{4}$, $V_d^4$ | $P\bar{4}2_1c$ | $C\bar{4}c2_1$ |
| 115 | $D_{2d}^{5}$, $V_d^5$ | $P\bar{4}m2$ | $C\bar{4}2m$ |
| 116 | $D_{2d}^{6}$, $V_d^6$ | $P\bar{4}c2$ | $C\bar{4}2c$ |
| 117[b] | $D_{2d}^{7}$, $C_d^7$ | $P\bar{4}b2$ | $C\bar{4}2b$ |
| 118[b] | $D_{2d}^{8}$, $V_d^8$ | $P\bar{4}n2$ | $C\bar{4}2n$ |
| 119 | $D_{2d}^{9}$, $V_d^9$ | $I\bar{4}m2$ | $F\bar{4}2m$ |
| 120 | $D_{2d}^{10}$, $V_d^{10}$ | $I\bar{4}c2$ | $F\bar{4}2c$ |
| 121 | $D_{2d}^{11}$, $V_d^{11}$ | $I\bar{4}2m$ | $F\bar{4}m2$ |
| 122 | $D_{2d}^{12}$, $V_d^{13}$ | $I\bar{4}2d$ | $F\bar{4}d2$ |
| 123 | $D_{4h}^{1}$ | $P4/mmm$ | $C4/mmm$ |
| 124 | $D_{4h}^{2}$ | $P4/mcc$ | $C4/mcc$ |
| 125[b] | $D_{4h}^{3}$ | $P4/nbm$ | $C4/amb$ |
| 126[b] | $D_{4h}^{4}$ | $P4/nnc$ | $C4/acn$ |
| 127[b] | $D_{4h}^{5}$ | $P4/mbm$ | $C4/mmb$ |
| 128[b] | $D_{4h}^{6}$ | $P4/mnc$ | $C4/mcn$ |
| 129 | $D_{4h}^{7}$ | $P4/nmm$ | $C4/amm$ |
| 130 | $D_{4h}^{8}$ | $P4/ncc$ | $C4/acc$ |

[a]Tetragonal: a- and b-axes in same plane but 45° to those in the standard orientation.

[b]See footnote, p. 204.

| No. | Schoenflies symbol | Standard symbol | Other orientations[a,c] |
|---|---|---|---|
| 131 | $D_{4h}^{9}$ | $P4_2/mmc$ | $C4_2/mcm$ |
| 132 | $D_{4h}^{10}$ | $P4_2/mcm$ | $C4_2/mmc$ |
| 133[b] | $D_{4h}^{11}$ | $P4_2/nbc$ | $C4_2/acb$ |
| 134[b] | $D_{4h}^{12}$ | $P4_2/nnm$ | $C4_2/amn$ |
| 135[b] | $D_{4h}^{13}$ | $P4_2/mbc$ | $C4_2/mcb$ |
| 136[b] | $D_{4h}^{14}$ | $P4_2/mnm$ | $C4_2/mmn$ |
| 137 | $D_{4h}^{15}$ | $P4_2/nmc$ | $C4_2/acm$ |
| 138 | $D_{4h}^{16}$ | $P4_2/ncm$ | $C4_2/amc$ |
| 139 | $D_{4h}^{17}$ | $I4/mmm$ | $F4/mmm$ |
| 140 | $D_{4h}^{18}$ | $I4/mcm$ | $F4/mmc$ |
| 141 | $D_{4h}^{19}$ | $I4_1/amd$ | $F4_1/ddm$ |
| 142 | $D_{4h}^{20}$ | $I4_1/acd$ | $F4_1/ddc$ |
| Rhombohedral (Trigonal) | | | |
| 143 | $C_3^1$ | $P3$ | $H3$ |
| 144 | $C_3^2$ | $P3_1$ | $H3_1$ |
| 145 | $C_3^3$ | $P3_2$ | $H3_2$ |
| 146 | $C_3^4$ | $R3$ | |
| 147 | $C_{3i}^1$, $S_6^1$ | $P\bar{3}$ | $H\bar{3}$ |
| 148 | $C_{3i}^2$, $S_6^2$ | $R\bar{3}$ | |
| 149 | $D_3^1$ | $P312$ | $H32$ |

[a]Tetragonal: a- and b-axes in same plane but 45° to those in the standard orientation.

[b]See footnote, p. 204.

[c]Rhombohedral: orientation in the Internationale Tabellen (1935).

| No. | Schoenflies symbol | Standard symbol | Other orientations[a,b] |
|---|---|---|---|
| 150 | $D_3^2$ | P321 | H312 |
| 151 | $D_3^3$ | $P3_112$ | $H3_12$ |
| 152 | $D_3^4$ | $P3_121$ | $H3_112$ |
| 153 | $D_3^5$ | $P3_212$ | $H3_22$ |
| 154 | $D_3^6$ | $P3_221$ | $H3_212$ |
| 155 | $D_3^7$ | R32 | |
| 156 | $C_{3v}^1$ | P3m1 | H31m |
| 157 | $C_{3v}^2$ | P31m | H3m |
| 158 | $C_{3v}^3$ | P3c1 | H31c |
| 159 | $C_{3v}^4$ | P31c | H3c |
| 160 | $C_{3v}^5$ | R3m | |
| 161 | $C_{3v}^6$ | | |
| 162 | $D_{3d}^1$ | $P\bar{3}1m$ | $H\bar{3}m$ |
| 163 | $D_{3d}^2$ | $P\bar{3}1c$ | $H\bar{3}c$ |
| 164 | $D_{3d}^3$ | $P\bar{3}m1$ | $H\bar{3}1m$ |
| 165 | $D_{3d}^4$ | $P\bar{3}c1$ | $H\bar{3}1c$ |
| 166 | $D_{3d}^5$ | $R\bar{3}m$ | |
| 167 | $D_{3d}^6$ | $R\bar{3}c$ | |
| Hexagonal | | | |
| 168 | $C_6^1$ | P6 | H6 |
| 169 | $C_6^2$ | $P6_1$ | $H6_1$ |

[a]Rhombohedral: orientation in the Internationale Tabellen (1935).
[b]Hexagonal: ibid.

| No. | Schoenflies symbol | Standard symbol | Other orientations[a] |
|---|---|---|---|
| 170 | $C_6^3$ | $P6_5$ | $H6_5$ |
| 171 | $C_6^4$ | $P6_2$ | $H6_2$ |
| 172 | $C_6^5$ | $P6_4$ | $H6_4$ |
| 173 | $C_6^6$ | $P6_3$ | $H6_3$ |
| 174 | $C_{3h}^1$ | $P\bar{6}$ | $H\bar{6}$ |
| 175 | $C_{6h}^1$ | $P6/m$ | $H6/m$ |
| 176 | $C_{6h}^2$ | $P6_3/m$ | $H6_3/m$ |
| 177 | $D_6^1$ | P622 | H62 |
| 178 | $D_6^2$ | $P6_122$ | $H6_12$ |
| 179 | $D_6^3$ | $P6_522$ | $H6_52$ |
| 180 | $D_6^4$ | $P6_222$ | $H6_22$ |
| 181 | $D_6^5$ | $P6_422$ | $H6_42$ |
| 182 | $D_6^6$ | $P6_322$ | $H6_32$ |
| 183 | $C_{6v}^1$ | P6mm | H6mm |
| 184 | $C_{6v}^2$ | P6cc | H6cc |
| 185 | $C_{6v}^3$ | $P6_3cm$ | H6mc |
| 186 | $C_{6v}^4$ | $P6_3mc$ | H6mc |
| 187 | $D_{3h}^1$ | $P\bar{6}m2$ | $H\bar{6}2m$ |
| 188 | $D_{3h}^2$ | $P\bar{6}c2$ | $H\bar{6}2c$ |
| 189 | $D_{3h}^3$ | $P\bar{6}2m$ | $H\bar{6}m2$ |
| 190 | $D_{3h}^4$ | $P\bar{6}2c$ | $H\bar{6}c2$ |

[a]Hexagonal: orientation in the Internationale Tabellen (1935).

| No. | Schoenflies symbol | Standard symbol | Other orientations |
|---|---|---|---|
| 191 | $D^{1}_{6h}$ | P6/mmm | H6/mmm |
| 192 | $D^{2}_{6h}$ | P6/mcc | H6/mcc |
| 193 | $D^{3}_{6h}$ | $P6_3/mcm$ | H6/mmc |
| 194 | $D^{4}_{6h}$ | $P6_3/mmc$ | $H6_3/mcm$ |
| Cubic | | | |
| 195 | $T^{1}$ | P23 | |
| 196 | $T^{2}$ | F23 | |
| 197 | $T^{3}$ | I23 | |
| 198 | $T^{4}$ | $P2_13$ | |
| 199 | $T^{5}$ | $I2_13$ | |
| 200 | $T^{1}_{h}$ | Pm3 | |
| 201 | $T^{2}_{h}$ | Pn3 | |
| 202 | $T^{3}_{h}$ | Fm3 | |
| 203 | $T^{4}_{h}$ | Fd3 | |
| 204 | $T^{5}_{h}$ | Im3 | |
| 205 | $T^{6}_{h}$ | Pa3 | |
| 206 | $T^{7}_{h}$ | Ia3 | |
| 207 | $O^{1}$ | P432 | |
| 208 | $O^{2}$ | $P4_232$ | |
| 209 | $O^{3}$ | F432 | |
| 210 | $O^{4}$ | $F4_132$ | |
| 211 | $O^{5}$ | I432 | |

| No. | Schoenflies symbol | Standard symbol | Other orientations |
|---|---|---|---|
| 212 | $O^6$ | $P4_332$ | |
| 213 | $O^7$ | $P4_132$ | |
| 214 | $O^8$ | $I4_132$ | |
| 215 | $T_d^1$ | $P\bar{4}3m$ | |
| 216 | $T_d^2$ | $F\bar{4}3m$ | |
| 217 | $T_d^3$ | $I\bar{4}3m$ | |
| 218 | $T_d^4$ | $P\bar{4}3n$ | |
| 219 | $T_d^5$ | $F\bar{4}3c$ | |
| 220 | $T_d^6$ | $I\bar{4}3d$ | |
| 221 | $O_h^1$ | $Pm3m$ | |
| 222 | $O_h^2$ | $Pn3n$ | |
| 223 | $O_h^3$ | $Pm3n$ | |
| 224 | $O_h^4$ | $Pn3m$ | |
| 225 | $O_h^5$ | $Fm3m$ | |
| 226 | $O_h^6$ | $Fm3c$ | |
| 227 | $O_h^7$ | $Fd3m$ | |
| 228 | $O_h^8$ | $Fd3c$ | |
| 229 | $O_h^9$ | $Im3m$ | |
| 230 | $O_h^{10}$ | $Ia3d$ | |

According to the Errata of January 1962 for The International Tables for X-Ray Crystallography, Vol. I (1952), "there is ... some ambiguity in using the notation C4mb for space group 100 when it is referred to the C lattice because the glide plane parallel to the (110) now involves a translation of (a+b)/4 for which there is at present no separate symbol. Similarly in space group 102, now called $C4_2mn$, the glide after reflection across (110) is [(a+b)/4 + c/2]. Corresponding glides occur in space groups 104, 106, 117, 118, 125, 126, 128, 133, 134, 135, 136 when referred to a C lattice."